(1)H (28)Si (19)F page 2
(2)H (28)Si (19)F 9
(1)H (28)Si (35)Cl 16
(2)H (28)Si (35)Cl 23
(1)H (28)Si (79)Br 30
(2)H (28)Si (79)Br 37
(1)H (28)Si (127)I 45
(2)H (28)Si (127)I 52
(1)H (74)Ge (19)F 59
(2)H (74)Ge (19)F 66
(1)H (74)Ge (35)Cl 73
(2)H (74)Ge (35)Cl 80
(1)H (74)Ge (79)Br 88
(2)H (74)Ge (79)Br 95
(1)H (74)Ge (127)I 102
(2)H (74)Ge (127)I 109
(1)H (120)Sn (19)F 116
(2)H (120)Sn (19)F 123
(1)H (120)Sn (35)Cl 130
(2)H (120)Sn (35)Cl 138
(1)H (120)Sn (79)Br 145
(2)H (120)Sn (79)Br 152
(1)H (120)Sn (127)I 159
(2)H (120)Sn (127)I 166

```
--------------------------------------------------------------------------------
------------------------------------------ (1)H (28)Si (19)F     GROUND STATE
--------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     1.621945 A    (     3.065033 A.U.)
 R20:     1.527002 A    (     2.885617 A.U.)
 R30:     1.683453 RAD  (    96.454771 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      4.7226307   2   0   0
      2.3018106   0   2   0
      0.9656376   0   0   2
      0.1213225   1   1   0
      0.2053669   1   0   1
     -0.0166955   0   1   1
    -26.9192688   3   0   0
    -10.4948502   0   3   0
     -1.4442195   0   0   3
     -0.4115862   2   1   0
      0.1299280   1   2   0
     -0.4588098   2   0   1
     -0.0315302   0   2   1
     -0.4025977   1   1   1
     -1.0844338   1   0   2
     -0.5414563   0   1   2
    122.7889563   4   0   0
     45.3400757   0   4   0
      5.6784503   0   0   4
      3.0760429   3   1   0
     -1.4250101   1   3   0
     -0.5069261   2   2   0
     -0.2371891   3   0   1
     -0.4728919   0   3   1
      1.1269584   2   1   1
      0.3699110   1   2   1
      1.4036970   2   0   2
     -0.4663979   0   2   2
      1.1317230   1   1   2
      1.6145882   1   0   3
      0.3015970   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:              A             B             C
 CENTER  1:     0.68051852     0.00822023     0.00000000    MASS: 27.976927 AMU
 CENTER  2:    -0.93851245    -0.08728626     0.00000000    MASS: 18.998403 AMU
 CENTER  3:    -1.19919558     1.41723284     0.00000000    MASS:  1.007825 AMU
 MOMENTS:       3.60485190    51.70809096    55.31294287    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
           A           B           C        UNIT
         7.7656      0.5414      0.5061    1/CM
      232808.2     16230.3     15172.6    MHZ

 PROLATE          ASYMMETRIC ROTOR (K=-0.990)           OBLATE
 -------------------------------+-------------------------------
 ^

 ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)
```

HARMONIC FORCE FIELD

F11:	4.7226 AJ/A**2	F12:	0.1213 AJ/A**2	F1A:	0.2054 AJ/A
		F22:	2.3018 AJ/A**2	F2A:	-0.0167 AJ/A
				FAA:	0.9656 AJ

WILSON FG ANALYSIS

ATOMIC MASSES:	27.976927	18.998403	1.007825	AMU
FUNDAMENTAL FREQUENCIES:	819.53413	898.02264	2021.30334	1/CM

NORMAL COORDINATE DISPLACEMENTS

	R1	R2	R3	FREQUENCY	
Q1:	0.97506447	0.01067194	0.22166502	819.53413395	S
Q2:	-0.68562770	0.03177564	0.72725853	898.02263718	B
Q3:	0.04694825	0.99856040	-0.02594206	2021.30334113	A

CORIOLIS COUPLING MATRICES

		S	B	A
ZETA-C	S	0.00000000	-0.27152178	-0.31937868
	B	0.27152178	0.00000000	-0.90789492
	A	0.31937868	0.90789492	0.00000000

TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION

AAAA:	-0.00202570 1/CM	AABB:	0.00000484 1/CM	ABAB:	-0.00004208 1/CM
BBBB:	-0.00000372 1/CM	BBCC:	-0.00000323 1/CM		
CCCC:	-0.00000284 1/CM	CCAA:	-0.00000437 1/CM		
AAAA:	-60.72903 MHZ	AABB:	0.14510 MHZ	ABAB:	-1.26144 MHZ
BBBB:	-0.11165 MHZ	BBCC:	-0.09695 MHZ		
CCCC:	-0.08528 MHZ	CCAA:	-0.13114 MHZ		

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION

AXIS	A:	0.77656448E+01 1/CM	232808.18006 MHZ
	B:	0.54139048E+00 1/CM	16230.47857 MHZ
	C:	0.50609699E+00 1/CM	15172.40634 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS

DJ:	0.81796231E-06 1/CM	0.02452 MHZ
DJK:	0.19286154E-04 1/CM	0.57818 MHZ
DK:	0.48632144E-03 1/CM	14.57955 MHZ
R5:	-0.46562637E-05 1/CM	-0.13959 MHZ
R6:	-0.15772490E-08 1/CM	-0.00005 MHZ
DEL-J:	0.54961068E-07 1/CM	0.00165 MHZ

A-REDUCTION DISTORTION CONSTANTS

DELTA-J:	0.82111681E-06 1/CM	0.02462 MHZ
DELTA-JK:	0.19267227E-04 1/CM	0.57762 MHZ
DELTA-K:	0.48633721E-03 1/CM	14.58002 MHZ
DEL-J:	0.54961068E-07 1/CM	0.00165 MHZ
DEL-K:	0.11901624E-04 1/CM	0.35680 MHZ

S-REDUCTION DISTORTION CONSTANTS

~DJ:	0.80661613E-06 1/CM	0.02418 MHZ
~DJK:	0.19354231E-04 1/CM	0.58023 MHZ
~DK:	0.48626471E-03 1/CM	14.57785 MHZ

```
  ~DEL-J:  0.54961068E-07 1/CM        0.00165 MHZ
     ~R6: -0.72503380E-08 1/CM       -0.00022 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 --------------------------------------------------
                      A              B              C
 ALPHA    S    -0.01445551     0.00346780     0.00437707  1/CM
          B    -0.10599918     0.00093668     0.00187361  1/CM
          A     0.22342833    -0.00059330     0.00020466  1/CM

                      A              B              C
 ALPHA    S     -433.36520      103.96217      131.22115  MHZ
          B    -3177.77566       28.08106       56.16946  MHZ
          A     6698.21310      -17.78669        6.13545  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S              B              A
 X(I,J):  S    -3.96629450    -6.04450000    -4.56557752  1/CM
          B    -6.04450000    -1.96396448   -11.77637969  1/CM
          A    -4.56557752   -11.77637969   -32.99758748  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -3.73568003  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (1)H (28)Si (19)F     EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     1.619027 A    (     3.059519 A.U.)
 R20:     1.527614 A    (     2.886773 A.U.)
 R30:     2.051363 RAD  (   117.534453 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      4.8432219   2   0   0
      1.8876004   0   2   0
      0.2992732   0   0   2
      0.0004270   1   1   0
      0.0550450   1   0   1
      0.0867223   0   1   1
    -27.7522033   3   0   0
    -11.9156190   0   3   0
     -0.1802556   0   0   3
     -0.2254769   2   1   0
     -0.1156739   1   2   0
      0.0614650   2   0   1
      0.1018133   0   2   1
      0.0864356   1   1   1
      0.1535337   1   0   2
      0.0644235   0   1   2
    142.2075948   4   0   0
     53.0844035   0   4   0
      9.1418675   0   0   4
     -1.8248301   3   1   0
     -0.9552482   1   3   0
     -1.1350376   2   2   0
     -1.9020289   3   0   1
     -2.5976135   0   3   1
     -1.5139281   2   1   1
     -1.8532984   1   2   1
     -0.6330040   2   0   2
     -3.2287038   0   2   2
```

```
    -0.3596767   1   1   2
     4.3438954   1   0   3
     2.6952208   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      0.69007475     0.02153459     0.00000000    MASS: 27.976927 AMU
CENTER  2:     -0.92466172    -0.09564649     0.00000000    MASS: 18.998403 AMU
CENTER  3:     -1.72557223     1.20522799     0.00000000    MASS:  1.007825 AMU
MOMENTS:        2.74106693    54.07888214    56.81994906    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
        10.2128       0.5177       0.4927     1/CM
       306172.4      15518.8      14770.1     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.995)           OBLATE
------------------------------+-----------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     4.8432 AJ/A**2    F12:      0.0004 AJ/A**2    F1A:      0.0550 AJ/A
                           F22:      1.8876 AJ/A**2    F2A:      0.0867 AJ/A
                                                       FAA:      0.2993 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                  27.976927      18.998403       1.007825  AMU
FUNDAMENTAL FREQUENCIES:        495.09918      848.65662     1830.08964  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
                R1             R2             R3             FREQUENCY
Q1:         0.39866814     0.01611034     0.91695375        495.09918204 B
Q2:         0.99941584     0.03122766    -0.01388563        848.65662465 S
Q3:        -0.07988158     0.99582280     0.04422529       1830.08964363 A


CORIOLIS COUPLING MATRICES
--------------------------
                     B              S              A
ZETA-C   B      0.00000000     0.23341968    -0.95586474
         S     -0.23341968     0.00000000     0.17843167
         A      0.95586474    -0.17843167     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:     -0.02495878 1/CM   AABB:      0.00009785 1/CM   ABAB:  -0.00011096 1/CM
BBBB:     -0.00000364 1/CM   BBCC:     -0.00000307 1/CM
CCCC:     -0.00000271 1/CM   CCAA:      0.00003055 1/CM

AAAA:      -748.24534 MHZ    AABB:         2.93354 MHZ    ABAB:     -3.32664 MHZ
BBBB:        -0.10902 MHZ    BBCC:        -0.09193 MHZ
CCCC:        -0.08114 MHZ    CCAA:         0.91600 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.10212811E+02 1/CM   306172.38901 MHZ
```

```
       B:  0.51767169E+00 1/CM    15519.40716 MHZ
       C:  0.49265866E+00 1/CM    14769.53532 MHZ

 FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
 -------------------------------------------
      DJ:  0.78632016E-06 1/CM        0.02357 MHZ
     DJK:  0.21808055E-04 1/CM        0.65379 MHZ
      DK:  0.62170999E-02 1/CM      186.38397 MHZ
      R5: -0.96354301E-05 1/CM       -0.28886 MHZ
      R6: -0.32858962E-08 1/CM       -0.00010 MHZ
   DEL-J:  0.58121944E-07 1/CM        0.00174 MHZ

 A-REDUCTION DISTORTION CONSTANTS
 --------------------------------
  DELTA-J:  0.79289195E-06 1/CM        0.02377 MHZ
 DELTA-JK:  0.21768624E-04 1/CM        0.65261 MHZ
  DELTA-K:  0.62171328E-02 1/CM      186.38496 MHZ
    DEL-J:  0.58121944E-07 1/CM        0.00174 MHZ
    DEL-K:  0.29473004E-04 1/CM        0.88358 MHZ

 S-REDUCTION DISTORTION CONSTANTS
 --------------------------------
     ~DJ:  0.77390668E-06 1/CM        0.02320 MHZ
    ~DJK:  0.21882535E-04 1/CM        0.65602 MHZ
     ~DK:  0.62170379E-02 1/CM      186.38211 MHZ
  ~DEL-J:  0.58121944E-07 1/CM        0.00174 MHZ
     ~R6: -0.94926355E-08 1/CM       -0.00028 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                     A              B              C
 ALPHA    B    -0.73970888    -0.00262281     0.00009321  1/CM
          S    -0.00458475     0.00420858     0.00383014  1/CM
          A     0.80722104     0.00028320     0.00204930  1/CM

                     A              B              C
 ALPHA    B   -22175.91478      -78.62994        2.79438  MHZ
          S     -137.44737      126.17008      114.82457  MHZ
          A    24199.87859        8.49005       61.43655  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                     B              S              A
 X(I,J):  B    29.71198298    -5.59404787   -31.54799658  1/CM
          S    -5.59404787    -4.79991542    -2.22222116  1/CM
          A   -31.54799658    -2.22222116   -87.19041713  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -1.45023888  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (1)H (28)Si (19)F     TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     1.618028 A    (     3.057630 A.U.)
 R20:     1.488876 A    (     2.813569 A.U.)
 R30:     2.014286 RAD  (   115.410102 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      4.9347001   2   0   0
      2.6405334   0   2   0
      0.3918776   0   0   2
```

```
     0.0356762   1   1   0
     0.0297303   1   0   1
    -0.0040856   0   1   1
   -27.7421241   3   0   0
   -12.9561032   0   3   0
    -0.8982364   0   0   3
    -0.1049097   2   1   0
     0.0707219   1   2   0
     0.1550375   2   0   1
     0.2255432   0   2   1
     0.1798907   1   1   1
    -0.0858780   1   0   2
     0.1602900   0   1   2
   131.9880766   4   0   0
    49.8403978   0   4   0
    10.4486538   0   0   4
    -3.1419133   3   1   0
    -2.8610800   1   3   0
    -1.7213666   2   2   0
    -0.7835872   3   0   1
    -1.3955146   0   3   1
    -1.1387150   2   1   1
    -1.5668097   1   2   1
     1.1951559   2   0   2
    -2.1211612   0   2   2
     1.1414614   1   1   2
     6.0666507   1   0   3
     5.6993339   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      0.68829454     0.01961963     0.00000000    MASS: 27.976927 AMU
CENTER  2:     -0.92576872    -0.09281492     0.00000000    MASS: 18.998403 AMU
CENTER  3:     -1.65528633     1.20500927     0.00000000    MASS:  1.007825 AMU
MOMENTS:        2.71968850    53.63183620    56.35152469    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         10.2931       0.5220       0.4968    1/CM
        308579.1     15648.1      14892.9     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.995)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     4.9347 AJ/A**2    F12:      0.0357 AJ/A**2    F1A:      0.0297 AJ/A
                           F22:      2.6405 AJ/A**2    F2A:     -0.0041 AJ/A
                                                       FAA:      0.3919 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      18.998403       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       579.21791      863.10509     2164.67529  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.52589380     0.03839581     0.84968316        579.21791071 B
```

```
Q2:        0.99880190     0.02270435    -0.04335055        863.10509473 S
Q3:       -0.03176191     0.99947552    -0.00631398       2164.67528606 A


CORIOLIS COUPLING MATRICES
--------------------------
                      B             S             A
ZETA-C   B     0.00000000     0.24116748    -0.93630461
         S    -0.24116748     0.00000000     0.25528791
         A     0.93630461    -0.25528791     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.01519697 1/CM   AABB:     0.00006793 1/CM   ABAB:  -0.00008976 1/CM
BBBB:    -0.00000356 1/CM   BBCC:    -0.00000306 1/CM
CCCC:    -0.00000271 1/CM   CCAA:     0.00002613 1/CM

AAAA:     -455.59363 MHZ    AABB:        2.03649 MHZ    ABAB:     -2.69100 MHZ
BBBB:       -0.10660 MHZ    BBCC:       -0.09182 MHZ
CCCC:       -0.08134 MHZ    CCAA:        0.78344 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.10293090E+02 1/CM   308579.09355 MHZ
       B:  0.52198006E+00 1/CM    15648.56907 MHZ
       C:  0.49676054E+00 1/CM    14892.50662 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.77914737E-06 1/CM        0.02336 MHZ
     DJK:  0.19806948E-04 1/CM        0.59380 MHZ
      DK:  0.37786557E-02 1/CM      113.28125 MHZ
      R5: -0.85815886E-05 1/CM       -0.25727 MHZ
      R6: -0.22470962E-08 1/CM       -0.00007 MHZ
   DEL-J:  0.52658796E-07 1/CM        0.00158 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.78364157E-06 1/CM        0.02349 MHZ
DELTA-JK:  0.19779983E-04 1/CM        0.59299 MHZ
 DELTA-K:  0.37786782E-02 1/CM      113.28193 MHZ
   DEL-J:  0.52658796E-07 1/CM        0.00158 MHZ
   DEL-K:  0.24137125E-04 1/CM        0.72361 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.76808698E-06 1/CM        0.02303 MHZ
    ~DJK:  0.19873310E-04 1/CM        0.59579 MHZ
     ~DK:  0.37786004E-02 1/CM      113.27959 MHZ
  ~DEL-J:  0.52658796E-07 1/CM        0.00158 MHZ
     ~R6: -0.77772937E-08 1/CM       -0.00023 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                      A             B             C
ALPHA    B    -0.84971753    -0.00025011     0.00137346  1/CM
         S    -0.02788040     0.00413007     0.00374434  1/CM
         A     0.35245899     0.00037575     0.00108845  1/CM

                      A             B             C
ALPHA    B   -25473.89151       -7.49799       41.17536  MHZ
         S     -835.83326      123.81649      112.25249  MHZ
         A    10566.45498       11.26480       32.63083  MHZ
```

ANHARMONIC VIBRATIONAL CONSTANTS

		B	S	A	
X(I,J):	B	21.12880823	-6.28595806	-14.81303965	1/CM
	S	-6.28595806	-4.92414028	-0.01415768	1/CM
	A	-14.81303965	-0.01415768	-46.79218532	1/CM

DARLING-DENNISON RESONANCE PARAMETER: -2.97525874 1/CM

---------- (2)H (28)Si (19)F GROUND STATE

REFERENCE GEOMETRY

R10: 1.621945 A (3.065033 A.U.)
R20: 1.527002 A (2.885617 A.U.)
R30: 1.683453 RAD (96.454771 DEGREES)

INTERNAL FORCE FIELD

POWERS OF	R1	R2	R3	(FACTORIALS EXCLUDED!)
4.7226307	2	0	0	
2.3018106	0	2	0	
0.9656376	0	0	2	
0.1213225	1	1	0	
0.2053669	1	0	1	
-0.0166955	0	1	1	
-26.9192688	3	0	0	
-10.4948502	0	3	0	
-1.4442195	0	0	3	
-0.4115862	2	1	0	
0.1299280	1	2	0	
-0.4588098	2	0	1	
-0.0315302	0	2	1	
-0.4025977	1	1	1	
-1.0844338	1	0	2	
-0.5414563	0	1	2	
122.7889563	4	0	0	
45.3400757	0	4	0	
5.6784503	0	0	4	
3.0760429	3	1	0	
-1.4250101	1	3	0	
-0.5069261	2	2	0	
-0.2371891	3	0	1	
-0.4728919	0	3	1	
1.1269584	2	1	1	
0.3699110	1	2	1	
1.4036970	2	0	2	
-0.4663979	0	2	2	
1.1317230	1	1	2	
1.6145882	1	0	3	
0.3015970	0	1	3	

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)

AXES:	A	B	C	
CENTER 1:	0.70516195	0.02051200	0.00000000	MASS: 27.976927 AMU
CENTER 2:	-0.90547797	-0.16980832	0.00000000	MASS: 18.998403 AMU
CENTER 3:	-1.25397277	1.31682708	0.00000000	MASS: 2.014102 AMU
MOMENTS:	6.72865094	54.22513755	60.95378849	10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE

A	B	C	UNIT

```
          4.1604      0.5163      0.4593    1/CM
         124726.2     15476.9     13768.4    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.969)           OBLATE
-------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     4.7226 AJ/A**2    F12:     0.1213 AJ/A**2    F1A:     0.2054 AJ/A
                           F22:     2.3018 AJ/A**2    F2A:    -0.0167 AJ/A
                                                      FAA:     0.9656 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      18.998403       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       644.79048      843.64904     1466.59308  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
                R1             R2             R3            FREQUENCY
Q1:        0.54267176     0.06939363     0.83707340        644.79048239 B
Q2:        0.99592634    -0.00609649    -0.08996419        843.64903730 A
Q3:        0.04263746     0.99822006    -0.04169851       1466.59307824 S


CORIOLIS COUPLING MATRICES
--------------------------
                     B              A              S
ZETA-C   B     0.00000000     0.35457671    -0.85516365
         A    -0.35457671     0.00000000     0.37811439
         S     0.85516365    -0.37811439     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00062801 1/CM   AABB:     0.00000613 1/CM   ABAB:  -0.00003321 1/CM
BBBB:    -0.00000358 1/CM   BBCC:    -0.00000276 1/CM
CCCC:    -0.00000222 1/CM   CCAA:    -0.00000280 1/CM

AAAA:      -18.82725 MHZ    AABB:        0.18388 MHZ    ABAB:     -0.99566 MHZ
BBBB:       -0.10726 MHZ    BBCC:       -0.08264 MHZ
CCCC:       -0.06643 MHZ    CCAA:       -0.08390 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.41604178E+01 1/CM   124726.19062 MHZ
       B:  0.51625957E+00 1/CM    15477.07290 MHZ
       C:  0.45926147E+00 1/CM    13768.31288 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.71542429E-06 1/CM        0.02145 MHZ
     DJK:  0.14341254E-04 1/CM        0.42994 MHZ
      DK:  0.14194568E-03 1/CM        4.25542 MHZ
      R5: -0.35506210E-05 1/CM       -0.10644 MHZ
      R6: -0.43766400E-08 1/CM       -0.00013 MHZ
   DEL-J:  0.85120842E-07 1/CM        0.00255 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.72417757E-06 1/CM        0.02171 MHZ
```

```
DELTA-JK:  0.14288735E-04 1/CM        0.42837 MHZ
 DELTA-K:  0.14198945E-03 1/CM        4.25674 MHZ
   DEL-J:  0.85120842E-07 1/CM        0.00255 MHZ
   DEL-K:  0.93573030E-05 1/CM        0.28052 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.68787222E-06 1/CM        0.02062 MHZ
    ~DJK:  0.14506567E-04 1/CM        0.43490 MHZ
     ~DK:  0.14180792E-03 1/CM        4.25129 MHZ
  ~DEL-J:  0.85120842E-07 1/CM        0.00255 MHZ
     ~R6: -0.18152676E-07 1/CM       -0.00054 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                     A              B              C
ALPHA    B    -0.05037666    -0.00022835     0.00236894  1/CM
         A    -0.00300639     0.00395602     0.00316835  1/CM
         S     0.08383771    -0.00012287     0.00064143  1/CM

                     A              B              C
ALPHA    B    -1510.25437       -6.84574       71.01911  MHZ
         A      -90.12937      118.59842       94.98479  MHZ
         S     2513.39125       -3.68364       19.22948  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                     B              A              S
X(I,J):  B    -0.49510610    10.75919723   -25.12399332  1/CM
         A    10.75919723    -4.91835315   -12.64209220  1/CM
         S   -25.12399332   -12.64209220   -17.28041143  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -2.74235047  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (2)H (28)Si (19)F     EXCITED STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     1.619027 A    (     3.059519 A.U.)
R20:     1.527614 A    (     2.886773 A.U.)
R30:     2.051363 RAD  (   117.534453 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     4.8432219   2   0   0
     1.8876004   0   2   0
     0.2992732   0   0   2
     0.0004270   1   1   0
     0.0550450   1   0   1
     0.0867223   0   1   1
   -27.7522033   3   0   0
   -11.9156190   0   3   0
    -0.1802556   0   0   3
    -0.2254769   2   1   0
    -0.1156739   1   2   0
     0.0614650   2   0   1
     0.1018133   0   2   1
     0.0864356   1   1   1
     0.1535337   1   0   2
     0.0644235   0   1   2
   142.2075948   4   0   0
    53.0844035   0   4   0
```

```
     9.1418675   0   0   4
    -1.8248301   3   1   0
    -0.9552482   1   3   0
    -1.1350376   2   2   0
    -1.9020289   3   0   1
    -2.5976135   0   3   1
    -1.5139281   2   1   1
    -1.8532984   1   2   1
    -0.6330040   2   0   2
    -3.2287038   0   2   2
    -0.3596767   1   1   2
     4.3438954   1   0   3
     2.6952208   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
--------------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      0.72428727     0.04238450     0.00000000    MASS: 27.976927 AMU
CENTER  2:     -0.87989175    -0.17605304     0.00000000    MASS: 18.998403 AMU
CENTER  3:     -1.76098031     1.07191130     0.00000000    MASS:  2.014102 AMU
MOMENTS:        4.90404489    59.16646713    64.07051202    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         5.7083       0.4731       0.4369     1/CM
      171132.0     14184.4      13098.7       MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.986)           OBLATE
-------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     4.8432 AJ/A**2    F12:      0.0004 AJ/A**2    F1A:      0.0550 AJ/A
                           F22:      1.8876 AJ/A**2    F2A:      0.0867 AJ/A
                                                       FAA:      0.2993 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                  27.976927      18.998403       2.014102  AMU
FUNDAMENTAL FREQUENCIES:        372.09731      842.72505     1330.30155  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:         0.37184110     0.04755837     0.92707734        372.09730641 B
Q2:         0.99690448     0.07795572    -0.01021628        842.72504764 S
Q3:        -0.19756496     0.97948497     0.03971504       1330.30154956 A


CORIOLIS COUPLING MATRICES
--------------------------
                    B              S              A
ZETA-C   B      0.00000000     0.25812545    -0.94000650
         S     -0.25812545     0.00000000     0.22306731
         A      0.94000650    -0.22306731     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00891933 1/CM   AABB:     0.00010226 1/CM   ABAB:  -0.00007249 1/CM
```

```
BBBB:    -0.00000400 1/CM   BBCC:    -0.00000281 1/CM
CCCC:    -0.00000219 1/CM   CCAA:     0.00003495 1/CM

AAAA:     -267.39492 MHZ    AABB:        3.06566 MHZ    ABAB:     -2.17329 MHZ
BBBB:       -0.11978 MHZ    BBCC:       -0.08419 MHZ
CCCC:       -0.06565 MHZ    CCAA:        1.04777 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.57083488E+01 1/CM   171131.99644 MHZ
       B:  0.47316033E+00 1/CM    14184.99009 MHZ
       C:  0.43690429E+00 1/CM    13098.06148 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.75539341E-06 1/CM        0.02265 MHZ
     DJK:  0.43348135E-06 1/CM        0.01300 MHZ
      DK:  0.22286447E-02 1/CM       66.81309 MHZ
      R5: -0.47983661E-05 1/CM       -0.14385 MHZ
      R6: -0.88928505E-08 1/CM       -0.00027 MHZ
   DEL-J:  0.11284427E-06 1/CM        0.00338 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.77317911E-06 1/CM        0.02318 MHZ
DELTA-JK:  0.32676714E-06 1/CM        0.00980 MHZ
 DELTA-K:  0.22287336E-02 1/CM       66.81575 MHZ
   DEL-J:  0.11284427E-06 1/CM        0.00338 MHZ
   DEL-K:  0.19904965E-04 1/CM        0.59674 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.73883533E-06 1/CM        0.02215 MHZ
    ~DJK:  0.53282986E-06 1/CM        0.01597 MHZ
     ~DK:  0.22285619E-02 1/CM       66.81061 MHZ
  ~DEL-J:  0.11284427E-06 1/CM        0.00338 MHZ
     ~R6: -0.17171893E-07 1/CM       -0.00051 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    B    -0.32158480    -0.00272051     0.00007018  1/CM
         S    -0.00843072     0.00379903     0.00331170  1/CM
         A     0.33000666     0.00039295     0.00214408  1/CM

                    A              B              C
ALPHA    B    -9640.87003      -81.55883        2.10393  MHZ
         S     -252.74663      113.89195       99.28239  MHZ
         A     9893.35115       11.78037       64.27786  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    B              S              A
X(I,J):  B    16.20092371    -2.14067677   -16.23491811  1/CM
         S    -2.14067677    -4.52147583    -2.81083251  1/CM
         A   -16.23491811    -2.81083251   -45.11172614  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -1.23004374  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H (28)Si (19)F     TRIPLET STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
```

```
R10:     1.618028 A    (     3.057630 A.U.)
R20:     1.488876 A    (     2.813569 A.U.)
R30:     2.014286 RAD  (   115.410102 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     4.9347001   2   0   0
     2.6405334   0   2   0
     0.3918776   0   0   2
     0.0356762   1   1   0
     0.0297303   1   0   1
    -0.0040856   0   1   1
   -27.7421241   3   0   0
   -12.9561032   0   3   0
    -0.8982364   0   0   3
    -0.1049097   2   1   0
     0.0707219   1   2   0
     0.1550375   2   0   1
     0.2255432   0   2   1
     0.1798907   1   1   1
    -0.0858780   1   0   2
     0.1602900   0   1   2
   131.9880766   4   0   0
    49.8403978   0   4   0
    10.4486538   0   0   4
    -3.1419133   3   1   0
    -2.8610800   1   3   0
    -1.7213666   2   2   0
    -0.7835872   3   0   1
    -1.3955146   0   3   1
    -1.1387150   2   1   1
    -1.5668097   1   2   1
     1.1951559   2   0   2
    -2.1211612   0   2   2
     1.1414614   1   1   2
     6.0666507   1   0   3
     5.6993339   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:     0.72125449     0.03909937     0.00000000    MASS: 27.976927 AMU
CENTER  2:    -0.88289716    -0.17194375     0.00000000    MASS: 18.998403 AMU
CENTER  3:    -1.69050430     1.07878176     0.00000000    MASS:  2.014102 AMU
MOMENTS:       4.89591458    58.31640298    63.21231756    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         5.7178      0.4800      0.4429    1/CM
      171416.2     14391.1     13276.5    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.986)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     4.9347 AJ/A**2    F12:     0.0357 AJ/A**2    F1A:     0.0297 AJ/A
                           F22:     2.6405 AJ/A**2    F2A:    -0.0041 AJ/A
                                                      FAA:     0.3919 AJ
```

WILSON FG ANALYSIS

ATOMIC MASSES:	27.976927	18.998403	2.014102	AMU
FUNDAMENTAL FREQUENCIES:	433.86363	858.75293	1571.60076	1/CM

NORMAL COORDINATE DISPLACEMENTS

	R1	R2	R3	FREQUENCY	
Q1:	0.43595724	0.07193324	0.89708801	433.86363183	B
Q2:	0.99805933	0.05268973	-0.03318685	858.75293467	S
Q3:	-0.08878903	0.99599933	-0.01009185	1571.60076461	A

CORIOLIS COUPLING MATRICES

		B	S	A
ZETA-C	B	0.00000000	0.29267443	-0.91612872
	S	-0.29267443	0.00000000	0.27395227
	A	0.91612872	-0.27395227	0.00000000

TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION

AAAA:	-0.00544182 1/CM	AABB:	0.00007065 1/CM	ABAB:	-0.00006106 1/CM
BBBB:	-0.00000374 1/CM	BBCC:	-0.00000276 1/CM		
CCCC:	-0.00000218 1/CM	CCAA:	0.00002748 1/CM		
AAAA:	-163.14166 MHZ	AABB:	2.11789 MHZ	ABAB:	-1.83060 MHZ
BBBB:	-0.11212 MHZ	BBCC:	-0.08272 MHZ		
CCCC:	-0.06546 MHZ	CCAA:	0.82387 MHZ		

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION

AXIS	A:	0.57178283E+01 1/CM	171416.18495 MHZ
	B:	0.48005082E+00 1/CM	14391.56193 MHZ
	C:	0.44284246E+00 1/CM	13276.08318 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS

DJ:	0.72775106E-06 1/CM	0.02182 MHZ
DJK:	0.45439774E-05 1/CM	0.13623 MHZ
DK:	0.13551833E-02 1/CM	40.62737 MHZ
R5:	-0.48863976E-05 1/CM	-0.14649 MHZ
R6:	-0.63274424E-08 1/CM	-0.00019 MHZ
DEL-J:	0.97272954E-07 1/CM	0.00292 MHZ

A-REDUCTION DISTORTION CONSTANTS

DELTA-J:	0.74040594E-06 1/CM	0.02220 MHZ
DELTA-JK:	0.44680481E-05 1/CM	0.13395 MHZ
DELTA-K:	0.13552465E-02 1/CM	40.62927 MHZ
DEL-J:	0.97272954E-07 1/CM	0.00292 MHZ
DEL-K:	0.16923758E-04 1/CM	0.50736 MHZ

S-REDUCTION DISTORTION CONSTANTS

~DJ:	0.71045638E-06 1/CM	0.02130 MHZ
~DJK:	0.46477455E-05 1/CM	0.13934 MHZ
~DK:	0.13550968E-02 1/CM	40.62478 MHZ
~DEL-J:	0.97272954E-07 1/CM	0.00292 MHZ
~R6:	-0.14974782E-07 1/CM	-0.00045 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS

```
                    A             B             C
ALPHA     B    -0.37669824    -0.00009934     0.00135716  1/CM
          S    -0.01186246     0.00375440     0.00326604  1/CM
          A     0.13755034     0.00074028     0.00135417  1/CM

                    A             B             C
ALPHA     B   -11293.12950       -2.97826       40.68672  MHZ
          S     -355.62756      112.55419       97.91345  MHZ
          A     4123.65556       22.19307       40.59694  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XBB PERTURBED BY MODE S
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XBS PERTURBED BY MODE B
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XSB PERTURBED BY MODE B
                    B             S             A
 X(I,J):  B    18.30753249   -29.69248913    -8.19436188  1/CM
          S   -29.69248913    -4.55822692    -0.98687422  1/CM
          A    -8.19436188    -0.98687422   -24.42464998  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -1.19513577  1/CM
-------------------------------------------------------------------------------
------------------------------------------ (1)H (28)Si (35)Cl    GROUND STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.078305 A    (     3.927428 A.U.)
 R20:     1.518326 A    (     2.869222 A.U.)
 R30:     1.664529 RAD  (    95.370465 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.5368332   2   0   0
      2.4030217   0   2   0
      0.8605981   0   0   2
      0.0449417   1   1   0
      0.2024918   1   0   1
     -0.0319303   0   1   1
    -12.0982433   3   0   0
    -11.0973463   0   3   0
     -1.0056564   0   0   3
     -0.1811498   2   1   0
      0.1553007   1   2   0
     -0.5062081   2   0   1
     -0.0297656   0   2   1
     -0.1960710   1   1   1
     -0.9107586   1   0   2
     -0.1597367   0   1   2
     51.7945851   4   0   0
     44.2331956   0   4   0
      2.6413737   0   0   4
      0.6342032   3   1   0
     -0.2623771   1   3   0
     -0.0447021   2   2   0
      0.3370488   3   0   1
      0.2555347   0   3   1
      0.5316282   2   1   1
     -0.0200271   1   2   1
      0.7548093   2   0   2
     -0.7752164   0   2   2
      0.2599161   1   1   2
      1.9161912   1   0   3
     -0.2447999   0   1   3
```

```
EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A              B              C
CENTER  1:     1.17160913     0.00452287     0.00000000    MASS: 27.976927 AMU
CENTER  2:    -0.90609253    -0.04575456     0.00000000    MASS: 34.968853 AMU
CENTER  3:    -1.08452025     1.46200830     0.00000000    MASS:  1.007825 AMU
MOMENTS:       3.69961811   113.41090869   117.11052681    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        7.5667      0.2468      0.2390    1/CM
     226844.8      7400.0      7166.2    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.998)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.5368 AJ/A**2    F12:     0.0449 AJ/A**2    F1A:     0.2025 AJ/A
                           F22:     2.4030 AJ/A**2    F2A:    -0.0319 AJ/A
                                                      FAA:     0.8606 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      34.968853       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       521.06560      813.99439     2041.08973  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99990988     0.00155999     0.01333424        521.06560098 S
Q2:        0.19400147     0.02329957     0.98072451        813.99438584 B
Q3:        0.01539506     0.99964384    -0.02179854       2041.08973368 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S              B              A
ZETA-C   S    -0.00000000    -0.18264152     0.07899220
         B     0.18264152    -0.00000000    -0.98000118
         A    -0.07899220     0.98000118     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00175998 1/CM   AABB:    -0.00000008 1/CM   ABAB:  -0.00001083 1/CM
BBBB:    -0.00000088 1/CM   BBCC:    -0.00000083 1/CM
CCCC:    -0.00000078 1/CM   CCAA:    -0.00000184 1/CM

AAAA:      -52.76299 MHZ    AABB:       -0.00252 MHZ    ABAB:     -0.32478 MHZ
BBBB:       -0.02641 MHZ    BBCC:       -0.02477 MHZ
CCCC:       -0.02329 MHZ    CCAA:       -0.05502 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.75667268E+01 1/CM   226844.76826 MHZ
       B:  0.24683813E+00 1/CM     7400.02118 MHZ
       C:  0.23903793E+00 1/CM     7166.17706 MHZ
```

```
FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.20704576E-06 1/CM        0.00621 MHZ
     DJK:  0.54823657E-05 1/CM        0.16436 MHZ
      DK:  0.43430656E-03 1/CM       13.02018 MHZ
      R5: -0.12414685E-05 1/CM       -0.03722 MHZ
      R6: -0.80452042E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.65153074E-08 1/CM        0.00020 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.20720666E-06 1/CM        0.00621 MHZ
DELTA-JK:  0.54814003E-05 1/CM        0.16433 MHZ
 DELTA-K:  0.43430737E-03 1/CM       13.02021 MHZ
   DEL-J:  0.65153074E-08 1/CM        0.00020 MHZ
   DEL-K:  0.30872434E-05 1/CM        0.09255 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.20638464E-06 1/CM        0.00619 MHZ
    ~DJK:  0.54863324E-05 1/CM        0.16448 MHZ
     ~DK:  0.43430325E-03 1/CM       13.02008 MHZ
  ~DEL-J:  0.65153074E-08 1/CM        0.00020 MHZ
     ~R6: -0.41100850E-09 1/CM       -0.00001 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    S     0.00096406     0.00162775     0.00158293  1/CM
         B    -0.11934556     0.00029416     0.00078509  1/CM
         A     0.21744505    -0.00027429    -0.00008101  1/CM

                    A              B              C
ALPHA    S       28.90187       48.79870       47.45500  MHZ
         B    -3577.88999        8.81861       23.53650  MHZ
         A     6518.83890       -8.22309       -2.42850  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -2.34118941    -3.76413505     1.25172448  1/CM
         B    -3.76413505    -2.21616438   -14.15398915  1/CM
         A     1.25172448   -14.15398915   -37.03290195  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -0.60543860  1/CM

--------------------------------------------------------------------------------
------------------------------------------ (1)H (28)Si (35)Cl    EXCITED STATE
--------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.050782 A    (     3.875417 A.U.)
R20:     1.508979 A    (     2.851559 A.U.)
R30:     2.055201 RAD  (   117.754352 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     2.7301929   2   0   0
     2.1727334   0   2   0
     0.4286463   0   0   2
    -0.0747081   1   1   0
     0.0683806   1   0   1
     0.0620148   0   1   1
```

```
  -13.8007781   3   0   0
  -12.4420008   0   3   0
   -0.0631386   0   0   3
   -0.0727291   2   1   0
    0.0137081   1   2   0
   -0.2658714   2   0   1
    0.0527505   0   2   1
   -0.1170195   1   1   1
   -0.3681164   1   0   2
   -0.3497423   0   1   2
   53.7267638   4   0   0
   43.9234446   0   4   0
   -0.2178247   0   0   4
    0.4100530   3   1   0
   -0.6491132   1   3   0
   -0.1076049   2   2   0
    0.3059156   3   0   1
   -0.1533549   0   3   1
    0.0542154   2   1   1
   -0.0880056   1   2   1
    0.0371926   2   0   2
   -0.5823864   0   2   2
    0.2463799   1   1   2
    0.4777541   1   0   3
    0.4525833   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
--------------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      1.16477334     0.01653485     0.00000000    MASS: 27.976927 AMU
CENTER  2:     -0.88490036    -0.04961580     0.00000000    MASS: 34.968853 AMU
CENTER  3:     -1.63007273     1.26253409     0.00000000    MASS:  1.007825 AMU
MOMENTS:        2.82323165   112.94343251   115.76666416    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         9.9156      0.2479      0.2418    1/CM
      297261.8      7430.6      7249.4    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.7302 AJ/A**2    F12:    -0.0747 AJ/A**2    F1A:     0.0684 AJ/A
                           F22:     2.1727 AJ/A**2    F2A:     0.0620 AJ/A
                                                      FAA:     0.4286 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      34.968853       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       540.96944      584.91312     1941.29290  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99542518     0.01674732     0.09406512        540.96943782 S
Q2:       -0.40400085    -0.00865438     0.91471767        584.91312377 B
Q3:       -0.05555144     0.99805417     0.02831814       1941.29289735 A
```

CORIOLIS COUPLING MATRICES

		S	B	A
ZETA-C	S	0.00000000	-0.16522546	-0.15585853
	B	0.16522546	-0.00000000	-0.97386276
	A	0.15585853	0.97386276	0.00000000

TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION

AAAA:	-0.01528883 1/CM	AABB:	0.00000652 1/CM	ABAB:	-0.00002105 1/CM
BBBB:	-0.00000083 1/CM	BBCC:	-0.00000079 1/CM		
CCCC:	-0.00000075 1/CM	CCAA:	-0.00000289 1/CM		
AAAA:	-458.34762 MHZ	AABB:	0.19548 MHZ	ABAB:	-0.63105 MHZ
BBBB:	-0.02491 MHZ	BBCC:	-0.02359 MHZ		
CCCC:	-0.02251 MHZ	CCAA:	-0.08654 MHZ		

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION

AXIS	A:	0.99155872E+01 1/CM	297261.83231 MHZ
	B:	0.24786167E+00 1/CM	7430.70615 MHZ
	C:	0.24181091E+00 1/CM	7249.30894 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS

DJ:	0.19746279E-06 1/CM	0.00592 MHZ
DJK:	0.92213854E-05 1/CM	0.27645 MHZ
DK:	0.38127888E-02 1/CM	114.30453 MHZ
R5:	-0.20407471E-05 1/CM	-0.06118 MHZ
R6:	-0.12047240E-09 1/CM	-0.00000 MHZ
DEL-J:	0.50067358E-08 1/CM	0.00015 MHZ

A-REDUCTION DISTORTION CONSTANTS

DELTA-J:	0.19770374E-06 1/CM	0.00593 MHZ
DELTA-JK:	0.92199397E-05 1/CM	0.27641 MHZ
DELTA-K:	0.38127900E-02 1/CM	114.30457 MHZ
DEL-J:	0.50067358E-08 1/CM	0.00015 MHZ
DEL-K:	0.56218742E-05 1/CM	0.16854 MHZ

S-REDUCTION DISTORTION CONSTANTS

~DJ:	0.19682437E-06 1/CM	0.00590 MHZ
~DJK:	0.92252159E-05 1/CM	0.27657 MHZ
~DK:	0.38127856E-02 1/CM	114.30444 MHZ
~DEL-J:	0.50067358E-08 1/CM	0.00015 MHZ
~R6:	-0.43968416E-09 1/CM	-0.00001 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS

		A	B	C	
ALPHA	S	-0.01214559	0.00163228	0.00173243	1/CM
	B	-0.41852704	-0.00001694	0.00044006	1/CM
	A	0.53155988	0.00048895	0.00075822	1/CM
ALPHA	S	-364.11556	48.93457	51.93694	MHZ
	B	-12547.12527	-0.50784	13.19253	MHZ
	A	15935.76486	14.65821	22.73073	MHZ

ANHARMONIC VIBRATIONAL CONSTANTS

```
                    S              B              A
X(I,J):  S    -2.98379220    -2.61582075    -3.70846712  1/CM
         B    -2.61582075    -3.14729467   -27.38483146  1/CM
         A    -3.70846712   -27.38483146   -74.89023820  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -1.50091538  1/CM

--------------------------------------------------------------------------------
----------------------------------------- (1)H (28)Si (35)Cl    TRIPLET STATE
--------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.048596 A    (     3.871286 A.U.)
 R20:     1.482851 A    (     2.802183 A.U.)
 R30:     2.018465 RAD  (   115.649502 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.8678859   2   0   0
      2.7061763   0   2   0
      0.5162505   0   0   2
     -0.0251028   1   1   0
      0.0718188   1   0   1
      0.0079052   0   1   1
    -13.7378336   3   0   0
    -13.1559118   0   3   0
     -0.3106039   0   0   3
     -0.1045351   2   1   0
      0.0641925   1   2   0
     -0.2333141   2   0   1
     -0.0112889   0   2   1
     -0.0925595   1   1   1
     -0.4414531   1   0   2
     -0.2478638   0   1   2
     53.1418452   4   0   0
     49.2372428   0   4   0
      0.4211429   0   0   4
     -0.1526074   3   1   0
     -1.0233241   1   3   0
     -0.6492596   2   2   0
      0.3402664   3   0   1
      0.0156110   0   3   1
      0.2420289   2   1   1
      0.0518867   1   2   1
      0.1948300   2   0   2
     -0.2965227   0   2   2
      0.3175563   1   1   2
      0.6548047   1   0   3
      0.2038637   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:              A             B             C
 CENTER  1:     1.16290503     0.01522989     0.00000000    MASS: 27.976927 AMU
 CENTER  2:    -0.88518634    -0.04871733     0.00000000    MASS: 34.968853 AMU
 CENTER  3:    -1.56828605     1.26758462     0.00000000    MASS:  1.007825 AMU
 MOMENTS:       2.83756077   112.44007952   115.27764028    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
           A           B           C        UNIT
         9.8655      0.2490      0.2428    1/CM
      295760.7      7463.9      7280.2    MHZ
```

```
PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.8679 AJ/A**2    F12:    -0.0251 AJ/A**2    F1A:     0.0718 AJ/A
                           F22:     2.7062 AJ/A**2    F2A:     0.0079 AJ/A
                                                      FAA:     0.5163 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      34.968853       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       555.42695      653.22280     2165.83900  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99780988     0.01436739     0.06456801        555.42694884 S
Q2:       -0.21683242     0.00852418     0.97617163        653.22280069 B
Q3:       -0.02403188     0.99971114     0.00031540       2165.83899871 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S     0.00000000    -0.17025923    -0.07517412
         B     0.17025923    -0.00000000    -0.98252768
         A     0.07517412     0.98252768     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.01042728 1/CM   AABB:     0.00000532 1/CM   ABAB:  -0.00001795 1/CM
BBBB:    -0.00000080 1/CM   BBCC:    -0.00000076 1/CM
CCCC:    -0.00000072 1/CM   CCAA:    -0.00000126 1/CM

AAAA:     -312.60201 MHZ    AABB:        0.15944 MHZ    ABAB:     -0.53807 MHZ
BBBB:       -0.02397 MHZ    BBCC:       -0.02271 MHZ
CCCC:       -0.02162 MHZ    CCAA:       -0.03772 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.98655154E+01 1/CM   295760.71907 MHZ
       B:  0.24897053E+00 1/CM     7463.94878 MHZ
       C:  0.24283744E+00 1/CM     7280.08341 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.18991207E-06 1/CM        0.00569 MHZ
     DJK:  0.75791832E-05 1/CM        0.22722 MHZ
      DK:  0.25990510E-02 1/CM       77.91759 MHZ
      R5: -0.18300423E-05 1/CM       -0.05486 MHZ
      R6: -0.94243572E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.48850935E-08 1/CM        0.00015 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.19010056E-06 1/CM        0.00570 MHZ
DELTA-JK:  0.75780523E-05 1/CM        0.22718 MHZ
 DELTA-K:  0.25990520E-02 1/CM       77.91762 MHZ
   DEL-J:  0.48850935E-08 1/CM        0.00015 MHZ
```

```
   DEL-K:  0.48426360E-05 1/CM        0.14518 MHZ

 S-REDUCTION DISTORTION CONSTANTS
 --------------------------------
     ~DJ:  0.18932869E-06 1/CM        0.00568 MHZ
    ~DJK:  0.75826835E-05 1/CM        0.22732 MHZ
     ~DK:  0.25990481E-02 1/CM       77.91750 MHZ
  ~DEL-J:  0.48850935E-08 1/CM        0.00015 MHZ
     ~R6: -0.38593445E-09 1/CM       -0.00001 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                     A              B              C
 ALPHA    S    -0.00153475     0.00151635     0.00153571  1/CM
          B    -0.43523071     0.00005387     0.00049987  1/CM
          A     0.29977021     0.00020084     0.00035158  1/CM

                     A              B              C
 ALPHA    S      -46.01070       45.45911       46.03954  MHZ
          B   -13047.88868        1.61494       14.98571  MHZ
          A     8986.88512        6.02104       10.54001  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                     S              B              A
 X(I,J):  S    -2.60959525    -2.46920183    -1.45414994  1/CM
          B    -2.46920183    -1.66604016   -15.98820254  1/CM
          A    -1.45414994   -15.98820254   -45.55438797  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.54323098  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (2)H (28)Si (35)Cl    GROUND STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.078305 A    (     3.927428 A.U.)
 R20:     1.518326 A    (     2.869222 A.U.)
 R30:     1.664529 RAD  (    95.370465 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.5368332   2   0   0
      2.4030217   0   2   0
      0.8605981   0   0   2
      0.0449417   1   1   0
      0.2024918   1   0   1
     -0.0319303   0   1   1
    -12.0982433   3   0   0
    -11.0973463   0   3   0
     -1.0056564   0   0   3
     -0.1811498   2   1   0
      0.1553007   1   2   0
     -0.5062081   2   0   1
     -0.0297656   0   2   1
     -0.1960710   1   1   1
     -0.9107586   1   0   2
     -0.1597367   0   1   2
     51.7945851   4   0   0
     44.2331956   0   4   0
      2.6413737   0   0   4
      0.6342032   3   1   0
     -0.2623771   1   3   0
```

```
    -0.0447021   2   2   0
     0.3370488   3   0   1
     0.2555347   0   3   1
     0.5316282   2   1   1
    -0.0200271   1   2   1
     0.7548093   2   0   2
    -0.7752164   0   2   2
     0.2599161   1   1   2
     1.9161912   1   0   3
    -0.2447999   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      1.18850077     0.01052319     0.00000000    MASS: 27.976927 AMU
CENTER  2:     -0.88738557    -0.08981573     0.00000000    MASS: 34.968853 AMU
CENTER  3:     -1.10210107     1.41320874     0.00000000    MASS:  2.014102 AMU
MOMENTS:        7.15301803   115.40869859   122.56171662    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         3.9136       0.2426       0.2284     1/CM
      117326.6       7271.9       6847.5     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.992)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.5368 AJ/A**2    F12:      0.0449 AJ/A**2    F1A:      0.2025 AJ/A
                           F22:      2.4030 AJ/A**2    F2A:     -0.0319 AJ/A
                                                       FAA:      0.8606 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      34.968853       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       520.25840      590.86477     1464.30663  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
                R1             R2             R3             FREQUENCY
Q1:         0.99775866     0.00516810     0.06671546        520.25840333 S
Q2:         0.03984868     0.03939367     0.99842888        590.86476698 B
Q3:         0.01268392     0.99953939    -0.02757038       1464.30662551 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S     -0.00000000    -0.24790654     0.03375124
         B      0.24790654     0.00000000    -0.96819585
         A     -0.03375124     0.96819585     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:     -0.00048399 1/CM   AABB:      0.00000030 1/CM   ABAB:  -0.00000982 1/CM
BBBB:     -0.00000084 1/CM   BBCC:     -0.00000075 1/CM
CCCC:     -0.00000067 1/CM   CCAA:     -0.00000138 1/CM
```

```
AAAA:      -14.50960 MHZ    AABB:        0.00901 MHZ    ABAB:     -0.29427 MHZ
BBBB:       -0.02526 MHZ    BBCC:       -0.02237 MHZ
CCCC:       -0.01997 MHZ    CCAA:       -0.04143 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.39135927E+01 1/CM   117326.56186 MHZ
       B:  0.24256512E+00 1/CM     7271.91951 MHZ
       C:  0.22840629E+00 1/CM     6847.44851 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.18809008E-06 1/CM        0.00564 MHZ
     DJK:  0.48020881E-05 1/CM        0.14396 MHZ
      DK:  0.11600685E-03 1/CM        3.47780 MHZ
      R5: -0.11162932E-05 1/CM       -0.03347 MHZ
      R6: -0.26042964E-09 1/CM       -0.00001 MHZ
   DEL-J:  0.11021807E-07 1/CM        0.00033 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.18861094E-06 1/CM        0.00565 MHZ
DELTA-JK:  0.47989629E-05 1/CM        0.14387 MHZ
 DELTA-K:  0.11600946E-03 1/CM        3.47788 MHZ
   DEL-J:  0.11021807E-07 1/CM        0.00033 MHZ
   DEL-K:  0.27738108E-05 1/CM        0.08316 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.18594150E-06 1/CM        0.00557 MHZ
    ~DJK:  0.48149795E-05 1/CM        0.14435 MHZ
     ~DK:  0.11599611E-03 1/CM        3.47748 MHZ
  ~DEL-J:  0.11021807E-07 1/CM        0.00033 MHZ
     ~R6: -0.13347189E-08 1/CM       -0.00004 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A             B             C
ALPHA    S     0.00123032    0.00157409    0.00162035  1/CM
         B    -0.04822413    0.00005002    0.00052124  1/CM
         A     0.07975067   -0.00014772    0.00008865  1/CM

                    A             B             C
ALPHA    S       36.88393      47.19008      48.57700  MHZ
         B    -1445.72315       1.49969      15.62636  MHZ
         A     2390.86506      -4.42854       2.65780  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S             B             A
X(I,J):  S    -2.34338825   -2.72718261    0.72488873  1/CM
         B    -2.72718261   -1.18142106   -6.68226508  1/CM
         A     0.72488873   -6.68226508  -19.04564600  1/CM

DARLING-DENNISON RESONANCE PARAMETER:      -0.18161667  1/CM

-------------------------------------------------------------------------------
----------------------------------------- (2)H (28)Si (35)Cl    EXCITED STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.050782 A    (     3.875417 A.U.)
R20:     1.508979 A    (     2.851559 A.U.)
R30:     2.055201 RAD  (   117.754352 DEGREES)
```

```
INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     2.7301929   2   0   0
     2.1727334   0   2   0
     0.4286463   0   0   2
    -0.0747081   1   1   0
     0.0683806   1   0   1
     0.0620148   0   1   1
   -13.8007781   3   0   0
   -12.4420008   0   3   0
    -0.0631386   0   0   3
    -0.0727291   2   1   0
     0.0137081   1   2   0
    -0.2658714   2   0   1
     0.0527505   0   2   1
    -0.1170195   1   1   1
    -0.3681164   1   0   2
    -0.3497423   0   1   2
    53.7267638   4   0   0
    43.9234446   0   4   0
    -0.2178247   0   0   4
     0.4100530   3   1   0
    -0.6491132   1   3   0
    -0.1076049   2   2   0
     0.3059156   3   0   1
    -0.1533549   0   3   1
     0.0542154   2   1   1
    -0.0880056   1   2   1
     0.0371926   2   0   2
    -0.5823864   0   2   2
     0.2463799   1   1   2
     0.4777541   1   0   3
     0.4525833   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      1.18957213     0.03294399     0.00000000    MASS: 27.976927 AMU
CENTER  2:     -0.85716605    -0.09512243     0.00000000    MASS: 34.968853 AMU
CENTER  3:     -1.64165429     1.19390720     0.00000000    MASS:  2.014102 AMU
MOMENTS:        5.34309310   117.41697601   122.76006912    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        5.2393      0.2384      0.2280    1/CM
     157069.9      7147.5      6836.4     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.996)           OBLATE
-------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.7302 AJ/A**2    F12:    -0.0747 AJ/A**2    F1A:     0.0684 AJ/A
                           F22:     2.1727 AJ/A**2    F2A:     0.0620 AJ/A
                                                      FAA:     0.4286 AJ

WILSON FG ANALYSIS
------------------
```

```
ATOMIC MASSES:                  27.976927      34.968853       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       424.72583      543.29257    1393.26389  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3            FREQUENCY
Q1:        0.38936287     0.02178384     0.92082681       424.72583492 B
Q2:        0.99856556     0.03549251    -0.04008882       543.29257317 S
Q3:       -0.07938558     0.99651459     0.02562412      1393.26388790 A


CORIOLIS COUPLING MATRICES
--------------------------
                     B              S              A
ZETA-C   B     0.00000000     0.21553376    -0.95376404
         S    -0.21553376     0.00000000     0.20947398
         A     0.95376404    -0.20947398     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00458278 1/CM   AABB:     0.00001062 1/CM   ABAB:  -0.00001750 1/CM
BBBB:    -0.00000078 1/CM   BBCC:    -0.00000070 1/CM
CCCC:    -0.00000064 1/CM   CCAA:     0.00000104 1/CM

AAAA:     -137.38820 MHZ    AABB:        0.31852 MHZ    ABAB:     -0.52470 MHZ
BBBB:       -0.02349 MHZ    BBCC:       -0.02088 MHZ
CCCC:       -0.01905 MHZ    CCAA:        0.03112 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.52392872E+01 1/CM   157069.88379 MHZ
       B:  0.23841835E+00 1/CM     7147.60252 MHZ
       C:  0.22803524E+00 1/CM     6836.32462 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.17654664E-06 1/CM        0.00529 MHZ
     DJK:  0.54823122E-05 1/CM        0.16436 MHZ
      DK:  0.11400354E-02 1/CM       34.17740 MHZ
      R5: -0.15839962E-05 1/CM       -0.04749 MHZ
      R6: -0.39930158E-09 1/CM       -0.00001 MHZ
   DEL-J:  0.92579539E-08 1/CM        0.00028 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.17734525E-06 1/CM        0.00532 MHZ
DELTA-JK:  0.54775205E-05 1/CM        0.16421 MHZ
 DELTA-K:  0.11400394E-02 1/CM       34.17752 MHZ
   DEL-J:  0.92579539E-08 1/CM        0.00028 MHZ
   DEL-K:  0.47081300E-05 1/CM        0.14115 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.17490395E-06 1/CM        0.00524 MHZ
    ~DJK:  0.54921683E-05 1/CM        0.16465 MHZ
     ~DK:  0.11400272E-02 1/CM       34.17716 MHZ
  ~DEL-J:  0.92579539E-08 1/CM        0.00028 MHZ
     ~R6: -0.12206466E-08 1/CM       -0.00004 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                     A              B              C
ALPHA    B    -0.17340294    -0.00031349     0.00048401  1/CM
         S     0.00385339     0.00155429     0.00141295  1/CM
```

```
          A     0.20151628     0.00042152     0.00073720  1/CM

                     A              B              C
 ALPHA    B    -5198.48963       -9.39817       14.51037  MHZ
          S      115.52165       46.59630       42.35908  MHZ
          A     6041.30614       12.63685       22.10074  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                     B              S              A
 X(I,J):  B    -1.28581717    -2.91728526   -14.59167531  1/CM
          S    -2.91728526    -3.00686334    -1.98011808  1/CM
          A   -14.59167531    -1.98011808   -38.47822848  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -1.15278424  1/CM

-------------------------------------------------------------------------------
----------------------------------------- (2)H (28)Si (35)Cl    TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.048596 A    (     3.871286 A.U.)
 R20:     1.482851 A    (     2.802183 A.U.)
 R30:     2.018465 RAD  (   115.649502 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.8678859   2   0   0
      2.7061763   0   2   0
      0.5162505   0   0   2
     -0.0251028   1   1   0
      0.0718188   1   0   1
      0.0079052   0   1   1
    -13.7378336   3   0   0
    -13.1559118   0   3   0
     -0.3106039   0   0   3
     -0.1045351   2   1   0
      0.0641925   1   2   0
     -0.2333141   2   0   1
     -0.0112889   0   2   1
     -0.0925595   1   1   1
     -0.4414531   1   0   2
     -0.2478638   0   1   2
     53.1418452   4   0   0
     49.2372428   0   4   0
      0.4211429   0   0   4
     -0.1526074   3   1   0
     -1.0233241   1   3   0
     -0.6492596   2   2   0
      0.3402664   3   0   1
      0.0156110   0   3   1
      0.2420289   2   1   1
      0.0518867   1   2   1
      0.1948300   2   0   2
     -0.2965227   0   2   2
      0.3175563   1   1   2
      0.6548047   1   0   3
      0.2038637   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:                A              B              C
 CENTER  1:     1.18681460     0.03052622     0.00000000    MASS: 27.976927 AMU
```

```
CENTER  2:    -0.85850860    -0.09365309     0.00000000    MASS: 34.968853 AMU
CENTER  3:    -1.58004134     1.20198055     0.00000000    MASS:  2.014102 AMU
MOMENTS:       5.38454941   116.58242519   121.96697459    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        5.1989      0.2401      0.2295     1/CM
     155860.6      7198.7      6880.9     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.996)           OBLATE
------------------------------+-----------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.8679 AJ/A**2    F12:    -0.0251 AJ/A**2    F1A:     0.0718 AJ/A
                           F22:     2.7062 AJ/A**2    F2A:     0.0079 AJ/A
                                                      FAA:     0.5163 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      34.968853       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       471.74815      560.39235     1553.97668  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
              R1             R2             R3            FREQUENCY
Q1:       0.52933540     0.03518178     0.84768289       471.74815038 B
Q2:       0.99572546     0.02612324    -0.08859116       560.39235120 S
Q3:      -0.03991506     0.99920027    -0.00236892      1553.97668119 A


CORIOLIS COUPLING MATRICES
--------------------------
                   B              S              A
ZETA-C   B     0.00000000     0.22536686    -0.92560541
         S    -0.22536686     0.00000000     0.30407960
         A     0.92560541    -0.30407960     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00312051 1/CM   AABB:     0.00000800 1/CM   ABAB:  -0.00001514 1/CM
BBBB:    -0.00000075 1/CM   BBCC:    -0.00000067 1/CM
CCCC:    -0.00000061 1/CM   CCAA:     0.00000122 1/CM

AAAA:      -93.55062 MHZ    AABB:        0.23973 MHZ    ABAB:     -0.45388 MHZ
BBBB:       -0.02258 MHZ    BBCC:       -0.02016 MHZ
CCCC:       -0.01835 MHZ    CCAA:        0.03670 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.51989493E+01 1/CM   155860.58359 MHZ
       B:  0.24012431E+00 1/CM     7198.74604 MHZ
       C:  0.22951879E+00 1/CM     6880.80028 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.17003713E-06 1/CM        0.00510 MHZ
     DJK:  0.49246760E-05 1/CM        0.14764 MHZ
      DK:  0.77503349E-03 1/CM       23.23492 MHZ
```

```
      R5: -0.14647990E-05 1/CM       -0.04391 MHZ
      R6: -0.31501359E-09 1/CM       -0.00001 MHZ
   DEL-J:  0.88177211E-08 1/CM        0.00026 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.17066715E-06 1/CM        0.00512 MHZ
DELTA-JK:  0.49208959E-05 1/CM        0.14752 MHZ
 DELTA-K:  0.77503664E-03 1/CM       23.23501 MHZ
   DEL-J:  0.88177211E-08 1/CM        0.00026 MHZ
   DEL-K:  0.41091847E-05 1/CM        0.12319 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.16847240E-06 1/CM        0.00505 MHZ
    ~DJK:  0.49340644E-05 1/CM        0.14792 MHZ
     ~DK:  0.77502567E-03 1/CM       23.23469 MHZ
  ~DEL-J:  0.88177211E-08 1/CM        0.00026 MHZ
     ~R6: -0.10973750E-08 1/CM       -0.00003 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    B    -0.16810115    -0.00010725     0.00057319  1/CM
         S    -0.00398264     0.00136961     0.00123061  1/CM
         A     0.11165038     0.00025212     0.00042063  1/CM

                    A              B              C
ALPHA    B    -5039.54585       -3.21532       17.18392  MHZ
         S     -119.39658       41.05985       36.89276  MHZ
         A     3347.19439        7.55848       12.61007  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    B              S              A
X(I,J):  B    -0.56193033    -2.75363584    -8.19445719  1/CM
         S    -2.75363584    -2.54420731    -0.81174414  1/CM
         A    -8.19445719    -0.81174414   -23.40358806  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -2.40315601  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (1)H (28)Si (79)Br    GROUND STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.247456 A    (     4.247078 A.U.)
R20:     1.517214 A    (     2.867119 A.U.)
R30:     1.649954 RAD  (    94.535424 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     2.1219198   2   0   0
     2.4178930   0   2   0
     0.7939644   0   0   2
     0.0289750   1   1   0
     0.1695695   1   0   1
    -0.0411747   0   1   1
    -8.9905042   3   0   0
   -11.1509559   0   3   0
    -0.9118501   0   0   3
    -0.1345410   2   1   0
     0.1519593   1   2   0
```

```
    -0.4925659   2   0   1
    -0.0196050   0   2   1
    -0.1208062   1   1   1
    -0.8358981   1   0   2
    -0.1114489   0   1   2
    33.4300158   4   0   0
    44.1452046   0   4   0
     2.1102510   0   0   4
     0.5071698   3   1   0
    -0.1899533   1   3   0
    -0.1309880   2   2   0
     0.8498682   3   0   1
     0.2285553   0   3   1
     0.4169534   2   1   1
    -0.0675039   1   2   1
     0.6951919   2   0   2
    -0.6179421   0   2   2
     0.0830256   1   1   2
     1.8445115   1   0   3
    -0.3078366   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      1.66633567     0.00321446     0.00000000    MASS: 27.976927 AMU
CENTER  2:     -0.58157915    -0.02018359     0.00000000    MASS: 78.918338 AMU
CENTER  3:     -0.71608775     1.49125565     0.00000000    MASS:  1.007825 AMU
MOMENTS:        3.77552221   174.17726183   177.95278404    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         7.4146      0.1607      0.1573     1/CM
      222284.2      4818.3      4716.1     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.1219 AJ/A**2    F12:     0.0290 AJ/A**2    F1A:     0.1696 AJ/A
                           F22:     2.4179 AJ/A**2    F2A:    -0.0412 AJ/A
                                                      FAA:     0.7940 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      78.918338       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       413.88900      774.13191     2031.19275  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
              R1             R2             R3             FREQUENCY
Q1:        0.99997909     0.00019072    -0.00646393        413.88900063 S
Q2:        0.22559128     0.01518106     0.97410375        774.13191260 B
Q3:        0.01063394     0.99969849    -0.02213253       2031.19275384 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S              B              A
ZETA-C   S     0.00000000    -0.14849231     0.07877885
```

```
         B     0.14849231    -0.00000000    -0.98577073
         A    -0.07877885     0.98577073     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00163291 1/CM   AABB:    -0.00000021 1/CM   ABAB:  -0.00000508 1/CM
BBBB:    -0.00000039 1/CM   BBCC:    -0.00000037 1/CM
CCCC:    -0.00000035 1/CM   CCAA:    -0.00000093 1/CM

AAAA:      -48.95350 MHZ    AABB:       -0.00620 MHZ    ABAB:     -0.15239 MHZ
BBBB:       -0.01155 MHZ    BBCC:       -0.01107 MHZ
CCCC:       -0.01062 MHZ    CCAA:       -0.02798 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.74146033E+01 1/CM   222284.22087 MHZ
       B:  0.16072185E+00 1/CM     4818.32008 MHZ
       C:  0.15731086E+00 1/CM     4716.06092 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.92428129E-07 1/CM        0.00277 MHZ
     DJK:  0.26417202E-05 1/CM        0.07920 MHZ
      DK:  0.40549405E-03 1/CM       12.15641 MHZ
      R5: -0.58900671E-06 1/CM       -0.01766 MHZ
      R6: -0.15662082E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.19483533E-08 1/CM        0.00006 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.92459453E-07 1/CM        0.00277 MHZ
DELTA-JK:  0.26415323E-05 1/CM        0.07919 MHZ
 DELTA-K:  0.40549421E-03 1/CM       12.15641 MHZ
   DEL-J:  0.19483533E-08 1/CM        0.00006 MHZ
   DEL-K:  0.14445338E-05 1/CM        0.04331 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.92289677E-07 1/CM        0.00277 MHZ
    ~DJK:  0.26425510E-05 1/CM        0.07922 MHZ
     ~DK:  0.40549336E-03 1/CM       12.15639 MHZ
  ~DEL-J:  0.19483533E-08 1/CM        0.00006 MHZ
     ~R6: -0.84888080E-10 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    S    -0.00024762     0.00080532     0.00078926  1/CM
         B    -0.11669050     0.00026868     0.00049336  1/CM
         A     0.21140808    -0.00017549    -0.00008908  1/CM

                    A              B              C
ALPHA    S       -7.42348       24.14281       23.66150  MHZ
         B    -3498.29318        8.05483       14.79056  MHZ
         A     6337.85482       -5.26111       -2.67064  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -1.38822141    -3.22560163     0.67920126  1/CM
         B    -3.22560163    -2.30178089   -13.18770104  1/CM
         A     0.67920126   -13.18770104   -36.57692452  1/CM
```

```
 DARLING-DENNISON RESONANCE PARAMETER:       -0.63430306  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (1)H (28)Si (79)Br    EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.218631 A    (     4.192606 A.U.)
 R20:     1.508861 A    (     2.851334 A.U.)
 R30:     2.057549 RAD  (   117.888881 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.1898313   2   0   0
      2.2162165   0   2   0
      0.3926972   0   0   2
     -0.0690467   1   1   0
      0.0551624   1   0   1
      0.0501401   0   1   1
    -10.3711335   3   0   0
    -12.3906198   0   3   0
     -0.0089100   0   0   3
     -0.0332389   2   1   0
      0.0213965   1   2   0
     -0.2479494   2   0   1
      0.0449337   0   2   1
     -0.1042665   1   1   1
     -0.3419624   1   0   2
     -0.2907058   0   1   2
     36.5401074   4   0   0
     44.2549675   0   4   0
     -0.5754438   0   0   4
      0.5830542   3   1   0
     -0.0719978   1   3   0
      0.1905676   2   2   0
      0.1929196   3   0   1
     -0.1543368   0   3   1
      0.0666344   2   1   1
     -0.1069379   1   2   1
      0.1487099   2   0   2
     -0.5687179   0   2   2
      0.1777731   1   1   2
      0.3649217   1   0   3
      0.3593679   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------------
 AXES:               A              B              C
 CENTER  1:     1.64994238     0.01536876     0.00000000    MASS: 27.976927 AMU
 CENTER  2:    -0.56835346    -0.02204285     0.00000000    MASS: 78.918338 AMU
 CENTER  3:    -1.29666104     1.29944629     0.00000000    MASS:  1.007825 AMU
 MOMENTS:       2.90049469   171.61422007   174.51471476    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
           A           B           C        UNIT
         9.6515      0.1631      0.1604     1/CM
      289343.4      4890.3      4809.0     MHZ

 PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
 ------------------------------+-------------------------------
 ^

 ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)
```

```
HARMONIC FORCE FIELD
--------------------
F11:     2.1898 AJ/A**2    F12:    -0.0690 AJ/A**2    F1A:     0.0552 AJ/A
                           F22:     2.2162 AJ/A**2    F2A:     0.0501 AJ/A
                                                      FAA:     0.3927 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      78.918338       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       422.94027      549.06847     1944.75207  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
              R1             R2             R3             FREQUENCY
Q1:        0.99996613     0.00792972     0.00220466       422.94027447 S
Q2:        0.13261231    -0.00477384     0.99115649       549.06846630 B
Q3:       -0.03880257     0.99897205     0.02343518      1944.75207122 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S              B              A
ZETA-C   S     0.00000000    -0.13840207     0.04193481
         B     0.13840207    -0.00000000    -0.98948792
         A    -0.04193481     0.98948792     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.01484748 1/CM   AABB:     0.00000009 1/CM   ABAB:  -0.00001042 1/CM
BBBB:    -0.00000039 1/CM   BBCC:    -0.00000037 1/CM
CCCC:    -0.00000036 1/CM   CCAA:    -0.00000402 1/CM

AAAA:     -445.11640 MHZ    AABB:        0.00259 MHZ    ABAB:     -0.31238 MHZ
BBBB:       -0.01157 MHZ    BBCC:       -0.01119 MHZ
CCCC:       -0.01086 MHZ    CCAA:       -0.12045 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.96514569E+01 1/CM   289343.40602 MHZ
       B:  0.16312304E+00 1/CM     4890.30577 MHZ
       C:  0.16040918E+00 1/CM     4808.94635 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.93478878E-07 1/CM        0.00280 MHZ
     DJK:  0.60057741E-05 1/CM        0.18005 MHZ
      DK:  0.37057719E-02 1/CM      111.09625 MHZ
      R5: -0.10452017E-05 1/CM       -0.03133 MHZ
      R6: -0.24282327E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.14967332E-08 1/CM        0.00004 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.93527442E-07 1/CM        0.00280 MHZ
DELTA-JK:  0.60054827E-05 1/CM        0.18004 MHZ
 DELTA-K:  0.37057721E-02 1/CM      111.09626 MHZ
   DEL-J:  0.14967332E-08 1/CM        0.00004 MHZ
   DEL-K:  0.27696776E-05 1/CM        0.08303 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.93329424E-07 1/CM        0.00280 MHZ
```

```
    ~DJK:  0.60066708E-05 1/CM        0.18008 MHZ
     ~DK:  0.37057711E-02 1/CM      111.09623 MHZ
  ~DEL-J:  0.14967332E-08 1/CM        0.00004 MHZ
     ~R6: -0.99008925E-10 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                      A              B              C
 ALPHA    S     0.00796647     0.00094628     0.00094111  1/CM
          B    -0.43448257     0.00009188     0.00035721  1/CM
          A     0.48112130     0.00027734     0.00039211  1/CM

                      A              B              C
 ALPHA    S      238.82863       28.36867       28.21373  MHZ
          B   -13025.46020        2.75437       10.70903  MHZ
          A    14423.65405        8.31431       11.75518  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S              B              A
 X(I,J):  S    -2.08086892    -2.51908748    -1.47123705  1/CM
          B    -2.51908748    -3.32366143   -25.17565933  1/CM
          A    -1.47123705   -25.17565933   -68.63637114  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.04303669  1/CM

-------------------------------------------------------------------------------------
------------------------------------------ (1)H (28)Si (79)Br    TRIPLET STATE
-------------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.213293 A    (     4.182519 A.U.)
 R20:     1.485139 A    (     2.806507 A.U.)
 R30:     2.022955 RAD  (   115.906774 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.3645325   2   0   0
      2.6909361   0   2   0
      0.4763023   0   0   2
     -0.0256804   1   1   0
      0.0568267   1   0   1
      0.0032369   0   1   1
    -10.3484126   3   0   0
    -13.0616082   0   3   0
     -0.2534833   0   0   3
     -0.0941531   2   1   0
      0.0244310   1   2   0
     -0.2228876   2   0   1
     -0.0009344   0   2   1
     -0.0684006   1   1   1
     -0.3917085   1   0   2
     -0.1987026   0   1   2
     37.9913864   4   0   0
     49.7329383   0   4   0
      0.2614547   0   0   4
      0.1738036   3   1   0
     -0.2041424   1   3   0
     -0.1854035   2   2   0
      0.2476241   3   0   1
     -0.0493797   0   3   1
      0.1966211   2   1   1
     -0.0065469   1   2   1
```

```
     0.2886773   2   0   2
    -0.3485024   0   2   2
     0.2019007   1   1   2
     0.4763233   1   0   3
     0.1148340   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
------------------------------------------------------------------------------
AXES:                A             B             C
CENTER  1:     1.64577262     0.01422754     0.00000000    MASS: 27.976927 AMU
CENTER  2:    -0.56762111    -0.02169028     0.00000000    MASS: 78.918338 AMU
CENTER  3:    -1.23825626     1.30351808     0.00000000    MASS:  1.007825 AMU
MOMENTS:       2.91464223   170.61901039   173.53365262    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        9.6046      0.1641      0.1613     1/CM
     287938.9      4918.8      4836.2     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.3645 AJ/A**2    F12:    -0.0257 AJ/A**2    F1A:     0.0568 AJ/A
                           F22:     2.6909 AJ/A**2    F2A:     0.0032 AJ/A
                                                      FAA:     0.4763 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      78.918338       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       439.90940      614.91363     2142.55807  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
              R1             R2             R3             FREQUENCY
Q1:        0.99994464     0.00628138     0.00844105        439.90940070 S
Q2:        0.07727475     0.00538103     0.99699531        614.91363211 B
Q3:       -0.01512784     0.99988555     0.00020136       2142.55807424 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S             B             A
ZETA-C   S     0.00000000    -0.14165138     0.02568394
         B     0.14165138     0.00000000    -0.98958336
         A    -0.02568394     0.98958336     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.01023744 1/CM   AABB:     0.00000059 1/CM   ABAB:  -0.00000879 1/CM
BBBB:    -0.00000036 1/CM   BBCC:    -0.00000035 1/CM
CCCC:    -0.00000034 1/CM   CCAA:    -0.00000232 1/CM

AAAA:     -306.91077 MHZ    AABB:        0.01771 MHZ    ABAB:     -0.26360 MHZ
BBBB:       -0.01090 MHZ    BBCC:       -0.01053 MHZ
CCCC:       -0.01020 MHZ    CCAA:       -0.06946 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
```

```
-----------------------------------------------------
AXIS   A:  0.96046092E+01 1/CM   287938.94699 MHZ
       B:  0.16407421E+00 1/CM     4918.82117 MHZ
       C:  0.16131636E+00 1/CM     4836.14287 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
-------------------------------------------
      DJ:  0.87938641E-07 1/CM        0.00264 MHZ
     DJK:  0.46519666E-05 1/CM        0.13946 MHZ
      DK:  0.25546204E-02 1/CM       76.58559 MHZ
      R5: -0.91663325E-06 1/CM       -0.02748 MHZ
      R6: -0.19206184E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.14578086E-08 1/CM        0.00004 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.87977053E-07 1/CM        0.00264 MHZ
DELTA-JK:  0.46517361E-05 1/CM        0.13946 MHZ
 DELTA-K:  0.25546206E-02 1/CM       76.58560 MHZ
   DEL-J:  0.14578086E-08 1/CM        0.00004 MHZ
   DEL-K:  0.23593083E-05 1/CM        0.07073 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.87804773E-07 1/CM        0.00263 MHZ
    ~DJK:  0.46527698E-05 1/CM        0.13949 MHZ
     ~DK:  0.25546197E-02 1/CM       76.58557 MHZ
  ~DEL-J:  0.14578086E-08 1/CM        0.00004 MHZ
     ~R6: -0.86140124E-10 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A             B             C
ALPHA    S     0.00462038    0.00082153    0.00081524  1/CM
         B    -0.44012844    0.00010303    0.00032962  1/CM
         A     0.29013426    0.00010160    0.00017152  1/CM

                    A             B             C
ALPHA    S      138.51543      24.62876      24.44035  MHZ
         B   -13194.71918       3.08883       9.88188  MHZ
         A     8698.00658       3.04599       5.14209  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S             B             A
X(I,J):  S    -1.60488973   -2.00947576   -0.75699894  1/CM
         B    -2.00947576   -1.43329283  -15.27478178  1/CM
         A    -0.75699894  -15.27478178  -44.01201992  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -0.10557918  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (2)H (28)Si (79)Br    GROUND STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.247456 A    (     4.247078 A.U.)
R20:     1.517214 A    (     2.867119 A.U.)
R30:     1.649954 RAD  (    94.535424 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     2.1219198   2   0   0
```

```
     2.4178930   0   2   0
     0.7939644   0   0   2
     0.0289750   1   1   0
     0.1695695   1   0   1
    -0.0411747   0   1   1
    -8.9905042   3   0   0
   -11.1509559   0   3   0
    -0.9118501   0   0   3
    -0.1345410   2   1   0
     0.1519593   1   2   0
    -0.4925659   2   0   1
    -0.0196050   0   2   1
    -0.1208062   1   1   1
    -0.8358981   1   0   2
    -0.1114489   0   1   2
    33.4300158   4   0   0
    44.1452046   0   4   0
     2.1102510   0   0   4
     0.5071698   3   1   0
    -0.1899533   1   3   0
    -0.1309880   2   2   0
     0.8498682   3   0   1
     0.2285553   0   3   1
     0.4169534   2   1   1
    -0.0675039   1   2   1
     0.6951919   2   0   2
    -0.6179421   0   2   2
     0.0830256   1   1   2
     1.8445115   1   0   3
    -0.3078366   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:     1.67297038     0.00708338     0.00000000    MASS: 27.976927 AMU
CENTER  2:    -0.57457257    -0.04002520     0.00000000    MASS: 78.918338 AMU
CENTER  3:    -0.72501690     1.46991111     0.00000000    MASS:  2.014102 AMU
MOMENTS:       7.43847974   175.04482895   182.48330869    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         3.7634      0.1599      0.1534    1/CM
      112824.0      4794.4      4599.0    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.996)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.1219 AJ/A**2    F12:     0.0290 AJ/A**2    F1A:     0.1696 AJ/A
                           F22:     2.4179 AJ/A**2    F2A:    -0.0412 AJ/A
                                                      FAA:     0.7940 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      78.918338       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       413.77028      556.30294     1446.01748  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
```

```
              R1            R2            R3            FREQUENCY
Q1:        0.99979888    0.00016280   -0.02005402        413.77028084 S
Q2:        0.25812077    0.02166173    0.96586978        556.30294174 B
Q3:        0.00988025    0.99965430   -0.02436536       1446.01747865 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S             B             A
ZETA-C   S     0.00000000   -0.20574361    0.12618447
         B     0.20574361    0.00000000   -0.97043652
         A    -0.12618447    0.97043652    0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00042476 1/CM   AABB:    -0.00000005 1/CM   ABAB:  -0.00000483 1/CM
BBBB:    -0.00000038 1/CM   BBCC:    -0.00000035 1/CM
CCCC:    -0.00000032 1/CM   CCAA:    -0.00000076 1/CM

AAAA:      -12.73404 MHZ    AABB:       -0.00162 MHZ    ABAB:     -0.14468 MHZ
BBBB:       -0.01135 MHZ    BBCC:       -0.01044 MHZ
CCCC:       -0.00965 MHZ    CCAA:       -0.02265 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.37634033E+01 1/CM   112823.99671 MHZ
       B:  0.15992524E+00 1/CM     4794.43817 MHZ
       C:  0.15340531E+00 1/CM     4598.97576 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.87431606E-07 1/CM        0.00262 MHZ
     DJK:  0.24404563E-05 1/CM        0.07316 MHZ
      DK:  0.10366258E-03 1/CM        3.10773 MHZ
      R5: -0.55761959E-06 1/CM       -0.01672 MHZ
      R6: -0.55823077E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.35442961E-08 1/CM        0.00011 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.87543252E-07 1/CM        0.00262 MHZ
DELTA-JK:  0.24397864E-05 1/CM        0.07314 MHZ
 DELTA-K:  0.10366314E-03 1/CM        3.10774 MHZ
   DEL-J:  0.35442961E-08 1/CM        0.00011 MHZ
   DEL-K:  0.13622840E-05 1/CM        0.04084 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.86927600E-07 1/CM        0.00261 MHZ
    ~DJK:  0.24434803E-05 1/CM        0.07325 MHZ
     ~DK:  0.10366006E-03 1/CM        3.10765 MHZ
  ~DEL-J:  0.35442961E-08 1/CM        0.00011 MHZ
     ~R6: -0.30782623E-09 1/CM       -0.00001 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                     A             B             C
ALPHA    S    -0.00024865    0.00079361    0.00078082  1/CM
         B    -0.04409733    0.00010252    0.00037740  1/CM
         A     0.07605902   -0.00011291    0.00000100  1/CM

                     A             B             C
ALPHA    S       -7.45432      23.79185      23.40831  MHZ
         B    -1322.00459       3.07345      11.31410  MHZ
```

```
          A     2280.19198       -3.38484        0.03012  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S               B               A
 X(I,J):  S    -1.39675741    -2.37927867     0.52378155  1/CM
          B    -2.37927867    -1.11748266    -6.63303528  1/CM
          A     0.52378155    -6.63303528   -18.53104000  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.57058065  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H (28)Si (79)Br    EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.218631 A    (     4.192606 A.U.)
 R20:     1.508861 A    (     2.851334 A.U.)
 R30:     2.057549 RAD  (   117.888881 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.1898313   2   0   0
      2.2162165   0   2   0
      0.3926972   0   0   2
     -0.0690467   1   1   0
      0.0551624   1   0   1
      0.0501401   0   1   1
    -10.3711335   3   0   0
    -12.3906198   0   3   0
     -0.0089100   0   0   3
     -0.0332389   2   1   0
      0.0213965   1   2   0
     -0.2479494   2   0   1
      0.0449337   0   2   1
     -0.1042665   1   1   1
     -0.3419624   1   0   2
     -0.2907058   0   1   2
     36.5401074   4   0   0
     44.2549675   0   4   0
     -0.5754438   0   0   4
      0.5830542   3   1   0
     -0.0719978   1   3   0
      0.1905676   2   2   0
      0.1929196   3   0   1
     -0.1543368   0   3   1
      0.0666344   2   1   1
     -0.1069379   1   2   1
      0.1487099   2   0   2
     -0.5687179   0   2   2
      0.1777731   1   1   2
      0.3649217   1   0   3
      0.3593679   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:                A               B               C
 CENTER  1:      1.66164040      0.03083023      0.00000000    MASS: 27.976927 AMU
 CENTER  2:     -0.55573409     -0.04324027      0.00000000    MASS: 78.918338 AMU
 CENTER  3:     -1.30578376      1.26603089      0.00000000    MASS:  2.014102 AMU
 MOMENTS:        5.64982238    174.44379760    180.09361999    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
```

```
--------------------------
          A           B           C        UNIT
        4.9548      0.1605      0.1554     1/CM
     148542.5      4810.9      4660.0     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.998)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.1898 AJ/A**2    F12:    -0.0690 AJ/A**2    F1A:     0.0552 AJ/A
                           F22:     2.2162 AJ/A**2    F2A:     0.0501 AJ/A
                                                      FAA:     0.3927 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      78.918338       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       395.92042      422.68328     1384.57016  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.21047453     0.00228211     0.97759668        395.92042125 B
Q2:        0.99978817     0.01647994    -0.01232984        422.68328425 S
Q3:       -0.04730698     0.99862952     0.02238606       1384.57016275 A


CORIOLIS COUPLING MATRICES
--------------------------
                     B              S              A
ZETA-C   B     0.00000000     0.18879908    -0.97739973
         S    -0.18879908     0.00000000     0.09510346
         A     0.97739973    -0.09510346     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00408157 1/CM   AABB:     0.00000274 1/CM   ABAB:  -0.00000946 1/CM
BBBB:    -0.00000037 1/CM   BBCC:    -0.00000035 1/CM
CCCC:    -0.00000033 1/CM   CCAA:    -0.00000145 1/CM

AAAA:     -122.36227 MHZ    AABB:        0.08202 MHZ    ABAB:     -0.28351 MHZ
BBBB:       -0.01113 MHZ    BBCC:       -0.01037 MHZ
CCCC:       -0.00977 MHZ    CCAA:       -0.04347 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.49548459E+01 1/CM   148542.54817 MHZ
       B:  0.16047711E+00 1/CM     4810.98287 MHZ
       C:  0.15544001E+00 1/CM     4659.97454 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.86978181E-07 1/CM        0.00261 MHZ
     DJK:  0.42330046E-05 1/CM        0.12690 MHZ
      DK:  0.10160715E-02 1/CM       30.46106 MHZ
      R5: -0.91906860E-06 1/CM       -0.02755 MHZ
      R6: -0.89103319E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.28473670E-08 1/CM        0.00009 MHZ

A-REDUCTION DISTORTION CONSTANTS
```

```
--------------------------------
 DELTA-J:  0.87156388E-07 1/CM        0.00261 MHZ
DELTA-JK:  0.42319354E-05 1/CM        0.12687 MHZ
 DELTA-K:  0.10160724E-02 1/CM       30.46108 MHZ
   DEL-J:  0.28473670E-08 1/CM        0.00009 MHZ
   DEL-K:  0.25169706E-05 1/CM        0.07546 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.86495635E-07 1/CM        0.00259 MHZ
    ~DJK:  0.42358999E-05 1/CM        0.12699 MHZ
     ~DK:  0.10160691E-02 1/CM       30.46099 MHZ
  ~DEL-J:  0.28473670E-08 1/CM        0.00009 MHZ
     ~R6: -0.33037625E-09 1/CM       -0.00001 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    B    -0.16411767    -0.00008362     0.00040987  1/CM
         S     0.00428069     0.00091572     0.00075130  1/CM
         A     0.17561993     0.00022065     0.00036786  1/CM

                    A              B              C
ALPHA    B    -4920.12415       -2.50700       12.28766  MHZ
         S      128.33190       27.45245       22.52352  MHZ
         A     5264.95326        6.61485       11.02803  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    B              S              A
X(I,J):  B    -1.67078891    -1.97919746   -12.79536772  1/CM
         S    -1.97919746    -2.05847327    -1.06304506  1/CM
         A   -12.79536772    -1.06304506   -34.77446150  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -0.18489633  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H (28)Si (79)Br    TRIPLET STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.213293 A    (     4.182519 A.U.)
R20:     1.485139 A    (     2.806507 A.U.)
R30:     2.022955 RAD  (   115.906774 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     2.3686255   2   0   0
     2.6922017   0   2   0
     0.4765005   0   0   2
    -0.0256390   1   1   0
     0.0569598   1   0   1
     0.0032836   0   1   1
   -10.3633548   3   0   0
   -13.0663773   0   3   0
    -0.2537073   0   0   3
    -0.0942227   2   1   0
     0.0245243   1   2   0
    -0.2230326   2   0   1
    -0.0008923   0   2   1
    -0.0684971   1   1   1
    -0.3918888   1   0   2
    -0.1987592   0   1   2
```

```
    37.9913864   4   0   0
    49.7329383   0   4   0
     0.2614547   0   0   4
     0.1738036   3   1   0
    -0.2041424   1   3   0
    -0.1854035   2   2   0
     0.2476241   3   0   1
    -0.0493797   0   3   1
     0.1966211   2   1   1
    -0.0065469   1   2   1
     0.2886773   2   0   2
    -0.3485024   0   2   2
     0.2019007   1   1   2
     0.4763233   1   0   3
     0.1148340   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      1.65667317     0.02861962     0.00000000    MASS: 27.976927 AMU
CENTER  2:     -0.55547356    -0.04260175     0.00000000    MASS: 78.918338 AMU
CENTER  3:     -1.24699451     1.27171844     0.00000000    MASS:  2.014102 AMU
MOMENTS:        5.68480697   173.13819773   178.82300469    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         4.9244       0.1617       0.1565     1/CM
      147628.4       4847.2       4693.1     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.998)           OBLATE
-------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.3686 AJ/A**2    F12:     -0.0256 AJ/A**2    F1A:      0.0570 AJ/A
                           F22:      2.6922 AJ/A**2    F2A:      0.0033 AJ/A
                                                       FAA:      0.4765 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927      78.918338       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       437.42127      445.95150     1525.63033  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:         0.95817609     0.01523737     0.28577333        437.42127178 S
Q2:        -0.81619556    -0.00459853     0.57775745        445.95149554 B
Q3:        -0.02104549     0.99977815    -0.00085849       1525.63032644 A


CORIOLIS COUPLING MATRICES
--------------------------
                   S              B              A
ZETA-C   S     0.00000000    -0.19421941    -0.50239540
         B     0.19421941    -0.00000000    -0.84254239
         A     0.50239540     0.84254239    -0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
```

```
-----------------------------------------------
AAAA:    -0.00280798 1/CM   AABB:     0.00000222 1/CM   ABAB:  -0.00000804 1/CM
BBBB:    -0.00000035 1/CM   BBCC:    -0.00000033 1/CM
CCCC:    -0.00000031 1/CM   CCAA:    -0.00000076 1/CM

AAAA:      -84.18124 MHZ    AABB:        0.06641 MHZ    ABAB:     -0.24105 MHZ
BBBB:       -0.01050 MHZ    BBCC:       -0.00978 MHZ
CCCC:       -0.00919 MHZ    CCAA:       -0.02282 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.49243536E+01 1/CM   147628.40999 MHZ
       B:  0.16168691E+00 1/CM     4847.25188 MHZ
       C:  0.15654480E+00 1/CM     4693.09529 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.81979651E-07 1/CM        0.00246 MHZ
     DJK:  0.34927862E-05 1/CM        0.10471 MHZ
      DK:  0.69842119E-03 1/CM       20.93814 MHZ
      R5: -0.81768429E-06 1/CM       -0.02451 MHZ
      R6: -0.70622100E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.27378083E-08 1/CM        0.00008 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.82120895E-07 1/CM        0.00246 MHZ
DELTA-JK:  0.34919388E-05 1/CM        0.10469 MHZ
 DELTA-K:  0.69842190E-03 1/CM       20.93816 MHZ
   DEL-J:  0.27378083E-08 1/CM        0.00008 MHZ
   DEL-K:  0.21589374E-05 1/CM        0.06472 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.81538474E-07 1/CM        0.00244 MHZ
    ~DJK:  0.34954333E-05 1/CM        0.10479 MHZ
     ~DK:  0.69841899E-03 1/CM       20.93808 MHZ
  ~DEL-J:  0.27378083E-08 1/CM        0.00008 MHZ
     ~R6: -0.29121040E-09 1/CM       -0.00001 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
*** WARNING *** CORIOLIS RESONANCE EXPECTED: AXIS C MODE S PERTURBED BY MODE B
*** WARNING *** CORIOLIS RESONANCE EXPECTED: AXIS C MODE B PERTURBED BY MODE S
                    A              B              C
ALPHA    S    -0.05461513     0.00057640     0.00105460  1/CM
         B    -0.10886822     0.00018009    -0.00002104  1/CM
         A     0.10495057     0.00010795     0.00019584  1/CM

                    A              B              C
ALPHA    S    -1637.32047       17.28009       31.61613  MHZ
         B    -3263.78710        5.39910       -0.63077  MHZ
         A     3146.33902        3.23635        5.87099  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -1.17009466    -1.91811908    -3.03942705  1/CM
         B    -1.91811908    -0.94236864    -5.19804401  1/CM
         A    -3.03942705    -5.19804401   -22.29628562  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -7.42721809  1/CM

-------------------------------------------------------------------------------
```

```
------------------------------------------- (1)H (28)Si (127)I    GROUND STATE
------------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.477409 A    (     4.681626 A.U.)
 R20:     1.516561 A    (     2.865885 A.U.)
 R30:     1.627742 RAD  (    93.262742 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.7067182   2   0   0
      2.4271603   0   2   0
      0.7047821   0   0   2
      0.0104821   1   1   0
      0.1414484   1   0   1
     -0.0378216   0   1   1
     -6.7520068   3   0   0
    -11.1778767   0   3   0
     -0.7170937   0   0   3
     -0.0592131   2   1   0
      0.1395978   1   2   0
     -0.3922480   2   0   1
     -0.0252722   0   2   1
     -0.0673508   1   1   1
     -0.7476909   1   0   2
     -0.0709981   0   1   2
     22.7210320   4   0   0
     44.2218773   0   4   0
      1.6020836   0   0   4
      0.3017841   3   1   0
     -0.0982303   1   3   0
     -0.2163678   2   2   0
      0.7585769   3   0   1
      0.1708259   0   3   1
      0.2427988   2   1   1
     -0.0482226   1   2   1
      0.6384516   2   0   2
     -0.3855190   0   2   2
     -0.0336465   1   1   2
      1.5195298   1   0   3
     -0.4505470   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:              A              B              C
 CENTER  1:     2.03287179     0.00208040     0.00000000    MASS: 27.976927 AMU
 CENTER  2:    -0.44387836    -0.01238306     0.00000000    MASS:126.904468 AMU
 CENTER  3:    -0.53913931     1.50151288     0.00000000    MASS:  1.007825 AMU
 MOMENTS:       3.80554417   233.99078342   237.79632759    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
           A            B            C        UNIT
         7.3561       0.1196       0.1177     1/CM
      220530.6       3586.6       3529.2     MHZ

 PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
 -------------------------------+-------------------------------
 ^

 ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


 HARMONIC FORCE FIELD
```

```
--------------------
F11:     1.7067 AJ/A**2    F12:     0.0105 AJ/A**2    F1A:     0.1414 AJ/A
                           F22:     2.4272 AJ/A**2    F2A:    -0.0378 AJ/A
                                                      FAA:     0.7048 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927     126.904468       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       352.35561      726.56628     2030.08614  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
              R1             R2             R3             FREQUENCY
Q1:        0.99994342     0.00007465    -0.01063727        352.35560884 S
Q2:        0.22087470     0.01132562     0.97523643        726.56627557 B
Q3:        0.00350417     0.99981436    -0.01894641       2030.08613604 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S     0.00000000    -0.12745826     0.07272586
         B     0.12745826     0.00000000    -0.98917407
         A    -0.07272586     0.98917407     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00157250 1/CM   AABB:    -0.00000021 1/CM   ABAB:  -0.00000320 1/CM
BBBB:    -0.00000022 1/CM   BBCC:    -0.00000021 1/CM
CCCC:    -0.00000021 1/CM   CCAA:    -0.00000061 1/CM

AAAA:      -47.14236 MHZ    AABB:       -0.00637 MHZ    ABAB:     -0.09586 MHZ
BBBB:       -0.00658 MHZ    BBCC:       -0.00638 MHZ
CCCC:       -0.00618 MHZ    CCAA:       -0.01824 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.73561095E+01 1/CM   220530.61940 MHZ
       B:  0.11963749E+00 1/CM     3586.64187 MHZ
       C:  0.11772229E+00 1/CM     3529.22545 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.53192115E-07 1/CM        0.00159 MHZ
     DJK:  0.16976176E-05 1/CM        0.05089 MHZ
      DK:  0.39137414E-03 1/CM       11.73310 MHZ
      R5: -0.37450728E-06 1/CM       -0.01123 MHZ
      R6: -0.50160815E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.84454615E-09 1/CM        0.00003 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.53202148E-07 1/CM        0.00159 MHZ
DELTA-JK:  0.16975574E-05 1/CM        0.05089 MHZ
 DELTA-K:  0.39137419E-03 1/CM       11.73310 MHZ
   DEL-J:  0.84454615E-09 1/CM        0.00003 MHZ
   DEL-K:  0.90065795E-06 1/CM        0.02700 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.53142563E-07 1/CM        0.00159 MHZ
    ~DJK:  0.16979149E-05 1/CM        0.05090 MHZ
     ~DK:  0.39137389E-03 1/CM       11.73309 MHZ
  ~DEL-J:  0.84454615E-09 1/CM        0.00003 MHZ
```

```
     ~R6: -0.29792091E-10 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 --------------------------------------------------
                      A              B              C
 ALPHA    S    -0.00056962     0.00054538     0.00053632  1/CM
          B    -0.12110454     0.00025786     0.00038914  1/CM
          A     0.20937445    -0.00010391    -0.00005484  1/CM

                      A              B              C
 ALPHA    S      -17.07664       16.35010       16.07841  MHZ
          B    -3630.62275        7.73055       11.66610  MHZ
          A     6276.88819       -3.11501       -1.64416  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S              B              A
 X(I,J):  S    -1.18520707    -2.80441463     0.42876194  1/CM
          B    -2.80441463    -1.96218629   -11.61963172  1/CM
          A     0.42876194   -11.61963172   -36.23527653  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.62524584  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (1)H (28)Si (127)I    EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.441326 A    (     4.613439 A.U.)
 R20:     1.507096 A    (     2.847999 A.U.)
 R30:     2.054533 RAD  (   117.716051 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.6697206   2   0   0
      2.2958239   0   2   0
      0.3479765   0   0   2
     -0.0698777   1   1   0
      0.0559207   1   0   1
      0.0414482   0   1   1
     -7.9477305   3   0   0
    -12.3112718   0   3   0
      0.0794554   0   0   3
     -0.0073986   2   1   0
      0.0480003   1   2   0
     -0.1984167   2   0   1
      0.0240067   0   2   1
     -0.0903829   1   1   1
     -0.3397647   1   0   2
     -0.2315593   0   1   2
     24.7171360   4   0   0
     44.5989630   0   4   0
     -1.1424493   0   0   4
      0.3819643   3   1   0
      0.0407290   1   3   0
      0.4772143   2   2   0
      0.3777884   3   0   1
     -0.1223795   0   3   1
      0.0193858   2   1   1
     -0.1577610   1   2   1
     -0.0765316   2   0   2
     -0.4498110   0   2   2
      0.0831880   1   1   2
```

```
     0.4286363   1   0   3
     0.3673616   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A              B              C
CENTER  1:     2.00751776     0.01386846     0.00000000    MASS: 27.976927 AMU
CENTER  2:    -0.43344407    -0.01348415     0.00000000    MASS:126.904468 AMU
CENTER  3:    -1.14919699     1.31292791     0.00000000    MASS:  1.007825 AMU
MOMENTS:       2.93203824   229.02640636   231.95844460    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A            B            C        UNIT
        9.5476       0.1222       0.1207     1/CM
     286230.6       3664.4       3618.1     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
-------------------------------+-----------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.6697 AJ/A**2    F12:    -0.0699 AJ/A**2    F1A:     0.0559 AJ/A
                           F22:     2.2958 AJ/A**2    F2A:     0.0414 AJ/A
                                                      FAA:     0.3480 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927     126.904468       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       350.18310      514.61388     1974.49228  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99992956     0.00529826    -0.01062077        350.18309505 S
Q2:        0.21107213    -0.00451233     0.97746007        514.61387644 B
Q3:       -0.03407131     0.99924298     0.01877813       1974.49228266 A


CORIOLIS COUPLING MATRICES
--------------------------
                   S              B              A
ZETA-C   S     0.00000000    -0.12045279     0.06563368
         B     0.12045279    -0.00000000    -0.99054699
         A    -0.06563368     0.99054699     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.01539411 1/CM   AABB:    -0.00000209 1/CM   ABAB:  -0.00000675 1/CM
BBBB:    -0.00000024 1/CM   BBCC:    -0.00000023 1/CM
CCCC:    -0.00000023 1/CM   CCAA:    -0.00000450 1/CM

AAAA:     -461.50376 MHZ    AABB:       -0.06260 MHZ    ABAB:     -0.20231 MHZ
BBBB:       -0.00708 MHZ    BBCC:       -0.00691 MHZ
CCCC:       -0.00676 MHZ    CCAA:       -0.13477 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.95476243E+01 1/CM   286230.58214 MHZ
       B:  0.12223125E+00 1/CM     3664.40066 MHZ
```

```
       C:  0.12068461E+00 1/CM     3618.03358 MHZ

 FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
 --------------------------------------------
      DJ:  0.57707023E-07 1/CM        0.00173 MHZ
     DJK:  0.49047357E-05 1/CM        0.14704 MHZ
      DK:  0.38435646E-02 1/CM      115.22717 MHZ
      R5: -0.69277805E-06 1/CM       -0.02077 MHZ
      R6: -0.82080206E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.66725711E-09 1/CM        0.00002 MHZ

 A-REDUCTION DISTORTION CONSTANTS
 --------------------------------
  DELTA-J:  0.57723439E-07 1/CM        0.00173 MHZ
 DELTA-JK:  0.49046372E-05 1/CM        0.14704 MHZ
  DELTA-K:  0.38435646E-02 1/CM      115.22717 MHZ
    DEL-J:  0.66725711E-09 1/CM        0.00002 MHZ
    DEL-K:  0.17857537E-05 1/CM        0.05354 MHZ

 S-REDUCTION DISTORTION CONSTANTS
 --------------------------------
     ~DJ:  0.57650188E-07 1/CM        0.00173 MHZ
    ~DJK:  0.49050767E-05 1/CM        0.14705 MHZ
     ~DK:  0.38435643E-02 1/CM      115.22716 MHZ
  ~DEL-J:  0.66725711E-09 1/CM        0.00002 MHZ
     ~R6: -0.36625664E-10 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                      A             B             C
 ALPHA    S     0.01360583    0.00073110    0.00072538  1/CM
          B    -0.42135450    0.00017559    0.00033938  1/CM
          A     0.43135754    0.00020576    0.00026528  1/CM

                      A             B             C
 ALPHA    S      407.89267      21.91796      21.74644  MHZ
          B   -12631.89044       5.26409      10.17423  MHZ
          A    12931.77399       6.16852       7.95303  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S             B             A
 X(I,J):  S    -2.08966024   -3.57150110   -1.01431346  1/CM
          B    -3.57150110   -4.89707003  -21.28584328  1/CM
          A    -1.01431346  -21.28584328  -60.50247790  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.19121050  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (1)H (28)Si (127)I    TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.432950 A    (     4.597611 A.U.)
 R20:     1.487007 A    (     2.810036 A.U.)
 R30:     2.032387 RAD  (   116.447188 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.8975705   2   0   0
      2.6809449   0   2   0
      0.4354930   0   0   2
     -0.0308247   1   1   0
```

```
     0.0453792   1   0   1
     0.0023994   0   1   1
    -7.8811484   3   0   0
   -12.9047838   0   3   0
    -0.2026184   0   0   3
    -0.0757772   2   1   0
     0.0182618   1   2   0
    -0.1964002   2   0   1
     0.0002234   0   2   1
    -0.0509632   1   1   1
    -0.3321586   1   0   2
    -0.1537636   0   1   2
    26.1694021   4   0   0
    49.3113344   0   4   0
    -0.0030342   0   0   4
     0.1242602   3   1   0
    -0.0729509   1   3   0
    -0.0556659   2   2   0
     0.2882069   3   0   1
    -0.0923915   0   3   1
     0.1209364   2   1   1
    -0.0260804   1   2   1
     0.1621498   2   0   2
    -0.3181371   0   2   2
     0.1022023   1   1   2
     0.3349286   1   0   3
     0.1023299   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A             B             C
CENTER  1:     2.00007116     0.01315211     0.00000000    MASS: 27.976927 AMU
CENTER  2:    -0.43211621    -0.01330736     0.00000000    MASS:126.904468 AMU
CENTER  3:    -1.10968412     1.31055317     0.00000000    MASS:  1.007825 AMU
MOMENTS:       2.91971478   227.24843673   230.16815151    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        9.5879      0.1232      0.1216    1/CM
       287438.7    3693.0      3646.2    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.8976 AJ/A**2    F12:    -0.0308 AJ/A**2    F1A:     0.0454 AJ/A
                           F22:     2.6809 AJ/A**2    F2A:     0.0024 AJ/A
                                                      FAA:     0.4355 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927     126.904468       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       374.26713      583.74291     2133.42866  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99999110     0.00414832     0.00076264        374.26712949 S
Q2:        0.10041249     0.00305155     0.99494121        583.74291205 B
```

```
Q3:       -0.01447515     0.99989515     0.00039449       2133.42865525 A


CORIOLIS COUPLING MATRICES
--------------------------
                      S              B              A
ZETA-C   S     0.00000000    -0.12331311     0.03127996
         B     0.12331311    -0.00000000    -0.99187471
         A    -0.03127996     0.99187471     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.01117600 1/CM   AABB:    -0.00000035 1/CM   ABAB:  -0.00000550 1/CM
BBBB:    -0.00000021 1/CM   BBCC:    -0.00000021 1/CM
CCCC:    -0.00000020 1/CM   CCAA:    -0.00000214 1/CM

AAAA:     -335.04820 MHZ    AABB:       -0.01051 MHZ    ABAB:     -0.16499 MHZ
BBBB:       -0.00637 MHZ    BBCC:       -0.00621 MHZ
CCCC:       -0.00607 MHZ    CCAA:       -0.06416 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.95879226E+01 1/CM   287438.69728 MHZ
       B:  0.12318740E+00 1/CM     3693.06551 MHZ
       C:  0.12162348E+00 1/CM     3646.18043 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.51839353E-07 1/CM        0.00155 MHZ
     DJK:  0.32706897E-05 1/CM        0.09805 MHZ
      DK:  0.27906786E-02 1/CM       83.66244 MHZ
      R5: -0.57575093E-06 1/CM       -0.01726 MHZ
      R6: -0.65871957E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.63622128E-09 1/CM        0.00002 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.51852527E-07 1/CM        0.00155 MHZ
DELTA-JK:  0.32706107E-05 1/CM        0.09805 MHZ
 DELTA-K:  0.27906787E-02 1/CM       83.66244 MHZ
   DEL-J:  0.63622128E-09 1/CM        0.00002 MHZ
   DEL-K:  0.14704506E-05 1/CM        0.04408 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.51791789E-07 1/CM        0.00155 MHZ
    ~DJK:  0.32709751E-05 1/CM        0.09806 MHZ
     ~DK:  0.27906784E-02 1/CM       83.66244 MHZ
  ~DEL-J:  0.63622128E-09 1/CM        0.00002 MHZ
     ~R6: -0.30368971E-10 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                      A              B              C
ALPHA    S     0.00361791     0.00057525     0.00056981  1/CM
         B    -0.46250767     0.00010966     0.00024590  1/CM
         A     0.28602507     0.00008022     0.00011980  1/CM

                      A              B              C
ALPHA    S      108.46225       17.24547       17.08250  MHZ
         B   -13865.63163        3.28750        7.37201  MHZ
         A     8574.81625        2.40489        3.59162  MHZ
```

```
ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                     S              B              A
X(I,J):  S    -1.35963737    -1.90809409    -0.71376207  1/CM
         B    -1.90809409    -1.69421476   -13.74125122  1/CM
         A    -0.71376207   -13.74125122   -42.62609299  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -0.09915371  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (2)H (28)Si (127)I    GROUND STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.477409 A    (     4.681626 A.U.)
R20:     1.516561 A    (     2.865885 A.U.)
R30:     1.627742 RAD  (    93.262742 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     1.7067182   2   0   0
     2.4271603   0   2   0
     0.7047821   0   0   2
     0.0104821   1   1   0
     0.1414484   1   0   1
    -0.0378216   0   1   1
    -6.7520068   3   0   0
   -11.1778767   0   3   0
    -0.7170937   0   0   3
    -0.0592131   2   1   0
     0.1395978   1   2   0
    -0.3922480   2   0   1
    -0.0252722   0   2   1
    -0.0673508   1   1   1
    -0.7476909   1   0   2
    -0.0709981   0   1   2
    22.7210320   4   0   0
    44.2218773   0   4   0
     1.6020836   0   0   4
     0.3017841   3   1   0
    -0.0982303   1   3   0
    -0.2163678   2   2   0
     0.7585769   3   0   1
     0.1708259   0   3   1
     0.2427988   2   1   1
    -0.0482226   1   2   1
     0.6384516   2   0   2
    -0.3855190   0   2   2
    -0.0336465   1   1   2
     1.5195298   1   0   3
    -0.4505470   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A              B              C
CENTER  1:     2.03633865     0.00451021     0.00000000    MASS: 27.976927 AMU
CENTER  2:    -0.44028240    -0.02462122     0.00000000    MASS:126.904468 AMU
CENTER  3:    -0.54450753     1.48868399     0.00000000    MASS:  2.014102 AMU
MOMENTS:       7.54065715   234.48132637   242.02198352    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
       3.7124      0.1194      0.1157    1/CM
```

```
        111295.2      3579.1      3467.6    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.998)           OBLATE
-----------------------------+-----------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.7067 AJ/A**2    F12:     0.0105 AJ/A**2    F1A:     0.1414 AJ/A
                           F22:     2.4272 AJ/A**2    F2A:    -0.0378 AJ/A
                                                      FAA:     0.7048 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927     126.904468       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       352.08511      520.17754     1441.76518  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99956676    -0.00003883    -0.02943274        352.08510812 A
Q2:        0.26152872     0.01490854     0.96508055        520.17754402 B
Q3:        0.00313329     0.99979405    -0.02005101       1441.76517704 S


CORIOLIS COUPLING MATRICES
--------------------------
                     A              B              S
ZETA-C   A     0.00000000    -0.17778496     0.12077171
         B     0.17778496     0.00000000    -0.97663028
         S    -0.12077171     0.97663028    -0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00040223 1/CM   AABB:    -0.00000010 1/CM   ABAB:  -0.00000309 1/CM
BBBB:    -0.00000022 1/CM   BBCC:    -0.00000020 1/CM
CCCC:    -0.00000019 1/CM   CCAA:    -0.00000048 1/CM

AAAA:      -12.05867 MHZ    AABB:       -0.00291 MHZ    ABAB:     -0.09250 MHZ
BBBB:       -0.00652 MHZ    BBCC:       -0.00612 MHZ
CCCC:       -0.00576 MHZ    CCAA:       -0.01444 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.37124085E+01 1/CM   111295.20905 MHZ
       B:  0.11938719E+00 1/CM     3579.13801 MHZ
       C:  0.11566689E+00 1/CM     3467.60622 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.51173480E-07 1/CM        0.00153 MHZ
     DJK:  0.15851125E-05 1/CM        0.04752 MHZ
      DK:  0.98922193E-04 1/CM        2.96561 MHZ
      R5: -0.36087047E-06 1/CM       -0.01082 MHZ
      R6: -0.18529969E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.15818362E-08 1/CM        0.00005 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.51210540E-07 1/CM        0.00154 MHZ
DELTA-JK:  0.15848902E-05 1/CM        0.04751 MHZ
```

```
 DELTA-K:  0.98922378E-04 1/CM        2.96562 MHZ
   DEL-J:  0.15818362E-08 1/CM        0.00005 MHZ
   DEL-K:  0.86498324E-06 1/CM        0.02593 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.50986750E-07 1/CM        0.00153 MHZ
    ~DJK:  0.15862329E-05 1/CM        0.04755 MHZ
     ~DK:  0.98921259E-04 1/CM        2.96558 MHZ
  ~DEL-J:  0.15818362E-08 1/CM        0.00005 MHZ
     ~R6: -0.11189511E-09 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    A    -0.00051513     0.00053897     0.00052785  1/CM
         B    -0.04463566     0.00012499     0.00029412  1/CM
         S     0.07488783    -0.00006948    -0.00000318  1/CM

                    A              B              C
ALPHA    A      -15.44328       16.15790       15.82469  MHZ
         B    -1338.14346        3.74719        8.81751  MHZ
         S     2245.08071       -2.08282       -0.09537  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    A              B              S
X(I,J):  A    -1.14007277    -2.19183695     0.32016680  1/CM
         B    -2.19183695    -0.95461596    -5.83479940  1/CM
         S     0.32016680    -5.83479940   -18.27270913  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -0.71352468  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (2)H (28)Si (127)I    EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.441326 A    (     4.613439 A.U.)
 R20:     1.507096 A    (     2.847999 A.U.)
 R30:     2.054533 RAD  (   117.716051 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.6697206   2   0   0
      2.2958239   0   2   0
      0.3479765   0   0   2
     -0.0698777   1   1   0
      0.0559207   1   0   1
      0.0414482   0   1   1
     -7.9477305   3   0   0
    -12.3112718   0   3   0
      0.0794554   0   0   3
     -0.0073986   2   1   0
      0.0480003   1   2   0
     -0.1984167   2   0   1
      0.0240067   0   2   1
     -0.0903829   1   1   1
     -0.3397647   1   0   2
     -0.2315593   0   1   2
     24.7171360   4   0   0
     44.5989630   0   4   0
     -1.1424493   0   0   4
```

```
     0.3819643   3   1   0
     0.0407290   1   3   0
     0.4772143   2   2   0
     0.3777884   3   0   1
    -0.1223795   0   3   1
     0.0193858   2   1   1
    -0.1577610   1   2   1
    -0.0765316   2   0   2
    -0.4498110   0   2   2
     0.0831880   1   1   2
     0.4286363   1   0   3
     0.3673616   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A             B             C
CENTER  1:     2.01470346     0.02783329     0.00000000    MASS: 27.976927 AMU
CENTER  2:    -0.42580382    -0.02663726     0.00000000    MASS:126.904468 AMU
CENTER  3:    -1.15624931     1.29174075     0.00000000    MASS:  2.014102 AMU
MOMENTS:       5.76608879   231.24683753   237.01292632    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         4.8549      0.1211      0.1181    1/CM
      145547.4      3629.2      3540.9    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.6697 AJ/A**2    F12:    -0.0699 AJ/A**2    F1A:     0.0559 AJ/A
                           F22:     2.2958 AJ/A**2    F2A:     0.0414 AJ/A
                                                      FAA:     0.3480 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                27.976927     126.904468       2.014102  AMU
FUNDAMENTAL FREQUENCIES:      349.09164      370.01112     1402.35145  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99421642     0.01099414    -0.10683086        349.09163960 S
Q2:        0.55629161     0.00343162     0.83098007        370.01112253 B
Q3:       -0.03811762     0.99910692     0.01823194       1402.35144697 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S             B             A
ZETA-C   S     0.00000000    -0.16660663     0.27759214
         B     0.16660663     0.00000000    -0.94614208
         A    -0.27759214     0.94614208     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00410319 1/CM   AABB:     0.00000043 1/CM   ABAB:  -0.00000632 1/CM
BBBB:    -0.00000023 1/CM   BBCC:    -0.00000022 1/CM
```

```
CCCC:    -0.00000021 1/CM   CCAA:    -0.00000202 1/CM

AAAA:     -123.01059 MHZ    AABB:        0.01296 MHZ    ABAB:     -0.18955 MHZ
BBBB:       -0.00688 MHZ    BBCC:       -0.00654 MHZ
CCCC:       -0.00626 MHZ    CCAA:       -0.06047 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.48549373E+01 1/CM   145547.36221 MHZ
       B:  0.12105759E+00 1/CM     3629.21532 MHZ
       C:  0.11811090E+00 1/CM     3540.87576 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.54717178E-07 1/CM        0.00164 MHZ
     DJK:  0.34481305E-05 1/CM        0.10337 MHZ
      DK:  0.10222950E-02 1/CM       30.64763 MHZ
      R5: -0.63662969E-06 1/CM       -0.01909 MHZ
      R6: -0.31123488E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.12857633E-08 1/CM        0.00004 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.54779425E-07 1/CM        0.00164 MHZ
DELTA-JK:  0.34477570E-05 1/CM        0.10336 MHZ
 DELTA-K:  0.10222953E-02 1/CM       30.64764 MHZ
   DEL-J:  0.12857633E-08 1/CM        0.00004 MHZ
   DEL-K:  0.16733848E-05 1/CM        0.05017 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.54519099E-07 1/CM        0.00163 MHZ
    ~DJK:  0.34493189E-05 1/CM        0.10341 MHZ
     ~DK:  0.10222940E-02 1/CM       30.64760 MHZ
  ~DEL-J:  0.12857633E-08 1/CM        0.00004 MHZ
     ~R6: -0.13016313E-09 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A             B             C
ALPHA    S     0.00242482    0.00065990    0.00073664  1/CM
         B    -0.15136485    0.00008032    0.00020926  1/CM
         A     0.15562294    0.00015664    0.00023548  1/CM

                    A             B             C
ALPHA    S       72.69418      19.78328      22.08395  MHZ
         B    -4537.80416       2.40788       6.27337  MHZ
         A     4665.45848       4.69596       7.05959  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S             B             A
X(I,J):  S    -1.99108300   -3.68342092   -1.17200240  1/CM
         B    -3.68342092   -2.03742354  -10.31765752  1/CM
         A    -1.17200240  -10.31765752  -30.51334137  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -2.63344113  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H (28)Si (127)I    TRIPLET STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.432950 A    (     4.597611 A.U.)
```

```
R20:     1.487007 A    (     2.810036 A.U.)
R30:     2.032387 RAD  (   116.447188 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     1.8975705   2   0   0
     2.6809449   0   2   0
     0.4354930   0   0   2
    -0.0308247   1   1   0
     0.0453792   1   0   1
     0.0023994   0   1   1
    -7.8811484   3   0   0
   -12.9047838   0   3   0
    -0.2026184   0   0   3
    -0.0757772   2   1   0
     0.0182618   1   2   0
    -0.1964002   2   0   1
     0.0002234   0   2   1
    -0.0509632   1   1   1
    -0.3321586   1   0   2
    -0.1537636   0   1   2
    26.1694021   4   0   0
    49.3113344   0   4   0
    -0.0030342   0   0   4
     0.1242602   3   1   0
    -0.0729509   1   3   0
    -0.0556659   2   2   0
     0.2882069   3   0   1
    -0.0923915   0   3   1
     0.1209364   2   1   1
    -0.0260804   1   2   1
     0.1621498   2   0   2
    -0.3181371   0   2   2
     0.1022023   1   1   2
     0.3349286   1   0   3
     0.1023299   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A             B             C
CENTER  1:     2.00701998     0.02642425     0.00000000    MASS: 27.976927 AMU
CENTER  2:    -0.42473976    -0.02630160     0.00000000    MASS:126.904468 AMU
CENTER  3:    -1.11656602     1.29016390     0.00000000    MASS:  2.014102 AMU
MOMENTS:       5.74517638   229.31892919   235.06410557    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        4.8726      0.1221      0.1191    1/CM
     146077.2      3659.7      3570.3     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.8976 AJ/A**2    F12:    -0.0308 AJ/A**2    F1A:     0.0454 AJ/A
                           F22:     2.6809 AJ/A**2    F2A:     0.0024 AJ/A
                                                      FAA:     0.4355 AJ
```

```
WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 27.976927     126.904468       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       374.18856      418.40965     1515.15770  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99995297     0.00851159     0.00464835        374.18856156 S
Q2:        0.08368176     0.00635241     0.99647228        418.40964971 B
Q3:       -0.01759536     0.99984518    -0.00016840       1515.15769697 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S     0.00000000    -0.17091200     0.03691298
         B     0.17091200    -0.00000000    -0.98459460
         A    -0.03691298     0.98459460     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00297478 1/CM   AABB:     0.00000090 1/CM   ABAB:  -0.00000517 1/CM
BBBB:    -0.00000021 1/CM   BBCC:    -0.00000020 1/CM
CCCC:    -0.00000019 1/CM   CCAA:    -0.00000092 1/CM

AAAA:      -89.18158 MHZ    AABB:        0.02694 MHZ    ABAB:     -0.15511 MHZ
BBBB:       -0.00621 MHZ    BBCC:       -0.00589 MHZ
CCCC:       -0.00562 MHZ    CCAA:       -0.02763 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.48726092E+01 1/CM   146077.15381 MHZ
       B:  0.12207516E+00 1/CM     3659.72136 MHZ
       C:  0.11909028E+00 1/CM     3570.23687 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.49292112E-07 1/CM        0.00148 MHZ
     DJK:  0.24941022E-05 1/CM        0.07477 MHZ
      DK:  0.74115087E-03 1/CM       22.21914 MHZ
      R5: -0.53235326E-06 1/CM       -0.01596 MHZ
      R6: -0.24940561E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.12173489E-08 1/CM        0.00004 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.49341993E-07 1/CM        0.00148 MHZ
DELTA-JK:  0.24938029E-05 1/CM        0.07476 MHZ
 DELTA-K:  0.74115112E-03 1/CM       22.21915 MHZ
   DEL-J:  0.12173489E-08 1/CM        0.00004 MHZ
   DEL-K:  0.13823559E-05 1/CM        0.04144 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.49124919E-07 1/CM        0.00147 MHZ
    ~DJK:  0.24951054E-05 1/CM        0.07480 MHZ
     ~DK:  0.74115004E-03 1/CM       22.21912 MHZ
  ~DEL-J:  0.12173489E-08 1/CM        0.00004 MHZ
     ~R6: -0.10853707E-09 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
```

```
 ALPHA     S      0.00178927      0.00056762      0.00058597  1/CM
           B     -0.17099724      0.00000208      0.00015277  1/CM
           A      0.10262311      0.00007429      0.00012600  1/CM

                       A               B               C
 ALPHA     S        53.64095        17.01694        17.56683  MHZ
           B     -5126.36831         0.06237         4.58003  MHZ
           A      3076.56360         2.22702         3.77743  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                       S               B               A
 X(I,J):   S     -1.36372377     -1.37595634     -0.50660099  1/CM
           B     -1.37595634     -0.85837564     -6.91254823  1/CM
           A     -0.50660099     -6.91254823    -21.49503469  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:        -0.03982517  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (1)H (74)Ge (19)F     GROUND STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:      1.764256 A    (      3.333961 A.U.)
 R20:      1.604165 A    (      3.031433 A.U.)
 R30:      1.645124 RAD  (     94.258679 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      3.8166093   2   0   0
      2.0389502   0   2   0
      0.8529392   0   0   2
      0.0894843   1   1   0
      0.1204236   1   0   1
     -0.0557621   0   1   1
    -20.7011911   3   0   0
     -8.9479070   0   3   0
     -1.4846530   0   0   3
     -0.2682941   2   1   0
      0.0899105   1   2   0
     -0.3454128   2   0   1
      0.0092882   0   2   1
     -0.2964489   1   1   1
     -1.0684001   1   0   2
     -0.4802399   0   1   2
    100.7426988   4   0   0
     58.1171261   0   4   0
     11.6203682   0   0   4
     -0.3400319   3   1   0
     -1.6359785   1   3   0
      0.0286499   2   2   0
      0.3177456   3   0   1
     -0.2161715   0   3   1
      1.0408932   2   1   1
      0.8541115   1   2   1
      1.8054573   2   0   2
     -0.2062982   0   2   2
      1.4640119   1   1   2
      3.3855096   1   0   3
      0.7932258   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
```

```
AXES:                A              B              C
CENTER  1:      0.37735671     0.00233612     0.00000000    MASS: 73.921178 AMU
CENTER  2:     -1.38417667    -0.08877914     0.00000000    MASS: 18.998403 AMU
CENTER  3:     -1.58510300     1.50221821     0.00000000    MASS:  1.007825 AMU
MOMENTS:        4.02589396    82.12711339    86.15300735    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         6.9535      0.3409      0.3249    1/CM
      208460.3     10218.8      9741.3    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.995)           OBLATE
------------------------------+-----------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     3.8166 AJ/A**2    F12:     0.0895 AJ/A**2    F1A:     0.1204 AJ/A
                           F22:     2.0390 AJ/A**2    F2A:    -0.0558 AJ/A
                                                      FAA:     0.8529 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      18.998403       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       633.90414      794.67829     1904.07299  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.98755901     0.00735662     0.15707669        633.90414418 S
Q2:       -0.50241733     0.04293801     0.86355843        794.67828687 B
Q3:        0.04161098     0.99798700    -0.04785889       1904.07298817 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S              B              A
ZETA-C   S     0.00000000    -0.22738156    -0.18759357
         B     0.22738156     0.00000000    -0.95556595
         A     0.18759357     0.95556595     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00155257 1/CM   AABB:     0.00000244 1/CM   ABAB:  -0.00001968 1/CM
BBBB:    -0.00000156 1/CM   BBCC:    -0.00000141 1/CM
CCCC:    -0.00000129 1/CM   CCAA:    -0.00000117 1/CM

AAAA:      -46.54484 MHZ    AABB:        0.07320 MHZ    ABAB:     -0.59012 MHZ
BBBB:       -0.04675 MHZ    BBCC:       -0.04233 MHZ
CCCC:       -0.03854 MHZ    CCAA:       -0.03512 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.69534865E+01 1/CM   208460.28754 MHZ
       B:  0.34086407E+00 1/CM    10218.84799 MHZ
       C:  0.32493130E+00 1/CM     9741.19547 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.35495942E-06 1/CM        0.01064 MHZ
```

```
     DJK:  0.88146547E-05 1/CM        0.26426 MHZ
      DK:  0.37897257E-03 1/CM       11.36131 MHZ
      R5: -0.22261628E-05 1/CM       -0.06674 MHZ
      R6: -0.33389205E-09 1/CM       -0.00001 MHZ
   DEL-J:  0.17123963E-07 1/CM        0.00051 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.35562720E-06 1/CM        0.01066 MHZ
DELTA-JK:  0.88106480E-05 1/CM        0.26414 MHZ
 DELTA-K:  0.37897591E-03 1/CM       11.36141 MHZ
   DEL-J:  0.17123963E-07 1/CM        0.00051 MHZ
   DEL-K:  0.55622703E-05 1/CM        0.16675 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.35228073E-06 1/CM        0.01056 MHZ
    ~DJK:  0.88307269E-05 1/CM        0.26474 MHZ
     ~DK:  0.37895918E-03 1/CM       11.36091 MHZ
  ~DEL-J:  0.17123963E-07 1/CM        0.00051 MHZ
     ~R6: -0.16732346E-08 1/CM       -0.00005 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    S    -0.00567812     0.00215849     0.00219123  1/CM
         B    -0.09586357     0.00072135     0.00152527  1/CM
         A     0.19573765    -0.00032180     0.00004761  1/CM

                    A              B              C
ALPHA    S     -170.22588       64.71001       65.69154  MHZ
         B    -2873.91751       21.62549       45.72650  MHZ
         A     5868.06739       -9.64739        1.42731  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -2.67259204    -2.10587223    -1.03913233  1/CM
         B    -2.10587223     3.10537532   -16.03800932  1/CM
         A    -1.03913233   -16.03800932    -8.19633873  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -1.26734630  1/CM

-------------------------------------------------------------------------------
----------------------------------------- (1)H (74)Ge (19)F     EXCITED STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     1.758417 A    (     3.322927 A.U.)
R20:     1.640350 A    (     3.099813 A.U.)
R30:     2.000230 RAD  (   114.604716 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     3.8899877   2   0   0
     1.0465791   0   2   0
     0.2324469   0   0   2
    -0.0578509   1   1   0
     0.0738237   1   0   1
     0.1128786   0   1   1
   -21.8655393   3   0   0
    -8.5267927   0   3   0
     0.3629284   0   0   3
```

```
    -0.1149903   2   1   0
    -0.0836556   1   2   0
    -0.3095334   2   0   1
    -0.1929674   0   2   1
    -0.2096827   1   1   1
     0.1667693   1   0   2
    -0.1698798   0   1   2
   108.5797316   4   0   0
    25.5826275   0   4   0
     5.5217362   0   0   4
     1.1128784   3   1   0
     1.5759018   1   3   0
     0.6634255   2   2   0
    -0.9204755   3   0   1
    -0.5183802   0   3   1
     0.0893022   2   1   1
     0.2520985   1   2   1
    -2.6355138   2   0   2
    -2.5453945   0   2   2
    -1.7038188   1   1   2
    -0.3684284   1   0   3
    -1.0620005   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
--------------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      0.38211697     0.00807428     0.00000000    MASS: 73.921178 AMU
CENTER  2:     -1.37289417    -0.10264737     0.00000000    MASS: 18.998403 AMU
CENTER  3:     -2.14693966     1.34276837     0.00000000    MASS:  1.007825 AMU
MOMENTS:        3.35781151    85.09859362    88.45640513    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
        8.3370       0.3290       0.3165      1/CM
      249936.3       9862.0       9487.6      MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.997)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     3.8900 AJ/A**2    F12:     -0.0579 AJ/A**2    F1A:      0.0738 AJ/A
                           F22:      1.0466 AJ/A**2    F2A:      0.1129 AJ/A
                                                       FAA:      0.2324 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      18.998403       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       392.52043      653.27259     1366.19717  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:         0.43303422    -0.00610010     0.90135684        392.52042630 B
Q2:         0.99935619     0.03577193    -0.00275221        653.27259195 S
Q3:        -0.18136840     0.97750326     0.10767026       1366.19717139 A


CORIOLIS COUPLING MATRICES
--------------------------
```

```
                    B              S              A
ZETA-C   B      0.00000000     0.17513971    -0.96836551
         S     -0.17513971     0.00000000     0.17774789
         A      0.96836551    -0.17774789     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.02083155 1/CM   AABB:     0.00004714 1/CM   ABAB:  -0.00006163 1/CM
BBBB:    -0.00000153 1/CM   BBCC:    -0.00000135 1/CM
CCCC:    -0.00000123 1/CM   CCAA:     0.00001361 1/CM

AAAA:     -624.51405 MHZ    AABB:        1.41308 MHZ    ABAB:     -1.84769 MHZ
BBBB:       -0.04581 MHZ    BBCC:       -0.04036 MHZ
CCCC:       -0.03677 MHZ    CCAA:        0.40793 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.83369776E+01 1/CM   249936.30811 MHZ
       B:  0.32896953E+00 1/CM     9862.25875 MHZ
       C:  0.31646236E+00 1/CM     9487.30301 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.34238311E-06 1/CM        0.01026 MHZ
     DJK:  0.14945829E-04 1/CM        0.44806 MHZ
      DK:  0.51925983E-02 1/CM      155.67018 MHZ
      R5: -0.55990926E-05 1/CM       -0.16786 MHZ
      R6: -0.96637544E-09 1/CM       -0.00003 MHZ
   DEL-J:  0.18850680E-07 1/CM        0.00057 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.34431586E-06 1/CM        0.01032 MHZ
DELTA-JK:  0.14934233E-04 1/CM        0.44772 MHZ
 DELTA-K:  0.51926079E-02 1/CM      155.67047 MHZ
   DEL-J:  0.18850680E-07 1/CM        0.00057 MHZ
   DEL-K:  0.16152004E-04 1/CM        0.48422 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.33801409E-06 1/CM        0.01013 MHZ
    ~DJK:  0.14972043E-04 1/CM        0.44885 MHZ
     ~DK:  0.51925764E-02 1/CM      155.66953 MHZ
  ~DEL-J:  0.18850680E-07 1/CM        0.00057 MHZ
     ~R6: -0.31508824E-08 1/CM       -0.00009 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    B    -0.10102129    -0.00297127    -0.00071117  1/CM
         S    -0.01687425     0.00242809     0.00225191  1/CM
         A     1.24004722     0.00054640     0.00223760  1/CM

                    A              B              C
ALPHA    B    -3028.54209      -89.07636      -21.32026  MHZ
         S     -505.87730       72.79219       67.51055  MHZ
         A    37175.68141       16.38061       67.08146  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    B              S              A
X(I,J):  B    14.87790219    -2.40022296   -83.36233126  1/CM
         S    -2.40022296    -3.49687335    -5.13903471  1/CM
```

```
         A   -83.36233126    -5.13903471  -198.56536355  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -3.60778442  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (1)H (74)Ge (19)F     TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     1.752891 A    (     3.312485 A.U.)
 R20:     1.558421 A    (     2.944990 A.U.)
 R30:     2.026812 RAD  (   116.127749 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      4.0947745   2   0   0
      2.1649172   0   2   0
      0.3307558   0   0   2
     -0.0009013   1   1   0
      0.1022451   1   0   1
      0.0645418   0   1   1
    -22.6604692   3   0   0
    -11.4515393   0   3   0
      0.5183923   0   0   3
     -0.2881660   2   1   0
     -0.1684203   1   2   0
     -0.2985319   2   0   1
     -0.3085009   0   2   1
     -0.2375048   1   1   1
      0.3131487   1   0   2
      0.1637269   0   1   2
    111.2515869   4   0   0
     38.9733764   0   4   0
      8.3193178   0   0   4
     -0.9512342   3   1   0
      1.8256941   1   3   0
     -0.3697819   2   2   0
     -0.9211250   3   0   1
      2.3667134   0   3   1
     -0.2656168   2   1   1
     -0.0045792   1   2   1
     -4.1995020   2   0   2
     -4.0962709   0   2   2
     -3.0371871   1   1   2
     -1.2027900   1   0   3
     -3.3778513   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------------
 AXES:                A             B             C
 CENTER  1:     0.38094162     0.00753449     0.00000000    MASS: 73.921178 AMU
 CENTER  2:    -1.36888358    -0.09615810     0.00000000    MASS: 18.998403 AMU
 CENTER  3:    -2.13633466     1.26003212     0.00000000    MASS:  1.007825 AMU
 MOMENTS:       2.95569111    84.56558650    87.52127761    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
           A           B           C        UNIT
         9.4712      0.3310      0.3199    1/CM
      283940.0      9924.1      9589.0    MHZ

 PROLATE          ASYMMETRIC ROTOR (K=-0.998)           OBLATE
 -------------------------------+-------------------------------
 ^
```

```
ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     4.0948 AJ/A**2    F12:    -0.0008 AJ/A**2    F1A:     0.1022 AJ/A
                           F22:     2.1666 AJ/A**2    F2A:     0.0645 AJ/A
                                                      FAA:     0.3306 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      18.998403       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       502.31545      673.78298     1960.31899  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
                R1             R2             R3             FREQUENCY
Q1:         0.55321373     0.02475060     0.83267159        502.31545381 B
Q2:         0.99926980     0.02575673    -0.02822152        673.78298233 S
Q3:        -0.05027289     0.99838024     0.02663718       1960.31898868 A


CORIOLIS COUPLING MATRICES
--------------------------
                      B              S              A
ZETA-C   B     0.00000000     0.19794725    -0.94858945
         S    -0.19794725     0.00000000     0.24697154
         A     0.94858945    -0.24697154     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:     -0.01656208 1/CM   AABB:      0.00003292 1/CM   ABAB:  -0.00004491 1/CM
BBBB:     -0.00000140 1/CM   BBCC:     -0.00000127 1/CM
CCCC:     -0.00000117 1/CM   CCAA:      0.00001185 1/CM

AAAA:      -496.51866 MHZ    AABB:         0.98695 MHZ    ABAB:     -1.34641 MHZ
BBBB:        -0.04189 MHZ    BBCC:        -0.03799 MHZ
CCCC:        -0.03506 MHZ    CCAA:         0.35514 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.94712196E+01 1/CM   283940.02662 MHZ
       B:  0.33103969E+00 1/CM     9924.32039 MHZ
       C:  0.31984696E+00 1/CM     9588.77092 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.31983900E-06 1/CM        0.00959 MHZ
     DJK:  0.10624175E-04 1/CM        0.31850 MHZ
      DK:  0.41295758E-02 1/CM      123.80157 MHZ
      R5: -0.42896011E-05 1/CM       -0.12860 MHZ
      R6: -0.51078613E-09 1/CM       -0.00002 MHZ
   DEL-J:  0.14249119E-07 1/CM        0.00043 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.32086058E-06 1/CM        0.00962 MHZ
DELTA-JK:  0.10618045E-04 1/CM        0.31832 MHZ
 DELTA-K:  0.41295810E-02 1/CM      123.80173 MHZ
   DEL-J:  0.14249119E-07 1/CM        0.00043 MHZ
   DEL-K:  0.11918182E-04 1/CM        0.35730 MHZ

S-REDUCTION DISTORTION CONSTANTS
```

```
--------------------------------
     ~DJ:  0.31721417E-06 1/CM        0.00951 MHZ
    ~DJK:  0.10639924E-04 1/CM        0.31898 MHZ
     ~DK:  0.41295627E-02 1/CM      123.80118 MHZ
  ~DEL-J:  0.14249119E-07 1/CM        0.00043 MHZ
     ~R6: -0.18232042E-08 1/CM       -0.00005 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                     A              B              C
ALPHA    B    -0.22665894    -0.00234519    -0.00073508  1/CM
         S    -0.03649495     0.00227201     0.00210399  1/CM
         A     0.36991095     0.00065745     0.00100586  1/CM

                     A              B              C
ALPHA    B    -6795.06418      -70.30703      -22.03720  MHZ
         S    -1094.09122       68.11327       63.07605  MHZ
         A    11089.65163       19.70981       30.15491  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                     B              S              A
X(I,J):  B    18.51912022     2.36276092   -28.65407766  1/CM
         S     2.36276092    -3.30016318    -1.25432429  1/CM
         A   -28.65407766    -1.25432429   -63.04243044  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -4.17427701  1/CM

------------------------------------------------------------------------------------
------------------------------------------ (2)H (74)Ge (19)F     GROUND STATE
------------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     1.764256 A    (     3.333961 A.U.)
R20:     1.604165 A    (     3.031433 A.U.)
R30:     1.645124 RAD  (    94.258679 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     3.8166093   2   0   0
     2.0389502   0   2   0
     0.8529392   0   0   2
     0.0894843   1   1   0
     0.1204236   1   0   1
    -0.0557621   0   1   1
   -20.7011911   3   0   0
    -8.9479070   0   3   0
    -1.4846530   0   0   3
    -0.2682941   2   1   0
     0.0899105   1   2   0
    -0.3454128   2   0   1
     0.0092882   0   2   1
    -0.2964489   1   1   1
    -1.0684001   1   0   2
    -0.4802399   0   1   2
   100.7426988   4   0   0
    58.1171261   0   4   0
    11.6203682   0   0   4
    -0.3400319   3   1   0
    -1.6359785   1   3   0
     0.0286499   2   2   0
     0.3177456   3   0   1
    -0.2161715   0   3   1
```

```
     1.0408932   2   1   1
     0.8541115   1   2   1
     1.8054573   2   0   2
    -0.2062982   0   2   2
     1.4640119   1   1   2
     3.3855096   1   0   3
     0.7932258   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
------------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      0.39434515     0.00611619     0.00000000    MASS: 73.921178 AMU
CENTER  2:     -1.36043900    -0.17286541     0.00000000    MASS: 18.998403 AMU
CENTER  3:     -1.64057718     1.40611102     0.00000000    MASS:  2.014102 AMU
MOMENTS:        7.55983690    86.47783259    94.03766950    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         3.7030      0.3237      0.2977     1/CM
      111012.8      9704.7      8924.5     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.985)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     3.8166 AJ/A**2    F12:      0.0895 AJ/A**2    F1A:      0.1204 AJ/A
                           F22:      2.0390 AJ/A**2    F2A:     -0.0558 AJ/A
                                                       FAA:      0.8529 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                  73.921178      18.998403       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       538.86086      680.40154    1382.30532  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.78000287     0.05061372     0.62372573        538.86086030 B
Q2:        0.96882033    -0.02214980    -0.24677227        680.40153633 A
Q3:        0.04186987     0.99721316    -0.06174814       1382.30532115 S


CORIOLIS COUPLING MATRICES
--------------------------
                    B              A              S
ZETA-C   B      0.00000000     0.29960669    -0.73179811
         A     -0.29960669     0.00000000     0.61213345
         S      0.73179811    -0.61213345     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00046437 1/CM   AABB:     0.00000275 1/CM   ABAB:  -0.00001608 1/CM
BBBB:    -0.00000149 1/CM   BBCC:    -0.00000124 1/CM
CCCC:    -0.00000105 1/CM   CCAA:    -0.00000068 1/CM

AAAA:      -13.92151 MHZ    AABB:       0.08230 MHZ    ABAB:     -0.48192 MHZ
BBBB:       -0.04457 MHZ    BBCC:      -0.03716 MHZ
CCCC:       -0.03156 MHZ    CCAA:      -0.02037 MHZ
```

```
 ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
 -----------------------------------------------------
 AXIS   A:  0.37029899E+01 1/CM   111012.84600 MHZ
        B:  0.32371498E+00 1/CM     9704.73126 MHZ
        C:  0.29768725E+00 1/CM     8924.43955 MHZ

 FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
 --------------------------------------------
       DJ:  0.31552557E-06 1/CM        0.00946 MHZ
      DJK:  0.68900862E-05 1/CM        0.20656 MHZ
       DK:  0.10888729E-03 1/CM        3.26436 MHZ
       R5: -0.17817861E-05 1/CM       -0.05342 MHZ
       R6: -0.94181933E-09 1/CM       -0.00003 MHZ
    DEL-J:  0.27128348E-07 1/CM        0.00081 MHZ

 A-REDUCTION DISTORTION CONSTANTS
 --------------------------------
  DELTA-J:  0.31740921E-06 1/CM        0.00952 MHZ
 DELTA-JK:  0.68787844E-05 1/CM        0.20622 MHZ
  DELTA-K:  0.10889670E-03 1/CM        3.26464 MHZ
    DEL-J:  0.27128348E-07 1/CM        0.00081 MHZ
    DEL-K:  0.45455781E-05 1/CM        0.13627 MHZ

 S-REDUCTION DISTORTION CONSTANTS
 --------------------------------
      ~DJ:  0.30869009E-06 1/CM        0.00925 MHZ
     ~DJK:  0.69310991E-05 1/CM        0.20779 MHZ
      ~DK:  0.10885311E-03 1/CM        3.26333 MHZ
   ~DEL-J:  0.27128348E-07 1/CM        0.00081 MHZ
      ~R6: -0.43595594E-08 1/CM       -0.00013 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                     A              B              C
 ALPHA    B    -0.03149262     0.00059035     0.00144334  1/CM
          A    -0.01322326     0.00188507     0.00186660  1/CM
          S     0.07322232    -0.00006688     0.00030599  1/CM

                     A              B              C
 ALPHA    B     -944.12512       17.69810       43.27032  MHZ
          A     -396.42333       56.51297       55.95940  MHZ
          S     2195.15002       -2.00509        9.17342  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                     B              A              S
 X(I,J):  B     1.06376713    -1.64387000    -7.64346052  1/CM
          A    -1.64387000    -4.93669608    10.11411103  1/CM
          S    -7.64346052    10.11411103    -4.32422863  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -7.53107801  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (2)H (74)Ge (19)F     EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     1.758417 A    (     3.322927 A.U.)
 R20:     1.640350 A    (     3.099813 A.U.)
 R30:     2.000230 RAD  (   114.604716 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
```

```
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     3.8899877   2   0   0
     1.0465791   0   2   0
     0.2324469   0   0   2
    -0.0578509   1   1   0
     0.0738237   1   0   1
     0.1128786   0   1   1
   -21.8655393   3   0   0
    -8.5267927   0   3   0
     0.3629284   0   0   3
    -0.1149903   2   1   0
    -0.0836556   1   2   0
    -0.3095334   2   0   1
    -0.1929674   0   2   1
    -0.2096827   1   1   1
     0.1667693   1   0   2
    -0.1698798   0   1   2
   108.5797316   4   0   0
    25.5826275   0   4   0
     5.5217362   0   0   4
     1.1128784   3   1   0
     1.5759018   1   3   0
     0.6634255   2   2   0
    -0.9204755   3   0   1
    -0.5183802   0   3   1
     0.0893022   2   1   1
     0.2520985   1   2   1
    -2.6355138   2   0   2
    -2.5453945   0   2   2
    -1.7038188   1   1   2
    -0.3684284   1   0   3
    -1.0620005   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
--------------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      0.40460118     0.01608825     0.00000000    MASS: 73.921178 AMU
CENTER  2:     -1.34167934    -0.19086035     0.00000000    MASS: 18.998403 AMU
CENTER  3:     -2.19394594     1.20985901     0.00000000    MASS:  2.014102 AMU
MOMENTS:        6.07648143    92.98113715    99.05761858    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B           C        UNIT
         4.6069       0.3011      0.2826     1/CM
      138112.7       9025.9      8472.2     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.991)           OBLATE
-------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     3.8900 AJ/A**2    F12:    -0.0579 AJ/A**2    F1A:     0.0738 AJ/A
                           F22:     1.0466 AJ/A**2    F2A:     0.1129 AJ/A
                                                      FAA:     0.2324 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      18.998403       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       291.65610      645.27970      996.23544  1/CM
```

NORMAL COORDINATE DISPLACEMENTS

	R1	R2	R3	FREQUENCY	
Q1:	0.42654800	0.02383330	0.90415086	291.65609515	B
Q2:	0.99582333	0.09125280	0.00296930	645.27969858	S
Q3:	-0.36338192	0.92660231	0.09675609	996.23544446	A

CORIOLIS COUPLING MATRICES

		B	S	A
ZETA-C	B	-0.00000000	0.16209417	-0.95776913
	S	-0.16209417	-0.00000000	0.23749477
	A	0.95776913	-0.23749477	0.00000000

TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION

AAAA:	-0.00717521 1/CM	AABB:	0.00005343 1/CM	ABAB:	-0.00004233 1/CM
BBBB:	-0.00000167 1/CM	BBCC:	-0.00000127 1/CM		
CCCC:	-0.00000104 1/CM	CCAA:	0.00002008 1/CM		
AAAA:	-215.10732 MHZ	AABB:	1.60185 MHZ	ABAB:	-1.26903 MHZ
BBBB:	-0.05009 MHZ	BBCC:	-0.03811 MHZ		
CCCC:	-0.03131 MHZ	CCAA:	0.60192 MHZ		

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION

AXIS	A:	0.46069423E+01 1/CM	138112.65864 MHZ
	B:	0.30108194E+00 1/CM	9026.20979 MHZ
	C:	0.28259311E+00 1/CM	8471.92848 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS

DJ:	0.33400312E-06 1/CM	0.01001 MHZ
DJK:	0.21196239E-05 1/CM	0.06354 MHZ
DK:	0.17913483E-02 1/CM	53.70327 MHZ
R5:	-0.31870623E-05 1/CM	-0.09555 MHZ
R6:	-0.27039392E-08 1/CM	-0.00008 MHZ
DEL-J:	0.39155378E-07 1/CM	0.00117 MHZ

A-REDUCTION DISTORTION CONSTANTS

DELTA-J:	0.33941100E-06 1/CM	0.01018 MHZ
DELTA-JK:	0.20871766E-05 1/CM	0.06257 MHZ
DELTA-K:	0.17913753E-02 1/CM	53.70408 MHZ
DEL-J:	0.39155378E-07 1/CM	0.00117 MHZ
DEL-K:	0.11422699E-04 1/CM	0.34244 MHZ

S-REDUCTION DISTORTION CONSTANTS

~DJ:	0.32717535E-06 1/CM	0.00981 MHZ
~DJK:	0.21605905E-05 1/CM	0.06477 MHZ
~DK:	0.17913141E-02 1/CM	53.70225 MHZ
~DEL-J:	0.39155378E-07 1/CM	0.00117 MHZ
~R6:	-0.61178231E-08 1/CM	-0.00018 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS

		A	B	C	
ALPHA	B	-0.03476291	-0.00350727	-0.00095075	1/CM
	S	-0.01548770	0.00230002	0.00205775	1/CM
	A	0.50644725	0.00018465	0.00198713	1/CM

	A	B	C

```
ALPHA    B    -1042.16587     -105.14541      -28.50264  MHZ
         S     -464.30968       68.95299       61.68987  MHZ
         A    15182.90698        5.53568       59.57277  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                     B              S              A
X(I,J):  B     7.96648629    -2.55100708   -42.40046198  1/CM
         S    -2.55100708    -3.27852376   -10.55677937  1/CM
         A   -42.40046198   -10.55677937  -101.16630186  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -6.91355656  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (2)H (74)Ge (19)F     TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
R10:     1.752891 A    (     3.312485 A.U.)
R20:     1.558421 A    (     2.944990 A.U.)
R30:     2.026812 RAD  (   116.127749 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     4.0947998   2   0   0
     2.1666239   0   2   0
     0.3306064   0   0   2
    -0.0008201   1   1   0
     0.1022006   1   0   1
     0.0645444   0   1   1
   -22.6596708   3   0   0
   -11.4576655   0   3   0
     0.5168238   0   0   3
    -0.2880517   2   1   0
    -0.1686807   1   2   0
    -0.2974654   2   0   1
    -0.3078311   0   2   1
    -0.2367587   1   1   1
     0.3138605   1   0   2
     0.1651288   0   1   2
   111.2515869   4   0   0
    38.9733764   0   4   0
     8.3193178   0   0   4
    -0.9512342   3   1   0
     1.8256941   1   3   0
    -0.3697819   2   2   0
    -0.9211250   3   0   1
     2.3667134   0   3   1
    -0.2656168   2   1   1
    -0.0045792   1   2   1
    -4.1995020   2   0   2
    -4.0962709   0   2   2
    -3.0371871   1   1   2
    -1.2027900   1   0   3
    -3.3778513   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
AXES:                A             B             C
CENTER  1:     0.40335464     0.01486083     0.00000000    MASS: 73.921178 AMU
CENTER  2:    -1.33886112    -0.17833499     0.00000000    MASS: 18.998403 AMU
CENTER  3:    -2.17477894     1.13675986     0.00000000    MASS:  2.014102 AMU
MOMENTS:       5.35223558    92.33913930    97.69137488    10**(-40) G*CM**2
```

```
ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        5.2303      0.3032      0.2866    1/CM
     156801.6      9088.7      8590.7     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.993)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     4.0948 AJ/A**2    F12:    -0.0008 AJ/A**2    F1A:     0.1022 AJ/A
                           F22:     2.1666 AJ/A**2    F2A:     0.0645 AJ/A
                                                      FAA:     0.3306 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      18.998403       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       372.03988      669.67922     1422.88551  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.48437939     0.05545243     0.87309887        372.03988322 B
Q2:        0.99827786     0.05557528    -0.01878014        669.67922110 S
Q3:       -0.10771000     0.99393681     0.02209462       1422.88550513 A


CORIOLIS COUPLING MATRICES
--------------------------
                    B              S              A
ZETA-C   B     0.00000000     0.23967599    -0.92953469
         S    -0.23967599     0.00000000     0.28021543
         A     0.92953469    -0.28021543     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00572377 1/CM   AABB:     0.00003794 1/CM   ABAB:  -0.00003164 1/CM
BBBB:    -0.00000138 1/CM   BBCC:    -0.00000112 1/CM
CCCC:    -0.00000095 1/CM   CCAA:     0.00001672 1/CM

AAAA:     -171.59429 MHZ    AABB:        1.13755 MHZ    ABAB:     -0.94842 MHZ
BBBB:       -0.04137 MHZ    BBCC:       -0.03354 MHZ
CCCC:       -0.02846 MHZ    CCAA:        0.50126 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.52303377E+01 1/CM   156801.58268 MHZ
       B:  0.30317186E+00 1/CM     9088.86385 MHZ
       C:  0.28654870E+00 1/CM     8590.51413 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.28829681E-06 1/CM        0.00864 MHZ
     DJK:  0.15752198E-05 1/CM        0.04722 MHZ
      DK:  0.14290788E-02 1/CM       42.84270 MHZ
      R5: -0.26145140E-05 1/CM       -0.07838 MHZ
      R6: -0.14299703E-08 1/CM       -0.00004 MHZ
   DEL-J:  0.26898432E-07 1/CM        0.00081 MHZ
```

```
A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.29115675E-06 1/CM        0.00873 MHZ
DELTA-JK:  0.15580602E-05 1/CM        0.04671 MHZ
 DELTA-K:  0.14290931E-02 1/CM       42.84313 MHZ
   DEL-J:  0.26898432E-07 1/CM        0.00081 MHZ
   DEL-K:  0.86255359E-05 1/CM        0.25859 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.28389385E-06 1/CM        0.00851 MHZ
    ~DJK:  0.16016376E-05 1/CM        0.04802 MHZ
     ~DK:  0.14290567E-02 1/CM       42.84204 MHZ
  ~DEL-J:  0.26898432E-07 1/CM        0.00081 MHZ
     ~R6: -0.36314532E-08 1/CM       -0.00011 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    B    -0.08877109    -0.00272911    -0.00092042  1/CM
         S    -0.02251811     0.00213366     0.00191247  1/CM
         A     0.14660757     0.00075402     0.00107414  1/CM

                    A              B              C
ALPHA    B    -2661.29054      -81.81662      -27.59361  MHZ
         S     -675.07608       63.96564       57.33433  MHZ
         A     4395.18437       22.60498       32.20184  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    B              S              A
X(I,J):  B    10.45993961    -0.55515754   -13.65453314  1/CM
         S    -0.55515754    -3.82106456     1.49361444  1/CM
         A   -13.65453314     1.49361444   -33.06307406  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -2.01868176  1/CM

--------------------------------------------------------------------------------
------------------------------------------ (1)H (74)Ge (35)Cl    GROUND STATE
--------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.193162 A    (     4.144477 A.U.)
R20:     1.599399 A    (     3.022427 A.U.)
R30:     1.637892 RAD  (    93.844295 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     2.2376382   2   0   0
     2.0965631   0   2   0
     0.7891246   0   0   2
     0.0480481   1   1   0
     0.1522620   1   0   1
    -0.0607094   0   1   1
    -9.2643380   3   0   0
    -9.3737492   0   3   0
    -0.9395319   0   0   3
    -0.0854305   2   1   0
     0.0789967   1   2   0
    -0.5466743   2   0   1
     0.0147234   0   2   1
    -0.1881576   1   1   1
```

```
    -0.7824830   1   0   2
    -0.1855179   0   1   2
    34.8425126   4   0   0
    36.9369679   0   4   0
     2.9687272   0   0   4
     0.2776664   3   1   0
    -0.0465385   1   3   0
    -0.1273117   2   2   0
     0.5453372   3   0   1
     0.1511376   0   3   1
     0.7677108   2   1   1
     0.1279416   1   2   1
     1.2211838   2   0   2
    -0.6034673   0   2   2
     0.1299338   1   1   2
     1.1603017   1   0   3
     0.0071825   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      0.71908060     0.00137161     0.00000000    MASS: 73.921178 AMU
CENTER  2:     -1.47349454    -0.04744034     0.00000000    MASS: 34.968853 AMU
CENTER  3:     -1.61622406     1.54544997     0.00000000    MASS:  1.007825 AMU
MOMENTS:        4.12798787   193.91589304   198.04388091    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B           C        UNIT
         6.7815       0.1444      0.1414     1/CM
      203304.6       4327.9      4237.6     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.2376 AJ/A**2    F12:      0.0480 AJ/A**2    F1A:      0.1523 AJ/A
                           F22:      2.0966 AJ/A**2    F2A:     -0.0607 AJ/A
                                                       FAA:      0.7891 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      34.968853       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       395.67063      734.60672     1907.22850  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:         0.99944052     0.00130949     0.03342056        395.67063403 S
Q2:         0.10086209     0.02894233     0.99447935        734.60672023 B
Q3:         0.02040800     0.99899728    -0.03984910       1907.22849646 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S              B              A
ZETA-C   S     -0.00000000    -0.14887945     0.03865896
         B      0.14887945     0.00000000    -0.98809939
         A     -0.03865896     0.98809939     0.00000000
```

```
TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00140449 1/CM   AABB:     0.00000024 1/CM   ABAB:  -0.00000411 1/CM
BBBB:    -0.00000031 1/CM   BBCC:    -0.00000029 1/CM
CCCC:    -0.00000028 1/CM   CCAA:    -0.00000038 1/CM

AAAA:      -42.10565 MHZ    AABB:        0.00717 MHZ    ABAB:     -0.12326 MHZ
BBBB:       -0.00920 MHZ    BBCC:       -0.00882 MHZ
CCCC:       -0.00846 MHZ    CCAA:       -0.01142 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.67815120E+01 1/CM   203304.62198 MHZ
       B:  0.14436199E+00 1/CM     4327.86376 MHZ
       C:  0.14135207E+00 1/CM     4237.62857 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.73608657E-07 1/CM        0.00221 MHZ
     DJK:  0.19439648E-05 1/CM        0.05828 MHZ
      DK:  0.34910571E-03 1/CM       10.46593 MHZ
      R5: -0.47441354E-06 1/CM       -0.01422 MHZ
      R6: -0.12437116E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.15458191E-08 1/CM        0.00005 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.73633531E-07 1/CM        0.00221 MHZ
DELTA-JK:  0.19438156E-05 1/CM        0.05827 MHZ
 DELTA-K:  0.34910583E-03 1/CM       10.46593 MHZ
   DEL-J:  0.15458191E-08 1/CM        0.00005 MHZ
   DEL-K:  0.11682765E-05 1/CM        0.03502 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.73501109E-07 1/CM        0.00220 MHZ
    ~DJK:  0.19446101E-05 1/CM        0.05830 MHZ
     ~DK:  0.34910517E-03 1/CM       10.46591 MHZ
  ~DEL-J:  0.15458191E-08 1/CM        0.00005 MHZ
     ~R6: -0.66211101E-10 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A             B             C
ALPHA    S    -0.00078642    0.00064056    0.00062704  1/CM
         B    -0.09823476    0.00022369    0.00041926  1/CM
         A     0.19465093   -0.00015613   -0.00007938  1/CM

                    A             B             C
ALPHA    S      -23.57633      19.20360      18.79821  MHZ
         B    -2945.00404       6.70604      12.56916  MHZ
         A     5835.48837      -4.68065      -2.37975  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S             B             A
X(I,J):  S    -1.10526020   -1.81481183    0.75636072  1/CM
         B    -1.81481183   -1.28403009  -14.76387795  1/CM
         A     0.75636072  -14.76387795  -34.03117043  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -0.28104359  1/CM
```

```
------------------------------------------ (1)H (74)Ge (35)Cl    EXCITED STATE
--------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.165805 A    (     4.092780 A.U.)
 R20:     1.607764 A    (     3.038234 A.U.)
 R30:     2.007766 RAD  (   115.036511 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.2538866   2   0   0
      1.4595505   0   2   0
      0.3373848   0   0   2
     -0.0831177   1   1   0
      0.0428819   1   0   1
      0.0774215   0   1   1
    -11.0742330   3   0   0
    -10.0192627   0   3   0
      0.0882249   0   0   3
      0.0932693   2   1   0
      0.0006900   1   2   0
     -0.3495215   2   0   1
      0.0392002   0   2   1
     -0.1525383   1   1   1
     -0.3596400   1   0   2
     -0.4141630   0   1   2
     41.9127652   4   0   0
     34.6578431   0   4   0
     -0.9449498   0   0   4
      1.1467417   3   1   0
     -0.0221535   1   3   0
      0.7483732   2   2   0
      0.3169879   3   0   1
     -0.1049847   0   3   1
      0.2455197   2   1   1
      0.1197173   1   2   1
      0.1161844   2   0   2
     -0.8527596   0   2   2
      0.1451553   1   1   2
      0.2426312   1   0   3
      0.3514911   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:                A              B              C
 CENTER  1:     0.71528880     0.00628301     0.00000000    MASS: 73.921178 AMU
 CENTER  2:    -1.44949760    -0.05314676     0.00000000    MASS: 34.968853 AMU
 CENTER  3:    -2.17073586     1.38320986     0.00000000    MASS:  1.007825 AMU
 MOMENTS:       3.37076384   192.68956408   196.06032792    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
           A            B            C        UNIT
        8.3049       0.1453       0.1428     1/CM
      248975.9       4355.4       4280.5     MHZ

 PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
 -------------------------------+-------------------------------
 ^

 ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


 HARMONIC FORCE FIELD
```

```
--------------------
F11:     2.2539 AJ/A**2    F12:    -0.0831 AJ/A**2    F1A:     0.0429 AJ/A
                           F22:     1.4596 AJ/A**2    F2A:     0.0774 AJ/A
                                                      FAA:     0.3374 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      34.968853       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       395.58511      483.03457     1591.76662  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99696782     0.01515215     0.07632544        395.58511495 S
Q2:       -0.34844414    -0.01667062     0.93718129        483.03456910 B
Q3:       -0.08094978     0.99520233     0.05494954       1591.76662246 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S     0.00000000    -0.13020613    -0.11708049
         B     0.13020613     0.00000000    -0.98454991
         A     0.11708049     0.98454991     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.01205579 1/CM   AABB:     0.00000291 1/CM   ABAB:  -0.00000929 1/CM
BBBB:    -0.00000031 1/CM   BBCC:    -0.00000030 1/CM
CCCC:    -0.00000029 1/CM   CCAA:    -0.00000075 1/CM

AAAA:     -361.42343 MHZ    AABB:        0.08738 MHZ    ABAB:     -0.27864 MHZ
BBBB:       -0.00939 MHZ    BBCC:       -0.00904 MHZ
CCCC:       -0.00874 MHZ    CCAA:       -0.02243 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.83049424E+01 1/CM   248975.91563 MHZ
       B:  0.14528152E+00 1/CM     4355.43037 MHZ
       C:  0.14278137E+00 1/CM     4280.47804 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.75526854E-07 1/CM        0.00226 MHZ
     DJK:  0.39545714E-05 1/CM        0.11856 MHZ
      DK:  0.30099168E-02 1/CM       90.23504 MHZ
      R5: -0.93221455E-06 1/CM       -0.02795 MHZ
      R6: -0.23060448E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.13495735E-08 1/CM        0.00004 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.75572975E-07 1/CM        0.00227 MHZ
DELTA-JK:  0.39542947E-05 1/CM        0.11855 MHZ
 DELTA-K:  0.30099170E-02 1/CM       90.23505 MHZ
   DEL-J:  0.13495735E-08 1/CM        0.00004 MHZ
   DEL-K:  0.24666170E-05 1/CM        0.07395 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.75384059E-07 1/CM        0.00226 MHZ
    ~DJK:  0.39554282E-05 1/CM        0.11858 MHZ
     ~DK:  0.30099161E-02 1/CM       90.23502 MHZ
  ~DEL-J:  0.13495735E-08 1/CM        0.00004 MHZ
```

```
     ~R6: -0.94457723E-10 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 --------------------------------------------------
                      A              B              C
 ALPHA    S    -0.01403740     0.00082072     0.00081585  1/CM
          B    -0.24379003     0.00004433     0.00031959  1/CM
          A     0.72182639     0.00043948     0.00062769  1/CM

                      A              B              C
 ALPHA    S     -420.83068       24.60469       24.45845  MHZ
          B    -7308.64136        1.32902        9.58112  MHZ
          A    21639.81123       13.17521       18.81763  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S              B              A
 X(I,J):  S    -1.92959484    -2.11972878    -2.56840179  1/CM
          B    -2.11972878    -6.32416127   -48.74252215  1/CM
          A    -2.56840179   -48.74252215  -120.83803445  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.58696359  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (1)H (74)Ge (35)Cl    TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.155776 A    (     4.073828 A.U.)
 R20:     1.557275 A    (     2.942825 A.U.)
 R30:     1.998288 RAD  (   114.493475 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.4712703   2   0   0
      2.2434114   0   2   0
      0.4513081   0   0   2
     -0.0545285   1   1   0
      0.0698745   1   0   1
      0.0049681   0   1   1
    -11.3097953   3   0   0
    -11.6143944   0   3   0
     -0.1942164   0   0   3
     -0.0077979   2   1   0
     -0.0482843   1   2   0
     -0.2656971   2   0   1
      0.0087205   0   2   1
     -0.1246859   1   1   1
     -0.4260814   1   0   2
     -0.2715442   0   1   2
     48.7765980   4   0   0
     42.3150211   0   4   0
     -0.0351712   0   0   4
      0.9231861   3   1   0
     -0.3851255   1   3   0
     -0.1750171   2   2   0
     -0.2599343   3   0   1
      0.0845403   0   3   1
      0.2924952   2   1   1
      0.2195831   1   2   1
      0.1179795   2   0   2
     -0.6215855   0   2   2
      0.2566593   1   1   2
```

```
     0.4396613   1   0   3
     0.1383445   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A             B             C
CENTER  1:     0.71182623     0.00583228     0.00000000    MASS: 73.921178 AMU
CENTER  2:    -1.44342709    -0.05117863     0.00000000    MASS: 34.968853 AMU
CENTER  3:    -2.12739706     1.34798079     0.00000000    MASS:  1.007825 AMU
MOMENTS:       3.19714888   190.75152637   193.94867525    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A            B            C        UNIT
        8.7559       0.1468       0.1443     1/CM
     262496.1       4399.6       4327.1     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.4713 AJ/A**2    F12:    -0.0545 AJ/A**2    F1A:     0.0699 AJ/A
                           F22:     2.2434 AJ/A**2    F2A:     0.0050 AJ/A
                                                      FAA:     0.4513 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      34.968853       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       415.88007      577.57905     1972.35406  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99867564     0.01378441     0.04956768        415.88006716 S
Q2:       -0.11676438     0.00975712     0.99311172        577.57905063 B
Q3:       -0.03920109     0.99923122    -0.00048684       1972.35405697 A


CORIOLIS COUPLING MATRICES
--------------------------
                   S              B              A
ZETA-C   S     0.00000000    -0.13481378    -0.03317257
         B     0.13481378    -0.00000000    -0.99031552
         A     0.03317257     0.99031552     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00855102 1/CM   AABB:     0.00000161 1/CM   ABAB:  -0.00000731 1/CM
BBBB:    -0.00000029 1/CM   BBCC:    -0.00000028 1/CM
CCCC:    -0.00000027 1/CM   CCAA:    -0.00000077 1/CM

AAAA:     -256.35322 MHZ    AABB:        0.04819 MHZ    ABAB:     -0.21901 MHZ
BBBB:       -0.00876 MHZ    BBCC:       -0.00846 MHZ
CCCC:       -0.00819 MHZ    CCAA:       -0.02305 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.87559261E+01 1/CM   262496.06907 MHZ
       B:  0.14675722E+00 1/CM     4399.67102 MHZ
```

```
       C:  0.14433629E+00 1/CM     4327.09315 MHZ

 FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
 --------------------------------------------
      DJ:  0.70633004E-07 1/CM        0.00212 MHZ
     DJK:  0.33018308E-05 1/CM        0.09899 MHZ
      DK:  0.21343832E-02 1/CM       63.98720 MHZ
      R5: -0.76406991E-06 1/CM       -0.02291 MHZ
      R6: -0.15192760E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.11879174E-08 1/CM        0.00004 MHZ

 A-REDUCTION DISTORTION CONSTANTS
 --------------------------------
  DELTA-J:  0.70663389E-07 1/CM        0.00212 MHZ
 DELTA-JK:  0.33016485E-05 1/CM        0.09898 MHZ
  DELTA-K:  0.21343834E-02 1/CM       63.98721 MHZ
    DEL-J:  0.11879174E-08 1/CM        0.00004 MHZ
    DEL-K:  0.19604201E-05 1/CM        0.05877 MHZ

 S-REDUCTION DISTORTION CONSTANTS
 --------------------------------
     ~DJ:  0.70525589E-07 1/CM        0.00211 MHZ
    ~DJK:  0.33024753E-05 1/CM        0.09901 MHZ
     ~DK:  0.21343827E-02 1/CM       63.98719 MHZ
  ~DEL-J:  0.11879174E-08 1/CM        0.00004 MHZ
     ~R6: -0.68900183E-10 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                      A             B             C
 ALPHA    S     0.00123626    0.00071689    0.00070938  1/CM
          B    -0.35176588    0.00011760    0.00032206  1/CM
          A     0.32312871    0.00024795    0.00031987  1/CM

                      A             B             C
 ALPHA    S       37.06208      21.49194      21.26657  MHZ
          B   -10545.67597       3.52561       9.65520  MHZ
          A     9687.15536       7.43323       9.58940  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S             B             A
 X(I,J):  S    -1.33237436   -2.10232979   -1.51607400  1/CM
          B    -2.10232979   -2.14019481  -21.11348276  1/CM
          A    -1.51607400  -21.11348276  -55.54420719  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.10013038  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (2)H (74)Ge (35)Cl    GROUND STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.193162 A    (     4.144477 A.U.)
 R20:     1.599399 A    (     3.022427 A.U.)
 R30:     1.637892 RAD  (    93.844295 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.2376382   2   0   0
      2.0965631   0   2   0
      0.7891246   0   0   2
      0.0480481   1   1   0
```

```
 0.1522620   1   0   1
-0.0607094   0   1   1
-9.2643380   3   0   0
-9.3737492   0   3   0
-0.9395319   0   0   3
-0.0854305   2   1   0
 0.0789967   1   2   0
-0.5466743   2   0   1
 0.0147234   0   2   1
-0.1881576   1   1   1
-0.7824830   1   0   2
-0.1855179   0   1   2
34.8425126   4   0   0
36.9369679   0   4   0
 2.9687272   0   0   4
 0.2776664   3   1   0
-0.0465385   1   3   0
-0.1273117   2   2   0
 0.5453372   3   0   1
 0.1511376   0   3   1
 0.7677108   2   1   1
 0.1279416   1   2   1
 1.2211838   2   0   2
-0.6034673   0   2   2
 0.1299338   1   1   2
 1.1603017   1   0   3
 0.0071825   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      0.73384687     0.00329932     0.00000000    MASS: 73.921178 AMU
CENTER  2:     -1.45714948    -0.09315446     0.00000000    MASS: 34.968853 AMU
CENTER  3:     -1.63446512     1.49625750     0.00000000    MASS:  2.014102 AMU
MOMENTS:        7.99280040   198.33103190   206.32383230    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         3.5024       0.1411       0.1357     1/CM
      104999.4       4231.5       4067.6     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.997)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.2376 AJ/A**2    F12:      0.0480 AJ/A**2    F1A:      0.1523 AJ/A
                           F22:      2.0966 AJ/A**2    F2A:     -0.0607 AJ/A
                                                       FAA:      0.7891 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      34.968853       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       392.50171      531.91331     1368.56424  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99495906     0.00498075     0.10015813        392.50171248 S
Q2:       -0.09193764     0.04374490     0.99480342        531.91331190 B
```

```
Q3:        0.01906023     0.99878446    -0.04545669       1368.56424422 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S             B             A
ZETA-C   S     0.00000000    -0.20286588    -0.02539079
         B     0.20286588     0.00000000    -0.97887729
         A     0.02539079     0.97887729     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00038137 1/CM   AABB:     0.00000024 1/CM   ABAB:  -0.00000377 1/CM
BBBB:    -0.00000029 1/CM   BBCC:    -0.00000027 1/CM
CCCC:    -0.00000025 1/CM   CCAA:    -0.00000035 1/CM

AAAA:      -11.43306 MHZ    AABB:        0.00717 MHZ    ABAB:     -0.11304 MHZ
BBBB:       -0.00875 MHZ    BBCC:       -0.00808 MHZ
CCCC:       -0.00748 MHZ    CCAA:       -0.01053 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.35024019E+01 1/CM   104999.37080 MHZ
       B:  0.14114825E+00 1/CM     4231.51831 MHZ
       C:  0.13567951E+00 1/CM     4067.56958 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.67602514E-07 1/CM        0.00203 MHZ
     DJK:  0.17781396E-05 1/CM        0.05331 MHZ
      DK:  0.93495720E-04 1/CM        2.80293 MHZ
      R5: -0.43308295E-06 1/CM       -0.01298 MHZ
      R6: -0.40607535E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.26553892E-08 1/CM        0.00008 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.67683729E-07 1/CM        0.00203 MHZ
DELTA-JK:  0.17776523E-05 1/CM        0.05329 MHZ
 DELTA-K:  0.93496126E-04 1/CM        2.80294 MHZ
   DEL-J:  0.26553892E-08 1/CM        0.00008 MHZ
   DEL-K:  0.10659973E-05 1/CM        0.03196 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.67250488E-07 1/CM        0.00202 MHZ
    ~DJK:  0.17802517E-05 1/CM        0.05337 MHZ
     ~DK:  0.93493960E-04 1/CM        2.80288 MHZ
  ~DEL-J:  0.26553892E-08 1/CM        0.00008 MHZ
     ~R6: -0.21662023E-09 1/CM       -0.00001 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A             B             C
ALPHA    S    -0.00024789     0.00061680     0.00060373  1/CM
         B    -0.03890606     0.00010912     0.00034132  1/CM
         A     0.07129864    -0.00008421     0.00001084  1/CM

                    A             B             C
ALPHA    S       -7.43142       18.49111       18.09928  MHZ
         B    -1166.37432        3.27121       10.23265  MHZ
         A     2137.47958       -2.52445        0.32486  MHZ
```

```
 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                        S              B              A
 X(I,J):  S    -1.12354503    -1.31716180     0.25862502  1/CM
          B    -1.31716180    -0.59744725    -6.96365652  1/CM
          A     0.25862502    -6.96365652   -17.50091647  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.13004686  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H (74)Ge (35)Cl    EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.165805 A    (     4.092780 A.U.)
 R20:     1.607764 A    (     3.038234 A.U.)
 R30:     2.007766 RAD  (   115.036511 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.2538866   2   0   0
      1.4595505   0   2   0
      0.3373848   0   0   2
     -0.0831177   1   1   0
      0.0428819   1   0   1
      0.0774215   0   1   1
    -11.0742330   3   0   0
    -10.0192627   0   3   0
      0.0882249   0   0   3
      0.0932693   2   1   0
      0.0006900   1   2   0
     -0.3495215   2   0   1
      0.0392002   0   2   1
     -0.1525383   1   1   1
     -0.3596400   1   0   2
     -0.4141630   0   1   2
     41.9127652   4   0   0
     34.6578431   0   4   0
     -0.9449498   0   0   4
      1.1467417   3   1   0
     -0.0221535   1   3   0
      0.7483732   2   2   0
      0.3169879   3   0   1
     -0.1049847   0   3   1
      0.2455197   2   1   1
      0.1197173   1   2   1
      0.1161844   2   0   2
     -0.8527596   0   2   2
      0.1451553   1   1   2
      0.2426312   1   0   3
      0.3514911   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:                A              B              C
 CENTER  1:     0.73490420     0.01255620     0.00000000    MASS: 73.921178 AMU
 CENTER  2:    -1.42765039    -0.10229009     0.00000000    MASS: 34.968853 AMU
 CENTER  3:    -2.18543445     1.31512597     0.00000000    MASS:  2.014102 AMU
 MOMENTS:       6.41138575   200.61917277   207.03055852    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
           A           B           C        UNIT
        4.3663      0.1395      0.1352    1/CM
```

```
        130898.2      4183.2      4053.7    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.998)           OBLATE
-----------------------------+-----------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.2539 AJ/A**2    F12:    -0.0831 AJ/A**2    F1A:     0.0429 AJ/A
                           F22:     1.4596 AJ/A**2    F2A:     0.0774 AJ/A
                                                      FAA:     0.3374 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      34.968853       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       341.41634      404.62981     1142.45713  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
                R1             R2             R3             FREQUENCY
Q1:         0.72840950     0.02259163     0.68476947        341.41633718 B
Q2:         0.98992084     0.03334099    -0.13764121        404.62981292 S
Q3:        -0.10736250     0.99285107     0.05215410       1142.45713283 A


CORIOLIS COUPLING MATRICES
--------------------------
                     B              S              A
ZETA-C   B      0.00000000     0.16927523    -0.88258278
         S     -0.16927523     0.00000000     0.43862688
         A      0.88258278    -0.43862688     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:     -0.00354986 1/CM   AABB:      0.00000504 1/CM   ABAB:  -0.00000791 1/CM
BBBB:     -0.00000030 1/CM   BBCC:     -0.00000027 1/CM
CCCC:     -0.00000025 1/CM   CCAA:      0.00000133 1/CM

AAAA:      -106.42210 MHZ    AABB:         0.15123 MHZ    ABAB:      -0.23704 MHZ
BBBB:        -0.00884 MHZ    BBCC:        -0.00816 MHZ
CCCC:        -0.00762 MHZ    CCAA:         0.03994 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.43662947E+01 1/CM   130898.22482 MHZ
       B:  0.13953922E+00 1/CM     4183.28065 MHZ
       C:  0.13521554E+00 1/CM     4053.66002 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.68509816E-07 1/CM        0.00205 MHZ
     DJK:  0.22221912E-05 1/CM        0.06662 MHZ
      DK:  0.88517408E-03 1/CM       26.53685 MHZ
      R5: -0.75507337E-06 1/CM       -0.02264 MHZ
      R6: -0.77373310E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.25438407E-08 1/CM        0.00008 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.68664562E-07 1/CM        0.00206 MHZ
DELTA-JK:  0.22212627E-05 1/CM        0.06659 MHZ
```

```
 DELTA-K:  0.88517485E-03 1/CM       26.53688 MHZ
   DEL-J:  0.25438407E-08 1/CM        0.00008 MHZ
   DEL-K:  0.21155670E-05 1/CM        0.06342 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.68123819E-07 1/CM        0.00204 MHZ
    ~DJK:  0.22245072E-05 1/CM        0.06669 MHZ
     ~DK:  0.88517215E-03 1/CM       26.53679 MHZ
  ~DEL-J:  0.25438407E-08 1/CM        0.00008 MHZ
     ~R6: -0.27037157E-09 1/CM       -0.00001 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    B    -0.09140967     0.00000199     0.00032326  1/CM
         S    -0.00916930     0.00062656     0.00063348  1/CM
         A     0.27388448     0.00032140     0.00055115  1/CM

                    A              B              C
ALPHA    B    -2740.39312        0.05964        9.69119  MHZ
         S     -274.88865       18.78383       18.99133  MHZ
         A     8210.85038        9.63526       16.52311  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    B              S              A
X(I,J):  B    -2.20562037    -4.44575196   -21.97395156  1/CM
         S    -4.44575196    -1.65251170    -5.07962453  1/CM
         A   -21.97395156    -5.07962453   -62.13112679  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -6.34025721  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (2)H (74)Ge (35)Cl    TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.155776 A    (     4.073828 A.U.)
 R20:     1.557275 A    (     2.942825 A.U.)
 R30:     1.998288 RAD  (   114.493475 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.4712703   2   0   0
      2.2434114   0   2   0
      0.4513081   0   0   2
     -0.0545285   1   1   0
      0.0698745   1   0   1
      0.0049681   0   1   1
    -11.3097953   3   0   0
    -11.6143944   0   3   0
     -0.1942164   0   0   3
     -0.0077979   2   1   0
     -0.0482843   1   2   0
     -0.2656971   2   0   1
      0.0087205   0   2   1
     -0.1246859   1   1   1
     -0.4260814   1   0   2
     -0.2715442   0   1   2
     48.7765980   4   0   0
     42.3150211   0   4   0
     -0.0351712   0   0   4
```

```
 0.9231861   3   1   0
-0.3851255   1   3   0
-0.1750171   2   2   0
-0.2599343   3   0   1
 0.0845403   0   3   1
 0.2924952   2   1   1
 0.2195831   1   2   1
 0.1179795   2   0   2
-0.6215855   0   2   2
 0.2566593   1   1   2
 0.4396613   1   0   3
 0.1383445   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A             B             C
CENTER  1:     0.73106389    0.01166456    0.00000000    MASS: 73.921178 AMU
CENTER  2:    -1.42212338   -0.09857020    0.00000000    MASS: 34.968853 AMU
CENTER  3:    -2.14044807    1.28326613    0.00000000    MASS:  2.014102 AMU
MOMENTS:       6.08847802  198.36267756  204.45115558    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        4.5979      0.1411      0.1369     1/CM
     137840.5      4230.8      4104.8      MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.998)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.4713 AJ/A**2    F12:    -0.0545 AJ/A**2    F1A:     0.0699 AJ/A
                           F22:     2.2434 AJ/A**2    F2A:     0.0050 AJ/A
                                                      FAA:     0.4513 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                73.921178      34.968853       2.014102  AMU
FUNDAMENTAL FREQUENCIES:      394.64580      439.73780     1415.39184  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
              R1             R2             R3             FREQUENCY
Q1:       0.92837839     0.03330511     0.37014096        394.64579970 S
Q2:      -0.90705163    -0.01484379     0.42075766        439.73779685 B
Q3:      -0.05448092     0.99850979    -0.00316542       1415.39184291 A


CORIOLIS COUPLING MATRICES
--------------------------
                   S             B             A
ZETA-C   S     0.00000000    -0.17880523    -0.59930589
         B     0.17880523     0.00000000    -0.78029554
         A     0.59930589     0.78029554     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00251983 1/CM   AABB:     0.00000333 1/CM   ABAB:  -0.00000628 1/CM
BBBB:    -0.00000027 1/CM   BBCC:    -0.00000025 1/CM
```

```
CCCC:    -0.00000024 1/CM   CCAA:     0.00000090 1/CM

AAAA:      -75.54249 MHZ    AABB:        0.09974 MHZ    ABAB:     -0.18837 MHZ
BBBB:       -0.00816 MHZ    BBCC:       -0.00759 MHZ
CCCC:       -0.00712 MHZ    CCAA:        0.02689 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.45978649E+01 1/CM   137840.52606 MHZ
       B:  0.14112620E+00 1/CM     4230.85721 MHZ
       C:  0.13692181E+00 1/CM     4104.81274 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.63584475E-07 1/CM        0.00191 MHZ
     DJK:  0.19585806E-05 1/CM        0.05872 MHZ
      DK:  0.62793438E-03 1/CM       18.82500 MHZ
      R5: -0.63248680E-06 1/CM       -0.01896 MHZ
      R6: -0.51005994E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.21598127E-08 1/CM        0.00006 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.63686487E-07 1/CM        0.00191 MHZ
DELTA-JK:  0.19579685E-05 1/CM        0.05870 MHZ
 DELTA-K:  0.62793489E-03 1/CM       18.82501 MHZ
   DEL-J:  0.21598127E-08 1/CM        0.00006 MHZ
   DEL-K:  0.16977166E-05 1/CM        0.05090 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.63286279E-07 1/CM        0.00190 MHZ
    ~DJK:  0.19603697E-05 1/CM        0.05877 MHZ
     ~DK:  0.62793289E-03 1/CM       18.82495 MHZ
  ~DEL-J:  0.21598127E-08 1/CM        0.00006 MHZ
     ~R6: -0.20010425E-09 1/CM       -0.00001 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A             B             C
ALPHA    S    -0.06423640    0.00035610    0.00048870  1/CM
         B    -0.07171297    0.00030359    0.00040690  1/CM
         A     0.12066020    0.00023016    0.00031356  1/CM

                    A             B             C
ALPHA    S    -1925.75885      10.67568      14.65073  MHZ
         B    -2149.90086       9.10151      12.19846  MHZ
         A     3617.30178       6.90012       9.40036  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S             B             A
X(I,J):  S    -0.90667663   -2.08998790   -5.89502394  1/CM
         B    -2.08998790   -1.30593958   -5.89720215  1/CM
         A    -5.89502394   -5.89720215  -28.53011731  1/CM

DARLING-DENNISON RESONANCE PARAMETER:     -11.04438238  1/CM

-------------------------------------------------------------------------------
----------------------------------------- (1)H (74)Ge (79)Br    GROUND STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.345921 A    (     4.433150 A.U.)
```

```
R20:     1.597327 A    (     3.018512 A.U.)
R30:     1.631765 RAD  (    93.493243 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     1.9221268   2   0   0
     2.1061261   0   2   0
     0.7509848   0   0   2
     0.0407795   1   1   0
     0.1243519   1   0   1
    -0.0642889   0   1   1
    -7.8581366   3   0   0
    -9.4032245   0   3   0
    -0.9310149   0   0   3
    -0.0669234   2   1   0
     0.1137660   1   2   0
    -0.4488260   2   0   1
     0.0091631   0   2   1
    -0.1271337   1   1   1
    -0.7197847   1   0   2
    -0.1744997   0   1   2
    27.5590051   4   0   0
    37.2006882   0   4   0
     2.5923571   0   0   4
     0.4388148   3   1   0
     0.0433005   1   3   0
     0.0230698   2   2   0
     0.7387443   3   0   1
     0.0721580   0   3   1
     0.4665368   2   1   1
    -0.0473276   1   2   1
     0.8854092   2   0   2
    -0.2447048   0   2   2
     0.0972258   1   1   2
     1.2530599   1   0   3
     0.0579708   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A             B             C
CENTER  1:     1.21955420     0.00102086     0.00000000    MASS: 73.921178 AMU
CENTER  2:    -1.12651838    -0.02103682     0.00000000    MASS: 78.918338 AMU
CENTER  3:    -1.23823568     1.57242354     0.00000000    MASS:  1.007825 AMU
MOMENTS:       4.19593845   351.43467394   355.63061239    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        6.6717      0.0797      0.0787    1/CM
     200012.2      2388.0      2359.9     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.9221 AJ/A**2    F12:     0.0408 AJ/A**2    F1A:     0.1244 AJ/A
                           F22:     2.1061 AJ/A**2    F2A:    -0.0643 AJ/A
                                                      FAA:     0.7510 AJ
```

```
WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      78.918338       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       290.48876      710.28212     1896.14091  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99994333     0.00021092     0.01064380        290.48875737 S
Q2:        0.13967999     0.02031273     0.98998833        710.28211777 B
Q3:        0.01813034     0.99912145    -0.03778393       1896.14090670 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S     0.00000000    -0.11173290     0.03943013
         B     0.11173290     0.00000000    -0.99295570
         A    -0.03943013     0.99295570     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00133885 1/CM   AABB:     0.00000011 1/CM   ABAB:  -0.00000134 1/CM
BBBB:    -0.00000010 1/CM   BBCC:    -0.00000009 1/CM
CCCC:    -0.00000009 1/CM   CCAA:    -0.00000008 1/CM

AAAA:      -40.13783 MHZ    AABB:        0.00317 MHZ    ABAB:     -0.04009 MHZ
BBBB:       -0.00287 MHZ    BBCC:       -0.00280 MHZ
CCCC:       -0.00273 MHZ    CCAA:       -0.00249 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.66716897E+01 1/CM   200012.23169 MHZ
       B:  0.79656478E-01 1/CM     2388.04119 MHZ
       C:  0.78716368E-01 1/CM     2359.85740 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.23357178E-07 1/CM        0.00070 MHZ
     DJK:  0.61632226E-06 1/CM        0.01848 MHZ
      DK:  0.33407379E-03 1/CM       10.01528 MHZ
      R5: -0.15522387E-06 1/CM       -0.00465 MHZ
      R6: -0.12386453E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.27737608E-09 1/CM        0.00001 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.23359655E-07 1/CM        0.00070 MHZ
DELTA-JK:  0.61630740E-06 1/CM        0.01848 MHZ
 DELTA-K:  0.33407380E-03 1/CM       10.01528 MHZ
   DEL-J:  0.27737608E-09 1/CM        0.00001 MHZ
   DEL-K:  0.37993554E-06 1/CM        0.01139 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.23346110E-07 1/CM        0.00070 MHZ
    ~DJK:  0.61638867E-06 1/CM        0.01848 MHZ
     ~DK:  0.33407373E-03 1/CM       10.01528 MHZ
  ~DEL-J:  0.27737608E-09 1/CM        0.00001 MHZ
     ~R6: -0.67724896E-11 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
```

```
 ALPHA     S     -0.00082265      0.00028550      0.00028152  1/CM
           B     -0.09531075      0.00014896      0.00021206  1/CM
           A      0.19030838     -0.00010278     -0.00007809  1/CM

                       A               B               C
 ALPHA     S       -24.66248         8.55912         8.43975  MHZ
           B     -2857.34433         4.46562         6.35743  MHZ
           A      5705.30175        -3.08133        -2.34099  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                       S               B               A
 X(I,J):   S     -0.72703577     -1.59642128      0.77898703  1/CM
           B     -1.59642128     -1.69056842    -13.51507925  1/CM
           A      0.77898703    -13.51507925    -33.24959659  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.20650004  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (1)H (74)Ge (79)Br    EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:      2.324578 A    (     4.392818 A.U.)
 R20:      1.604226 A    (     3.031548 A.U.)
 R30:      2.024232 RAD  (   115.979951 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.8232299   2   0   0
      1.5530358   0   2   0
      0.3176025   0   0   2
     -0.0723624   1   1   0
      0.0397807   1   0   1
      0.0488442   0   1   1
     -8.7925926   3   0   0
    -10.0713422   0   3   0
      0.1232611   0   0   3
      0.1673906   2   1   0
      0.0928113   1   2   0
     -0.2872277   2   0   1
      0.0575262   0   2   1
     -0.1519647   1   1   1
     -0.3517514   1   0   2
     -0.3545586   0   1   2
     28.9602759   4   0   0
     36.0987728   0   4   0
     -1.2125903   0   0   4
      0.7481964   3   1   0
      0.3871046   1   3   0
      0.9476484   2   2   0
      0.5282496   3   0   1
     -0.2374064   0   3   1
      0.1504492   2   1   1
      0.0685913   1   2   1
      0.0834868   2   0   2
     -0.7351420   0   2   2
      0.2446485   1   1   2
      0.1969941   1   0   3
      0.2886154   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
```

```
AXES:                A              B              C
CENTER  1:      1.21170915     0.00583528     0.00000000    MASS: 73.921178 AMU
CENTER  2:     -1.11183603    -0.02359058     0.00000000    MASS: 78.918338 AMU
CENTER  3:     -1.81253313     1.41927293     0.00000000    MASS:  1.007825 AMU
MOMENTS:        3.44814943   347.71879647   351.16694590    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         8.1186      0.0805      0.0797    1/CM
      243388.2      2413.6      2389.9     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.8232 AJ/A**2    F12:    -0.0724 AJ/A**2    F1A:     0.0398 AJ/A
                           F22:     1.5530 AJ/A**2    F2A:     0.0488 AJ/A
                                                      FAA:     0.3176 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      78.918338       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       283.49526      461.58226     1628.17073  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99986640     0.00689347     0.01482081        283.49525572 S
Q2:        0.04948506    -0.00819931     0.99874121        461.58225635 B
Q3:       -0.05447450     0.99797187     0.03293437       1628.17072989 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S              B              A
ZETA-C   S     0.00000000    -0.10128833     0.01111660
         B     0.10128833     0.00000000    -0.99479500
         A    -0.01111660     0.99479500     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.01099948 1/CM   AABB:    -0.00000050 1/CM   ABAB:  -0.00000318 1/CM
BBBB:    -0.00000010 1/CM   BBCC:    -0.00000010 1/CM
CCCC:    -0.00000010 1/CM   CCAA:    -0.00000155 1/CM

AAAA:     -329.75627 MHZ    AABB:       -0.01498 MHZ    ABAB:     -0.09528 MHZ
BBBB:       -0.00311 MHZ    BBCC:       -0.00305 MHZ
CCCC:       -0.00299 MHZ    CCAA:       -0.04648 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.81185575E+01 1/CM   243388.23798 MHZ
       B:  0.80507938E-01 1/CM     2413.56732 MHZ
       C:  0.79716713E-01 1/CM     2389.84699 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.25428272E-07 1/CM        0.00076 MHZ
```

```
     DJK:  0.20507534E-05 1/CM        0.06148 MHZ
      DK:  0.27477950E-02 1/CM       82.37682 MHZ
      R5: -0.33147487E-06 1/CM       -0.00994 MHZ
      R6: -0.21866267E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.23838961E-09 1/CM        0.00001 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.25432645E-07 1/CM        0.00076 MHZ
DELTA-JK:  0.20507272E-05 1/CM        0.06148 MHZ
 DELTA-K:  0.27477950E-02 1/CM       82.37682 MHZ
   DEL-J:  0.23838961E-09 1/CM        0.00001 MHZ
   DEL-K:  0.84066991E-06 1/CM        0.02520 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.25411959E-07 1/CM        0.00076 MHZ
    ~DJK:  0.20508513E-05 1/CM        0.06148 MHZ
     ~DK:  0.27477949E-02 1/CM       82.37682 MHZ
  ~DEL-J:  0.23838961E-09 1/CM        0.00001 MHZ
     ~R6: -0.10343402E-10 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A             B             C
ALPHA    S    -0.00117718    0.00037562    0.00037115  1/CM
         B    -0.26303039    0.00012494    0.00021497  1/CM
         A     0.58869563    0.00018177    0.00023228  1/CM

                    A             B             C
ALPHA    S      -35.29101      11.26088      11.12667  MHZ
         B    -7885.45290       3.74553       6.44473  MHZ
         A    17648.65153       5.44930       6.96345  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S             B             A
X(I,J):  S    -1.23567896   -2.07004880    0.27253750  1/CM
         B    -2.07004880   -6.23008279  -39.51459470  1/CM
         A     0.27253750  -39.51459470 -100.57153672  1/CM

DARLING-DENNISON RESONANCE PARAMETER:        0.38320339  1/CM

--------------------------------------------------------------------------------
----------------------------------------- (1)H (74)Ge (79)Br    TRIPLET STATE
--------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.306845 A    (     4.359307 A.U.)
R20:     1.558577 A    (     2.945285 A.U.)
R30:     2.005346 RAD  (   114.897836 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     2.0876347   2   0   0
     2.2487556   0   2   0
     0.4244278   0   0   2
    -0.0435062   1   1   0
     0.0509958   1   0   1
    -0.0039183   0   1   1
    -9.1070362   3   0   0
   -11.5289971   0   3   0
    -0.1758012   0   0   3
```

```
    -0.0304283   2   1   0
    -0.0484634   1   2   0
    -0.2549263   2   0   1
     0.0438556   0   2   1
    -0.0969909   1   1   1
    -0.3768995   1   0   2
    -0.2202337   0   1   2
    32.3429795   4   0   0
    42.3689924   0   4   0
    -0.0878202   0   0   4
     0.3282607   3   1   0
     0.0824975   1   3   0
     0.1179845   2   2   0
     0.3674652   3   0   1
    -0.1069539   0   3   1
     0.2430023   2   1   1
     0.1440904   1   2   1
     0.2465394   2   0   2
    -0.6410700   0   2   2
     0.1877069   1   1   2
     0.3207011   1   0   3
     0.1522472   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      1.20309210     0.00550715     0.00000000    MASS: 73.921178 AMU
CENTER  2:     -1.10420258    -0.02281629     0.00000000    MASS: 78.918338 AMU
CENTER  3:     -1.77823848     1.38270899     0.00000000    MASS:  1.007825 AMU
MOMENTS:        3.27152865   342.74172119   346.01324984    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         8.5569       0.0817       0.0809     1/CM
      256528.1       2448.6       2425.5      MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
-------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.0876 AJ/A**2    F12:     -0.0435 AJ/A**2    F1A:      0.0510 AJ/A
                           F22:      2.2488 AJ/A**2    F2A:     -0.0039 AJ/A
                                                       FAA:      0.4244 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      78.918338       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       303.62005      550.27930     1958.76273  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
                R1             R2             R3             FREQUENCY
Q1:         0.99987566     0.00602838     0.01457123        303.62005394 S
Q2:         0.04814990     0.00631562     0.99882015        550.27929912 B
Q3:        -0.02498810     0.99968320    -0.00301520       1958.76273163 A


CORIOLIS COUPLING MATRICES
--------------------------
```

```
                    S              B              A
ZETA-C   S    -0.00000000    -0.10371918     0.01293190
         B     0.10371918    -0.00000000    -0.99452255
         A    -0.01293190     0.99452255    -0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00833449 1/CM   AABB:    -0.00000025 1/CM   ABAB:  -0.00000249 1/CM
BBBB:    -0.00000009 1/CM   BBCC:    -0.00000009 1/CM
CCCC:    -0.00000009 1/CM   CCAA:    -0.00000099 1/CM

AAAA:     -249.86184 MHZ    AABB:       -0.00742 MHZ    ABAB:     -0.07477 MHZ
BBBB:       -0.00283 MHZ    BBCC:       -0.00278 MHZ
CCCC:       -0.00273 MHZ    CCAA:       -0.02962 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.85568560E+01 1/CM   256528.09543 MHZ
       B:  0.81676933E-01 1/CM     2448.61293 MHZ
       C:  0.80904143E-01 1/CM     2425.44524 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.23153194E-07 1/CM        0.00069 MHZ
     DJK:  0.15096334E-05 1/CM        0.04526 MHZ
      DK:  0.20820907E-02 1/CM       62.41951 MHZ
      R5: -0.26538508E-06 1/CM       -0.00796 MHZ
      R6: -0.15497633E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.21294856E-09 1/CM        0.00001 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.23156294E-07 1/CM        0.00069 MHZ
DELTA-JK:  0.15096148E-05 1/CM        0.04526 MHZ
 DELTA-K:  0.20820907E-02 1/CM       62.41951 MHZ
   DEL-J:  0.21294856E-09 1/CM        0.00001 MHZ
   DEL-K:  0.66674611E-06 1/CM        0.01999 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.23141095E-07 1/CM        0.00069 MHZ
    ~DJK:  0.15097060E-05 1/CM        0.04526 MHZ
     ~DK:  0.20820906E-02 1/CM       62.41951 MHZ
  ~DEL-J:  0.21294856E-09 1/CM        0.00001 MHZ
     ~R6: -0.75991285E-11 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    S     0.00144425     0.00031187     0.00030882  1/CM
         B    -0.35881287     0.00010371     0.00017141  1/CM
         A     0.30758670     0.00010201     0.00012532  1/CM

                    A              B              C
ALPHA    S       43.29754        9.34948        9.25825  MHZ
         B   -10756.93942        3.10904        5.13888  MHZ
         A     9221.21757        3.05829        3.75715  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -0.88437718    -1.55887761    -0.76760268  1/CM
         B    -1.55887761    -1.93028455   -19.41248683  1/CM
```

```
          A    -0.76760268   -19.41248683   -52.92020448  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:        0.02713348  1/CM

--------------------------------------------------------------------------------
----------------------------------------- (2)H (74)Ge (79)Br    GROUND STATE
--------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.345921 A    (     4.433150 A.U.)
 R20:     1.597327 A    (     3.018512 A.U.)
 R30:     1.631765 RAD  (    93.493243 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.9221268   2   0   0
      2.1061261   0   2   0
      0.7509848   0   0   2
      0.0407795   1   1   0
      0.1243519   1   0   1
     -0.0642889   0   1   1
     -7.8581366   3   0   0
     -9.4032245   0   3   0
     -0.9310149   0   0   3
     -0.0669234   2   1   0
      0.1137660   1   2   0
     -0.4488260   2   0   1
      0.0091631   0   2   1
     -0.1271337   1   1   1
     -0.7197847   1   0   2
     -0.1744997   0   1   2
     27.5590051   4   0   0
     37.2006882   0   4   0
      2.5923571   0   0   4
      0.4388148   3   1   0
      0.0433005   1   3   0
      0.0230698   2   2   0
      0.7387443   3   0   1
      0.0721580   0   3   1
      0.4665368   2   1   1
     -0.0473276   1   2   1
      0.8854092   2   0   2
     -0.2447048   0   2   2
      0.0972258   1   1   2
      1.2530599   1   0   3
      0.0579708   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------------
 AXES:              A             B             C
 CENTER  1:     1.22763290     0.00228038     0.00000000    MASS: 73.921178 AMU
 CENTER  2:    -1.11813093    -0.04171029     0.00000000    MASS: 78.918338 AMU
 CENTER  3:    -1.24474096     1.55063596     0.00000000    MASS:  2.014102 AMU
 MOMENTS:       8.27033144   354.01019925   362.28053069    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
           A           B           C        UNIT
         3.3849      0.0791      0.0773    1/CM
      101475.9      2370.7      2316.5     MHZ

 PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
 -------------------------------+-------------------------------
 ^
```

```
ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.9221 AJ/A**2    F12:     0.0408 AJ/A**2    F1A:     0.1244 AJ/A
                           F22:     2.1061 AJ/A**2    F2A:    -0.0643 AJ/A
                                                      FAA:     0.7510 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      78.918338       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       290.19111      507.66492     1349.98055  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
                R1             R2             R3             FREQUENCY
Q1:         0.99966875     0.00066240     0.02572835        290.19111310 S
Q2:         0.10206755     0.02682642     0.99441569        507.66491958 B
Q3:         0.01776657     0.99903884    -0.04007165       1349.98055306 A


CORIOLIS COUPLING MATRICES
--------------------------
                      S              B              A
ZETA-C   S     0.00000000    -0.15540044     0.04261394
         B     0.15540044    -0.00000000    -0.98693199
         A    -0.04261394     0.98693199     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00034658 1/CM   AABB:     0.00000007 1/CM   ABAB:  -0.00000129 1/CM
BBBB:    -0.00000009 1/CM   BBCC:    -0.00000009 1/CM
CCCC:    -0.00000009 1/CM   CCAA:    -0.00000012 1/CM

AAAA:      -10.39024 MHZ    AABB:        0.00196 MHZ    ABAB:     -0.03860 MHZ
BBBB:       -0.00281 MHZ    BBCC:       -0.00268 MHZ
CCCC:       -0.00256 MHZ    CCAA:       -0.00355 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.33848703E+01 1/CM   101475.86224 MHZ
       B:  0.79076948E-01 1/CM     2370.66733 MHZ
       C:  0.77271477E-01 1/CM     2316.54066 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.22401811E-07 1/CM        0.00067 MHZ
     DJK:  0.61225664E-06 1/CM        0.01835 MHZ
      DK:  0.86010624E-04 1/CM        2.57853 MHZ
      R5: -0.14922081E-06 1/CM       -0.00447 MHZ
      R6: -0.45034642E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.51526124E-09 1/CM        0.00002 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.22410818E-07 1/CM        0.00067 MHZ
DELTA-JK:  0.61220260E-06 1/CM        0.01835 MHZ
 DELTA-K:  0.86010669E-04 1/CM        2.57854 MHZ
   DEL-J:  0.51526124E-09 1/CM        0.00002 MHZ
   DEL-K:  0.36442588E-06 1/CM        0.01093 MHZ

S-REDUCTION DISTORTION CONSTANTS
```

```
--------------------------------
     ~DJ:  0.22361073E-07 1/CM        0.00067 MHZ
    ~DJK:  0.61250107E-06 1/CM        0.01836 MHZ
     ~DK:  0.86010421E-04 1/CM        2.57853 MHZ
  ~DEL-J:  0.51526124E-09 1/CM        0.00002 MHZ
     ~R6: -0.24872277E-10 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    S    -0.00030883     0.00028351     0.00027677  1/CM
         B    -0.03583195     0.00008349     0.00016669  1/CM
         A     0.06843295    -0.00006706    -0.00003405  1/CM

                    A              B              C
ALPHA    S       -9.25838        8.49942        8.29737  MHZ
         B    -1074.21487        2.50299        4.99725  MHZ
         A     2051.56825       -2.01054       -1.02091  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -0.72527700    -1.17512685     0.53826975  1/CM
         B    -1.17512685    -0.81920879    -6.75115251  1/CM
         A     0.53826975    -6.75115251   -16.84309393  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -0.11635294  1/CM

-------------------------------------------------------------------------------
----------------------------------------- (2)H (74)Ge (79)Br    EXCITED STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.324578 A    (     4.392818 A.U.)
R20:     1.604226 A    (     3.031548 A.U.)
R30:     2.024232 RAD  (   115.979951 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     1.8232299   2   0   0
     1.5530358   0   2   0
     0.3176025   0   0   2
    -0.0723624   1   1   0
     0.0397807   1   0   1
     0.0488442   0   1   1
    -8.7925926   3   0   0
   -10.0713422   0   3   0
     0.1232611   0   0   3
     0.1673906   2   1   0
     0.0928113   1   2   0
    -0.2872277   2   0   1
     0.0575262   0   2   1
    -0.1519647   1   1   1
    -0.3517514   1   0   2
    -0.3545586   0   1   2
    28.9602759   4   0   0
    36.0987728   0   4   0
    -1.2125903   0   0   4
     0.7481964   3   1   0
     0.3871046   1   3   0
     0.9476484   2   2   0
     0.5282496   3   0   1
    -0.2374064   0   3   1
```

```
     0.1504492   2   1   1
     0.0685913   1   2   1
     0.0834868   2   0   2
    -0.7351420   0   2   2
     0.2446485   1   1   2
     0.1969941   1   0   3
     0.2886154   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      1.22343624     0.01169382     0.00000000    MASS: 73.921178 AMU
CENTER  2:     -1.09956970    -0.04637051     0.00000000    MASS: 78.918338 AMU
CENTER  3:     -1.81799873     1.38774639     0.00000000    MASS:  2.014102 AMU
MOMENTS:        6.73949564   353.22531454   359.96481018    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         4.1537       0.0793       0.0778     1/CM
      124525.5       2375.9       2331.4     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.8232 AJ/A**2    F12:    -0.0724 AJ/A**2    F1A:     0.0398 AJ/A
                           F22:     1.5530 AJ/A**2    F2A:     0.0488 AJ/A
                                                      FAA:     0.3176 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      78.918338       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       282.21283      332.09712     1159.20758  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
              R1             R2             R3             FREQUENCY
Q1:        0.99777198     0.01398428     0.06523438        282.21283439 S
Q2:       -0.23546236    -0.00732319     0.97185588        332.09711917 B
Q3:       -0.06304850     0.99750328     0.03181336       1159.20757917 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S              B              A
ZETA-C   S     0.00000000    -0.13859832    -0.08508591
         B     0.13859832     0.00000000    -0.98668683
         A     0.08508591     0.98668683    -0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00297763 1/CM   AABB:     0.00000067 1/CM   ABAB:  -0.00000296 1/CM
BBBB:    -0.00000010 1/CM   BBCC:    -0.00000010 1/CM
CCCC:    -0.00000009 1/CM   CCAA:    -0.00000040 1/CM

AAAA:      -89.26710 MHZ    AABB:        0.02019 MHZ    ABAB:     -0.08864 MHZ
BBBB:       -0.00300 MHZ    BBCC:       -0.00288 MHZ
CCCC:       -0.00278 MHZ    CCAA:       -0.01185 MHZ
```

```
 ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
 -----------------------------------------------------
 AXIS   A:  0.41537232E+01 1/CM   124525.49247 MHZ
        B:  0.79252887E-01 1/CM     2375.94183 MHZ
        C:  0.77768354E-01 1/CM     2331.43666 MHZ

 FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
 --------------------------------------------
       DJ:  0.24048358E-07 1/CM        0.00072 MHZ
      DJK:  0.13607618E-05 1/CM        0.04079 MHZ
       DK:  0.74302262E-03 1/CM       22.27526 MHZ
       R5: -0.30255976E-06 1/CM       -0.00907 MHZ
       R6: -0.81392828E-11 1/CM       -0.00000 MHZ
    DEL-J:  0.46036024E-09 1/CM        0.00001 MHZ

 A-REDUCTION DISTORTION CONSTANTS
 --------------------------------
  DELTA-J:  0.24064637E-07 1/CM        0.00072 MHZ
 DELTA-JK:  0.13606641E-05 1/CM        0.04079 MHZ
  DELTA-K:  0.74302270E-03 1/CM       22.27526 MHZ
    DEL-J:  0.46036024E-09 1/CM        0.00001 MHZ
    DEL-K:  0.78386562E-06 1/CM        0.02350 MHZ

 S-REDUCTION DISTORTION CONSTANTS
 --------------------------------
      ~DJ:  0.23993249E-07 1/CM        0.00072 MHZ
     ~DJK:  0.13610925E-05 1/CM        0.04080 MHZ
      ~DK:  0.74302235E-03 1/CM       22.27525 MHZ
   ~DEL-J:  0.46036024E-09 1/CM        0.00001 MHZ
      ~R6: -0.35693666E-10 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                     A              B              C
 ALPHA    S    -0.00439810     0.00036861     0.00036656  1/CM
          B    -0.09361031     0.00002586     0.00013934  1/CM
          A     0.21476744     0.00013603     0.00020262  1/CM

                     A              B              C
 ALPHA    S     -131.85163       11.05057       10.98933  MHZ
          B    -2806.36655        0.77536        4.17721  MHZ
          A     6438.56601        4.07814        6.07432  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                     S              B              A
 X(I,J):  S    -1.25315511    -1.33212199    -0.21866150  1/CM
          B    -1.33212199    -3.27876802   -19.69170243  1/CM
          A    -0.21866150   -19.69170243   -50.98655629  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:        0.07195996  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H (74)Ge (79)Br    TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.306845 A    (     4.359307 A.U.)
 R20:     1.558577 A    (     2.945285 A.U.)
 R30:     2.005346 RAD  (   114.897836 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
```

```
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     2.0934098   2   0   0
     2.2512240   0   2   0
     0.4247693   0   0   2
    -0.0434438   1   1   0
     0.0513035   1   0   1
    -0.0037924   0   1   1
    -9.1273875   3   0   0
   -11.5380235   0   3   0
    -0.1760036   0   0   3
    -0.0307405   2   1   0
    -0.0486034   1   2   0
    -0.2552907   2   0   1
     0.0440061   0   2   1
    -0.0972367   1   1   1
    -0.3772019   1   0   2
    -0.2202660   0   1   2
    32.3429795   4   0   0
    42.3689924   0   4   0
    -0.0878202   0   0   4
     0.3282607   3   1   0
     0.0824975   1   3   0
     0.1179845   2   2   0
     0.3674652   3   0   1
    -0.1069539   0   3   1
     0.2430023   2   1   1
     0.1440904   1   2   1
     0.2465394   2   0   2
    -0.6410700   0   2   2
     0.1877069   1   1   2
     0.3207011   1   0   3
     0.1522472   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
--------------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      1.21426934     0.01102971     0.00000000    MASS: 73.921178 AMU
CENTER  2:     -1.09189904    -0.04485053     0.00000000    MASS: 78.918338 AMU
CENTER  3:     -1.78211540     1.35256282     0.00000000    MASS:  2.014102 AMU
MOMENTS:        6.39701902   347.84740829   354.24442731    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B           C        UNIT
         4.3761       0.0805      0.0790     1/CM
      131192.2       2412.7      2369.1     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
-------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.0934 AJ/A**2    F12:     -0.0434 AJ/A**2    F1A:      0.0513 AJ/A
                           F22:      2.2512 AJ/A**2    F2A:     -0.0038 AJ/A
                                                       FAA:      0.4248 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178      78.918338       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       302.98600      395.58118     1395.28240  1/CM
```

NORMAL COORDINATE DISPLACEMENTS

	R1	R2	R3	FREQUENCY	
Q1:	0.99877064	0.01250961	0.04796590	302.98600027	S
Q2:	-0.11620896	0.00959524	0.99317844	395.58117590	B
Q3:	-0.03068052	0.99952107	-0.00404266	1395.28239863	A

CORIOLIS COUPLING MATRICES

		S	B	A
ZETA-C	S	0.00000000	-0.14269460	-0.03724007
	B	0.14269460	-0.00000000	-0.98906594
	A	0.03724007	0.98906594	0.00000000

TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION

AAAA:	-0.00225079 1/CM	AABB:	0.00000055 1/CM	ABAB:	-0.00000233 1/CM
BBBB:	-0.00000009 1/CM	BBCC:	-0.00000009 1/CM		
CCCC:	-0.00000008 1/CM	CCAA:	-0.00000020 1/CM		
AAAA:	-67.47687 MHZ	AABB:	0.01645 MHZ	ABAB:	-0.06984 MHZ
BBBB:	-0.00272 MHZ	BBCC:	-0.00262 MHZ		
CCCC:	-0.00253 MHZ	CCAA:	-0.00614 MHZ		

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION

AXIS	A:	0.43761007E+01 1/CM	131192.20230 MHZ
	B:	0.80478088E-01 1/CM	2412.67243 MHZ
	C:	0.79024258E-01 1/CM	2369.08772 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS

DJ:	0.21869285E-07 1/CM	0.00066 MHZ
DJK:	0.10351593E-05 1/CM	0.03103 MHZ
DK:	0.56163946E-03 1/CM	16.83753 MHZ
R5:	-0.24391189E-06 1/CM	-0.00731 MHZ
R6:	-0.57566478E-11 1/CM	-0.00000 MHZ
DEL-J:	0.40541143E-09 1/CM	0.00001 MHZ

A-REDUCTION DISTORTION CONSTANTS

DELTA-J:	0.21880798E-07 1/CM	0.00066 MHZ
DELTA-JK:	0.10350902E-05 1/CM	0.03103 MHZ
DELTA-K:	0.56163952E-03 1/CM	16.83753 MHZ
DEL-J:	0.40541143E-09 1/CM	0.00001 MHZ
DEL-K:	0.62391990E-06 1/CM	0.01870 MHZ

S-REDUCTION DISTORTION CONSTANTS

~DJ:	0.21828016E-07 1/CM	0.00065 MHZ
~DJK:	0.10354069E-05 1/CM	0.03104 MHZ
~DK:	0.56163925E-03 1/CM	16.83752 MHZ
~DEL-J:	0.40541143E-09 1/CM	0.00001 MHZ
~R6:	-0.26390812E-10 1/CM	-0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS

		A	B	C	
ALPHA	S	-0.00078956	0.00030495	0.00030214	1/CM
	B	-0.13153545	0.00003605	0.00012256	1/CM
	A	0.11134566	0.00008638	0.00011653	1/CM

	A	B	C

```
ALPHA    S      -23.67037        9.14210        9.05787  MHZ
         B    -3943.33374        1.08063        3.67418  MHZ
         A     3338.05902        2.58949        3.49349  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                     S              B              A
 X(I,J):  S    -0.89113999    -1.06798731    -0.64115728  1/CM
          B    -1.06798731    -1.00730343    -9.70600074  1/CM
          A    -0.64115728    -9.70600074   -26.79869528  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:        0.00698259  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (1)H (74)Ge (127)I    GROUND STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.564907 A    (     4.846973 A.U.)
 R20:     1.595601 A    (     3.015250 A.U.)
 R30:     1.613592 RAD  (    92.452038 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.5426990   2   0   0
      2.1175231   0   2   0
      0.6770920   0   0   2
      0.0230819   1   1   0
      0.1100861   1   0   1
     -0.0558410   0   1   1
     -6.0212248   3   0   0
     -9.4437108   0   3   0
     -0.7641428   0   0   3
     -0.0391641   2   1   0
      0.1358017   1   2   0
     -0.3640771   2   0   1
     -0.0055766   0   2   1
     -0.0736107   1   1   1
     -0.6467723   1   0   2
     -0.1516144   0   1   2
     19.3282292   4   0   0
     37.6174595   0   4   0
      1.8732613   0   0   4
      0.0317823   3   1   0
      0.0754046   1   3   0
     -0.0543788   2   2   0
      0.6798078   3   0   1
     -0.0578420   0   3   1
      0.3748415   2   1   1
     -0.0602027   1   2   1
      0.8327193   2   0   2
     -0.0118325   0   2   2
     -0.0331570   1   1   2
      1.0804500   1   0   3
     -0.0732507   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:                A              B              C
 CENTER  1:     1.62576150     0.00064538     0.00000000    MASS: 73.921178 AMU
 CENTER  2:    -0.93893096    -0.01293106     0.00000000    MASS:126.904468 AMU
 CENTER  3:    -1.01572413     1.58093068     0.00000000    MASS:  1.007825 AMU
 MOMENTS:       4.21799781   511.93964294   516.15764075    10**(-40) G*CM**2
```

```
ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
     6.6368      0.0547      0.0542    1/CM
  198966.2      1639.3      1625.9    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.5427 AJ/A**2    F12:     0.0231 AJ/A**2    F1A:     0.1101 AJ/A
                           F22:     2.1175 AJ/A**2    F2A:    -0.0558 AJ/A
                                                      FAA:     0.6771 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178     126.904468       1.007825  AMU
FUNDAMENTAL FREQUENCIES:      235.31651      672.99605     1896.42959  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
              R1             R2             R3             FREQUENCY
Q1:       0.99999156     0.00003032     0.00410917       235.31651360 S
Q2:       0.15295502     0.01533564     0.98811415       672.99604508 B
Q3:       0.01010805     0.99945881    -0.03130371      1896.42959233 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S              B              A
ZETA-C   S     0.00000000    -0.09194716     0.03804826
         B     0.09194716    -0.00000000    -0.99503671
         A    -0.03804826     0.99503671     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00130770 1/CM   AABB:     0.00000003 1/CM   ABAB:  -0.00000070 1/CM
BBBB:    -0.00000005 1/CM   BBCC:    -0.00000005 1/CM
CCCC:    -0.00000005 1/CM   CCAA:    -0.00000005 1/CM

AAAA:      -39.20396 MHZ    AABB:        0.00103 MHZ    ABAB:     -0.02108 MHZ
BBBB:       -0.00141 MHZ    BBCC:       -0.00139 MHZ
CCCC:       -0.00137 MHZ    CCAA:       -0.00161 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.66367980E+01 1/CM   198966.20434 MHZ
       B:  0.54682294E-01 1/CM     1639.33398 MHZ
       C:  0.54235300E-01 1/CM     1625.93343 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
     DJ:  0.11601116E-07 1/CM        0.00035 MHZ
    DJK:  0.33312640E-06 1/CM        0.00999 MHZ
     DK:  0.32658109E-03 1/CM        9.79066 MHZ
     R5: -0.82337343E-07 1/CM       -0.00247 MHZ
     R6: -0.28754884E-12 1/CM       -0.00000 MHZ
  DEL-J:  0.95104916E-10 1/CM        0.00000 MHZ
```

```
A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.11601691E-07 1/CM        0.00035 MHZ
DELTA-JK:  0.33312295E-06 1/CM        0.00999 MHZ
 DELTA-K:  0.32658109E-03 1/CM        9.79066 MHZ
   DEL-J:  0.95104916E-10 1/CM        0.00000 MHZ
   DEL-K:  0.19854974E-06 1/CM        0.00595 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.11598321E-07 1/CM        0.00035 MHZ
    ~DJK:  0.33314317E-06 1/CM        0.00999 MHZ
     ~DK:  0.32658108E-03 1/CM        9.79065 MHZ
  ~DEL-J:  0.95104916E-10 1/CM        0.00000 MHZ
     ~R6: -0.16853921E-11 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    S    -0.00065284     0.00017613     0.00017433  1/CM
         B    -0.09907704     0.00012195     0.00015292  1/CM
         A     0.18910678    -0.00006737    -0.00005541  1/CM

                    A              B              C
ALPHA    S      -19.57152        5.28036        5.22639  MHZ
         B    -2970.25489        3.65609        4.58440  MHZ
         A     5669.27894       -2.01962       -1.66123  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -0.56556842    -1.41827927     0.58789355  1/CM
         B    -1.41827927    -1.70326667   -12.04813557  1/CM
         A     0.58789355   -12.04813557   -32.68132286  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -0.22561320  1/CM

-------------------------------------------------------------------------------
----------------------------------------- (1)H (74)Ge (127)I    EXCITED STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.543755 A    (     4.807002 A.U.)
R20:     1.595748 A    (     3.015528 A.U.)
R30:     2.000040 RAD  (   114.593839 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     1.3171222   2   0   0
     1.7304002   0   2   0
     0.2682579   0   0   2
    -0.0652271   1   1   0
     0.0540635   1   0   1
     0.0346487   0   1   1
    -6.7483875   3   0   0
   -10.2586354   0   3   0
     0.2654789   0   0   3
     0.1605112   2   1   0
     0.1918999   1   2   0
    -0.1738901   2   0   1
     0.0425798   0   2   1
    -0.1399070   1   1   1
```

```
    -0.3948212   1   0   2
    -0.2874075   0   1   2
    19.2488698   4   0   0
    36.5257421   0   4   0
    -1.9944702   0   0   4
     0.4163340   3   1   0
     0.6538067   1   3   0
     1.0161271   2   2   0
     0.8249896   3   0   1
    -0.2472566   0   3   1
     0.1162463   2   1   1
    -0.1489952   1   2   1
    -0.2298395   2   0   2
    -0.5379226   0   2   2
     0.1686264   1   1   2
     0.4646218   1   0   3
     0.4505342   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:     1.61589419     0.00517939     0.00000000    MASS: 73.921178 AMU
CENTER  2:    -0.92851451    -0.01438774     0.00000000    MASS:126.904468 AMU
CENTER  3:    -1.60361406     1.43179739     0.00000000    MASS:  1.007825 AMU
MOMENTS:       3.47771406   506.49126378   509.96897784    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        8.0495      0.0553      0.0549     1/CM
     241319.2      1657.0      1645.7      MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.3171 AJ/A**2    F12:    -0.0652 AJ/A**2    F1A:     0.0541 AJ/A
                           F22:     1.7304 AJ/A**2    F2A:     0.0346 AJ/A
                                                      FAA:     0.2683 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178     126.904468       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       217.52130      424.39798     1714.20309  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99999098     0.00424136     0.00022440        217.52129781 S
Q2:        0.20220628    -0.00464335     0.97933195        424.39798311 B
Q3:       -0.04069504     0.99895645     0.02073451       1714.20308673 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S              B              A
ZETA-C   S     0.00000000    -0.08513650     0.04691397
         B     0.08513650    -0.00000000    -0.99526421
         A    -0.04691397     0.99526421     0.00000000
```

```
TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.01121842 1/CM   AABB:    -0.00000172 1/CM   ABAB:  -0.00000182 1/CM
BBBB:    -0.00000006 1/CM   BBCC:    -0.00000006 1/CM
CCCC:    -0.00000006 1/CM   CCAA:    -0.00000221 1/CM

AAAA:     -336.31972 MHZ    AABB:       -0.05142 MHZ    ABAB:     -0.05456 MHZ
BBBB:       -0.00170 MHZ    BBCC:       -0.00168 MHZ
CCCC:       -0.00166 MHZ    CCAA:       -0.06636 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.80495403E+01 1/CM   241319.15347 MHZ
       B:  0.55270622E-01 1/CM     1656.97160 MHZ
       C:  0.54893361E-01 1/CM     1645.66162 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.14026796E-07 1/CM        0.00042 MHZ
     DJK:  0.18640652E-05 1/CM        0.05588 MHZ
      DK:  0.28027264E-02 1/CM       84.02363 MHZ
      R5: -0.19629172E-06 1/CM       -0.00588 MHZ
      R6: -0.50914950E-12 1/CM       -0.00000 MHZ
   DEL-J:  0.84477126E-10 1/CM        0.00000 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.14027814E-07 1/CM        0.00042 MHZ
DELTA-JK:  0.18640591E-05 1/CM        0.05588 MHZ
 DELTA-K:  0.28027264E-02 1/CM       84.02363 MHZ
   DEL-J:  0.84477126E-10 1/CM        0.00000 MHZ
   DEL-K:  0.47889783E-06 1/CM        0.01436 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.14022164E-07 1/CM        0.00042 MHZ
    ~DJK:  0.18640930E-05 1/CM        0.05588 MHZ
     ~DK:  0.28027264E-02 1/CM       84.02363 MHZ
  ~DEL-J:  0.84477126E-10 1/CM        0.00000 MHZ
     ~R6: -0.28249121E-11 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A             B             C
ALPHA    S     0.01194476    0.00028141    0.00027948  1/CM
         B    -0.22206336    0.00019327    0.00024010  1/CM
         A     0.47496322    0.00008587    0.00010588  1/CM

                    A             B             C
ALPHA    S      358.09491       8.43643       8.37851  MHZ
         B    -6657.29215       5.79395       7.19811  MHZ
         A    14239.03959       2.57418       3.17410  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S             B             A
X(I,J):  S    -1.32564575   -4.25500662    0.91771433  1/CM
         B    -4.25500662  -10.45552900  -30.95443562  1/CM
         A     0.91771433  -30.95443562  -79.63148673  1/CM

DARLING-DENNISON RESONANCE PARAMETER:        0.13733030  1/CM
```

```
------------------------------------------ (1)H (74)Ge (127)I    TRIPLET STATE
--------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.517404 A    (     4.757205 A.U.)
 R20:     1.559635 A    (     2.947284 A.U.)
 R30:     2.015500 RAD  (   115.479669 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.6621410   2   0   0
      2.2706493   0   2   0
      0.3920816   0   0   2
     -0.0487252   1   1   0
      0.0429238   1   0   1
     -0.0076278   0   1   1
     -7.0339356   3   0   0
    -11.4191776   0   3   0
     -0.1440906   0   0   3
     -0.0267527   2   1   0
     -0.0141675   1   2   0
     -0.2081067   2   0   1
      0.0528286   0   2   1
     -0.0789279   1   1   1
     -0.3283655   1   0   2
     -0.1719948   0   1   2
     22.3260007   4   0   0
     42.6704256   0   4   0
     -0.1912257   0   0   4
      0.1668945   3   1   0
      0.2487799   1   3   0
      0.1799071   2   2   0
      0.3786953   3   0   1
     -0.2599910   0   3   1
      0.1778723   2   1   1
      0.0734603   1   2   1
      0.1471873   2   0   2
     -0.5933312   0   2   2
      0.0753878   1   1   2
      0.2584390   1   0   3
      0.2286619   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:              A             B             C
 CENTER  1:     1.59843209     0.00513127     0.00000000    MASS: 73.921178 AMU
 CENTER  2:    -0.91836787    -0.01401736     0.00000000    MASS:126.904468 AMU
 CENTER  3:    -1.60047366     1.38869007     0.00000000    MASS:  1.007825 AMU
 MOMENTS:       3.27196292   495.63570586   498.90766878    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
           A           B           C        UNIT
         8.5557      0.0565      0.0561    1/CM
      256494.0      1693.3      1682.2    MHZ

 PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
 -------------------------------+-------------------------------
 ^

 ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


 HARMONIC FORCE FIELD
```

```
--------------------
F11:     1.6621 AJ/A**2    F12:    -0.0487 AJ/A**2    F1A:     0.0429 AJ/A
                           F22:     2.2706 AJ/A**2    F2A:    -0.0076 AJ/A
                                                      FAA:     0.3921 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178     126.904468       1.007825  AMU
FUNDAMENTAL FREQUENCIES:      245.16199      525.83172     1963.49827  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
              R1             R2             R3             FREQUENCY
Q1:        0.99996863     0.00392476     0.00688058        245.16199445 S
Q2:        0.07955120     0.00475869     0.99681942        525.83172275 B
Q3:       -0.02438378     0.99969384    -0.00420187       1963.49826866 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S     0.00000000    -0.08642964     0.01864136
         B     0.08642964    -0.00000000    -0.99608354
         A    -0.01864136     0.99608354     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00902390 1/CM   AABB:    -0.00000058 1/CM   ABAB:  -0.00000131 1/CM
BBBB:    -0.00000005 1/CM   BBCC:    -0.00000005 1/CM
CCCC:    -0.00000005 1/CM   CCAA:    -0.00000096 1/CM

AAAA:     -270.52966 MHZ    AABB:       -0.01725 MHZ    ABAB:     -0.03923 MHZ
BBBB:       -0.00143 MHZ    BBCC:       -0.00142 MHZ
CCCC:       -0.00140 MHZ    CCAA:       -0.02866 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.85557203E+01 1/CM   256494.04763 MHZ
       B:  0.56481137E-01 1/CM     1693.26194 MHZ
       C:  0.56110443E-01 1/CM     1682.14880 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.11811513E-07 1/CM        0.00035 MHZ
     DJK:  0.10134936E-05 1/CM        0.03038 MHZ
      DK:  0.22549491E-02 1/CM       67.60168 MHZ
      R5: -0.13973358E-06 1/CM       -0.00419 MHZ
      R6: -0.37847716E-12 1/CM       -0.00000 MHZ
   DEL-J:  0.73567793E-10 1/CM        0.00000 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.11812270E-07 1/CM        0.00035 MHZ
DELTA-JK:  0.10134891E-05 1/CM        0.03038 MHZ
 DELTA-K:  0.22549492E-02 1/CM       67.60168 MHZ
   DEL-J:  0.73567793E-10 1/CM        0.00000 MHZ
   DEL-K:  0.34889008E-06 1/CM        0.01046 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.11808466E-07 1/CM        0.00035 MHZ
    ~DJK:  0.10135119E-05 1/CM        0.03038 MHZ
     ~DK:  0.22549491E-02 1/CM       67.60168 MHZ
  ~DEL-J:  0.73567793E-10 1/CM        0.00000 MHZ
```

```
     ~R6: -0.19020651E-11 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 --------------------------------------------------
                      A              B              C
 ALPHA    S      0.00192937     0.00019910     0.00019760  1/CM
          B     -0.37999668     0.00008844     0.00012204  1/CM
          A      0.29550548     0.00006956     0.00008038  1/CM

                      A              B              C
 ALPHA    S        57.84119        5.96891        5.92385  MHZ
          B    -11392.01416        2.65136        3.65859  MHZ
          A      8859.03155        2.08543        2.40972  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S              B              A
 X(I,J):  S     -0.74103732    -1.42307020    -0.64430891  1/CM
          B     -1.42307020    -1.94872134   -17.23389620  1/CM
          A     -0.64430891   -17.23389620   -49.29785441  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:         0.01797062  1/CM

--------------------------------------------------------------------------------
------------------------------------------ (2)H (74)Ge (127)I    GROUND STATE
--------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:      2.564907 A    (     4.846973 A.U.)
 R20:      1.595601 A    (     3.015250 A.U.)
 R30:      1.613592 RAD  (    92.452038 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.5426990   2   0   0
      2.1175231   0   2   0
      0.6770920   0   0   2
      0.0230819   1   1   0
      0.1100861   1   0   1
     -0.0558410   0   1   1
     -6.0212248   3   0   0
     -9.4437108   0   3   0
     -0.7641428   0   0   3
     -0.0391641   2   1   0
      0.1358017   1   2   0
     -0.3640771   2   0   1
     -0.0055766   0   2   1
     -0.0736107   1   1   1
     -0.6467723   1   0   2
     -0.1516144   0   1   2
     19.3282292   4   0   0
     37.6174595   0   4   0
      1.8732613   0   0   4
      0.0317823   3   1   0
      0.0754046   1   3   0
     -0.0543788   2   2   0
      0.6798078   3   0   1
     -0.0578420   0   3   1
      0.3748415   2   1   1
     -0.0602027   1   2   1
      0.8327193   2   0   2
     -0.0118325   0   2   2
     -0.0331570   1   1   2
```

```
     1.0804500   1   0   3
    -0.0732507   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A              B              C
CENTER  1:     1.63081572     0.00141930     0.00000000    MASS: 73.921178 AMU
CENTER  2:    -0.93376920    -0.02570812     0.00000000    MASS:126.904468 AMU
CENTER  3:    -1.01898286     1.56772561     0.00000000    MASS:  2.014102 AMU
MOMENTS:       8.35945796   513.66911384   522.02857180    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A            B            C        UNIT
        3.3488       0.0545       0.0536     1/CM
     100394.0       1633.8       1607.6     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
-------------------------------+-----------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.5427 AJ/A**2    F12:     0.0231 AJ/A**2    F1A:     0.1101 AJ/A
                           F22:     2.1175 AJ/A**2    F2A:    -0.0558 AJ/A
                                                      FAA:     0.6771 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178     126.904468       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       235.27525      479.30565     1346.89067  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99995620     0.00010849     0.00935920        235.27524863 S
Q2:        0.14150091     0.01894753     0.98975678        479.30565203 B
Q3:        0.00994543     0.99942366    -0.03245663       1346.89067427 A


CORIOLIS COUPLING MATRICES
--------------------------
                   S              B              A
ZETA-C   S     0.00000000    -0.12869643     0.05001972
         B     0.12869643     0.00000000    -0.99042176
         A    -0.05001972     0.99042176     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00033369 1/CM   AABB:     0.00000002 1/CM   ABAB:  -0.00000069 1/CM
BBBB:    -0.00000005 1/CM   BBCC:    -0.00000005 1/CM
CCCC:    -0.00000004 1/CM   CCAA:    -0.00000007 1/CM

AAAA:      -10.00372 MHZ    AABB:        0.00053 MHZ    ABAB:     -0.02060 MHZ
BBBB:       -0.00140 MHZ    BBCC:       -0.00135 MHZ
CCCC:       -0.00131 MHZ    CCAA:       -0.00205 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.33487817E+01 1/CM   100393.95111 MHZ
       B:  0.54498182E-01 1/CM     1633.81445 MHZ
```

```
       C:  0.53625351E-01 1/CM     1607.64762 MHZ

 FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
 --------------------------------------------
      DJ:  0.11302489E-07 1/CM        0.00034 MHZ
     DJK:  0.33364179E-06 1/CM        0.01000 MHZ
      DK:  0.83077070E-04 1/CM        2.49059 MHZ
      R5: -0.80433588E-07 1/CM       -0.00241 MHZ
      R6: -0.10834474E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.18158357E-09 1/CM        0.00001 MHZ

 A-REDUCTION DISTORTION CONSTANTS
 --------------------------------
  DELTA-J:  0.11304656E-07 1/CM        0.00034 MHZ
 DELTA-JK:  0.33362879E-06 1/CM        0.01000 MHZ
  DELTA-K:  0.83077081E-04 1/CM        2.49059 MHZ
    DEL-J:  0.18158357E-09 1/CM        0.00001 MHZ
    DEL-K:  0.19358511E-06 1/CM        0.00580 MHZ

 S-REDUCTION DISTORTION CONSTANTS
 --------------------------------
      ~DJ:  0.11291835E-07 1/CM        0.00034 MHZ
     ~DJK:  0.33370571E-06 1/CM        0.01000 MHZ
      ~DK:  0.83077017E-04 1/CM        2.49059 MHZ
   ~DEL-J:  0.18158357E-09 1/CM        0.00001 MHZ
      ~R6: -0.64105299E-11 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                     A             B             C
 ALPHA    S    -0.00028503     0.00017552     0.00017226  1/CM
          B    -0.03638679     0.00007374     0.00011573  1/CM
          A     0.06761908    -0.00004573    -0.00002937  1/CM

                     A             B             C
 ALPHA    S       -8.54507        5.26193        5.16410  MHZ
          B    -1090.84868        2.21077        3.46941  MHZ
          A     2027.16903       -1.37097       -0.88046  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XSS PERTURBED BY MODE B
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XSB PERTURBED BY MODE S
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XBS PERTURBED BY MODE S
                     S             B             A
 X(I,J):  S    -0.58844185    -0.93175421     0.41731104  1/CM
          B    -0.93175421    -0.83844774    -6.04606030  1/CM
          A     0.41731104    -6.04606030   -16.47824583  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.15288899  1/CM

-------------------------------------------------------------------------------
----------------------------------------- (2)H (74)Ge (127)I    EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.543755 A    (     4.807002 A.U.)
 R20:     1.595748 A    (     3.015528 A.U.)
 R30:     2.000040 RAD  (   114.593839 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.3171222   2   0   0
```

```
     1.7304002   0   2   0
     0.2682579   0   0   2
    -0.0652271   1   1   0
     0.0540635   1   0   1
     0.0346487   0   1   1
    -6.7483875   3   0   0
   -10.2586354   0   3   0
     0.2654789   0   0   3
     0.1605112   2   1   0
     0.1918999   1   2   0
    -0.1738901   2   0   1
     0.0425798   0   2   1
    -0.1399070   1   1   1
    -0.3948212   1   0   2
    -0.2874075   0   1   2
    19.2488698   4   0   0
    36.5257421   0   4   0
    -1.9944702   0   0   4
     0.4163340   3   1   0
     0.6538067   1   3   0
     1.0161271   2   2   0
     0.8249896   3   0   1
    -0.2472566   0   3   1
     0.1162463   2   1   1
    -0.1489952   1   2   1
    -0.2298395   2   0   2
    -0.5379226   0   2   2
     0.1686264   1   1   2
     0.4646218   1   0   3
     0.4505342   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:     1.62381761     0.01037813     0.00000000    MASS: 73.921178 AMU
CENTER  2:    -0.92036984    -0.02846404     0.00000000    MASS:126.904468 AMU
CENTER  3:    -1.60640584     1.41256526     0.00000000    MASS:  2.014102 AMU
MOMENTS:       6.85732802   510.79585722   517.65318524    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        4.0823      0.0548      0.0541    1/CM
     122385.7      1643.0      1621.2     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.3171 AJ/A**2    F12:    -0.0652 AJ/A**2    F1A:     0.0541 AJ/A
                           F22:     1.7304 AJ/A**2    F2A:     0.0346 AJ/A
                                                      FAA:     0.2683 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                73.921178     126.904468       2.014102  AMU
FUNDAMENTAL FREQUENCIES:      217.42977      302.87871     1217.47688  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
```

```
              R1            R2            R3          FREQUENCY
Q1:        0.99996321    0.00854683    0.00073234      217.42977199 S
Q2:        0.20013141   -0.00116714    0.97976837      302.87870683 B
Q3:       -0.04404187    0.99882584    0.02018041     1217.47688144 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S             B             A
ZETA-C   S     0.00000000   -0.11829578    0.06525697
         B     0.11829578   -0.00000000   -0.99083179
         A    -0.06525697    0.99083179    0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00295351 1/CM   AABB:    -0.00000042 1/CM   ABAB:  -0.00000174 1/CM
BBBB:    -0.00000006 1/CM   BBCC:    -0.00000005 1/CM
CCCC:    -0.00000005 1/CM   CCAA:    -0.00000093 1/CM

AAAA:      -88.54401 MHZ    AABB:       -0.01273 MHZ    ABAB:     -0.05226 MHZ
BBBB:       -0.00166 MHZ    BBCC:       -0.00162 MHZ
CCCC:       -0.00158 MHZ    CCAA:       -0.02794 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.40823480E+01 1/CM   122385.71811 MHZ
       B:  0.54804846E-01 1/CM     1643.00799 MHZ
       C:  0.54078503E-01 1/CM     1621.23279 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.13495971E-07 1/CM        0.00040 MHZ
     DJK:  0.11838132E-05 1/CM        0.03549 MHZ
      DK:  0.73718020E-03 1/CM       22.10011 MHZ
      R5: -0.18614216E-06 1/CM       -0.00558 MHZ
      R6: -0.19584965E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.16483617E-09 1/CM        0.00000 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.13499888E-07 1/CM        0.00040 MHZ
DELTA-JK:  0.11837897E-05 1/CM        0.03549 MHZ
 DELTA-K:  0.73718022E-03 1/CM       22.10011 MHZ
   DEL-J:  0.16483617E-09 1/CM        0.00000 MHZ
   DEL-K:  0.45917048E-06 1/CM        0.01377 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.13479187E-07 1/CM        0.00040 MHZ
    ~DJK:  0.11839139E-05 1/CM        0.03549 MHZ
     ~DK:  0.73718012E-03 1/CM       22.10010 MHZ
  ~DEL-J:  0.16483617E-09 1/CM        0.00000 MHZ
     ~R6: -0.10350139E-10 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                     A             B             C
ALPHA    S     0.00605967    0.00027686    0.00027422  1/CM
         B    -0.08068605    0.00009977    0.00016267  1/CM
         A     0.17126452    0.00006394    0.00009106  1/CM

                     A             B             C
ALPHA    S      181.66446       8.30019       8.22095  MHZ
         B    -2418.90713       2.99104       4.87687  MHZ
```

```
         A     5134.38129        1.91679        2.72994  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S              B              A
 X(I,J):  S    -1.32374343    -3.05340883     0.65416061  1/CM
          B    -3.05340883    -5.32430503   -15.66691430  1/CM
          A     0.65416061   -15.66691430   -40.18598600  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:         0.11576490  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H (74)Ge (127)I    TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.517404 A    (     4.757205 A.U.)
 R20:     1.559635 A    (     2.947284 A.U.)
 R30:     2.015500 RAD  (   115.479669 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.6584738   2   0   0
      2.2720694   0   2   0
      0.3919718   0   0   2
     -0.0487141   1   1   0
      0.0429210   1   0   1
     -0.0076252   0   1   1
     -7.0222125   3   0   0
    -11.4243603   0   3   0
     -0.1439254   0   0   3
     -0.0267398   2   1   0
     -0.0141252   1   2   0
     -0.2079718   2   0   1
      0.0530771   0   2   1
     -0.0788651   1   1   1
     -0.3283738   1   0   2
     -0.1719479   0   1   2
     22.3260007   4   0   0
     42.6704256   0   4   0
     -0.1912257   0   0   4
      0.1668945   3   1   0
      0.2487799   1   3   0
      0.1799071   2   2   0
      0.3786953   3   0   1
     -0.2599910   0   3   1
      0.1778723   2   1   1
      0.0734603   1   2   1
      0.1471873   2   0   2
     -0.5933312   0   2   2
      0.0753878   1   1   2
      0.2584390   1   0   3
      0.2286619   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:              A              B              C
 CENTER  1:     1.60667297     0.01026323     0.00000000    MASS: 73.921178 AMU
 CENTER  2:    -0.91044434    -0.02772057     0.00000000    MASS:126.904468 AMU
 CENTER  3:    -1.60255239     1.36993772     0.00000000    MASS:  2.014102 AMU
 MOMENTS:       6.45154164   500.12669328   506.57823492    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
```

```
--------------------------
          A           B           C        UNIT
     4.3391      0.0560      0.0553    1/CM
  130083.5      1678.1      1656.7    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.6585 AJ/A**2    F12:    -0.0487 AJ/A**2    F1A:     0.0429 AJ/A
                           F22:     2.2721 AJ/A**2    F2A:    -0.0076 AJ/A
                                                      FAA:     0.3920 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 73.921178     126.904468       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       244.65299      375.42975     1394.97122  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99979767     0.00796894     0.01846904        244.65298563 S
Q2:        0.03071491     0.00760182     0.99949928        375.42974902 B
Q3:       -0.02728254     0.99961637    -0.00477188       1394.97121858 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S    -0.00000000    -0.12016517     0.01108971
         B     0.12016517    -0.00000000    -0.99269197
         A    -0.01108971     0.99269197     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00237008 1/CM   AABB:     0.00000003 1/CM   ABAB:  -0.00000125 1/CM
BBBB:    -0.00000005 1/CM   BBCC:    -0.00000005 1/CM
CCCC:    -0.00000004 1/CM   CCAA:    -0.00000036 1/CM

AAAA:      -71.05316 MHZ    AABB:        0.00088 MHZ    ABAB:     -0.03758 MHZ
BBBB:       -0.00140 MHZ    BBCC:       -0.00137 MHZ
CCCC:       -0.00133 MHZ    CCAA:       -0.01067 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.43391178E+01 1/CM   130083.48388 MHZ
       B:  0.55973955E-01 1/CM     1678.05700 MHZ
       C:  0.55260821E-01 1/CM     1656.67777 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.11399551E-07 1/CM        0.00034 MHZ
     DJK:  0.68552093E-06 1/CM        0.02055 MHZ
      DK:  0.59182262E-03 1/CM       17.74240 MHZ
      R5: -0.13253217E-06 1/CM       -0.00397 MHZ
      R6: -0.14458779E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.14271476E-09 1/CM        0.00000 MHZ

A-REDUCTION DISTORTION CONSTANTS
```

```
--------------------------------
 DELTA-J:  0.11402443E-07 1/CM        0.00034 MHZ
DELTA-JK:  0.68550358E-06 1/CM        0.02055 MHZ
 DELTA-K:  0.59182263E-03 1/CM       17.74240 MHZ
   DEL-J:  0.14271476E-09 1/CM        0.00000 MHZ
   DEL-K:  0.33454263E-06 1/CM        0.01003 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.11388519E-07 1/CM        0.00034 MHZ
    ~DJK:  0.68558713E-06 1/CM        0.02055 MHZ
     ~DK:  0.59182256E-03 1/CM       17.74239 MHZ
  ~DEL-J:  0.14271476E-09 1/CM        0.00000 MHZ
     ~R6: -0.69619982E-11 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    S     0.00069529     0.00019740     0.00019504  1/CM
         B    -0.13835603     0.00004284     0.00008776  1/CM
         A     0.10603834     0.00005532     0.00006977  1/CM

                    A              B              C
ALPHA    S       20.84441        5.91796        5.84708  MHZ
         B    -4147.80953        1.28440        2.63089  MHZ
         A     3178.94956        1.65833        2.09156  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -0.73573508    -1.03112126    -0.47021618  1/CM
         B    -1.03112126    -0.99329565    -8.66471609  1/CM
         A    -0.47021618    -8.66471609   -24.85696965  1/CM

DARLING-DENNISON RESONANCE PARAMETER:        0.05090187  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (1)H (120)Sn (19)F    GROUND STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     1.962453 A    (     3.708499 A.U.)
R20:     1.790257 A    (     3.383096 A.U.)
R30:     1.621974 RAD  (    92.932249 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     3.1944740   2   0   0
     1.7210709   0   2   0
     0.6703978   0   0   2
     0.0538943   1   1   0
     0.0269198   1   0   1
    -0.0676106   0   1   1
   -16.3821477   3   0   0
    -7.0263911   0   3   0
    -1.3100321   0   0   3
    -0.0837172   2   1   0
     0.0902840   1   2   0
    -0.0191586   2   0   1
     0.0484395   0   2   1
    -0.1169546   1   1   1
    -0.7166629   1   0   2
    -0.3131150   0   1   2
```

```
    75.8269837   4   0   0
    17.2477900   0   4   0
    11.4786562   0   0   4
     0.8111442   3   1   0
    -2.7517195   1   3   0
    -0.2052767   2   2   0
     0.5548443   3   0   1
     1.2904097   0   3   1
     0.3903715   2   1   1
    -0.2478085   1   2   1
     1.5014070   2   0   2
    -0.0157077   0   2   2
     0.9833263   1   1   2
     4.0533615   1   0   3
     1.4203934   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:     0.28150987     0.00130852     0.00000000    MASS:119.902197 AMU
CENTER  2:    -1.67802728    -0.09754692     0.00000000    MASS: 18.998403 AMU
CENTER  3:    -1.85926420     1.68317076     0.00000000    MASS:  1.007825 AMU
MOMENTS:       5.04172970   110.39399344   115.43572315    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         5.5525       0.2536       0.2425     1/CM
      166458.5       7602.2       7270.2     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.996)           OBLATE
-------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     3.1945 AJ/A**2    F12:      0.0539 AJ/A**2    F1A:      0.0269 AJ/A
                           F22:      1.7211 AJ/A**2    F2A:     -0.0676 AJ/A
                                                       FAA:      0.6704 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197      18.998403       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       534.72359       654.86750     1749.87894  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.95716576     0.01219229     0.28928370        534.72358557 S
Q2:       -0.81837650     0.02665620     0.57406389        654.86749791 B
Q3:        0.03216279     0.99787697    -0.05663140       1749.87894146 A


CORIOLIS COUPLING MATRICES
--------------------------
                   S              B              A
ZETA-C   S     0.00000000    -0.21700712    -0.43839450
         B     0.21700712     0.00000000    -0.87219159
         A     0.43839450     0.87219159     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
```

```
-----------------------------------------------
AAAA:    -0.00092579 1/CM   AABB:     0.00000153 1/CM   ABAB:  -0.00001388 1/CM
BBBB:    -0.00000085 1/CM   BBCC:    -0.00000078 1/CM
CCCC:    -0.00000071 1/CM   CCAA:    -0.00000036 1/CM

AAAA:      -27.75442 MHZ    AABB:        0.04598 MHZ    ABAB:     -0.41625 MHZ
BBBB:       -0.02562 MHZ    BBCC:       -0.02334 MHZ
CCCC:       -0.02137 MHZ    CCAA:       -0.01089 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.55524594E+01 1/CM   166458.54951 MHZ
       B:  0.25358384E+00 1/CM     7602.25259 MHZ
       C:  0.24250604E+00 1/CM     7270.14833 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.19559297E-06 1/CM        0.00586 MHZ
     DJK:  0.62584008E-05 1/CM        0.18762 MHZ
      DK:  0.22499296E-03 1/CM        6.74512 MHZ
      R5: -0.16125659E-05 1/CM       -0.04834 MHZ
      R6: -0.15792649E-09 1/CM       -0.00000 MHZ
   DEL-J:  0.88607166E-08 1/CM        0.00027 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.19590882E-06 1/CM        0.00587 MHZ
DELTA-JK:  0.62565057E-05 1/CM        0.18757 MHZ
 DELTA-K:  0.22499454E-03 1/CM        6.74517 MHZ
   DEL-J:  0.88607166E-08 1/CM        0.00027 MHZ
   DEL-K:  0.38300946E-05 1/CM        0.11482 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.19390912E-06 1/CM        0.00581 MHZ
    ~DJK:  0.62685039E-05 1/CM        0.18793 MHZ
     ~DK:  0.22498454E-03 1/CM        6.74487 MHZ
  ~DEL-J:  0.88607166E-08 1/CM        0.00027 MHZ
     ~R6: -0.99985219E-09 1/CM       -0.00003 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A             B             C
ALPHA    S    -0.02373591     0.00112028     0.00129012  1/CM
         B    -0.06598344     0.00086787     0.00123569  1/CM
         A     0.14594924    -0.00013335     0.00011782  1/CM

                    A             B             C
ALPHA    S     -711.58463       33.58518       38.67696  MHZ
         B    -1978.13377       26.01805       37.04520  MHZ
         A     4375.44831       -3.99768        3.53218  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S             B             A
X(I,J):  S    -0.50406045     3.15792304    -5.49329705  1/CM
         B     3.15792304     0.78426117    -7.20155157  1/CM
         A    -5.49329705    -7.20155157   -39.58239066  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -7.75619176  1/CM

-------------------------------------------------------------------------------
----------------------------------------- (1)H (120)Sn (19)F    EXCITED STATE
-------------------------------------------------------------------------------
```

```
REFERENCE GEOMETRY
------------------
R10:     1.959168 A    (     3.702292 A.U.)
R20:     1.858484 A    (     3.512027 A.U.)
R30:     1.974630 RAD  (   113.137957 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     3.2171686   2   0   0
     0.6264716   0   2   0
     0.1832124   0   0   2
    -0.0580727   1   1   0
     0.0375920   1   0   1
     0.0775720   0   1   1
   -16.8763606   3   0   0
    -5.6246464   0   3   0
     0.2545823   0   0   3
     0.0071759   2   1   0
    -0.0681466   1   2   0
    -0.2029830   2   0   1
    -0.1005414   0   2   1
    -0.1219102   1   1   1
     0.0189990   1   0   2
    -0.2883600   0   1   2
    75.8987598   4   0   0
    24.7870671   0   4   0
     1.1587333   0   0   4
     0.3289192   3   1   0
     0.6119103   1   3   0
     0.5842295   2   2   0
    -0.1961953   3   0   1
    -0.3698767   0   3   1
     0.1409485   2   1   1
     0.1589281   1   2   1
    -1.2017340   2   0   2
    -0.8224460   0   2   2
    -0.4652858   1   1   2
    -0.6080126   1   0   3
    -0.6188973   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A             B             C
CENTER  1:     0.28562554     0.00554085     0.00000000    MASS:119.902197 AMU
CENTER  2:    -1.66975272    -0.11684552     0.00000000    MASS: 18.998403 AMU
CENTER  3:    -2.50489362     1.54344023     0.00000000    MASS:  1.007825 AMU
MOMENTS:       4.42350939   114.70018663   119.12369601    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
      6.3285      0.2441      0.2350    1/CM
    189722.4      7316.8      7045.1    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.997)           OBLATE
------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     3.2172 AJ/A**2    F12:    -0.0581 AJ/A**2    F1A:     0.0376 AJ/A
```

```
                          F22:     0.6265 AJ/A**2    F2A:     0.0776 AJ/A
                                                     FAA:     0.1832 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197      18.998403       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       306.07583      570.53686     1059.07423  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
                R1             R2             R3             FREQUENCY
Q1:         0.44124930    -0.00376435     0.89737667        306.07583153 B
Q2:         0.99916131     0.04021724    -0.00769721        570.53685820 S
Q3:        -0.28089839     0.95202372     0.12143695       1059.07423396 A


CORIOLIS COUPLING MATRICES
--------------------------
                     B              S              A
ZETA-C   B      0.00000000     0.14659880    -0.96883004
         S     -0.14659880     0.00000000     0.19969261
         A      0.96883004    -0.19969261     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:     -0.01402724 1/CM   AABB:      0.00003481 1/CM   ABAB:  -0.00004302 1/CM
BBBB:     -0.00000088 1/CM   BBCC:     -0.00000076 1/CM
CCCC:     -0.00000069 1/CM   CCAA:      0.00001293 1/CM

AAAA:      -420.52622 MHZ    AABB:         1.04355 MHZ    ABAB:      -1.28985 MHZ
BBBB:        -0.02627 MHZ    BBCC:        -0.02292 MHZ
CCCC:        -0.02072 MHZ    CCAA:         0.38762 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.63284594E+01 1/CM   189722.44412 MHZ
       B:  0.24406881E+00 1/CM     7316.99912 MHZ
       C:  0.23499299E+00 1/CM     7044.91273 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.19473239E-06 1/CM        0.00584 MHZ
     DJK:  0.91881933E-05 1/CM        0.27546 MHZ
      DK:  0.34974282E-02 1/CM      104.85026 MHZ
      R5: -0.40048276E-05 1/CM       -0.12006 MHZ
      R6: -0.59882752E-09 1/CM       -0.00002 MHZ
   DEL-J:  0.11589865E-07 1/CM        0.00035 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.19593005E-06 1/CM        0.00587 MHZ
DELTA-JK:  0.91810074E-05 1/CM        0.27524 MHZ
 DELTA-K:  0.34974342E-02 1/CM      104.85044 MHZ
   DEL-J:  0.11589865E-07 1/CM        0.00035 MHZ
   DEL-K:  0.11223660E-04 1/CM        0.33648 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.19174770E-06 1/CM        0.00575 MHZ
    ~DJK:  0.92061014E-05 1/CM        0.27599 MHZ
     ~DK:  0.34974133E-02 1/CM      104.84981 MHZ
  ~DEL-J:  0.11589865E-07 1/CM        0.00035 MHZ
     ~R6: -0.20911720E-08 1/CM       -0.00006 MHZ
```

```
 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 --------------------------------------------------
                      A              B              C
 ALPHA    B    -0.00600054    -0.00206444    -0.00040036  1/CM
          S    -0.00039885     0.00161332     0.00153195  1/CM
          A     1.21955428     0.00039504     0.00200542  1/CM

                      A              B              C
 ALPHA    B     -179.89153      -61.89021      -12.00250  MHZ
          S      -11.95733       48.36604       45.92685  MHZ
          A    36561.31846       11.84287       60.12093  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      B              S              A
 X(I,J):  B    -4.09645521    -2.40728742   -93.22444559  1/CM
          S    -2.40728742    -2.73914589   -12.34886649  1/CM
          A   -93.22444559   -12.34886649  -219.26179507  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -6.62279116  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (1)H (120)Sn (19)F    TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     1.951604 A    (     3.687999 A.U.)
 R20:     1.746351 A    (     3.300127 A.U.)
 R30:     2.005609 RAD  (   114.912944 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      3.3853299   2   0   0
      1.7121679   0   2   0
      0.2958259   0   0   2
     -0.0066585   1   1   0
      0.0561150   1   0   1
      0.0247861   0   1   1
    -17.5546232   3   0   0
     -8.6469277   0   3   0
      0.2302752   0   0   3
     -0.1345809   2   1   0
     -0.1298227   1   2   0
     -0.1905428   2   0   1
     -0.1300980   0   2   1
     -0.1363392   1   1   1
      0.0409765   1   0   2
     -0.0903959   0   1   2
     77.1530854   4   0   0
     30.1255406   0   4   0
      0.8012066   0   0   4
     -0.9397969   3   1   0
     -0.5059702   1   3   0
     -0.4343192   2   2   0
      0.3486297   3   0   1
      0.6956260   0   3   1
      0.1728659   2   1   1
      0.2895236   1   2   1
     -1.4076327   2   0   2
     -1.2711218   0   2   2
     -0.7151663   1   1   2
     -1.4528945   1   0   3
     -1.5980237   0   1   3
```

```
EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A             B             C
CENTER  1:     0.28455791     0.00509495     0.00000000    MASS:119.902197 AMU
CENTER  2:    -1.66383473    -0.10804016     0.00000000    MASS: 18.998403 AMU
CENTER  3:    -2.48943619     1.43050087     0.00000000    MASS:  1.007825 AMU
MOMENTS:       3.79799976   113.82741870   117.62541847    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         7.3707      0.2459      0.2380    1/CM
       220968.7      7372.9      7134.8    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.998)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     3.3853 AJ/A**2    F12:    -0.0067 AJ/A**2    F1A:     0.0561 AJ/A
                           F22:     1.7122 AJ/A**2    F2A:     0.0248 AJ/A
                                                      FAA:     0.2958 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:               119.902197      18.998403       1.007825  AMU
FUNDAMENTAL FREQUENCIES:      421.34194      592.10398     1743.19970  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.59592023     0.02929259     0.80250920        421.34193572 B
Q2:        0.99853884     0.02363209    -0.04859740        592.10397764 S
Q3:       -0.05297115     0.99854082     0.01050194       1743.19969864 A


CORIOLIS COUPLING MATRICES
--------------------------
                    B              S              A
ZETA-C   B     0.00000000     0.19073136    -0.93521894
         S    -0.19073136    -0.00000000     0.29830703
         A     0.93521894    -0.29830703     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00974901 1/CM   AABB:     0.00002236 1/CM   ABAB:  -0.00002778 1/CM
BBBB:    -0.00000078 1/CM   BBCC:    -0.00000070 1/CM
CCCC:    -0.00000065 1/CM   CCAA:     0.00001077 1/CM

AAAA:     -292.26784 MHZ    AABB:        0.67021 MHZ    ABAB:     -0.83291 MHZ
BBBB:       -0.02330 MHZ    BBCC:       -0.02113 MHZ
CCCC:       -0.01945 MHZ    CCAA:        0.32292 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.73707218E+01 1/CM   220968.68495 MHZ
       B:  0.24593746E+00 1/CM     7373.01976 MHZ
       C:  0.23798903E+00 1/CM     7134.73174 MHZ
```

```
FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.17772952E-06 1/CM        0.00533 MHZ
     DJK:  0.52541493E-05 1/CM        0.15752 MHZ
      DK:  0.24318195E-02 1/CM       72.90412 MHZ
      R5: -0.27447934E-05 1/CM       -0.08229 MHZ
      R6: -0.26088268E-09 1/CM       -0.00001 MHZ
   DEL-J:  0.80435912E-08 1/CM        0.00024 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.17825128E-06 1/CM        0.00534 MHZ
DELTA-JK:  0.52510187E-05 1/CM        0.15742 MHZ
 DELTA-K:  0.24318221E-02 1/CM       72.90420 MHZ
   DEL-J:  0.80435912E-08 1/CM        0.00024 MHZ
   DEL-K:  0.73614221E-05 1/CM        0.22069 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.17619932E-06 1/CM        0.00528 MHZ
    ~DJK:  0.52633304E-05 1/CM        0.15779 MHZ
     ~DK:  0.24318119E-02 1/CM       72.90389 MHZ
  ~DEL-J:  0.80435912E-08 1/CM        0.00024 MHZ
     ~R6: -0.10259810E-08 1/CM       -0.00003 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                     A              B              C
ALPHA    B    -0.22228326    -0.00110205    -0.00018555  1/CM
         S    -0.02592010     0.00150611     0.00143181  1/CM
         A     0.27737491     0.00048998     0.00073091  1/CM

                     A              B              C
ALPHA    B    -6663.88466      -33.03859       -5.56264  MHZ
         S     -777.06505       45.15190       42.92468  MHZ
         A     8315.49087       14.68911       21.91203  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                     B              S              A
X(I,J):  B    -0.13518910     0.85514653   -18.70350529  1/CM
         S     0.85514653    -2.76307908    -1.88277466  1/CM
         A   -18.70350529    -1.88277466   -54.61193834  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -4.68696280  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (2)H (120)Sn (19)F    GROUND STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     1.962453 A    (     3.708499 A.U.)
R20:     1.790257 A    (     3.383096 A.U.)
R30:     1.621974 RAD  (    92.932249 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     3.1944740   2   0   0
     1.7210709   0   2   0
     0.6703978   0   0   2
     0.0538943   1   1   0
     0.0269198   1   0   1
    -0.0676106   0   1   1
```

```
  -16.3821477   3   0   0
   -7.0263911   0   3   0
   -1.3100321   0   0   3
   -0.0837172   2   1   0
    0.0902840   1   2   0
   -0.0191586   2   0   1
    0.0484395   0   2   1
   -0.1169546   1   1   1
   -0.7166629   1   0   2
   -0.3131150   0   1   2
   75.8269837   4   0   0
   17.2477900   0   4   0
   11.4786562   0   0   4
    0.8111442   3   1   0
   -2.7517195   1   3   0
   -0.2052767   2   2   0
    0.5548443   3   0   1
    1.2904097   0   3   1
    0.3903715   2   1   1
   -0.2478085   1   2   1
    1.5014070   2   0   2
   -0.0157077   0   2   2
    0.9833263   1   1   2
    4.0533615   1   0   3
    1.4203934   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
--------------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      0.29495905     0.00363654     0.00000000    MASS:119.902197 AMU
CENTER  2:     -1.65745272    -0.19039054     0.00000000    MASS: 18.998403 AMU
CENTER  3:     -1.92506818     1.57940725     0.00000000    MASS:  2.014102 AMU
MOMENTS:        9.48907600   116.38177383   125.87084982    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         2.9501      0.2405      0.2224    1/CM
        88442.6      7211.1      6667.5    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.987)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     3.1945 AJ/A**2    F12:     0.0539 AJ/A**2    F1A:     0.0269 AJ/A
                           F22:     1.7211 AJ/A**2    F2A:    -0.0676 AJ/A
                                                      FAA:     0.6704 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:               119.902197      18.998403       2.014102  AMU
FUNDAMENTAL FREQUENCIES:      423.51303      599.34907     1270.43587  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
              R1             R2             R3            FREQUENCY
Q1:       0.70843805     0.05005367     0.70399586       423.51302792 B
Q2:       0.98023001    -0.01708037    -0.19712276       599.34906620 A
Q3:       0.03478362     0.99710870    -0.06755997      1270.43587082 S
```

```
CORIOLIS COUPLING MATRICES
--------------------------
                    B             A             S
ZETA-C   B     0.00000000    0.28686011   -0.78167070
         A    -0.28686011    0.00000000    0.55380699
         S     0.78167070   -0.55380699    0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00027701 1/CM   AABB:     0.00000189 1/CM   ABAB:  -0.00001137 1/CM
BBBB:    -0.00000085 1/CM   BBCC:    -0.00000071 1/CM
CCCC:    -0.00000061 1/CM   CCAA:     0.00000004 1/CM

AAAA:       -8.30456 MHZ    AABB:        0.05657 MHZ    ABAB:     -0.34078 MHZ
BBBB:       -0.02537 MHZ    BBCC:       -0.02137 MHZ
CCCC:       -0.01826 MHZ    CCAA:        0.00117 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.29501291E+01 1/CM    88442.64834 MHZ
       B:  0.24053706E+00 1/CM     7211.11997 MHZ
       C:  0.22240145E+00 1/CM     6667.42779 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.18102017E-06 1/CM        0.00543 MHZ
     DJK:  0.48400507E-05 1/CM        0.14510 MHZ
      DK:  0.64231527E-04 1/CM        1.92561 MHZ
      R5: -0.12979775E-05 1/CM       -0.03891 MHZ
      R6: -0.46683718E-09 1/CM       -0.00001 MHZ
   DEL-J:  0.14824053E-07 1/CM        0.00044 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.18195384E-06 1/CM        0.00545 MHZ
DELTA-JK:  0.48344486E-05 1/CM        0.14493 MHZ
 DELTA-K:  0.64236196E-04 1/CM        1.92575 MHZ
   DEL-J:  0.14824053E-07 1/CM        0.00044 MHZ
   DEL-K:  0.31558130E-05 1/CM        0.09461 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.17669090E-06 1/CM        0.00530 MHZ
    ~DJK:  0.48660263E-05 1/CM        0.14588 MHZ
     ~DK:  0.64209881E-04 1/CM        1.92496 MHZ
  ~DEL-J:  0.14824053E-07 1/CM        0.00044 MHZ
     ~R6: -0.26314721E-08 1/CM       -0.00008 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A             B             C
ALPHA    B    -0.03099316    0.00031852    0.00089198  1/CM
         A    -0.00828136    0.00142311    0.00137584  1/CM
         S     0.05447987    0.00002286    0.00027802  1/CM

                    A             B             C
ALPHA    B     -929.15146       9.54897      26.74101  MHZ
         A     -248.26879      42.66379      41.24679  MHZ
         S     1633.26541       0.68527       8.33495  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
```

```
                    B              A              S
X(I,J):  B     2.54647013    -1.21172134    -6.84677204  1/CM
         A    -1.21172134    -2.85237517     2.59758398  1/CM
         S    -6.84677204     2.59758398   -20.87224148  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -4.99947677  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H (120)Sn (19)F    EXCITED STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     1.959168 A    (     3.702292 A.U.)
R20:     1.858484 A    (     3.512027 A.U.)
R30:     1.974630 RAD  (   113.137957 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     3.2171686   2   0   0
     0.6264716   0   2   0
     0.1832124   0   0   2
    -0.0580727   1   1   0
     0.0375920   1   0   1
     0.0775720   0   1   1
   -16.8763606   3   0   0
    -5.6246464   0   3   0
     0.2545823   0   0   3
     0.0071759   2   1   0
    -0.0681466   1   2   0
    -0.2029830   2   0   1
    -0.1005414   0   2   1
    -0.1219102   1   1   1
     0.0189990   1   0   2
    -0.2883600   0   1   2
    75.8987598   4   0   0
    24.7870671   0   4   0
     1.1587333   0   0   4
     0.3289192   3   1   0
     0.6119103   1   3   0
     0.5842295   2   2   0
    -0.1961953   3   0   1
    -0.3698767   0   3   1
     0.1409485   2   1   1
     0.1589281   1   2   1
    -1.2017340   2   0   2
    -0.8224460   0   2   2
    -0.4652858   1   1   2
    -0.6080126   1   0   3
    -0.6188973   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A             B             C
CENTER  1:     0.30335848     0.01112909     0.00000000    MASS:119.902197 AMU
CENTER  2:    -1.64239799    -0.21803088     0.00000000    MASS: 18.998403 AMU
CENTER  3:    -2.56710422     1.39408807     0.00000000    MASS:  2.014102 AMU
MOMENTS:       8.02427822   125.46107195   133.48535017    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
     3.4887      0.2231      0.2097    1/CM
   104587.5      6689.2      6287.1    MHZ
```

```
PROLATE          ASYMMETRIC ROTOR (K=-0.992)           OBLATE
-----------------------------+-----------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     3.2172 AJ/A**2    F12:    -0.0581 AJ/A**2    F1A:     0.0376 AJ/A
                           F22:     0.6265 AJ/A**2    F2A:     0.0776 AJ/A
                                                      FAA:     0.1832 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197      18.998403       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       226.72298      559.87162      777.30056  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.42477573     0.02373276     0.90498748        226.72298006 B
Q2:        0.99325980     0.11589633     0.00173665        559.87162169 S
Q3:       -0.55978772     0.82239800     0.10148515        777.30055628 A


CORIOLIS COUPLING MATRICES
--------------------------
                     B              S              A
ZETA-C   B     0.00000000     0.07516693    -0.96292657
         S    -0.07516693     0.00000000     0.25907981
         A     0.96292657    -0.25907981     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00482323 1/CM   AABB:     0.00003784 1/CM   ABAB:  -0.00002968 1/CM
BBBB:    -0.00000104 1/CM   BBCC:    -0.00000078 1/CM
CCCC:    -0.00000063 1/CM   CCAA:     0.00001600 1/CM

AAAA:     -144.59690 MHZ    AABB:        1.13456 MHZ    ABAB:     -0.88968 MHZ
BBBB:       -0.03108 MHZ    BBCC:       -0.02336 MHZ
CCCC:       -0.01890 MHZ    CCAA:        0.47973 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.34886626E+01 1/CM   104587.47613 MHZ
       B:  0.22313563E+00 1/CM     6689.43802 MHZ
       C:  0.20970926E+00 1/CM     6286.92563 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.20501891E-06 1/CM        0.00615 MHZ
     DJK:  0.96649849E-06 1/CM        0.02897 MHZ
      DK:  0.12046368E-02 1/CM       36.11410 MHZ
      R5: -0.23317119E-05 1/CM       -0.06990 MHZ
      R6: -0.17028035E-08 1/CM       -0.00005 MHZ
   DEL-J:  0.25397764E-07 1/CM        0.00076 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.20842452E-06 1/CM        0.00625 MHZ
DELTA-JK:  0.94606485E-06 1/CM        0.02836 MHZ
 DELTA-K:  0.12046538E-02 1/CM       36.11461 MHZ
   DEL-J:  0.25397764E-07 1/CM        0.00076 MHZ
```

```
   DEL-K:  0.79834473E-05 1/CM        0.23934 MHZ

 S-REDUCTION DISTORTION CONSTANTS
 --------------------------------
     ~DJ:  0.20023527E-06 1/CM        0.00600 MHZ
    ~DJK:  0.99520032E-06 1/CM        0.02984 MHZ
     ~DK:  0.12046129E-02 1/CM       36.11339 MHZ
  ~DEL-J:  0.25397764E-07 1/CM        0.00076 MHZ
     ~R6: -0.40946222E-08 1/CM       -0.00012 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                     A              B              C
 ALPHA    B     0.00213598    -0.00251484    -0.00063063  1/CM
          S     0.01017654     0.00151716     0.00146398  1/CM
          A     0.48252698     0.00004058     0.00170774  1/CM

                     A              B              C
 ALPHA    B       64.03500      -75.39316      -18.90569  MHZ
          S      305.08493       45.48327       43.88890  MHZ
          A    14465.79545        1.21654       51.19677  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XBS PERTURBED BY MODE A
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XBA PERTURBED BY MODE S
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XSB PERTURBED BY MODE A
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XSA PERTURBED BY MODE B
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XAB PERTURBED BY MODE S
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XAS PERTURBED BY MODE B
                     B              S              A
 X(I,J):  B    -2.28631715    -3.58985235   -47.33185828  1/CM
          S    -3.58985235    -3.05672189   -28.71221872  1/CM
          A   -47.33185828   -28.71221872  -104.99268120  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:      -16.72089648  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H (120)Sn (19)F    TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     1.951604 A    (     3.687999 A.U.)
 R20:     1.746351 A    (     3.300127 A.U.)
 R30:     2.005609 RAD  (   114.912944 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      3.3853299   2   0   0
      1.7121679   0   2   0
      0.2958259   0   0   2
     -0.0066585   1   1   0
      0.0561150   1   0   1
      0.0247861   0   1   1
    -17.5546232   3   0   0
     -8.6469277   0   3   0
      0.2302752   0   0   3
     -0.1345809   2   1   0
     -0.1298227   1   2   0
     -0.1905428   2   0   1
     -0.1300980   0   2   1
     -0.1363392   1   1   1
      0.0409765   1   0   2
```

```
    -0.0903959   0   1   2
    77.1530854   4   0   0
    30.1255406   0   4   0
     0.8012066   0   0   4
    -0.9397969   3   1   0
    -0.5059702   1   3   0
    -0.4343192   2   2   0
     0.3486297   3   0   1
     0.6956260   0   3   1
     0.1728659   2   1   1
     0.2895236   1   2   1
    -1.4076327   2   0   2
    -1.2711218   0   2   2
    -0.7151663   1   1   2
    -1.4528945   1   0   3
    -1.5980237   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:     0.30220951     0.01010568     0.00000000    MASS:119.902197 AMU
CENTER  2:    -1.63801766    -0.20096774     0.00000000    MASS: 18.998403 AMU
CENTER  3:    -2.54002227     1.29406200     0.00000000    MASS:  2.014102 AMU
MOMENTS:       6.89512471   124.40664823   131.30177294    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         4.0600       0.2250       0.2132     1/CM
      121714.8       6745.9       6391.7     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.994)           OBLATE
-------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     3.3853 AJ/A**2    F12:    -0.0067 AJ/A**2    F1A:     0.0561 AJ/A
                           F22:     1.7122 AJ/A**2    F2A:     0.0248 AJ/A
                                                      FAA:     0.2958 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:               119.902197      18.998403       2.014102  AMU
FUNDAMENTAL FREQUENCIES:      311.14872      588.01776     1265.67487  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.50174857     0.05788801     0.86307436       311.14871825 B
Q2:        0.99809737     0.05121057    -0.03433837       588.01776163 S
Q3:       -0.10840735     0.99408590     0.00640888      1265.67486617 A


CORIOLIS COUPLING MATRICES
--------------------------
                   B              S              A
ZETA-C   B     0.00000000     0.23156502    -0.91922538
         S    -0.23156502    -0.00000000     0.31843733
         A     0.91922538    -0.31843733     0.00000000
```

```
TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00337763 1/CM   AABB:     0.00002420 1/CM   ABAB:  -0.00001972 1/CM
BBBB:    -0.00000079 1/CM   BBCC:    -0.00000065 1/CM
CCCC:    -0.00000055 1/CM   CCAA:     0.00001241 1/CM

AAAA:     -101.25890 MHZ    AABB:        0.72543 MHZ    ABAB:     -0.59128 MHZ
BBBB:       -0.02383 MHZ    BBCC:       -0.01939 MHZ
CCCC:       -0.01638 MHZ    CCAA:        0.37200 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.40599700E+01 1/CM   121714.84142 MHZ
       B:  0.22502400E+00 1/CM     6746.05006 MHZ
       C:  0.21319965E+00 1/CM     6391.56485 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.16617024E-06 1/CM        0.00498 MHZ
     DJK:  0.37752182E-06 1/CM        0.01132 MHZ
      DK:  0.84386463E-03 1/CM       25.29843 MHZ
      R5: -0.17207865E-05 1/CM       -0.05159 MHZ
      R6: -0.74450124E-09 1/CM       -0.00002 MHZ
   DEL-J:  0.15524039E-07 1/CM        0.00047 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.16765924E-06 1/CM        0.00503 MHZ
DELTA-JK:  0.36858780E-06 1/CM        0.01105 MHZ
 DELTA-K:  0.84387207E-03 1/CM       25.29865 MHZ
   DEL-J:  0.15524039E-07 1/CM        0.00047 MHZ
   DEL-K:  0.53762402E-05 1/CM        0.16118 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.16352146E-06 1/CM        0.00490 MHZ
    ~DJK:  0.39341451E-06 1/CM        0.01179 MHZ
     ~DK:  0.84385138E-03 1/CM       25.29803 MHZ
  ~DEL-J:  0.15524039E-07 1/CM        0.00047 MHZ
     ~R6: -0.20688920E-08 1/CM       -0.00006 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A             B             C
ALPHA    B    -0.09119570    -0.00136304    -0.00033702  1/CM
         S    -0.01436189     0.00142276     0.00130473  1/CM
         A     0.10995372     0.00054872     0.00077219  1/CM

                    A             B             C
ALPHA    B    -2733.97830      -40.86277      -10.10373  MHZ
         S     -430.55879       42.65340       39.11477  MHZ
         A     3296.32957       16.45030       23.14957  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    B             S             A
X(I,J):  B     0.01501107    -0.18506682    -9.37828315  1/CM
         S    -0.18506682    -3.16166446     0.32021694  1/CM
         A    -9.37828315     0.32021694   -28.47792511  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -2.11149409  1/CM

--------------------------------------------------------------------------------
------------------------------------------ (1)H (120)Sn (35)Cl   GROUND STATE
```

```
--------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.381128 A    (     4.499680 A.U.)
 R20:     1.793849 A    (     3.389884 A.U.)
 R30:     1.620862 RAD  (    92.868571 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.1551821   2   0   0
      1.7385235   0   2   0
      0.6870276   0   0   2
      0.0464385   1   1   0
      0.0925673   1   0   1
     -0.0670835   0   1   1
     -6.9959663   3   0   0
     -7.0690068   0   3   0
     -0.8635152   0   0   3
      0.2341554   2   1   0
     -0.0166298   1   2   0
     -0.4951679   2   0   1
      0.0179518   0   2   1
     -0.2008431   1   1   1
     -0.4336567   1   0   2
     -0.1017145   0   1   2
      7.2939281   4   0   0
     29.4329229   0   4   0
      4.2624983   0   0   4
      2.1439994   3   1   0
      0.5936032   1   3   0
     -0.3053067   2   2   0
     -3.3491722   3   0   1
      0.1458912   0   3   1
      0.2785830   2   1   1
      0.2968607   1   2   1
      3.3215551   2   0   2
     -0.8008194   0   2   2
      0.5007239   1   1   2
     -0.7019288   1   0   3
     -0.1890888   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------------
 AXES:                A             B             C
 CENTER  1:     0.55024335     0.00079758     0.00000000    MASS:119.902197 AMU
 CENTER  2:    -1.83019328    -0.05277537     0.00000000    MASS: 34.968853 AMU
 CENTER  3:    -1.96028693     1.73627578     0.00000000    MASS:  1.007825 AMU
 MOMENTS:       5.20695403   261.21355916   266.42051319    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
           A           B           C        UNIT
         5.3763      0.1072      0.1051    1/CM
      161176.6      3212.8      3150.1     MHZ

 PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
 -------------------------------+-------------------------------
 ^

 ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


 HARMONIC FORCE FIELD
 --------------------
```

```
F11:     2.1552 AJ/A**2    F12:     0.0464 AJ/A**2    F1A:     0.0926 AJ/A
                           F22:     1.7385 AJ/A**2    F2A:    -0.0671 AJ/A
                                                      FAA:     0.6870 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197      34.968853       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       363.54320      611.47426     1737.03958  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99864816     0.00115413     0.05196661        363.54319973 S
Q2:       -0.02553652     0.02786462     0.99928547        611.47425921 B
Q3:        0.02552544     0.99845004    -0.04945675       1737.03958353 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S     0.00000000    -0.14477836    -0.00149860
         B     0.14477836     0.00000000    -0.98946298
         A     0.00149860     0.98946298     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00083595 1/CM   AABB:     0.00000025 1/CM   ABAB:  -0.00000259 1/CM
BBBB:    -0.00000015 1/CM   BBCC:    -0.00000014 1/CM
CCCC:    -0.00000014 1/CM   CCAA:    -0.00000008 1/CM

AAAA:      -25.06102 MHZ    AABB:        0.00762 MHZ    ABAB:     -0.07752 MHZ
BBBB:       -0.00447 MHZ    BBCC:       -0.00429 MHZ
CCCC:       -0.00413 MHZ    CCAA:       -0.00225 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.53762717E+01 1/CM   161176.57439 MHZ
       B:  0.10716924E+00 1/CM     3212.85294 MHZ
       C:  0.10507427E+00 1/CM     3150.04739 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.35811877E-07 1/CM        0.00107 MHZ
     DJK:  0.11765193E-05 1/CM        0.03527 MHZ
      DK:  0.20777405E-03 1/CM        6.22891 MHZ
      R5: -0.30230123E-06 1/CM       -0.00906 MHZ
      R6: -0.55105798E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.71089187E-09 1/CM        0.00002 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.35822898E-07 1/CM        0.00107 MHZ
DELTA-JK:  0.11764532E-05 1/CM        0.03527 MHZ
 DELTA-K:  0.20777410E-03 1/CM        6.22891 MHZ
   DEL-J:  0.71089187E-09 1/CM        0.00002 MHZ
   DEL-K:  0.71550282E-06 1/CM        0.02145 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.35751792E-07 1/CM        0.00107 MHZ
    ~DJK:  0.11768798E-05 1/CM        0.03528 MHZ
     ~DK:  0.20777375E-03 1/CM        6.22890 MHZ
  ~DEL-J:  0.71089187E-09 1/CM        0.00002 MHZ
     ~R6: -0.35552954E-10 1/CM       -0.00000 MHZ
```

```
 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 --------------------------------------------------
                      A              B              C
 ALPHA     S    -0.00236705     0.00030198     0.00029727  1/CM
           B    -0.07877428     0.00005193     0.00017960  1/CM
           A     0.13950401    -0.00006534    -0.00001656  1/CM

                      A              B              C
 ALPHA     S      -70.96239        9.05328        8.91191  MHZ
           B    -2361.59366        1.55683        5.38417  MHZ
           A     4182.22504       -1.95871       -0.49650  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S              B              A
 X(I,J):   S    -1.11615749     1.43945665     0.93118877  1/CM
           B     1.43945665     1.32282474   -12.64996585  1/CM
           A     0.93118877   -12.64996585   -23.14744871  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.17288774  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (1)H (120)Sn (35)Cl   EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:      2.364413 A    (     4.468094 A.U.)
 R20:      1.832218 A    (     3.462391 A.U.)
 R30:      1.958935 RAD  (   112.238697 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.1481112   2   0   0
      0.8848852   0   2   0
      0.2664681   0   0   2
     -0.0728413   1   1   0
      0.0493070   1   0   1
      0.0582775   0   1   1
     -8.3269710   3   0   0
     -6.6281943   0   3   0
      0.0634806   0   0   3
      0.3779691   2   1   0
     -0.0280196   1   2   0
     -0.1578614   2   0   1
      0.0433690   0   2   1
     -0.0903336   1   1   1
     -0.2345949   1   0   2
     -0.4049673   0   1   2
      9.0956074   4   0   0
     24.2643908   0   4   0
     -0.9330710   0   0   4
      3.3056643   3   1   0
      0.3350091   1   3   0
      0.3991937   2   2   0
     -4.1824820   3   0   1
     -0.6914233   0   3   1
      0.4741557   2   1   1
      0.2323149   1   2   1
     -0.3094157   2   0   2
     -0.4707625   0   2   2
      0.4055808   1   1   2
     -0.0861174   1   0   3
```

```
     0.1595906   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A              B              C
CENTER  1:     0.55032802     0.00425453     0.00000000    MASS:119.902197 AMU
CENTER  2:    -1.81337954    -0.06116171     0.00000000    MASS: 34.968853 AMU
CENTER  3:    -2.55375235     1.61598246     0.00000000    MASS:  1.007825 AMU
MOMENTS:       4.59105908   262.15806397   266.74912305    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         6.0975       0.1068       0.1049     1/CM
      182798.6       3201.3       3146.2     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.1481 AJ/A**2    F12:    -0.0728 AJ/A**2    F1A:     0.0493 AJ/A
                           F22:     0.8849 AJ/A**2    F2A:     0.0583 AJ/A
                                                      FAA:     0.2665 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:               119.902197      34.968853       1.007825  AMU
FUNDAMENTAL FREQUENCIES:      355.90664      380.35341     1239.86886  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3            FREQUENCY
Q1:        0.97237522     0.01269919     0.23307758       355.90663773 S
Q2:       -0.87737253    -0.01963391     0.47940792       380.35340916 B
Q3:       -0.11887843     0.99059429     0.06775599      1239.86885852 A


CORIOLIS COUPLING MATRICES
--------------------------
                   S              B              A
ZETA-C   S     0.00000000    -0.12080635    -0.49476759
         B     0.12080635    -0.00000000    -0.86058751
         A     0.49476759     0.86058751    -0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00700103 1/CM   AABB:     0.00000165 1/CM   ABAB:  -0.00000637 1/CM
BBBB:    -0.00000015 1/CM   BBCC:    -0.00000014 1/CM
CCCC:    -0.00000014 1/CM   CCAA:    -0.00000048 1/CM

AAAA:     -209.88548 MHZ    AABB:        0.04933 MHZ    ABAB:     -0.19100 MHZ
BBBB:       -0.00450 MHZ    BBCC:       -0.00433 MHZ
CCCC:       -0.00418 MHZ    CCAA:       -0.01452 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.60975036E+01 1/CM   182798.56545 MHZ
       B:  0.10678357E+00 1/CM     3201.29112 MHZ
       C:  0.10494438E+00 1/CM     3146.15338 MHZ
```

```
 FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
 --------------------------------------------
       DJ:  0.36164811E-07 1/CM        0.00108 MHZ
      DJK:  0.28228620E-05 1/CM        0.08463 MHZ
       DK:  0.17473974E-02 1/CM       52.38566 MHZ
       R5: -0.66292330E-06 1/CM       -0.01987 MHZ
       R6: -0.12847458E-10 1/CM       -0.00000 MHZ
    DEL-J:  0.64921973E-09 1/CM        0.00002 MHZ

 A-REDUCTION DISTORTION CONSTANTS
 --------------------------------
  DELTA-J:  0.36190506E-07 1/CM        0.00108 MHZ
 DELTA-JK:  0.28227078E-05 1/CM        0.08462 MHZ
  DELTA-K:  0.17473976E-02 1/CM       52.38566 MHZ
    DEL-J:  0.64921973E-09 1/CM        0.00002 MHZ
    DEL-K:  0.16606768E-05 1/CM        0.04979 MHZ

 S-REDUCTION DISTORTION CONSTANTS
 --------------------------------
      ~DJ:  0.36063066E-07 1/CM        0.00108 MHZ
     ~DJK:  0.28234725E-05 1/CM        0.08465 MHZ
      ~DK:  0.17473969E-02 1/CM       52.38564 MHZ
   ~DEL-J:  0.64921973E-09 1/CM        0.00002 MHZ
      ~R6: -0.63720278E-10 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                      A             B             C
 ALPHA    S    -0.05137300     0.00026745     0.00033818  1/CM
          B    -0.08982169     0.00007625     0.00021263  1/CM
          A     0.68824344     0.00038574     0.00056942  1/CM

                      A             B             C
 ALPHA    S    -1540.12380       8.01781       10.13846  MHZ
          B    -2692.78660       2.28600        6.37461  MHZ
          A    20633.01972      11.56420       17.07081  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S             B             A
 X(I,J):  S    -1.96064686    -5.36331250   -14.45604904  1/CM
          B    -5.36331250    -3.73656753   -42.28328175  1/CM
          A   -14.45604904   -42.28328175  -146.69738020  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:      -14.99436062  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (1)H (120)Sn (35)Cl   TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.350950 A    (     4.442653 A.U.)
 R20:     1.753639 A    (     3.313899 A.U.)
 R30:     1.958091 RAD  (   112.190374 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.3127676   2   0   0
      1.7439160   0   2   0
      0.3826403   0   0   2
     -0.0402633   1   1   0
      0.0626173   1   0   1
```

```
    -0.0071109   0   1   1
    -8.8052331   3   0   0
    -8.6369110   0   3   0
    -0.1961708   0   0   3
     0.1790450   2   1   0
    -0.0999146   1   2   0
    -0.0817951   2   0   1
     0.0188621   0   2   1
    -0.0659042   1   1   1
    -0.2951313   1   0   2
    -0.2527973   0   1   2
    14.9152293   4   0   0
    28.6016748   0   4   0
    -0.1590055   0   0   4
     3.0491163   3   1   0
    -0.4722628   1   3   0
    -0.0371436   2   2   0
    -3.0899473   3   0   1
     0.0301257   0   3   1
     0.2806006   2   1   1
     0.2553257   1   2   1
    -0.1792738   2   0   2
    -0.4414853   0   2   2
     0.3066867   1   1   2
     0.2022326   1   0   3
     0.0558871   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:     0.54693047     0.00390319     0.00000000    MASS:119.902197 AMU
CENTER  2:    -1.80304562    -0.05799055     0.00000000    MASS: 34.968853 AMU
CENTER  3:    -2.50810218     1.54775107     0.00000000    MASS:  1.007825 AMU
MOMENTS:       4.20729086   258.85904183   263.06633269    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         6.6537       0.1081       0.1064     1/CM
      199472.5       3242.1       3190.2     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.3128 AJ/A**2    F12:    -0.0403 AJ/A**2    F1A:     0.0626 AJ/A
                           F22:     1.7439 AJ/A**2    F2A:    -0.0071 AJ/A
                                                      FAA:     0.3826 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:               119.902197      34.968853       1.007825  AMU
FUNDAMENTAL FREQUENCIES:      375.55665      472.57774     1739.03135  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3            FREQUENCY
Q1:        0.99715783     0.01281621     0.07424292       375.55664886 S
Q2:       -0.27917760     0.00908285     0.96019653       472.57773908 B
Q3:       -0.03927719     0.99920147    -0.00733034      1739.03135239 A
```

CORIOLIS COUPLING MATRICES

		S	B	A
ZETA-C	S	0.00000000	-0.13056706	-0.08884237
	B	0.13056706	0.00000000	-0.98745090
	A	0.08884237	0.98745090	0.00000000

TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION

AAAA:	-0.00473284 1/CM	AABB:	0.00000129 1/CM	ABAB:	-0.00000467 1/CM
BBBB:	-0.00000014 1/CM	BBCC:	-0.00000014 1/CM		
CCCC:	-0.00000013 1/CM	CCAA:	0.00000004 1/CM		
AAAA:	-141.88707 MHZ	AABB:	0.03880 MHZ	ABAB:	-0.13989 MHZ
BBBB:	-0.00430 MHZ	BBCC:	-0.00415 MHZ		
CCCC:	-0.00402 MHZ	CCAA:	0.00127 MHZ		

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION

AXIS	A:	0.66536877E+01 1/CM	199472.54470 MHZ
	B:	0.10814425E+00 1/CM	3242.08301 MHZ
	C:	0.10641377E+00 1/CM	3190.20477 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS

DJ:	0.34660069E-07 1/CM	0.00104 MHZ
DJK:	0.19296166E-05 1/CM	0.05785 MHZ
DK:	0.11812465E-02 1/CM	35.41288 MHZ
R5:	-0.50475205E-06 1/CM	-0.01513 MHZ
R6:	-0.74215447E-11 1/CM	-0.00000 MHZ
DEL-J:	0.58023249E-09 1/CM	0.00002 MHZ

A-REDUCTION DISTORTION CONSTANTS

DELTA-J:	0.34674913E-07 1/CM	0.00104 MHZ
DELTA-JK:	0.19295275E-05 1/CM	0.05785 MHZ
DELTA-K:	0.11812466E-02 1/CM	35.41288 MHZ
DEL-J:	0.58023249E-09 1/CM	0.00002 MHZ
DEL-K:	0.12341109E-05 1/CM	0.03700 MHZ

S-REDUCTION DISTORTION CONSTANTS

~DJ:	0.34593357E-07 1/CM	0.00104 MHZ
~DJK:	0.19300169E-05 1/CM	0.05786 MHZ
~DK:	0.11812462E-02 1/CM	35.41287 MHZ
~DEL-J:	0.58023249E-09 1/CM	0.00002 MHZ
~R6:	-0.40777971E-10 1/CM	-0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS

		A	B	C	
ALPHA	S	-0.00175283	0.00036005	0.00036133	1/CM
	B	-0.24007625	0.00003824	0.00017184	1/CM
	A	0.24004200	0.00018013	0.00023174	1/CM
		A	B	C	
ALPHA	S	-52.54839	10.79390	10.83242	MHZ
	B	-7197.30525	1.14655	5.15169	MHZ
	A	7196.27820	5.40005	6.94738	MHZ

ANHARMONIC VIBRATIONAL CONSTANTS

```
 --------------------------------
                      S              B              A
 X(I,J):  S    -1.38299314    -1.01883219    -0.76429822  1/CM
          B    -1.01883219    -1.83870779   -18.44643995  1/CM
          A    -0.76429822   -18.44643995   -52.65470740  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.50483511  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (2)H (120)Sn (35)Cl   GROUND STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.381128 A    (     4.499680 A.U.)
 R20:     1.793849 A    (     3.389884 A.U.)
 R30:     1.620862 RAD  (    92.868571 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.1551821   2   0   0
      1.7385235   0   2   0
      0.6870276   0   0   2
      0.0464385   1   1   0
      0.0925673   1   0   1
     -0.0670835   0   1   1
     -6.9959663   3   0   0
     -7.0690068   0   3   0
     -0.8635152   0   0   3
      0.2341554   2   1   0
     -0.0166298   1   2   0
     -0.4951679   2   0   1
      0.0179518   0   2   1
     -0.2008431   1   1   1
     -0.4336567   1   0   2
     -0.1017145   0   1   2
      7.2939281   4   0   0
     29.4329229   0   4   0
      4.2624983   0   0   4
      2.1439994   3   1   0
      0.5936032   1   3   0
     -0.3053067   2   2   0
     -3.3491722   3   0   1
      0.1458912   0   3   1
      0.2785830   2   1   1
      0.2968607   1   2   1
      3.3215551   2   0   2
     -0.8008194   0   2   2
      0.5007239   1   1   2
     -0.7019288   1   0   3
     -0.1890888   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------------
 AXES:                A              B              C
 CENTER  1:      0.56290819     0.00201108     0.00000000    MASS:119.902197 AMU
 CENTER  2:     -1.81578016    -0.10377345     0.00000000    MASS: 34.968853 AMU
 CENTER  3:     -1.98509254     1.68199297     0.00000000    MASS:  2.014102 AMU
 MOMENTS:       10.08798958   267.71739380   277.80538338    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
            A           B           C        UNIT
          2.7750      0.1046      0.1008    1/CM
         83191.9      3134.8      3021.0    MHZ
```

```
PROLATE          ASYMMETRIC ROTOR (K=-0.997)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.1552 AJ/A**2    F12:     0.0464 AJ/A**2    F1A:     0.0926 AJ/A
                           F22:     1.7385 AJ/A**2    F2A:    -0.0671 AJ/A
                                                      FAA:     0.6870 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197      34.968853       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       356.00489      447.47384     1246.53665  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.98325549     0.00682301     0.18210459        356.00489165 S
Q2:       -0.41582417     0.03786639     0.90865637        447.47383570 B
Q3:        0.02531312     0.99818200    -0.05469859       1246.53665317 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S     0.00000000    -0.19748226    -0.17876201
         B     0.19748226     0.00000000    -0.96386975
         A     0.17876201     0.96386975     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00022642 1/CM   AABB:     0.00000021 1/CM   ABAB:  -0.00000237 1/CM
BBBB:    -0.00000014 1/CM   BBCC:    -0.00000013 1/CM
CCCC:    -0.00000012 1/CM   CCAA:    -0.00000010 1/CM

AAAA:       -6.78785 MHZ    AABB:        0.00631 MHZ    ABAB:     -0.07095 MHZ
BBBB:       -0.00428 MHZ    BBCC:       -0.00397 MHZ
CCCC:       -0.00369 MHZ    CCAA:       -0.00309 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.27749830E+01 1/CM    83191.89930 MHZ
       B:  0.10456569E+00 1/CM     3134.80062 MHZ
       C:  0.10076818E+00 1/CM     3020.95412 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.33186576E-07 1/CM        0.00099 MHZ
     DJK:  0.10901834E-05 1/CM        0.03268 MHZ
      DK:  0.55481166E-04 1/CM        1.66328 MHZ
      R5: -0.27562146E-06 1/CM       -0.00826 MHZ
      R6: -0.18112726E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.12347939E-08 1/CM        0.00004 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.33222801E-07 1/CM        0.00100 MHZ
DELTA-JK:  0.10899660E-05 1/CM        0.03268 MHZ
 DELTA-K:  0.55481347E-04 1/CM        1.66329 MHZ
```

```
   DEL-J:  0.12347939E-08 1/CM        0.00004 MHZ
   DEL-K:  0.65321062E-06 1/CM        0.01958 MHZ

 S-REDUCTION DISTORTION CONSTANTS
 --------------------------------
     ~DJ:  0.32990739E-07 1/CM        0.00099 MHZ
    ~DJK:  0.10913584E-05 1/CM        0.03272 MHZ
     ~DK:  0.55480187E-04 1/CM        1.66325 MHZ
  ~DEL-J:  0.12347939E-08 1/CM        0.00004 MHZ
     ~R6: -0.11603110E-09 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                      A              B              C
 ALPHA    S    -0.00225009     0.00027898     0.00028830  1/CM
          B    -0.03007894     0.00002013     0.00016043  1/CM
          A     0.05100300    -0.00002711     0.00003294  1/CM

                      A              B              C
 ALPHA    S      -67.45615        8.36351        8.64305  MHZ
          B     -901.74411        0.60351        4.80956  MHZ
          A     1529.03139       -0.81264        0.98752  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S              B              A
 X(I,J):  S    -1.10779324     0.29757507    -0.20708667  1/CM
          B     0.29757507     1.22279857    -5.18823735  1/CM
          A    -0.20708667    -5.18823735   -11.91069255  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -0.72751046  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H (120)Sn (35)Cl   EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.364413 A    (     4.468094 A.U.)
 R20:     1.832218 A    (     3.462391 A.U.)
 R30:     1.958935 RAD  (   112.238697 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      2.1481112   2   0   0
      0.8848852   0   2   0
      0.2664681   0   0   2
     -0.0728413   1   1   0
      0.0493070   1   0   1
      0.0582775   0   1   1
     -8.3269710   3   0   0
     -6.6281943   0   3   0
      0.0634806   0   0   3
      0.3779691   2   1   0
     -0.0280196   1   2   0
     -0.1578614   2   0   1
      0.0433690   0   2   1
     -0.0903336   1   1   1
     -0.2345949   1   0   2
     -0.4049673   0   1   2
      9.0956074   4   0   0
     24.2643908   0   4   0
     -0.9330710   0   0   4
      3.3056643   3   1   0
```

```
     0.3350091   1   3   0
     0.3991937   2   2   0
    -4.1824820   3   0   1
    -0.6914233   0   3   1
     0.4741557   2   1   1
     0.2323149   1   2   1
    -0.3094157   2   0   2
    -0.4707625   0   2   2
     0.4055808   1   1   2
    -0.0861174   1   0   3
     0.1595906   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      0.56667601     0.00858097     0.00000000    MASS:119.902197 AMU
CENTER  2:     -1.79454171    -0.11808220     0.00000000    MASS: 34.968853 AMU
CENTER  3:     -2.57813848     1.53930748     0.00000000    MASS:  2.014102 AMU
MOMENTS:        8.74894448   273.16320245   281.91214693    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         3.1997      0.1025      0.0993    1/CM
        95924.6      3072.3      2977.0    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.998)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.1481 AJ/A**2    F12:    -0.0728 AJ/A**2    F1A:     0.0493 AJ/A
                           F22:     0.8849 AJ/A**2    F2A:     0.0583 AJ/A
                                                      FAA:     0.2665 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:               119.902197      34.968853       2.014102  AMU
FUNDAMENTAL FREQUENCIES:      267.56413      364.78057      890.31402  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.52499379     0.01441637     0.85098395        267.56412932 B
Q2:        0.99819963     0.03397916    -0.04942577        364.78056534 S
Q3:       -0.16127705     0.98483337     0.06397609        890.31401943 A


CORIOLIS COUPLING MATRICES
--------------------------
                    B              S              A
ZETA-C   B     0.00000000     0.15256229    -0.94700503
         S    -0.15256229    -0.00000000     0.28267689
         A     0.94700503    -0.28267689     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00206351 1/CM   AABB:     0.00000310 1/CM   ABAB:  -0.00000543 1/CM
BBBB:    -0.00000014 1/CM   BBCC:    -0.00000013 1/CM
CCCC:    -0.00000012 1/CM   CCAA:     0.00000092 1/CM
```

```
AAAA:      -61.86261 MHZ    AABB:        0.09286 MHZ    ABAB:     -0.16282 MHZ
BBBB:       -0.00433 MHZ    BBCC:       -0.00397 MHZ
CCCC:       -0.00370 MHZ    CCAA:        0.02761 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.31997002E+01 1/CM    95924.60160 MHZ
       B:  0.10248155E+00 1/CM     3072.31951 MHZ
       C:  0.99299751E-01 1/CM     2976.93173 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.33388285E-07 1/CM        0.00100 MHZ
     DJK:  0.16441893E-05 1/CM        0.04929 MHZ
      DK:  0.51420107E-03 1/CM       15.41536 MHZ
      R5: -0.54220340E-06 1/CM       -0.01625 MHZ
      R6: -0.44024003E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.12989959E-08 1/CM        0.00004 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.33476333E-07 1/CM        0.00100 MHZ
DELTA-JK:  0.16436610E-05 1/CM        0.04928 MHZ
 DELTA-K:  0.51420151E-03 1/CM       15.41537 MHZ
   DEL-J:  0.12989959E-08 1/CM        0.00004 MHZ
   DEL-K:  0.14274133E-05 1/CM        0.04279 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.33109923E-07 1/CM        0.00099 MHZ
    ~DJK:  0.16458594E-05 1/CM        0.04934 MHZ
     ~DK:  0.51419967E-03 1/CM       15.41532 MHZ
  ~DEL-J:  0.12989959E-08 1/CM        0.00004 MHZ
     ~R6: -0.18320482E-09 1/CM       -0.00001 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    B    -0.05440785    -0.00014355     0.00011833  1/CM
         S    -0.00035470     0.00034054     0.00033429  1/CM
         A     0.26080466     0.00026654     0.00049212  1/CM

                    A              B              C
ALPHA    B    -1631.10628       -4.30338        3.54755  MHZ
         S      -10.63373       10.20916       10.02190  MHZ
         A     7818.72730        7.99061       14.75343  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    B              S              A
X(I,J):  B    -2.90527466    -2.36752340   -27.73163402  1/CM
         S    -2.36752340    -1.10728681    -2.22603274  1/CM
         A   -27.73163402    -2.22603274   -75.28619395  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -2.95427410  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H (120)Sn (35)Cl   TRIPLET STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.350950 A    (     4.442653 A.U.)
R20:     1.753639 A    (     3.313899 A.U.)
```

```
R30:     1.958091 RAD  (   112.190374 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     2.3127676   2   0   0
     1.7439160   0   2   0
     0.3826403   0   0   2
    -0.0402633   1   1   0
     0.0626173   1   0   1
    -0.0071109   0   1   1
    -8.8052331   3   0   0
    -8.6369110   0   3   0
    -0.1961708   0   0   3
     0.1790450   2   1   0
    -0.0999146   1   2   0
    -0.0817951   2   0   1
     0.0188621   0   2   1
    -0.0659042   1   1   1
    -0.2951313   1   0   2
    -0.2527973   0   1   2
    14.9152293   4   0   0
    28.6016748   0   4   0
    -0.1590055   0   0   4
     3.0491163   3   1   0
    -0.4722628   1   3   0
    -0.0371436   2   2   0
    -3.0899473   3   0   1
     0.0301257   0   3   1
     0.2806006   2   1   1
     0.2553257   1   2   1
    -0.1792738   2   0   2
    -0.4414853   0   2   2
     0.3066867   1   1   2
     0.2022326   1   0   3
     0.0558871   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      0.56299504     0.00786126     0.00000000    MASS:119.902197 AMU
CENTER  2:     -1.78474019    -0.11196264     0.00000000    MASS: 34.968853 AMU
CENTER  3:     -2.52917896     1.47590443     0.00000000    MASS:  2.014102 AMU
MOMENTS:        8.02546716   269.46186251   277.48732967    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         3.4881       0.1039       0.1009     1/CM
      104572.0       3114.5       3024.4     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.998)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     2.3128 AJ/A**2    F12:    -0.0403 AJ/A**2    F1A:     0.0626 AJ/A
                           F22:     1.7439 AJ/A**2    F2A:    -0.0071 AJ/A
                                                      FAA:     0.3826 AJ

WILSON FG ANALYSIS
```

```
------------------
ATOMIC MASSES:                119.902197      34.968853       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       330.51126      387.03294    1247.98432  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.77835612     0.03343917     0.62693187        330.51125879 B
Q2:        0.98308675     0.01953634    -0.18209551        387.03294253 S
Q3:       -0.05587760     0.99838718    -0.01003695       1247.98431560 A


CORIOLIS COUPLING MATRICES
--------------------------
                     B              S              A
ZETA-C   B      0.00000000     0.17291429    -0.83662306
         S     -0.17291429     0.00000000     0.51977159
         A      0.83662306    -0.51977159    -0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:     -0.00140052 1/CM   AABB:      0.00000219 1/CM   ABAB:   -0.00000402 1/CM
BBBB:     -0.00000014 1/CM   BBCC:     -0.00000013 1/CM
CCCC:     -0.00000012 1/CM   CCAA:      0.00000089 1/CM

AAAA:       -41.98645 MHZ    AABB:         0.06552 MHZ    ABAB:      -0.12056 MHZ
BBBB:        -0.00405 MHZ    BBCC:        -0.00377 MHZ
CCCC:        -0.00353 MHZ    CCAA:         0.02666 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.34881458E+01 1/CM   104571.98274 MHZ
       B:  0.10388900E+00 1/CM     3114.51391 MHZ
       C:  0.10088343E+00 1/CM     3024.40909 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.31550209E-07 1/CM        0.00095 MHZ
     DJK:  0.11789509E-05 1/CM        0.03534 MHZ
      DK:  0.34891876E-03 1/CM       10.46032 MHZ
      R5: -0.42113357E-06 1/CM       -0.01263 MHZ
      R6: -0.25429407E-10 1/CM       -0.00000 MHZ
   DEL-J:  0.10896533E-08 1/CM        0.00003 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.31601068E-07 1/CM        0.00095 MHZ
DELTA-JK:  0.11786457E-05 1/CM        0.03533 MHZ
 DELTA-K:  0.34891902E-03 1/CM       10.46033 MHZ
   DEL-J:  0.10896533E-08 1/CM        0.00003 MHZ
   DEL-K:  0.10714357E-05 1/CM        0.03212 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.31363286E-07 1/CM        0.00094 MHZ
    ~DJK:  0.11800724E-05 1/CM        0.03538 MHZ
     ~DK:  0.34891783E-03 1/CM       10.46029 MHZ
  ~DEL-J:  0.10896533E-08 1/CM        0.00003 MHZ
     ~R6: -0.11889055E-09 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                     A              B              C
ALPHA    B     -0.07626478     0.00001026     0.00015852  1/CM
```

```
          S    -0.01730185     0.00029363     0.00030836  1/CM
          A     0.08944728     0.00016706     0.00022704  1/CM

                     A              B              C
 ALPHA    B    -2286.36053        0.30766        4.75236  MHZ
          S     -518.69647        8.80284        9.24440  MHZ
          A     2681.56195        5.00838        6.80644  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                     B              S              A
 X(I,J):  B    -0.66852681    -2.19287804    -7.86708939  1/CM
          S    -2.19287804    -0.93451116    -2.07662643  1/CM
          A    -7.86708939    -2.07662643   -27.02469086  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -6.64158589  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (1)H (120)Sn (79)Br   GROUND STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.522455 A    (     4.766751 A.U.)
 R20:     1.788396 A    (     3.379579 A.U.)
 R30:     1.624584 RAD  (    93.081783 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.8521353   2   0   0
      1.7596629   0   2   0
      0.7105093   0   0   2
      0.0776576   1   1   0
      0.0332532   1   0   1
     -0.0840226   0   1   1
     -7.0517160   3   0   0
     -7.0538390   0   3   0
     -1.3001909   0   0   3
      0.1246261   2   1   0
      0.0808662   1   2   0
     -0.5308108   2   0   1
      0.0296523   0   2   1
     -0.1738000   1   1   1
     -0.2003385   1   0   2
     -0.0890752   0   1   2
     22.8797283   4   0   0
     26.0084449   0   4   0
      6.0752740   0   0   4
      0.4486086   3   1   0
      0.6659613   1   3   0
      0.5338740   2   2   0
     -0.4226385   3   0   1
     -0.2632606   0   3   1
      0.2687354   2   1   1
     -0.0288562   1   2   1
      1.8618697   2   0   2
     -0.2341181   0   2   2
      0.3136685   1   1   2
     -1.5319206   1   0   3
      0.3922338   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:               A              B              C
```

```
CENTER  1:     1.00933852     0.00066823     0.00000000    MASS:119.902197 AMU
CENTER  2:    -1.51273625    -0.02351355     0.00000000    MASS: 78.918338 AMU
CENTER  3:    -1.62654704     1.76174222     0.00000000    MASS:  1.007825 AMU
MOMENTS:       5.26672100   507.14753811   512.41425911    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
     5.3153      0.0552      0.0546    1/CM
   159347.5      1654.8      1637.8    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
------------------------------+-----------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.8521 AJ/A**2    F12:     0.0777 AJ/A**2    F1A:     0.0333 AJ/A
                           F22:     1.7597 AJ/A**2    F2A:    -0.0840 AJ/A
                                                      FAA:     0.7105 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:               119.902197      78.918338       1.007825  AMU
FUNDAMENTAL FREQUENCIES:      255.80741      616.38839     1733.68252  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
              R1             R2             R3            FREQUENCY
Q1:       0.99974160    -0.00011604     0.02273133       255.80740565 A
Q2:      -0.00614734     0.02334288     0.99970862       616.38839324 B
Q3:       0.04420580     0.99739791    -0.05694963      1733.68252216 S


CORIOLIS COUPLING MATRICES
--------------------------
                   A             B             S
ZETA-C   A     0.00000000    -0.10784623     0.00265082
         B     0.10784623     0.00000000    -0.99416405
         S    -0.00265082     0.99416405     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00080613 1/CM   AABB:     0.00000024 1/CM   ABAB:  -0.00000067 1/CM
BBBB:    -0.00000004 1/CM   BBCC:    -0.00000004 1/CM
CCCC:    -0.00000004 1/CM   CCAA:     0.00000015 1/CM

AAAA:      -24.16710 MHZ    AABB:        0.00728 MHZ    ABAB:     -0.02022 MHZ
BBBB:       -0.00123 MHZ    BBCC:       -0.00121 MHZ
CCCC:       -0.00118 MHZ    CCAA:        0.00458 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.53152615E+01 1/CM   159347.53580 MHZ
       B:  0.55198989E-01 1/CM     1654.82411 MHZ
       C:  0.54631515E-01 1/CM     1637.81165 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.10064238E-07 1/CM        0.00030 MHZ
     DJK:  0.21816850E-06 1/CM        0.00654 MHZ
```

```
      DK:  0.20130368E-03 1/CM        6.03493 MHZ
      R5: -0.78618193E-07 1/CM       -0.00236 MHZ
      R6: -0.42564540E-12 1/CM       -0.00000 MHZ
   DEL-J:  0.10660508E-09 1/CM        0.00000 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.10065089E-07 1/CM        0.00030 MHZ
DELTA-JK:  0.21816339E-06 1/CM        0.00654 MHZ
 DELTA-K:  0.20130368E-03 1/CM        6.03493 MHZ
   DEL-J:  0.10660508E-09 1/CM        0.00000 MHZ
   DEL-K:  0.18880139E-06 1/CM        0.00566 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.10059997E-07 1/CM        0.00030 MHZ
    ~DJK:  0.21819395E-06 1/CM        0.00654 MHZ
     ~DK:  0.20130366E-03 1/CM        6.03493 MHZ
  ~DEL-J:  0.10660508E-09 1/CM        0.00000 MHZ
     ~R6: -0.25459347E-11 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                   A             B             C
ALPHA    A    -0.00214366     0.00015864     0.00015648  1/CM
         B    -0.07441793     0.00000805     0.00004376  1/CM
         S     0.13376919    -0.00009037    -0.00007636  1/CM

                   A             B             C
ALPHA    A      -64.26523        4.75600        4.69128  MHZ
         B    -2230.99355        0.24134        1.31177  MHZ
         S     4010.29959       -2.70917       -2.28916  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                   A             B             S
X(I,J):  A    -0.55314084     0.35553061     1.52151289  1/CM
         B     0.35553061     0.70383139   -11.22315471  1/CM
         S     1.52151289   -11.22315471   -25.89939977  1/CM

DARLING-DENNISON RESONANCE PARAMETER:        0.08649386  1/CM

--------------------------------------------------------------------------------
----------------------------------------- (1)H (120)Sn (79)Br   EXCITED STATE
--------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.510934 A    (     4.744978 A.U.)
R20:     1.815586 A    (     3.430961 A.U.)
R30:     1.981257 RAD  (   113.517649 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     1.7158997   2   0   0
     1.0590497   0   2   0
     0.2635784   0   0   2
    -0.0229066   1   1   0
     0.0169894   1   0   1
     0.0394523   0   1   1
    -7.6876934   3   0   0
    -7.1049971   0   3   0
     0.0436487   0   0   3
     0.3187774   2   1   0
```

```
 0.0980025   1   2   0
-0.2816920   2   0   1
 0.0954310   0   2   1
-0.1011364   1   1   1
-0.2271639   1   0   2
-0.3196407   0   1   2
23.6871221   4   0   0
25.1891245   0   4   0
-1.0937331   0   0   4
 0.5246312   3   1   0
 0.4875413   1   3   0
 1.0350830   2   2   0
 0.3190736   3   0   1
-0.4528045   0   3   1
 0.0531524   2   1   1
 0.2362704   1   2   1
 0.3361943   2   0   2
-0.5722206   0   2   2
 0.4025601   1   1   2
-0.0588274   1   0   3
 0.2604666   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
--------------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      1.00781570     0.00406676     0.00000000    MASS:119.902197 AMU
CENTER  2:     -1.50248680    -0.02698473     0.00000000    MASS: 78.918338 AMU
CENTER  3:     -2.24796492     1.62922760     0.00000000    MASS:  1.007825 AMU
MOMENTS:        4.54089240   506.51536943   511.05626183    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        6.1649      0.0553      0.0548     1/CM
     184818.1      1656.9      1642.2     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
-------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.7159 AJ/A**2    F12:     -0.0229 AJ/A**2    F1A:      0.0170 AJ/A
                           F22:      1.0590 AJ/A**2    F2A:      0.0395 AJ/A
                                                       FAA:      0.2636 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197      78.918338       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       246.22790      371.53883     1344.29378  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:         0.99957422     0.00571069     0.02861421       246.22789993 S
Q2:        -0.11705234    -0.00828603     0.99309118       371.53882508 B
Q3:        -0.03106632     0.99875635     0.03899530      1344.29377538 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
```

```
ZETA-C   S     0.00000000    -0.09881373    -0.03173729
         B     0.09881373     0.00000000    -0.99459971
         A     0.03173729     0.99459971     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00676312 1/CM   AABB:     0.00000052 1/CM   ABAB:  -0.00000179 1/CM
BBBB:    -0.00000004 1/CM   BBCC:    -0.00000004 1/CM
CCCC:    -0.00000004 1/CM   CCAA:    -0.00000002 1/CM

AAAA:     -202.75326 MHZ    AABB:        0.01558 MHZ    ABAB:     -0.05368 MHZ
BBBB:       -0.00134 MHZ    BBCC:       -0.00131 MHZ
CCCC:       -0.00129 MHZ    CCAA:       -0.00071 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.61648674E+01 1/CM   184818.07968 MHZ
       B:  0.55267997E-01 1/CM     1656.89292 MHZ
       C:  0.54776568E-01 1/CM     1642.16024 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.10931573E-07 1/CM        0.00033 MHZ
     DJK:  0.74938412E-06 1/CM        0.02247 MHZ
      DK:  0.16900199E-02 1/CM       50.66552 MHZ
      R5: -0.18981667E-06 1/CM       -0.00569 MHZ
      R6: -0.89912567E-12 1/CM       -0.00000 MHZ
   DEL-J:  0.10001514E-09 1/CM        0.00000 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.10933371E-07 1/CM        0.00033 MHZ
DELTA-JK:  0.74937333E-06 1/CM        0.02247 MHZ
 DELTA-K:  0.16900199E-02 1/CM       50.66552 MHZ
   DEL-J:  0.10001514E-09 1/CM        0.00000 MHZ
   DEL-K:  0.46906253E-06 1/CM        0.01406 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.10923939E-07 1/CM        0.00033 MHZ
    ~DJK:  0.74942992E-06 1/CM        0.02247 MHZ
     ~DK:  0.16900198E-02 1/CM       50.66552 MHZ
  ~DEL-J:  0.10001514E-09 1/CM        0.00000 MHZ
     ~R6: -0.47159788E-11 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    S    -0.01025091     0.00020696     0.00020429  1/CM
         B    -0.19328681     0.00002884     0.00008178  1/CM
         A     0.53078596     0.00003045     0.00007036  1/CM

                    A              B              C
ALPHA    S     -307.31468        6.20460        6.12450  MHZ
         B    -5794.59280        0.86473        2.45161  MHZ
         A    15912.56321        0.91295        2.10926  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -0.88375607    -0.54481359     2.82713320  1/CM
         B    -0.54481359    -4.92767690   -39.13816058  1/CM
         A     2.82713320   -39.13816058  -110.35860750  1/CM
```

```
 DARLING-DENNISON RESONANCE PARAMETER:        0.44378691  1/CM

--------------------------------------------------------------------------------
---------------------------------------- (1)H (120)Sn (79)Br   TRIPLET STATE
--------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.493988 A    (     4.712955 A.U.)
 R20:     1.753021 A    (     3.312730 A.U.)
 R30:     1.967860 RAD  (   112.750046 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.9116969   2   0   0
      1.7728547   0   2   0
      0.3648346   0   0   2
     -0.0057150   1   1   0
      0.0353873   1   0   1
     -0.0152195   0   1   1
     -7.9892394   3   0   0
     -8.6330347   0   3   0
     -0.2084848   0   0   3
      0.1209886   2   1   0
     -0.0411611   1   2   0
     -0.2438378   2   0   1
      0.0749239   0   2   1
     -0.0752502   1   1   1
     -0.2801501   1   0   2
     -0.1796516   0   1   2
     25.2251517   4   0   0
     29.6534307   0   4   0
     -0.2643661   0   0   4
      0.0669519   3   1   0
      0.1404484   1   3   0
      0.3090539   2   2   0
      0.1960627   3   0   1
     -0.1327991   0   3   1
      0.1169614   2   1   1
      0.2383493   1   2   1
      0.3648542   2   0   2
     -0.4739404   0   2   2
      0.3548785   1   1   2
      0.0853287   1   0   3
      0.0759294   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------------
 AXES:                A              B              C
 CENTER  1:     1.00093717     0.00371796     0.00000000    MASS:119.902197 AMU
 CENTER  2:    -1.49277925    -0.02585904     0.00000000    MASS: 78.918338 AMU
 CENTER  3:    -2.18977311     1.58257718     0.00000000    MASS:  1.007825 AMU
 MOMENTS:       4.28180875   499.52176783   503.80357658    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
           A           B           C        UNIT
         6.5379      0.0560      0.0556    1/CM
      196001.1      1680.1      1665.8    MHZ

 PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
 -------------------------------+-------------------------------
 ^
```

```
ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.9117 AJ/A**2    F12:    -0.0057 AJ/A**2    F1A:     0.0354 AJ/A
                           F22:     1.7729 AJ/A**2    F2A:    -0.0152 AJ/A
                                                      FAA:     0.3648 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197      78.918338       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       260.11344      453.34180     1739.10640  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3            FREQUENCY
Q1:        0.99976769     0.00515709     0.02092767        260.11344420 S
Q2:       -0.01315322     0.00795842     0.99988182        453.34180080 B
Q3:       -0.00876340     0.99990820    -0.01033397       1739.10639541 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S              B              A
ZETA-C   S     0.00000000    -0.09913009    -0.00187628
         B     0.09913009    -0.00000000    -0.99507271
         A     0.00187628     0.99507271     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00462456 1/CM   AABB:     0.00000020 1/CM   ABAB:  -0.00000136 1/CM
BBBB:    -0.00000004 1/CM   BBCC:    -0.00000004 1/CM
CCCC:    -0.00000004 1/CM   CCAA:    -0.00000014 1/CM

AAAA:     -138.64072 MHZ    AABB:        0.00605 MHZ    ABAB:     -0.04078 MHZ
BBBB:       -0.00125 MHZ    BBCC:       -0.00122 MHZ
CCCC:       -0.00120 MHZ    CCAA:       -0.00406 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.65378911E+01 1/CM   196001.05050 MHZ
       B:  0.56041725E-01 1/CM     1680.08869 MHZ
       C:  0.55565181E-01 1/CM     1665.80226 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.10217193E-07 1/CM        0.00031 MHZ
     DJK:  0.64314093E-06 1/CM        0.01928 MHZ
      DK:  0.11554858E-02 1/CM       34.64059 MHZ
      R5: -0.14890515E-06 1/CM       -0.00446 MHZ
      R6: -0.57081695E-12 1/CM       -0.00000 MHZ
   DEL-J:  0.87496869E-10 1/CM        0.00000 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.10218335E-07 1/CM        0.00031 MHZ
DELTA-JK:  0.64313408E-06 1/CM        0.01928 MHZ
 DELTA-K:  0.11554858E-02 1/CM       34.64059 MHZ
   DEL-J:  0.87496869E-10 1/CM        0.00000 MHZ
   DEL-K:  0.35992559E-06 1/CM        0.01079 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
```

```
     ~DJ:  0.10211720E-07 1/CM        0.00031 MHZ
    ~DJK:  0.64317377E-06 1/CM        0.01928 MHZ
     ~DK:  0.11554857E-02 1/CM       34.64059 MHZ
  ~DEL-J:  0.87496869E-10 1/CM        0.00000 MHZ
     ~R6: -0.33075849E-11 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 --------------------------------------------------
                      A              B              C
 ALPHA    S    -0.00255913     0.00018024     0.00017840  1/CM
          B    -0.25565926     0.00004408     0.00008249  1/CM
          A     0.22837996     0.00002948     0.00004445  1/CM

                      A              B              C
 ALPHA    S      -76.72067        5.40357        5.34828  MHZ
          B    -7664.47210        1.32155        2.47294  MHZ
          A     6846.65925        0.88375        1.33261  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S              B              A
 X(I,J):  S    -0.69994769    -0.77800585     0.39773087  1/CM
          B    -0.77800585    -1.85248776   -15.83442684  1/CM
          A     0.39773087   -15.83442684   -48.27402687  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:        0.11361190  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H  (120)Sn (79)Br  GROUND STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.522455 A    (     4.766751 A.U.)
 R20:     1.788396 A    (     3.379579 A.U.)
 R30:     1.624584 RAD  (    93.081783 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.8521353   2   0   0
      1.7596629   0   2   0
      0.7105093   0   0   2
      0.0776576   1   1   0
      0.0332532   1   0   1
     -0.0840226   0   1   1
     -7.0517160   3   0   0
     -7.0538390   0   3   0
     -1.3001909   0   0   3
      0.1246261   2   1   0
      0.0808662   1   2   0
     -0.5308108   2   0   1
      0.0296523   0   2   1
     -0.1738000   1   1   1
     -0.2003385   1   0   2
     -0.0890752   0   1   2
     22.8797283   4   0   0
     26.0084449   0   4   0
      6.0752740   0   0   4
      0.4486086   3   1   0
      0.6659613   1   3   0
      0.5338740   2   2   0
     -0.4226385   3   0   1
     -0.2632606   0   3   1
      0.2687354   2   1   1
```

```
    -0.0288562   1   2   1
     1.8618697   2   0   2
    -0.2341181   0   2   2
     0.3136685   1   1   2
    -1.5319206   1   0   3
     0.3922338   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
------------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      1.01751988     0.00151355     0.00000000    MASS:119.902197 AMU
CENTER  2:     -1.50421107    -0.04664166     0.00000000    MASS: 78.918338 AMU
CENTER  3:     -1.63498714     1.73745157     0.00000000    MASS:  2.014102 AMU
MOMENTS:       10.38164565   511.59144690   521.97309255    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         2.6965      0.0547      0.0536     1/CM
        80838.7      1640.4      1607.8     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.8521 AJ/A**2    F12:      0.0777 AJ/A**2    F1A:      0.0333 AJ/A
                           F22:      1.7597 AJ/A**2    F2A:     -0.0840 AJ/A
                                                       FAA:      0.7105 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                 119.902197      78.918338       2.014102  AMU
FUNDAMENTAL FREQUENCIES:        254.61278      441.45678     1234.43252  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:         0.99848066     0.00029223     0.05510249        254.61278313 S
Q2:        -0.09081260     0.02947606     0.99543168        441.45677854 B
Q3:         0.04478942     0.99723019    -0.05937895       1234.43252260 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S              B              A
ZETA-C   S     0.00000000    -0.15017821    -0.02464432
         B     0.15017821     0.00000000    -0.98835174
         A     0.02464432     0.98835174     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00020842 1/CM   AABB:      0.00000013 1/CM   ABAB:  -0.00000065 1/CM
BBBB:    -0.00000004 1/CM   BBCC:     -0.00000004 1/CM
CCCC:    -0.00000004 1/CM   CCAA:      0.00000004 1/CM

AAAA:       -6.24835 MHZ    AABB:         0.00396 MHZ    ABAB:     -0.01946 MHZ
BBBB:       -0.00121 MHZ    BBCC:        -0.00116 MHZ
CCCC:       -0.00112 MHZ    CCAA:         0.00134 MHZ
```

```
 ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
 -----------------------------------------------------
 AXIS   A:  0.26964896E+01 1/CM    80838.72652 MHZ
        B:  0.54719504E-01 1/CM     1640.44951 MHZ
        C:  0.53631056E-01 1/CM     1607.81864 MHZ

 FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
 --------------------------------------------
       DJ:  0.97025987E-08 1/CM        0.00029 MHZ
      DJK:  0.26099142E-06 1/CM        0.00782 MHZ
       DK:  0.51834925E-04 1/CM        1.55397 MHZ
       R5: -0.75569044E-07 1/CM       -0.00227 MHZ
       R6: -0.15534677E-11 1/CM       -0.00000 MHZ
    DEL-J:  0.19929172E-09 1/CM        0.00001 MHZ

 A-REDUCTION DISTORTION CONSTANTS
 --------------------------------
  DELTA-J:  0.97057056E-08 1/CM        0.00029 MHZ
 DELTA-JK:  0.26097277E-06 1/CM        0.00782 MHZ
  DELTA-K:  0.51834940E-04 1/CM        1.55397 MHZ
    DEL-J:  0.19929172E-09 1/CM        0.00001 MHZ
    DEL-K:  0.18130763E-06 1/CM        0.00544 MHZ

 S-REDUCTION DISTORTION CONSTANTS
 --------------------------------
      ~DJ:  0.96870341E-08 1/CM        0.00029 MHZ
     ~DJK:  0.26108480E-06 1/CM        0.00783 MHZ
      ~DK:  0.51834847E-04 1/CM        1.55397 MHZ
   ~DEL-J:  0.19929172E-09 1/CM        0.00001 MHZ
      ~R6: -0.93357572E-11 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                      A             B             C
 ALPHA    S    -0.00110301     0.00015847     0.00015490  1/CM
          B    -0.02803263    -0.00000289     0.00004393  1/CM
          A     0.04803715    -0.00005964    -0.00004096  1/CM

                      A             B             C
 ALPHA    S      -33.06738        4.75083        4.64393  MHZ
          B     -840.39706       -0.08673        1.31695  MHZ
          A     1440.11760       -1.78802       -1.22799  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      S             B             A
 X(I,J):  S    -0.55350339     0.10212120     1.00070862  1/CM
          B     0.10212120     0.52702535    -5.48565645  1/CM
          A     1.00070862    -5.48565645   -13.11547458  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:        0.02326045  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H  (120)Sn (79)Br  EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.510934 A    (     4.744978 A.U.)
 R20:     1.815586 A    (     3.430961 A.U.)
 R30:     1.981257 RAD  (   113.517649 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
```

```
     1.7158997   2   0   0
     1.0590497   0   2   0
     0.2635784   0   0   2
    -0.0229066   1   1   0
     0.0169894   1   0   1
     0.0394523   0   1   1
    -7.6876934   3   0   0
    -7.1049971   0   3   0
     0.0436487   0   0   3
     0.3187774   2   1   0
     0.0980025   1   2   0
    -0.2816920   2   0   1
     0.0954310   0   2   1
    -0.1011364   1   1   1
    -0.2271639   1   0   2
    -0.3196407   0   1   2
    23.6871221   4   0   0
    25.1891245   0   4   0
    -1.0937331   0   0   4
     0.5246312   3   1   0
     0.4875413   1   3   0
     1.0350830   2   2   0
     0.3190736   3   0   1
    -0.4528045   0   3   1
     0.0531524   2   1   1
     0.2362704   1   2   1
     0.3361943   2   0   2
    -0.5722206   0   2   2
     0.4025601   1   1   2
    -0.0588274   1   0   3
     0.2604666   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:      1.01905459     0.00816551     0.00000000    MASS:119.902197 AMU
CENTER  2:     -1.49069258    -0.05308793     0.00000000    MASS: 78.918338 AMU
CENTER  3:     -2.25604444     1.59403484     0.00000000    MASS:  2.014102 AMU
MOMENTS:        8.88075075   514.99024179   523.87099254    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
         3.1522      0.0544      0.0534     1/CM
       94500.9      1629.6      1602.0     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.7159 AJ/A**2    F12:     -0.0229 AJ/A**2    F1A:      0.0170 AJ/A
                           F22:      1.0590 AJ/A**2    F2A:      0.0395 AJ/A
                                                       FAA:      0.2636 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:               119.902197      78.918338       2.014102  AMU
FUNDAMENTAL FREQUENCIES:      241.61115      270.83554      956.92084  1/CM

NORMAL COORDINATE DISPLACEMENTS
```

```
------------------------------
                R1             R2             R3              FREQUENCY
Q1:         0.98483211     0.01134856     0.17313846        241.61114854 S
Q2:        -0.73758347    -0.01117239     0.67516353        270.83553653 B
Q3:        -0.04111237     0.99843882     0.03781119        956.92083653 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S    -0.00000000    -0.13510051    -0.34987094
         B     0.13510051    -0.00000000    -0.92700495
         A     0.34987094     0.92700495     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00183024 1/CM   AABB:     0.00000080 1/CM   ABAB:  -0.00000167 1/CM
BBBB:    -0.00000004 1/CM   BBCC:    -0.00000004 1/CM
CCCC:    -0.00000004 1/CM   CCAA:     0.00000025 1/CM

AAAA:      -54.86936 MHZ    AABB:        0.02398 MHZ    ABAB:     -0.05001 MHZ
BBBB:       -0.00130 MHZ    BBCC:       -0.00124 MHZ
CCCC:       -0.00120 MHZ    CCAA:        0.00741 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.31522109E+01 1/CM    94500.90847 MHZ
       B:  0.54358492E-01 1/CM     1629.62663 MHZ
       C:  0.53436638E-01 1/CM     1601.99015 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.10400807E-07 1/CM        0.00031 MHZ
     DJK:  0.55148866E-06 1/CM        0.01653 MHZ
      DK:  0.45699927E-03 1/CM       13.70049 MHZ
      R5: -0.17385655E-06 1/CM       -0.00521 MHZ
      R6: -0.33661258E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.19682167E-09 1/CM        0.00001 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.10407539E-07 1/CM        0.00031 MHZ
DELTA-JK:  0.55144827E-06 1/CM        0.01653 MHZ
 DELTA-K:  0.45699930E-03 1/CM       13.70049 MHZ
   DEL-J:  0.19682167E-09 1/CM        0.00001 MHZ
   DEL-K:  0.43822042E-06 1/CM        0.01314 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.10374943E-07 1/CM        0.00031 MHZ
    ~DJK:  0.55164385E-06 1/CM        0.01654 MHZ
     ~DK:  0.45699914E-03 1/CM       13.70049 MHZ
  ~DEL-J:  0.19682167E-09 1/CM        0.00001 MHZ
     ~R6: -0.16298184E-10 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                     A              B              C
ALPHA    S    -0.01806384     0.00018139     0.00019092  1/CM
         B    -0.05862119     0.00000644     0.00006217  1/CM
         A     0.19364022     0.00002477     0.00007760  1/CM

                     A              B              C
ALPHA    S     -541.54024        5.43805        5.72361  MHZ
```

```
          B    -1757.41919        0.19310        1.86384  MHZ
          A     5805.18798        0.74246        2.32625  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                       S              B              A
 X(I,J):  S    -0.82486487    -1.76186919    -1.33994223  1/CM
          B    -1.76186919    -1.87998897   -16.52387511  1/CM
          A    -1.33994223   -16.52387511   -55.98382262  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:       -3.78724154  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H  (120)Sn (79)Br  TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.493988 A    (     4.712955 A.U.)
 R20:     1.753021 A    (     3.312730 A.U.)
 R30:     1.967860 RAD  (   112.750046 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.9116969   2   0   0
      1.7728547   0   2   0
      0.3648346   0   0   2
     -0.0057150   1   1   0
      0.0353873   1   0   1
     -0.0152195   0   1   1
     -7.9892394   3   0   0
     -8.6330347   0   3   0
     -0.2084848   0   0   3
      0.1209886   2   1   0
     -0.0411611   1   2   0
     -0.2438378   2   0   1
      0.0749239   0   2   1
     -0.0752502   1   1   1
     -0.2801501   1   0   2
     -0.1796516   0   1   2
     25.2251517   4   0   0
     29.6534307   0   4   0
     -0.2643661   0   0   4
      0.0669519   3   1   0
      0.1404484   1   3   0
      0.3090539   2   2   0
      0.1960627   3   0   1
     -0.1327991   0   3   1
      0.1169614   2   1   1
      0.2383493   1   2   1
      0.3648542   2   0   2
     -0.4739404   0   2   2
      0.3548785   1   1   2
      0.0853287   1   0   3
      0.0759294   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:                A              B              C
 CENTER  1:      1.01189017     0.00746922     0.00000000    MASS:119.902197 AMU
 CENTER  2:     -1.48131870    -0.05089072     0.00000000    MASS: 78.918338 AMU
 CENTER  3:     -2.19683227     1.54939296     0.00000000    MASS:  2.014102 AMU
 MOMENTS:        8.37931812   507.56053586   515.93985399    10**(-40) G*CM**2
```

```
ROTATIONAL CONSTANTS AT RE
--------------------------
           A           B           C        UNIT
        3.3408      0.0552      0.0543    1/CM
      100156.0      1653.5      1626.6    MHZ

PROLATE          ASYMMETRIC ROTOR (K=-0.999)           OBLATE
-------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.9117 AJ/A**2    F12:    -0.0057 AJ/A**2    F1A:     0.0354 AJ/A
                           F22:     1.7729 AJ/A**2    F2A:    -0.0152 AJ/A
                                                      FAA:     0.3648 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197      78.918338       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       258.35881      326.29100     1238.05635  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99715801     0.01099242     0.07453232        258.35881085 S
Q2:       -0.28532138     0.00945146     0.95838530        326.29100432 B
Q3:       -0.01432660     0.99983206    -0.01142800       1238.05635220 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S    -0.00000000    -0.13649083    -0.09774856
         B     0.13649083    -0.00000000    -0.98580702
         A     0.09774856     0.98580702     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00125230 1/CM   AABB:     0.00000047 1/CM   ABAB:  -0.00000127 1/CM
BBBB:    -0.00000004 1/CM   BBCC:    -0.00000004 1/CM
CCCC:    -0.00000004 1/CM   CCAA:     0.00000012 1/CM

AAAA:      -37.54286 MHZ    AABB:        0.01402 MHZ    ABAB:     -0.03818 MHZ
BBBB:       -0.00120 MHZ    BBCC:       -0.00116 MHZ
CCCC:       -0.00112 MHZ    CCAA:        0.00367 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.33408446E+01 1/CM   100156.00333 MHZ
       B:  0.55154137E-01 1/CM     1653.47946 MHZ
       C:  0.54258136E-01 1/CM     1626.61804 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.96988601E-08 1/CM        0.00029 MHZ
     DJK:  0.46996610E-06 1/CM        0.01409 MHZ
      DK:  0.31259409E-03 1/CM        9.37134 MHZ
      R5: -0.13753946E-06 1/CM       -0.00412 MHZ
      R6: -0.21368914E-11 1/CM       -0.00000 MHZ
   DEL-J:  0.16861104E-09 1/CM        0.00001 MHZ
```

```
A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.97031339E-08 1/CM        0.00029 MHZ
DELTA-JK:  0.46994046E-06 1/CM        0.01409 MHZ
 DELTA-K:  0.31259412E-03 1/CM        9.37134 MHZ
   DEL-J:  0.16861104E-09 1/CM        0.00001 MHZ
   DEL-K:  0.33777638E-06 1/CM        0.01013 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.96801093E-08 1/CM        0.00029 MHZ
    ~DJK:  0.47007860E-06 1/CM        0.01409 MHZ
     ~DK:  0.31259400E-03 1/CM        9.37133 MHZ
  ~DEL-J:  0.16861104E-09 1/CM        0.00001 MHZ
     ~R6: -0.11512291E-10 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    S    -0.00370739     0.00017491     0.00017376  1/CM
         B    -0.09230522     0.00001279     0.00006115  1/CM
         A     0.08263721     0.00003038     0.00004981  1/CM

                    A              B              C
ALPHA    S     -111.14467        5.24367        5.20920  MHZ
         B    -2767.24090        0.38332        1.83320  MHZ
         A     2477.40137        0.91078        1.49327  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -0.70044003    -0.60727184     0.08959529  1/CM
         B    -0.60727184    -0.91003743    -7.80434105  1/CM
         A     0.08959529    -7.80434105   -24.45906468  1/CM

DARLING-DENNISON RESONANCE PARAMETER:       -0.20567056  1/CM

--------------------------------------------------------------------------------
------------------------------------------ (1)H (120)Sn (127)I   GROUND STATE
--------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.739003 A    (     5.175966 A.U.)
R20:     1.783213 A    (     3.369785 A.U.)
R30:     1.620307 RAD  (    92.836746 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     1.4241720   2   0   0
     1.7971466   0   2   0
     0.6937948   0   0   2
     0.0820464   1   1   0
     0.0022002   1   0   1
    -0.0904109   0   1   1
    -5.5949499   3   0   0
    -7.0962666   0   3   0
    -1.3336879   0   0   3
     0.1005528   2   1   0
     0.2109965   1   2   0
    -0.4603005   2   0   1
    -0.0055946   0   2   1
    -0.1652944   1   1   1
    -0.0540536   1   0   2
```

```
    -0.0969832   0   1   2
    14.8873149   4   0   0
    27.9526703   0   4   0
     4.1173172   0   0   4
    -0.4358545   3   1   0
     0.9015196   1   3   0
     0.7454530   2   2   0
     0.4697013   3   0   1
    -0.5929769   0   3   1
     0.0378819   2   1   1
    -0.4221565   1   2   1
     2.1669305   2   0   2
     0.4108180   0   2   2
     0.2704397   1   1   2
    -1.7574435   1   0   3
     0.6317557   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:               A              B              C
CENTER  1:     1.41406351     0.00053623     0.00000000    MASS:119.902197 AMU
CENTER  2:    -1.32473293    -0.01453388     0.00000000    MASS:126.904468 AMU
CENTER  3:    -1.42365491     1.76629674     0.00000000    MASS:  1.007825 AMU
MOMENTS:       5.26563961   771.32167237   776.58731198    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         5.3164       0.0363       0.0360     1/CM
      159380.3       1088.1       1080.7     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.4242 AJ/A**2    F12:      0.0820 AJ/A**2    F1A:      0.0022 AJ/A
                           F22:      1.7971 AJ/A**2    F2A:     -0.0904 AJ/A
                                                       FAA:      0.6938 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197     126.904468       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       197.35748      608.36226     1747.75320  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:         0.99988686    -0.00028640     0.01503939        197.35747997 A
Q2:        -0.02081090     0.02163057     0.99954941        608.36225699 B
Q3:         0.04593320     0.99723426    -0.05842923       1747.75320474 S


CORIOLIS COUPLING MATRICES
--------------------------
                    A              B              S
ZETA-C   A     0.00000000    -0.08823911    -0.00151274
         B     0.08823911    -0.00000000    -0.99609817
         S     0.00151274     0.99609817     0.00000000
```

```
 TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
 ------------------------------------------------
 AAAA:    -0.00079190 1/CM   AABB:     0.00000020 1/CM   ABAB:  -0.00000030 1/CM
 BBBB:    -0.00000002 1/CM   BBCC:    -0.00000002 1/CM
 CCCC:    -0.00000002 1/CM   CCAA:     0.00000016 1/CM

 AAAA:      -23.74067 MHZ    AABB:        0.00611 MHZ    ABAB:     -0.00901 MHZ
 BBBB:       -0.00059 MHZ    BBCC:       -0.00058 MHZ
 CCCC:       -0.00057 MHZ    CCAA:        0.00493 MHZ

 ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
 -----------------------------------------------------
 AXIS   A:  0.53163531E+01 1/CM   159380.26061 MHZ
        B:  0.36293577E-01 1/CM     1088.05409 MHZ
        C:  0.36047430E-01 1/CM     1080.67478 MHZ

 FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
 --------------------------------------------
       DJ:  0.48403730E-08 1/CM        0.00015 MHZ
      DJK:  0.48477291E-07 1/CM        0.00145 MHZ
       DK:  0.19792254E-03 1/CM        5.93357 MHZ
       R5: -0.35098365E-07 1/CM       -0.00105 MHZ
       R6: -0.86146073E-13 1/CM       -0.00000 MHZ
    DEL-J:  0.33995881E-10 1/CM        0.00000 MHZ

 A-REDUCTION DISTORTION CONSTANTS
 --------------------------------
  DELTA-J:  0.48405453E-08 1/CM        0.00015 MHZ
 DELTA-JK:  0.48476257E-07 1/CM        0.00145 MHZ
  DELTA-K:  0.19792254E-03 1/CM        5.93357 MHZ
    DEL-J:  0.33995881E-10 1/CM        0.00000 MHZ
    DEL-K:  0.84980315E-07 1/CM        0.00255 MHZ

 S-REDUCTION DISTORTION CONSTANTS
 --------------------------------
      ~DJ:  0.48395549E-08 1/CM        0.00015 MHZ
     ~DJK:  0.48482199E-07 1/CM        0.00145 MHZ
      ~DK:  0.19792253E-03 1/CM        5.93357 MHZ
   ~DEL-J:  0.33995881E-10 1/CM        0.00000 MHZ
      ~R6: -0.49519248E-12 1/CM       -0.00000 MHZ

 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 -------------------------------------------------
                     A             B             C
 ALPHA    A    -0.00203230    0.00010494    0.00010389  1/CM
          B    -0.07365280   -0.00000403    0.00001192  1/CM
          S     0.12943918   -0.00009561   -0.00008918  1/CM

                     A             B             C
 ALPHA    A      -60.92681       3.14606       3.11449  MHZ
          B    -2208.05531      -0.12077       0.35723  MHZ
          S     3880.48924      -2.86633      -2.67358  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                     A             B             S
 X(I,J):  A    -0.54917838    0.70942411    1.86751184  1/CM
          B     0.70942411   -1.43594960   -9.45949727  1/CM
          S     1.86751184   -9.45949727  -22.81224447  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:        0.18378458  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (1)H (120)Sn (127)I   EXCITED STATE
```

```
--------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.732885 A    (     5.164405 A.U.)
 R20:     1.798556 A    (     3.398779 A.U.)
 R30:     1.992537 RAD  (   114.163950 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.1897271   2   0   0
      1.2833229   0   2   0
      0.2448502   0   0   2
     -0.0052331   1   1   0
      0.0194824   1   0   1
      0.0146178   0   1   1
     -5.9106747   3   0   0
     -7.5204713   0   3   0
      0.0751241   0   0   3
      0.2466576   2   1   0
      0.2352541   1   2   0
     -0.1589854   2   0   1
      0.0903208   0   2   1
     -0.1324164   1   1   1
     -0.2401163   1   0   2
     -0.2182273   0   1   2
     15.4478873   4   0   0
     24.9511061   0   4   0
     -1.1290149   0   0   4
     -0.2151470   3   1   0
      0.5724456   1   3   0
      1.2528659   2   2   0
      0.7496755   3   0   1
     -0.4098706   0   3   1
     -0.0468919   2   1   1
     -0.0541657   1   2   1
      0.0596420   2   0   2
     -0.5872157   0   2   2
      0.3584795   1   1   2
      0.0146972   1   0   3
      0.2546923   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------------
 AXES:              A              B              C
 CENTER  1:     1.41332293     0.00372912     0.00000000    MASS:119.902197 AMU
 CENTER  2:    -1.31891953    -0.01638215     0.00000000    MASS:126.904468 AMU
 CENTER  3:    -2.06756403     1.61916876     0.00000000    MASS:  1.007825 AMU
 MOMENTS:       4.44681533   771.42829161   775.87510694    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
           A           B           C        UNIT
         6.2953      0.0363      0.0361    1/CM
      188728.1      1087.9      1081.7    MHZ

 PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
 ------------------------------+-------------------------------
 ^

 ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


 HARMONIC FORCE FIELD
 --------------------
```

```
F11:     1.1897 AJ/A**2    F12:    -0.0052 AJ/A**2    F1A:     0.0195 AJ/A
                           F22:     1.2833 AJ/A**2    F2A:     0.0146 AJ/A
                                                      FAA:     0.2449 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197     126.904468       1.007825  AMU
FUNDAMENTAL FREQUENCIES:       180.62578      360.09227     1475.99694  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99992718     0.00337755     0.01158549        180.62577620 S
Q2:        0.02374109    -0.00092104     0.99971772        360.09227392 B
Q3:       -0.00720390     0.99990759     0.01152890       1475.99694158 A


CORIOLIS COUPLING MATRICES
--------------------------
                     S              B              A
ZETA-C   S     0.00000000    -0.08229767     0.00523332
         B     0.08229767     0.00000000    -0.99659405
         A    -0.00523332     0.99659405     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:     -0.00701990 1/CM   AABB:      0.00000002 1/CM   ABAB:  -0.00000085 1/CM
BBBB:     -0.00000002 1/CM   BBCC:     -0.00000002 1/CM
CCCC:     -0.00000002 1/CM   CCAA:     -0.00000021 1/CM

AAAA:      -210.45122 MHZ    AABB:         0.00068 MHZ    ABAB:     -0.02550 MHZ
BBBB:        -0.00070 MHZ    BBCC:        -0.00069 MHZ
CCCC:        -0.00069 MHZ    CCAA:        -0.00624 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.62952917E+01 1/CM   188728.10120 MHZ
       B:  0.36288611E-01 1/CM     1087.90522 MHZ
       C:  0.36080468E-01 1/CM     1081.66526 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.57845260E-08 1/CM        0.00017 MHZ
     DJK:  0.45996930E-06 1/CM        0.01379 MHZ
      DK:  0.17545085E-02 1/CM       52.59884 MHZ
      R5: -0.91865211E-07 1/CM       -0.00275 MHZ
      R6: -0.16639169E-12 1/CM       -0.00000 MHZ
   DEL-J:  0.32863869E-10 1/CM        0.00000 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.57848588E-08 1/CM        0.00017 MHZ
DELTA-JK:  0.45996730E-06 1/CM        0.01379 MHZ
 DELTA-K:  0.17545085E-02 1/CM       52.59884 MHZ
   DEL-J:  0.32863869E-10 1/CM        0.00000 MHZ
   DEL-K:  0.22375925E-06 1/CM        0.00671 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.57829986E-08 1/CM        0.00017 MHZ
    ~DJK:  0.45997846E-06 1/CM        0.01379 MHZ
     ~DK:  0.17545085E-02 1/CM       52.59884 MHZ
  ~DEL-J:  0.32863869E-10 1/CM        0.00000 MHZ
     ~R6: -0.93012166E-12 1/CM       -0.00000 MHZ
```

```
 VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
 --------------------------------------------------
                      A              B              C
 ALPHA     S    -0.00383196     0.00015430     0.00015293  1/CM
           B    -0.22773169     0.00005599     0.00007835  1/CM
           A     0.38147680    -0.00004414    -0.00003155  1/CM

                      A              B              C
 ALPHA     S     -114.87932        4.62578        4.58482  MHZ
           B    -6827.22456        1.67854        2.34876  MHZ
           A    11436.38709       -1.32325       -0.94576  MHZ


 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XSS PERTURBED BY MODE B
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XSB PERTURBED BY MODE S
 *** WARNING *** FERMI RESONANCE EXPECTED: 1XBS PERTURBED BY MODE S
                      S              B              A
 X(I,J):   S    -0.83046999    -1.80862690     3.30867262  1/CM
           B    -1.80862690    -4.50931666   -25.39564441  1/CM
           A     3.30867262   -25.39564441   -80.20475360  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:        0.49239727  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (1)H (120)Sn (127)I   TRIPLET STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.704780 A    (     5.111295 A.U.)
 R20:     1.752181 A    (     3.311144 A.U.)
 R30:     1.981244 RAD  (   113.516934 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.4633317   2   0   0
      1.8188693   0   2   0
      0.3429339   0   0   2
     -0.0014376   1   1   0
      0.0277448   1   0   1
     -0.0240547   0   1   1
     -6.1521171   3   0   0
     -8.6016352   0   3   0
     -0.2160315   0   0   3
      0.0636368   2   1   0
      0.0262366   1   2   0
     -0.1772754   2   0   1
      0.0941945   0   2   1
     -0.0838538   1   1   1
     -0.2333292   1   0   2
     -0.1104516   0   1   2
     17.3698117   4   0   0
     29.7417341   0   4   0
      0.1642635   0   0   4
     -0.1777194   3   1   0
      0.1697362   1   3   0
      0.4063190   2   2   0
      0.5399377   3   0   1
     -0.4565188   0   3   1
      0.0796777   2   1   1
      0.1053686   1   2   1
      0.3282576   2   0   2
```

```
    -0.5803748   0   2   2
     0.2271726   1   1   2
    -0.0011562   1   0   3
     0.1238946   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A             B             C
CENTER  1:     1.39886581    0.00350084    0.00000000    MASS:119.902197 AMU
CENTER  2:    -1.30566877   -0.01589951    0.00000000    MASS:126.904468 AMU
CENTER  3:    -2.01610634    1.58555360    0.00000000    MASS:  1.007825 AMU
MOMENTS:       4.26291921  755.65325192  759.91617113    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A           B           C        UNIT
        6.5669      0.0370      0.0368     1/CM
     196869.6      1110.6      1104.4     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.4633 AJ/A**2    F12:    -0.0014 AJ/A**2    F1A:     0.0277 AJ/A
                           F22:     1.8189 AJ/A**2    F2A:    -0.0241 AJ/A
                                                      FAA:     0.3429 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:               119.902197     126.904468       1.007825  AMU
FUNDAMENTAL FREQUENCIES:      200.31229      437.34201     1757.30527  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
              R1            R2            R3            FREQUENCY
Q1:       0.99993585    0.00321935    0.01085920       200.31229119 S
Q2:       0.03434584    0.00759610    0.99938114       437.34200573 B
Q3:      -0.00342870    0.99988633   -0.01468253      1757.30526835 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S             B             A
ZETA-C   S     0.00000000   -0.08145133    0.00865862
         B     0.08145133    0.00000000   -0.99663971
         A    -0.00865862    0.99663971   -0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00500466 1/CM   AABB:    -0.00000003 1/CM   ABAB:  -0.00000064 1/CM
BBBB:    -0.00000002 1/CM   BBCC:    -0.00000002 1/CM
CCCC:    -0.00000002 1/CM   CCAA:    -0.00000019 1/CM

AAAA:     -150.03603 MHZ    AABB:       -0.00085 MHZ    ABAB:     -0.01926 MHZ
BBBB:       -0.00061 MHZ    BBCC:       -0.00060 MHZ
CCCC:       -0.00059 MHZ    CCAA:       -0.00556 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
```

```
AXIS   A:  0.65668614E+01 1/CM   196869.55638 MHZ
       B:  0.37046150E-01 1/CM     1110.61567 MHZ
       C:  0.36838214E-01 1/CM     1104.38192 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
-------------------------------------------
      DJ:  0.50050530E-08 1/CM        0.00015 MHZ
     DJK:  0.36463097E-06 1/CM        0.01093 MHZ
      DK:  0.12507961E-02 1/CM       37.49793 MHZ
      R5: -0.70462066E-07 1/CM       -0.00211 MHZ
      R6: -0.11671892E-12 1/CM       -0.00000 MHZ
   DEL-J:  0.27731579E-10 1/CM        0.00000 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.50052864E-08 1/CM        0.00015 MHZ
DELTA-JK:  0.36462957E-06 1/CM        0.01093 MHZ
 DELTA-K:  0.12507962E-02 1/CM       37.49793 MHZ
   DEL-J:  0.27731579E-10 1/CM        0.00000 MHZ
   DEL-K:  0.17024724E-06 1/CM        0.00510 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.50039311E-08 1/CM        0.00015 MHZ
    ~DJK:  0.36463770E-06 1/CM        0.01093 MHZ
     ~DK:  0.12507961E-02 1/CM       37.49793 MHZ
  ~DEL-J:  0.27731579E-10 1/CM        0.00000 MHZ
     ~R6: -0.67765912E-12 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    S    -0.00135887     0.00011482     0.00011395  1/CM
         B    -0.28072284     0.00003767     0.00005465  1/CM
         A     0.21261957     0.00000171     0.00000798  1/CM

                    A              B              C
ALPHA    S      -40.73797        3.44227        3.41624  MHZ
         B    -8415.85921        1.12928        1.63851  MHZ
         A     6374.17448        0.05130        0.23916  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -0.60208423    -0.64070307     0.53690541  1/CM
         B    -0.64070307    -0.91820219   -13.72024006  1/CM
         A     0.53690541   -13.72024006   -44.09514131  1/CM

DARLING-DENNISON RESONANCE PARAMETER:        0.12118490  1/CM

-------------------------------------------------------------------------------
------------------------------------------ (2)H (120)Sn (127)I   GROUND STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.739003 A    (     5.175966 A.U.)
R20:     1.783213 A    (     3.369785 A.U.)
R30:     1.620307 RAD  (    92.836746 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     1.4241720   2   0   0
     1.7971466   0   2   0
```

```
 0.6937948   0   0   2
 0.0820464   1   1   0
 0.0022002   1   0   1
-0.0904109   0   1   1
-5.5949499   3   0   0
-7.0962666   0   3   0
-1.3336879   0   0   3
 0.1005528   2   1   0
 0.2109965   1   2   0
-0.4603005   2   0   1
-0.0055946   0   2   1
-0.1652944   1   1   1
-0.0540536   1   0   2
-0.0969832   0   1   2
14.8873149   4   0   0
27.9526703   0   4   0
 4.1173172   0   0   4
-0.4358545   3   1   0
 0.9015196   1   3   0
 0.7454530   2   2   0
 0.4697013   3   0   1
-0.5929769   0   3   1
 0.0378819   2   1   1
-0.4221565   1   2   1
 2.1669305   2   0   2
 0.4108180   0   2   2
 0.2704397   1   1   2
-1.7574435   1   0   3
 0.6317557   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------
AXES:                A              B              C
CENTER  1:     1.41983593     0.00116736     0.00000000    MASS:119.902197 AMU
CENTER  2:    -1.31883694    -0.02889886     0.00000000    MASS:126.904468 AMU
CENTER  3:    -1.42750841     1.75136342     0.00000000    MASS:  2.014102 AMU
MOMENTS:      10.43469277   774.71756901   785.15226179    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
          A            B            C        UNIT
        2.6828       0.0361       0.0357     1/CM
       80427.8       1083.3       1068.9     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
-------------------------------+-------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.4242 AJ/A**2    F12:      0.0820 AJ/A**2    F1A:      0.0022 AJ/A
                           F22:      1.7971 AJ/A**2    F2A:     -0.0904 AJ/A
                                                       FAA:      0.6938 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197     126.904468       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       196.87907      433.73968     1241.40262  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
```

```
Q1:        0.99944352    -0.00039838     0.03335409        196.87906608 A
Q2:       -0.05836525     0.02524415     0.99797607        433.73968046 B
Q3:        0.04641054     0.99713135    -0.05979234       1241.40261845 S


CORIOLIS COUPLING MATRICES
--------------------------
                     A             B             S
ZETA-C   A     0.00000000    -0.12363279    -0.01316189
         B     0.12363279    -0.00000000    -0.99224075
         S     0.01316189     0.99224075     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00020205 1/CM   AABB:     0.00000011 1/CM   ABAB:  -0.00000029 1/CM
BBBB:    -0.00000002 1/CM   BBCC:    -0.00000002 1/CM
CCCC:    -0.00000002 1/CM   CCAA:     0.00000007 1/CM

AAAA:       -6.05735 MHZ    AABB:        0.00316 MHZ    ABAB:     -0.00881 MHZ
BBBB:       -0.00058 MHZ    BBCC:       -0.00057 MHZ
CCCC:       -0.00055 MHZ    CCAA:        0.00200 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.26827814E+01 1/CM    80427.76456 MHZ
       B:  0.36134487E-01 1/CM     1083.28469 MHZ
       C:  0.35654201E-01 1/CM     1068.88610 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.47360693E-08 1/CM        0.00014 MHZ
     DJK:  0.94422396E-07 1/CM        0.00283 MHZ
      DK:  0.50413686E-04 1/CM        1.51136 MHZ
      R5: -0.34292087E-07 1/CM       -0.00103 MHZ
      R6: -0.32590416E-12 1/CM       -0.00000 MHZ
   DEL-J:  0.65277034E-10 1/CM        0.00000 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.47367211E-08 1/CM        0.00014 MHZ
DELTA-JK:  0.94418486E-07 1/CM        0.00283 MHZ
 DELTA-K:  0.50413690E-04 1/CM        1.51136 MHZ
   DEL-J:  0.65277034E-10 1/CM        0.00000 MHZ
   DEL-K:  0.82952824E-07 1/CM        0.00249 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.47329581E-08 1/CM        0.00014 MHZ
    ~DJK:  0.94441064E-07 1/CM        0.00283 MHZ
     ~DK:  0.50413671E-04 1/CM        1.51136 MHZ
  ~DEL-J:  0.65277034E-10 1/CM        0.00000 MHZ
     ~R6: -0.18815038E-11 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                     A             B             C
ALPHA    A    -0.00103935     0.00010509     0.00010313  1/CM
         B    -0.02713667    -0.00000747     0.00001413  1/CM
         S     0.04621999    -0.00006593    -0.00005715  1/CM

                     A             B             C
ALPHA    A      -31.15899        3.15051        3.09191  MHZ
         B     -813.53686       -0.22402        0.42370  MHZ
         S     1385.64039       -1.97662       -1.71332  MHZ
```

```
 ANHARMONIC VIBRATIONAL CONSTANTS
 --------------------------------
                      A              B              S
 X(I,J):  A    -0.55814562     0.48145994     1.28809324  1/CM
          B     0.48145994    -0.63398558    -4.66623859  1/CM
          S     1.28809324    -4.66623859   -11.49415809  1/CM

 DARLING-DENNISON RESONANCE PARAMETER:        0.11917011  1/CM

-------------------------------------------------------------------------------
---------------------------------------- (2)H (120)Sn (127)I   EXCITED STATE
-------------------------------------------------------------------------------
 REFERENCE GEOMETRY
 ------------------
 R10:     2.732885 A    (     5.164405 A.U.)
 R20:     1.798556 A    (     3.398779 A.U.)
 R30:     1.992537 RAD  (   114.163950 DEGREES)

 INTERNAL FORCE FIELD
 --------------------
    POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
      1.1897271   2   0   0
      1.2833229   0   2   0
      0.2448502   0   0   2
     -0.0052331   1   1   0
      0.0194824   1   0   1
      0.0146178   0   1   1
     -5.9106747   3   0   0
     -7.5204713   0   3   0
      0.0751241   0   0   3
      0.2466576   2   1   0
      0.2352541   1   2   0
     -0.1589854   2   0   1
      0.0903208   0   2   1
     -0.1324164   1   1   1
     -0.2401163   1   0   2
     -0.2182273   0   1   2
     15.4478873   4   0   0
     24.9511061   0   4   0
     -1.1290149   0   0   4
     -0.2151470   3   1   0
      0.5724456   1   3   0
      1.2528659   2   2   0
      0.7496755   3   0   1
     -0.4098706   0   3   1
     -0.0468919   2   1   1
     -0.0541657   1   2   1
      0.0596420   2   0   2
     -0.5872157   0   2   2
      0.3584795   1   1   2
      0.0146972   1   0   3
      0.2546923   0   1   3

 EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
 -------------------------------------------------------------------
 AXES:              A              B              C
 CENTER  1:     1.42166770     0.00747026     0.00000000    MASS:119.902197 AMU
 CENTER  2:    -1.31035764    -0.03241478     0.00000000    MASS:126.904468 AMU
 CENTER  3:    -2.07081965     1.59767507     0.00000000    MASS:  2.014102 AMU
 MOMENTS:       8.76952925   778.58275663   787.35228588    10**(-40) G*CM**2

 ROTATIONAL CONSTANTS AT RE
 --------------------------
```

```
          A           B           C        UNIT
        3.1922      0.0360      0.0356     1/CM
       95699.4      1077.9      1065.9     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
-----------------------------+-----------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.1897 AJ/A**2    F12:    -0.0052 AJ/A**2    F1A:      0.0195 AJ/A
                           F22:     1.2833 AJ/A**2    F2A:      0.0146 AJ/A
                                                      FAA:      0.2449 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197     126.904468       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       180.22760      257.20003     1048.18736  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99941302     0.00687172     0.03356186        180.22759677 S
Q2:       -0.08297518     0.00109631     0.99655101        257.20002548 B
Q3:       -0.01042415     0.99988552     0.01096746       1048.18736431 A


CORIOLIS COUPLING MATRICES
--------------------------
                    S              B              A
ZETA-C   S     0.00000000    -0.11446815    -0.02587993
         B     0.11446815    -0.00000000    -0.99308976
         A     0.02587993     0.99308976     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
AAAA:    -0.00184661 1/CM   AABB:     0.00000024 1/CM   ABAB:  -0.00000082 1/CM
BBBB:    -0.00000002 1/CM   BBCC:    -0.00000002 1/CM
CCCC:    -0.00000002 1/CM   CCAA:     0.00000001 1/CM

AAAA:      -55.36009 MHZ    AABB:        0.00724 MHZ    ABAB:     -0.02445 MHZ
BBBB:       -0.00069 MHZ    BBCC:       -0.00067 MHZ
CCCC:       -0.00065 MHZ    CCAA:        0.00022 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.31921895E+01 1/CM    95699.43722 MHZ
       B:  0.35955153E-01 1/CM     1077.90841 MHZ
       C:  0.35554524E-01 1/CM     1065.89785 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.55894411E-08 1/CM        0.00017 MHZ
     DJK:  0.33447835E-06 1/CM        0.01003 MHZ
      DK:  0.46131338E-03 1/CM       13.82983 MHZ
      R5: -0.87281342E-07 1/CM       -0.00262 MHZ
      R6: -0.64021528E-12 1/CM       -0.00000 MHZ
   DEL-J:  0.64538370E-10 1/CM        0.00000 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
```

```
 DELTA-J:  0.55907215E-08 1/CM        0.00017 MHZ
DELTA-JK:  0.33447067E-06 1/CM        0.01003 MHZ
 DELTA-K:  0.46131339E-03 1/CM       13.82983 MHZ
   DEL-J:  0.64538370E-10 1/CM        0.00000 MHZ
   DEL-K:  0.21491518E-06 1/CM        0.00644 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.55839020E-08 1/CM        0.00017 MHZ
    ~DJK:  0.33451158E-06 1/CM        0.01003 MHZ
     ~DK:  0.46131335E-03 1/CM       13.82983 MHZ
  ~DEL-J:  0.64538370E-10 1/CM        0.00000 MHZ
     ~R6: -0.34097515E-11 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    S    -0.00272352     0.00015263     0.00015039  1/CM
         B    -0.08196119     0.00002323     0.00005332  1/CM
         A     0.13738864    -0.00002794    -0.00001089  1/CM

                    A              B              C
ALPHA    S      -81.64897        4.57566        4.50864  MHZ
         B    -2457.13485        0.69650        1.59837  MHZ
         A     4118.80786       -0.83761       -0.32638  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -0.95619451    -0.92435537     2.23510931  1/CM
         B    -0.92435537    -2.30168030   -12.67120124  1/CM
         A     2.23510931   -12.67120124   -40.48694006  1/CM

DARLING-DENNISON RESONANCE PARAMETER:        0.32420014  1/CM

-------------------------------------------------------------------------------
----------------------------------------- (2)H (120)Sn (127)I   TRIPLET STATE
-------------------------------------------------------------------------------
REFERENCE GEOMETRY
------------------
R10:     2.704780 A    (     5.111295 A.U.)
R20:     1.752181 A    (     3.311144 A.U.)
R30:     1.981244 RAD  (   113.516934 DEGREES)

INTERNAL FORCE FIELD
--------------------
   POWERS OF    R1  R2  R3  (FACTORIALS EXCLUDED!)
     1.4633317   2   0   0
     1.8188693   0   2   0
     0.3429339   0   0   2
    -0.0014376   1   1   0
     0.0277448   1   0   1
    -0.0240547   0   1   1
    -6.1521171   3   0   0
    -8.6016352   0   3   0
    -0.2160315   0   0   3
     0.0636368   2   1   0
     0.0262366   1   2   0
    -0.1772754   2   0   1
     0.0941945   0   2   1
    -0.0838538   1   1   1
    -0.2333292   1   0   2
    -0.1104516   0   1   2
    17.3698117   4   0   0
```

```
    29.7417341   0   4   0
     0.1642635   0   0   4
    -0.1777194   3   1   0
     0.1697362   1   3   0
     0.4063190   2   2   0
     0.5399377   3   0   1
    -0.4565188   0   3   1
     0.0796777   2   1   1
     0.1053686   1   2   1
     0.3282576   2   0   2
    -0.5803748   0   2   2
     0.2271726   1   1   2
    -0.0011562   1   0   3
     0.1238946   0   1   3

EQUILIBRIUM GEOMETRY IN MOLECULE FIXED AXES SYSTEM (ASYMMETRIC TOP)
-------------------------------------------------------------------------
AXES:              A              B              C
CENTER  1:     1.40700483     0.00701550     0.00000000    MASS:119.902197 AMU
CENTER  2:    -1.29732556    -0.03146551     0.00000000    MASS:126.904468 AMU
CENTER  3:    -2.01904408     1.56493543     0.00000000    MASS:  2.014102 AMU
MOMENTS:       8.40914267   762.45522001   770.86436268    10**(-40) G*CM**2

ROTATIONAL CONSTANTS AT RE
--------------------------
           A            B            C        UNIT
         3.3290       0.0367       0.0363     1/CM
        99800.8       1100.7       1088.7     MHZ

PROLATE          ASYMMETRIC ROTOR (K=-1.000)           OBLATE
------------------------------+------------------------------
^

ASSIGNMENT OF MOLECULE FIXED AXES: A-->Z  B-->X  C-->Y    CASE I(R)


HARMONIC FORCE FIELD
--------------------
F11:     1.4633 AJ/A**2    F12:    -0.0014 AJ/A**2    F1A:     0.0277 AJ/A
                           F22:     1.8189 AJ/A**2    F2A:    -0.0241 AJ/A
                                                      FAA:     0.3429 AJ

WILSON FG ANALYSIS
------------------
ATOMIC MASSES:                119.902197     126.904468       2.014102  AMU
FUNDAMENTAL FREQUENCIES:       199.93427      312.20103     1248.02753  1/CM

NORMAL COORDINATE DISPLACEMENTS
-------------------------------
               R1             R2             R3             FREQUENCY
Q1:        0.99956624     0.00659428     0.02870278        199.93427185 S
Q2:       -0.04221789     0.01005173     0.99905786        312.20102647 B
Q3:       -0.00601525     0.99986540    -0.01526414       1248.02753005 A


CORIOLIS COUPLING MATRICES
--------------------------
                   S              B              A
ZETA-C   S     0.00000000    -0.11341236    -0.01093759
         B     0.11341236     0.00000000    -0.99348780
         A     0.01093759     0.99348780     0.00000000


TAU CONSTANTS AND QUARTIC CENTRIFUGAL DISTORTION
------------------------------------------------
```

```
AAAA:     -0.00131585 1/CM   AABB:      0.00000015 1/CM   ABAB:  -0.00000062 1/CM
BBBB:     -0.00000002 1/CM   BBCC:     -0.00000002 1/CM
CCCC:     -0.00000002 1/CM   CCAA:     -0.00000001 1/CM

AAAA:       -39.44831 MHZ    AABB:         0.00436 MHZ    ABAB:     -0.01851 MHZ
BBBB:        -0.00059 MHZ    BBCC:        -0.00058 MHZ
CCCC:        -0.00057 MHZ    CCAA:        -0.00043 MHZ

ROTATIONAL CONSTANTS INCLUDING CENTRIFUGAL DISTORTION
-----------------------------------------------------
AXIS   A:  0.33289957E+01 1/CM    99800.78185 MHZ
       B:  0.36715657E-01 1/CM     1100.70774 MHZ
       C:  0.36315019E-01 1/CM     1088.69691 MHZ

FIRST ORDER CENTRIFUGAL DISTORTION CONSTANTS
--------------------------------------------
      DJ:  0.48383157E-08 1/CM        0.00015 MHZ
     DJK:  0.26624744E-06 1/CM        0.00798 MHZ
      DK:  0.32869240E-03 1/CM        9.85395 MHZ
      R5: -0.67162597E-07 1/CM       -0.00201 MHZ
      R6: -0.44846849E-12 1/CM       -0.00000 MHZ
   DEL-J:  0.54043450E-10 1/CM        0.00000 MHZ

A-REDUCTION DISTORTION CONSTANTS
--------------------------------
 DELTA-J:  0.48392127E-08 1/CM        0.00015 MHZ
DELTA-JK:  0.26624206E-06 1/CM        0.00798 MHZ
 DELTA-K:  0.32869240E-03 1/CM        9.85395 MHZ
   DEL-J:  0.54043450E-10 1/CM        0.00000 MHZ
   DEL-K:  0.16380963E-06 1/CM        0.00491 MHZ

S-REDUCTION DISTORTION CONSTANTS
--------------------------------
     ~DJ:  0.48342295E-08 1/CM        0.00014 MHZ
    ~DJK:  0.26627196E-06 1/CM        0.00798 MHZ
     ~DK:  0.32869237E-03 1/CM        9.85395 MHZ
  ~DEL-J:  0.54043450E-10 1/CM        0.00000 MHZ
     ~R6: -0.24916011E-11 1/CM       -0.00000 MHZ

VIBRATIONAL DEPENDENCE OF THE ROTATIONAL CONSTANTS
--------------------------------------------------
                    A              B              C
ALPHA    S    -0.00101340     0.00011366     0.00011223  1/CM
         B    -0.10197940     0.00001728     0.00004005  1/CM
         A     0.07625091     0.00000519     0.00001359  1/CM

                    A              B              C
ALPHA    S      -30.38099        3.40751        3.36464  MHZ
         B    -3057.26566        0.51811        1.20069  MHZ
         A     2285.94481        0.15555        0.40750  MHZ


ANHARMONIC VIBRATIONAL CONSTANTS
--------------------------------
                    S              B              A
X(I,J):  S    -0.59752635    -0.48983908     0.35324221  1/CM
         B    -0.48983908    -0.44709895    -6.86922245  1/CM
         A     0.35324221    -6.86922245   -22.24034002  1/CM

DARLING-DENNISON RESONANCE PARAMETER:        0.09464644  1/CM
```