Supplementary Materials: Completing the spectral mosaic of chloromethane by adding the CHD₂Cl missing piece through the interplay of rotational/vibrational spectroscopy and quantum chemical calculations

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List of supporting material available

Table S.1. Fit of the rotational transitions of $^{12}CHD_2^{35}Cl$ in PIFORM format

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CHD2Cl -- 35Cl                                 Tue Mar 18 09:42:24 2025


------------------------------------------------------------------=========
                                    obs       o-c    error   blends   Notes
                                                             o-c    wt
    / instead of : below denotes (o-c)>3*err
------------------------------------------------------------------=========
!Mallinson-TableII
   1:  5  0  5 10  7    4  1  3 10  6   29771.6170  -0.1104  0.020   0.0432 0.50
!Mallinson-TableII
   2:  5  0  5 10  4    4  1  3 10  3   29771.6170   0.1967  0.020   0.0432 0.50
!Mallinson-TableII
   3:  5  0  5 10  6    4  1  3 10  5   29768.8270  -0.1306  0.020   0.0221 0.50
!Mallinson-TableII
   4:  5  0  5 10  5    4  1  3 10  4   29768.8270   0.1748  0.020   0.0221 0.50
!Mallinson-TableII
   5:  8  2  6 10 10    9  1  8 10 11   37515.0420  -0.0778  0.035  -0.0280 0.50
!Mallinson-TableII
   6:  8  2  6 10  7    9  1  8 10  8   37515.0420   0.0218  0.035  -0.0280 0.50
!Mallinson-TableII
   7:  8  2  6 10  9    9  1  8 10 10   37517.5820  -0.0394  0.035   0.0109 0.50
!Mallinson-TableII
   8:  8  2  6 10  8    9  1  8 10  9   37517.5820   0.0611  0.035   0.0109 0.50
!Mallinson-TableII
   9:  9  2  8 10 11   10  1 10 10 12   29773.7720  -0.0105  0.010   0.0049 0.50
!Mallinson-TableII
  10:  9  2  8 10  8   10  1 10 10  9   29773.7720   0.0203  0.010   0.0049 0.50
!Mallinson-TableII
  11:  9  2  8 10 10   10  1 10 10 11   29775.7120  -0.0223  0.010  -0.0066 0.50
!Mallinson-TableII
  12:  9  2  8 10  9   10  1 10 10 10   29775.7120   0.0091  0.010  -0.0066 0.50
!Mallinson-TableII
  13: 12  1 11 10 14   11  2  9 10 13   36198.3260  -0.0222  0.042  -0.0135 0.50
!Mallinson-TableII
  14: 12  1 11 10 11   11  2  9 10 10   36198.3260  -0.0047  0.042  -0.0135 0.50
!Mallinson-TableII
  15: 12  1 11 10 13   11  2  9 10 12   36197.0360   0.0382  0.042   0.0468 0.50
!Mallinson-TableII
  16: 12  1 11 10 12   11  2  9 10 11   36197.0360   0.0554  0.042   0.0468 0.50
!Mallinson-TableII
  17: 13  1 13 10 15   12  2 11 10 14   33688.0350  -0.0380  0.062  -0.0218 0.50
!Mallinson-TableII
  18: 13  1 13 10 12   12  2 11 10 11   33688.0350  -0.0055  0.062  -0.0218 0.50
!Mallinson-TableII
  19: 13  1 13 10 14   12  2 11 10 13   33687.0250   0.0539  0.062   0.0701 0.50
!Mallinson-TableII
  20: 13  1 13 10 13   12  2 11 10 12   33687.0250   0.0862  0.062   0.0701 0.50
!Mallinson-TableII
  21: 12  2 10 10 14   13  0 13 10 15   37861.0280   0.0636  0.088   0.0650 0.50
!Mallinson-TableII
  22: 12  2 10 10 11   13  0 13 10 12   37861.0280   0.0663  0.088   0.0650 0.50
!Mallinson-TableII
  23: 12  2 10 10 13   13  0 13 10 14   37862.3280  -0.0548  0.088  -0.0534 0.50
!Mallinson-TableII
  24: 12  2 10 10 12   13  0 13 10 13   37862.3280  -0.0518  0.088  -0.0534 0.50
!Mallinson-TableII
  25: 16  3 14 10 18   17  2 16 10 19   28537.1450   0.0218  0.157   0.0257 0.50
!Mallinson-TableII
  26: 16  3 14 10 15   17  2 16 10 16   28537.1450   0.0295  0.157   0.0257 0.50
!Mallinson-TableII
  27: 16  3 14 10 17   17  2 16 10 18   28538.0360  -0.2016  0.157  -0.1977 0.50
!Mallinson-TableII
  28: 16  3 14 10 16   17  2 16 10 17   28538.0360  -0.1937  0.157  -0.1977 0.50
!Mallinson-TableII
  29: 20  2 19 10 22   19  3 17 10 21   39760.3040  -0.0491  0.091  -0.0452 0.50
!Mallinson-TableII
  30: 20  2 19 10 19   19  3 17 10 18   39760.3040  -0.0413  0.091  -0.0452 0.50
!Mallinson-TableII
  31: 20  2 19 10 21   19  3 17 10 20   39759.6440   0.0769  0.091   0.0808 0.50
!Mallinson-TableII
  32: 20  2 19 10 20   19  3 17 10 19   39759.6440   0.0846  0.091   0.0808 0.50
!Mallinson-TableII
  33:  1  1  0 10  3    2  0  2 10  4   37949.1890  -0.0118  0.050
!Mallinson-TableV
  34:  1  0  1  0  1    0  0  0  0  0   23049.8900   0.172 UNFITTD   23049.7176
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!Mallinson-TableV
  35:  1  1  0  0  1    2  0  2  0  2      37956.3250  -0.0548  0.500
!Mallinson-TableV
  36:  2  0  2  0  2    1  0  1  0  1      46097.8000  -0.4767  0.200
!Mallinson-TableV
  37:  2  1  1  0  2    1  1  0  0  1      46406.2100  -1.7971  1.000
!Mallinson-TableV
  38:  2  1  2  0  2    1  1  1  0  1      45788.2100  -1.0281  1.000
!Mallinson-TableV
  39:  5  0  5  0  5    4  1  3  0  4      29770.3620   0.0323  0.020
!Mallinson-TableV
  40:  8  2  6  0  8    9  1  8  0  9      37516.3000  -0.0086  0.035
!Mallinson-TableV
  41:  9  2  8  0  9   10  1 10  0 10      29774.7310  -0.0004  0.010
!Mallinson-TableV
  42: 12  1 11  0 12   11  2  9  0 11      36197.6890   0.0162  0.042
!Mallinson-TableV
  43: 12  2 10  0 12   13  0 13  0 13      37861.6720   0.0058  0.088
!Mallinson-TableV
  44: 13  1 13  0 13   12  2 11  0 12      33687.5380   0.0247  0.062
!Mallinson-TableV
  45: 16  0 16  0 16   15  2 13  0 15      28822.1500   0.172 UNFITTD   28821.9776
!Mallinson-TableV
  46: 16  3 14  0 16   17  2 16  0 17      28537.5880  -0.0860  0.157
!Mallinson-TableV
  47: 20  2 19  0 20   19  3 17  0 19      39759.9760   0.0179  0.091
!Mallinson-TableV
  48: 23  4 19  0 23   24  3 21  0 24      33108.9480   0.0421  0.020
!Mallinson-TableV
  49: 23  4 20  0 23   24  3 22  0 24      33534.5580  -0.0227  0.020
!Mallinson-TableV
  50: 27  3 24  0 27   26  4 22  0 26      36580.5870  -0.0491  0.020
!Mallinson-TableV
  51: 27  3 25  0 27   26  4 23  0 26      35733.9270   0.0118  0.020
!Mallinson-TableV
  52: 30  5 25  0 30   31  4 27  0 31      39700.0210   0.100 UNFITTD   39699.9206
!Mallinson-TableV
  53: 30  5 26  0 30   31  4 28  0 31      39747.7760  -0.0168  0.020
!Mallinson-TableV
  54: 34  4 30  0 34   33  5 28  0 33      29642.2000   0.0117  0.020
!Mallinson-TableV
  55: 34  4 31  0 34   33  5 29  0 33      29543.4250  -0.0033  0.020
!Mallinson-TableV
  56: 13  1 12  0 13   13  1 13  0 13      28122.5740  -0.0063  0.020
!Mallinson-TableV
  57: 14  1 13  0 14   14  1 14  0 14      32440.8800  -0.0087  0.020
!Mallinson-TableV
  58: 15  1 14  0 15   15  1 15  0 15      37064.3570  -0.0074  0.020
!Mallinson-TableV
  59: 28  1 28  0 28   28  0 28  0 28      37983.7950  -0.0529  0.020
!Mallinson-TableV
  60: 29  1 29  0 29   29  0 29  0 29      35849.2880  -0.0167  0.020
!Mallinson-TableV
  61: 30  1 30  0 30   30  0 30  0 30      33770.1490  -0.0115  0.020
!Mallinson-TableV
  62: 30  2 28  0 30   30  2 29  0 30      28396.7500   0.0058  0.020
!Mallinson-TableV
  63: 31  1 31  0 31   31  0 31  0 31      31752.4170   0.0085  0.020
!Mallinson-TableV
  64: 31  2 29  0 31   31  2 30  0 31      32015.0000  -0.0008  0.020
!Mallinson-TableV
  65: 32  1 32  0 32   32  0 32  0 32      29801.2100   0.0202  0.020
!Mallinson-TableV
  66: 33  1 33  0 33   33  0 33  0 33      27920.8150   0.0330  0.020
  67:  4  1  4 10  5    3  1  3 10  5      91559.6990  -0.0078  0.010
  68:  4  1  4 10  4    3  1  3 10  3      91572.6800  -0.0008  0.010
  69:  4  1  4 10  5    3  1  3 10  4      91573.6470   0.0017  0.010
  70:  4  1  4 10  3    3  1  3 10  2      91574.5380  -0.0037  0.010
  71:  4  1  4 10  6    3  1  3 10  5      91575.5120   0.0042  0.010
  72:  4  1  4 10  4    3  1  3 10  4      91579.1870  -0.0009  0.010
  73:  4  1  4 10  3    3  1  3 10  3      91588.4770  -0.0061  0.020
  74:  4  0  4 10  5    3  0  3 10  5      92169.2350  -0.0014  0.010
  75:  4  3  1 10  4    3  3  0 10  4      92174.7190  -0.0117  0.010  -0.0074 0.50
  76:  4  3  2 10  4    3  3  1 10  4      92174.7190  -0.0029  0.010  -0.0074 0.50
  77:  4  3  1 10  5    3  3  0 10  4      92177.0190  -0.0000  0.010   0.0044 0.50
  78:  4  3  2 10  5    3  3  1 10  4      92177.0190   0.0087  0.010   0.0044 0.50
  79:  4  3  1 10  3    3  3  0 10  3      92179.0780  -0.0051  0.010  -0.0007 0.50
  80:  4  3  2 10  3    3  3  1 10  3      92179.0780   0.0037  0.010  -0.0007 0.50
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 81:  4  3  2 10   4    3  3  1 10   3      92185.6580   0.0733  0.010  -0.0023 0.15
 82:  4  3  1 10   4    3  3  0 10   3      92185.6580   0.0644  0.010  -0.0023 0.15
 83:  4  0  4 10   4    3  0  3 10   3      92185.6580  -0.0336  0.010  -0.0023 0.40
 84:  4  0  4 10   3    3  0  3 10   2      92185.6580  -0.0342  0.010  -0.0023 0.30
 85:  4  2  3 10   5    3  2  2 10   5      92186.3580  -0.0131  0.020
 86:  4  2  3 10   5    3  2  2 10   4      92186.3800   0.0131  0.020
 87:  4  0  4 10   6    3  0  3 10   5      92187.8610   0.0084  0.010   0.0084 0.50
 88:  4  0  4 10   5    3  0  3 10   4      92187.8610   0.0082  0.010   0.0084 0.50
 89:  4  2  3 10   4    3  2  2 10   4      92188.9660  -0.0110  0.020
 90:  4  2  3 10   4    3  2  2 10   3      92188.9860   0.0060  0.020
 91:  4  2  3 10   6    3  2  2 10   5      92193.7940  -0.0212  0.010   0.0101 0.33
 92:  4  3  1 10   6    3  3  0 10   5      92193.7940   0.0213  0.010   0.0101 0.33
 93:  4  3  2 10   6    3  3  1 10   5      92193.7940   0.0301  0.010   0.0101 0.33
 94:  4  0  4 10   4    3  0  3 10   4      92194.3970   0.0136  0.080
 95:  4  2  2 10   5    3  2  1 10   5      92194.8990  -0.0137  0.010
 96:  4  2  2 10   5    3  2  1 10   4      92194.9190   0.0100  0.010
 97:  4  2  3 10   3    3  2  2 10   3      92196.4270  -0.0031  0.010
 98:  4  2  3 10   3    3  2  2 10   2      92196.4290   0.0051  0.010
 99:  4  2  2 10   4    3  2  1 10   4      92197.5080  -0.0113  0.010
100:  4  2  2 10   4    3  2  1 10   3      92197.5250   0.0029  0.010
101:  4  3  1 10   5    3  3  0 10   5      92200.2740  -0.0183  0.010  -0.0139 0.50
102:  4  3  2 10   5    3  3  1 10   5      92200.2740  -0.0095  0.010  -0.0139 0.50
103:  4  3  2 10   6    3  3  1 10   2      92202.3480   0.0057  0.010
104:  4  2  2 10   6    3  2  1 10   5      92202.3520  -0.0056  0.010
105:  4  3  1 10   3    3  3  0 10   2      92202.3570   0.0059  0.010
106:  4  0  4 10   3    3  0  3 10   3      92204.2860  -0.0212  0.010
107:  4  2  2 10   3    3  2  1 10   2      92204.9620  -0.0043  0.010
108:  4  2  2 10   3    3  2  1 10   3      92204.9690  -0.0040  0.010
109:  4  1  3 10   5    3  1  2 10   5      92797.0700  -0.0030  0.010
110:  4  1  3 10   4    3  1  2 10   3      92810.0870   0.0001  0.010
111:  4  1  3 10   5    3  1  2 10   4      92811.0600   0.0035  0.010
112:  4  1  3 10   3    3  1  2 10   2      92811.9500   0.0022  0.010
113:  4  1  3 10   6    3  1  2 10   5      92812.9280   0.0090  0.010
114:  4  1  3 10   4    3  1  2 10   4      92816.6140  -0.0008  0.020
115:  4  1  3 10   3    3  1  2 10   3      92825.9310  -0.0032  0.020
116: 11  8  3 10  12   10  8  2 10  11     253302.6470  -0.0136  0.025  -0.0137 0.50
117: 11  8  4 10  12   10  8  3 10  11     253302.6470  -0.0136  0.025  -0.0137 0.50
118: 11  8  3 10  11   10  8  2 10  10     253303.5400  -0.0094  0.025  -0.0094 0.50
119: 11  8  4 10  11   10  8  3 10  10     253303.5400  -0.0094  0.025  -0.0094 0.50
120: 11  8  3 10  13   10  8  2 10  12     253308.0800   0.0033  0.025   0.0033 0.50
121: 11  8  4 10  13   10  8  3 10  12     253308.0800   0.0033  0.025   0.0033 0.50
122: 11  8  3 10  10   10  8  2 10   9     253308.9700   0.0047  0.025   0.0048 0.50
123: 11  8  4 10  10   10  8  3 10   9     253308.9700   0.0047  0.025   0.0048 0.50
124: 11  7  4 10  12   10  7  3 10  11     253346.2690  -0.0129  0.025  -0.0130 0.50
125: 11  7  5 10  12   10  7  4 10  11     253346.2690  -0.0129  0.025  -0.0130 0.50
126: 11  7  4 10  11   10  7  3 10  10     253346.9320   0.0249  0.025   0.0250 0.50
127: 11  7  5 10  11   10  7  4 10  10     253346.9320   0.0249  0.025   0.0250 0.50
128: 11  7  4 10  13   10  7  3 10  12     253350.4300   0.0011  0.025   0.0012 0.50
129: 11  7  5 10  13   10  7  4 10  12     253350.4300   0.0011  0.025   0.0012 0.50
130: 11  7  4 10  10   10  7  3 10   9     253351.0910   0.0376  0.025   0.0377 0.50
131: 11  7  5 10  10   10  7  4 10   9     253351.0910   0.0376  0.025   0.0377 0.50
132: 11  6  5 10  12   10  6  4 10  11     253384.7820   0.0183  0.025   0.0183 0.50
133: 11  6  6 10  12   10  6  5 10  11     253384.7820   0.0183  0.025   0.0183 0.50
134: 11  6  5 10  11   10  6  4 10  10     253385.1410  -0.0191  0.025  -0.0191 0.50
135: 11  6  6 10  11   10  6  5 10  10     253385.1410  -0.0191  0.025  -0.0191 0.50
136: 11  6  5 10  13   10  6  4 10  12     253387.8280   0.0175  0.025   0.0175 0.50
137: 11  6  6 10  13   10  6  5 10  12     253387.8280   0.0175  0.025   0.0175 0.50
138: 11  6  5 10  10   10  6  4 10   9     253388.1810  -0.0252  0.025  -0.0253 0.50
139: 11  6  6 10  10   10  6  5 10   9     253388.1810  -0.0252  0.025  -0.0253 0.50
140: 11  5  6 10  11   10  5  5 10  10     253418.6790  -0.1084  0.025  -0.0022 0.24
141: 11  5  6 10  12   10  5  5 10  11     253418.6790   0.0945  0.025  -0.0022 0.26
142: 11  5  7 10  11   10  5  6 10  10     253418.6790  -0.1083  0.025  -0.0022 0.24
143: 11  5  7 10  12   10  5  6 10  11     253418.6790   0.0945  0.025  -0.0022 0.26
144: 11  5  6 10  13   10  5  5 10  12     253420.7910   0.0905  0.025   0.0034 0.28
145: 11  5  6 10  10   10  5  5 10   9     253420.7910  -0.1117  0.025   0.0034 0.22
146: 11  5  7 10  13   10  5  6 10  12     253420.7910   0.0906  0.025   0.0034 0.28
147: 11  5  7 10  10   10  5  6 10   9     253420.7910  -0.1117  0.025   0.0034 0.22
148: 11  2 10 10  11   10  2  9 10  10     253439.9800   0.2598  0.025  -0.0011 0.24
149: 11  2 10 10  12   10  2  9 10  11     253439.9800   0.0930  0.025  -0.0011 0.26
150: 11  2 10 10  13   10  2  9 10  12     253439.9800  -0.2453  0.025  -0.0011 0.29
151: 11  2 10 10  10   10  2  9 10   9     253439.9800  -0.0784  0.025  -0.0011 0.22
152: 11  4  7 10  11   10  4  6 10  10     253448.9790  -0.0462  0.025  -0.0194 0.24
153: 11  4  7 10  12   10  4  6 10  11     253448.9790  -0.0017  0.025  -0.0194 0.26
154: 11  4  8 10  10   10  4  7 10  10     253448.9790  -0.0391  0.025  -0.0194 0.24
155: 11  4  8 10  12   10  4  7 10  11     253448.9790   0.0054  0.025  -0.0194 0.26
156: 11  4  7 10  13   10  4  6 10  12     253450.3360   0.0009  0.025  -0.0144 0.28
157: 11  4  7 10  10   10  4  6 10   9     253450.3360  -0.0430  0.025  -0.0144 0.22
158: 11  4  8 10  13   10  4  7 10  12     253450.3360   0.0081  0.025  -0.0144 0.28
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159: 11   4   8 10 10    10   4   7 10   9     253450.3360  -0.0359  0.025  -0.0144 0.22
160: 11   3   9 10 11    10   3   8 10 10      253479.0100   0.0316  0.025  -0.0096 0.48
161: 11   3   9 10 12    10   3   8 10 11      253479.0100  -0.0471  0.025  -0.0096 0.52
162: 11   3   9 10 13    10   3   8 10 12      253479.7880  -0.0309  0.025   0.0031 0.57
163: 11   3   9 10 10    10   3   8 10   9     253479.7880   0.0480  0.025   0.0031 0.43
164: 11   3   8 10 11    10   3   7 10 10      253480.8840   0.0168  0.025  -0.0243 0.48
165: 11   3   8 10 12    10   3   7 10 11      253480.8840  -0.0618  0.025  -0.0243 0.52
166: 11   3   8 10 13    10   3   7 10 12      253481.6650  -0.0427  0.025  -0.0086 0.57
167: 11   3   8 10 10    10   3   7 10   9     253481.6650   0.0362  0.025  -0.0086 0.43
168: 11   2   9 10 11    10   2   8 10 10      253627.2360   0.2886  0.025   0.0272 0.24
169: 11   2   9 10 12    10   2   8 10 11      253627.2360   0.1218  0.025   0.0272 0.26
170: 11   2   9 10 13    10   2   8 10 12      253627.2360  -0.2174  0.025   0.0272 0.29
171: 11   2   9 10 10    10   2   8 10   9     253627.2360  -0.0506  0.025   0.0272 0.22
172: 11   1 10 10 11     10   1   9 10 10      255130.7090   0.1471  0.025  -0.0153 0.24
173: 11   1 10 10 12     10   1   9 10 11      255130.7090  -0.0727  0.025  -0.0153 0.26
174: 11   1 10 10 13     10   1   9 10 12      255130.7090  -0.1571  0.025  -0.0153 0.29
175: 11   1 10 10 10     10   1   9 10   9     255130.7090   0.0628  0.025  -0.0153 0.22
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177: 11   2   9 10 10    11   1 11 10 10       262506.4530   0.1161  0.025   0.0239 0.43
178: 11   2   9 10 11    11   1 11 10 11       262507.6890   0.1117  0.025   0.0264 0.48
179: 11   2   9 10 12    11   1 11 10 12       262507.6890  -0.0515  0.025   0.0264 0.52
180: 16   0 16 10 15     15   1 14 10 14       264087.4500  -0.0399  0.025   0.0121 0.23
181: 16   0 16 10 16     15   1 14 10 15       264087.4500   0.1611  0.025   0.0121 0.24
182: 16   0 16 10 17     15   1 14 10 16       264087.4500   0.0702  0.025   0.0121 0.26
183: 16   0 16 10 18     15   1 14 10 17       264087.4500  -0.1308  0.025   0.0121 0.27
184: 12   1 12 10 11     11   1 11 10 10       274594.4200   0.0886  0.025   0.0202 0.22
185: 12   1 12 10 12     11   1 11 10 11       274594.4200   0.1535  0.025   0.0202 0.24
186: 12   1 12 10 13     11   1 11 10 12       274594.4200  -0.0323  0.025   0.0202 0.26
187: 12   1 12 10 14     11   1 11 10 13       274594.4200  -0.0972  0.025   0.0202 0.28
188: 12 11   1 10 13     11 11   0 10 12       276140.3770  -0.0169  0.025  -0.0170 0.50
189: 12 11   2 10 13     11 11   1 10 12       276140.3770  -0.0169  0.025  -0.0170 0.50
190: 12 11   1 10 12     11 11   0 10 11       276141.6790  -0.0127  0.025  -0.0127 0.50
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192: 12 11   1 10 14     11 11   0 10 13       276148.2630  -0.0068  0.025  -0.0069 0.50
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205: 12   9   3 10 13    11   9   2 10 12      276264.6220  -0.0286  0.025  -0.0287 0.50
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212: 12   0 12 10 14     11   0 11 10 13       276266.5900  -0.0859  0.025   0.0045 0.28
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226: 12   7   5 10 12    11   7   4 10 11      276365.6260  -0.2367  0.025  -0.0241 0.24
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228: 12   7   6 10 12    11   7   5 10 11      276365.6260  -0.2367  0.025  -0.0241 0.24
229: 12   7   6 10 13    11   7   5 10 12      276365.6260   0.1713  0.025  -0.0241 0.26
230: 12   7   5 10 11    11   7   4 10 10      276368.7660  -0.2861  0.025  -0.0567 0.22
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232: 12   7   6 10 10    11   7   5 10 10      276368.7660  -0.2861  0.025  -0.0567 0.22
233: 12   7   6 10 14    11   7   5 10 13      276368.7660   0.1214  0.025  -0.0567 0.28
234: 12   6   6 10 12    11   6   5 10 11      276407.6280  -0.1396  0.025  -0.0108 0.24
235: 12   6   6 10 13    11   6   5 10 12      276407.6280   0.1075  0.025  -0.0108 0.26
236: 12   6   7 10 12    11   6   6 10 11      276407.6280  -0.1396  0.025  -0.0108 0.24
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239: 12   6   6 10 14    11   6   5 10 13    276409.9560   0.0918  0.025  -0.0159 0.28
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244: 12   5   8 10 12    11   5   7 10 11    276444.7920  -0.0645  0.025  -0.0067 0.24
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277: 12   1 11 10 14     11   1 10 10 13     278299.9320  -0.0909  0.025   0.0267 0.28
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332: 13   5   9 10 13    12   5   8 10 12    299467.6370  -0.0341  0.025  -0.0053 0.24
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335: 13   5   8 10 15    12   5   7 10 14    299468.9160   0.0214  0.025  -0.0029 0.28
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337: 13   5   9 10 15    12   5   8 10 14    299468.9160   0.0215  0.025  -0.0029 0.28
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366: 14   1 14 10 12     13   1 13 10 12     320299.9150   0.0582  0.025   0.0045 0.22
367: 14   1 14 10 14     13   1 13 10 13     320299.9150   0.0989  0.025   0.0045 0.24
368: 14   1 14 10 15     13   1 13 10 14     320299.9150  -0.0392  0.025   0.0045 0.26
369: 14   1 14 10 16     13   1 13 10 15     320299.9150  -0.0798  0.025   0.0045 0.28
370: 14 13   1 10 15     13 13   0 10 14     321958.4440   0.0054  0.025   0.0054 0.50
371: 14 13   2 10 15     13 13   1 10 14     321958.4440   0.0054  0.025   0.0054 0.50
372: 14 13   1 10 14     13 13   0 10 13     321959.4520   0.0365  0.025   0.0365 0.50
373: 14 13   2 10 14     13 13   1 10 13     321959.4520   0.0365  0.025   0.0365 0.50
374: 14 13   1 10 16     13 13   0 10 15     321965.3610   0.0079  0.025   0.0080 0.50
375: 14 13   2 10 16     13 13   1 10 15     321965.3610   0.0079  0.025   0.0080 0.50
376: 14 13   1 10 13     13 13   0 10 12     321966.3700   0.0389  0.025   0.0389 0.50
377: 14 13   2 10 13     13 13   1 10 12     321966.3700   0.0389  0.025   0.0389 0.50
378: 14 12   2 10 15     13 12   1 10 14     322047.8950  -0.0325  0.025  -0.0326 0.50
379: 14 12   3 10 15     13 12   2 10 14     322047.8950  -0.0325  0.025  -0.0326 0.50
380: 14 12   2 10 14     13 12   1 10 13     322048.7520   0.0132  0.025   0.0132 0.50
381: 14 12   3 10 14     13 12   2 10 13     322048.7520   0.0132  0.025   0.0132 0.50
382: 14 12   2 10 16     13 12   1 10 15     322053.7960  -0.0233  0.025  -0.0234 0.50
383: 14 12   3 10 16     13 12   2 10 15     322053.7960  -0.0233  0.025  -0.0234 0.50
384: 14 12   2 10 13     13 12   1 10 12     322054.6640   0.0328  0.025   0.0329 0.50
385: 14 12   3 10 13     13 12   2 10 12     322054.6640   0.0328  0.025   0.0329 0.50
386: 14 11   3 10 15     13 11   2 10 14     322130.4600  -0.0399  0.025  -0.0400 0.50
387: 14 11   4 10 15     13 11   3 10 14     322130.4600  -0.0399  0.025  -0.0400 0.50
388: 14 11   3 10 14     13 11   2 10 13     322131.1900   0.0313  0.025   0.0313 0.50
389: 14 11   4 10 14     13 11   3 10 13     322131.1900   0.0313  0.025   0.0313 0.50
390: 14 11   3 10 16     13 11   2 10 15     322135.4220  -0.0289  0.025  -0.0289 0.50
391: 14 11   4 10 16     13 11   3 10 15     322135.4220  -0.0289  0.025  -0.0289 0.50
392: 14 11   3 10 13     13 11   2 10 12     322136.1530   0.0433  0.025   0.0433 0.50
```

7

```
393: 14 11   4 10 13    13 11   3 10 12       322136.1530    0.0433  0.025   0.0433 0.50
394: 14  0  14 10 13    13  0  13 10 12       322172.4680    0.0835  0.025   0.0052 0.22
395: 14  0  14 10 14    13  0  13 10 13       322172.4680    0.0823  0.025   0.0052 0.24
396: 14  0  14 10 15    13  0  13 10 14       322172.4680   -0.0626  0.025   0.0052 0.26
397: 14  0  14 10 16    13  0  13 10 15       322172.4680   -0.0614  0.025   0.0052 0.28
398: 14 10   4 10 15    13 10   3 10 14       322206.1750   -0.0078  0.025  -0.0078 0.50
399: 14 10   5 10 15    13 10   4 10 14       322206.1750   -0.0078  0.025  -0.0078 0.50
400: 14 10   4 10 14    13 10   3 10 13       322206.6710   -0.0312  0.025  -0.0312 0.50
401: 14 10   5 10 14    13 10   4 10 13       322206.6710   -0.0312  0.025  -0.0312 0.50
402: 14 10   4 10 16    13 10   3 10 15       322210.2700   -0.0046  0.025  -0.0046 0.50
403: 14 10   5 10 16    13 10   4 10 15       322210.2700   -0.0046  0.025  -0.0046 0.50
404: 14 10   4 10 13    13 10   3 10 12       322210.7720   -0.0218  0.025  -0.0218 0.50
405: 14 10   5 10 13    13 10   4 10 12       322210.7720   -0.0218  0.025  -0.0218 0.50
406: 14  9   5 10 14    13  9   4 10 13       322275.2020   -0.2259  0.025  -0.0223 0.24
407: 14  9   5 10 15    13  9   4 10 14       322275.2020    0.1672  0.025  -0.0223 0.26
408: 14  9   6 10 14    13  9   5 10 13       322275.2020   -0.2259  0.025  -0.0223 0.24
409: 14  9   6 10 15    13  9   5 10 14       322275.2020    0.1672  0.025  -0.0223 0.26
410: 14  9   5 10 13    13  9   4 10 12       322278.4670   -0.2750  0.025  -0.0575 0.22
411: 14  9   5 10 16    13  9   4 10 15       322278.4670    0.1178  0.025  -0.0575 0.28
412: 14  9   6 10 13    13  9   5 10 12       322278.4670   -0.2750  0.025  -0.0575 0.22
413: 14  9   6 10 16    13  9   5 10 15       322278.4670    0.1178  0.025  -0.0575 0.28
414: 14  8   6 10 14    13  8   5 10 13       322337.3170   -0.1337  0.025   0.0115 0.24
415: 14  8   6 10 15    13  8   5 10 14       322337.3170    0.1466  0.025   0.0115 0.26
416: 14  8   7 10 14    13  8   6 10 13       322337.3170   -0.1337  0.025   0.0115 0.24
417: 14  8   7 10 15    13  8   6 10 14       322337.3170    0.1466  0.025   0.0115 0.26
418: 14  8   6 10 13    13  8   5 10 12       322339.9270   -0.1422  0.025   0.0129 0.22
419: 14  8   6 10 16    13  8   5 10 15       322339.9270    0.1377  0.025   0.0129 0.28
420: 14  8   7 10 13    13  8   6 10 12       322339.9270   -0.1422  0.025   0.0129 0.22
421: 14  8   7 10 16    13  8   6 10 15       322339.9270    0.1377  0.025   0.0129 0.28
422: 14  7   7 10 14    13  7   6 10 13       322392.8880   -0.1047  0.025  -0.0111 0.24
423: 14  7   7 10 15    13  7   6 10 14       322392.8880    0.0760  0.025  -0.0111 0.26
424: 14  7   8 10 14    13  7   7 10 13       322392.8880   -0.1047  0.025  -0.0111 0.24
425: 14  7   8 10 15    13  7   7 10 14       322392.8880    0.0760  0.025  -0.0111 0.26
426: 14  7   7 10 13    13  7   6 10 12       322394.8810   -0.1164  0.025  -0.0166 0.22
427: 14  7   7 10 16    13  7   6 10 15       322394.8810    0.0638  0.025  -0.0166 0.28
428: 14  7   8 10 13    13  7   7 10 12       322394.8810   -0.1164  0.025  -0.0166 0.22
429: 14  7   8 10 16    13  7   7 10 15       322394.8810    0.0638  0.025  -0.0166 0.28
430: 14  6   8 10 14    13  6   7 10 13       322442.4420   -0.0618  0.025  -0.0129 0.24
431: 14  6   8 10 15    13  6   7 10 14       322442.4420    0.0325  0.025  -0.0129 0.26
432: 14  6   9 10 14    13  6   8 10 13       322442.4420   -0.0618  0.025  -0.0129 0.24
433: 14  6   9 10 15    13  6   8 10 14       322442.4420    0.0325  0.025  -0.0129 0.26
434: 14  6   8 10 13    13  6   7 10 12       322443.9150   -0.0616  0.025  -0.0096 0.22
435: 14  6   8 10 16    13  6   7 10 15       322443.9150    0.0323  0.025  -0.0096 0.28
436: 14  6   9 10 13    13  6   8 10 12       322443.9150   -0.0616  0.025  -0.0096 0.22
437: 14  6   9 10 16    13  6   8 10 15       322443.9150    0.0323  0.025  -0.0096 0.28
438: 14  2  13 10 13    13  2  12 10 12       322482.2510   -0.0249  0.025  -0.0068 0.22
439: 14  2  13 10 14    13  2  12 10 13       322482.2510    0.1385  0.025  -0.0068 0.24
440: 14  2  13 10 15    13  2  12 10 14       322482.2510    0.0202  0.025  -0.0068 0.26
441: 14  2  13 10 16    13  2  12 10 15       322482.2510   -0.1432  0.025  -0.0068 0.28
442: 14  5   9 10 14    13  5   8 10 13       322486.9610   -0.0173  0.025  -0.0063 0.24
443: 14  5   9 10 15    13  5   8 10 14       322486.9610    0.0039  0.025  -0.0063 0.26
444: 14  5  10 10 14    13  5   9 10 13       322486.9610   -0.0172  0.025  -0.0063 0.24
445: 14  5  10 10 15    13  5   9 10 14       322486.9610    0.0040  0.025  -0.0063 0.26
446: 14  5   9 10 13    13  5   8 10 12       322488.0030    0.0017  0.025   0.0135 0.22
447: 14  5   9 10 16    13  5   8 10 15       322488.0030    0.0227  0.025   0.0135 0.28
448: 14  5  10 10 13    13  5   9 10 12       322488.0030    0.0019  0.025   0.0135 0.22
449: 14  5  10 10 16    13  5   9 10 15       322488.0030    0.0229  0.025   0.0135 0.28
450: 14  4  10 10 14    13  4   9 10 13       322528.9620   -0.0223  0.025  -0.0220 0.24
451: 14  4  10 10 15    13  4   9 10 14       322528.9620   -0.0608  0.025  -0.0220 0.26
452: 14  4  11 10 14    13  4  10 10 13       322528.9620    0.0181  0.025  -0.0220 0.24
453: 14  4  11 10 15    13  4  10 10 14       322528.9620   -0.0203  0.025  -0.0220 0.26
454: 14  4  10 10 13    13  4   9 10 12       322529.6920    0.0530  0.025   0.0518 0.22
455: 14  4  10 10 16    13  4   9 10 15       322529.6920    0.0142  0.025   0.0518 0.28
456: 14  4  11 10 13    13  4  10 10 12       322529.6920    0.0935  0.025   0.0518 0.22
457: 14  4  11 10 16    13  4  10 10 15       322529.6920    0.0547  0.025   0.0518 0.28
458: 14  3  12 10 13    13  3  11 10 12       322573.9230   -0.0897  0.025   0.0483 0.22
459: 14  3  12 10 14    13  3  11 10 13       322573.9230    0.2786  0.025   0.0483 0.24
460: 14  3  12 10 15    13  3  11 10 14       322573.9230    0.1935  0.025   0.0483 0.26
461: 14  3  12 10 16    13  3  11 10 15       322573.9230   -0.1749  0.025   0.0483 0.28
462: 14  3  11 10 13    13  3  10 10 12       322580.3010   -0.1120  0.025   0.0261 0.22
463: 14  3  11 10 14    13  3  10 10 13       322580.3010    0.2563  0.025   0.0261 0.24
464: 14  3  11 10 15    13  3  10 10 14       322580.3010    0.1712  0.025   0.0261 0.26
465: 14  3  11 10 16    13  3  10 10 15       322580.3010   -0.1972  0.025   0.0261 0.28
466: 14  2  12 10 13    13  2  11 10 12       322867.4800   -0.0170  0.025   0.0016 0.22
467: 14  2  12 10 14    13  2  11 10 13       322867.4800    0.1475  0.025   0.0016 0.24
468: 14  2  12 10 15    13  2  11 10 14       322867.4800    0.0292  0.025   0.0016 0.26
469: 14  2  12 10 16    13  2  11 10 15       322867.4800   -0.1354  0.025   0.0016 0.28
470: 14  1  13 10 13    13  1  12 10 12       324618.2210    0.0561  0.025   0.0021 0.22
```

```
471: 14  1 13 10 14    13  1 12 10 13       324618.2210   0.0967  0.025   0.0021 0.24
472: 14  1 13 10 15    13  1 12 10 14       324618.2210  -0.0417  0.025   0.0021 0.26
473: 14  1 13 10 16    13  1 12 10 15       324618.2210  -0.0823  0.025   0.0021 0.28
-------------------------------------------------------------------------------------=========
   3 Lines rejected from fit


PARAMETERS IN FIT (values truncated and Nlines statistics):

       1000000           A  /MHz        95426.0587(24)                      1
      -1001010           .  /MHz        95426.0587(24)        =  1.00000 *  1
       2000000           B  /MHz        11679.70195(18)                     2
      -2001010           .  /MHz        11679.70195(18)       =  1.00000 *  2
       3000000           C  /MHz        11370.06627(18)                     3
      -3001010           .  /MHz        11370.06627(18)       =  1.00000 *  3
         20000      Delta_J  /kHz           12.66567(43)                    4
        -21010           .  /kHz           12.66567(43)       =  1.00000 *  4
        110000     Delta_JK  /kHz          127.1323(17)                     5
       -111010           .  /kHz          127.1323(17)        =  1.00000 *  5
        200000      Delta_K  /kHz          959.74(19)                       6
       -201010           .  /kHz          959.74(19)          =  1.00000 *  6
       4010000      delta_J  /kHz            0.310662(41)                   7
      -4011010           .  /kHz            0.310662(41)       =  1.00000 *  7
       4100000      delta_K  /kHz           60.346(24)                      8
      -4101010           .  /kHz           60.346(24)          =  1.00000 *  8
         30000        Phi_J  /Hz       [-0.002427853123]                    9
        -31010           .  /Hz       [-0.002427853123]       =  1.00000 *  9
        120000       Phi_JK  /Hz       [ 0.332733965]                      10
       -121010           .  /Hz       [ 0.332733965]          =  1.00000 * 10
        210000       Phi_KJ  /Hz       [ 2.649427203]                      11
       -211010           .  /Hz       [ 2.649427203]          =  1.00000 * 11
        300000        Phi_K  /Hz       [31.602872]                         12
       -301010           .  /Hz       [31.602872]             =  1.00000 * 12
       4020000        phi_J  /Hz       [ 0.000160615029]                   13
      -4021010           .  /Hz       [ 0.000160615029]       =  1.00000 * 13
       4110000       phi_JK  /Hz       [ 0.267288418]                      14
      -4111010           .  /Hz       [ 0.267288418]          =  1.00000 * 14
       4200000        phi_K  /Hz       [23.8537]                           15
      -4201010           .  /Hz       [23.8537]               =  1.00000 * 15

    11001001010       X_aa  /MHz          -74.469(15)                      16
   -11003001010       X_cc  /MHz           74.469(15)         = -1.00000 * 16
    11002001010       X_bb  /MHz           37.324(24)                      17
   -11003001010       X_cc  /MHz          -37.324(24)         = -1.00000 * 17


 MICROWAVE AVG =       -0.016000 MHz, IR AVG =         0.00000
 MICROWAVE RMS =        0.148567 MHz, IR RMS =         0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.94172          0.94172

   distinct frequency lines in fit:   212
        distinct parameters of fit:    10
          lines rejected from fit:     3   (ERRTST =  3.00E+00)

MICROWAVE        lines fitted        lines    lines      RMS       RMS ERROR    J range  Ka range
freq. range
           total   dv=0  dv.ne.0    UNFITTD   e>900
v"= 0        30     30      0          2        0      0.388879    1.13912    1  34    0   5
27921   46406
v"=10       182    182      0          1        0      0.027943    0.90450    1  20    0  13
28537   324618
----------------------------------------------------------------------------------------------
total:      212    212      0          3        0      0.148561    0.94126

NOTE: the RMS values above are for Nlines statistics, but the 'total' values may differ slightly
from
     those in the .FIT file since the o-c values for this evaluation are as rounded in the .FIT.


 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
 (values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

       1000000           A  /MHz        95426.0588(23)                      1
      -1001010           .  /MHz        95426.0588(23)        =  1.00000 *  1
       2000000           B  /MHz        11679.70196(17)                     2
      -2001010           .  /MHz        11679.70196(17)       =  1.00000 *  2
       3000000           C  /MHz        11370.06627(17)                     3
      -3001010           .  /MHz        11370.06627(17)       =  1.00000 *  3
         20000      Delta_J  /kHz           12.66567(41)                    4
        -21010           .  /kHz           12.66567(41)       =  1.00000 *  4
```

9

```
       110000      Delta_JK  /kHz        127.1323(16)                            5
      -111010         .      /kHz        127.1323(16)        =  1.00000 *  5
       200000      Delta_K   /kHz        959.74(19)                              6
      -201010         .      /kHz        959.74(19)          =  1.00000 *  6
      4010000      delta_J   /kHz          0.310662(40)                          7
     -4011010         .      /kHz          0.310662(40)      =  1.00000 *  7
      4100000      delta_K   /kHz         60.346(23)                             8
     -4101010         .      /kHz         60.346(23)         =  1.00000 *  8
        30000      Phi_J     /Hz         [-0.002427853123]                       9
       -31010         .      /Hz         [-0.002427853123]  =  1.00000 *  9
       120000      Phi_JK    /Hz         [ 0.332733965]                         10
      -121010         .      /Hz         [ 0.332733965]      =  1.00000 * 10
       210000      Phi_KJ    /Hz         [ 2.649427203]                         11
      -211010         .      /Hz         [ 2.649427203]      =  1.00000 * 11
       300000      Phi_K     /Hz         [31.602872]                            12
      -301010         .      /Hz         [31.602872]         =  1.00000 * 12
      4020000      phi_J     /Hz         [ 0.000160615029]                      13
     -4021010         .      /Hz         [ 0.000160615029]   =  1.00000 * 13
      4110000      phi_JK    /Hz         [ 0.267288418]                         14
     -4111010         .      /Hz         [ 0.267288418]      =  1.00000 * 14
      4200000      phi_K     /Hz         [23.8537]                              15
     -4201010         .      /Hz         [23.8537]           =  1.00000 * 15

   11001001010       X_aa    /MHz        -74.469(14)                            16
  -11003001010       X_cc    /MHz         74.469(14)         = -1.00000 * 16
   11002001010       X_bb    /MHz         37.325(23)                            17
  -11003001010       X_cc    /MHz        -37.325(23)         = -1.00000 * 17


  CORRELATION COEFFICIENTS, C.ij:

            A         B         C       -Delta_J -Delta_J -Delta_K -delta_J -delta_K

A         1.0000
B         0.4479    1.0000
C         0.6306    0.6733    1.0000
-Delta_J -0.4934   -0.6598   -0.6383    1.0000
-Delta_JK -0.1529  -0.3326   -0.3791   -0.1437   1.0000
-Delta_K -0.6293   -0.4689   -0.5327    0.9245  -0.3364   1.0000
-delta_J  0.3683   -0.1360    0.2348   -0.1271   0.1160  -0.2144   1.0000
-delta_K -0.1129   -0.2590    0.1818    0.1289  -0.1445   0.1012  -0.4324   1.0000
X_aa     -0.0069   -0.0123   -0.0113    0.0074   0.0090   0.0046   0.0014  -0.0001
X_bb      0.0040    0.0245    0.0157   -0.0134  -0.0114  -0.0067  -0.0123   0.0016


          X_aa      X_bb

X_aa      1.0000
X_bb     -0.3569    1.0000

 Mean value of |C.ij|, i.ne.j =   0.2333
 Mean value of  C.ij,  i.ne.j =  -0.0611


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

    59:    -2.6        354:    2.5         50:    -2.5         36:    -2.4
   410:    -2.3        230:   -2.3        352:    -2.2          1:     2.2
   106:    -2.1         48:    2.1        454:     2.1        310:    -2.0
   458:     1.9        264:    1.9        350:     1.8         37:    -1.8
   224:     1.8        392:    1.7        220:     1.7         66:     1.7
    39:     1.6        386:   -1.6        376:     1.6        356:    -1.5
   284:     1.5        130:    1.5        372:     1.5        292:     1.4
   304:     1.4        268:    1.4        286:    -1.4        101:    -1.4
    95:    -1.4        266:   -1.3        384:     1.3        378:    -1.3
    27:    -1.3        388:    1.3        400:    -1.2        390:    -1.2
   205:    -1.1         49:   -1.1         19:     1.1         99:    -1.1
    15:     1.1          3:    1.1        168:     1.1        280:     1.1
   274:     1.1        178:    1.1


   59: 28  1 28  0 28   28  0 28  0 28      37983.7950  -0.0529  0.020
  354: 13  3 10 10 13   12  3  9 10 12     299549.3460   0.1079  0.025   0.0623 0.48
   50: 27  3 24  0 27   26  4 22  0 26      36580.5870  -0.0491  0.020
   36:  2  0  2  0  2    1  0  1  0  1      46097.8000  -0.4767  0.200
  410: 14  9  5 10 13   13  9  4 10 12     322278.4670  -0.2750  0.025  -0.0575 0.22
  230: 12  7  5 10 11   11  7  4 10 10     276368.7660  -0.2861  0.025  -0.0567 0.22
  352: 13  3 11 10 12   12  3 10 10 11     299545.2900  -0.0056  0.025  -0.0548 0.44
```

10

```
    1:  5  0  5 10  7     4  1  3 10  6        29771.6170  -0.1104  0.020   0.0432 0.50
  106:  4  0  4 10  3     3  0  3 10  3        92204.2860  -0.0212  0.010
   48: 23  4 19  0 23    24  3 21  0 24        33108.9480   0.0421  0.020
```
/ SPFIT output reformatted with PIFORM

Table S.2. Fit of the rotational transitions of $^{12}CHD_2^{37}Cl$ in PIFORM format

```
chd2cl -- 37cl                                    Tue Mar 18 09:41:13 2025


----------------------------------------------------------------------=========
                                        obs       o-c    error    blends   Notes
                                                                  o-c    wt
    / instead of : below denotes (o-c)>3*err
----------------------------------------------------------------------=========
!Mallinson-TableII
   1:  1  0  1 10  3    0  0  0 10  2     22673.8000   0.2004  0.090
!Mallinson-TableII
   2:  1  0  1 10  2    0  0  0 10  2     22659.2900   0.367 UNFITTD   22658.9229
!Mallinson-TableII
   3:  1  0  1 10  1    0  0  0 10  2     22685.6000   0.2563  0.090
!Mallinson-TableII
   4:  5  0  5 10  6    4  1  3 10  5     27737.9070   0.1022  0.161   0.2271 0.50
!Mallinson-TableII
   5:  5  0  5 10  5    4  1  3 10  4     27737.9070   0.3519  0.161   0.2271 0.50
!Mallinson-TableII
   6:  5  0  5 10  7    4  1  3 10  6     27739.7370  -0.2263  0.161  -0.1009 0.50
!Mallinson-TableII
   7:  5  0  5 10  4    4  1  3 10  3     27739.7370   0.0244  0.161  -0.1009 0.50
!Mallinson-TableII
   8:  9  2  8 10  8   10  1 10 10  9     33848.3030  -0.0142  0.110  -0.0247 0.50
!Mallinson-TableII
   9:  9  2  8 10 11   10  1 10 10 12     33848.3030  -0.0351  0.110  -0.0247 0.50
!Mallinson-TableII
  10:  9  2  8 10  9   10  1 10 10 10     33849.6880  -0.1428  0.110  -0.1535 0.50
!Mallinson-TableII
  11:  9  2  8 10 10   10  1 10 10 11     33849.6880  -0.1641  0.110  -0.1535 0.50
!Mallinson-TableV
  12:  1  0  1  0  1    0  0  0  0  0     22670.9400   0.277 UNFITTD   22670.6627
!Mallinson-TableV
  13:  5  0  5  0  5    4  1  3  0  4     27738.9920   0.1215  0.161
!Mallinson-TableV
  14:  9  2  8  0  9   10  1 10  0 10     33848.9870  -0.0884  0.110
!Mallinson-TableV
  15: 12  1 11  0 12   11  2  9  0 11     30739.6280   0.0268  0.050
!Mallinson-TableV
  16: 13  1 13  0 13   12  2 11  0 12     28664.1200  -0.1252  0.050
!Mallinson-TableV
  17: 16  3 13  0 16   17  2 15  0 17     32840.6690   0.0661  0.050
!Mallinson-TableV
  18: 16  3 14  0 16   17  2 16  0 17     35866.0620   0.231 UNFITTD   35865.8302
!Mallinson-TableV
  19: 20  2 18  0 20   19  3 16  0 19     36980.9920   0.0529  0.050
!Mallinson-TableV
  20: 20  2 19  0 20   19  3 17  0 19     31346.8190  -0.0075  0.050
!Mallinson-TableV
  21: 31  5 27  0 31   32  4 29  0 32     30534.0040  -0.260 UNFITTD   30534.2644
!Mallinson-TableV
  22: 31  5 26  0 31   32  4 28  0 32     30480.7990  -0.0034  0.050
!Mallinson-TableV
  23: 35  4 31  0 35   34  5 29  0 34     37719.5020  -0.0311  0.050
!Mallinson-TableV
  24: 35  4 32  0 35   34  5 30  0 34     37611.6570   0.0326  0.050
!Mallinson-TableV
  25: 13  1 12  0 13   13  1 13  0 13     27206.1010  -0.0081  0.020
!Mallinson-TableV
  26: 14  1 13  0 14   14  1 14  0 14     31384.0340  -0.0111  0.020
!Mallinson-TableV
  27: 15  1 14  0 15   15  1 15  0 15     35857.3680  -0.0214  0.020
!Mallinson-TableV
  28: 28  1 28  0 28   28  0 28  0 28     39159.6070  -0.069 UNFITTD   39159.6761
!Mallinson-TableV
  29: 29  1 29  0 29   29  0 29  0 29     37032.7810  -0.0433  0.020
!Mallinson-TableV
  30: 30  1 30  0 30   30  0 30  0 30     34956.2310  -0.0166  0.020
!Mallinson-TableV
  31: 30  2 28  0 30   30  2 29  0 30     26635.4680   0.0324  0.020
!Mallinson-TableV
  32: 31  1 31  0 31   31  0 31  0 31     32936.0400  -0.0158  0.020
!Mallinson-TableV
  33: 31  2 29  0 31   31  2 30  0 31     30044.1950   0.0147  0.020
!Mallinson-TableV
  34: 32  1 32  0 32   32  0 32  0 32     30977.5940   0.0175  0.020
```

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!Mallinson-TableV
 35: 32   2 30   0 32    32   2 31   0 32       33731.3860  -0.0099  0.020
!Mallinson-TableV
 36: 33   1 33   0 33    33   0 33   0 33       29085.3650   0.0303  0.020
!Mallinson-TableV
 37: 33   2 31   0 33    33   2 32   0 33       37704.0680  -0.0254  0.020
 38:  4   1  4 10  4     3   1  3 10  3         90077.2440  -0.0064  0.010
 39:  4   1  4 10  5     3   1  3 10  4         90078.0080   0.0000  0.010
 40:  4   1  4 10  3     3   1  3 10  2         90078.7100  -0.0076  0.010
 41:  4   1  4 10  6     3   1  3 10  5         90079.4830   0.0067  0.010
 42:  4   0  4 10  5     3   0  3 10  5         90657.4950  -0.0021  0.010
 43:  4   3  1 10  4     3   3  0 10  4         90661.6450  -0.0078  0.010  -0.0039 0.50
 44:  4   3  2 10  4     3   3  1 10  4         90661.6450   0.0000  0.010  -0.0039 0.50
 45:  4   3  1 10  5     3   3  0 10  4         90663.4580   0.0016  0.010   0.0056 0.50
 46:  4   3  2 10  5     3   3  1 10  4         90663.4580   0.0095  0.010   0.0056 0.50
 47:  4   3  1 10  3     3   3  0 10  3         90665.0790  -0.0040  0.010  -0.0000 0.50
 48:  4   3  2 10  3     3   3  1 10  3         90665.0790   0.0039  0.010  -0.0000 0.50
 49:  4   3  1 10  4     3   3  0 10  3         90670.2220   0.0054  0.010   0.0094 0.50
 50:  4   3  2 10  4     3   3  1 10  3         90670.2220   0.0133  0.010   0.0094 0.50
 51:  4   0  4 10  4     3   0  3 10  3         90670.4580  -0.0124  0.010  -0.0125 0.50
 52:  4   0  4 10  3     3   0  3 10  2         90670.4580  -0.0125  0.010  -0.0125 0.50
 53:  4   2  3 10  5     3   2  2 10  4         90671.4130   0.0043  0.010   0.0030 0.50
 54:  4   2  3 10  5     3   2  2 10  5         90671.4130   0.0016  0.010   0.0030 0.50
 55:  4   0  4 10  6     3   0  3 10  5         90672.1740   0.0002  0.010   0.0001 0.50
 56:  4   0  4 10  5     3   0  3 10  4         90672.1740  -0.0000  0.010   0.0001 0.50
 57:  4   2  3 10  4     3   2  2 10  3         90673.4720   0.0035  0.010   0.0045 0.50
 58:  4   2  3 10  4     3   2  2 10  4         90673.4720   0.0053  0.010   0.0045 0.50
 59:  4   3  1 10  6     3   3  0 10  5         90676.6600  -0.0051  0.010  -0.0012 0.50
 60:  4   3  2 10  6     3   3  1 10  5         90676.6600   0.0027  0.010  -0.0012 0.50
 61:  4   2  3 10  6     3   2  2 10  5         90677.2970   0.0163  0.010  -0.0044 0.50
 62:  4   0  4 10  4     3   0  3 10  4         90677.2970  -0.0252  0.010  -0.0044 0.50
 63:  4   2  2 10  5     3   2  1 10  4         90679.3690  -0.0153  0.010   0.0065 0.25
 64:  4   2  3 10  3     3   2  2 10  2         90679.3690   0.0313  0.010   0.0065 0.25
 65:  4   2  2 10  5     3   2  1 10  5         90679.3690  -0.0174  0.010   0.0065 0.25
 66:  4   2  3 10  3     3   2  2 10  3         90679.3690   0.0273  0.010   0.0065 0.25
 67:  4   2  2 10  4     3   2  1 10  3         90681.4370  -0.0072  0.010  -0.0065 0.50
 68:  4   2  2 10  4     3   2  1 10  4         90681.4370  -0.0056  0.010  -0.0065 0.50
 69:  4   3  1 10  3     3   3  0 10  2         90683.4220  -0.0059  0.010  -0.0019 0.50
 70:  4   3  2 10  3     3   3  1 10  2         90683.4220   0.0020  0.010  -0.0019 0.50
 71:  4   0  4 10  3     3   0  3 10  3         90685.2450   0.0983  0.010  -0.0021 0.09
 72:  4   2  2 10  6     3   2  1 10  5         90685.2450  -0.0117  0.010  -0.0021 0.91
 73:  4   2  2 10  3     3   2  1 10  2         90687.3080  -0.0059  0.010  -0.0082 0.50
 74:  4   2  2 10  3     3   2  1 10  3         90687.3080  -0.0104  0.010  -0.0082 0.50
 75:  4   1  3 10  4     3   1  2 10  3         91274.2850   0.0011  0.010
 76:  4   1  3 10  5     3   1  2 10  4         91275.0590   0.0078  0.010
 77:  4   1  3 10  3     3   1  2 10  2         91275.7490  -0.0020  0.010
 78:  4   1  3 10  6     3   1  2 10  5         91276.5200   0.0006  0.010
 79: 11   1 11 10 11    10   1 10 10 10        247623.4850   0.1132  0.025  -0.0143 0.24
 80: 11   1 11 10 12    10   1 10 10 11        247623.4850  -0.0593  0.025  -0.0143 0.26
 81: 11   1 11 10 13    10   1 10 10 12        247623.4850  -0.1258  0.025  -0.0143 0.29
 82: 11   1 11 10 10    10   1 10 10  9        247623.4850   0.0468  0.025  -0.0143 0.22
 83: 11  10  1 10 13    10  10  0 10 12        249047.5800   0.0403  0.025   0.0404 0.50
 84: 11  10  2 10 13    10  10  1 10 12        249047.5800   0.0403  0.025   0.0404 0.50
 85: 11  10  1 10 10    10  10  0 10  9        249048.7660   0.0260  0.025   0.0261 0.50
 86: 11  10  2 10 10    10  10  1 10  9        249048.7660   0.0260  0.025   0.0261 0.50
 87: 11   9  2 10 12    10   9  1 10 11        249093.4950   0.0170  0.025   0.0171 0.50
 88: 11   9  3 10 12    10   9  2 10 11        249093.4950   0.0170  0.025   0.0171 0.50
 89: 11   9  2 10 11    10   9  1 10 10        249094.4310   0.0169  0.025   0.0169 0.50
 90: 11   9  3 10 11    10   9  2 10 10        249094.4310   0.0169  0.025   0.0169 0.50
 91: 11   9  2 10 13    10   9  1 10 12        249098.8850   0.0031  0.025   0.0031 0.50
 92: 11   9  3 10 13    10   9  2 10 12        249098.8850   0.0031  0.025   0.0031 0.50
 93: 11   9  2 10 10    10   9  1 10  9        249099.8220   0.0036  0.025   0.0036 0.50
 94: 11   9  3 10 10    10   9  2 10  9        249099.8220   0.0036  0.025   0.0036 0.50
 95: 11   0 11 10 11    10   0 10 10 10        249137.6080   0.0939  0.025  -0.0076 0.24
 96: 11   0 11 10 12    10   0 10 10 11        249137.6080  -0.0931  0.025  -0.0076 0.26
 97: 11   0 11 10 13    10   0 10 10 12        249137.6080  -0.0919  0.025  -0.0076 0.29
 98: 11   0 11 10 10    10   0 10 10  9        249137.6080   0.0951  0.025  -0.0076 0.22
 99: 11   8  3 10 12    10   8  2 10 11        249140.7960  -0.0123  0.025  -0.0124 0.50
100: 11   8  4 10 12    10   8  3 10 11        249140.7960  -0.0123  0.025  -0.0124 0.50
101: 11   8  3 10 11    10   8  2 10 10        249141.5210   0.0119  0.025   0.0120 0.50
102: 11   8  4 10 11    10   8  3 10 10        249141.5210   0.0119  0.025   0.0120 0.50
103: 11   8  3 10 13    10   8  2 10 12        249145.0630  -0.0153  0.025  -0.0154 0.50
104: 11   8  4 10 13    10   8  3 10 12        249145.0630  -0.0153  0.025  -0.0154 0.50
105: 11   8  3 10 10    10   8  2 10  9        249145.7920   0.0131  0.025   0.0131 0.50
106: 11   8  4 10 10    10   8  3 10  9        249145.7920   0.0131  0.025   0.0131 0.50
107: 11   7  4 10 12    10   7  3 10 11        249182.9300  -0.0245  0.025  -0.0246 0.50
108: 11   7  5 10 12    10   7  4 10 11        249182.9300  -0.0245  0.025  -0.0246 0.50
109: 11   7  4 10 11    10   7  3 10 10        249183.4730   0.0256  0.025   0.0257 0.50
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13

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110: 11   7   5 10 11     10   7   4 10 10      249183.4730   0.0256   0.025    0.0257 0.50
111: 11   7   4 10 13     10   7   3 10 12      249186.2180  -0.0058   0.025   -0.0059 0.50
112: 11   7   5 10 13     10   7   4 10 12      249186.2180  -0.0058   0.025   -0.0059 0.50
113: 11   7   4 10 10     10   7   3 10  9      249186.7550   0.0387   0.025    0.0387 0.50
114: 11   7   5 10 10     10   7   4 10  9      249186.7550   0.0387   0.025    0.0387 0.50
115: 11   6   5 10 11     10   6   4 10 10      249220.2510  -0.1765   0.025   -0.0131 0.24
116: 11   6   5 10 12     10   6   4 10 11      249220.2510   0.1359   0.025   -0.0131 0.26
117: 11   6   6 10 11     10   6   5 10 10      249220.2510  -0.1765   0.025   -0.0131 0.24
118: 11   6   6 10 12     10   6   5 10 11      249220.2510   0.1359   0.025   -0.0131 0.26
119: 11   6   5 10 13     10   6   4 10 12      249222.6210   0.1039   0.025   -0.0307 0.28
120: 11   6   5 10 10     10   6   4 10  9      249222.6210  -0.2081   0.025   -0.0307 0.22
121: 11   6   6 10 13     10   6   5 10 12      249222.6210   0.1039   0.025   -0.0307 0.28
122: 11   6   6 10 10     10   6   5 10  9      249222.6210  -0.2081   0.025   -0.0307 0.22
123: 11   5   6 10 11     10   5   5 10 10      249252.8010  -0.0947   0.025   -0.0111 0.24
124: 11   5   6 10 12     10   5   5 10 11      249252.8010   0.0651   0.025   -0.0111 0.26
125: 11   5   7 10 11     10   5   6 10 10      249252.8010  -0.0947   0.025   -0.0111 0.24
126: 11   5   7 10 12     10   5   6 10 11      249252.8010   0.0652   0.025   -0.0111 0.26
127: 11   5   6 10 13     10   5   5 10 12      249254.4570   0.0530   0.025   -0.0158 0.28
128: 11   5   6 10 10     10   5   5 10  9      249254.4570  -0.1065   0.025   -0.0158 0.22
129: 11   5   7 10 13     10   5   6 10 12      249254.4570   0.0530   0.025   -0.0158 0.28
130: 11   5   7 10 10     10   5   6 10  9      249254.4570  -0.1065   0.025   -0.0158 0.22
131: 11   2 10 10 11      10   2   9 10 10      249274.7130   0.2252   0.025    0.0196 0.24
132: 11   2 10 10 12      10   2   9 10 11      249274.7130   0.0937   0.025    0.0196 0.26
133: 11   2 10 10 13      10   2   9 10 12      249274.7130  -0.1729   0.025    0.0196 0.29
134: 11   2 10 10 10      10   2   9 10  9      249274.7130  -0.0414   0.025    0.0196 0.22
135: 11   4   7 10 11     10   4   6 10 10      249281.9880  -0.0174   0.025    0.0040 0.24
136: 11   4   7 10 12     10   4   6 10 11      249281.9880   0.0175   0.025    0.0040 0.26
137: 11   4   8 10 11     10   4   7 10 10      249281.9880  -0.0112   0.025    0.0040 0.24
138: 11   4   8 10 12     10   4   7 10 11      249281.9880   0.0238   0.025    0.0040 0.26
139: 11   4   7 10 13     10   4   6 10 12      249283.0540   0.0158   0.025    0.0040 0.28
140: 11   4   7 10 10     10   4   6 10  9      249283.0540  -0.0188   0.025    0.0040 0.22
141: 11   4   8 10 13     10   4   7 10 12      249283.0540   0.0221   0.025    0.0040 0.28
142: 11   4   8 10 10     10   4   7 10  9      249283.0540  -0.0126   0.025    0.0040 0.22
143: 11   3   9 10 11     10   3   8 10 10      249310.7180   0.0318   0.025   -0.0006 0.48
144: 11   3   9 10 12     10   3   8 10 11      249310.7180  -0.0302   0.025   -0.0006 0.52
145: 11   3   9 10 13     10   3   8 10 12      249311.3590   0.0101   0.025    0.0370 0.57
146: 11   3   9 10 10     10   3   8 10  9      249311.3590   0.0723   0.025    0.0370 0.43
147: 11   3   8 10 11     10   3   7 10 10      249312.4080   0.0197   0.025   -0.0128 0.48
148: 11   3   8 10 12     10   3   7 10 11      249312.4080  -0.0423   0.025   -0.0128 0.52
149: 11   3   8 10 13     10   3   7 10 12      249313.0540   0.0029   0.025    0.0298 0.57
150: 11   3   8 10 10     10   3   7 10  9      249313.0540   0.0651   0.025    0.0298 0.43
151: 11   2   9 10 11     10   2   8 10 10      249449.5300   0.1926   0.025   -0.0136 0.24
152: 11   2   9 10 12     10   2   8 10 11      249449.5300   0.0612   0.025   -0.0136 0.26
153: 11   2   9 10 13     10   2   8 10 12      249449.5300  -0.2067   0.025   -0.0136 0.29
154: 11   2   9 10 10     10   2   8 10  9      249449.5300  -0.0752   0.025   -0.0136 0.22
155: 11   1 10 10 11      10   1   9 10 10      250910.9680   0.1498   0.025    0.0217 0.24
156: 11   1 10 10 12      10   1   9 10 11      250910.9680  -0.0238   0.025    0.0217 0.26
157: 11   1 10 10 13      10   1   9 10 12      250910.9680  -0.0902   0.025    0.0217 0.29
158: 11   1 10 10 10      10   1   9 10  9      250910.9680   0.0834   0.025    0.0217 0.22
159: 12   1 12 10 11      11   1 11 10 10       270112.7690   0.0360   0.025   -0.0179 0.22
160: 12   1 12 10 12      11   1 11 10 11       270112.7690   0.0870   0.025   -0.0179 0.24
161: 12   1 12 10 13      11   1 11 10 12       270112.7690  -0.0592   0.025   -0.0179 0.26
162: 12   1 12 10 14      11   1 11 10 13       270112.7690  -0.1102   0.025   -0.0179 0.28
163: 12 10   2 10 13      11 10   1 10 12       271669.1440   0.0103   0.025    0.0103 0.50
164: 12 10   3 10 13      11 10   2 10 12       271669.1440   0.0103   0.025    0.0103 0.50
165: 12 10   2 10 12      11 10   1 10 11       271669.9610   0.0085   0.025    0.0086 0.50
166: 12 10   3 10 12      11 10   2 10 11       271669.9610   0.0085   0.025    0.0086 0.50
167: 12 10   2 10 14      11 10   1 10 13       271674.2690   0.0033   0.025    0.0034 0.50
168: 12 10   3 10 14      11 10   2 10 13       271674.2690   0.0033   0.025    0.0034 0.50
169: 12 10   2 10 11      11 10   1 10 10       271675.0940   0.0092   0.025    0.0093 0.50
170: 12 10   3 10 11      11 10   2 10 10       271675.0940   0.0092   0.025    0.0093 0.50
171: 12   9   3 10 13     11   9   2 10 12      271726.3550  -0.0061   0.025   -0.0062 0.50
172: 12   9   4 10 13     11   9   3 10 12      271726.3550  -0.0061   0.025   -0.0062 0.50
173: 12   9   3 10 12     11   9   2 10 11      271727.0260   0.0312   0.025    0.0312 0.50
174: 12   9   4 10 12     11   9   3 10 11      271727.0260   0.0312   0.025    0.0312 0.50
175: 12   9   3 10 14     11   9   2 10 13      271730.5200   0.0018   0.025    0.0018 0.50
176: 12   9   4 10 14     11   9   3 10 13      271730.5200   0.0018   0.025    0.0018 0.50
177: 12   9   3 10 11     11   9   2 10 10      271731.1970   0.0452   0.025    0.0452 0.50
178: 12   9   4 10 11     11   9   3 10 10      271731.1970   0.0452   0.025    0.0452 0.50
179: 12   0 12 10 11      11   0 11 10 10       271736.6760   0.0922   0.025    0.0067 0.22
180: 12   0 12 10 12      11   0 11 10 11       271736.6760   0.0909   0.025    0.0067 0.24
181: 12   0 12 10 13      11   0 11 10 12       271736.6760  -0.0655   0.025    0.0067 0.26
182: 12   0 12 10 14      11   0 11 10 13       271736.6760  -0.0642   0.025    0.0067 0.28
183: 12   8   4 10 13     11   8   3 10 12      271777.8930   0.0010   0.025    0.0010 0.50
184: 12   8   5 10 13     11   8   4 10 12      271777.8930   0.0010   0.025    0.0010 0.50
185: 12   8   4 10 12     11   8   3 10 11      271778.3900   0.0301   0.025    0.0301 0.50
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233: 12  3   9 10 11    11  3   8 10 10    271969.2560   0.0571  0.025   0.0185 0.44
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253: 13 12   1 10 12    12 12   0 10 11    294157.8990  -0.0393  0.025  -0.0393 0.50
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263: 13 10   3 10 14    12 10   2 10 13    294293.6790  -0.0257  0.025  -0.0258 0.50
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265: 13 10   3 10 13    12 10   2 10 12    294294.3150   0.0371  0.025   0.0371 0.50
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273: 13  0 13 10 14     12  0 12 10 13       294322.8750  -0.0840   0.025   -0.0220 0.26
274: 13  0 13 10 15     12  0 12 10 14       294322.8750  -0.0826   0.025   -0.0220 0.28
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287: 13  8   5 10 12    12  8   4 10 11      294414.1710  -0.1629   0.025    0.0150 0.22
288: 13  8   5 10 15    12  8   4 10 14      294414.1710   0.1558   0.025    0.0150 0.28
289: 13  8   6 10 12    12  8   5 10 11      294414.1710  -0.1629   0.025    0.0150 0.22
290: 13  8   6 10 15    12  8   5 10 14      294414.1710   0.1558   0.025    0.0150 0.28
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309: 13  5   9 10 13    12  5   8 10 12      294544.9230  -0.0392   0.025   -0.0166 0.24
310: 13  5   9 10 14    12  5   8 10 13      294544.9230   0.0044   0.025   -0.0166 0.26
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372: 14   9   5 10 16     13   9   4 10 15      316983.7890    0.1137   0.025   -0.0245 0.28
373: 14   9   6 10 13     13   9   5 10 12      316983.7890   -0.1960   0.025   -0.0245 0.22
374: 14   9   6 10 16     13   9   5 10 15      316983.7890    0.1137   0.025   -0.0245 0.28
375: 14   8   6 10 14     13   8   5 10 13      317041.3360   -0.1002   0.025    0.0143 0.24
376: 14   8   6 10 15     13   8   5 10 14      317041.3360    0.1207   0.025    0.0143 0.26
377: 14   8   7 10 14     13   8   6 10 13      317041.3360   -0.1002   0.025    0.0143 0.24
378: 14   8   7 10 15     13   8   6 10 14      317041.3360    0.1207   0.025    0.0143 0.26
379: 14   8   6 10 13     13   8   5 10 12      317043.3870   -0.1137   0.025    0.0086 0.22
380: 14   8   6 10 16     13   8   5 10 15      317043.3870    0.1070   0.025    0.0086 0.28
381: 14   8   7 10 13     13   8   6 10 12      317043.3870   -0.1137   0.025    0.0086 0.22
382: 14   8   7 10 16     13   8   6 10 15      317043.3870    0.1070   0.025    0.0086 0.28
383: 14   7   7 10 14     13   7   6 10 13      317095.1130   -0.0863   0.025   -0.0125 0.24
384: 14   7   7 10 15     13   7   6 10 14      317095.1130    0.0561   0.025   -0.0125 0.26
385: 14   7   8 10 14     13   7   7 10 13      317095.1130   -0.0863   0.025   -0.0125 0.24
386: 14   7   8 10 15     13   7   7 10 14      317095.1130    0.0561   0.025   -0.0125 0.26
387: 14   7   7 10 13     13   7   6 10 12      317096.6890   -0.0909   0.025   -0.0121 0.22
388: 14   7   7 10 16     13   7   6 10 15      317096.6890    0.0512   0.025   -0.0121 0.28
389: 14   7   8 10 13     13   7   7 10 12      317096.6890   -0.0909   0.025   -0.0121 0.22
390: 14   7   8 10 16     13   7   7 10 15      317096.6890    0.0512   0.025   -0.0121 0.28
391: 14   6   8 10 14     13   6   7 10 13      317143.0490   -0.0311   0.025    0.0074 0.24
392: 14   6   8 10 15     13   6   7 10 14      317143.0490    0.0432   0.025    0.0074 0.26
393: 14   6   9 10 14     13   6   8 10 13      317143.0490   -0.0311   0.025    0.0074 0.24
394: 14   6   9 10 15     13   6   8 10 14      317143.0490    0.0432   0.025    0.0074 0.26
395: 14   6   8 10 13     13   6   7 10 12      317144.2170   -0.0244   0.025    0.0167 0.22
396: 14   6   8 10 16     13   6   7 10 15      317144.2170    0.0497   0.025    0.0167 0.28
397: 14   6   9 10 13     13   6   8 10 12      317144.2170   -0.0244   0.025    0.0167 0.22
398: 14   6   9 10 16     13   6   8 10 15      317144.2170    0.0497   0.025    0.0167 0.28
399: 14   2 13 10 13     13   2 12 10 12      317184.2640   -0.0034   0.025    0.0108 0.22
400: 14   2 13 10 14     13   2 12 10 13      317184.2640    0.1253   0.025    0.0108 0.24
401: 14   2 13 10 15     13   2 12 10 14      317184.2640    0.0320   0.025    0.0108 0.26
402: 14   2 13 10 16     13   2 12 10 15      317184.2640   -0.0967   0.025    0.0108 0.28
403: 14   5   9 10 14     13   5   8 10 13      317185.9930   -0.0131   0.025   -0.0044 0.24
404: 14   5   9 10 15     13   5   8 10 14      317185.9930    0.0036   0.025   -0.0044 0.26
405: 14   5 10 10 14     13   5   9 10 13      317185.9930   -0.0130   0.025   -0.0044 0.24
406: 14   5 10 10 15     13   5   9 10 14      317185.9930    0.0037   0.025   -0.0044 0.26
407: 14   5   9 10 13     13   5   8 10 12      317186.8480    0.0354   0.025    0.0447 0.22
408: 14   5   9 10 16     13   5   8 10 15      317186.8480    0.0519   0.025    0.0447 0.28
409: 14   5 10 10 13     13   5   9 10 12      317186.8480    0.0355   0.025    0.0447 0.22
410: 14   5 10 10 16     13   5   9 10 15      317186.8480    0.0521   0.025    0.0447 0.28
411: 14   4 10 10 14     13   4   9 10 13      317226.3850    0.0123   0.025    0.0142 0.24
412: 14   4 10 10 15     13   4   9 10 14      317226.3850   -0.0180   0.025    0.0142 0.26
413: 14   4 11 10 14     13   4 10 10 13      317226.3850    0.0475   0.025    0.0142 0.24
414: 14   4 11 10 15     13   4 10 10 14      317226.3850    0.0171   0.025    0.0142 0.26
415: 14   4 10 10 13     13   4   9 10 12      317226.9100    0.0211   0.025    0.0219 0.22
416: 14   4 10 10 16     13   4   9 10 15      317226.9100   -0.0093   0.025    0.0219 0.28
417: 14   4 11 10 13     13   4 10 10 12      317226.9100    0.0564   0.025    0.0219 0.22
418: 14   4 11 10 16     13   4 10 10 15      317226.9100    0.0258   0.025    0.0219 0.28
419: 14   3 12 10 13     13   3 11 10 12      317269.2640   -0.0949   0.025    0.0139 0.22
420: 14   3 12 10 14     13   3 11 10 13      317269.2640    0.1955   0.025    0.0139 0.24
421: 14   3 12 10 15     13   3 11 10 14      317269.2640    0.1284   0.025    0.0139 0.26
```

```
 422: 14  3 12 10 16    13  3 11 10 15        317269.2640  -0.1621  0.025   0.0139 0.28
 423: 14  3 11 10 13    13  3 10 10 12        317275.0120  -0.1153  0.025  -0.0064 0.22
 424: 14  3 11 10 14    13  3 10 10 13        317275.0120   0.1751  0.025  -0.0064 0.24
 425: 14  3 11 10 15    13  3 10 10 14        317275.0120   0.1081  0.025  -0.0064 0.26
 426: 14  3 11 10 16    13  3 10 10 15        317275.0120  -0.1824  0.025  -0.0064 0.28
 427: 14  2 12 10 13    13  2 11 10 12        317544.1170  -0.0161  0.025  -0.0012 0.22
 428: 14  2 12 10 14    13  2 11 10 13        317544.1170   0.1141  0.025  -0.0012 0.24
 429: 14  2 12 10 15    13  2 11 10 14        317544.1170   0.0209  0.025  -0.0012 0.26
 430: 14  2 12 10 16    13  2 11 10 15        317544.1170  -0.1094  0.025  -0.0012 0.28
 431: 14  1 13 10 13    13  1 12 10 12        319251.9550   0.0415  0.025  -0.0012 0.22
 432: 14  1 13 10 14    13  1 12 10 13        319251.9550   0.0733  0.025  -0.0012 0.24
 433: 14  1 13 10 15    13  1 12 10 14        319251.9550  -0.0359  0.025  -0.0012 0.26
 434: 14  1 13 10 16    13  1 12 10 15        319251.9550  -0.0678  0.025  -0.0012 0.28
----------------------------------------------------------------------------------=========
    5 Lines rejected from fit

PARAMETERS IN FIT (values truncated and Nlines statistics):

      1000000            A   /MHz        95425.1307(71)                      1
     -1001010            .   /MHz        95425.1307(71)           =  1.00000 *  1
      2000000            B   /MHz        11485.12341(25)                     2
     -2001010            .   /MHz        11485.12341(25)          =  1.00000 *  2
      3000000            C   /MHz        11185.58835(24)                     3
     -3001010            .   /MHz        11185.58835(24)          =  1.00000 *  3
        20000        Delta_J /kHz           12.27402(76)                    4
       -21010            .   /kHz           12.27402(76)          =  1.00000 *  4
       110000        Delta_JK /kHz         123.3619(21)                     5
      -111010            .   /kHz          123.3619(21)           =  1.00000 *  5
       200000        Delta_K /kHz          963.28(39)                       6
      -201010            .   /kHz          963.28(39)             =  1.00000 *  6
      4010000        delta_J /kHz            0.296208(43)                    7
     -4011010            .   /kHz            0.296208(43)          =  1.00000 *  7
      4100000        delta_K /kHz           58.785(24)                      8
     -4101010            .   /kHz           58.785(24)            =  1.00000 *  8
        30000         Phi_J  /Hz         [-0.002322]                        9
       -31010            .   /Hz         [-0.002322]              =  1.00000 *  9
       120000         Phi_JK /Hz         [ 0.346]                          10
      -121010            .   /Hz         [ 0.346]                 =  1.00000 * 10
       210000         Phi_KJ /Hz         [ 2.717]                          11
      -211010            .   /Hz         [ 2.717]                 =  1.00000 * 11
       300000         Phi_K  /Hz         [32.]                             12
      -301010            .   /Hz         [32.]                    =  1.00000 * 12
      4020000         phi_J  /Hz         [ 0.000153]                       13
     -4021010            .   /Hz         [ 0.000153]              =  1.00000 * 13
      4110000         phi_JK /Hz         [ 0.254]                          14
     -4111010            .   /Hz         [ 0.254]                 =  1.00000 * 14
      4200000         phi_K  /Hz         [24.]                             15
     -4201010            .   /Hz         [24.]                    =  1.00000 * 15

   11001001010         X_aa  /MHz          -58.711(22)                     16
  -11003001010         X_cc  /MHz           58.711(22)           = -1.00000 * 16
   11002001010         X_bb  /MHz           29.52(20)                      17
  -11003001010         X_cc  /MHz          -29.52(20)            = -1.00000 * 17

 MICROWAVE AVG =        0.002619 MHz, IR AVG =        0.00000
 MICROWAVE RMS =        0.042450 MHz, IR RMS =        0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=         0.91556         0.91556

   distinct frequency lines in fit:   168
         distinct parameters of fit:    10
           lines rejected from fit:     5     (ERRTST =  3.00E+00)

MICROWAVE        lines fitted      lines    lines      RMS       RMS ERROR   J range  Ka range
freq. range
           total  dv=0 dv.ne.0  UNFITTD  e>900
v"= 0        22    22     0        3       0      0.049779    1.11150      4  35    0   5
26635   37720
v"=10       146   146     0        2       0      0.041222    0.88188      0  14    0  12
22674  319252
------------------------------------------------------------------------------------------
total:      168   168     0        5       0      0.042441    0.91523

NOTE: the RMS values above are for Nlines statistics, but the 'total' values may differ slightly
from
      those in the .FIT file since the o-c values for this evaluation are as rounded in the .FIT.


  PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
```

```
  (values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

       1000000          A    /MHz      95425.1307(67)                            1
      -1001010          .    /MHz      95425.1307(67)              =  1.00000 *  1
       2000000          B    /MHz      11485.12342(23)                           2
      -2001010          .    /MHz      11485.12342(23)             =  1.00000 *  2
       3000000          C    /MHz      11185.58835(23)                           3
      -3001010          .    /MHz      11185.58835(23)             =  1.00000 *  3
         20000      Delta_J  /kHz         12.27402(72)                           4
        -21010          .    /kHz         12.27402(72)             =  1.00000 *  4
        110000      Delta_JK /kHz        123.3620(20)                            5
       -111010          .    /kHz        123.3620(20)              =  1.00000 *  5
        200000      Delta_K  /kHz        963.28(37)                              6
       -201010          .    /kHz        963.28(37)                =  1.00000 *  6
       4010000      delta_J  /kHz          0.296208(41)                          7
      -4011010          .    /kHz          0.296208(41)            =  1.00000 *  7
       4100000      delta_K  /kHz         58.785(22)                             8
      -4101010          .    /kHz         58.785(22)                =  1.00000 *  8
         30000       Phi_J   /Hz         [-0.002322]                             9
        -31010          .    /Hz         [-0.002322]               =  1.00000 *  9
        120000       Phi_JK  /Hz         [ 0.346]                               10
       -121010          .    /Hz         [ 0.346]                  =  1.00000 * 10
        210000       Phi_KJ  /Hz         [ 2.717]                               11
       -211010          .    /Hz         [ 2.717]                  =  1.00000 * 11
        300000       Phi_K   /Hz         [32.]                                  12
       -301010          .    /Hz         [32.]                     =  1.00000 * 12
       4020000       phi_J   /Hz         [ 0.000153]                            13
      -4021010          .    /Hz         [ 0.000153]               =  1.00000 * 13
       4110000       phi_JK  /Hz         [ 0.254]                               14
      -4111010          .    /Hz         [ 0.254]                  =  1.00000 * 14
       4200000       phi_K   /Hz         [24.]                                  15
      -4201010          .    /Hz         [24.]                     =  1.00000 * 15

    11001001010       X_aa   /MHz        -58.711(21)                            16
   -11003001010       X_cc   /MHz         58.711(21)               = -1.00000 * 16
    11002001010       X_bb   /MHz         29.52(19)                             17
   -11003001010       X_cc   /MHz        -29.52(19)                = -1.00000 * 17

  CORRELATION COEFFICIENTS, C.ij:

            A         B         C       -Delta_J -Delta_J -Delta_K -delta_J -delta_K

A          1.0000
B          0.3133   1.0000
C          0.2139   0.8121   1.0000
-Delta_J  -0.2379  -0.8032  -0.7817   1.0000
-Delta_JK -0.0249  -0.1174  -0.1618  -0.2913   1.0000
-Delta_K  -0.6166  -0.6660  -0.6053   0.8659  -0.3754   1.0000
-delta_J   0.3084  -0.0596   0.1831  -0.1084   0.1205  -0.2182   1.0000
-delta_K  -0.3644  -0.2220   0.0627   0.1462  -0.1572   0.2656  -0.5953   1.0000
X_aa      -0.0447  -0.1534  -0.1533   0.1282   0.0381   0.1008  -0.0085   0.0120
X_bb      -0.0042   0.0037  -0.0101   0.0033  -0.0014   0.0042  -0.0250   0.0056

            X_aa      X_bb

X_aa       1.0000
X_bb      -0.0815   1.0000

 Mean value of |C.ij|, i.ne.j =   0.2328
 Mean value of  C.ij,  i.ne.j =  -0.0734


 No correlations with absolute value greater than 0.9950


 Worst fitted lines (obs-calc/error):

     3:    2.8       251:   -2.8        16:   -2.5         1:    2.2
    29:   -2.2       269:    2.1       257:    1.9       281:   -1.9
   277:   -1.8       177:    1.8       407:    1.8       275:    1.7
   247:   -1.6       319:   -1.6        31:    1.6        83:    1.6
   253:   -1.6       113:    1.5        36:    1.5       265:    1.5
   145:    1.5         4:    1.4        10:   -1.4        17:    1.3
   279:    1.3       195:   -1.3        37:   -1.3        51:   -1.2
   173:    1.2       119:   -1.2       259:   -1.2       185:    1.2
   149:    1.2        27:   -1.1        19:    1.1        85:    1.0
   263:   -1.0       189:    1.0       109:    1.0       107:   -1.0
   371:   -1.0       229:    1.0       261:    1.0        49:    0.9
```

```
  239:    -0.9          323:     0.9       271:    -0.9          34:    0.9
  415:     0.9          155:     0.9


    3:  1  0  1 10  1    0  0  0 10  2      22685.6000    0.2563  0.090
  251: 13 12  1 10 15   12 12  0 10 14     294156.9840   -0.0701  0.025   -0.0702 0.50
   16: 13  1 13  0 13   12  2 11  0 12      28664.1200   -0.1252  0.050
    1:  1  0  1 10  3    0  0  0 10  2      22673.8000    0.2004  0.090
   29: 29  1 29  0 29   29  0 29  0 29      37032.7810   -0.0433  0.020
  269: 13 10  3 10 12   12 10  2 10 11     294298.3620    0.0517  0.025    0.0517 0.50
  257: 13 11  2 10 13   12 11  1 10 12     294226.3620    0.0483  0.025    0.0484 0.50
  281: 13  9  4 10 12   12  9  3 10 11     294359.2820   -0.0479  0.025   -0.0479 0.50
  277: 13  9  4 10 13   12  9  3 10 12     294356.0180   -0.0458  0.025   -0.0458 0.50
  177: 12  9  3 10 11   11  9  2 10 10     271731.1970    0.0452  0.025    0.0452 0.50
                                         _____
                                         / SPFIT output reformatted with PIFORM
```

Table S.3. Fit of the rotational transitions of $^{13}CHD_2^{35}Cl$ in PIFORM format

```
13CHD2Cl -- 35Cl                                 Tue Mar 18 09:44:02 2025


-------------------------------------------------------------------------=========
                                        obs       o-c     error    blends    Notes
                                                                    o-c    wt
      / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------=========
   1:  4  1  4  5    3  1  3  5       88881.1581   0.0325  0.020
   2:  4  1  4  4    3  1  3  3       88894.0946  -0.0063  0.020
   3:  4  1  4  5    3  1  3  4       88895.0652  -0.0005  0.020
   4:  4  1  4  3    3  1  3  2       88895.9632   0.0015  0.020
   5:  4  1  4  6    3  1  3  5       88896.9389   0.0108  0.020
   6:  4  1  4  4    3  1  3  4       88900.5830  -0.0259  0.020
   7:  4  1  4  3    3  1  3  3       88909.9442   0.0392  0.020
   8:  4  0  4  5    3  0  3  5       89453.3750  -0.0047  0.020
   9:  4  3  1  4    3  3  0  4       89457.9513   0.0148  0.020   0.0185 0.50
  10:  4  3  2  4    3  3  1  4       89457.9513   0.0221  0.020   0.0185 0.50
  11:  4  3  1  5    3  3  0  4       89460.2320   0.0074  0.020   0.0110 0.50
  12:  4  3  2  5    3  3  1  4       89460.2320   0.0146  0.020   0.0110 0.50
  13:  4  3  1  3    3  3  0  3       89462.3082   0.0196  0.020   0.0233 0.50
  14:  4  3  2  3    3  3  1  3       89462.3082   0.0269  0.020   0.0233 0.50
  15:  4  3  1  4    3  3  0  3       89468.7855  -0.0125  0.020  -0.0090 0.50
  16:  4  3  2  4    3  3  1  3       89468.7855  -0.0053  0.020  -0.0090 0.50
  17:  4  0  4  3    3  0  3  2       89469.7996  -0.0342  0.020   0.0208 0.27
  18:  4  0  4  4    3  0  3  3       89469.7996  -0.0336  0.020   0.0208 0.36
  19:  4  2  3  5    3  2  2  4       89469.7996   0.1137  0.020   0.0208 0.34
  20:  4  2  3  5    3  2  2  5       89469.7996   0.1093  0.020   0.0208 0.03
  21:  4  0  4  5    3  0  3  4       89472.0167   0.0226  0.020  -0.0416 0.34
  22:  4  0  4  6    3  0  3  5       89472.0167   0.0227  0.020  -0.0416 0.45
  23:  4  2  3  4    3  2  2  3       89472.0167  -0.2819  0.020  -0.0416 0.18
  24:  4  2  3  4    3  2  2  4       89472.0167  -0.2789  0.020  -0.0416 0.03
  25:  4  2  2  5    3  2  1  4       89477.0636  -0.1200  0.020  -0.0243 0.26
  26:  4  2  2  5    3  2  1  5       89477.0636  -0.1240  0.020  -0.0243 0.02
  27:  4  2  3  6    3  2  2  5       89477.0636  -0.0698  0.020  -0.0243 0.34
  28:  4  3  1  6    3  3  0  5       89477.0636   0.0873  0.020  -0.0243 0.19
  29:  4  3  2  6    3  3  1  5       89477.0636   0.0945  0.020  -0.0243 0.19
  30:  4  2  2  4    3  2  1  3       89479.7847  -0.0118  0.020   0.0115 0.49
  31:  4  2  2  4    3  2  1  4       89479.7847  -0.0089  0.020   0.0115 0.08
  32:  4  2  3  3    3  2  2  2       89479.7847   0.0429  0.020   0.0115 0.37
  33:  4  2  3  3    3  2  2  3       89479.7847   0.0365  0.020   0.0115 0.06
  34:  4  3  1  5    3  3  0  5       89483.5196   0.0241  0.020   0.0278 0.50
  35:  4  3  2  5    3  3  1  5       89483.5196   0.0314  0.020   0.0278 0.50
  36:  4  2  2  6    3  2  1  5       89484.6339   0.0023  0.020
  37:  4  3  1  3    3  3  0  2       89485.5797   0.0257  0.020   0.0294 0.50
  38:  4  3  2  3    3  3  1  2       89485.5797   0.0330  0.020   0.0294 0.50
  39:  4  2  2  3    3  2  1  2       89487.2541   0.0142  0.020   0.0133 0.86
  40:  4  2  2  3    3  2  1  3       89487.2541   0.0074  0.020   0.0133 0.14
  41:  4  0  4  3    3  0  3  3       89488.4169  -0.0299  0.020
  42:  4  1  3  4    3  1  2  3       90055.3541   0.0057  0.020
  43:  4  1  3  5    3  1  2  4       90056.3265   0.0089  0.020
  44:  4  1  3  3    3  1  2  2       90057.2233   0.0141  0.020
  45:  4  1  3  6    3  1  2  5       90058.1940   0.0141  0.020
  46:  4  1  3  4    3  1  2  4       90061.8633  -0.0109  0.020
  47:  8  1  8  7    7  1  7  6      177761.7880   0.0982  0.040  -0.0146 0.20
  48:  8  1  8  8    7  1  7  7      177761.7880   0.3196  0.040  -0.0146 0.23
  49:  8  1  8  9    7  1  7  8      177761.7880  -0.0750  0.040  -0.0146 0.26
  50:  8  1  8 10    7  1  7  9      177761.7880  -0.2965  0.040  -0.0146 0.30
  51:  8  7  1  9    7  7  0  8      178838.9450   0.0251  0.040   0.0252 0.50
  52:  8  7  2  9    7  7  1  8      178838.9450   0.0251  0.040   0.0252 0.50
  53:  8  7  1  8    7  7  0  7      178841.6330   0.0247  0.040   0.0247 0.50
  54:  8  7  2  8    7  7  1  7      178841.6330   0.0247  0.040   0.0247 0.50
  55:  8  7  1 10    7  7  0  9      178849.7650  -0.0126  0.040  -0.0126 0.50
  56:  8  7  2 10    7  7  1  9      178849.7650  -0.0126  0.040  -0.0126 0.50
  57:  8  7  1  7    7  7  0  6      178852.4100  -0.0585  0.040  -0.0586 0.50
  58:  8  7  2  7    7  7  1  6      178852.4100  -0.0585  0.040  -0.0586 0.50
  59:  8  6  2  9    7  6  1  8      178866.7670   0.0292  0.040   0.0293 0.50
  60:  8  6  3  9    7  6  2  8      178866.7670   0.0292  0.040   0.0293 0.50
  61:  8  6  2  8    7  6  1  7      178868.5330  -0.0590  0.040  -0.0590 0.50
  62:  8  6  3  8    7  6  2  7      178868.5330  -0.0590  0.040  -0.0590 0.50
  63:  8  6  2 10    7  6  1  9      178874.7420   0.0263  0.040   0.0263 0.50
  64:  8  6  3 10    7  6  2  9      178874.7420   0.0263  0.040   0.0263 0.50
  65:  8  0  8  7    7  0  7  6      178876.5560   0.3778  0.040   0.1053 0.18
  66:  8  0  8  8    7  0  7  7      178876.5560   0.3773  0.040   0.1053 0.21
  67:  8  6  2  7    7  6  1  6      178876.5560  -0.0139  0.040   0.1053 0.05
  68:  8  6  3  7    7  6  2  6      178876.5560  -0.0139  0.040   0.1053 0.05
```

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 69:   8   0   8 10     7   0   7   9        178876.5560   -0.0816   0.040    0.1053  0.27
 70:   8   0   8  9     7   0   7   8        178876.5560   -0.0822   0.040    0.1053  0.24
 71:   8   5   3  9     7   5   2   8        178890.7220    0.0134   0.040    0.0135  0.50
 72:   8   5   4  9     7   5   3   8        178890.7220    0.0134   0.040    0.0135  0.50
 73:   8   5   3  8     7   5   2   7        178891.8620    0.0055   0.040    0.0056  0.50
 74:   8   5   4  8     7   5   3   7        178891.8620    0.0055   0.040    0.0056  0.50
 75:   8   5   3 10     7   5   2   9        178896.2300   -0.0192   0.040   -0.0193  0.50
 76:   8   5   4 10     7   5   3   9        178896.2300   -0.0192   0.040   -0.0193  0.50
 77:   8   5   3  7     7   5   2   6        178897.3860   -0.0100   0.040   -0.0100  0.50
 78:   8   5   4  7     7   5   3   6        178897.3860   -0.0100   0.040   -0.0100  0.50
 79:   8   4   4  9     7   4   3   8        178911.3010    0.0555   0.040    0.0558  0.50
 80:   8   4   5  9     7   4   4   8        178911.3010    0.0560   0.040    0.0558  0.50
 81:   8   4   4  8     7   4   3   7        178911.8810    0.0659   0.040    0.0663  0.50
 82:   8   4   5  8     7   4   4   7        178911.8810    0.0665   0.040    0.0663  0.50
 83:   8   4   4 10     7   4   3   9        178914.8110    0.0191   0.040    0.0194  0.50
 84:   8   4   5 10     7   4   4   9        178914.8110    0.0197   0.040    0.0194  0.50
 85:   8   4   4  7     7   4   3   6        178915.3840    0.0239   0.040    0.0242  0.50
 86:   8   4   5  7     7   4   4   6        178915.3840    0.0244   0.040    0.0242  0.50
 87:   8   2   7  8     7   2   6   7        178921.9890    0.0816   0.040   -0.0260  0.47
 88:   8   2   7  9     7   2   6   8        178921.9890   -0.1205   0.040   -0.0260  0.53
 89:   8   2   7  7     7   2   6   6        178922.9420    0.1485   0.040    0.0279  0.40
 90:   8   2   7 10     7   2   6   9        178922.9420   -0.0541   0.040    0.0279  0.60
 91:   8   3   5  8     7   3   4   7        178929.7700   -0.2168   0.040   -0.0013  0.23
 92:   8   3   5  9     7   3   4   8        178929.7700   -0.0973   0.040   -0.0013  0.27
 93:   8   3   6  8     7   3   5   7        178929.7700    0.0870   0.040   -0.0013  0.23
 94:   8   3   6  9     7   3   5   8        178929.7700    0.2065   0.040   -0.0013  0.27
 95:   8   3   5  7     7   3   4   6        178931.7510   -0.2298   0.040   -0.0074  0.20
 96:   8   3   5 10     7   3   4   9        178931.7510   -0.1113   0.040   -0.0074  0.30
 97:   8   3   6  7     7   3   5   6        178931.7510    0.0740   0.040   -0.0074  0.20
 98:   8   3   6 10     7   3   5   9        178931.7510    0.1925   0.040   -0.0074  0.30
 99:   8   2   6  8     7   2   5   7        178984.9130    0.0919   0.040   -0.0156  0.47
100:   8   2   6  9     7   2   5   8        178984.9130   -0.1101   0.040   -0.0156  0.53
101:   8   2   6  7     7   2   5   6        178985.8680    0.1602   0.040    0.0397  0.40
102:   8   2   6 10     7   2   5   9        178985.8680   -0.0423   0.040    0.0397  0.60
103:   8   1   7  7     7   1   6   6        180083.1990    0.1655   0.040    0.0522  0.20
104:   8   1   7  8     7   1   6   7        180083.1990    0.3869   0.040    0.0522  0.23
105:   8   1   7  9     7   1   6   8        180083.1990   -0.0086   0.040    0.0522  0.26
106:   8   1   7 10     7   1   6   9        180083.1990   -0.2301   0.040    0.0522  0.30
107:   9   1   9 11     8   1   8  10        199970.2160   -0.2081   0.040    0.0103  0.29
108:   9   1   9  8     8   1   8   7        199970.2160    0.1108   0.040    0.0103  0.21
109:   9   1   9  9     8   1   8   8        199970.2160    0.2658   0.040    0.0103  0.23
110:   9   1   9 10     8   1   8   9        199970.2160   -0.0531   0.040    0.0103  0.26
111:   9   8   1 11     8   8   0  10        201164.7500    0.0558   0.040    0.0558  0.50
112:   9   8   2 11     8   8   1  10        201164.7500    0.0558   0.040    0.0558  0.50
113:   9   8   1  8     8   8   0   7        201166.9370    0.0581   0.040    0.0582  0.50
114:   9   8   2  8     8   8   1   7        201166.9370    0.0581   0.040    0.0582  0.50
115:   9   7   2 10     8   7   1   9        201189.6930   -0.0641   0.040   -0.0641  0.50
116:   9   7   3 10     8   7   2   9        201189.6930   -0.0641   0.040   -0.0641  0.50
117:   9   7   2  9     8   7   1   8        201191.2550   -0.0896   0.040   -0.0897  0.50
118:   9   7   3  9     8   7   2   8        201191.2550   -0.0896   0.040   -0.0897  0.50
119:   9   7   2 11     8   7   1  10        201197.3270   -0.0312   0.040   -0.0312  0.50
120:   9   7   3 11     8   7   2  10        201197.3270   -0.0312   0.040   -0.0312  0.50
121:   9   7   2  8     8   7   1   7        201198.8980   -0.0480   0.040   -0.0480  0.50
122:   9   7   3  8     8   7   2   7        201198.8980   -0.0480   0.040   -0.0480  0.50
123:   9   0   9 11     8   0   8  10        201209.6200   -0.1327   0.040    0.0262  0.29
124:   9   0   9  8     8   0   8   7        201209.6200    0.2263   0.040    0.0262  0.21
125:   9   0   9  9     8   0   8   8        201209.6200    0.2257   0.040    0.0262  0.23
126:   9   0   9 10     8   0   8   9        201209.6200   -0.1334   0.040    0.0262  0.26
127:   9   6   3 10     8   6   2   9        201220.3580   -0.0576   0.040   -0.0576  0.50
128:   9   6   4 10     8   6   3   9        201220.3580   -0.0576   0.040   -0.0576  0.50
129:   9   6   3  9     8   6   2   8        201221.4630   -0.0242   0.040   -0.0242  0.50
130:   9   6   4  9     8   6   3   8        201221.4630   -0.0242   0.040   -0.0242  0.50
131:   9   6   3 11     8   6   2  10        201225.9350   -0.0655   0.040   -0.0655  0.50
132:   9   6   4 11     8   6   3  10        201225.9350   -0.0655   0.040   -0.0655  0.50
133:   9   6   3  8     8   6   2   7        201227.0400   -0.0313   0.040   -0.0314  0.50
134:   9   6   4  8     8   6   3   7        201227.0400   -0.0313   0.040   -0.0314  0.50
135:   9   5   4 10     8   5   3   9        201246.9940    0.0248   0.040    0.0248  0.50
136:   9   5   5 10     8   5   4   9        201246.9940    0.0248   0.040    0.0248  0.50
137:   9   5   4  9     8   5   3   8        201247.6010   -0.0029   0.040   -0.0029  0.50
138:   9   5   5  9     8   5   4   8        201247.6010   -0.0029   0.040   -0.0029  0.50
139:   9   5   4 11     8   5   3  10        201250.8440   -0.0038   0.040   -0.0038  0.50
140:   9   5   5 11     8   5   4  10        201250.8440   -0.0038   0.040   -0.0038  0.50
141:   9   5   4  8     8   5   3   7        201251.4960    0.0144   0.040    0.0145  0.50
142:   9   5   5  8     8   5   4   7        201251.4960    0.0144   0.040    0.0145  0.50
143:   9   4   5  9     8   4   4   8        201270.0980   -0.1874   0.040   -0.0404  0.24
144:   9   4   5 10     8   4   4   9        201270.0980    0.0896   0.040   -0.0404  0.26
145:   9   4   6  9     8   4   5   8        201270.0980   -0.1861   0.040   -0.0404  0.24
146:   9   4   6 10     8   4   5   9        201270.0980    0.0909   0.040   -0.0404  0.26
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147:  9   4   5  11     8   4   4  10        201272.5680    0.0771   0.040   -0.0369 0.29
148:  9   4   5   8     8   4   4   7        201272.5680   -0.1989   0.040   -0.0369 0.21
149:  9   4   6  11     8   4   5  10        201272.5680    0.0784   0.040   -0.0369 0.29
150:  9   4   6   8     8   4   5   7        201272.5680   -0.1977   0.040   -0.0369 0.21
151:  9   2   8   9     8   2   7   8        201277.0020    0.1442   0.040    0.0386 0.47
152:  9   2   8  10     8   2   7   9        201277.0020   -0.0557   0.040    0.0386 0.53
153:  9   2   8  11     8   2   7  10        201277.5510   -0.1273   0.040   -0.0440 0.58
154:  9   2   8   8     8   2   7   7        201277.5510    0.0730   0.040   -0.0440 0.42
155:  9   3   6   9     8   3   5   8        201291.3880   -0.3694   0.040   -0.0916 0.24
156:  9   3   6  10     8   3   5   9        201291.3880   -0.3706   0.040   -0.0916 0.26
157:  9   3   7   9     8   3   6   8        201291.3880    0.1874   0.040   -0.0916 0.24
158:  9   3   7  10     8   3   6   9        201291.3880    0.1862   0.040   -0.0916 0.26
159:  9   3   6  11     8   3   5  10        201292.9090   -0.2461   0.040    0.0331 0.29
160:  9   3   6   8     8   3   5   7        201292.9090   -0.2443   0.040    0.0331 0.21
161:  9   3   7  11     8   3   6  10        201292.9090    0.3107   0.040    0.0331 0.29
162:  9   3   7   8     8   3   6   7        201292.9090    0.3125   0.040    0.0331 0.21
163:  9   2   7   9     8   2   6   8        201366.8450    0.1616   0.040    0.0560 0.47
164:  9   2   7  10     8   2   6   9        201366.8450   -0.0383   0.040    0.0560 0.53
165:  9   2   7  11     8   2   6  10        201367.4010   -0.1035   0.040   -0.0203 0.58
166:  9   2   7   8     8   2   6   7        201367.4010    0.0967   0.040   -0.0203 0.42
167:  9   1   8  11     8   1   7  10        202581.1740   -0.2019   0.040    0.0169 0.29
168:  9   1   8   8     8   1   7   7        202581.1740    0.1178   0.040    0.0169 0.21
169:  9   1   8   9     8   1   7   8        202581.1740    0.2727   0.040    0.0169 0.23
170:  9   1   8  10     8   1   7   9        202581.1740   -0.0469   0.040    0.0169 0.26
171: 10   1  10  11     9   1   9  10        222174.4480   -0.0792   0.040   -0.0179 0.26
172: 10   1  10  12     9   1   9  11        222174.4480   -0.1918   0.040   -0.0179 0.29
173: 10   1  10   9     9   1   9   8        222174.4480    0.0706   0.040   -0.0179 0.21
174: 10   1  10  10     9   1   9   9        222174.4480    0.1832   0.040   -0.0179 0.24
175: 10   9   1  11     9   9   0  10        223455.6890    0.0029   0.040    0.0030 0.50
176: 10   9   2  11     9   9   1  10        223455.6890    0.0029   0.040    0.0030 0.50
177: 10   9   1  10     9   9   0   9        223457.4490   -0.0441   0.040   -0.0441 0.50
178: 10   9   2  10     9   9   1   9        223457.4490   -0.0441   0.040   -0.0441 0.50
179: 10   9   1  12     9   9   0  11        223464.8150   -0.0085   0.040   -0.0086 0.50
180: 10   9   2  12     9   9   1  11        223464.8150   -0.0085   0.040   -0.0086 0.50
181: 10   9   1   9     9   9   0   8        223466.6700    0.0374   0.040    0.0375 0.50
182: 10   9   2   9     9   9   1   8        223466.6700    0.0374   0.040    0.0375 0.50
183: 10   8   2  11     9   8   1  10        223498.9170   -0.0126   0.040   -0.0127 0.50
184: 10   8   3  11     9   8   2  10        223498.9170   -0.0126   0.040   -0.0127 0.50
185: 10   8   2  10     9   8   1   9        223500.2760   -0.0215   0.040   -0.0215 0.50
186: 10   8   3  10     9   8   2   9        223500.2760   -0.0215   0.040   -0.0215 0.50
187: 10   8   2  12     9   8   1  11        223506.1430   -0.0069   0.040   -0.0070 0.50
188: 10   8   3  12     9   8   2  11        223506.1430   -0.0069   0.040   -0.0070 0.50
189: 10   8   2   9     9   8   1   8        223507.5400    0.0218   0.040    0.0218 0.50
190: 10   8   3   9     9   8   2   8        223507.5400    0.0218   0.040    0.0218 0.50
191: 10   0  10  11     9   0   9  10        223533.4350   -0.1627   0.040   -0.0327 0.26
192: 10   0  10  12     9   0   9  11        223533.4350   -0.1620   0.040   -0.0327 0.29
193: 10   0  10   9     9   0   9   8        223533.4350    0.1266   0.040   -0.0327 0.21
194: 10   0  10  10     9   0   9   9        223533.4350    0.1259   0.040   -0.0327 0.24
195: 10   7   3  11     9   7   2  10        223537.3490   -0.0142   0.040   -0.0143 0.50
196: 10   7   4  11     9   7   3  10        223537.3490   -0.0142   0.040   -0.0143 0.50
197: 10   7   3  10     9   7   2   9        223538.3670    0.0237   0.040    0.0237 0.50
198: 10   7   4  10     9   7   3   9        223538.3670    0.0237   0.040    0.0237 0.50
199: 10   7   3  12     9   7   2  11        223542.8580   -0.0336   0.040   -0.0336 0.50
200: 10   7   4  12     9   7   3  11        223542.8580   -0.0336   0.040   -0.0336 0.50
201: 10   7   3   9     9   7   2   8        223543.9360    0.0648   0.040    0.0648 0.50
202: 10   7   4   9     9   7   3   8        223543.9360    0.0648   0.040    0.0648 0.50
203: 10   6   4  11     9   6   3  10        223571.1270    0.0022   0.040    0.0022 0.50
204: 10   6   5  11     9   6   4  10        223571.1270    0.0022   0.040    0.0022 0.50
205: 10   6   4  10     9   6   3   9        223571.7260   -0.0424   0.040   -0.0424 0.50
206: 10   6   5  10     9   6   4   9        223571.7260   -0.0424   0.040   -0.0424 0.50
207: 10   6   4  12     9   6   3  11        223575.1790   -0.0076   0.040   -0.0076 0.50
208: 10   6   5  12     9   6   4  11        223575.1790   -0.0076   0.040   -0.0076 0.50
209: 10   6   4   9     9   6   3   8        223575.7340   -0.0955   0.040   -0.0955 0.50
210: 10   6   5   9     9   6   4   8        223575.7340   -0.0955   0.040   -0.0955 0.50
211: 10   5   5  11     9   5   4  10        223600.6880    0.1606   0.040   -0.0097 0.26
212: 10   5   5  10     9   5   4   9        223600.6880   -0.1982   0.040   -0.0097 0.24
213: 10   5   6  11     9   5   5  10        223600.6880    0.1606   0.040   -0.0097 0.26
214: 10   5   6  10     9   5   5   9        223600.6880   -0.1982   0.040   -0.0097 0.24
215: 10   5   5  12     9   5   4  11        223603.4650    0.1167   0.040   -0.0351 0.29
216: 10   5   5   9     9   5   4   8        223603.4650   -0.2413   0.040   -0.0351 0.21
217: 10   5   6  12     9   5   5  11        223603.4650    0.1167   0.040   -0.0351 0.29
218: 10   5   6   9     9   5   5   8        223603.4650   -0.2413   0.040   -0.0351 0.21
219: 10   4   6  11     9   4   5  10        223626.4300    0.0466   0.040   -0.0117 0.26
220: 10   4   6  10     9   4   5   9        223626.4300   -0.0792   0.040   -0.0117 0.24
221: 10   4   7  11     9   4   6  10        223626.4300    0.0493   0.040   -0.0117 0.26
222: 10   4   7  10     9   4   6   9        223626.4300   -0.0765   0.040   -0.0117 0.24
223: 10   2   9  11     9   2   8  10        223628.2970    0.0525   0.040   -0.0279 0.15
224: 10   2   9  12     9   2   8  11        223628.2970   -0.3986   0.040   -0.0279 0.17
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225: 10	2	9	9	9	2	8	8	223628.2970	-0.2134	0.040	-0.0279	0.12
226: 10	2	9	10	9	2	8	9	223628.2970	0.2375	0.040	-0.0279	0.14
227: 10	4	6	12	9	4	5	11	223628.2970	0.1081	0.040	-0.0279	0.12
228: 10	4	6	9	9	4	5	8	223628.2970	-0.0170	0.040	-0.0279	0.09
229: 10	4	7	12	9	4	6	11	223628.2970	0.1109	0.040	-0.0279	0.12
230: 10	4	7	9	9	4	6	8	223628.2970	-0.0143	0.040	-0.0279	0.09
231: 10	3	8	11	9	3	7	10	223650.8020	-0.0847	0.040	-0.0584	0.53
232: 10	3	8	10	9	3	7	9	223650.8020	-0.0293	0.040	-0.0584	0.47
233: 10	3	7	11	9	3	6	10	223651.8250	-0.0161	0.040	-0.0219	0.26
234: 10	3	7	10	9	3	6	9	223651.8250	0.0392	0.040	-0.0219	0.24
235: 10	3	8	12	9	3	7	11	223651.8250	-0.0774	0.040	-0.0219	0.29
236: 10	3	8	9	9	3	7	8	223651.8250	-0.0215	0.040	-0.0219	0.21
237: 10	3	7	12	9	3	6	11	223652.8620	0.0051	0.040	0.0289	0.58
238: 10	3	7	9	9	3	6	8	223652.8620	0.0610	0.040	0.0289	0.42
239: 10	2	8	11	9	2	7	10	223751.7870	0.1246	0.040	-0.0193	0.26
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242: 10	2	8	10	9	2	7	9	223751.7870	0.3096	0.040	-0.0193	0.24
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249: 11	1	11	13	10	1	10	12	244374.1580	-0.1275	0.040	0.0141	0.29
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263: 11	9	2	13	10	9	1	12	245799.3530	-0.0045	0.040	-0.0045	0.50
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275: 11	0	11	11	10	0	10	10	245847.0510	0.1171	0.040	-0.0120	0.24
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291: 11	6	5	13	10	6	4	12	245922.0160	0.1225	0.040	-0.0481	0.28
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293: 11	6	6	13	10	6	5	12	245922.0160	0.1225	0.040	-0.0481	0.28
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295: 11	5	6	11	10	5	5	10	245951.3950	-0.1058	0.040	0.0003	0.24
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421: 13   1  13 12   12   1  12 11        288758.0400   0.0758  0.040   0.0153 0.22
422: 13   1  13 13   12   1  12 12        288758.0400   0.1267  0.040   0.0153 0.24
423: 13   1  13 14   12   1  12 13        288758.0400  -0.0326  0.040   0.0153 0.26
424: 13   1  13 15   12   1  12 14        288758.0400  -0.0836  0.040   0.0153 0.28
425: 13  12   1 14   12  12   0 13        290251.7830  -0.0317  0.040  -0.0318 0.50
426: 13  12   2 14   12  12   1 13        290251.7830  -0.0317  0.040  -0.0318 0.50
427: 13  12   1 13   12  12   0 12        290252.9590   0.0240  0.040   0.0241 0.50
428: 13  12   2 13   12  12   1 12        290252.9590   0.0240  0.040   0.0241 0.50
429: 13  12   1 15   12  12   0 14        290259.1730  -0.0054  0.040  -0.0054 0.50
430: 13  12   2 15   12  12   1 14        290259.1730  -0.0054  0.040  -0.0054 0.50
431: 13  12   1 12   12  12   0 11        290260.3480   0.0480  0.040   0.0481 0.50
432: 13  12   2 12   12  12   1 11        290260.3480   0.0480  0.040   0.0481 0.50
433: 13  11   2 14   12  11   1 13        290325.8860  -0.0391  0.040  -0.0391 0.50
434: 13  11   3 14   12  11   2 13        290325.8860  -0.0391  0.040  -0.0391 0.50
435: 13  11   2 13   12  11   1 12        290326.8830   0.0432  0.040   0.0432 0.50
436: 13  11   3 13   12  11   2 12        290326.8830   0.0432  0.040   0.0432 0.50
437: 13  11   2 15   12  11   1 14        290332.0770  -0.0359  0.040  -0.0359 0.50
438: 13  11   3 15   12  11   2 14        290332.0770  -0.0359  0.040  -0.0359 0.50
439: 13  11   2 12   12  11   1 11        290333.0870   0.0588  0.040   0.0589 0.50
440: 13  11   3 12   12  11   2 11        290333.0870   0.0588  0.040   0.0589 0.50
441: 13  10   3 14   12  10   2 13        290393.7880  -0.0247  0.040  -0.0247 0.50
442: 13  10   4 14   12  10   3 13        290393.7880  -0.0247  0.040  -0.0247 0.50
443: 13  10   3 13   12  10   2 12        290394.5810   0.0413  0.040   0.0414 0.50
444: 13  10   4 13   12  10   3 12        290394.5810   0.0413  0.040   0.0414 0.50
445: 13  10   3 15   12  10   2 14        290398.9100  -0.0168  0.040  -0.0168 0.50
446: 13  10   4 15   12  10   3 14        290398.9100  -0.0168  0.040  -0.0168 0.50
447: 13  10   3 12   12  10   2 11        290399.7170   0.0632  0.040   0.0633 0.50
448: 13  10   4 12   12  10   3 11        290399.7170   0.0632  0.040   0.0633 0.50
449: 13   0  13 12   12   0  12 11        290439.5390   0.1037  0.040   0.0124 0.22
450: 13   0  13 13   12   0  12 12        290439.5390   0.1027  0.040   0.0124 0.24
451: 13   0  13 14   12   0  12 13        290439.5390  -0.0657  0.040   0.0124 0.26
452: 13   0  13 15   12   0  12 14        290439.5390  -0.0648  0.040   0.0124 0.28
453: 13   9   4 13   12   9   3 12        290455.7500  -0.3210  0.040  -0.0318 0.24
454: 13   9   4 14   12   9   3 13        290455.7500   0.2358  0.040  -0.0318 0.26
455: 13   9   5 13   12   9   4 12        290455.7500  -0.3210  0.040  -0.0318 0.24
456: 13   9   5 14   12   9   4 13        290455.7500   0.2358  0.040  -0.0318 0.26
457: 13   9   4 12   12   9   3 11        290459.8400  -0.3733  0.040  -0.0627 0.22
458: 13   9   4 15   12   9   3 14        290459.8400   0.1833  0.040  -0.0627 0.28
```

```
459: 13   9   5 12    12   9   4 11         290459.8400   -0.3733   0.040   -0.0627  0.22
460: 13   9   5 15    12   9   4 14         290459.8400    0.1833   0.040   -0.0627  0.28
461: 13   8   5 13    12   8   4 12         290511.3030   -0.2075   0.040    0.0027  0.24
462: 13   8   5 14    12   8   4 13         290511.3030    0.1972   0.040    0.0027  0.26
463: 13   8   6 13    12   8   5 12         290511.3030   -0.2075   0.040    0.0027  0.24
464: 13   8   6 14    12   8   5 13         290511.3030    0.1972   0.040    0.0027  0.26
465: 13   8   5 12    12   8   4 11         290514.5470   -0.2363   0.040   -0.0107  0.22
466: 13   8   5 15    12   8   4 14         290514.5470    0.1680   0.040   -0.0107  0.28
467: 13   8   6 12    12   8   5 11         290514.5470   -0.2363   0.040   -0.0107  0.22
468: 13   8   6 15    12   8   5 14         290514.5470    0.1680   0.040   -0.0107  0.28
469: 13   7   6 13    12   7   5 12         290560.8550   -0.1555   0.040   -0.0150  0.24
470: 13   7   6 14    12   7   5 13         290560.8550    0.1149   0.040   -0.0150  0.26
471: 13   7   7 13    12   7   6 12         290560.8550   -0.1555   0.040   -0.0150  0.24
472: 13   7   7 14    12   7   6 13         290560.8550    0.1149   0.040   -0.0150  0.26
473: 13   7   6 15    12   7   5 11         290563.3300   -0.1861   0.040   -0.0355  0.22
474: 13   7   6 15    12   7   5 14         290563.3300    0.0838   0.040   -0.0355  0.28
475: 13   7   7 12    12   7   6 11         290563.3300   -0.1861   0.040   -0.0355  0.22
476: 13   7   7 15    12   7   6 14         290563.3300    0.0838   0.040   -0.0355  0.28
477: 13   6   7 13    12   6   6 12         290604.7910   -0.0928   0.040   -0.0128  0.24
478: 13   6   7 14    12   6   6 13         290604.7910    0.0612   0.040   -0.0128  0.26
479: 13   6   8 13    12   6   7 12         290604.7910   -0.0928   0.040   -0.0128  0.24
480: 13   6   8 14    12   6   7 13         290604.7910    0.0612   0.040   -0.0128  0.26
481: 13   6   7 12    12   6   6 11         290606.6350   -0.0896   0.040   -0.0040  0.22
482: 13   6   7 15    12   6   6 14         290606.6350    0.0639   0.040   -0.0040  0.28
483: 13   6   8 12    12   6   7 11         290606.6350   -0.0896   0.040   -0.0040  0.22
484: 13   6   8 15    12   6   7 14         290606.6350    0.0639   0.040   -0.0040  0.28
485: 13   5   8 13    12   5   7 12         290643.7740   -0.0526   0.040   -0.0237  0.24
486: 13   5   8 14    12   5   7 13         290643.7740    0.0029   0.040   -0.0237  0.26
487: 13   5   9 13    12   5   8 12         290643.7740   -0.0525   0.040   -0.0237  0.24
488: 13   5   9 14    12   5   8 13         290643.7740    0.0029   0.040   -0.0237  0.26
489: 13   5   8 12    12   5   7 11         290645.0900   -0.0149   0.040    0.0158  0.22
490: 13   5   8 15    12   5   7 14         290645.0900    0.0402   0.040    0.0158  0.28
491: 13   5   9 12    12   5   8 11         290645.0900   -0.0149   0.040    0.0158  0.22
492: 13   5   9 15    12   5   8 14         290645.0900    0.0402   0.040    0.0158  0.28
493: 13   2 12 12    12   2 11 11         290655.3730   -0.0239   0.040    0.0064  0.22
494: 13   2 12 13    12   2 11 12         290655.3730    0.1804   0.040    0.0064  0.24
495: 13   2 12 14    12   2 11 13         290655.3730    0.0477   0.040    0.0064  0.26
496: 13   2 12 15    12   2 11 14         290655.3730   -0.1567   0.040    0.0064  0.28
497: 13   4   9 13    12   4   8 12         290679.5900   -0.0463   0.040   -0.0502  0.24
498: 13   4   9 14    12   4   8 13         290679.5900   -0.0714   0.040   -0.0502  0.26
499: 13   4 10 13    12   4   9 12         290679.5900   -0.0280   0.040   -0.0502  0.24
500: 13   4 10 14    12   4   9 13         290679.5900   -0.0531   0.040   -0.0502  0.26
501: 13   4   9 12    12   4   8 11         290680.5020    0.0475   0.040    0.0425  0.22
502: 13   4   9 15    12   4   8 14         290680.5020    0.0221   0.040    0.0425  0.28
503: 13   4 10 12    12   4   9 11         290680.5020    0.0657   0.040    0.0425  0.22
504: 13   4 10 15    12   4   9 14         290680.5020    0.0404   0.040    0.0425  0.28
505: 13   3 11 12    12   3 10 11         290716.6280   -0.1971   0.040   -0.0151  0.22
506: 13   3 11 13    12   3 10 12         290716.6280    0.2631   0.040   -0.0151  0.24
507: 13   3 11 14    12   3 10 13         290716.6280    0.1753   0.040   -0.0151  0.26
508: 13   3 11 15    12   3 10 14         290716.6280   -0.2851   0.040   -0.0151  0.28
509: 13   3 10 12    12   3   9 11         290720.2550   -0.1844   0.040   -0.0023  0.22
510: 13   3 10 13    12   3   9 12         290720.2550    0.2759   0.040   -0.0023  0.24
511: 13   3 10 14    12   3   9 13         290720.2550    0.1880   0.040   -0.0023  0.26
512: 13   3 10 15    12   3   9 14         290720.2550   -0.2724   0.040   -0.0023  0.28
513: 13   2 11 12    12   2 10 11         290926.6500   -0.0087   0.040    0.0221  0.22
514: 13   2 11 13    12   2 10 12         290926.6500    0.1965   0.040    0.0221  0.24
515: 13   2 11 14    12   2 10 13         290926.6500    0.0639   0.040    0.0221  0.26
516: 13   2 11 15    12   2 10 14         290926.6500   -0.1414   0.040    0.0221  0.28
517: 13   1 12 12    12   1 11 11         292524.0200    0.0762   0.040    0.0156  0.22
518: 13   1 12 13    12   1 11 12         292524.0200    0.1271   0.040    0.0156  0.24
519: 13   1 12 14    12   1 11 13         292524.0200   -0.0325   0.040    0.0156  0.26
520: 13   1 12 15    12   1 11 14         292524.0200   -0.0834   0.040    0.0156  0.28
521: 14   1 14 13    13   1 13 12         310941.3940    0.0678   0.040    0.0141  0.22
522: 14   1 14 14    13   1 13 13         310941.3940    0.1085   0.040    0.0141  0.24
523: 14   1 14 15    13   1 13 14         310941.3940   -0.0295   0.040    0.0141  0.26
524: 14   1 14 16    13   1 13 15         310941.3940   -0.0702   0.040    0.0141  0.28
525: 14 12   2 15    13 12   1 14         312562.2980   -0.0355   0.040   -0.0355  0.50
526: 14 12   3 15    13 12   2 14         312562.2980   -0.0355   0.040   -0.0355  0.50
527: 14 12   2 14    13 12   1 13         312563.1980    0.0533   0.040    0.0533  0.50
528: 14 12   3 14    13 12   2 13         312563.1980    0.0533   0.040    0.0533  0.50
529: 14 12   2 16    13 12   1 15         312568.1970   -0.0277   0.040   -0.0277  0.50
530: 14 12   3 16    13 12   2 15         312568.1970   -0.0277   0.040   -0.0277  0.50
531: 14 12   2 13    13 12   1 12         312569.1120    0.0756   0.040    0.0756  0.50
532: 14 12   3 13    13 12   2 12         312569.1120    0.0756   0.040    0.0756  0.50
533: 14 11   3 15    13 11   2 14         312642.0280    0.0204   0.040    0.0204  0.50
534: 14 11   4 15    13 11   3 14         312642.0280    0.0204   0.040    0.0204  0.50
535: 14 11   3 14    13 11   2 13         312642.6450   -0.0212   0.040   -0.0212  0.50
536: 14 11   4 14    13 11   3 13         312642.6450   -0.0212   0.040   -0.0212  0.50
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537: 14 11   3 16    13 11   2 15         312646.9870   0.0290  0.040   0.0290 0.50
538: 14 11   4 16    13 11   3 15         312646.9870   0.0290  0.040   0.0290 0.50
539: 14 11   3 13    13 11   2 12         312647.6190   0.0023  0.040   0.0023 0.50
540: 14 11   4 13    13 11   3 12         312647.6190   0.0023  0.040   0.0023 0.50
541: 14  0 14 13    13  0 13 12         312716.5200   0.0847  0.040   0.0065 0.22
542: 14  0 14 14    13  0 13 13         312716.5200   0.0837  0.040   0.0065 0.24
543: 14  0 14 15    13  0 13 14         312716.5200  -0.0612  0.040   0.0065 0.26
544: 14  0 14 16    13  0 13 15         312716.5200  -0.0602  0.040   0.0065 0.28
545: 14  9  5 14    13  9  4 13         312781.5910  -0.2155  0.040  -0.0118 0.24
546: 14  9  5 15    13  9  4 14         312781.5910   0.1777  0.040  -0.0118 0.26
547: 14  9  6 14    13  9  5 13         312781.5910  -0.2155  0.040  -0.0118 0.24
548: 14  9  6 15    13  9  5 14         312781.5910   0.1777  0.040  -0.0118 0.26
549: 14  9  5 13    13  9  4 12         312784.8900  -0.2302  0.040  -0.0127 0.22
550: 14  9  5 16    13  9  4 15         312784.8900   0.1626  0.040  -0.0127 0.28
551: 14  9  6 13    13  9  5 12         312784.8900  -0.2302  0.040  -0.0127 0.22
552: 14  9  6 16    13  9  5 15         312784.8900   0.1626  0.040  -0.0127 0.28
553: 14  8  6 14    13  8  5 13         312841.4280  -0.1446  0.040   0.0006 0.24
554: 14  8  6 15    13  8  5 14         312841.4280   0.1356  0.040   0.0006 0.26
555: 14  8  7 14    13  8  6 13         312841.4280  -0.1446  0.040   0.0006 0.24
556: 14  8  7 15    13  8  6 14         312841.4280   0.1356  0.040   0.0006 0.26
557: 14  8  6 13    13  8  5 12         312844.0360  -0.1548  0.040   0.0001 0.22
558: 14  8  6 16    13  8  5 15         312844.0360   0.1250  0.040   0.0001 0.28
559: 14  8  7 13    13  8  6 12         312844.0360  -0.1548  0.040   0.0001 0.22
560: 14  8  7 16    13  8  6 15         312844.0360   0.1250  0.040   0.0001 0.28
561: 14  7  7 14    13  7  6 13         312894.9310  -0.0978  0.040  -0.0042 0.24
562: 14  7  7 15    13  7  6 14         312894.9310   0.0829  0.040  -0.0042 0.26
563: 14  7  8 14    13  7  7 13         312894.9310  -0.0978  0.040  -0.0042 0.24
564: 14  7  8 15    13  7  7 14         312894.9310   0.0829  0.040  -0.0042 0.26
565: 14  7  7 13    13  7  6 12         312896.9350  -0.0983  0.040   0.0015 0.22
566: 14  7  7 16    13  7  6 15         312896.9350   0.0819  0.040   0.0015 0.28
567: 14  7  8 13    13  7  7 12         312896.9350  -0.0983  0.040   0.0015 0.22
568: 14  7  8 16    13  7  7 15         312896.9350   0.0819  0.040   0.0015 0.28
569: 14  6  8 14    13  6  7 13         312942.5110  -0.0569  0.040  -0.0080 0.24
570: 14  6  8 15    13  6  7 14         312942.5110   0.0374  0.040  -0.0080 0.26
571: 14  6  9 14    13  6  8 13         312942.5110  -0.0569  0.040  -0.0080 0.24
572: 14  6  9 15    13  6  8 14         312942.5110   0.0374  0.040  -0.0080 0.26
573: 14  6  8 13    13  6  7 12         312944.0050  -0.0356  0.040   0.0164 0.22
574: 14  6  8 16    13  6  7 15         312944.0050   0.0583  0.040   0.0164 0.28
575: 14  6  9 13    13  6  8 12         312944.0050  -0.0356  0.040   0.0164 0.22
576: 14  6  9 16    13  6  8 15         312944.0050   0.0583  0.040   0.0164 0.28
577: 14  5  9 14    13  5  8 13         312985.0160  -0.0454  0.040  -0.0344 0.24
578: 14  5  9 15    13  5  8 14         312985.0160  -0.0241  0.040  -0.0344 0.26
579: 14  5 10 14    13  5  9 13         312985.0160  -0.0453  0.040  -0.0344 0.24
580: 14  5 10 15    13  5  9 14         312985.0160  -0.0240  0.040  -0.0344 0.26
581: 14  5  9 13    13  5  8 12         312986.0970   0.0128  0.040   0.0245 0.22
582: 14  5  9 16    13  5  8 15         312986.0970   0.0338  0.040   0.0245 0.28
583: 14  5 10 13    13  5  9 12         312986.0970   0.0129  0.040   0.0245 0.22
584: 14  5 10 16    13  5  9 15         312986.0970   0.0339  0.040   0.0245 0.28
585: 14  2 13 13    13  2 12 12         312987.5480  -0.0158  0.040   0.0022 0.22
586: 14  2 13 14    13  2 12 13         312987.5480   0.1476  0.040   0.0022 0.24
587: 14  2 13 15    13  2 12 14         312987.5480   0.0293  0.040   0.0022 0.26
588: 14  2 13 16    13  2 12 15         312987.5480  -0.1342  0.040   0.0022 0.28
589: 14  4 10 14    13  4  9 13         313024.8040   0.0441  0.040   0.0397 0.24
590: 14  4 10 15    13  4  9 14         313024.8040   0.0055  0.040   0.0397 0.26
591: 14  4 11 14    13  4 10 13         313024.8040   0.0751  0.040   0.0397 0.24
592: 14  4 11 15    13  4 10 14         313024.8040   0.0366  0.040   0.0397 0.26
593: 14  4 10 13    13  4  9 12         313025.3640  -0.0504  0.040  -0.0564 0.22
594: 14  4 10 16    13  4  9 15         313025.3640  -0.0892  0.040  -0.0564 0.28
595: 14  4 11 13    13  4 10 12         313025.3640  -0.0193  0.040  -0.0564 0.22
596: 14  4 11 16    13  4 10 15         313025.3640  -0.0581  0.040  -0.0564 0.28
597: 14  3 12 13    13  3 11 12         313066.5820  -0.1321  0.040   0.0059 0.22
598: 14  3 12 14    13  3 11 13         313066.5820   0.2361  0.040   0.0059 0.24
599: 14  3 12 15    13  3 11 14         313066.5820   0.1510  0.040   0.0059 0.26
600: 14  3 12 16    13  3 11 15         313066.5820  -0.2173  0.040   0.0059 0.28
601: 14  3 11 13    13  3 10 12         313071.8230  -0.1453  0.040  -0.0073 0.22
602: 14  3 11 14    13  3 10 13         313071.8230   0.2230  0.040  -0.0073 0.24
603: 14  3 11 15    13  3 10 14         313071.8230   0.1379  0.040  -0.0073 0.26
604: 14  3 11 16    13  3 10 15         313071.8230  -0.2304  0.040  -0.0073 0.28
605: 14  2 12 13    13  2 11 12         313326.0200   0.0114  0.040   0.0300 0.22
606: 14  2 12 14    13  2 11 13         313326.0200   0.1758  0.040   0.0300 0.24
607: 14  2 12 15    13  2 11 14         313326.0200   0.0576  0.040   0.0300 0.26
608: 14  2 12 16    13  2 11 15         313326.0200  -0.1069  0.040   0.0300 0.28
609: 14  1 13 13    13  1 12 12         314994.8400   0.0595  0.040   0.0056 0.22
610: 14  1 13 14    13  1 12 13         314994.8400   0.1001  0.040   0.0056 0.24
611: 14  1 13 15    13  1 12 14         314994.8400  -0.0382  0.040   0.0056 0.26
612: 14  1 13 16    13  1 12 15         314994.8400  -0.0789  0.040   0.0056 0.28
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PARAMETERS IN FIT (values truncated and Nlines statistics):

      10000              A  /MHz        95358.5(55)                      1
      20000              B  /MHz        11330.5476(88)                   2
      30000              C  /MHz        11039.9541(88)                   3
        200        Delta_J  /kHz           12.0282(37)                   4
       1100       Delta_JK  /kHz          122.738(21)                    5
       2000        Delta_K  /kHz         [928.936]                       6
      40100        delta_J  /kHz            0.2827(30)                    7
      41000        delta_K  /kHz           60.7(43)                       8
        300          Phi_J  /Hz          [-0.002656]                     9
       1200         Phi_JK  /Hz          [ 0.306]                       10
       2100         Phi_KJ  /Hz          [ 2.655]                       11
       3000          Phi_K  /Hz          [32.]                          12
      40200          phi_J  /Hz          [ 0.000128]                    13
      41100         phi_JK  /Hz          [ 0.248]                       14
      42000          phi_K  /Hz          [23.]                          15
   110010000          X_aa  /MHz          -74.461(35)                   16
  -110030000          X_cc  /MHz           74.461(35)        = -1.00000 * 16
   110020000          X_bb  /MHz           37.307(70)                   17
  -110030000          X_cc  /MHz          -37.307(70)        = -1.00000 * 17

 MICROWAVE AVG =       -0.000531 MHz, IR AVG =          0.00000
 MICROWAVE RMS =        0.033418 MHz, IR RMS =          0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.88846          0.88846

  distinct frequency lines in fit:   221
        distinct parameters of fit:     9

                                upper state  lower state      overall
         limits of quantum number  1:    4   14       3   13       3   14
         limits of quantum number  2:    0   12       0   12       0   12
         limits of quantum number  3:    1   14       0   13       0   14
         limits of quantum number  4:    3   16       2   15       2   16

                  frequency range:      88881        314994


 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
 (values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

      10000              A  /MHz        95358.5(50)                      1
      20000              B  /MHz        11330.5476(80)                   2
      30000              C  /MHz        11039.9541(80)                   3
        200        Delta_J  /kHz           12.0282(34)                   4
       1100       Delta_JK  /kHz          122.738(19)                    5
       2000        Delta_K  /kHz         [928.936]                       6
      40100        delta_J  /kHz            0.2827(27)                    7
      41000        delta_K  /kHz           60.7(39)                       8
        300          Phi_J  /Hz          [-0.002656]                     9
       1200         Phi_JK  /Hz          [ 0.306]                       10
       2100         Phi_KJ  /Hz          [ 2.655]                       11
       3000          Phi_K  /Hz          [32.]                          12
      40200          phi_J  /Hz          [ 0.000128]                    13
      41100         phi_JK  /Hz          [ 0.248]                       14
      42000          phi_K  /Hz          [23.]                          15
   110010000          X_aa  /MHz          -74.461(32)                   16
  -110030000          X_cc  /MHz           74.461(32)        = -1.00000 * 16
   110020000          X_bb  /MHz           37.307(63)                   17
  -110030000          X_cc  /MHz          -37.307(63)        = -1.00000 * 17

 CORRELATION COEFFICIENTS, C.ij:

           A         B         C      -Delta_J -Delta_J -delta_J -delta_K X_aa

A         1.0000
B        -0.5199   1.0000
C         0.5219  -0.9968   1.0000
-Delta_J  0.4904  -0.9366   0.9132   1.0000
-Delta_JK -0.5235  0.9747  -0.9757  -0.9454   1.0000
-delta_J  0.0559  -0.1745   0.1708   0.0469  -0.0337   1.0000
-delta_K  0.5385  -0.9849   0.9857   0.9355  -0.9898   0.0346   1.0000
X_aa      0.0023   0.0048  -0.0033  -0.0020  -0.0034  -0.0356   0.0034   1.0000
X_bb     -0.0062  -0.0148   0.0133   0.0039   0.0020   0.0760  -0.0019  -0.6103

          X_bb

X_bb      1.0000
```

```
Mean value of |C.ij|, i.ne.j =   0.3759
Mean value of  C.ij,  i.ne.j =  -0.0551


Worst correlations, with absolute value greater than 0.9950:

     30000  C          <->       20000  B          -0.996809


Worst fitted lines (obs-calc/error):

  273:   -2.6         65:    2.6       209:   -2.4       155:   -2.3
  355:    2.3        117:   -2.2        21:   -2.1         7:    2.0
  531:    1.9         81:    1.7       131:   -1.6         1:    1.6
  201:    1.6        115:   -1.6       347:    1.6       447:    1.6
  457:   -1.6        351:    1.5        41:   -1.5        61:   -1.5
  439:    1.5         37:    1.5       401:    1.5        57:   -1.5
  231:   -1.5        113:    1.5       127:   -1.4       349:   -1.4
  593:   -1.4        163:    1.4       111:    1.4        79:    1.4
   34:    1.4        527:    1.3       405:    1.3       103:    1.3
    6:   -1.3        497:   -1.3       353:   -1.2        25:   -1.2
  321:    1.2        431:    1.2       291:   -1.2       121:   -1.2
  409:    1.2         13:    1.2       343:    1.1       177:   -1.1
  153:   -1.1        271:   -1.1

  273: 11  8  3 10   10  8  2  9          245845.9510  -0.1054   0.040  -0.1054 0.50
   65:  8  0  8  7    7  0  7  6          178876.5560   0.3778   0.040   0.1053 0.18
  209: 10  6  4  9    9  6  3  8          223575.7340  -0.0955   0.040  -0.0955 0.50
  155:  9  3  6  9    8  3  5  8          201291.3880  -0.3694   0.040  -0.0916 0.24
  355: 12  9  3 11   11  9  2 10          268131.9840   0.0907   0.040   0.0907 0.50
  117:  9  7  2  9    8  7  1  8          201191.2550  -0.0896   0.040  -0.0897 0.50
   21:  4  0  4  5    3  0  3  4           89472.0167   0.0226   0.020  -0.0416 0.34
    7:  4  1  4  3    3  1  3  3           88909.9442   0.0392   0.020
  531: 14 12  2 13   13 12  1 12          312569.1120   0.0756   0.040   0.0756 0.50
   81:  8  4  4  8    7  4  3  7          178911.8810   0.0659   0.040   0.0663 0.50

                              / SPFIT output reformatted with PIFORM
```

Table S.4. Fit of the rotational transitions of $^{13}CHD_2^{37}Cl$ in PIFORM format

```
13CHD2Cl -- 37Cl                                Tue Mar 18 09:44:55 2025


-------------------------------------------------------------------------=========
                                           obs       o-c    error    blends    Notes
                                                                     o-c    wt
     / instead of : below denotes (o-c)>3*err
-------------------------------------------------------------------------=========
   1:  4  1  4  4    3  1  3  3          87382.6597  -0.0125  0.020
   2:  4  1  4  5    3  1  3  4          87383.4362   0.0106  0.020
   3:  4  1  4  3    3  1  3  2          87384.1273  -0.0131  0.020
   4:  4  1  4  6    3  1  3  5          87384.9109   0.0162  0.020
   5:  4  1  4  4    3  1  3  4          87387.7713  -0.0035  0.020
   6:  4  3  1  5    3  3  0  4          87931.1715   0.0164  0.020   0.0197 0.50
   7:  4  3  2  5    3  3  1  4          87931.1715   0.0229  0.020   0.0197 0.50
   8:  4  3  1  4    3  3  0  3          87937.9193  -0.0005  0.020   0.0027 0.50
   9:  4  3  2  4    3  3  1  3          87937.9193   0.0059  0.020   0.0027 0.50
  10:  4  0  4  3    3  0  3  2          87939.1044   0.0549  0.020  -0.0014 0.28
  11:  4  0  4  4    3  0  3  3          87939.1044   0.0548  0.020  -0.0014 0.37
  12:  4  2  3  5    3  2  2  4          87939.1044  -0.1055  0.020  -0.0014 0.35
  13:  4  0  4  5    3  0  3  4          87940.7590   0.0046  0.020   0.0050 0.43
  14:  4  0  4  6    3  0  3  5          87940.7590   0.0051  0.020   0.0050 0.57
  15:  4  3  1  6    3  3  0  5          87944.3759   0.0029  0.020   0.0062 0.50
  16:  4  3  2  6    3  3  1  5          87944.3759   0.0094  0.020   0.0062 0.50
  17:  4  2  3  6    3  2  2  5          87945.1067   0.0207  0.020
  18:  4  2  2  5    3  2  1  4          87946.1664  -0.0250  0.020
  19:  4  2  3  3    3  2  2  2          87947.1648   0.0204  0.020
  20:  4  2  2  4    3  2  1  3          87948.2734   0.0205  0.020
  21:  4  3  1  3    3  3  0  2          87951.1208  -0.0195  0.020  -0.0163 0.50
  22:  4  3  2  3    3  3  1  2          87951.1208  -0.0130  0.020  -0.0163 0.50
  23:  4  2  2  6    3  2  1  5          87952.0796   0.0114  0.020
  24:  4  2  2  3    3  2  1  2          87954.1153  -0.0113  0.020
  25:  4  1  3  4    3  1  2  3          88504.4866  -0.0123  0.020
  26:  4  1  3  5    3  1  2  4          88505.2688  -0.0028  0.020
  27:  4  1  3  3    3  1  2  2          88505.9614  -0.0056  0.020
  28:  4  1  3  6    3  1  2  5          88506.7435   0.0027  0.020
  29:  8  1  8  7    7  1  7  6         174739.5820   0.0791  0.040  -0.0090 0.20
  30:  8  1  8  8    7  1  7  7         174739.5820   0.2536  0.040  -0.0090 0.23
  31:  8  1  8  9    7  1  7  8         174739.5820  -0.0560  0.040  -0.0090 0.26
  32:  8  1  8 10    7  1  7  9         174739.5820  -0.2306  0.040  -0.0090 0.30
  33:  8  7  1  9    7  7  0  8         175780.4500   0.0068  0.040   0.0069 0.50
  34:  8  7  2  9    7  7  1  8         175780.4500   0.0068  0.040   0.0069 0.50
  35:  8  7  1  8    7  7  0  7         175782.6150   0.0503  0.040   0.0504 0.50
  36:  8  7  2  8    7  7  1  7         175782.6150   0.0503  0.040   0.0504 0.50
  37:  8  7  1 10    7  7  0  9         175789.0190   0.0085  0.040   0.0086 0.50
  38:  8  7  2 10    7  7  1  9         175789.0190   0.0085  0.040   0.0086 0.50
  39:  8  7  1  7    7  7  0  6         175791.0820  -0.0514  0.040  -0.0514 0.50
  40:  8  7  2  7    7  7  1  6         175791.0820  -0.0514  0.040  -0.0514 0.50
  41:  8  6  2  9    7  6  1  8         175807.0630   0.0051  0.040   0.0051 0.50
  42:  8  6  3  9    7  6  2  8         175807.0630   0.0051  0.040   0.0051 0.50
  43:  8  6  2  8    7  6  1  7         175808.5040  -0.0169  0.040  -0.0169 0.50
  44:  8  6  3  8    7  6  2  7         175808.5040  -0.0169  0.040  -0.0169 0.50
  45:  8  6  2 10    7  6  1  9         175813.3370  -0.0157  0.040  -0.0157 0.50
  46:  8  6  3 10    7  6  2  9         175813.3370  -0.0157  0.040  -0.0157 0.50
  47:  8  6  2  7    7  6  1  6         175814.8070  -0.0087  0.040  -0.0088 0.50
  48:  8  6  3  7    7  6  2  6         175814.8070  -0.0087  0.040  -0.0088 0.50
  49:  8  0  8  7    7  0  7  6         175818.1070   0.2233  0.040   0.0181 0.20
  50:  8  0  8  8    7  0  7  7         175818.1070   0.2220  0.040   0.0181 0.23
  51:  8  0  8  9    7  0  7  8         175818.1070  -0.1406  0.040   0.0181 0.26
  52:  8  0  8 10    7  0  7  9         175818.1070  -0.1393  0.040   0.0181 0.30
  53:  8  5  3  9    7  5  2  8         175830.0010   0.0199  0.040   0.0200 0.50
  54:  8  5  4  9    7  5  3  8         175830.0010   0.0199  0.040   0.0200 0.50
  55:  8  5  3  8    7  5  2  7         175830.8940   0.0073  0.040   0.0073 0.50
  56:  8  5  4  8    7  5  3  7         175830.8940   0.0073  0.040   0.0073 0.50
  57:  8  5  3 10    7  5  2  9         175834.3300  -0.0227  0.040  -0.0228 0.50
  58:  8  5  4 10    7  5  3  9         175834.3300  -0.0227  0.040  -0.0228 0.50
  59:  8  5  3  7    7  5  2  6         175835.2800   0.0223  0.040   0.0223 0.50
  60:  8  5  4  7    7  5  3  6         175835.2800   0.0223  0.040   0.0223 0.50
  61:  8  4  4  8    7  4  3  7         175849.7930  -0.2535  0.040  -0.0141 0.23
  62:  8  4  4  9    7  4  3  8         175849.7930   0.1957  0.040  -0.0141 0.27
  63:  8  4  5  8    7  4  4  7         175849.7930  -0.2530  0.040  -0.0141 0.23
  64:  8  4  5  9    7  4  4  8         175849.7930   0.1962  0.040  -0.0141 0.27
  65:  8  4  4  7    7  4  3  6         175852.5380  -0.3058  0.040  -0.0387 0.20
  66:  8  4  4 10    7  4  3  9         175852.5380   0.1426  0.040  -0.0387 0.30
  67:  8  4  5  7    7  4  4  6         175852.5380  -0.3053  0.040  -0.0387 0.20
  68:  8  4  5 10    7  4  4  9         175852.5380   0.1430  0.040  -0.0387 0.30
```

```
 69:  8  2  7  8    7  2  6  7       175860.2370   0.0260   0.040   -0.0589 0.47
 70:  8  2  7  9    7  2  6  8       175860.2370  -0.1335   0.040   -0.0589 0.53
 71:  8  2  7  7    7  2  6  6       175861.0340   0.1239   0.040    0.0288 0.40
 72:  8  2  7 10    7  2  6  9       175861.0340  -0.0358   0.040    0.0288 0.60
 73:  8  3  5  8    7  3  4  7       175867.2140  -0.1957   0.040   -0.0093 0.23
 74:  8  3  5  9    7  3  4  8       175867.2140  -0.1015   0.040   -0.0093 0.27
 75:  8  3  6  8    7  3  5  7       175867.2140   0.0769   0.040   -0.0093 0.23
 76:  8  3  6  9    7  3  5  8       175867.2140   0.1711   0.040   -0.0093 0.27
 77:  8  3  5  7    7  3  4  6       175868.8000  -0.1833   0.040    0.0088 0.20
 78:  8  3  5 10    7  3  4  9       175868.8000  -0.0897   0.040    0.0088 0.30
 79:  8  3  6  7    7  3  5  6       175868.8000   0.0894   0.040    0.0088 0.20
 80:  8  3  6 10    7  3  5  9       175868.8000   0.1830   0.040    0.0088 0.30
 81:  8  2  6  8    7  2  5  7       175918.8610   0.0640   0.040   -0.0208 0.47
 82:  8  2  6  9    7  2  5  8       175918.8610  -0.0953   0.040   -0.0208 0.53
 83:  8  2  6  7    7  2  5  6       175919.6270   0.1296   0.040    0.0345 0.40
 84:  8  2  6 10    7  2  5  9       175919.6270  -0.0300   0.040    0.0345 0.60
 85:  8  1  7  7    7  1  6  6       176982.2270   0.1397   0.040    0.0493 0.20
 86:  8  1  7  8    7  1  6  7       176982.2270   0.3142   0.040    0.0493 0.23
 87:  8  1  7  9    7  1  6  8       176982.2270   0.0003   0.040    0.0493 0.26
 88:  8  1  7 10    7  1  6  9       176982.2270  -0.1741   0.040    0.0493 0.30
 89:  9  1  9 11    8  1  8 10       196570.7650  -0.1671   0.040    0.0045 0.29
 90:  9  1  9  8    8  1  8  7       196570.7650   0.0832   0.040    0.0045 0.21
 91:  9  1  9  9    8  1  8  8       196570.7650   0.2052   0.040    0.0045 0.23
 92:  9  1  9 10    8  1  8  9       196570.7650  -0.0451   0.040    0.0045 0.26
 93:  9  8  1 11    8  8  0 10       197722.8420   0.0772   0.040    0.0773 0.50
 94:  9  8  2 11    8  8  1 10       197722.8420   0.0772   0.040    0.0773 0.50
 95:  9  8  1  8    8  8  0  7       197724.5460   0.0577   0.040    0.0577 0.50
 96:  9  8  2  8    8  8  1  7       197724.5460   0.0577   0.040    0.0577 0.50
 97:  9  7  2 10    8  7  1  9       197748.6090   0.0439   0.040    0.0440 0.50
 98:  9  7  3 10    8  7  2  9       197748.6090   0.0439   0.040    0.0440 0.50
 99:  9  7  2  9    8  7  1  8       197749.8810   0.0633   0.040    0.0634 0.50
100:  9  7  3  9    8  7  2  8       197749.8810   0.0633   0.040    0.0634 0.50
101:  9  7  2 11    8  7  1 10       197754.5260  -0.0365   0.040   -0.0365 0.50
102:  9  7  3 11    8  7  2 10       197754.5260  -0.0365   0.040   -0.0365 0.50
103:  9  7  2  8    8  7  1  7       197755.8190   0.0036   0.040    0.0037 0.50
104:  9  7  3  8    8  7  2  7       197755.8190   0.0036   0.040    0.0037 0.50
105:  9  0  9 11    8  0  8 10       197770.5200  -0.0977   0.040    0.0272 0.29
106:  9  0  9  8    8  0  8  7       197770.5200   0.1857   0.040    0.0272 0.21
107:  9  0  9  9    8  0  8  8       197770.5200   0.1842   0.040    0.0272 0.23
108:  9  0  9 10    8  0  8  9       197770.5200  -0.0992   0.040    0.0272 0.26
109:  9  6  3 10    8  6  2  9       197777.9940  -0.0309   0.040   -0.0310 0.50
110:  9  6  4 10    8  6  3  9       197777.9940  -0.0309   0.040   -0.0310 0.50
111:  9  6  3  9    8  6  2  8       197778.9160   0.0455   0.040    0.0456 0.50
112:  9  6  4  9    8  6  3  8       197778.9160   0.0455   0.040    0.0456 0.50
113:  9  6  3 11    8  6  2 10       197782.3750  -0.0565   0.040   -0.0566 0.50
114:  9  6  4 11    8  6  3 10       197782.3750  -0.0565   0.040   -0.0566 0.50
115:  9  6  3  8    8  6  2  7       197783.3080   0.0314   0.040    0.0314 0.50
116:  9  6  4  8    8  6  3  7       197783.3080   0.0314   0.040    0.0314 0.50
117:  9  5  4  9    8  5  3  8       197803.7680  -0.2552   0.040    0.0094 0.24
118:  9  5  4 10    8  5  3  9       197803.7680   0.2454   0.040    0.0094 0.26
119:  9  5  5  9    8  5  4  8       197803.7680  -0.2552   0.040    0.0094 0.24
120:  9  5  5 10    8  5  4  9       197803.7680   0.2454   0.040    0.0094 0.26
121:  9  5  4 11    8  5  3 10       197806.7470   0.1641   0.040   -0.0437 0.29
122:  9  5  4  8    8  5  3  7       197806.7470  -0.3359   0.040   -0.0437 0.21
123:  9  5  5 11    8  5  4 10       197806.7470   0.1641   0.040   -0.0437 0.29
124:  9  5  5  8    8  5  4  7       197806.7470  -0.3359   0.040   -0.0437 0.21
125:  9  4  5  9    8  4  4  8       197825.6840  -0.1418   0.040   -0.0258 0.24
126:  9  4  5 10    8  4  4  9       197825.6840   0.0766   0.040   -0.0258 0.26
127:  9  4  6  9    8  4  5  8       197825.6840  -0.1407   0.040   -0.0258 0.24
128:  9  4  6 10    8  4  5  9       197825.6840   0.0777   0.040   -0.0258 0.26
129:  9  4  5 11    8  4  4 10       197827.6330   0.0669   0.040   -0.0231 0.29
130:  9  4  5  8    8  4  4  7       197827.6330  -0.1510   0.040   -0.0231 0.21
131:  9  4  6 11    8  4  5 10       197827.6330   0.0680   0.040   -0.0231 0.29
132:  9  4  6  8    8  4  5  7       197827.6330  -0.1499   0.040   -0.0231 0.21
133:  9  2  8 11    8  2  7 10       197833.1780  -0.3247   0.040   -0.0115 0.29
134:  9  2  8  8    8  2  7  7       197833.1780  -0.1667   0.040   -0.0115 0.21
135:  9  2  8  9    8  2  7  8       197833.1780   0.3225   0.040   -0.0115 0.23
136:  9  2  8 10    8  2  7  9       197833.1780   0.1646   0.040   -0.0115 0.26
137:  9  3  6  9    8  3  5  8       197846.0250  -0.3163   0.040   -0.0670 0.24
138:  9  3  6 10    8  3  5  9       197846.0250  -0.3173   0.040   -0.0670 0.26
139:  9  3  7  9    8  3  6  8       197846.0250   0.1834   0.040   -0.0670 0.24
140:  9  3  7 10    8  3  6  9       197846.0250   0.1825   0.040   -0.0670 0.26
141:  9  3  6 11    8  3  5 10       197847.2850  -0.1593   0.040    0.0912 0.29
142:  9  3  6  8    8  3  5  7       197847.2850  -0.1579   0.040    0.0912 0.21
143:  9  3  7 11    8  3  6 10       197847.2850   0.3405   0.040    0.0912 0.29
144:  9  3  7  8    8  3  6  7       197847.2850   0.3419   0.040    0.0912 0.21
145:  9  2  7 11    8  2  6 10       197916.8930  -0.2603   0.040    0.0536 0.29
146:  9  2  7  8    8  2  6  7       197916.8930  -0.1024   0.040    0.0536 0.21
```

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147:  9  2  7  9     8  2  6  8        197916.8930   0.3883   0.040    0.0536 0.23
148:  9  2  7 10     8  2  6  9        197916.8930   0.2305   0.040    0.0536 0.26
149:  9  1  8 11     8  1  7 10        199093.1460  -0.1719   0.040    0.0011 0.29
150:  9  1  8  8     8  1  7  7        199093.1460   0.0817   0.040    0.0011 0.21
151:  9  1  8  9     8  1  7  8        199093.1460   0.2037   0.040    0.0011 0.23
152:  9  1  8 10     8  1  7  9        199093.1460  -0.0499   0.040    0.0011 0.26
153: 10  1 10 11     9  1  9 10        218397.9580  -0.0665   0.040   -0.0185 0.26
154: 10  1 10 12     9  1  9 11        218397.9580  -0.1551   0.040   -0.0185 0.29
155: 10  1 10  9     9  1  9  8        218397.9580   0.0509   0.040   -0.0185 0.21
156: 10  1 10 10     9  1  9  9        218397.9580   0.1395   0.040   -0.0185 0.24
157: 10  8  2 11     9  8  1 10        219676.6190  -0.0390   0.040   -0.0391 0.50
158: 10  8  3 11     9  8  2 10        219676.6190  -0.0390   0.040   -0.0391 0.50
159: 10  8  2 10     9  8  1  9        219677.7410   0.0036   0.040    0.0036 0.50
160: 10  8  3 10     9  8  2  9        219677.7410   0.0036   0.040    0.0036 0.50
161: 10  8  2 12     9  8  1 11        219682.2990  -0.0561   0.040   -0.0561 0.50
162: 10  8  3 12     9  8  2 11        219682.2990  -0.0561   0.040   -0.0561 0.50
163: 10  8  2  9     9  8  1  8        219683.4690   0.0343   0.040    0.0344 0.50
164: 10  8  3  9     9  8  2  8        219683.4690   0.0343   0.040    0.0344 0.50
165: 10  0 10 11     9  0  9 10        219714.1890  -0.0688   0.040    0.0343 0.26
166: 10  0 10 12     9  0  9 11        219714.1890  -0.0672   0.040    0.0343 0.29
167: 10  0 10  9     9  0  9  8        219714.1890   0.1606   0.040    0.0343 0.21
168: 10  0 10 10     9  0  9  9        219714.1890   0.1589   0.040    0.0343 0.24
169: 10  7  3 12     9  7  2 11        219718.0340  -0.0221   0.040   -0.0221 0.50
170: 10  7  4 12     9  7  3 11        219718.0340  -0.0221   0.040   -0.0221 0.50
171: 10  7  3  9     9  7  2  8        219718.8840   0.0549   0.040    0.0550 0.50
172: 10  7  4  9     9  7  3  8        219718.8840   0.0549   0.040    0.0550 0.50
173: 10  6  4 11     9  6  3 10        219746.3960   0.1823   0.040   -0.0586 0.26
174: 10  6  4 10     9  6  3  9        219746.3960  -0.3254   0.040   -0.0586 0.24
175: 10  6  5 11     9  6  4 10        219746.3960   0.1823   0.040   -0.0586 0.26
176: 10  6  5 10     9  6  4  9        219746.3960  -0.3254   0.040   -0.0586 0.24
177: 10  6  4 12     9  6  3 11        219749.5780   0.1594   0.040   -0.0558 0.29
178: 10  6  4  9     9  6  3  8        219749.5780  -0.3478   0.040   -0.0558 0.21
179: 10  6  5 12     9  6  4 11        219749.5780   0.1594   0.040   -0.0558 0.29
180: 10  6  5  9     9  6  4  8        219749.5780  -0.3478   0.040   -0.0558 0.21
181: 10  5  5 11     9  5  4 10        219774.6230   0.1148   0.040   -0.0196 0.26
182: 10  5  5 10     9  5  4  9        219774.6230  -0.1683   0.040   -0.0196 0.24
183: 10  5  6 11     9  5  5 10        219774.6230   0.1148   0.040   -0.0196 0.26
184: 10  5  6 10     9  5  5  9        219774.6230  -0.1683   0.040   -0.0196 0.24
185: 10  5  5 12     9  5  4 11        219776.8520   0.1180   0.040   -0.0018 0.29
186: 10  5  5  9     9  5  4  8        219776.8520  -0.1645   0.040   -0.0018 0.21
187: 10  5  6 12     9  5  5 11        219776.8520   0.1180   0.040   -0.0018 0.29
188: 10  5  6  9     9  5  5  8        219776.8520  -0.1645   0.040   -0.0018 0.21
189: 10  4  6 11     9  4  5 10        219799.3530   0.0191   0.040   -0.0268 0.26
190: 10  4  6 10     9  4  5  9        219799.3530  -0.0801   0.040   -0.0268 0.24
191: 10  4  7 11     9  4  6 10        219799.3530   0.0215   0.040   -0.0268 0.26
192: 10  4  7 10     9  4  6  9        219799.3530  -0.0777   0.040   -0.0268 0.24
193: 10  4  6 12     9  4  5 11        219800.7800   0.0215   0.040   -0.0192 0.29
194: 10  4  6  9     9  4  5  8        219800.7800  -0.0773   0.040   -0.0192 0.21
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196: 10  4  7  9     9  4  6  8        219800.7800  -0.0749   0.040   -0.0192 0.21
197: 10  2  9 11     9  2  8 10        219802.1880   0.1223   0.040    0.0091 0.26
198: 10  2  9 12     9  2  8 11        219802.1880  -0.2335   0.040    0.0091 0.29
199: 10  2  9  9     9  2  8  8        219802.1880  -0.0874   0.040    0.0091 0.21
200: 10  2  9 10     9  2  8  9        219802.1880   0.2683   0.040    0.0091 0.24
201: 10  3  8 11     9  3  7 10        219822.6580  -0.0915   0.040   -0.0707 0.53
202: 10  3  8 10     9  3  7  9        219822.6580  -0.0477   0.040   -0.0707 0.47
203: 10  3  7 11     9  3  6 10        219823.5400  -0.0661   0.040   -0.0187 0.26
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206: 10  3  8  9     9  3  7  8        219823.5400   0.0330   0.040   -0.0187 0.21
207: 10  3  7 12     9  3  6 11        219824.4370   0.0293   0.040    0.0480 0.58
208: 10  3  7  9     9  3  6  8        219824.4370   0.0733   0.040    0.0480 0.42
209: 10  2  8 11     9  2  7 10        219917.1230   0.1210   0.040    0.0070 0.26
210: 10  2  8 12     9  2  7 11        219917.1230  -0.2364   0.040    0.0070 0.29
211: 10  2  8  9     9  2  7  8        219917.1230  -0.0905   0.040    0.0070 0.21
212: 10  2  8 10     9  2  7  9        219917.1230   0.2669   0.040    0.0070 0.24
213: 10  1  9 11     9  1  8 10        221199.9070  -0.0534   0.040   -0.0043 0.26
214: 10  1  9 12     9  1  8 11        221199.9070  -0.1421   0.040   -0.0043 0.29
215: 10  1  9  9     9  1  8  8        221199.9070   0.0665   0.040   -0.0043 0.21
216: 10  1  9 10     9  1  8  9        221199.9070   0.1551   0.040   -0.0043 0.24
217: 11  1 11 11    10  1 10 10        240220.8230   0.1319   0.040    0.0046 0.24
218: 11  1 11 12    10  1 10 11        240220.8230  -0.0402   0.040    0.0046 0.26
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220: 11  1 11 10    10  1 10  9        240220.8230   0.0656   0.040    0.0046 0.22
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222: 11  9  3 12    10  9  2 11        241589.5820  -0.0593   0.040   -0.0594 0.50
223: 11  9  2 11    10  9  1 10        241590.6340   0.0558   0.040    0.0558 0.50
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228: 11  9  3 10   10  9  2  9        241596.0770   0.0907  0.040   0.0908 0.50
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234: 11  8  4 13   10  8  3 12        241639.5310   0.0066  0.040   0.0066 0.50
235: 11  8  3 10   10  8  2  9        241640.2460   0.0206  0.040   0.0206 0.50
236: 11  8  4 10   10  8  3  9        241640.2460   0.0206  0.040   0.0206 0.50
237: 11  0 11 11   10  0 10 10        241648.1540   0.1214  0.040   0.0201 0.24
238: 11  0 11 12   10  0 10 11        241648.1540  -0.0658  0.040   0.0201 0.26
239: 11  0 11 13   10  0 10 12        241648.1540  -0.0640  0.040   0.0201 0.29
240: 11  0 11 10   10  0 10  9        241648.1540   0.1232  0.040   0.0201 0.22
241: 11  7  4 11   10  7  3 10        241676.0550  -0.2717  0.040  -0.0138 0.24
242: 11  7  4 12   10  7  3 11        241676.0550   0.2213  0.040  -0.0138 0.26
243: 11  7  5 11   10  7  4 10        241676.0550  -0.2717  0.040  -0.0138 0.24
244: 11  7  5 12   10  7  4 11        241676.0550   0.2213  0.040  -0.0138 0.26
245: 11  7  4 13   10  7  3 12        241679.2760   0.1707  0.040  -0.0418 0.28
246: 11  7  4 10   10  7  3  9        241679.2760  -0.3220  0.040  -0.0418 0.22
247: 11  7  5 13   10  7  4 12        241679.2760   0.1707  0.040  -0.0418 0.28
248: 11  7  5 10   10  7  4  9        241679.2760  -0.3220  0.040  -0.0418 0.22
249: 11  6  5 11   10  6  4 10        241711.6820  -0.1919  0.040  -0.0284 0.24
250: 11  6  5 12   10  6  4 11        241711.6820   0.1207  0.040  -0.0284 0.26
251: 11  6  6 11   10  6  5 10        241711.6820  -0.1919  0.040  -0.0284 0.24
252: 11  6  6 12   10  6  5 11        241711.6820   0.1207  0.040  -0.0284 0.26
253: 11  6  5 13   10  6  4 12        241714.0920   0.1270  0.040  -0.0076 0.28
254: 11  6  5 10   10  6  4  9        241714.0920  -0.1852  0.040  -0.0076 0.22
255: 11  6  6 13   10  6  5 12        241714.0920   0.1270  0.040  -0.0076 0.28
256: 11  6  6 10   10  6  5  9        241714.0920  -0.1852  0.040  -0.0076 0.22
257: 11  5  6 11   10  5  5 10        241742.8880  -0.0959  0.040  -0.0123 0.24
258: 11  5  6 12   10  5  5 11        241742.8880   0.0640  0.040  -0.0123 0.26
259: 11  5  7 11   10  5  6 10        241742.8880  -0.0959  0.040  -0.0123 0.24
260: 11  5  7 12   10  5  6 11        241742.8880   0.0640  0.040  -0.0123 0.26
261: 11  5  6 13   10  5  5 12        241744.5590   0.0657  0.040  -0.0031 0.28
262: 11  5  6 10   10  5  5  9        241744.5590  -0.0939  0.040  -0.0031 0.22
263: 11  5  7 13   10  5  6 12        241744.5590   0.0657  0.040  -0.0031 0.28
264: 11  5  7 10   10  5  6  9        241744.5590  -0.0939  0.040  -0.0031 0.22
265: 11  2 10 11   10  2  9 10        241767.2270   0.2044  0.040  -0.0014 0.24
266: 11  2 10 12   10  2  9 11        241767.2270   0.0728  0.040  -0.0014 0.26
267: 11  2 10 13   10  2  9 12        241767.2270  -0.1939  0.040  -0.0014 0.29
268: 11  2 10 10   10  2  9  9        241767.2270  -0.0622  0.040  -0.0014 0.22
269: 11  4  7 11   10  4  6 10        241770.6050  -0.0608  0.040  -0.0401 0.24
270: 11  4  7 12   10  4  6 11        241770.6050  -0.0257  0.040  -0.0401 0.26
271: 11  4  8 11   10  4  7 10        241770.6050  -0.0560  0.040  -0.0401 0.24
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273: 11  4  7 13   10  4  6 12        241771.7530   0.0538  0.040   0.0412 0.28
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277: 11  3  9 11   10  3  8 10        241797.7650   0.2315  0.040  -0.1042 0.24
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286: 11  2  9 12   10  2  8 11        241920.3540   0.0907  0.040   0.0156 0.26
287: 11  2  9 13   10  2  8 12        241920.3540  -0.1778  0.040   0.0156 0.29
288: 11  2  9 10   10  2  8  9        241920.3540  -0.0463  0.040   0.0156 0.22
289: 11  1 10 11   10  1  9 10        243301.9830   0.1165  0.040  -0.0120 0.24
290: 11  1 10 12   10  1  9 11        243301.9830  -0.0578  0.040  -0.0120 0.26
291: 11  1 10 13   10  1  9 12        243301.9830  -0.1241  0.040  -0.0120 0.29
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293: 12  1 12 11   11  1 11 10        262038.8770   0.0600  0.040   0.0063 0.22
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305: 12 10  2 13   11 10  1 12      263485.7780  -0.0549  0.040  -0.0549 0.50
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307: 12 10  2 12   11 10  1 11      263486.7250   0.0727  0.040   0.0727 0.50
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309: 12 10  2 14   11 10  1 13      263490.9180  -0.0504  0.040  -0.0505 0.50
310: 12 10  3 14   11 10  2 13      263490.9180  -0.0504  0.040  -0.0505 0.50
311: 12 10  2 11   11 10  1 10      263491.8700   0.0819  0.040   0.0819 0.50
312: 12 10  3 11   11 10  2 10      263491.8700   0.0819  0.040   0.0819 0.50
313: 12  0 12 11   11  0 11 10      263571.5050   0.0857  0.040  -0.0001 0.22
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322: 12  8  4 14   11  8  3 13      263594.0850   0.1695  0.040  -0.0350 0.28
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324: 12  8  5 14   11  8  4 13      263594.0850   0.1695  0.040  -0.0350 0.28
325: 12  7  5 12   11  7  4 11      263635.0010  -0.1813  0.040  -0.0136 0.24
326: 12  7  5 13   11  7  4 12      263635.0010   0.1405  0.040  -0.0136 0.26
327: 12  7  6 12   11  7  5 11      263635.0010  -0.1813  0.040  -0.0136 0.24
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342: 12  5  7 13   11  5  6 12      263708.2980   0.0067  0.040  -0.0352 0.26
343: 12  5  8 12   11  5  7 11      263708.2980  -0.0809  0.040  -0.0352 0.24
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346: 12  5  7 14   11  5  6 13      263709.6190   0.0435  0.040   0.0054 0.28
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377: 13  1 13 12   12  1 12 11      283851.7400   0.0637  0.040   0.0162 0.22
378: 13  1 13 13   12  1 12 12      283851.7400   0.1035  0.040   0.0162 0.24
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35

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401: 13 10   3 12   12 10   2 11        285433.4450  -0.3810  0.040  -0.0610 0.22
402: 13 10   3 15   12 10   2 14        285433.4450   0.1925  0.040  -0.0610 0.28
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414: 13  9   4 15   12  9   3 14        285492.3250   0.1748  0.040  -0.0193 0.28
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419: 13  8   6 13   12  8   5 12        285542.7710  -0.1732  0.040  -0.0074 0.24
420: 13  8   6 14   12  8   5 13        285542.7710   0.1460  0.040  -0.0074 0.26
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422: 13  8   5 15   12  8   4 14        285545.3330   0.1254  0.040  -0.0156 0.28
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424: 13  8   6 15   12  8   5 14        285545.3330   0.1254  0.040  -0.0156 0.28
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430: 13  7   6 15   12  7   5 14        285592.6530   0.0865  0.040  -0.0076 0.28
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435: 13  6   8 13   12  6   7 12        285633.1070  -0.0794  0.040  -0.0163 0.24
436: 13  6   8 14   12  6   7 13        285633.1070   0.0421  0.040  -0.0163 0.26
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443: 13  5   9 13   12  5   8 12        285670.6760  -0.0681  0.040  -0.0454 0.24
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458: 13  4   9 15   12  4   8 14        285705.7370  -0.0772  0.040  -0.0605 0.28
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480: 14   1 14 16    13   1 13 15         305658.9760  -0.0647  0.040   0.0014 0.28
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482: 14  10   4 15   13  10   3 14        307369.0960   0.1976  0.040   0.0001 0.26
483: 14  10   5 14   13  10   4 13        307369.0960  -0.2121  0.040   0.0001 0.24
484: 14  10   5 15   13  10   4 14        307369.0960   0.1976  0.040   0.0001 0.26
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492: 14   0 14 16    13   0 13 15         307382.8280  -0.0528  0.040  -0.0009 0.28
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495: 14   9   6 14   13   9   5 13        307433.2750  -0.1613  0.040  -0.0006 0.24
496: 14   9   6 15   13   9   5 14        307433.2750   0.1488  0.040  -0.0006 0.26
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499: 14   9   6 13   13   9   5 12        307435.8790  -0.1720  0.040  -0.0003 0.22
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504: 14   7   8 15   13   7   7 14        307542.8680   0.0660  0.040  -0.0027 0.26
505: 14   7   7 13   13   7   6 12        307544.4630  -0.0632  0.040   0.0156 0.22
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509: 14   6   8 14   13   6   7 13        307588.8090  -0.0606  0.040  -0.0221 0.24
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526: 14   2 13 14    13   2 12 13         307634.8170   0.1197  0.040   0.0052 0.24
527: 14   2 13 15    13   2 12 14         307634.8170   0.0263  0.040   0.0052 0.26
528: 14   2 13 16    13   2 12 15         307634.8170  -0.1024  0.040   0.0052 0.28
529: 14   4 10 13   13   4   9 12        307668.2420  -0.2296  0.040   0.0251 0.11
530: 14   4 10 14   13   4   9 13        307668.2420   0.2869  0.040   0.0251 0.12
531: 14   4 10 15   13   4   9 14        307668.2420   0.2565  0.040   0.0251 0.13
532: 14   4 10 16   13   4   9 15        307668.2420  -0.2602  0.040   0.0251 0.14
533: 14   4 11 13   13   4 10 12         307668.2420  -0.2027  0.040   0.0251 0.11
534: 14   4 11 14   13   4 10 13         307668.2420   0.3138  0.040   0.0251 0.12
535: 14   4 11 15   13   4 10 14         307668.2420   0.2834  0.040   0.0251 0.13
536: 14   4 11 16   13   4 10 15         307668.2420  -0.2333  0.040   0.0251 0.14
```

```
537: 14   3 12 13     13   3 11 12              307707.8570  -0.0932  0.040   0.0158 0.22
538: 14   3 12 14     13   3 11 13              307707.8570   0.1975  0.040   0.0158 0.24
539: 14   3 12 15     13   3 11 14              307707.8570   0.1304  0.040   0.0158 0.26
540: 14   3 12 16     13   3 11 15              307707.8570  -0.1604  0.040   0.0158 0.28
541: 14   3 11 13     13   3 10 12              307712.5670  -0.0996  0.040   0.0094 0.22
542: 14   3 11 14     13   3 10 13              307712.5670   0.1912  0.040   0.0094 0.24
543: 14   3 11 15     13   3 10 14              307712.5670   0.1240  0.040   0.0094 0.26
544: 14   3 11 16     13   3 10 15              307712.5670  -0.1668  0.040   0.0094 0.28
545: 14   2 12 13     13   2 11 12              307950.1040  -0.0126  0.040   0.0027 0.22
546: 14   2 12 14     13   2 11 13              307950.1040   0.1184  0.040   0.0027 0.24
547: 14   2 12 15     13   2 11 14              307950.1040   0.0251  0.040   0.0027 0.26
548: 14   2 12 16     13   2 11 15              307950.1040  -0.1059  0.040   0.0027 0.28
549: 14   1 13 13     13   1 12 12              309575.2490   0.0488  0.040   0.0058 0.22
550: 14   1 13 14     13   1 12 13              309575.2490   0.0805  0.040   0.0058 0.24
551: 14   1 13 15     13   1 12 14              309575.2490  -0.0292  0.040   0.0058 0.26
552: 14   1 13 16     13   1 12 15              309575.2490  -0.0609  0.040   0.0058 0.28
--------------------------------------------------------------------------------

PARAMETERS IN FIT (values truncated and Nlines statistics):

        10000           A  /MHz       95359.1(60)                         1
        20000           B  /MHz       11134.1477(92)                      2
        30000           C  /MHz       10853.4201(92)                      3
          200      Delta_J  /kHz          11.6429(38)                     4
         1100     Delta_JK  /kHz         118.942(22)                      5
         2000      Delta_K  /kHz        [932.871]                         6
        40100      delta_J  /kHz           0.2722(32)                     7
        41000      delta_K  /kHz          57.7(45)                        8
          300        Phi_J  /Hz        [-0.002532]                        9
         1200       Phi_JK  /Hz        [ 0.287]                          10
         2100       Phi_KJ  /Hz        [ 2.544]                          11
         3000        Phi_K  /Hz        [32.]                             12
        40200        phi_J  /Hz        [ 0.000122]                       13
        41100       phi_JK  /Hz        [ 0.235]                          14
        42000        phi_K  /Hz        [22.]                             15
     110010000        X_aa  /MHz         -58.751(57)                     16
    -110030000        X_cc  /MHz          58.751(57)       = -1.00000 * 16
     110020000        X_bb  /MHz          29.71(20)                      17
    -110030000        X_cc  /MHz         -29.71(20)        = -1.00000 * 17

 MICROWAVE AVG =       -0.000094 MHz, IR AVG =       0.00000
 MICROWAVE RMS =        0.035300 MHz, IR RMS =       0.00000
 END OF ITERATION  1 OLD, NEW RMS ERROR=        0.90468         0.90468

  distinct frequency lines in fit:   180
       distinct parameters of fit:     9

                              upper state  lower state       overall
        limits of quantum number  1:     4   14      3   13      3   14
        limits of quantum number  2:     0   12      0   12      0   12
        limits of quantum number  3:     1   14      0   13      0   14
        limits of quantum number  4:     3   16      2   15      2   16

                frequency range:       87382       309575


 PARAMETERS IN FIT WITH STANDARD ERRORS ON THOSE THAT ARE FITTED:
 (values rounded and degrees of freedom, Ndegf=Nlines-Nconst, statistics)

        10000           A  /MHz       95359.1(56)                         1
        20000           B  /MHz       11134.1477(85)                      2
        30000           C  /MHz       10853.4201(85)                      3
          200      Delta_J  /kHz          11.6429(35)                     4
         1100     Delta_JK  /kHz         118.943(20)                      5
         2000      Delta_K  /kHz        [932.871]                         6
        40100      delta_J  /kHz           0.2722(30)                     7
        41000      delta_K  /kHz          57.7(42)                        8
          300        Phi_J  /Hz        [-0.002532]                        9
         1200       Phi_JK  /Hz        [ 0.287]                          10
         2100       Phi_KJ  /Hz        [ 2.544]                          11
         3000        Phi_K  /Hz        [32.]                             12
        40200        phi_J  /Hz        [ 0.000122]                       13
        41100       phi_JK  /Hz        [ 0.235]                          14
        42000        phi_K  /Hz        [22.]                             15
     110010000        X_aa  /MHz         -58.751(53)                     16
    -110030000        X_cc  /MHz          58.751(53)       = -1.00000 * 16
     110020000        X_bb  /MHz          29.71(19)                      17
    -110030000        X_cc  /MHz         -29.71(19)        = -1.00000 * 17
```

```
 CORRELATION COEFFICIENTS, C.ij:

           A         B         C       -Delta_J -Delta_J -delta_J -delta_K X_aa

A          1.0000
B         -0.5172    1.0000
C          0.5184   -0.9963    1.0000
-Delta_J   0.4810   -0.9248    0.8967    1.0000
-Delta_JK -0.5164    0.9690   -0.9703   -0.9313    1.0000
-delta_J   0.0409   -0.1840    0.1826    0.0348   -0.0305    1.0000
-delta_K   0.5377   -0.9831    0.9834    0.9250   -0.9863    0.0318    1.0000
X_aa      -0.0050    0.0012    0.0058   -0.0315    0.0064    0.0267   -0.0036    1.0000
X_bb      -0.0004   -0.0158    0.0239   -0.0264   -0.0065    0.0770    0.0037   -0.2773

           X_bb

X_bb       1.0000

 Mean value of |C.ij|, i.ne.j =   0.3654
 Mean value of  C.ij,  i.ne.j =  -0.0461


 Worst correlations, with absolute value greater than 0.9950:

      30000  C         <->       20000  B          -0.996328


 Worst fitted lines (obs-calc/error):

   281:    2.9       277:   -2.6       141:    2.3       227:    2.3
   301:   -2.1       311:    2.0       453:    2.0       387:    1.9
    93:    1.9       307:    1.8       201:   -1.8       383:    1.7
   137:   -1.7       353:   -1.6        99:    1.6       391:    1.5
   401:   -1.5       457:   -1.5       221:   -1.5        69:   -1.5
   173:   -1.5        95:    1.4       113:   -1.4       161:   -1.4
   177:   -1.4       223:    1.4       171:    1.4       305:   -1.4
   297:   -1.3       357:    1.3       145:    1.3        39:   -1.3
   309:   -1.3        35:    1.3        18:   -1.2        85:    1.2
   207:    1.2       111:    1.1       521:    1.1       441:   -1.1
    97:    1.1       121:   -1.1       245:   -1.0        17:    1.0
   273:    1.0        20:    1.0        19:    1.0       269:   -1.0
   225:   -1.0         6:    1.0

   281: 11   3   8 11    10   3   7 10            241799.3780    0.4529   0.040    0.1172 0.24
   277: 11   3   9 11    10   3   8 10            241797.7650    0.2315   0.040   -0.1042 0.24
   141:  9   3   6 11     8   3   5 10            197847.2850   -0.1593   0.040    0.0912 0.29
   227: 11   9   2 10    10   9   1  9            241596.0770    0.0907   0.040    0.0908 0.50
   301: 12  11   1 14    11  11   0 13            263431.2350   -0.0853   0.040   -0.0853 0.50
   311: 12  10   2 11    11  10   1 10            263491.8700    0.0819   0.040    0.0819 0.50
   453: 13   4   9 13    12   4   8 12            285705.2290    0.0804   0.040    0.0781 0.24
   387: 13  12   1 12    12  12   0 11            285298.6530    0.0775   0.040    0.0776 0.50
    93:  9   8   1 11     8   8   0 10            197722.8420    0.0772   0.040    0.0773 0.50
   307: 12  10   2 12    11  10   1 11            263486.7250    0.0727   0.040    0.0727 0.50
                                              _____
                                             / SPFIT output reformatted with PIFORM
```

Table S.5. Part of the CFOUR output file of the CCSD(T)/V5Z-aV(5+*d*)Z harmonic frequency calculation for $^{12}CHD_2{}^{35}Cl$

```
   ***********************************************************************
      <<<    CCCCCC    CCCCCC   |||    CCCCCC    CCCCCC   >>>
       <<<     CCC       CCC    |||    CCC       CCC      >>>
        <<<    CCC       CCC    |||    CCC       CCC       >>>
      <<<      CCC       CCC    |||    CCC       CCC        >>>
        <<<    CCC       CCC    |||    CCC       CCC       >>>
       <<<     CCC       CCC    |||    CCC       CCC      >>>
        <<<    CCCCCC    CCCCCC  |||    CCCCCC    CCCCCC   >>>
   ***********************************************************************

    ******************************************************************
    * CFOUR Coupled-Cluster techniques for Computational Chemistry *
    ******************************************************************


   Department of Chemistry              Institut fuer Physikalische Chemie
   University of Texas at Austin        Universitaet Mainz
   Austin, TX  78712, USA               D-55099 Mainz, Germany

                   Version 1.0


                        Normal Coordinates

            A'                      A''                      A'
          719.17                  782.13                   883.84
          VIBRATION               VIBRATION                VIBRATION
C    0.062 0.6618  0.0000    0.0000  0.0000  0.3694    0.4286 -0.3572  0.0000
CL  -0.019-0.5637  0.0000    0.0000  0.0000 -0.1636   -0.1272  0.0910  0.0000
H   -0.030 0.3407  0.0108   -0.0287  0.6380 -0.0752   -0.2663  0.4025  0.0374
H   -0.030 0.3407 -0.0108    0.0287 -0.6380 -0.0752   -0.2663  0.4025 -0.0374
H   -0.014 0.0740  0.0000    0.0000  0.0000 -0.0985    0.0234 -0.4418  0.0000

            A'                      A'                       A''
         1073.53                 1279.36                  1332.59
          VIBRATION               VIBRATION                VIBRATION
C    0.271 0.2890  0.0000    0.0520 -0.2828  0.0000    0.0000  0.0000  0.2598
CL   0.002 0.0065  0.0000    0.0483 -0.0375  0.0000    0.0000  0.0000  0.0038
H   -0.345-0.3346  0.4314   -0.2531  0.1315  0.0572    0.3252 -0.1278 -0.0321
H   -0.345-0.3346 -0.4314   -0.2531  0.1315 -0.0572   -0.3252  0.1278 -0.0321
H    0.022-0.0897  0.0000    0.2517  0.8252  0.0000    0.0000  0.0000 -0.8284

            A'                      A''                      A'
         2252.79                 2363.83                  3152.90
          VIBRATION               VIBRATION                VIBRATION
C    0.231 0.1875  0.0000    0.0000  0.0000  0.4343    0.2745 -0.0620  0.0000
CL  -0.001-0.0036  0.0000    0.0000  0.0000 -0.0029   -0.0008 -0.0001  0.0000
H   -0.312-0.2121 -0.5552   -0.2979 -0.2011 -0.5258   -0.0058 -0.0118 -0.0288
H   -0.312-0.2121  0.5552    0.2979  0.2011 -0.5258   -0.0058 -0.0118  0.0288
H    0.093-0.0259  0.0000    0.0000  0.0000  0.0051   -0.9259  0.2481  0.0000
         Gradient vector in normal coordinate representation
         -------------------------------------------------------
  i    W(I)     dE/dQ(i)      dE/dq      dE/dq      [dE/dQ(i)]/w(i)
                              (cm-1)     (eV)          (relative)
         -------------------------------------------------------
   7   719.17  0.0000000000     0.00000    0.00000   0.0000000000
   8   782.13  0.0000000000     0.00000    0.00000   0.0000000000
   9   883.84  0.0000000000     0.00000    0.00000   0.0000000000
  10  1073.53  0.0000000000     0.00000    0.00000   0.0000000000
  11  1279.36  0.0000000000     0.00000    0.00000   0.0000000000
  12  1332.59  0.0000000000     0.00000    0.00000   0.0000000000
  13  2252.79  0.0000000000     0.00000    0.00000   0.0000000000
  14  2363.83  0.0000000000     0.00000    0.00000   0.0000000000
  15  3152.90  0.0000000000     0.00000    0.00000   0.0000000000
         -------------------------------------------------------


                 Normal modes in internal coordinates
---------------------------------------------------------------------------
           0.072        0.007        0.075        1.296        1.354
---------------------------------------------------------------------------
RCl      0.000000     0.000000     0.000000     0.000000     0.000000
RH       0.000000     0.000000     0.000000     0.000000     0.000000
TDA1     0.000000     0.000000     0.000000     0.000002     0.000003
RH       0.000000     0.000000     0.000000     0.000000     0.000000
```

```
TDA1      0.000000      0.000000      0.000000      0.000002     -0.000003
D120      0.000000      0.000000      0.000000      0.000003      0.000000
RH        0.000000      0.000000      0.000000      0.000001      0.000000
TDA1      0.000000      0.000000      0.000000     -0.000003      0.000000
D120      0.000000      0.000000      0.000000     -0.000001     -0.000002
---------------------------------------------------------------------------
           5.313       719.170       782.129       883.840      1073.533
---------------------------------------------------------------------------
RCl       0.000000      0.949091      0.000000     -0.236890      0.137008
RH        0.000000      0.014356      0.023541      0.013656     -0.008861
TDA1      0.000001      0.100392      0.646416      0.428477     -0.250074
RH        0.000000      0.014356     -0.023541      0.013656     -0.008861
TDA1     -0.000001      0.100392     -0.646416      0.428477     -0.250074
D120      0.000000      0.143335      0.000000      0.573441      0.808943
RH        0.000000     -0.003300      0.000000      0.005932      0.009294
TDA1      0.000000     -0.230140      0.000000     -0.406506     -0.194742
D120     -0.000003     -0.071668     -0.403961     -0.286720     -0.404472
---------------------------------------------------------------------------
        1279.362      1332.587      2252.792      2363.827      3152.903
---------------------------------------------------------------------------
RCl      -0.144280      0.000000      0.069503      0.000000     -0.020159
RH        0.004047     -0.007614     -0.697790     -0.696753     -0.049796
TDA1      0.179063     -0.051775     -0.005018      0.067346      0.025617
RH        0.004047      0.007614     -0.697790      0.696753     -0.049796
TDA1      0.179063      0.051775     -0.005018     -0.067346      0.025617
D120      0.357509      0.000000      0.098114      0.000000      0.073571
RH        0.045566      0.000000     -0.062810      0.000000      0.992706
TDA1      0.867860      0.000000     -0.072940      0.000000     -0.033026
D120     -0.178754     -0.997258     -0.049057     -0.141420     -0.036786
---------------------------------------------------------------------------


         -----------------------------------------------------------------
                        Dipole Moment Function
                        (Normal Coordinate Basis)
         -----------------------------------------------------------------
           Mode      Symmetry    d(Mu(x))/dQ   d(Mu(y))/dQ   d(Mu(z))/dQ
         -----------------------------------------------------------------
            Q7         A'         -0.008002      0.132310      0.000000
            Q8         A''         0.000000      0.000000     -0.014836
            Q9         A'         -0.024521     -0.075551      0.000000
            Q10        A'         -0.047857      0.061641      0.000000
            Q11        A'         -0.007183     -0.079667      0.000000
            Q12        A''         0.000000      0.000000     -0.077461
            Q13        A'          0.019207      0.109512      0.000000
            Q14        A''         0.000000      0.000000      0.047297
            Q15        A'          0.053949     -0.077611      0.000000
         -----------------------------------------------------------------
--------------------------------------------------------------------------
         --------------------------------------------------------------
         Parameter              (MHz)                 (CM-1)
         --------------------------------------------------------------

            R6             -.141944E-04           -.473474E-09
            R5             -.123279E-01           -.411214E-06
            SI                          0.555878E+03

   A-reduced centrifugal distortion parameters

            DJ              0.124356E-01           0.414806E-06
            DK              0.925514E+00           0.308718E-04
            DJK             0.126376E+00           0.421546E-05
            DELJ            0.124640E-01           0.415753E-06
            DELK            0.925656E+00           0.308766E-04
            DELJK           0.126206E+00           0.420978E-05
            delJ            0.299622E-03           0.999430E-08
            delK            0.562172E-01           0.187520E-05

   S-reduced centrifugal distortion parameters

            DJ              0.124134E-01           0.414066E-06
            DK              0.925403E+00           0.308681E-04
            DJK             0.126509E+00           0.421990E-05
            D1             -.299622E-03           -.999430E-08
            D2             -.252830E-04           -.843352E-09
         --------------------------------------------------------------
    Vibrational frequencies after rotational projection  of
    Cartesian force constants:
          1               0.0000i
```

```
     2              0.0000i
     3              0.0000i
     4              0.0000
     5              0.0000
     6              0.0000
     7            719.1695
     8            782.1286
     9            883.8401
    10           1073.5334
    11           1279.3616
    12           1332.5867
    13           2252.7922
    14           2363.8272
    15           3152.9030
 Zero-point vibrational energy:   19.7855 kcal/mol =   82.7825 kJ/mol.
             0.50 seconds walltime passed
--executable xjoda finished with status            0
```

Table S.6. Part of the CFOUR output file of the CCSD(T)/V5Z-aV(5+d)Z harmonic frequency calculation for $^{12}CHD_2{}^{37}Cl$

```
     ******************************************************************
     <<<    CCCCCC    CCCCCC   |||    CCCCCC    CCCCCC    >>>
      <<<     CCC       CCC    |||     CCC       CCC      >>>
       <<<    CCC       CCC    |||     CCC       CCC        >>>
      <<<     CCC       CCC    |||     CCC       CCC        >>>
       <<<    CCC       CCC    |||     CCC       CCC      >>>
        <<<   CCC       CCC    |||     CCC       CCC      >>>
         <<<  CCCCCC    CCCCCC  |||    CCCCCC    CCCCCC   >>>
     ******************************************************************


       ****************************************************************
       * CFOUR Coupled-Cluster techniques for Computational Chemistry *
       ****************************************************************


     Department of Chemistry            Institut fuer Physikalische Chemie
     University of Texas at Austin      Universitaet Mainz
     Austin, TX  78712, USA             D-55099 Mainz, Germany

                     Version 1.0

                        Normal Coordinates

              A'                     A''                     A'
            712.95                 781.56                  883.26
           VIBRATION              VIBRATION               VIBRATION
C      0.060 0.6697  0.0000   0.0000  0.0000  0.3697    0.4291 -0.3539  0.0000
CL    -0.018-0.5538  0.0000   0.0000  0.0000 -0.1592   -0.1240  0.0859  0.0000
H     -0.029 0.3409  0.0105  -0.0287  0.6385 -0.0753   -0.2663  0.4043  0.0375
H     -0.029 0.3409 -0.0105   0.0287 -0.6385 -0.0753   -0.2663  0.4043 -0.0375
H     -0.014 0.0794  0.0000   0.0000  0.0000 -0.0986    0.0231 -0.4425  0.0000

              A'                     A'                     A''
            1073.53                1279.23                1332.59
           VIBRATION              VIBRATION               VIBRATION
C      0.271 0.2891  0.0000   0.0521 -0.2834  0.0000    0.0000  0.0000  0.2598
CL     0.002 0.0063  0.0000   0.0469 -0.0362  0.0000    0.0000  0.0000  0.0037
H     -0.345-0.3345  0.4314  -0.2532  0.1316  0.0572    0.3252 -0.1279 -0.0321
H     -0.345-0.3345 -0.4314  -0.2532  0.1316 -0.0572   -0.3252  0.1279 -0.0321
H      0.022-0.0897  0.0000   0.2519  0.8250  0.0000    0.0000  0.0000 -0.8284

              A'                     A''                     A'
            2252.79                2363.83                3152.90
           VIBRATION              VIBRATION               VIBRATION
C      0.231 0.1874  0.0000   0.0000  0.0000  0.4343    0.2745 -0.0620  0.0000
CL    -0.001-0.0035  0.0000   0.0000  0.0000 -0.0028   -0.0008 -0.0001  0.0000
H     -0.312-0.2121 -0.5552  -0.2979 -0.2011 -0.5258   -0.0058 -0.0118 -0.0288
H     -0.312-0.2121  0.5552   0.2979  0.2011 -0.5258   -0.0058 -0.0118  0.0288
H      0.093-0.0259  0.0000   0.0000  0.0000  0.0051   -0.9258  0.2482  0.0000
           Gradient vector in normal coordinate representation
     ------------------------------------------------------------
   i   W(I)     dE/dQ(i)     dE/dq     dE/dq    [dE/dQ(i)]/w(i)
                             (cm-1)    (eV)        (relative)
     ------------------------------------------------------------
   7  712.95  0.0000000000    0.00000    0.00000  0.0000000000
   8  781.56  0.0000000000    0.00000    0.00000  0.0000000000
   9  883.26  0.0000000000    0.00000    0.00000  0.0000000000
  10 1073.53  0.0000000000    0.00000    0.00000  0.0000000000
  11 1279.23  0.0000000000    0.00000    0.00000  0.0000000000
  12 1332.59  0.0000000000    0.00000    0.00000  0.0000000000
  13 2252.79  0.0000000000    0.00000    0.00000  0.0000000000
  14 2363.83  0.0000000000    0.00000    0.00000  0.0000000000
  15 3152.90  0.0000000000    0.00000    0.00000  0.0000000000
     ------------------------------------------------------------


             Normal modes in internal coordinates
-------------------------------------------------------------------------------
             0.053        0.020        0.061        1.291        1.309
-------------------------------------------------------------------------------
RCl      0.000000     0.000000     0.000000     0.000000     0.000000
RH       0.000000     0.000000     0.000000     0.000000     0.000000
TDA1     0.000000     0.000000     0.000000     0.000003     0.000001
RH       0.000000     0.000000     0.000000     0.000000     0.000000
TDA1     0.000000     0.000000     0.000000    -0.000003     0.000001
```

D120	0.000000	0.000000	0.000000	0.000000	0.000003
RH	0.000000	0.000000	0.000000	0.000000	0.000001
TDA1	0.000000	0.000000	0.000000	0.000000	-0.000003
D120	0.000000	0.000000	0.000000	-0.000002	-0.000001

	5.217	712.954	781.562	883.261	1073.531
RCl	0.000000	0.951721	0.000000	-0.232639	0.137190
RH	0.000000	0.014231	0.023537	0.013715	-0.008858
TDA1	0.000001	0.096945	0.646423	0.428726	-0.250062
RH	0.000000	0.014231	-0.023537	0.013715	-0.008858
TDA1	-0.000001	0.096945	-0.646423	0.428726	-0.250062
D120	0.000000	0.138479	0.000000	0.573786	0.808918
RH	0.000000	-0.003318	0.000000	0.005896	0.009292
TDA1	0.000000	-0.225931	0.000000	-0.407821	-0.194774
D120	-0.000004	-0.069239	-0.403939	-0.286893	-0.404459

	1279.234	1332.586	2252.791	2363.826	3152.903
RCl	-0.145329	0.000000	0.069456	0.000000	-0.020160
RH	0.004044	-0.007613	-0.697793	-0.696754	-0.049796
TDA1	0.179334	-0.051751	-0.005022	0.067337	0.025616
RH	0.004044	0.007613	-0.697793	0.696754	-0.049796
TDA1	0.179334	0.051751	-0.005022	-0.067337	0.025616
D120	0.357849	0.000000	0.098111	0.000000	0.073570
RH	0.045560	0.000000	-0.062809	0.000000	0.992706
TDA1	0.867398	0.000000	-0.072934	0.000000	-0.033023
D120	-0.178925	-0.997260	-0.049055	-0.141415	-0.036785

Dipole Moment Function
(Normal Coordinate Basis)

Mode	Symmetry	d(Mu(x))/dQ	d(Mu(y))/dQ	d(Mu(z))/dQ
Q7	A'	-0.007830	0.131492	0.000000
Q8	A''	0.000000	0.000000	-0.015117
Q9	A'	-0.024806	-0.074464	0.000000
Q10	A'	-0.047845	0.061700	0.000000
Q11	A'	-0.007118	-0.079937	0.000000
Q12	A''	0.000000	0.000000	-0.077454
Q13	A'	0.019220	0.109493	0.000000
Q14	A''	0.000000	0.000000	0.047292
Q15	A'	0.053937	-0.077620	0.000000

Parameter	(MHz)	(CM-1)
R6	-.132919E-04	-.443371E-09
R5	-.119581E-01	-.398880E-06
SI	0.575974E+03	

A-reduced centrifugal distortion parameters

DJ	0.120525E-01	0.402029E-06
DK	0.929567E+00	0.310070E-04
DJK	0.122603E+00	0.408959E-05
DELJ	0.120791E-01	0.402916E-06
DELK	0.929700E+00	0.310115E-04
DELJK	0.122443E+00	0.408427E-05
delJ	0.285896E-03	0.953646E-08
delK	0.545395E-01	0.181924E-05

S-reduced centrifugal distortion parameters

DJ	0.120318E-01	0.401337E-06
DK	0.929464E+00	0.310036E-04
DJK	0.122728E+00	0.409375E-05
D1	-.285896E-03	-.953646E-08
D2	-.236727E-04	-.789637E-09

Vibrational frequencies after rotational projection of
Cartesian force constants:
```
     1          0.0000i
     2          0.0000i
```

```
         3                0.0000
         4                0.0000
         5                0.0000
         6                0.0000
         7              712.9536
         8              781.5625
         9              883.2610
        10             1073.5310
        11             1279.2338
        12             1332.5861
        13             2252.7908
        14             2363.8263
        15             3152.9027
 Zero-point vibrational energy:   19.7747 kcal/mol =   82.7376 kJ/mol.
            2.25 seconds walltime passed
--executable xjoda finished with status            0
```

Table S.7. Part of the CFOUR output file of the CCSD(T)/V5Z-aV(5+*d*)Z harmonic frequency calculation for $^{13}CHD_2^{35}Cl$

```
***********************************************************************
      <<<    CCCCCC    CCCCCC   |||    CCCCCC    CCCCCC   >>>
     <<<     CCC       CCC      |||    CCC       CCC       >>>
    <<<      CCC       CCC      |||    CCC       CCC        >>>
   <<<       CCC       CCC      |||    CCC       CCC         >>>
    <<<      CCC       CCC      |||    CCC       CCC        >>>
     <<<     CCC       CCC      |||    CCC       CCC       >>>
      <<<    CCCCCC    CCCCCC   |||    CCCCCC    CCCCCC   >>>
      ***********************************************************************


       ****************************************************************
       * CFOUR Coupled-Cluster techniques for Computational Chemistry *
       ****************************************************************


   Department of Chemistry             Institut fuer Physikalische Chemie
   University of Texas at Austin        Universitaet Mainz
   Austin, TX  78712, USA              D-55099 Mainz, Germany

                    Version 1.0



                         Normal Coordinates

              A'                       A''                      A'
            706.18                   777.90                   873.26
            VIBRATION                VIBRATION                VIBRATION
C    0.051 0.6801  0.0000     0.0000  0.0000  0.3656     0.4237 -0.3306  0.0000
CL  -0.015-0.5770  0.0000     0.0000  0.0000 -0.1644    -0.1283  0.0734  0.0000
H   -0.026 0.3114  0.0139    -0.0282  0.6372 -0.0835    -0.2766  0.4184  0.0390
H   -0.026 0.3114 -0.0139     0.0282 -0.6372 -0.0835    -0.2766  0.4184 -0.0390
H   -0.017 0.0754  0.0000     0.0000  0.0000 -0.1086     0.0162 -0.4276  0.0000

              A'                       A'                       A''
           1067.01                  1275.41                  1329.06
            VIBRATION                VIBRATION                VIBRATION
C    0.263 0.2775  0.0000     0.0494 -0.2632  0.0000     0.0000  0.0000  0.2542
CL   0.002 0.0145  0.0000     0.0493 -0.0420  0.0000     0.0000  0.0000  0.0045
H   -0.346-0.3462  0.4261    -0.2543  0.1279  0.0648     0.3220 -0.1339 -0.0387
H   -0.346-0.3462 -0.4261    -0.2543  0.1279 -0.0648    -0.3220  0.1339 -0.0387
H    0.015-0.1034  0.0000     0.2509  0.8311  0.0000     0.0000  0.0000 -0.8301

              A'                       A''                      A'
           2245.06                  2346.63                  3143.30
            VIBRATION                VIBRATION                VIBRATION
C    0.225 0.1780  0.0000     0.0000  0.0000  0.4186     0.2629 -0.0606  0.0000
CL  -0.001-0.0031  0.0000     0.0000  0.0000 -0.0027    -0.0007 -0.0003  0.0000
H   -0.313-0.2118 -0.5584    -0.3017 -0.2025 -0.5294    -0.0039 -0.0111 -0.0269
H   -0.313-0.2118  0.5584     0.3017  0.2025 -0.5294    -0.0039 -0.0111  0.0269
H    0.086-0.0225  0.0000     0.0000  0.0000  0.0088    -0.9288  0.2508  0.0000
          Gradient vector in normal coordinate representation
        -----------------------------------------------------------
  i    W(I)     dE/dQ(i)       dE/dq       dE/dq     [dE/dQ(i)]/w(i)
                              (cm-1)       (eV)         (relative)
        -----------------------------------------------------------
   7   706.18  0.0000000000       0.00000      0.00000   0.0000000000
   8   777.90  0.0000000000       0.00000      0.00000   0.0000000000
   9   873.26  0.0000000000       0.00000      0.00000   0.0000000000
  10  1067.01  0.0000000000       0.00000      0.00000   0.0000000000
  11  1275.41  0.0000000000       0.00000      0.00000   0.0000000000
  12  1329.06  0.0000000000       0.00000      0.00000   0.0000000000
  13  2245.06  0.0000000000       0.00000      0.00000   0.0000000000
  14  2346.63  0.0000000000       0.00000      0.00000   0.0000000000
  15  3143.30  0.0000000000       0.00000      0.00000   0.0000000000
        -----------------------------------------------------------


                  Normal modes in internal coordinates
--------------------------------------------------------------------------
          0.096         0.054         0.111         1.277         1.330
--------------------------------------------------------------------------
RCl      0.000000      0.000000      0.000000      0.000000      0.000000
RH       0.000000      0.000000      0.000000      0.000000      0.000000
TDA1     0.000000      0.000000      0.000000      0.000003      0.000002
```

RH	0.000000	0.000000	0.000000	0.000000	0.000000
TDA1	0.000000	0.000000	0.000000	-0.000003	0.000002
D120	0.000000	0.000000	0.000000	0.000000	0.000003
RH	0.000000	0.000000	0.000000	0.000000	0.000001
TDA1	0.000000	0.000000	0.000000	0.000000	-0.000003
D120	0.000000	0.000000	0.000000	-0.000002	-0.000001

	5.216	706.184	777.897	873.259	1067.010
RCl	0.000000	0.960052	0.000000	-0.210285	0.125590
RH	0.000000	0.011099	0.021345	0.013384	-0.011678
TDA1	0.000001	0.067444	0.644826	0.430020	-0.256372
RH	0.000000	0.011099	-0.021345	0.013384	-0.011678
TDA1	-0.000001	0.067444	-0.644826	0.430020	-0.256372
D120	0.000000	0.126702	0.000000	0.580792	0.806028
RH	0.000000	-0.004520	0.000000	0.007991	0.009702
TDA1	0.000000	-0.221064	0.000000	-0.404814	-0.200761
D120	-0.000004	-0.063351	-0.409252	-0.290396	-0.403014

	1275.411	1329.056	2245.063	2346.629	3143.304
RCl	-0.126870	0.000000	0.063771	0.000000	-0.018805
RH	0.005196	-0.011596	-0.699269	-0.698342	-0.045772
TDA1	0.168208	-0.056603	-0.003436	0.063294	0.023612
RH	0.005196	0.011596	-0.699269	0.698342	-0.045772
TDA1	0.168208	0.056603	-0.003436	-0.063294	0.023612
D120	0.365048	0.000000	0.090579	0.000000	0.067017
RH	0.046774	0.000000	-0.057029	0.000000	0.993860
TDA1	0.870918	0.000000	-0.066684	0.000000	-0.031116
D120	-0.182524	-0.996656	-0.045289	-0.128933	-0.033509

```
        -------------------------------------------------------
                    Dipole Moment Function
                   (Normal Coordinate Basis)
        -------------------------------------------------------

   Mode     Symmetry    d(Mu(x))/dQ   d(Mu(y))/dQ   d(Mu(z))/dQ
        -------------------------------------------------------

    Q7        A'        -0.007645      0.133632      0.000000
    Q8        A''        0.000000      0.000000     -0.016081
    Q9        A'        -0.026087     -0.068718      0.000000
    Q10       A'        -0.047793      0.058854      0.000000
    Q11       A'        -0.007955     -0.074512      0.000000
    Q12       A''        0.000000      0.000000     -0.077647
    Q13       A'         0.019557      0.106321      0.000000
    Q14       A''        0.000000      0.000000      0.046905
    Q15       A'         0.053225     -0.077325      0.000000
        -------------------------------------------------------
-------------------------------------------------------------------
        -----------------------------------------------------
        Parameter            (MHz)              (CM-1)
        -----------------------------------------------------

         R6             -.128349E-04        -.428126E-09
         R5             -.116901E-01        -.389940E-06
         SI                     0.594361E+03

  A-reduced centrifugal distortion parameters

         DJ              0.118072E-01        0.393845E-06
         DK              0.928660E+00        0.309768E-04
         DJK             0.122045E+00        0.407100E-05
         DELJ            0.118328E-01        0.394701E-06
         DELK            0.928789E+00        0.309811E-04
         DELJK           0.121891E+00        0.406586E-05
         delJ            0.274458E-03        0.915492E-08
         delK            0.538945E-01        0.179773E-05

  S-reduced centrifugal distortion parameters

         DJ              0.117875E-01        0.393189E-06
         DK              0.928562E+00        0.309735E-04
         DJK             0.122163E+00        0.407493E-05
         D1             -.274458E-03        -.915492E-08
         D2             -.226691E-04        -.756160E-09
        -----------------------------------------------------
   Vibrational frequencies after rotational projection  of
   Cartesian force constants:
```

```
      1              0.0000i
      2              0.0000i
      3              0.0000i
      4              0.0000
      5              0.0000
      6              0.0000
      7            706.1843
      8            777.8969
      9            873.2590
     10           1067.0098
     11           1275.4113
     12           1329.0561
     13           2245.0634
     14           2346.6288
     15           3143.3041
 Zero-point vibrational energy:   19.6763 kcal/mol =   82.3259 kJ/mol.
           0.12 seconds walltime passed
--executable xjoda finished with status            0
```

Table S.8. Part of the CFOUR output file of the CCSD(T)/V5Z-aV(5+*d*)Z harmonic frequency calculation for $^{13}CHD_2^{37}Cl$

```
--invoking executable xjoda


    *************************************************************************
        <<<     CCCCCC     CCCCCC   |||     CCCCCC     CCCCCC   >>>
       <<<       CCC         CCC    |||      CCC         CCC     >>>
      <<<        CCC         CCC    |||      CCC         CCC      >>>
     <<<         CCC         CCC    |||      CCC         CCC       >>>
      <<<        CCC         CCC    |||      CCC         CCC      >>>
       <<<       CCC         CCC    |||      CCC         CCC     >>>
        <<<     CCCCC       CCCCC   |||     CCCCCC     CCCCCC   >>>
    *************************************************************************


      ****************************************************************
      * CFOUR Coupled-Cluster techniques for Computational Chemistry *
      ****************************************************************


    Department of Chemistry            Institut fuer Physikalische Chemie
    University of Texas at Austin      Universitaet Mainz
    Austin, TX  78712, USA             D-55099 Mainz, Germany

                    Version 1.0



                        Normal Coordinates

            A'                        A''                       A'
          699.79                    777.33                    872.75
          VIBRATION                 VIBRATION                 VIBRATION
C     0.048 0.6877  0.0000    0.0000  0.0000  0.3659    0.4241 -0.3279  0.0000
CL   -0.014-0.5668  0.0000    0.0000  0.0000 -0.1601   -0.1250  0.0692  0.0000
H    -0.024 0.3122  0.0135   -0.0282  0.6376 -0.0836   -0.2766  0.4198  0.0390
H    -0.024 0.3122 -0.0135    0.0282 -0.6376 -0.0836   -0.2766  0.4198 -0.0390
H    -0.017 0.0803  0.0000    0.0000  0.0000 -0.1086    0.0158 -0.4283  0.0000

            A'                        A'                        A''
          1067.00                   1275.27                   1329.06
          VIBRATION                 VIBRATION                 VIBRATION
C     0.263 0.2778  0.0000    0.0495 -0.2637  0.0000    0.0000  0.0000  0.2542
CL    0.002 0.0139  0.0000    0.0479 -0.0405  0.0000    0.0000  0.0000  0.0043
H    -0.346-0.3461  0.4261   -0.2544  0.1280  0.0648    0.3220 -0.1340 -0.0387
H    -0.346-0.3461 -0.4261   -0.2544  0.1280 -0.0648   -0.3220  0.1340 -0.0387
H     0.015-0.1034  0.0000    0.2511  0.8309  0.0000    0.0000  0.0000 -0.8301

            A'                        A''                       A'
          2245.06                   2346.63                   3143.30
          VIBRATION                 VIBRATION                 VIBRATION
C     0.225 0.1780  0.0000    0.0000  0.0000  0.4186    0.2629 -0.0607  0.0000
CL   -0.001-0.0030  0.0000    0.0000  0.0000 -0.0026   -0.0007 -0.0003  0.0000
H    -0.313-0.2118 -0.5584   -0.3018 -0.2024 -0.5294   -0.0039 -0.0111 -0.0269
H    -0.313-0.2118  0.5584    0.3018  0.2024 -0.5294   -0.0039 -0.0111  0.0269
H     0.086-0.0225  0.0000    0.0000  0.0000  0.0088   -0.9287  0.2509  0.0000
        Gradient vector in normal coordinate representation
        --------------------------------------------------------
   i    W(I)     dE/dQ(i)      dE/dq      dE/dq    [dE/dQ(i)]/w(i)
                              (cm-1)      (eV)        (relative)
        --------------------------------------------------------
    7   699.79  0.0000000000     0.00000     0.00000   0.0000000000
    8   777.33  0.0000000000     0.00000     0.00000   0.0000000000
    9   872.75  0.0000000000     0.00000     0.00000   0.0000000000
   10  1067.00  0.0000000000     0.00000     0.00000   0.0000000000
   11  1275.27  0.0000000000     0.00000     0.00000   0.0000000000
   12  1329.06  0.0000000000     0.00000     0.00000   0.0000000000
   13  2245.06  0.0000000000     0.00000     0.00000   0.0000000000
   14  2346.63  0.0000000000     0.00000     0.00000   0.0000000000
   15  3143.30  0.0000000000     0.00000     0.00000   0.0000000000
        --------------------------------------------------------


              Normal modes in internal coordinates
--------------------------------------------------------------------------------
        0.100          0.044          0.109          1.288          1.322
--------------------------------------------------------------------------------
```

RCl	0.000000	0.000000	0.000000	0.000000	0.000000
RH	0.000000	0.000000	0.000000	0.000000	0.000000
TDA1	0.000000	0.000000	0.000000	0.000003	0.000002
RH	0.000000	0.000000	0.000000	0.000000	0.000000
TDA1	0.000000	0.000000	0.000000	-0.000003	0.000002
D120	0.000000	0.000000	0.000000	0.000000	0.000003
RH	0.000000	0.000000	0.000000	0.000000	0.000001
TDA1	0.000000	0.000000	0.000000	0.000000	-0.000003
D120	0.000000	0.000000	0.000000	-0.000002	-0.000001

	5.235	699.794	777.329	872.746	1067.004
RCl	0.000000	0.961930	0.000000	-0.206836	0.126010
RH	0.000000	0.011006	0.021342	0.013418	-0.011674
TDA1	0.000001	0.064815	0.644835	0.430102	-0.256383
RH	0.000000	0.011006	-0.021342	0.013418	-0.011674
TDA1	-0.000001	0.064815	-0.644835	0.430102	-0.256383
D120	0.000000	0.122537	0.000000	0.581060	0.805954
RH	0.000000	-0.004540	0.000000	0.007955	0.009697
TDA1	0.000000	-0.217388	0.000000	-0.405934	-0.200845
D120	-0.000004	-0.061268	-0.409225	-0.290530	-0.402977

	1275.268	1329.056	2245.063	2346.629	3143.305
RCl	-0.128011	0.000000	0.063730	0.000000	-0.018807
RH	0.005193	-0.011595	-0.699272	-0.698344	-0.045772
TDA1	0.168468	-0.056575	-0.003439	0.063285	0.023611
RH	0.005193	0.011595	-0.699272	0.698344	-0.045772
TDA1	0.168468	0.056575	-0.003439	-0.063285	0.023611
D120	0.365424	0.000000	0.090575	0.000000	0.067016
RH	0.046770	0.000000	-0.057029	0.000000	0.993861
TDA1	0.870454	0.000000	-0.066678	0.000000	-0.031114
D120	-0.182712	-0.996659	-0.045288	-0.128928	-0.033508

```
          -----------------------------------------------------------------
                          Dipole Moment Function
                        (Normal Coordinate Basis)
          -----------------------------------------------------------------
           Mode     Symmetry    d(Mu(x))/dQ  d(Mu(y))/dQ  d(Mu(z))/dQ
          -----------------------------------------------------------------
            Q7        A'         -0.007476     0.132633     0.000000
            Q8        A''         0.000000     0.000000    -0.016364
            Q9        A'         -0.026364    -0.067828     0.000000
            Q10       A'         -0.047781     0.058979     0.000000
            Q11       A'         -0.007890    -0.074802     0.000000
            Q12       A''         0.000000     0.000000    -0.077640
            Q13       A'          0.019570     0.106304     0.000000
            Q14       A''         0.000000     0.000000     0.046901
            Q15       A'          0.053213    -0.077334     0.000000
          -----------------------------------------------------------------
```

Parameter	(MHz)	(CM-1)
R6	-.119858E-04	-.399804E-09
R5	-.113241E-01	-.377730E-06
SI	0.616702E+03	

A-reduced centrifugal distortion parameters

DJ	0.114285E-01	0.381215E-06
DK	0.932701E+00	0.311116E-04
DJK	0.118277E+00	0.394529E-05
DELJ	0.114525E-01	0.382015E-06
DELK	0.932821E+00	0.311156E-04
DELJK	0.118133E+00	0.394049E-05
delJ	0.261359E-03	0.871800E-08
delK	0.522149E-01	0.174170E-05

S-reduced centrifugal distortion parameters

DJ	0.114102E-01	0.380603E-06
DK	0.932610E+00	0.311085E-04
DJK	0.118387E+00	0.394896E-05
D1	-.261359E-03	-.871800E-08
D2	-.211670E-04	-.706054E-09

```
 -----------------------------------------------------------
   Vibrational frequencies after rotational projection  of
   Cartesian force constants:
           1              0.0000i
           2              0.0000i
           3              0.0000i
           4              0.0000
           5              0.0000
           6              0.0000
           7            699.7944
           8            777.3288
           9            872.7463
          10           1067.0044
          11           1275.2679
          12           1329.0561
          13           2245.0630
          14           2346.6288
          15           3143.3049
  Zero-point vibrational energy:   19.6654 kcal/mol =   82.2803 kJ/mol.
             0.38 seconds walltime passed
 --executable xjoda finished with status             0
```

Table S.9. Part of the CFOUR output file of the CCSD(T)/VQZ-aV(Q+*d*)Z anharmonic frequency calculation for $^{12}CHD_2{}^{35}Cl$

```
     ****************************************************************
         <<<    CCCCCC    CCCCCC   |||     CCCCCC    CCCCCC   >>>
        <<<      CCC        CCC    |||      CCC        CCC     >>>
       <<<       CCC        CCC    |||      CCC        CCC      >>>
      <<<        CCC        CCC    |||      CCC        CCC       >>>
       <<<       CCC        CCC    |||      CCC        CCC      >>>
        <<<      CCC        CCC    |||      CCC        CCC     >>>
         <<<    CCCCCC    CCCCCC   |||     CCCCCC    CCCCCC   >>>
     ****************************************************************


        **************************************************************
        * CFOUR Coupled-Cluster techniques for Computational Chemistry *
        **************************************************************


     Department of Chemistry            Institut fuer Physikalische Chemie
     University of Texas at Austin      Universitaet Mainz
     Austin, TX  78712, USA             D-55099 Mainz, Germany

                     Version 1.0



                           Normal Coordinates

                A'                          A''                         A'
               718.57                      781.05                     881.33
             VIBRATION                   VIBRATION                  VIBRATION
C     0.067 0.6600  0.0000     0.0000  0.0000  0.3718     0.4306 -0.3570  0.0000
CL   -0.021-0.5628  0.0000     0.0000  0.0000 -0.1636    -0.1295  0.0967  0.0000
H    -0.031 0.3432  0.0113    -0.0233  0.6371 -0.0775    -0.2631  0.3951  0.0387
H    -0.031 0.3432 -0.0113     0.0233 -0.6371 -0.0775    -0.2631  0.3951 -0.0387
H    -0.015 0.0669  0.0000     0.0000  0.0000 -0.1001     0.0208 -0.4548  0.0000


                A'                          A'                          A''
              1073.05                     1269.13                    1324.63
             VIBRATION                   VIBRATION                  VIBRATION
C     0.268 0.2948  0.0000     0.0601 -0.2812  0.0000     0.0000  0.0000  0.2598
CL    0.002 0.0072  0.0000     0.0483 -0.0382  0.0000     0.0000  0.0000  0.0042
H    -0.338-0.3393  0.4306    -0.2635  0.1342  0.0651     0.3299 -0.1321 -0.0347
H    -0.338-0.3393 -0.4306    -0.2635  0.1342 -0.0651    -0.3299  0.1321 -0.0347
H     0.019-0.0999  0.0000     0.2528  0.8163  0.0000     0.0000  0.0000 -0.8231


                A'                          A''                         A'
              2251.67                     2361.61                    3202.70
             VIBRATION                   VIBRATION                  VIBRATION
C     0.232 0.1873  0.0000     0.0000  0.0000  0.4338     0.2741 -0.0631  0.0000
CL   -0.001-0.0037  0.0000     0.0000  0.0000 -0.0029    -0.0008 -0.0001  0.0000
H    -0.312-0.2124 -0.5550    -0.2983 -0.2013 -0.5257    -0.0053 -0.0110 -0.0270
H    -0.312-0.2124  0.5550     0.2983  0.2013 -0.5257    -0.0053 -0.0110  0.0270
H     0.090-0.0243  0.0000     0.0000  0.0000  0.0068    -0.9257  0.2494  0.0000
          Gradient vector in normal coordinate representation
      -----------------------------------------------------------
  i     W(I)     dE/dQ(i)      dE/dq      dE/dq    [dE/dQ(i)]/w(i)
                              (cm-1)      (eV)       (relative)
      -----------------------------------------------------------
   7   718.57 -0.0000002244    -0.02016    0.00000   0.0000000000
   8   781.05  0.0000000000     0.00000    0.00000   0.0000000000
   9   881.33  0.0000006107     0.04954    0.00001   0.0000000000
  10  1073.05  0.0000005087     0.03740    0.00000   0.0000000000
  11  1269.13  0.0000022090     0.14933    0.00002   0.0000000000
  12  1324.63  0.0000000000     0.00000    0.00000   0.0000000000
  13  2251.67 -0.0000074473    -0.37796   -0.00005   0.0000000000
  14  2361.61  0.0000000000     0.00000    0.00000   0.0000000000
  15  3202.70 -0.0037340810  -158.89939   -0.01970   0.0000021356
      -----------------------------------------------------------


                   Normal modes in internal coordinates
------------------------------------------------------------------------------
          95.671       35.741        0.011        0.013        0.045
------------------------------------------------------------------------------
RCl       0.000000    -0.000468     0.000000     0.000000     0.000000
RH        0.000100     0.000015     0.000000     0.000000     0.000000
TDA1     -0.001493    -0.000239     0.000000     0.000000     0.000000
```

```
RH        -0.000100      0.000015      0.000000      0.000000      0.000000
TDA1       0.001493     -0.000239      0.000000      0.000000      0.000000
D120       0.000000     -0.000808      0.000000      0.000000      0.000000
RH         0.000000      0.000089      0.000000      0.000000      0.000000
TDA1       0.000000      0.002633      0.000000      0.000000      0.000000
D120       0.006659      0.000404      0.000000      0.000000      0.000000
-------------------------------------------------------------------------
           10.402       718.574       781.047       881.330      1073.052
-------------------------------------------------------------------------
RCl        0.000000      0.943625      0.000000     -0.238483      0.140233
RH         0.000006      0.014511      0.023448      0.013727     -0.008865
TDA1       0.000149      0.104930      0.643991      0.423207     -0.255798
RH        -0.000006      0.014511     -0.023448      0.013727     -0.008865
TDA1      -0.000149      0.104930     -0.643991      0.423207     -0.255798
D120       0.000000      0.150919      0.000000      0.571906      0.803532
RH         0.000000     -0.003123      0.000000      0.004458      0.008122
TDA1       0.000000     -0.242178      0.000000     -0.419136     -0.205346
D120      -0.000177     -0.075459     -0.411645     -0.285953     -0.401766
-------------------------------------------------------------------------
          1269.134      1324.629      2251.671      2361.613      3202.695
-------------------------------------------------------------------------
RCl       -0.143013      0.000000      0.069421      0.000000     -0.020478
RH         0.005462     -0.009415     -0.697928     -0.696877     -0.048256
TDA1       0.180866     -0.054291     -0.004766      0.067453      0.025774
RH         0.005462      0.009415     -0.697928      0.696877     -0.048256
TDA1       0.180866      0.054291     -0.004766     -0.067453      0.025774
D120       0.379290      0.000000      0.098948      0.000000      0.073790
RH         0.044100      0.000000     -0.058648      0.000000      0.992837
TDA1       0.855740      0.000000     -0.072465      0.000000     -0.032600
D120      -0.189645     -0.996959     -0.049474     -0.140089     -0.036895
-------------------------------------------------------------------------


       -----------------------------------------------------------------
                       Dipole Moment Function
                     (Normal Coordinate Basis)
       -----------------------------------------------------------------

       Mode      Symmetry    d(Mu(x))/dQ   d(Mu(y))/dQ   d(Mu(z))/dQ
       -----------------------------------------------------------------

        Q7         A'         -0.008331      0.130930      0.000000
        Q8         A''         0.000000      0.000000     -0.016955
        Q9         A'         -0.026353     -0.075060      0.000000
        Q10        A'         -0.047419      0.064275      0.000000
        Q11        A'         -0.008076     -0.081295      0.000000
        Q12        A''         0.000000      0.000000     -0.076140
        Q13        A'          0.021483      0.109741      0.000000
        Q14        A''         0.000000      0.000000      0.052101
        Q15        A'          0.056871     -0.076301      0.000000

       -----------------------------------------------------------------
-------------------------------------------------------------------------------
       --------------------------------------------------------------
            Parameter              (MHz)              (CM-1)
       --------------------------------------------------------------


            R6            -.139874E-04         -.466570E-09
            R5            -.120508E-01         -.401970E-06
            SI                       0.553555E+03

  A-reduced centrifugal distortion parameters

            DJ             0.123981E-01         0.413557E-06
            DK             0.930803E+00         0.310483E-04
            DJK            0.128062E+00         0.427169E-05
            DELJ           0.124261E-01         0.414490E-06
            DELK           0.930943E+00         0.310529E-04
            DELJK          0.127894E+00         0.426609E-05
            delJ           0.300842E-03         0.100350E-07
            delK           0.550727E-01         0.183703E-05

  S-reduced centrifugal distortion parameters

            DJ             0.123764E-01         0.412831E-06
            DK             0.930694E+00         0.310446E-04
            DJK            0.128193E+00         0.427605E-05
            D1            -.300842E-03         -.100350E-07
            D2            -.248723E-04         -.829650E-09
       --------------------------------------------------------------
   Vibrational frequencies after rotational projection  of
   Cartesian force constants:
```

```
            1            0.0000i
            2            0.0000i
            3            0.0000i
            4            0.0000i
            5            0.0000
            6            0.0000
            7          718.5729
            8          781.0264
            9          881.3244
           10         1073.0511
           11         1269.1217
           12         1324.5462
           13         2251.6709
           14         2361.6132
           15         3202.6951
  Zero-point vibrational energy:  19.8190 kcal/mol =   82.9229 kJ/mol.
            0.00 seconds walltime passed
 --executable xjoda finished with status           0
 --invoking executable xcubic
  @GETMEM-I,  Allocated  13351 MB of main memory.
  back




 *******************************************************************************
         PARAMETERS RELEVANT TO MOLECULAR STRUCTURE
 *******************************************************************************


  Force Field from Numerical Differentiation of Analytic Second Derivatives
  ------------------------------------------------------------------------
 Cubic force constants written to file cubic.

 ------------------------------------------------------------------------------
  Mean and mean-square displacements in dimensionless normal coordinates

          Geometrical properties evaluated at     0.00 K

          Coordinate             <q>             <q**2>
 ------------------------------------------------------------------------------
              7              0.1320164107    0.4999999889
              8              0.0000000000    0.4999999889
              9             -0.0334764131    0.4999999889
             10              0.0058884200    0.4999999889
             11              0.0118353056    0.4999999889
             12              0.0000000000    0.4999999889
             13             -0.1290163300    0.4999999889
             14              0.0000000000    0.4999999889
             15              0.0784897075    0.4999999889
 ------------------------------------------------------------------------------


      ----------------------------------------------------
   ATOM              INTERNUCLEAR DISTANCE / Angstrom
      ----------------------------------------------------
   I   J        Re          Rg          Ra
      ----------------------------------------------------
   2   1      1.7826656   1.7908931   1.7905717
   3   1      1.0850773   1.1004835   1.0929730
   3   2      2.3617095   2.3756770   2.3739115
   4   1      1.0850773   1.1004835   1.0929730
   4   2      2.3617095   2.3756770   2.3739115
   4   3      1.7831251   1.8022929   1.7960215
   5   1      1.0850773   1.1062110   1.0942246
   5   2      2.3617095   2.3798912   2.3763141
   5   3      1.7831251   1.8062534   1.7970700
   5   4      1.7831251   1.8062534   1.7970700
      ----------------------------------------------------
 *******************************************************************************
      PARAMETERS RELEVANT TO ROTATIONAL SPECTROSCOPY
 *******************************************************************************


  ------------------------------------------------------------------------------
                          VIB-ROT CONSTANT / (cm-1)
                          ------------------------------
      AXIS      MODE     CORIOLIS     QUADRATIC     ANHARMONIC    TOTAL
  ------------------------------------------------------------------------------
       1         7      0.0006563    -0.0010991     0.0035170     0.0030742
       1         8      0.0003843    -0.0000001     0.0007751     0.0011593
```

```
    1      9      0.0000070    -0.0002227     0.0009862     0.0007705
    1     10      0.0001123    -0.0000297     0.0001810     0.0002636
    1     11      0.0060005    -0.0000750     0.0007627     0.0066882
    1     12     -0.0063108    -0.0000102    -0.0001027    -0.0064237
    1     13     -0.0002683    -0.0000276     0.0007256     0.0004296
    1     14     -0.0004188    -0.0000048     0.0005426     0.0001190
    1     15     -0.0000191    -0.0000040    -0.0000971    -0.0001202
    2      7      0.0009497    -0.0000578     0.0033571     0.0042490
    2      8      0.0248495    -0.0047677    -0.0185359     0.0015459
    2      9     -0.0096434    -0.0035625    -0.0146246    -0.0278305
    2     10      0.0237549    -0.0038711    -0.0057027     0.0141810
    2     11      0.0403636    -0.0024535    -0.0033257     0.0345843
    2     12     -0.0158126    -0.0001123    -0.0054433    -0.0213681
    2     13     -0.0028688    -0.0198078     0.0525677     0.0298912
    2     14     -0.0342059    -0.0001572     0.0504218     0.0160587
    2     15     -0.0199165    -0.0029719     0.0383398     0.0154513
    3      7      0.0002197    -0.0011584     0.0036851     0.0027464
    3      8      0.0002897    -0.0005801     0.0009985     0.0007081
    3      9      0.0016180    -0.0000313     0.0009877     0.0025744
    3     10     -0.0012216    -0.0000178     0.0001292    -0.0011103
    3     11      0.0000295    -0.0000005     0.0007238     0.0007528
    3     12     -0.0001655    -0.0000241     0.0000100    -0.0001797
    3     13     -0.0001879    -0.0000050     0.0002813     0.0000885
    3     14     -0.0000959    -0.0000241     0.0003470     0.0002271
    3     15     -0.0003518    -0.0000070     0.0002832    -0.0000756
-------------------------------------------------------------------------


-------------------------------------------------------------------------
 Be, B0 AND B-B0 SHIFTS FOR SINGLY EXCITED VIBRATIONAL STATES (CM-1)
 -------------------------------------------------------------
VIBRATION          X AXIS              Y AXIS               Z AXIS
-------------------------------------------------------------------------
  Be                0.38017121          3.20840528           0.39029061
  B0                0.37719095          3.17502387           0.38742477
  Be-B0             0.00298026          0.03338141           0.00286584
  B'                0.37718747          3.17502850           0.38742594
  Be-B'             0.00298374          0.03337677           0.00286467
  B''               0.37719416          3.17502932           0.38742931
  Be-B''            0.00297704          0.03337595           0.00286129
  B^A               0.37718537          3.17502849           0.38742804
  Be-B^A            0.00298583          0.03337678           0.00286256
  B^S               0.37718911          3.17502850           0.38742430
  Be-B^S            0.00298210          0.03337677           0.00286631
    7              -0.00307416         -0.00424905          -0.00274643
    8              -0.00115932         -0.00154585          -0.00070807
    9              -0.00077054          0.02783052          -0.00257442
   10              -0.00026364         -0.01418100           0.00111029
   11              -0.00668816         -0.03458432          -0.00075278
   12               0.00642372          0.02136810           0.00017966
   13              -0.00042962         -0.02989115          -0.00008847
   14              -0.00011896         -0.01605872          -0.00022706
   15               0.00012017         -0.01545133           0.00007561
-------------------------------------------------------------------------
-------------------------------------------------------------------------
 Be, B0 AND B-B0 SHIFTS FOR SINGLY EXCITED VIBRATIONAL STATES (MHz)
VIBRATION          X AXIS              Y AXIS               Z AXIS
-------------------------------------------------------------------------
  Be            11397.24608989      96185.57041048       11700.61803626
  B0            11307.90025843      95184.82089272       11614.70238667
  Be-B0            89.34583145       1000.74951776          85.91564959
  B'            11307.79583792      95184.95987365       11614.73750930
  Be-B'            89.45025197       1000.61053683          85.88052696
  B''           11307.99657534      95184.98447408       11614.83858772
  Be-B''           89.24951455       1000.58593640          85.77944854
  B^A           11307.73301344      95184.95964796       11614.80055948
  Be-B^A           89.51307645       1000.61076252          85.81747678
  B^S           11307.84508370      95184.95989936       11614.68828809
  Be-B^S           89.40100618       1000.61051112          85.92974817
    7               -92.16088932       -127.38330134         -82.33592820
    8               -34.75554915        -46.34350914         -21.22743550
    9               -23.10020403        834.33787236         -77.17915917
   10                -7.90371380       -425.13554512          33.28576198
   11              -200.50604902      -1036.81191401         -22.56788075
   12               192.57822935        640.59938712           5.38614289
   13               -12.87965860       -896.11421317          -2.65233496
   14                -3.56647283       -481.42844331          -6.80714394
   15                 3.60264449       -463.21936889           2.26667848
```

```
          -------------------------------------------------------------------------
                        Vibrationally averaged dipole moment
          -------------------------------------------------------------------------
                         a.u.                               Debye
                 x         y         z            x         y         z
          -------------------------------------------------------------------------
MU_e -0.03019   0.75412   0.00000       -0.07674   1.91665   0.00000
<MŪ> -0.02813   0.74862   0.00000       -0.07148   1.90268   0.00000

Equilibrium dipole moment:    0.75472 a.u. (   1.91818 D)
Equilibrium dipole moment:    0.74915 a.u. (   1.90402 D)
          -------------------------------------------------------------------------
          ****************************************************************************
              PARAMETERS RELEVANT TO VIBRATIONAL SPECTROSCOPY
          ****************************************************************************
            Quartic force constants written to file quartic
            =============================================================
            Performing F(IIJJ)/F(JJII) consistency check
            Differences greater than 1 cm-1 will be printed.
            =============================================================
             I    I    K    K       F(IIKK)       F(KKII)      Difference
            -------------------------------------------------------------
            -------------------------------------------------------------
            Largest absolute difference is    0.46814 cm-1.
            Largest relative difference is .32008D-01.
VPT2 vibrational analysis


 Thresholds for removing resonance denominators:
 Delta_omega = 50 cm-1; Phi(ijk) = 80 cm-1

          ------------------------------
            ANHARMONICITY CONSTANTS X(ij)
                          (cm-1)
          ------------------------------
            (*) Near-zero denominators were removed
          ------------------------------
                    I  J        X(IJ)
          ------------------------------
                    7   7      -3.4121
                    7   8      -3.7196
                    7   9      -4.0086
                    7  10      -1.4486
                    7  11      -5.5887
                    7  12      -0.9215
                    7  13      -0.1260
                    7  14       0.7965
                    7  15       2.3682
                    8   8      -0.5109
                    8   9      -1.3140
                    8  10      -4.0775
                    8  11      -0.5246
                    8  12      -3.4518
                    8  13      -4.0033
                    8  14      -3.2081
                    8  15       0.5008
                    9   9      -2.1739
                    9  10      -1.8309
                    9  11      -8.7608
                    9  12      -4.4351
                    9  13       5.4717
                    9  14      -2.9957
                    9  15      -2.9799
                   10  10      -5.5258
                   10  11      -1.9862
                   10  12       4.3094
                   10  13       3.6909
                   10  14     -18.7134
                   10  15      -1.0806
                   11  11      -5.2848
                   11  12       1.1528
                   11  13       1.3460
                   11  14      -2.3987
                   11  15     -17.9768
                   12  12      -5.5215
                   12  13      -6.0736
                   12  14     -12.6586
                   12  15     -21.9961
```

```
              13 13       -14.9604
              13 14       -62.3382
              13 15        -0.0204
              14 14       -19.6510
              14 15         1.4084
              15 15       -61.3604


--------------------------------------------------------------------------------
        HARMONIC AND FUNDAMENTAL FREQUENCIES (cm-1) AND INTENSITIES (km/mol)
--------------------------------------------------------------------------------


         Harmonic    Fundamental Anharmonic   Harmonic    Fundamental  Anharm
  Mode   Frequency    Frequency  Contribution Intensity   Intensity    Contrib
   7     719.1584     706.0100    -13.1484     16.8484      17.8539     1.0055
   8     781.6742     770.7533    -10.9209      0.2645       0.2670     0.0025
   9     883.4357     868.6612    -14.7744      6.2980       6.1323    -0.1658
  10    1073.3561    1051.7360    -21.6201      6.0395       5.6502    -0.3893
  11    1278.8086    1250.8706    -27.9380      6.4837       5.8193    -0.6644
  12    1332.5687    1299.4886    -33.0802      5.7344       5.8024     0.0680
  13    2253.3234    2192.3762    -60.9472     12.1905      11.2089    -0.9815
  14    2363.8797    2274.5239    -89.3558      2.5978       2.5673    -0.0305
  15    3153.1883    3010.5791   -142.6091      9.2611      10.1088     0.8476
--------------------------------------------------------------------------------

--------------------------------------------------------------------------------
                        ZERO-POINT VIBRATIONAL ENERGIES
--------------------------------------------------------------------------------
                        kcal/mol      kJ/mol      Hartree        cm-1
--------------------------------------------------------------------------------
Harmonic contribution :   19.7844      82.7779    0.03152846     6919.697
VPT2-correction       :   -0.2334      -0.9766   -0.00037199      -81.642
--------------------------------------------------------------------------------
Harm+VPT2             :   19.5510      81.8012    0.03115647     6838.055
--------------------------------------------------------------------------------
  MAXLEVEL set to                    3
 -------------------------------------------------------------------------------
                        All levels with up to three quanta
 -------------------------------------------------------------------------------
  MODE MODE MODE MODE MODE                  Anharmonic    Anharm      Harmonic
   I    J    K    L    M   NI  NJ  NK  NL  NM Frequency   Intensity   Transition
--------------------------------------------------------------------------------
   7    0    0    0    0    1   0   0   0   0   706.010   17.853576   719.158399
   8    0    0    0    0    1   0   0   0   0   770.753    0.266969   781.674223
   9    0    0    0    0    1   0   0   0   0   868.661    6.132139   883.435675
  10    0    0    0    0    1   0   0   0   0  1051.736    5.650042  1073.356127
  11    0    0    0    0    1   0   0   0   0  1250.870    5.819164  1278.808612
  12    0    0    0    0    1   0   0   0   0  1299.488    5.802245  1332.568742
   7    0    0    0    0    2   0   0   0   0  1405.195    0.129840  1438.316798
   8    7    0    0    0    1   1   0   0   0  1473.043    0.012255  1500.832622
   8    0    0    0    0    2   0   0   0   0  1540.484    0.001663  1563.348446
   9    7    0    0    0    1   1   0   0   0  1570.662    0.002643  1602.594075
   9    8    0    0    0    1   1   0   0   0  1638.100    0.020393  1665.109899
   9    0    0    0    0    2   0   0   0   0  1732.974    0.050132  1766.871351
  10    7    0    0    0    1   1   0   0   0  1756.297    0.043206  1792.514526
  10    8    0    0    0    1   1   0   0   0  1818.411    0.065701  1855.030350
  10    9    0    0    0    1   1   0   0   0  1918.566    0.043220  1956.791802
  11    7    0    0    0    1   1   0   0   0  1951.291    0.064394  1997.967011
  12    7    0    0    0    1   1   0   0   0  2004.577    0.002853  2051.727141
  11    8    0    0    0    1   1   0   0   0  2021.099    0.004763  2060.482835
  12    8    0    0    0    1   1   0   0   0  2066.790    0.083132  2114.242965
  10    0    0    0    0    2   0   0   0   0  2092.420    0.795687  2146.712254
   7    0    0    0    0    3   0   0   0   0  2097.557    0.000000  2157.475198
  11    9    0    0    0    1   1   0   0   0  2110.771    0.613857  2162.244287
  12    9    0    0    0    1   1   0   0   0  2163.714    0.000274  2216.004418
   8    7    0    0    0    1   2   0   0   0  2168.509    0.000000  2219.991022
  13    0    0    0    0    1   0   0   0   0  2192.376   11.208705  2253.323425
   8    7    0    0    0    2   1   0   0   0  2239.055    0.000000  2282.506845
   9    7    0    0    0    1   2   0   0   0  2265.839    0.000000  2321.752474
  14    0    0    0    0    1   0   0   0   0  2274.523    2.567247  2363.879670
  11   10    0    0    0    1   1   0   0   0  2300.620    0.218413  2352.164739
   8    0    0    0    0    3   0   0   0   0  2309.194    0.000000  2345.022669
   9    8    7    0    0    1   1   1   0   0  2336.382    0.000000  2384.268298
  12   10    0    0    0    1   1   0   0   0  2355.533    0.813133  2405.924869
   9    8    0    0    0    1   2   0   0   0  2406.518    0.000000  2446.784122
   9    7    0    0    0    2   1   0   0   0  2430.967    0.000000  2486.029750
  10    7    0    0    0    1   2   0   0   0  2454.034    0.000000  2511.672925
  11    0    0    0    0    2   0   0   0   0  2491.171    0.154296  2557.617224
   9    8    0    0    0    2   1   0   0   0  2501.099    0.000000  2548.545574
  10    8    7    0    0    1   1   1   0   0  2519.253    0.000000  2574.188749
```

57

12	11	0	0	0	1	1	0	0	0	2551.512	0.047841	2611.377354
10	8	0	0	0	1	2	0	0	0	2584.065	0.000000	2636.704573
12	0	0	0	0	2	0	0	0	0	2587.934	0.151023	2665.137484
9	0	0	0	0	3	0	0	0	0	2592.940	0.000000	2650.307026
10	9	7	0	0	1	1	1	0	0	2619.119	0.000000	2675.950202
11	7	0	0	0	1	2	0	0	0	2644.889	0.000000	2717.125410
10	9	8	0	0	1	1	1	0	0	2683.928	0.000000	2738.466026
12	7	0	0	0	1	2	0	0	0	2702.841	0.000000	2770.885541
11	8	7	0	0	1	1	1	0	0	2717.801	0.000000	2779.641234
12	8	7	0	0	1	1	1	0	0	2768.159	0.000000	2833.401365
10	9	0	0	0	1	2	0	0	0	2781.048	0.000000	2840.227478
11	8	0	0	0	1	2	0	0	0	2790.306	0.000000	2842.157058
10	7	0	0	0	2	1	0	0	0	2795.533	0.000000	2865.870653
11	9	7	0	0	1	1	1	0	0	2807.183	0.000000	2881.402686
12	8	0	0	0	1	2	0	0	0	2833.069	0.000000	2895.917188
10	8	0	0	0	2	1	0	0	0	2855.018	0.000000	2928.386477
12	9	7	0	0	1	1	1	0	0	2864.794	0.000000	2935.162817
11	9	8	0	0	1	1	1	0	0	2879.685	0.000000	2943.918510
13	7	0	0	0	1	1	0	0	0	2898.260	0.092466	2972.481824
12	9	8	0	0	1	1	1	0	0	2929.702	0.000000	2997.678641
10	9	0	0	0	2	1	0	0	0	2957.419	0.000000	3030.147929
13	8	0	0	0	1	1	0	0	0	2959.126	0.002985	3034.997648
11	9	0	0	0	1	2	0	0	0	2966.323	0.000000	3045.679963
14	7	0	0	0	1	1	0	0	0	2981.330	0.016787	3083.038070
11	10	7	0	0	1	1	1	0	0	2999.593	0.000000	3071.323138
15	0	0	0	0	1	0	0	0	0	3010.579	10.108554	3153.188268
12	9	0	0	0	1	2	0	0	0	3023.593	0.000000	3099.440093
14	8	0	0	0	1	1	0	0	0	3042.069	0.538831	3145.553893
12	10	7	0	0	1	1	1	0	0	3059.173	0.000000	3125.083268
13	9	0	0	0	1	1	0	0	0	3066.509	0.737065	3136.759101
11	10	8	0	0	1	1	1	0	0	3066.771	0.000000	3133.838962
12	10	8	0	0	1	1	1	0	0	3118.757	0.000000	3187.599092
10	0	0	0	0	3	0	0	0	0	3122.052	0.000000	3220.068381
14	9	0	0	0	1	1	0	0	0	3140.189	0.011316	3247.315346
11	10	9	0	0	1	1	1	0	0	3158.690	0.000000	3235.600414
11	7	0	0	0	2	1	0	0	0	3186.004	0.000000	3276.775623
12	10	9	0	0	1	1	1	0	0	3217.929	0.000000	3289.360545
13	10	0	0	0	1	1	0	0	0	3247.803	0.057767	3326.679552
12	11	7	0	0	1	1	1	0	0	3251.011	0.000000	3330.535753
11	8	0	0	0	2	1	0	0	0	3260.875	0.000000	3339.291447
12	7	0	0	0	2	1	0	0	0	3292.101	0.000000	3384.295884
14	10	0	0	0	1	1	0	0	0	3307.546	0.303655	3437.235797
12	11	8	0	0	1	1	1	0	0	3318.288	0.000000	3393.051577
11	10	0	0	0	1	2	0	0	0	3339.318	0.000000	3425.520866
11	9	0	0	0	2	1	0	0	0	3342.311	0.000000	3441.052899
12	8	0	0	0	2	1	0	0	0	3351.783	0.000000	3446.811708
12	10	0	0	0	1	2	0	0	0	3400.527	0.000000	3479.280996
12	11	9	0	0	1	1	1	0	0	3406.977	0.000000	3494.813029
13	11	0	0	0	1	1	0	0	0	3444.592	0.072097	3532.132037
12	9	0	0	0	2	1	0	0	0	3447.725	0.000000	3548.573160
13	12	0	0	0	1	1	0	0	0	3485.791	0.268558	3585.892167
14	11	0	0	0	1	1	0	0	0	3522.995	0.018733	3642.688282
11	10	0	0	0	2	1	0	0	0	3538.935	0.000000	3630.973351
14	12	0	0	0	1	1	0	0	0	3561.353	0.208368	3696.448413
13	7	0	0	0	1	2	0	0	0	3597.319	0.000000	3691.640224
12	11	10	0	0	1	1	1	0	0	3605.571	0.000000	3684.733481
12	10	0	0	0	2	1	0	0	0	3648.288	0.000000	3738.493611
13	8	7	0	0	1	1	1	0	0	3661.290	0.000000	3754.156048
14	7	0	0	0	1	2	0	0	0	3681.312	0.000000	3802.196469
15	7	0	0	0	1	1	0	0	0	3718.957	0.049644	3872.346667
11	0	0	0	0	3	0	0	0	0	3720.903	0.000000	3836.425835
13	8	0	0	0	1	2	0	0	0	3724.854	0.000000	3816.671871
14	8	7	0	0	1	1	1	0	0	3745.156	0.000000	3864.712293
13	9	7	0	0	1	1	1	0	0	3768.384	0.000000	3855.917500
15	8	0	0	0	1	1	0	0	0	3781.833	0.003397	3934.862491
12	11	0	0	0	1	2	0	0	0	3792.965	0.000000	3890.185966
14	8	0	0	0	1	2	0	0	0	3808.592	0.000000	3927.228117
13	9	8	0	0	1	1	1	0	0	3831.945	0.000000	3918.433324
12	11	0	0	0	2	1	0	0	0	3841.110	0.000000	3943.946096
14	9	7	0	0	1	1	1	0	0	3842.987	0.000000	3966.473745
12	0	0	0	0	3	0	0	0	0	3865.336	0.000000	3997.706227
15	9	0	0	0	1	1	0	0	0	3876.260	0.304073	4036.623943
14	9	8	0	0	1	1	1	0	0	3906.420	0.000000	4028.989569
13	9	0	0	0	1	2	0	0	0	3936.294	0.000000	4020.194776
13	10	7	0	0	1	1	1	0	0	3952.238	0.000000	4045.837951
14	9	0	0	0	1	2	0	0	0	4001.507	0.000000	4130.751021
13	10	8	0	0	1	1	1	0	0	4010.475	0.000000	4108.353775
14	10	7	0	0	1	1	1	0	0	4012.904	0.000000	4156.394197

15	10	0	0	0	1	1	0	0	0	4061.234	0.067941	4226.544395
14	10	8	0	0	1	1	1	0	0	4071.014	0.000000	4218.910020
13	10	9	0	0	1	1	1	0	0	4120.105	0.000000	4210.115228
13	11	7	0	0	1	1	1	0	0	4144.888	0.000000	4251.290436
14	10	9	0	0	1	1	1	0	0	4171.381	0.000000	4320.671473
13	12	7	0	0	1	1	1	0	0	4190.753	0.000000	4305.050567
13	11	8	0	0	1	1	1	0	0	4210.818	0.000000	4313.806260
14	11	7	0	0	1	1	1	0	0	4224.213	0.000000	4361.846681
15	11	0	0	0	1	1	0	0	0	4243.472	0.571554	4431.996880
13	12	8	0	0	1	1	1	0	0	4249.089	0.000000	4367.566391
14	12	7	0	0	1	1	1	0	0	4267.238	0.000000	4415.606812
15	12	0	0	0	1	1	0	0	0	4288.071	0.054579	4485.757010
14	11	8	0	0	1	1	1	0	0	4290.016	0.000000	4424.362505
13	10	0	0	0	1	2	0	0	0	4292.178	0.000000	4400.035679
13	11	9	0	0	1	1	1	0	0	4309.964	0.000000	4415.567712
14	12	8	0	0	1	1	1	0	0	4325.447	0.000000	4478.122636
14	10	0	0	0	1	2	0	0	0	4329.517	0.000000	4510.591924
13	0	0	0	0	2	0	0	0	0	4354.831	0.032388	4506.646850
13	12	9	0	0	1	1	1	0	0	4355.489	0.000000	4469.327843
14	11	9	0	0	1	1	1	0	0	4379.900	0.000000	4526.123958
14	13	0	0	0	1	1	0	0	0	4404.561	0.274181	4617.203096
15	7	0	0	0	1	2	0	0	0	4420.511	0.000000	4591.505066
14	12	9	0	0	1	1	1	0	0	4422.584	0.000000	4579.884088
15	8	7	0	0	1	1	1	0	0	4486.491	0.000000	4654.020890
13	11	10	0	0	1	1	1	0	0	4498.033	0.000000	4605.488164
14	0	0	0	0	2	0	0	0	0	4509.745	0.195644	4727.759341
13	12	10	0	0	1	1	1	0	0	4545.527	0.000000	4659.248294
15	8	0	0	0	1	2	0	0	0	4552.065	0.000000	4716.536714
14	11	10	0	0	1	1	1	0	0	4554.032	0.000000	4716.044409
15	9	7	0	0	1	1	1	0	0	4580.630	0.000000	4755.782342
14	12	10	0	0	1	1	1	0	0	4598.685	0.000000	4769.804540
15	9	8	0	0	1	1	1	0	0	4646.200	0.000000	4818.298166
13	11	0	0	0	1	2	0	0	0	4686.239	0.000000	4810.940649
15	9	0	0	0	1	2	0	0	0	4737.594	0.000000	4920.059619
13	12	11	0	0	1	1	1	0	0	4739.160	0.000000	4864.700779
14	11	0	0	0	1	2	0	0	0	4760.898	0.000000	4921.496894
13	12	0	0	0	1	2	0	0	0	4768.163	0.000000	4918.460910
15	10	7	0	0	1	1	1	0	0	4768.164	0.000000	4945.702794
14	12	11	0	0	1	1	1	0	0	4810.978	0.000000	4975.257024
15	10	8	0	0	1	1	1	0	0	4828.411	0.000000	5008.218618
14	12	0	0	0	1	2	0	0	0	4837.140	0.000000	5029.017155
15	10	9	0	0	1	1	1	0	0	4925.085	0.000000	5109.980070
15	11	7	0	0	1	1	1	0	0	4946.262	0.000000	5151.155279
15	12	7	0	0	1	1	1	0	0	4995.528	0.000000	5204.915409
15	11	8	0	0	1	1	1	0	0	5014.202	0.000000	5213.671103
15	12	8	0	0	1	1	1	0	0	5055.873	0.000000	5267.431233
13	7	0	0	0	2	1	0	0	0	5060.589	0.000000	5225.805250
15	11	9	0	0	1	1	1	0	0	5100.393	0.000000	5315.432555
15	10	0	0	0	1	2	0	0	0	5100.838	0.000000	5299.900522
14	13	7	0	0	1	1	1	0	0	5111.242	0.000000	5336.361495
13	8	0	0	0	2	1	0	0	0	5117.578	0.000000	5288.321073
15	12	9	0	0	1	1	1	0	0	5149.317	0.000000	5369.192685
14	13	8	0	0	1	1	1	0	0	5168.104	0.000000	5398.877319
15	13	0	0	0	1	1	0	0	0	5202.934	0.041933	5406.511693
14	7	0	0	0	2	1	0	0	0	5217.348	0.000000	5446.917740
13	9	0	0	0	2	1	0	0	0	5234.436	0.000000	5390.082526
14	8	0	0	0	2	1	0	0	0	5274.083	0.000000	5509.433564
14	13	9	0	0	1	1	1	0	0	5275.699	0.000000	5500.638771
15	14	0	0	0	1	1	0	0	0	5286.511	0.047033	5517.067938
15	11	10	0	0	1	1	1	0	0	5292.142	0.000000	5505.353007
15	12	10	0	0	1	1	1	0	0	5343.036	0.000000	5559.113137
14	9	0	0	0	2	1	0	0	0	5372.415	0.000000	5611.195016
13	10	0	0	0	2	1	0	0	0	5413.949	0.000000	5580.002977
14	13	10	0	0	1	1	1	0	0	5441.275	0.000000	5690.559223
15	11	0	0	0	1	2	0	0	0	5465.797	0.000000	5710.805491
15	12	11	0	0	1	1	1	0	0	5522.118	0.000000	5764.565622
14	10	0	0	0	2	1	0	0	0	5524.055	0.000000	5801.115468
15	12	0	0	0	1	2	0	0	0	5554.521	0.000000	5818.325752
13	11	0	0	0	2	1	0	0	0	5608.394	0.000000	5785.455462
13	12	0	0	0	2	1	0	0	0	5642.173	0.000000	5839.215593
14	13	11	0	0	1	1	1	0	0	5654.379	0.000000	5896.011707
14	13	12	0	0	1	1	1	0	0	5685.318	0.000000	5949.771838
14	11	0	0	0	2	1	0	0	0	5755.819	0.000000	6006.567952
14	12	0	0	0	2	1	0	0	0	5783.917	0.000000	6060.328083
15	0	0	0	0	2	0	0	0	0	5898.437	0.515631	6306.376535
15	13	7	0	0	1	1	1	0	0	5911.187	0.000000	6125.670092
15	13	8	0	0	1	1	1	0	0	5970.185	0.000000	6188.185916
15	14	7	0	0	1	1	1	0	0	5995.686	0.000000	6236.226337

```
 15   14    8    0    0   1   1   1   0   0   6054.557   0.000000   6298.742161
 15   13    9    0    0   1   1   1   0   0   6074.088   0.000000   6289.947368
 15   14    9    0    0   1   1   1   0   0   6149.197   0.000000   6400.503614
 15   13   10    0    0   1   1   1   0   0   6257.281   0.000000   6479.867820
 15   14   10    0    0   1   1   1   0   0   6318.453   0.000000   6590.424065
 15   13   11    0    0   1   1   1   0   0   6437.174   0.000000   6685.320305
 15   13   12    0    0   1   1   1   0   0   6474.353   0.000000   6739.080435
 13    0    0    0    0   3   0   0   0   0   6487.366   0.000000   6759.970276
 14   13    0    0    0   1   2   0   0   0   6504.679   0.000000   6870.526521
 15   14   11    0    0   1   1   1   0   0   6517.006   0.000000   6795.876550
 15   14   12    0    0   1   1   1   0   0   6551.345   0.000000   6849.636680
 14   13    0    0    0   2   1   0   0   0   6577.445   0.000000   6981.082766
 15    7    0    0    0   2   1   0   0   0   6609.183   0.000000   7025.534935
 15    8    0    0    0   2   1   0   0   0   6670.192   0.000000   7088.050759
 14    0    0    0    0   3   0   0   0   0   6705.666   0.000000   7091.639011
 15    9    0    0    0   2   1   0   0   0   6761.138   0.000000   7189.812211
 15   10    0    0    0   2   1   0   0   0   6948.012   0.000000   7379.732662
 15   11    0    0    0   2   1   0   0   0   7113.354   0.000000   7585.185147
 15   12    0    0    0   2   1   0   0   0   7153.933   0.000000   7638.945278
 15   13    0    0    0   1   2   0   0   0   7365.370   0.000000   7659.835118
 15   14   13    0    0   1   1   1   0   0   7416.529   0.000000   7770.391363
 15   14    0    0    0   1   2   0   0   0   7523.141   0.000000   7880.947608
 15   13    0    0    0   2   1   0   0   0   8090.772   0.000000   8559.699961
 15   14    0    0    0   2   1   0   0   0   8175.778   0.000000   8670.256206
 15    0    0    0    0   3   0   0   0   0   8663.574   0.000000   9459.564803
--------------------------------------------------------------------------------
 Dipole moment function written to files dipolex(y,z)
  @CHECKOUT-I, Total execution time :        0.0000 seconds.
  --executable xcubic finished with status            0
```

60

Table S.10. Part of the CFOUR output file of the CCSD(T)/VQZ-aV(Q+d)Z anharmonic frequency calculation for $^{12}CHD_2^{37}Cl$

```
   **************************************************************************
       <<<    CCCCCC    CCCCCC   |||    CCCCCC    CCCCCC    >>>
      <<<      CCC       CCC     |||    CCC        CCC       >>>
     <<<       CCC       CCC     |||    CCC        CCC        >>>
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     <<<       CCC       CCC     |||    CCC        CCC        >>>
      <<<      CCC       CCC     |||    CCC        CCC       >>>
       <<<    CCCCCC    CCCCCC   |||    CCCCCC    CCCCCC    >>>
   **************************************************************************


     ****************************************************************
     * CFOUR Coupled-Cluster techniques for Computational Chemistry *
     ****************************************************************


   Department of Chemistry              Institut fuer Physikalische Chemie
   University of Texas at Austin        Universitaet Mainz
   Austin, TX  78712, USA               D-55099 Mainz, Germany

                     Version 1.0


                        Normal Coordinates

             A'                        A''                       A'
           712.38                    780.48                    880.71
          VIBRATION                 VIBRATION                 VIBRATION
C     0.064 0.6681  0.0000    0.0000  0.0000  0.3721    0.4312 -0.3534  0.0000
CL   -0.020-0.5529  0.0000    0.0000  0.0000 -0.1592   -0.1262  0.0912  0.0000
H    -0.030 0.3433  0.0110   -0.0232  0.6376 -0.0776   -0.2631  0.3971  0.0388
H    -0.030 0.3433 -0.0110    0.0232 -0.6376 -0.0776   -0.2631  0.3971 -0.0388
H    -0.015 0.0726  0.0000    0.0000  0.0000 -0.1001    0.0204 -0.4556  0.0000

             A'                        A'                        A''
          1073.05                   1269.00                   1324.63
          VIBRATION                 VIBRATION                 VIBRATION
C     0.268 0.2949  0.0000    0.0602 -0.2818  0.0000    0.0000  0.0000  0.2598
CL    0.002 0.0069  0.0000    0.0470 -0.0369  0.0000    0.0000  0.0000  0.0041
H    -0.338-0.3392  0.4306   -0.2636  0.1342  0.0652    0.3299 -0.1322 -0.0347
H    -0.338-0.3392 -0.4306   -0.2636  0.1342 -0.0652   -0.3299  0.1322 -0.0347
H     0.019-0.0999  0.0000    0.2530  0.8160  0.0000    0.0000  0.0000 -0.8231

             A'                        A''                       A'
          2251.67                   2361.61                   3202.70
          VIBRATION                 VIBRATION                 VIBRATION
C     0.232 0.1873  0.0000    0.0000  0.0000  0.4338    0.2740 -0.0632  0.0000
CL   -0.001-0.0035  0.0000    0.0000  0.0000 -0.0028   -0.0008 -0.0001  0.0000
H    -0.312-0.2123 -0.5550   -0.2983 -0.2012 -0.5257   -0.0053 -0.0110 -0.0270
H    -0.312-0.2123  0.5550    0.2983  0.2012 -0.5257   -0.0053 -0.0110  0.0270
H     0.090-0.0243  0.0000    0.0000  0.0000  0.0068   -0.9257  0.2495  0.0000
          Gradient vector in normal coordinate representation
      -----------------------------------------------------------
    i   W(I)      dE/dQ(i)       dE/dq      dE/dq     [dE/dQ(i)]/w(i)
                               (cm-1)      (eV)        (relative)
      -----------------------------------------------------------
    7   712.38 -0.0000002243     -0.02024     0.00000    0.0000000000
    8   780.48  0.0000000000      0.00000     0.00000    0.0000000000
    9   880.71  0.0000006073      0.04928     0.00001    0.0000000000
   10  1073.05  0.0000005085      0.03738     0.00000    0.0000000000
   11  1269.00  0.0000022098      0.14939     0.00002    0.0000000000
   12  1324.63  0.0000000000      0.00000     0.00000    0.0000000000
   13  2251.67 -0.0000074472     -0.37795    -0.00005    0.0000000000
   14  2361.61  0.0000000000      0.00000     0.00000    0.0000000000
   15  3202.70 -0.0037340809   -158.89938    -0.01970    0.0000021628
      -----------------------------------------------------------


                Normal modes in internal coordinates
 --------------------------------------------------------------------------
          95.659        35.442        0.012        0.012        0.040
 --------------------------------------------------------------------------
RCl      0.000000     -0.000464     0.000000     0.000000     0.000000
```

RH	0.000100	0.000014	0.000000	0.000000	0.000000
TDA1	-0.001496	-0.000239	0.000000	0.000000	0.000000
RH	-0.000100	0.000014	0.000000	0.000000	0.000000
TDA1	0.001496	-0.000239	0.000000	0.000000	0.000000
D120	0.000000	-0.000803	0.000000	0.000000	0.000000
RH	0.000000	0.000088	0.000000	0.000000	0.000000
TDA1	0.000000	0.002613	0.000000	0.000000	0.000000
D120	0.006660	0.000402	0.000000	0.000000	0.000000

	10.319	712.382	780.482	880.714	1073.050
RCl	0.000000	0.946571	0.000000	-0.233946	0.140440
RH	0.000006	0.014382	0.023445	0.013789	-0.008862
TDA1	0.000149	0.101322	0.643997	0.423453	-0.255796
RH	-0.000006	0.014382	-0.023445	0.013789	-0.008862
TDA1	-0.000149	0.101322	-0.643997	0.423453	-0.255796
D120	0.000000	0.145789	0.000000	0.572269	0.803497
RH	0.000000	-0.003131	0.000000	0.004422	0.008120
TDA1	0.000000	-0.237652	0.000000	-0.420571	-0.205382
D120	-0.000176	-0.072895	-0.411628	-0.286135	-0.401748

	1269.005	1324.628	2251.670	2361.613	3202.695
RCl	-0.144084	0.000000	0.069373	0.000000	-0.020478
RH	0.005459	-0.009414	-0.697931	-0.696878	-0.048256
TDA1	0.181138	-0.054266	-0.004770	0.067444	0.025773
RH	0.005459	0.009414	-0.697931	0.696878	-0.048256
TDA1	0.181138	0.054266	-0.004770	-0.067444	0.025773
D120	0.379643	0.000000	0.098945	0.000000	0.073789
RH	0.044090	0.000000	-0.058648	0.000000	0.992838
TDA1	0.855250	0.000000	-0.072459	0.000000	-0.032597
D120	-0.189821	-0.996962	-0.049472	-0.140084	-0.036894

```
       ----------------------------------------------------------------
                          Dipole Moment Function
                       (Normal Coordinate Basis)
       ----------------------------------------------------------------
         Mode    Symmetry   d(Mu(x))/dQ   d(Mu(y))/dQ   d(Mu(z))/dQ
       ----------------------------------------------------------------
          Q7        A'       -0.008141      0.130147      0.000000
          Q8        A''       0.000000      0.000000     -0.017233
          Q9        A'       -0.026646     -0.073911      0.000000
          Q10       A'       -0.047407      0.064340      0.000000
          Q11       A'       -0.008015     -0.081570      0.000000
          Q12       A''       0.000000      0.000000     -0.076134
          Q13       A'        0.021496      0.109721      0.000000
          Q14       A''       0.000000      0.000000      0.052096
          Q15       A'        0.056859     -0.076309      0.000000
       ----------------------------------------------------------------
```

```
   -----------------------------------------------------------------------
   ----------------------------------------------------------------
          Parameter              (MHz)               (CM-1)
   ----------------------------------------------------------------

          R6              -.130982E-04        -.436909E-09
          R5              -.116881E-01        -.389873E-06
          SI                    0.573566E+03

   A-reduced centrifugal distortion parameters

          DJ               0.120161E-01        0.400814E-06
          DK               0.934898E+00        0.311848E-04
          DJK              0.124242E+00        0.414426E-05
          DELJ             0.120423E-01        0.401687E-06
          DELK             0.935029E+00        0.311892E-04
          DELJK            0.124085E+00        0.413902E-05
          delJ             0.287056E-03        0.957516E-08
          delK             0.534269E-01        0.178213E-05

   S-reduced centrifugal distortion parameters

          DJ               0.119957E-01        0.400134E-06
          DK               0.934796E+00        0.311814E-04
          DJK              0.124364E+00        0.414834E-05
          D1              -.287056E-03        -.957516E-08
          D2              -.232872E-04        -.776777E-09
   ----------------------------------------------------------------
```

```
    Vibrational frequencies after rotational projection  of
    Cartesian force constants:
              1              0.0000i
              2              0.0000i
              3              0.0000i
              4              0.0000
              5              0.0000
              6              0.0000
              7            712.3812
              8            780.4613
              9            880.7088
             10           1073.0495
             11           1268.9923
             12           1324.5456
             13           2251.6699
             14           2361.6126
             15           3202.6950
   Zero-point vibrational energy:   19.8083 kcal/mol =   82.8780 kJ/mol.
               0.38 seconds walltime passed
  --executable xjoda finished with status            0
  --invoking executable xcubic
   @GETMEM-I,  Allocated   13351 MB of main memory.
   back




  ********************************************************************************
        PARAMETERS RELEVANT TO MOLECULAR STRUCTURE
  ********************************************************************************

   Force Field from Numerical Differentiation of Analytic Second Derivatives
   --------------------------------------------------------------------------
  Cubic force constants written to file cubic.

  ------------------------------------------------------------------------------
   Mean and mean-square displacements in dimensionless normal coordinates

           Geometrical properties evaluated at     0.00 K

           Coordinate              <q>           <q**2>
  ------------------------------------------------------------------------------
               7              0.1321044667    0.4999999889
               8              0.0000000000    0.4999999889
               9             -0.0325827646    0.4999999889
              10              0.0058548311    0.4999999889
              11              0.0117484668    0.4999999889
              12              0.0000000000    0.4999999889
              13             -0.1289257363    0.4999999889
              14              0.0000000000    0.4999999889
              15              0.0784458787    0.4999999889
  ------------------------------------------------------------------------------


     --------------------------------------------------------
     ATOM              INTERNUCLEAR DISTANCE / Angstrom
     --------------------------------------------------------
     I   J        Re           Rg           Ra
     --------------------------------------------------------
     2   1      1.7826656    1.7908405    1.7905230
     3   1      1.0850773    1.1004844    1.0929669
     3   2      2.3617095    2.3756395    2.3738700
     4   1      1.0850773    1.1004844    1.0929669
     4   2      2.3617095    2.3756395    2.3738700
     4   3      1.7831251    1.8022880    1.7960060
     5   1      1.0850773    1.1062119    1.0942196
     5   2      2.3617095    2.3798556    2.3762750
     5   3      1.7831251    1.8062483    1.7970554
     5   4      1.7831251    1.8062483    1.7970554
     --------------------------------------------------------
  ********************************************************************************
       PARAMETERS RELEVANT TO ROTATIONAL SPECTROSCOPY
  ********************************************************************************


     ------------------------------------------------------------------------------
                             VIB-ROT CONSTANT / (cm-1)
                             ------------------------------
      AXIS      MODE      CORIOLIS     QUADRATIC    ANHARMONIC     TOTAL
     ------------------------------------------------------------------------------
```

```
     1        7       0.0005781     -0.0010753      0.0034441       0.0029469
     1        8       0.0004244     -0.0000001      0.0007660       0.0011902
     1        9       0.0000126     -0.0002156      0.0009607       0.0007576
     1       10       0.0001089     -0.0000286      0.0001796       0.0002599
     1       11       0.0057920     -0.0000722      0.0007530       0.0064729
     1       12      -0.0060931     -0.0000097     -0.0000994      -0.0062021
     1       13      -0.0002600     -0.0000264      0.0007028       0.0004165
     1       14      -0.0004053     -0.0000046      0.0005239       0.0001140
     1       15      -0.0000185     -0.0000039     -0.0000987      -0.0001210
     2        7       0.0008124     -0.0000524      0.0033943       0.0041543
     2        8       0.0248519     -0.0046983     -0.0185760       0.0015775
     2        9      -0.0095056     -0.0035376     -0.0147321      -0.0277752
     2       10       0.0237580     -0.0038669     -0.0057029       0.0141882
     2       11       0.0403189     -0.0024479     -0.0033261       0.0345449
     2       12      -0.0157676     -0.0001104     -0.0054424      -0.0213204
     2       13      -0.0028686     -0.0198081      0.0525688       0.0298921
     2       14      -0.0342101     -0.0001545      0.0504246       0.0160600
     2       15      -0.0199155     -0.0029708      0.0383356       0.0154493
     3        7       0.0002015     -0.0011337      0.0036063       0.0026741
     3        8       0.0002804     -0.0005621      0.0009825       0.0007008
     3        9       0.0015724     -0.0000282      0.0009613       0.0025055
     3       10      -0.0011777     -0.0000169      0.0001295      -0.0010651
     3       11       0.0000283     -0.0000005      0.0007154       0.0007433
     3       12      -0.0001602     -0.0000232      0.0000097      -0.0001736
     3       13      -0.0001817     -0.0000048      0.0002728       0.0000863
     3       14      -0.0000928     -0.0000232      0.0003343       0.0002183
     3       15      -0.0003402     -0.0000067      0.0002688      -0.0000781
------------------------------------------------------------------------------


------------------------------------------------------------------------------
 Be, B0 AND B-B0 SHIFTS FOR SINGLY EXCITED VIBRATIONAL STATES (CM-1)
 ------------------------------------------------------------------
VIBRATION          X AXIS               Y AXIS               Z AXIS
------------------------------------------------------------------------------
  Be               0.37398667           3.20837886           0.38377489
  B0               0.37106931           3.17499356           0.38096914
  Be-B0            0.00291737           0.03338530           0.00280576
  B'               0.37106593           3.17499805           0.38097027
  Be-B'            0.00292075           0.03338080           0.00280462
  B''              0.37107242           3.17499885           0.38097355
  Be-B''           0.00291425           0.03338001           0.00280135
  B^A              0.37106389           3.17499804           0.38097231
  Be-B^A           0.00292278           0.03338081           0.00280258
  B^S              0.37106752           3.17499805           0.38096868
  Be-B^S           0.00291915           0.03338080           0.00280621
   7              -0.00294691          -0.00415432          -0.00267408
   8              -0.00119022          -0.00157750          -0.00070081
   9              -0.00075762           0.02777524          -0.00250551
  10              -0.00025985          -0.01418821           0.00106506
  11              -0.00647286          -0.03454485          -0.00074325
  12               0.00620044           0.02132044           0.00017363
  13              -0.00041647          -0.02989207          -0.00008631
  14              -0.00011396          -0.01606001          -0.00021833
  15               0.00012101          -0.01544933           0.00007809
------------------------------------------------------------------------------
------------------------------------------------------------------------------
 Be, B0 AND B-B0 SHIFTS FOR SINGLY EXCITED VIBRATIONAL STATES (MHz)
VIBRATION          X AXIS               Y AXIS               Z AXIS
------------------------------------------------------------------------------
  Be           11211.83844253       96184.77834540       11505.28190683
  B0           11124.37790688       95183.91223521       11421.16745295
  Be-B0           87.46053565        1000.86611019          84.11445388
  B'           11124.27665565       95184.04700444       11421.20149975
  Be-B'           87.56178688        1000.73134096          84.08040708
  B''          11124.47135735       95184.07085256       11421.29955169
  Be-B''          87.36708517        1000.70749284          83.98235514
  B^A          11124.21569548       95184.04679310       11421.26267126
  Be-B^A          87.62274704        1000.73155230          84.01923557
  B^S          11124.32442335       95184.04702849       11421.15375508
  Be-B^S          87.51401918        1000.73131691          84.12815175
   7             -88.34618583        -124.54329642         -80.16682998
   8             -35.68202622         -47.29236440         -21.00989520
   9             -22.71279232         832.68088650         -75.11332186
  10              -7.79023205        -425.35171364          31.92970464
  11            -194.05143794       -1035.62869755         -22.28221090
  12             185.93550006         639.17079973           5.20539649
  13             -12.48532307        -896.14170414          -2.58754881
```

```
     14              -3.41638743        -481.46686079         -6.54541333
     15               3.62781349        -463.15926967          2.34121119
    ----------------------------------------------------------------------
                 Vibrationally averaged dipole moment
    ----------------------------------------------------------------------
                    a.u.                            Debye
          x        y        z            x        y        z
    ----------------------------------------------------------------------
MU_e -0.03009  0.75412  0.00000      -0.07647  1.91666  0.00000
<MU> -0.02801  0.74857  0.00000      -0.07120  1.90256  0.00000

Equilibrium dipole moment:   0.75472 a.u. (   1.91818 D)
Equilibrium dipole moment:   0.74910 a.u. (   1.90389 D)
    ----------------------------------------------------------------------
****************************************************************************
    PARAMETERS RELEVANT TO VIBRATIONAL SPECTROSCOPY
****************************************************************************
  Quartic force constants written to file quartic
  ================================================================
  Performing F(IIJJ)/F(JJII) consistency check
  Differences greater than 1 cm-1 will be printed.
  ================================================================
  I   I   K   K      F(IIKK)       F(KKII)        Difference
  ----------------------------------------------------------------
  ----------------------------------------------------------------
  Largest absolute difference is    0.31976 cm-1.
  Largest relative difference is .11429D+00.
VPT2 vibrational analysis


 Thresholds for removing resonance denominators:
 Delta_omega = 50 cm-1; Phi(ijk) = 80 cm-1

-------------------------------
  ANHARMONICITY CONSTANTS X(ij)
             (cm-1)
-------------------------------
  (*) Near-zero denominators were removed
-------------------------------
        I  J        X(IJ)
-------------------------------
        7   7      -3.3481
        7   8      -3.6948
        7   9      -3.9650
        7  10      -1.4534
        7  11      -5.6018
        7  12      -0.9055
        7  13      -0.1031
        7  14       0.8213
        7  15       2.3412
        8   8      -0.5079
        8   9      -1.2732
        8  10      -4.0820
        8  11      -0.5338
        8  12      -3.4636
        8  13      -4.0065
        8  14      -3.1567
        8  15       0.4467
        9   9      -2.1431
        9  10      -1.8274
        9  11      -8.7271
        9  12      -4.4679
        9  13       5.4542
        9  14      -3.0450
        9  15      -3.0390
       10  10      -5.5267
       10  11      -1.9890
       10  12       4.3066
       10  13       3.6906
       10  14     -18.7134
       10  15      -1.0802
       11  11      -5.2879
       11  12       1.1453
       11  13       1.3074
       11  14      -2.3990
       11  15     -17.9713
       12  12      -5.5249
       12  13      -6.0738
```

```
          12 14        -12.6646
          12 15        -21.9955
          13 13        -14.9604
          13 14        -62.3383
          13 15         -0.0810
          14 14        -19.6513
          14 15          1.3678
          15 15        -61.3604


--------------------------------------------------------------------------------
      HARMONIC AND FUNDAMENTAL FREQUENCIES (cm-1) AND INTENSITIES (km/mol)
--------------------------------------------------------------------------------


          Harmonic    Fundamental Anharmonic    Harmonic    Fundamental  Anharm
  Mode    Frequency    Frequency  Contribution  Intensity   Intensity    Contrib
   7      712.9446     699.9679    -12.9767      16.6408     17.6160      0.9751
   8      781.1097     770.2120    -10.8977       0.2735      0.2760      0.0025
   9      882.8539     868.1225    -14.7314       6.1520      5.9986     -0.1534
  10     1073.3548    1051.7272    -21.6276       6.0453      5.6577     -0.3875
  11     1278.6809    1250.7205    -27.9604       6.5254      5.8545     -0.6709
  12     1332.5682    1299.4589    -33.1093       5.7335      5.8010      0.0675
  13     2253.3224    2192.3264    -60.9961      12.1868     11.2170     -0.9698
  14     2363.8791    2274.5125    -89.3666       2.5973      2.5674     -0.0299
  15     3153.1882    3010.4616   -142.7266       9.2611     10.2584      0.9974
--------------------------------------------------------------------------------


--------------------------------------------------------------------------------
                      ZERO-POINT VIBRATIONAL ENERGIES
--------------------------------------------------------------------------------
                       kcal/mol      kJ/mol       Hartree        cm-1
--------------------------------------------------------------------------------
Harmonic contribution :   19.7737     82.7330     0.03151139     6915.951
VPT2-correction       :   -0.2334     -0.9764    -0.00037189      -81.620
--------------------------------------------------------------------------------
Harm+VPT2             :   19.5403     81.7567     0.03113950     6834.331
--------------------------------------------------------------------------------
   MAXLEVEL set to                    3
 --------------------------------------------------------------------------------
                   All levels with up to three quanta
--------------------------------------------------------------------------------
  MODE MODE MODE MODE MODE                    Anharmonic      Anharm      Harmonic
   I    J    K    L    M   NI  NJ  NK  NL  NM Frequency      Intensity   Transition
--------------------------------------------------------------------------------
    7    0    0    0    0   1   0   0   0   0   699.967      17.615627   712.944633
    8    0    0    0    0   1   0   0   0   0   770.211       0.275968   781.109677
    9    0    0    0    0   1   0   0   0   0   868.122       5.998515   882.853857
   10    0    0    0    0   1   0   0   0   0  1051.727       5.657621  1073.354769
   11    0    0    0    0   1   0   0   0   0  1250.720       5.854368  1278.680931
   12    0    0    0    0   1   0   0   0   0  1299.458       5.800851  1332.568230
    7    0    0    0    0   2   0   0   0   0  1393.239       0.136363  1425.889266
    8    7    0    0    0   1   1   0   0   0  1466.485       0.012819  1494.054310
    8    0    0    0    0   2   0   0   0   0  1539.408       0.001635  1562.219355
    9    7    0    0    0   1   1   0   0   0  1564.125       0.002722  1595.798490
    9    8    0    0    0   1   1   0   0   0  1637.061       0.020584  1663.963534
    9    0    0    0    0   2   0   0   0   0  1731.958       0.049948  1765.707714
   10    7    0    0    0   1   1   0   0   0  1750.241       0.041943  1786.299402
   10    8    0    0    0   1   1   0   0   0  1817.857       0.065377  1854.464446
   10    9    0    0    0   1   1   0   0   0  1918.022       0.043487  1956.208626
   11    7    0    0    0   1   1   0   0   0  1945.086       0.063661  1991.625564
   12    7    0    0    0   1   1   0   0   0  1998.521       0.002750  2045.512863
   11    8    0    0    0   1   1   0   0   0  2020.398       0.004672  2059.790609
   12    8    0    0    0   1   1   0   0   0  2066.207       0.082832  2113.677908
    7    0    0    0    0   3   0   0   0   0  2079.815       0.000000  2138.833899
   10    0    0    0    0   2   0   0   0   0  2092.400       0.795952  2146.709538
   11    9    0    0    0   1   1   0   0   0  2110.115       0.602942  2161.534788
    8    7    0    0    0   1   2   0   0   0  2156.062       0.000000  2206.998943
   12    9    0    0    0   1   1   0   0   0  2163.113       0.000308  2215.422087
   13    0    0    0    0   1   0   0   0   0  2192.326      11.216781  2253.322441
    8    7    0    0    0   2   1   0   0   0  2231.986       0.000000  2275.163987
    9    7    0    0    0   1   2   0   0   0  2253.432       0.000000  2308.743123
   14    0    0    0    0   1   0   0   0   0  2274.512       2.567300  2363.879130
   11   10    0    0    0   1   1   0   0   0  2300.458       0.218491  2352.035700
    8    0    0    0    0   3   0   0   0   0  2307.588       0.000000  2343.329032
    9    8    7    0    0   1   1   1   0   0  2329.369       0.000000  2376.908167
   12   10    0    0    0   1   1   0   0   0  2355.492       0.813067  2405.922999
    9    8    0    0    0   1   2   0   0   0  2404.984       0.000000  2445.073212
    9    7    0    0    0   2   1   0   0   0  2423.996       0.000000  2478.652347
   10    7    0    0    0   1   2   0   0   0  2442.060       0.000000  2499.244035
   11    0    0    0    0   2   0   0   0   0  2490.865       0.153707  2557.361863
```

9	8	0	0	0	2	1	0	0	0	2499.624	0.000000	2546.817391
10	8	7	0	0	1	1	1	0	0	2512.676	0.000000	2567.409079
12	11	0	0	0	1	1	0	0	0	2551.324	0.047762	2611.249162
10	8	0	0	0	1	2	0	0	0	2582.971	0.000000	2635.574123
12	0	0	0	0	2	0	0	0	0	2587.868	0.151044	2665.136461
9	0	0	0	0	3	0	0	0	0	2591.508	0.000000	2648.561571
10	9	7	0	0	1	1	1	0	0	2612.571	0.000000	2669.153259
11	7	0	0	0	1	2	0	0	0	2632.756	0.000000	2704.570197
10	9	8	0	0	1	1	1	0	0	2682.879	0.000000	2737.318303
12	7	0	0	0	1	2	0	0	0	2690.887	0.000000	2758.457496
11	8	7	0	0	1	1	1	0	0	2711.069	0.000000	2772.735242
12	8	7	0	0	1	1	1	0	0	2761.574	0.000000	2826.622541
10	9	0	0	0	1	2	0	0	0	2780.031	0.000000	2839.062483
11	8	0	0	0	1	2	0	0	0	2789.061	0.000000	2840.900286
10	7	0	0	0	2	1	0	0	0	2789.462	0.000000	2859.654171
11	9	7	0	0	1	1	1	0	0	2800.517	0.000000	2874.479421
12	8	0	0	0	1	2	0	0	0	2831.939	0.000000	2894.787585
10	8	0	0	0	2	1	0	0	0	2854.448	0.000000	2927.819215
12	9	7	0	0	1	1	1	0	0	2858.211	0.000000	2928.366720
11	9	8	0	0	1	1	1	0	0	2878.520	0.000000	2942.644466
13	7	0	0	0	1	1	0	0	0	2892.191	0.091639	2966.267073
12	9	8	0	0	1	1	1	0	0	2928.588	0.000000	2996.531765
10	9	0	0	0	2	1	0	0	0	2956.868	0.000000	3029.563395
13	8	0	0	0	1	1	0	0	0	2958.531	0.003002	3034.432118
11	9	0	0	0	1	2	0	0	0	2965.225	0.000000	3044.388646
14	7	0	0	0	1	1	0	0	0	2975.301	0.016703	3076.823763
11	10	7	0	0	1	1	1	0	0	2993.371	0.000000	3064.980333
15	0	0	0	0	1	0	0	0	0	3010.461	10.258234	3153.188205
12	9	0	0	0	1	2	0	0	0	3022.482	0.000000	3098.275944
14	8	0	0	0	1	1	0	0	0	3041.567	0.453122	3144.988807
12	10	7	0	0	1	1	1	0	0	3053.101	0.000000	3118.867632
13	9	0	0	0	1	1	0	0	0	3065.903	0.682443	3136.176298
11	10	8	0	0	1	1	1	0	0	3066.054	0.000000	3133.145378
12	10	8	0	0	1	1	1	0	0	3118.159	0.000000	3187.032677
10	0	0	0	0	3	0	0	0	0	3122.021	0.000000	3220.064307
14	9	0	0	0	1	1	0	0	0	3139.589	0.011129	3246.732987
11	10	9	0	0	1	1	1	0	0	3158.026	0.000000	3234.889557
11	7	0	0	0	2	1	0	0	0	3179.629	0.000000	3270.306496
12	10	9	0	0	1	1	1	0	0	3217.320	0.000000	3288.776856
12	11	7	0	0	1	1	1	0	0	3244.785	0.000000	3324.193795
13	10	0	0	0	1	1	0	0	0	3247.744	0.057780	3326.677209
11	8	0	0	0	2	1	0	0	0	3260.009	0.000000	3338.471540
12	7	0	0	0	2	1	0	0	0	3286.025	0.000000	3378.081094
14	10	0	0	0	1	1	0	0	0	3307.526	0.303881	3437.233899
12	11	8	0	0	1	1	0	0	0	3317.539	0.000000	3392.358839
11	10	0	0	0	1	2	0	0	0	3339.143	0.000000	3425.390469
11	9	0	0	0	2	1	0	0	0	3341.533	0.000000	3440.215720
12	8	0	0	0	2	1	0	0	0	3351.152	0.000000	3446.246138
12	10	0	0	0	1	2	0	0	0	3400.473	0.000000	3479.277768
12	11	9	0	0	1	1	1	0	0	3406.252	0.000000	3494.103019
13	11	0	0	0	1	1	0	0	0	3444.354	0.072345	3532.003372
12	9	0	0	0	2	1	0	0	0	3447.054	0.000000	3547.990318
13	12	0	0	0	1	1	0	0	0	3485.711	0.268554	3585.890671
14	11	0	0	0	1	1	0	0	0	3522.834	0.018815	3642.560061
11	10	0	0	0	2	1	0	0	0	3538.614	0.000000	3630.716632
14	12	0	0	0	1	1	0	0	0	3561.306	0.208402	3696.447360
13	7	0	0	0	1	2	0	0	0	3585.359	0.000000	3679.211706
12	11	10	0	0	1	1	1	0	0	3605.369	0.000000	3684.603931
12	10	0	0	0	2	1	0	0	0	3648.208	0.000000	3738.491230
13	8	7	0	0	1	1	1	0	0	3654.701	0.000000	3747.376751
14	7	0	0	0	1	2	0	0	0	3669.394	0.000000	3789.768396
15	7	0	0	0	1	1	0	0	0	3712.770	0.050255	3866.132837
11	0	0	0	0	3	0	0	0	0	3720.434	0.000000	3836.042794
13	8	0	0	0	1	2	0	0	0	3723.721	0.000000	3815.541795
14	8	7	0	0	1	1	1	0	0	3738.662	0.000000	3857.933440
13	9	7	0	0	1	1	1	0	0	3761.802	0.000000	3849.120930
15	8	0	0	0	1	1	0	0	0	3781.120	0.003430	3934.297882
12	11	0	0	0	1	2	0	0	0	3792.614	0.000000	3889.930093
14	8	0	0	0	1	2	0	0	0	3807.607	0.000000	3926.098484
13	9	8	0	0	1	1	1	0	0	3830.835	0.000000	3917.285975
14	9	7	0	0	1	1	1	0	0	3836.414	0.000000	3959.677620
12	11	0	0	0	2	1	0	0	0	3840.879	0.000000	3943.817392
12	0	0	0	0	3	0	0	0	0	3865.227	0.000000	3997.704691
15	9	0	0	0	1	1	0	0	0	3875.545	0.301901	4036.042062
14	9	8	0	0	1	1	1	0	0	3905.372	0.000000	4027.842664
13	9	0	0	0	1	2	0	0	0	3935.193	0.000000	4019.030155
13	10	7	0	0	1	1	1	0	0	3946.155	0.000000	4039.621842
14	9	0	0	0	1	2	0	0	0	4000.381	0.000000	4129.586844

14	10	7	0	0	1	1	1	0	0	4006.862	0.000000	4150.178532
13	10	8	0	0	1	1	1	0	0	4009.867	0.000000	4107.786887
15	10	0	0	0	1	1	0	0	0	4061.108	0.067870	4226.542973
14	10	8	0	0	1	1	1	0	0	4070.499	0.000000	4218.343576
13	10	9	0	0	1	1	1	0	0	4119.493	0.000000	4209.531066
13	11	7	0	0	1	1	1	0	0	4138.617	0.000000	4244.948005
14	10	9	0	0	1	1	1	0	0	4170.776	0.000000	4320.087756
13	12	7	0	0	1	1	1	0	0	4184.670	0.000000	4298.835304
13	11	8	0	0	1	1	1	0	0	4210.025	0.000000	4313.113049
14	11	7	0	0	1	1	1	0	0	4218.021	0.000000	4355.504694
15	11	0	0	0	1	1	0	0	0	4243.210	0.572439	4431.869136
13	12	8	0	0	1	1	1	0	0	4248.453	0.000000	4367.000348
14	12	7	0	0	1	1	1	0	0	4261.190	0.000000	4409.391993
15	12	0	0	0	1	1	0	0	0	4287.925	0.054615	4485.756435
14	11	8	0	0	1	1	1	0	0	4289.355	0.000000	4423.669739
13	10	0	0	0	1	2	0	0	0	4292.108	0.000000	4400.031978
13	11	9	0	0	1	1	1	0	0	4309.203	0.000000	4414.857229
14	12	8	0	0	1	1	1	0	0	4324.898	0.000000	4477.557038
14	10	0	0	0	1	2	0	0	0	4329.486	0.000000	4510.588668
13	0	0	0	0	2	0	0	0	0	4354.731	0.032386	4506.644881
13	12	9	0	0	1	1	1	0	0	4354.820	0.000000	4468.744528
14	11	9	0	0	1	1	1	0	0	4379.184	0.000000	4525.413918
14	13	0	0	0	1	1	0	0	0	4404.500	0.274182	4617.201570
15	7	0	0	0	1	2	0	0	0	4408.383	0.000000	4579.077470
14	12	9	0	0	1	1	1	0	0	4421.916	0.000000	4579.301217
15	8	7	0	0	1	1	1	0	0	4479.734	0.000000	4647.242515
13	11	10	0	0	1	1	1	0	0	4497.782	0.000000	4605.358141
14	0	0	0	0	2	0	0	0	0	4509.722	0.195675	4727.758260
13	12	10	0	0	1	1	1	0	0	4545.435	0.000000	4659.245440
15	8	0	0	0	1	2	0	0	0	4550.763	0.000000	4715.407559
14	11	10	0	0	1	1	1	0	0	4553.858	0.000000	4715.914830
15	9	7	0	0	1	1	1	0	0	4573.889	0.000000	4748.986694
14	12	10	0	0	1	1	1	0	0	4598.627	0.000000	4769.802129
15	9	8	0	0	1	1	1	0	0	4644.930	0.000000	4817.151739
13	11	0	0	0	1	2	0	0	0	4685.806	0.000000	4810.684303
15	9	0	0	0	1	2	0	0	0	4736.342	0.000000	4918.895919
13	12	11	0	0	1	1	1	0	0	4738.884	0.000000	4864.571602
14	11	0	0	0	1	2	0	0	0	4760.579	0.000000	4921.240993
15	10	7	0	0	1	1	1	0	0	4761.964	0.000000	4939.487606
13	12	0	0	0	1	2	0	0	0	4768.046	0.000000	4918.458901
14	12	11	0	0	1	1	1	0	0	4810.773	0.000000	4975.128292
15	10	8	0	0	1	1	1	0	0	4827.685	0.000000	5007.652651
14	12	0	0	0	1	2	0	0	0	4837.051	0.000000	5029.015591
15	10	9	0	0	1	1	1	0	0	4924.364	0.000000	5109.396831
15	11	7	0	0	1	1	1	0	0	4939.918	0.000000	5144.813769
15	12	7	0	0	1	1	1	0	0	4989.328	0.000000	5198.701068
15	11	8	0	0	1	1	1	0	0	5013.335	0.000000	5212.978813
13	7	0	0	0	2	1	0	0	0	5054.493	0.000000	5219.589514
15	12	8	0	0	1	1	1	0	0	5055.120	0.000000	5266.866112
15	11	9	0	0	1	1	1	0	0	5099.567	0.000000	5314.722993
15	10	0	0	0	1	2	0	0	0	5100.702	0.000000	5299.897742
14	13	7	0	0	1	1	1	0	0	5105.186	0.000000	5330.146203
13	8	0	0	0	2	1	0	0	0	5116.930	0.000000	5287.754558
15	12	9	0	0	1	1	1	0	0	5148.540	0.000000	5368.610292
14	13	8	0	0	1	1	1	0	0	5167.549	0.000000	5398.311248
15	13	0	0	0	1	1	0	0	0	5202.706	0.041943	5406.510645
14	7	0	0	0	2	1	0	0	0	5211.332	0.000000	5440.702893
13	9	0	0	0	2	1	0	0	0	5233.762	0.000000	5389.498738
14	8	0	0	0	2	1	0	0	0	5273.620	0.000000	5508.867937
14	13	9	0	0	1	1	1	0	0	5275.032	0.000000	5500.055428
15	14	0	0	0	1	1	0	0	0	5286.341	0.047032	5517.067335
15	11	10	0	0	1	1	1	0	0	5291.868	0.000000	5505.223905
15	12	10	0	0	1	1	1	0	0	5342.878	0.000000	5559.111204
14	9	0	0	0	2	1	0	0	0	5371.754	0.000000	5610.612117
13	10	0	0	0	2	1	0	0	0	5413.840	0.000000	5579.999650
14	13	10	0	0	1	1	1	0	0	5441.204	0.000000	5690.556339
15	11	0	0	0	1	2	0	0	0	5465.384	0.000000	5710.550067
15	12	11	0	0	1	1	1	0	0	5521.819	0.000000	5764.437366
14	10	0	0	0	2	1	0	0	0	5524.022	0.000000	5801.113029
15	12	0	0	0	1	2	0	0	0	5554.338	0.000000	5818.324665
13	11	0	0	0	2	1	0	0	0	5608.067	0.000000	5785.325813
13	12	0	0	0	2	1	0	0	0	5642.043	0.000000	5839.213111
14	13	11	0	0	1	1	1	0	0	5654.129	0.000000	5895.882502
14	13	12	0	0	1	1	1	0	0	5685.221	0.000000	5949.769801
14	11	0	0	0	2	1	0	0	0	5755.644	0.000000	6006.439191
14	12	0	0	0	2	1	0	0	0	5783.852	0.000000	6060.326490
15	0	0	0	0	2	0	0	0	0	5898.202	0.515636	6306.376409
15	13	7	0	0	1	1	1	0	0	5904.912	0.000000	6119.455278

```
  15   13    8    0    0    1    1    1    0    0   5969.359    0.000000   6187.620322
  15   14    7    0    0    1    1    1    0    0   5989.472    0.000000   6230.011967
  15   14    8    0    0    1    1    1    0    0   6053.843    0.000000   6298.177012
  15   13    9    0    0    1    1    1    0    0   6073.244    0.000000   6289.364502
  15   14    9    0    0    1    1    1    0    0   6148.380    0.000000   6399.921192
  15   13   10    0    0    1    1    1    0    0   6257.044    0.000000   6479.865414
  15   14   10    0    0    1    1    1    0    0   6318.275    0.000000   6590.422103
  15   13   11    0    0    1    1    1    0    0   6436.763    0.000000   6685.191577
  15   13   12    0    0    1    1    1    0    0   6474.096    0.000000   6739.078876
  13    0    0    0    0    3    0    0    0    0   6487.216    0.000000   6759.967322
  14   13    0    0    0    1    2    0    0    0   6504.567    0.000000   6870.524011
  15   14   11    0    0    1    1    1    0    0   6516.692    0.000000   6795.748266
  15   14   12    0    0    1    1    1    0    0   6551.140    0.000000   6849.635565
  14   13    0    0    0    2    1    0    0    0   6577.372    0.000000   6981.080700
  15    7    0    0    0    2    1    0    0    0   6602.852    0.000000   7019.321042
  15    8    0    0    0    2    1    0    0    0   6669.307    0.000000   7087.486086
  14    0    0    0    0    3    0    0    0    0   6705.629    0.000000   7091.637390
  15    9    0    0    0    2    1    0    0    0   6760.246    0.000000   7189.230266
  15   10    0    0    0    2    1    0    0    0   6947.769    0.000000   7379.731178
  15   11    0    0    0    2    1    0    0    0   7112.980    0.000000   7585.057341
  15   12    0    0    0    2    1    0    0    0   7153.670    0.000000   7638.944640
  15   13    0    0    0    1    2    0    0    0   7365.031    0.000000   7659.833086
  15   14   13    0    0    1    1    1    0    0   7416.249    0.000000   7770.389775
  15   14    0    0    0    1    2    0    0    0   7522.919    0.000000   7880.946464
  15   13    0    0    0    2    1    0    0    0   8090.366    0.000000   8559.698850
  15   14    0    0    0    2    1    0    0    0   8175.450    0.000000   8670.255539
  15    0    0    0    0    3    0    0    0    0   8663.222    0.000000   9459.564614
 -------------------------------------------------------------------------------
 Dipole moment function written to files dipolex(y,z)
  @CHECKOUT-I, Total execution time :        0.0000 seconds.
  --executable xcubic finished with status            0
```

Table S.11. Part of the CFOUR output file of the CCSD(T)/VQZ-aV(Q+*d*)Z anharmonic frequency calculation for $^{13}CHD_2^{35}Cl$

```
    *************************************************************************
      <<<     CCCCCC    CCCCCC    |||     CCCCCC    CCCCCC    >>>
       <<<      CCC       CCC     |||      CCC       CCC        >>>
        <<<     CCC       CCC     |||      CCC       CCC          >>>
     <<<        CCC       CCC     |||      CCC       CCC            >>>
        <<<     CCC       CCC     |||      CCC       CCC          >>>
       <<<      CCC       CCC     |||      CCC       CCC        >>>
        <<<    CCCCCC    CCCCCC   |||     CCCCCC    CCCCCC    >>>
    *************************************************************************


     ***************************************************************
     * CFOUR Coupled-Cluster techniques for Computational Chemistry *
     ***************************************************************


    Department of Chemistry              Institut fuer Physikalische Chemie
    University of Texas at Austin        Universitaet Mainz
    Austin, TX  78712, USA               D-55099 Mainz, Germany

                    Version 1.0




                          Normal Coordinates

              A'                       A''                       A'
             705.66                   776.73                   870.68
           VIBRATION                VIBRATION                VIBRATION
C      0.055 0.6785  0.0000    0.0000  0.0000  0.3681     0.4259 -0.3309  0.0000
CL    -0.017-0.5762  0.0000    0.0000  0.0000 -0.1645    -0.1307  0.0791  0.0000
H     -0.027 0.3140  0.0144   -0.0226  0.6362 -0.0859    -0.2736  0.4114  0.0401
H     -0.027 0.3140 -0.0144    0.0226 -0.6362 -0.0859    -0.2736  0.4114 -0.0401
H     -0.018 0.0686  0.0000    0.0000  0.0000 -0.1102     0.0136 -0.4406  0.0000


              A'                       A'                       A''
            1066.44                  1265.24                  1321.15
           VIBRATION                VIBRATION                VIBRATION
C      0.260 0.2828  0.0000    0.0572 -0.2612  0.0000     0.0000  0.0000  0.2542
CL     0.002 0.0153  0.0000    0.0494 -0.0428  0.0000     0.0000  0.0000  0.0048
H     -0.339-0.3510  0.4251   -0.2648  0.1303  0.0727     0.3267 -0.1383 -0.0412
H     -0.339-0.3510 -0.4251   -0.2648  0.1303 -0.0727    -0.3267  0.1383 -0.0412
H      0.011-0.1139  0.0000    0.2518  0.8222  0.0000     0.0000  0.0000 -0.8248


              A'                       A''                      A'
            2244.05                  2344.63                  3192.88
           VIBRATION                VIBRATION                VIBRATION
C      0.226 0.1779  0.0000    0.0000  0.0000  0.4182     0.2625 -0.0617  0.0000
CL    -0.001-0.0031  0.0000    0.0000  0.0000 -0.0027    -0.0007 -0.0002  0.0000
H     -0.313-0.2121 -0.5582   -0.3022 -0.2026 -0.5293    -0.0036 -0.0104 -0.0252
H     -0.313-0.2121  0.5582    0.3022  0.2026 -0.5293    -0.0036 -0.0104  0.0252
H      0.083-0.0210  0.0000    0.0000  0.0000  0.0104    -0.9286  0.2520  0.0000

 ...
 ...


  ----------------------------------------------------------------
                   Dipole Moment Function
                  (Normal Coordinate Basis)
  ----------------------------------------------------------------
   Mode     Symmetry    d(Mu(x))/dQ   d(Mu(y))/dQ   d(Mu(z))/dQ
  ----------------------------------------------------------------
    Q7         A'        -0.007921      0.132328      0.000000
    Q8         A''        0.000000      0.000000     -0.018180
    Q9         A'        -0.027896     -0.068388      0.000000
    Q10        A'        -0.047313      0.061442      0.000000
    Q11        A'        -0.008836     -0.076060      0.000000
    Q12        A''        0.000000      0.000000     -0.076288
    Q13        A'         0.021832      0.106563      0.000000
    Q14        A''        0.000000      0.000000      0.051678
    Q15        A'         0.056164     -0.075997      0.000000
  ----------------------------------------------------------------
 --------------------------------------------------------------------------
 ------------------------------------------------------------
```

```
         Parameter              (MHz)                  (CM-1)
----------------------------------------------------------------

         R6                 -.126541E-04           -.422094E-09
         R5                 -.114311E-01           -.381301E-06
         SI                           0.591847E+03

  A-reduced centrifugal distortion parameters

         DJ                  0.117713E-01           0.392650E-06
         DK                  0.934015E+00           0.311554E-04
         DJK                 0.123706E+00           0.412638E-05
         DELJ                0.117967E-01           0.393494E-06
         DELK                0.934141E+00           0.311596E-04
         DELJK               0.123554E+00           0.412132E-05
         delJ                0.275559E-03           0.919165E-08
         delK                0.528193E-01           0.176186E-05

  S-reduced centrifugal distortion parameters

         DJ                  0.117520E-01           0.392005E-06
         DK                  0.933918E+00           0.311522E-04
         DJK                 0.123822E+00           0.413025E-05
         D1                 -.275559E-03           -.919165E-08
         D2                 -.223112E-04           -.744222E-09
----------------------------------------------------------------
  Vibrational frequencies after rotational projection  of
  Cartesian force constants:
         1               0.0000i
         2               0.0000i
         3               0.0000i
         4               0.0000
         5               0.0000
         6               0.0000
         7             705.6551
         8             776.7056
         9             870.6713
        10            1066.4358
        11            1265.2273
        12            1321.0638
        13            2244.0510
        14            2344.6326
        15            3192.8838
  Zero-point vibrational energy:   19.7099 kcal/mol =   82.4665 kJ/mol.
             0.12 seconds walltime passed
 --executable xjoda finished with status            0
 --invoking executable xcubic
  @GETMEM-I,  Allocated  13351 MB of main memory.
  back




********************************************************************************
       PARAMETERS RELEVANT TO MOLECULAR STRUCTURE
********************************************************************************


  Force Field from Numerical Differentiation of Analytic Second Derivatives
  --------------------------------------------------------------------------
 Cubic force constants written to file cubic.

--------------------------------------------------------------------------
  Mean and mean-square displacements in dimensionless normal coordinates

          Geometrical properties evaluated at    0.00 K

       Coordinate           <q>             <q**2>
--------------------------------------------------------------------------
          7               0.1311925788    0.4999999889
          8               0.0000000000    0.4999999889
          9              -0.0278008593    0.4999999889
         10               0.0025194350    0.4999999889
         11               0.0141452783    0.4999999889
         12               0.0000000000    0.4999999889
         13              -0.1280562746    0.4999999889
         14               0.0000000000    0.4999999889
         15               0.0788742042    0.4999999889
--------------------------------------------------------------------------
```

```
        -------------------------------------------------------
         ATOM            INTERNUCLEAR DISTANCE / Angstrom
        -------------------------------------------------------
         I    J        Re         Rg         Ra
        -------------------------------------------------------
         2    1      1.7826656  1.7907040  1.7904117
         3    1      1.0850773  1.1004048  1.0929183
         3    2      2.3617095  2.3755677  2.3737726
         4    1      1.0850773  1.1004048  1.0929183
         4    2      2.3617095  2.3755677  2.3737726
         4    3      1.7831251  1.8022035  1.7959046
         5    1      1.0850773  1.1061524  1.0941738
         5    2      2.3617095  2.3797714  2.3761631
         5    3      1.7831251  1.8061640  1.7969527
         5    4      1.7831251  1.8061640  1.7969527
        -------------------------------------------------------
    ****************************************************************************
        PARAMETERS RELEVANT TO ROTATIONAL SPECTROSCOPY
    ****************************************************************************


        ------------------------------------------------------------------------
                                    VIB-ROT CONSTANT / (cm-1)
                                -------------------------------
          AXIS       MODE      CORIOLIS    QUADRATIC    ANHARMONIC    TOTAL
        ------------------------------------------------------------------------
           1          7       0.0005478   -0.0010600    0.0034618    0.0029495
           1          8       0.0004307   -0.0000001    0.0007531    0.0011836
           1          9       0.0000013   -0.0002077    0.0008831    0.0006768
           1         10       0.0001417   -0.0000256    0.0001792    0.0002952
           1         11       0.0055757   -0.0000742    0.0007529    0.0062543
           1         12      -0.0058904   -0.0000092   -0.0000902   -0.0059898
           1         13      -0.0002602   -0.0000259    0.0006545    0.0003684
           1         14      -0.0003913   -0.0000046    0.0004748    0.0000790
           1         15      -0.0000182   -0.0000038   -0.0001243   -0.0001463
           2          7       0.0006369   -0.0000356    0.0037281    0.0043294
           2          8       0.0272787   -0.0046298   -0.0187689    0.0038800
           2          9      -0.0112541   -0.0035610   -0.0152172   -0.0300323
           2         10       0.0225705   -0.0037830   -0.0057242    0.0130634
           2         11       0.0408410   -0.0023134   -0.0032037    0.0353239
           2         12      -0.0150175   -0.0001197   -0.0052745   -0.0204116
           2         13      -0.0034698   -0.0198774    0.0522981    0.0289510
           2         14      -0.0342978   -0.0001554    0.0503647    0.0159115
           2         15      -0.0197529   -0.0030404    0.0379118    0.0151184
           3          7       0.0002014   -0.0011185    0.0036226    0.0027055
           3          8       0.0002706   -0.0005468    0.0009650    0.0006887
           3          9       0.0015110   -0.0000197    0.0008783    0.0023697
           3         10      -0.0011370   -0.0000197    0.0001291   -0.0010277
           3         11       0.0000314   -0.0000007    0.0007165    0.0007473
           3         12      -0.0001499   -0.0000235    0.0000179   -0.0001556
           3         13      -0.0001745   -0.0000046    0.0002407    0.0000616
           3         14      -0.0000936   -0.0000230    0.0002867    0.0001701
           3         15      -0.0003317   -0.0000066    0.0002295   -0.0001088
        ------------------------------------------------------------------------


        ------------------------------------------------------------------------
         Be, B0 AND B-B0 SHIFTS FOR SINGLY EXCITED VIBRATIONAL STATES (CM-1)
        ----------------------------------------------------------------
         VIBRATION          X AXIS               Y AXIS               Z AXIS
        ------------------------------------------------------------------------
          Be                0.36907372          3.20583433          0.37856773
          B0                0.36623839          3.17276754          0.37584231
          Be-B0             0.00283533          0.03306679          0.00272542
          B'                0.36623510          3.17277194          0.37584341
          Be-B'             0.00283863          0.03306238          0.00272432
          B''               0.36624152          3.17277272          0.37584668
          Be-B''            0.00283220          0.03306160          0.00272105
          B^A               0.36623307          3.17277194          0.37584544
          Be-B^A            0.00284065          0.03306239          0.00272229
          B^S               0.36623666          3.17277194          0.37584185
          Be-B^S            0.00283707          0.03306238          0.00272588
           7               -0.00294953         -0.00432938         -0.00270552
           8               -0.00118362         -0.00387996         -0.00068871
           9               -0.00067676          0.03003230         -0.00236969
          10               -0.00029521         -0.01306338          0.00102769
          11               -0.00625435         -0.03532386         -0.00074725
          12                0.00598978          0.02041159          0.00015557
```

72

```
   13              -0.00036837         -0.02895096         -0.00006160
   14              -0.00007896         -0.01591149         -0.00017014
   15               0.00014634         -0.01511844          0.00010883
  --------------------------------------------------------------------------
  --------------------------------------------------------------------------
  Be, B0 AND B-B0 SHIFTS FOR SINGLY EXCITED VIBRATIONAL STATES (MHz)
  VIBRATION          X AXIS              Y AXIS              Z AXIS
  --------------------------------------------------------------------------
    Be             11064.55191046      96108.49529308      11349.17504372
    B0             10979.55081552      95117.17786932      11267.46898467
    Be-B0             85.00109494        991.31742376         81.70605905
    B'             10979.45202024      95117.30994995      11267.50190991
    Be-B'             85.09989022        991.18534313         81.67313381
    B''            10979.64459194      95117.33331453      11267.60001676
    Be-B''            84.90731852        991.16197855         81.57502696
    B^A            10979.39127325      95117.30974586      11267.56286098
    Be-B^A            85.16063721        991.18554722         81.61218274
    B^S            10979.49871862      95117.30997128      11267.45523528
    Be-B^S            85.05319184        991.18532180         81.71980844
     7               -88.42462801       -129.79163567        -81.10956897
     8               -35.48411736       -116.31836857        -20.64695858
     9               -20.28863936        900.34575510        -71.04163534
    10                -8.85016870       -391.63017476         30.80928506
    11              -187.50056591      -1058.98264133        -22.40212944
    12               179.56919542        611.92418253          4.66374050
    13               -11.04333311       -867.92790966         -1.84680797
    14                -2.36723808       -477.01458620         -5.10054933
    15                 4.38730524       -453.23946895          3.26250598
  --------------------------------------------------------------------------
                   Vibrationally averaged dipole moment
  --------------------------------------------------------------------------
                 a.u.                          Debye
         x         y         z           x         y         z
  --------------------------------------------------------------------------
MU_e -0.02877   0.75417   0.00000    -0.07313   1.91679   0.00000
<MU> -0.02669   0.74853   0.00000    -0.06784   1.90244   0.00000

Equilibrium dipole moment:   0.75472 a.u. (   1.91818 D)
Equilibrium dipole moment:   0.74900 a.u. (   1.90365 D)
  --------------------------------------------------------------------------
****************************************************************************
    PARAMETERS RELEVANT TO VIBRATIONAL SPECTROSCOPY
****************************************************************************
  Quartic force constants written to file quartic
     ========================================================
  Performing F(IIJJ)/F(JJII) consistency check
  Differences greater than 1 cm-1 will be printed.
     ========================================================
  I   I   K   K      F(IIKK)       F(KKII)        Difference
     --------------------------------------------------------
     --------------------------------------------------------
  Largest absolute difference is    0.13200 cm-1.
  Largest relative difference is .60311D-02.
VPT2 vibrational analysis


 Thresholds for removing resonance denominators:
 Delta_omega = 50 cm-1; Phi(ijk) = 80 cm-1

 -------------------------------
  ANHARMONICITY CONSTANTS X(ij)
                (cm-1)
 -------------------------------
  (*) Near-zero denominators were removed
 -------------------------------
        I  J       X(IJ)
 -------------------------------
        7  7       -3.4443
        7  8       -3.7800
        7  9       -3.8597
        7 10       -1.4719
        7 11       -5.5830
        7 12       -0.9482
        7 13        0.1176
        7 14        1.0455
        7 15        2.3086
        8  8       -0.4996
        8  9       -1.0790
```

```
              8 10        -4.0201
              8 11        -0.3109
              8 12        -3.5775
              8 13        -3.9050
              8 14        -2.8279
              8 15         0.0328
              9  9        -1.8942
              9 10        -1.6963
              9 11        -7.7765
              9 12        -4.5293
              9 13         4.4647
              9 14        -3.1586
              9 15        -3.3092
             10 10        -5.1547
             10 11        -1.9946
             10 12         3.1032
             10 13         2.5110
             10 14       -17.1795
             10 15        -1.0973
             11 11        -5.2294
             11 12         1.1098
             11 13         0.7759
             11 14        -2.4499
             11 15       -17.9381
             12 12        -5.5046
             12 13        -6.0792
             12 14       -11.3850
             12 15       -21.5671
             13 13       -14.8593
             13 14       -61.9911
             13 15        -0.1415
             14 14       -19.1776
             14 15         1.1385
             15 15       -60.9724


--------------------------------------------------------------------------------
      HARMONIC AND FUNDAMENTAL FREQUENCIES (cm-1) AND INTENSITIES (km/mol)
--------------------------------------------------------------------------------

          Harmonic    Fundamental Anharmonic   Harmonic   Fundamental   Anharm
  Mode    Frequency    Frequency   Contribution Intensity  Intensity    Contrib
    7     706.1993     693.2252    -12.9741      17.2023    18.1372      0.9349
    8     777.4431     766.7101    -10.7330       0.3050     0.3070      0.0019
    9     872.8407     858.5804    -14.2603       5.4155     5.2405     -0.1750
   10    1066.8187    1045.5865    -21.2322       5.7027     5.3312     -0.3715
   11    1274.8609    1247.3184    -27.5425       5.6992     5.0872     -0.6119
   12    1329.0386    1296.0926    -32.9459       5.7563     5.8193      0.0630
   13    2245.5778    2183.7352    -61.8426      11.5298    10.9347     -0.5951
   14    2346.6818    2259.9226    -86.7592       2.5575     2.7143      0.1568
   15    3143.5899    3001.3585   -142.2314       9.1337    10.9405      1.8068
--------------------------------------------------------------------------------
--------------------------------------------------------------------------------
                    ZERO-POINT VIBRATIONAL ENERGIES
--------------------------------------------------------------------------------
                         kcal/mol      kJ/mol       Hartree        cm-1
--------------------------------------------------------------------------------
Harmonic contribution :   19.6752      82.3212     0.03135453     6881.525
VPT2-correction       :   -0.2309      -0.9659    -0.00036789      -80.743
--------------------------------------------------------------------------------
Harm+VPT2             :   19.4444      81.3553     0.03098664     6800.782
--------------------------------------------------------------------------------
   MAXLEVEL set to                    3
 --------------------------------------------------------------------------------
             All levels with up to three quanta
--------------------------------------------------------------------------------
  MODE MODE MODE MODE MODE             Anharmonic    Anharm     Harmonic
   I    J    K    L    M   NI NJ NK NL NM Frequency   Intensity  Transition
--------------------------------------------------------------------------------
    7    0    0    0    0   1  0  0  0  0   693.225   18.136805   706.199306
    8    0    0    0    0   1  0  0  0  0   766.710    0.306982   777.443141
    9    0    0    0    0   1  0  0  0  0   858.580    5.240395   872.840664
   10    0    0    0    0   1  0  0  0  0  1045.586    5.331136  1066.818661
   11    0    0    0    0   1  0  0  0  0  1247.318    5.087146  1274.860892
   12    0    0    0    0   1  0  0  0  0  1296.092    5.819221  1329.038582
    7    0    0    0    0   2  0  0  0  0  1379.561    0.115520  1412.398611
    8    7    0    0    0   1  1  0  0  0  1456.155    0.012279  1483.642447
    8    0    0    0    0   2  0  0  0  0  1532.421    0.001884  1554.886282
    9    7    0    0    0   1  1  0  0  0  1547.945    0.003517  1579.039969
```

74

9	8	0	0	0	1	1	0	0	0	1624.211	0.021054	1650.283805
9	0	0	0	0	2	0	0	0	0	1713.372	0.043297	1745.681328
10	7	0	0	0	1	1	0	0	0	1737.339	0.039930	1773.017967
10	8	0	0	0	1	1	0	0	0	1808.276	0.062890	1844.261802
10	9	0	0	0	1	1	0	0	0	1902.470	0.045468	1939.659325
11	7	0	0	0	1	1	0	0	0	1934.960	0.056656	1981.060198
12	7	0	0	0	1	1	0	0	0	1988.369	0.002654	2035.237887
11	8	0	0	0	1	1	0	0	0	2013.717	0.004013	2052.304033
7	0	0	0	0	3	0	0	0	0	2059.010	0.000000	2118.597917
12	8	0	0	0	1	1	0	0	0	2059.225	0.077002	2106.481723
10	0	0	0	0	2	0	0	0	0	2080.863	0.618706	2133.637323
11	9	0	0	0	1	1	0	0	0	2098.122	0.445147	2147.701556
8	7	0	0	0	1	2	0	0	0	2138.711	0.000000	2189.841752
12	9	0	0	0	1	1	0	0	0	2150.143	0.000170	2201.879246
13	0	0	0	0	1	0	0	0	0	2183.735	10.934464	2245.577792
8	7	0	0	0	2	1	0	0	0	2218.086	0.000000	2261.085588
9	7	0	0	0	1	2	0	0	0	2230.422	0.000000	2285.239275
14	0	0	0	0	1	0	0	0	0	2259.922	2.714252	2346.681846
11	10	0	0	0	1	1	0	0	0	2290.910	0.196328	2341.679553
8	0	0	0	0	3	0	0	0	0	2297.132	0.000000	2332.329423
9	8	7	0	0	1	1	1	0	0	2309.796	0.000000	2356.483111
12	10	0	0	0	1	1	0	0	0	2344.782	0.611380	2395.857243
9	8	0	0	0	1	2	0	0	0	2388.843	0.000000	2427.726946
9	7	0	0	0	2	1	0	0	0	2398.878	0.000000	2451.880633
10	7	0	0	0	1	2	0	0	0	2422.204	0.000000	2479.217273
9	8	0	0	0	2	1	0	0	0	2477.924	0.000000	2523.124469
11	0	0	0	0	2	0	0	0	0	2484.177	0.139390	2549.721784
10	8	7	0	0	1	1	1	0	0	2496.249	0.000000	2550.461108
12	11	0	0	0	1	1	0	0	0	2544.520	0.044213	2603.899474
9	0	0	0	0	3	0	0	0	0	2564.375	0.000000	2618.521992
10	8	0	0	0	1	2	0	0	0	2569.967	0.000000	2621.704943
12	0	0	0	0	2	0	0	0	0	2581.176	0.146784	2658.077163
10	9	7	0	0	1	1	1	0	0	2590.364	0.000000	2645.858631
11	7	0	0	0	1	2	0	0	0	2615.714	0.000000	2687.259503
10	9	8	0	0	1	1	1	0	0	2664.081	0.000000	2717.102466
12	7	0	0	0	1	2	0	0	0	2673.758	0.000000	2741.437193
11	8	7	0	0	1	1	1	0	0	2697.579	0.000000	2758.503339
12	8	7	0	0	1	1	1	0	0	2747.722	0.000000	2812.681028
10	9	0	0	0	1	2	0	0	0	2755.566	0.000000	2812.499989
10	7	0	0	0	2	1	0	0	0	2771.145	0.000000	2839.836628
11	8	0	0	0	1	2	0	0	0	2779.117	0.000000	2829.747174
11	9	7	0	0	1	1	1	0	0	2781.904	0.000000	2853.900862
12	8	0	0	0	1	2	0	0	0	2821.358	0.000000	2883.924864
12	9	7	0	0	1	1	1	0	0	2838.561	0.000000	2908.078551
10	8	0	0	0	2	1	0	0	0	2839.533	0.000000	2911.080464
11	9	8	0	0	1	1	1	0	0	2863.442	0.000000	2925.144697
13	7	0	0	0	1	1	0	0	0	2877.078	0.092500	2951.777097
12	9	8	0	0	1	1	1	0	0	2912.197	0.000000	2979.322387
10	9	0	0	0	2	1	0	0	0	2936.051	0.000000	3006.477987
11	9	0	0	0	1	2	0	0	0	2945.137	0.000000	3020.542220
13	8	0	0	0	1	1	0	0	0	2946.540	0.003892	3023.020933
14	7	0	0	0	1	1	0	0	0	2954.193	0.020158	3052.881154
11	10	7	0	0	1	1	1	0	0	2977.080	0.000000	3047.878859
12	9	0	0	0	1	2	0	0	0	3000.406	0.000000	3074.719909
15	0	0	0	0	1	0	0	0	0	3001.358	10.940258	3143.589896
14	8	0	0	0	1	1	0	0	0	3023.804	0.046757	3124.124987
12	10	7	0	0	1	1	1	0	0	3035.587	0.000000	3102.056549
13	9	0	0	0	1	1	0	0	0	3046.780	0.327968	3118.418456
11	10	8	0	0	1	1	1	0	0	3053.289	0.000000	3119.122694
12	10	8	0	0	1	1	1	0	0	3103.894	0.000000	3173.300384
10	0	0	0	0	3	0	0	0	0	3105.831	0.000000	3200.455984
14	9	0	0	0	1	1	0	0	0	3115.344	0.009531	3219.522510
11	10	9	0	0	1	1	1	0	0	3140.017	0.000000	3214.520217
11	7	0	0	0	2	1	0	0	0	3166.237	0.000000	3255.921090
12	10	9	0	0	1	1	1	0	0	3197.137	0.000000	3268.697907
12	11	7	0	0	1	1	1	0	0	3231.214	0.000000	3310.098779
13	10	0	0	0	1	1	0	0	0	3231.832	0.054257	3312.396453
11	8	0	0	0	2	1	0	0	0	3250.266	0.000000	3327.164925
12	7	0	0	0	2	1	0	0	0	3272.504	0.000000	3364.276469
14	10	0	0	0	1	1	0	0	0	3288.329	0.311145	3413.500508
12	11	8	0	0	1	1	1	0	0	3307.342	0.000000	3381.342615
11	10	0	0	0	1	2	0	0	0	3324.192	0.000000	3408.498215
11	9	0	0	0	2	1	0	0	0	3327.205	0.000000	3422.562448
12	8	0	0	0	2	1	0	0	0	3340.731	0.000000	3435.520304
12	10	0	0	0	1	2	0	0	0	3383.162	0.000000	3462.675905
12	11	9	0	0	1	1	1	0	0	3390.795	0.000000	3476.740138
12	9	0	0	0	2	1	0	0	0	3430.697	0.000000	3530.917827
13	11	0	0	0	1	1	0	0	0	3431.829	0.064190	3520.438684

13	12	0	0	0	1	1	0	0	0	3473.748	0.274987	3574.616373
14	11	0	0	0	1	1	0	0	0	3504.791	0.016698	3621.542738
11	10	0	0	0	2	1	0	0	0	3525.775	0.000000	3616.540446
14	12	0	0	0	1	1	0	0	0	3544.630	0.216222	3675.720428
13	7	0	0	0	1	2	0	0	0	3563.532	0.000000	3657.976403
12	11	10	0	0	1	1	1	0	0	3591.215	0.000000	3670.718135
12	10	0	0	0	2	1	0	0	0	3632.968	0.000000	3724.895825
13	8	7	0	0	1	1	1	0	0	3636.103	0.000000	3729.220238
14	7	0	0	0	1	2	0	0	0	3641.575	0.000000	3759.080458
15	7	0	0	0	1	1	0	0	0	3696.892	0.057035	3849.789202
13	8	0	0	0	1	2	0	0	0	3708.346	0.000000	3800.464074
11	0	0	0	0	3	0	0	0	0	3710.578	0.000000	3824.582676
14	8	7	0	0	1	1	1	0	0	3714.295	0.000000	3830.324293
13	9	7	0	0	1	1	1	0	0	3736.263	0.000000	3824.617761
15	8	0	0	0	1	1	0	0	0	3768.101	0.003322	3921.033038
12	11	0	0	0	1	2	0	0	0	3782.490	0.000000	3878.760366
14	8	0	0	0	1	2	0	0	0	3786.687	0.000000	3901.568128
14	9	7	0	0	1	1	1	0	0	3805.755	0.000000	3925.721816
13	9	8	0	0	1	1	1	0	0	3808.506	0.000000	3895.861597
12	11	0	0	0	2	1	0	0	0	3830.714	0.000000	3932.938055
12	0	0	0	0	3	0	0	0	0	3855.250	0.000000	3987.115745
15	9	0	0	0	1	1	0	0	0	3856.629	0.298736	4016.430560
14	9	8	0	0	1	1	1	0	0	3878.147	0.000000	3996.965651
13	9	0	0	0	1	2	0	0	0	3906.036	0.000000	3991.259120
13	10	7	0	0	1	1	1	0	0	3923.703	0.000000	4018.595759
14	9	0	0	0	1	2	0	0	0	3966.977	0.000000	4092.363174
14	10	7	0	0	1	1	1	0	0	3981.128	0.000000	4119.699813
13	10	8	0	0	1	1	1	0	0	3990.617	0.000000	4089.839594
15	10	0	0	0	1	1	0	0	0	4045.847	0.065020	4210.408558
14	10	8	0	0	1	1	1	0	0	4048.191	0.000000	4190.943649
13	10	9	0	0	1	1	1	0	0	4093.181	0.000000	4185.237117
13	11	7	0	0	1	1	1	0	0	4119.589	0.000000	4226.637989
14	10	9	0	0	1	1	1	0	0	4142.055	0.000000	4286.341172
13	12	7	0	0	1	1	1	0	0	4166.143	0.000000	4280.815679
14	11	7	0	0	1	1	1	0	0	4193.478	0.000000	4327.742044
13	11	8	0	0	1	1	1	0	0	4194.323	0.000000	4297.881825
15	11	0	0	0	1	1	0	0	0	4230.738	0.568254	4418.450789
13	12	8	0	0	1	1	1	0	0	4232.976	0.000000	4352.059515
14	12	7	0	0	1	1	1	0	0	4237.952	0.000000	4381.919734
14	11	8	0	0	1	1	1	0	0	4268.362	0.000000	4398.985879
13	10	0	0	0	1	2	0	0	0	4269.620	0.000000	4379.215115
15	12	0	0	0	1	1	0	0	0	4275.884	0.054785	4472.628478
13	11	9	0	0	1	1	1	0	0	4287.098	0.000000	4393.279348
14	12	8	0	0	1	1	1	0	0	4304.934	0.000000	4453.163569
14	10	0	0	0	1	2	0	0	0	4306.427	0.000000	4480.319169
13	12	9	0	0	1	1	1	0	0	4332.264	0.000000	4447.457037
13	0	0	0	0	2	0	0	0	0	4337.751	0.031431	4491.155584
14	11	9	0	0	1	1	1	0	0	4352.436	0.000000	4494.383402
14	13	0	0	0	1	1	0	0	0	4381.666	0.261157	4592.259638
15	7	0	0	0	1	2	0	0	0	4385.537	0.000000	4555.988508
14	12	9	0	0	1	1	1	0	0	4395.522	0.000000	4548.561092
15	8	7	0	0	1	1	1	0	0	4459.855	0.000000	4627.232343
13	11	10	0	0	1	1	1	0	0	4477.932	0.000000	4587.257345
14	0	0	0	0	2	0	0	0	0	4481.490	0.186380	4693.363693
13	12	10	0	0	1	1	1	0	0	4524.949	0.000000	4641.435035
14	11	10	0	0	1	1	1	0	0	4531.203	0.000000	4688.361400
15	8	0	0	0	1	2	0	0	0	4533.845	0.000000	4698.476179
15	9	7	0	0	1	1	1	0	0	4548.303	0.000000	4722.629866
14	12	10	0	0	1	1	1	0	0	4576.140	0.000000	4742.539089
15	9	8	0	0	1	1	1	0	0	4622.293	0.000000	4793.873701
13	11	0	0	0	1	2	0	0	0	4669.464	0.000000	4795.299576
15	9	0	0	0	1	2	0	0	0	4708.112	0.000000	4889.271224
13	12	11	0	0	1	1	1	0	0	4722.952	0.000000	4849.477266
14	11	0	0	0	1	2	0	0	0	4739.200	0.000000	4896.403630
15	10	7	0	0	1	1	1	0	0	4739.909	0.000000	4916.607863
13	12	0	0	0	1	2	0	0	0	4752.752	0.000000	4903.654955
14	12	11	0	0	1	1	1	0	0	4790.608	0.000000	4950.581320
15	10	8	0	0	1	1	1	0	0	4808.570	0.000000	4987.851699
14	12	0	0	0	1	2	0	0	0	4818.328	0.000000	5004.759010
15	10	9	0	0	1	1	1	0	0	4899.422	0.000000	5083.249222
15	11	7	0	0	1	1	1	0	0	4920.689	0.000000	5124.650094
15	12	7	0	0	1	1	1	0	0	4970.469	0.000000	5178.827784
15	11	8	0	0	1	1	1	0	0	4997.170	0.000000	5195.893930
13	7	0	0	0	2	1	0	0	0	5031.212	0.000000	5197.354889
15	12	8	0	0	1	1	1	0	0	5039.049	0.000000	5250.071619
14	13	7	0	0	1	1	1	0	0	5076.055	0.000000	5298.458944
15	11	9	0	0	1	1	1	0	0	5078.233	0.000000	5291.291452
15	10	0	0	0	1	2	0	0	0	5080.027	0.000000	5277.227219

```
  13    8    0    0    0    2    1    0    0    0    5096.651    0.000000    5268.598725
  15   12    9    0    0    1    1    1    0    0    5126.625    0.000000    5345.469142
  14   13    8    0    0    1    1    1    0    0    5141.643    0.000000    5369.702779
  14    7    0    0    0    2    1    0    0    0    5176.806    0.000000    5399.562998
  15   13    0    0    0    1    1    0    0    0    5184.952    0.041488    5389.167688
  13    9    0    0    0    2    1    0    0    0    5205.261    0.000000    5363.996248
  14   13    9    0    0    1    1    1    0    0    5241.553    0.000000    5465.100302
  14    8    0    0    0    2    1    0    0    0    5242.544    0.000000    5470.806834
  15   14    0    0    0    1    1    0    0    0    5262.419    0.043044    5490.271743
  15   11   10    0    0    1    1    1    0    0    5273.233    0.000000    5485.269450
  15   12   10    0    0    1    1    1    0    0    5323.476    0.000000    5539.447140
  14    9    0    0    0    2    1    0    0    0    5333.753    0.000000    5566.204357
  13   10    0    0    0    2    1    0    0    0    5388.360    0.000000    5557.974245
  14   13   10    0    0    1    1    1    0    0    5412.584    0.000000    5659.078300
  15   11    0    0    0    1    2    0    0    0    5449.660    0.000000    5693.311681
  14   10    0    0    0    2    1    0    0    0    5492.717    0.000000    5760.182354
  15   12   11    0    0    1    1    1    0    0    5506.374    0.000000    5747.489370
  15   12    0    0    0    1    2    0    0    0    5539.400    0.000000    5801.667060
  13   11    0    0    0    2    1    0    0    0    5586.621    0.000000    5766.016476
  13   12    0    0    0    2    1    0    0    0    5621.685    0.000000    5820.194165
  14   13   11    0    0    1    1    1    0    0    5627.311    0.000000    5867.120530
  14   13   12    0    0    1    1    1    0    0    5660.295    0.000000    5921.298220
  14   11    0    0    0    2    1    0    0    0    5723.908    0.000000    5968.224585
  14   12    0    0    0    2    1    0    0    0    5754.812    0.000000    6022.402274
  15   13    7    0    0    1    1    1    0    0    5880.603    0.000000    6095.366994
  15    0    0    0    0    2    0    0    0    0    5880.772    0.500211    6287.179793
  15   13    8    0    0    1    1    1    0    0    5947.789    0.000000    6166.610829
  15   14    7    0    0    1    1    1    0    0    5958.998    0.000000    6196.471048
  15   14    8    0    0    1    1    1    0    0    6026.334    0.000000    6267.714884
  15   13    9    0    0    1    1    1    0    0    6044.687    0.000000    6262.008352
  15   14    9    0    0    1    1    1    0    0    6114.532    0.000000    6363.112407
  15   13   10    0    0    1    1    1    0    0    6231.952    0.000000    6455.986350
  15   14   10    0    0    1    1    1    0    0    6289.729    0.000000    6557.090404
  15   13   11    0    0    1    1    1    0    0    6415.108    0.000000    6664.028580
  15   13   12    0    0    1    1    1    0    0    6453.398    0.000000    6718.206270
  13    0    0    0    0    3    0    0    0    0    6462.049    0.000000    6736.733375
  14   13    0    0    0    1    2    0    0    0    6473.692    0.000000    6837.837430
  15   14   11    0    0    1    1    1    0    0    6489.350    0.000000    6765.132635
  15   14   12    0    0    1    1    1    0    0    6525.560    0.000000    6819.310325
  14   13    0    0    0    2    1    0    0    0    6541.243    0.000000    6938.941485
  15    7    0    0    0    2    1    0    0    0    6578.614    0.000000    6993.379099
  15    8    0    0    0    2    1    0    0    0    6647.547    0.000000    7064.622934
  14    0    0    0    0    3    0    0    0    0    6664.702    0.000000    7040.045539
  15    9    0    0    0    2    1    0    0    0    6732.734    0.000000    7160.020457
  15   10    0    0    0    2    1    0    0    0    6924.164    0.000000    7353.998454
  15   11    0    0    0    2    1    0    0    0    7092.214    0.000000    7562.040685
  15   12    0    0    0    2    1    0    0    0    7133.730    0.000000    7616.218375
  15   13    0    0    0    1    2    0    0    0    7338.827    0.000000    7634.745480
  15   14   13    0    0    1    1    1    0    0    7384.022    0.000000    7735.849535
  15   14    0    0    0    1    2    0    0    0    7485.125    0.000000    7836.953589
  15   13    0    0    0    2    1    0    0    0    8064.224    0.000000    8532.757585
  15   14    0    0    0    2    1    0    0    0    8142.971    0.000000    8633.861639
  15    0    0    0    0    3    0    0    0    0    8638.241    0.000000    9430.769689
 --------------------------------------------------------------------------------
 Dipole moment function written to files dipolex(y,z)
  @CHECKOUT-I, Total execution time :        0.0000 seconds.
  --executable xcubic finished with status           0
```

Table S.12. Part of the CFOUR output file of the CCSD(T)/VQZ-aV(Q+*d*)Z anharmonic frequency calculation for $^{13}CHD_2^{37}Cl$

```
    ********************************************************************
        <<<    CCCCCC    CCCCCC   |||    CCCCCC    CCCCCC   >>>
       <<<    CCC       CCC      |||    CCC       CCC       >>>
      <<<    CCC       CCC      |||    CCC       CCC        >>>
    <<<     CCC       CCC      |||    CCC       CCC          >>>
      <<<    CCC       CCC      |||    CCC       CCC        >>>
       <<<    CCC       CCC      |||    CCC       CCC       >>>
        <<<    CCCCCC    CCCCCC   |||    CCCCCC    CCCCCC   >>>
    ********************************************************************


      ****************************************************************
      * CFOUR Coupled-Cluster techniques for Computational Chemistry *
      ****************************************************************


   Department of Chemistry            Institut fuer Physikalische Chemie
   University of Texas at Austin       Universitaet Mainz
   Austin, TX  78712, USA             D-55099 Mainz, Germany

                     Version 1.0



                        Normal Coordinates

           A'                      A''                      A'
         699.29                  776.16                   870.13
          VIBRATION               VIBRATION               VIBRATION
C     0.053 0.6862  0.0000   0.0000  0.0000  0.3684    0.4263 -0.3279  0.0000
CL   -0.016-0.5661  0.0000   0.0000  0.0000 -0.1601   -0.1273  0.0746  0.0000
H    -0.025 0.3147  0.0140  -0.0225  0.6367 -0.0860   -0.2736  0.4129  0.0402
H    -0.025 0.3147 -0.0140   0.0225 -0.6367 -0.0860   -0.2736  0.4129 -0.0402
H    -0.017 0.0738  0.0000   0.0000  0.0000 -0.1102    0.0132 -0.4414  0.0000


           A'                      A'                       A''
        1066.43                 1265.09                  1321.14
          VIBRATION               VIBRATION               VIBRATION
C     0.261 0.2831  0.0000   0.0574 -0.2618  0.0000    0.0000  0.0000  0.2542
CL    0.001 0.0147  0.0000   0.0480 -0.0413  0.0000    0.0000  0.0000  0.0047
H    -0.339-0.3509  0.4251  -0.2649  0.1303  0.0727    0.3267 -0.1383 -0.0412
H    -0.339-0.3509 -0.4251  -0.2649  0.1303 -0.0727   -0.3267  0.1383 -0.0412
H     0.011-0.1139  0.0000   0.2520  0.8220  0.0000    0.0000  0.0000 -0.8248


           A'                      A''                      A'
        2244.05                 2344.63                  3192.88
          VIBRATION               VIBRATION               VIBRATION
C     0.226 0.1779  0.0000   0.0000  0.0000  0.4182    0.2625 -0.0617  0.0000
CL   -0.001-0.0030  0.0000   0.0000  0.0000 -0.0026   -0.0007 -0.0002  0.0000
H    -0.313-0.2121 -0.5582  -0.3022 -0.2026 -0.5293   -0.0036 -0.0104 -0.0252
H    -0.313-0.2121  0.5582   0.3022  0.2026 -0.5293   -0.0036 -0.0104  0.0252
H     0.083-0.0210  0.0000   0.0000  0.0000  0.0104   -0.9285  0.2522  0.0000

 ...
 ...


  ------------------------------------------------------------------
              Dipole Moment Function
              (Normal Coordinate Basis)
  ------------------------------------------------------------------
   Mode     Symmetry    d(Mu(x))/dQ    d(Mu(y))/dQ    d(Mu(z))/dQ
  ------------------------------------------------------------------
    Q7         A'       -0.007736       0.131361       0.000000
    Q8         A''       0.000000       0.000000      -0.018460
    Q9         A'       -0.028180      -0.067431       0.000000
    Q10        A'       -0.047301       0.061575       0.000000
    Q11        A'       -0.008774      -0.076354       0.000000
    Q12        A''       0.000000       0.000000      -0.076280
    Q13        A'        0.021846       0.106546       0.000000
    Q14        A''       0.000000       0.000000       0.051673
    Q15        A'        0.056152      -0.076006       0.000000
  ------------------------------------------------------------------
-------------------------------------------------------------------------
  ------------------------------------------------------------------
     Parameter                  (MHz)                 (CM-1)
```

```
          ---------------------------------------------------------
          R6              -.118171E-04            -.394176E-09
          R5              -.110721E-01            -.369326E-06
          SI                          0.614094E+03

   A-reduced centrifugal distortion parameters

          DJ              0.113937E-01            0.380053E-06
          DK              0.938099E+00            0.312916E-04
          DJK             0.119890E+00            0.399909E-05
          DELJ            0.114173E-01            0.380842E-06
          DELK            0.938217E+00            0.312955E-04
          DELJK           0.119748E+00            0.399436E-05
          delJ            0.262404E-03            0.875285E-08
          delK            0.511714E-01            0.170690E-05

   S-reduced centrifugal distortion parameters

          DJ              0.113757E-01            0.379452E-06
          DK              0.938008E+00            0.312886E-04
          DJK             0.119998E+00            0.400270E-05
          D1              -.262404E-03            -.875285E-08
          D2              -.208321E-04            -.694884E-09
          ---------------------------------------------------------
   Vibrational frequencies after rotational projection  of
   Cartesian force constants:
          1               0.0000i
          2               0.0000i
          3               0.0000i
          4               0.0000
          5               0.0000
          6               0.0000
          7             699.2864
          8             776.1374
          9             870.1265
         10            1066.4291
         11            1265.0819
         12            1321.0630
         13            2244.0502
         14            2344.6322
         15            3192.8838
   Zero-point vibrational energy:  19.6990 kcal/mol =   82.4209 kJ/mol.
              0.12 seconds walltime passed
  --executable xjoda finished with status            0
  --invoking executable xcubic
   @GETMEM-I,   Allocated   13351 MB of main memory.
   back




**********************************************************************************
        PARAMETERS RELEVANT TO MOLECULAR STRUCTURE
**********************************************************************************

 Force Field from Numerical Differentiation of Analytic Second Derivatives
 --------------------------------------------------------------------------
 Cubic force constants written to file cubic.

 --------------------------------------------------------------------------
  Mean and mean-square displacements in dimensionless normal coordinates

          Geometrical properties evaluated at      0.00 K

        Coordinate          <q>           <q**2>
 --------------------------------------------------------------------------
          7            0.1312022034   0.4999999889
          8            0.0000000000   0.4999999889
          9           -0.0270787460   0.4999999889
         10            0.0025262379   0.4999999889
         11            0.0140444010   0.4999999889
         12            0.0000000000   0.4999999889
         13           -0.1279622719   0.4999999889
         14            0.0000000000   0.4999999889
         15            0.0788287507   0.4999999889
 --------------------------------------------------------------------------


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

```
    ATOM              INTERNUCLEAR DISTANCE / Angstrom
    -------------------------------------------------------
    I    J         Re          Rg          Ra
    -------------------------------------------------------
    2    1       1.7826656   1.7906503   1.7903618
    3    1       1.0850773   1.1004058   1.0929121
    3    2       2.3617095   2.3755295   2.3737302
    4    1       1.0850773   1.1004058   1.0929121
    4    2       2.3617095   2.3755295   2.3737302
    4    3       1.7831251   1.8021984   1.7958888
    5    1       1.0850773   1.1061533   1.0941687
    5    2       2.3617095   2.3797351   2.3761231
    5    3       1.7831251   1.8061588   1.7969378
    5    4       1.7831251   1.8061588   1.7969378
    -------------------------------------------------------
****************************************************************************
     PARAMETERS RELEVANT TO ROTATIONAL SPECTROSCOPY
****************************************************************************


    --------------------------------------------------------------------
                            VIB-ROT CONSTANT / (cm-1)
                            ----------------------------
    AXIS       MODE      CORIOLIS     QUADRATIC    ANHARMONIC    TOTAL
    --------------------------------------------------------------------
     1          7       0.0004846   -0.0010357    0.0033834    0.0028322
     1          8       0.0004573   -0.0000001    0.0007437    0.0012009
     1          9       0.0000059   -0.0002011    0.0008624    0.0006672
     1         10       0.0001374   -0.0000247    0.0001779    0.0002906
     1         11       0.0053732   -0.0000713    0.0007427    0.0060446
     1         12      -0.0056781   -0.0000087   -0.0000871   -0.0057738
     1         13      -0.0002518   -0.0000247    0.0006327    0.0003562
     1         14      -0.0003782   -0.0000043    0.0004570    0.0000745
     1         15      -0.0000176   -0.0000037   -0.0001253   -0.0001467
     2          7       0.0005503   -0.0000329    0.0037414    0.0042588
     2          8       0.0271967   -0.0045594   -0.0188098    0.0038276
     2          9      -0.0110817   -0.0035325   -0.0153029   -0.0299171
     2         10       0.0225715   -0.0037795   -0.0057234    0.0130687
     2         11       0.0407914   -0.0023072   -0.0032044    0.0352798
     2         12      -0.0149663   -0.0001176   -0.0052736   -0.0203575
     2         13      -0.0034696   -0.0198777    0.0522993    0.0289519
     2         14      -0.0343021   -0.0001527    0.0503675    0.0159128
     2         15      -0.0197519   -0.0030392    0.0379076    0.0151164
     3          7       0.0001844   -0.0010929    0.0035380    0.0026295
     3          8       0.0002615   -0.0005292    0.0009489    0.0006813
     3          9       0.0014670   -0.0000177    0.0008572    0.0023064
     3         10      -0.0010952   -0.0000187    0.0001296   -0.0009842
     3         11       0.0000302   -0.0000007    0.0007076    0.0007371
     3         12      -0.0001449   -0.0000226    0.0000174   -0.0001500
     3         13      -0.0001686   -0.0000043    0.0002326    0.0000597
     3         14      -0.0000904   -0.0000222    0.0002750    0.0001624
     3         15      -0.0003204   -0.0000062    0.0002160   -0.0001106
    --------------------------------------------------------------------


    --------------------------------------------------------------------
     Be, B0 AND B-B0 SHIFTS FOR SINGLY EXCITED VIBRATIONAL STATES (CM-1)
     --------------------------------------------------------------
    VIBRATION       X AXIS              Y AXIS              Z AXIS
    --------------------------------------------------------------------
    Be              0.36282140          3.20580736          0.37199210
    B0              0.36004854          3.17273669          0.36932632
    Be-B0           0.00277285          0.03307067          0.00266578
    B'              0.36004535          3.17274096          0.36932738
    Be-B'           0.00277604          0.03306640          0.00266472
    B''             0.36005158          3.17274171          0.36933055
    Be-B''          0.00276982          0.03306564          0.00266155
    B^A             0.36004339          3.17274095          0.36932935
    Be-B^A          0.00277801          0.03306641          0.00266275
    B^S             0.36004686          3.17274096          0.36932587
    Be-B^S          0.00277453          0.03306640          0.00266623
     7             -0.00283224         -0.00425877         -0.00262947
     8             -0.00120092         -0.00382755         -0.00068126
     9             -0.00066721          0.02991711         -0.00230644
    10             -0.00029057         -0.01306865          0.00098424
    11             -0.00604458         -0.03527983         -0.00073713
    12              0.00577385          0.02035752          0.00015000
    13             -0.00035619         -0.02895194         -0.00005971
```

```
    14                 -0.00007449            -0.01591280            -0.00016238
    15                  0.00014666            -0.01511642             0.00011060
    --------------------------------------------------------------------------------
    --------------------------------------------------------------------------------
  Be, B0 AND B-B0 SHIFTS FOR SINGLY EXCITED VIBRATIONAL STATES (MHz)
  VIBRATION          X AXIS                 Y AXIS                 Z AXIS
    --------------------------------------------------------------------------------
    Be              10877.11179173        96107.68676687        11152.04253561
    B0              10793.98378386        95116.25315455        11072.12445102
    Be-B0              83.12800787          991.43361232           79.91808459
    B'              10793.88811594        95116.38106059        11072.15632479
    Be-B'              83.22367579          991.30570628           79.88621082
    B''             10794.07468242        95116.40368103        11072.25140244
    Be-B''             83.03710931          991.28308584           79.79113316
    B^A             10793.82925196        95116.38087001        11072.21537935
    Be-B^A             83.28253977          991.30589686           79.82715625
    B^S             10793.93335159        95116.38108049        11072.11111135
    Be-B^S             83.17844014          991.30568638           79.93142426
     7                -84.90838911         -127.67466944          -78.82957416
     8                -36.00275537         -114.74712255          -20.42366407
     9                -20.00251139          896.89240601          -69.14545447
    10                 -8.71104958         -391.78830211           29.50679051
    11               -181.21194371        -1057.66281883          -22.09858052
    12                173.09559065          610.30318938            4.49701089
    13                -10.67837820         -867.95724962           -1.79008378
    14                 -2.23325965         -477.05367813           -4.86817214
    15                  4.39668062         -453.17897935            3.31555856
    --------------------------------------------------------------------------------
                    Vibrationally averaged dipole moment
  --------------------------------------------------------------------------------
                    a.u.                          Debye
          x         y         z             x         y         z
  --------------------------------------------------------------------------------
  MU_e -0.02866   0.75418   0.00000      -0.07285   1.91680   0.00000
  <MU> -0.02658   0.74847   0.00000      -0.06756   1.90231   0.00000

  Equilibrium dipole moment:    0.75472 a.u. (   1.91818 D)
  Equilibrium dipole moment:    0.74895 a.u. (   1.90351 D)
  --------------------------------------------------------------------------------
  ********************************************************************************
     PARAMETERS RELEVANT TO VIBRATIONAL SPECTROSCOPY
  ********************************************************************************
   Quartic force constants written to file quartic
     ============================================================
   Performing F(IIJJ)/F(JJII) consistency check
   Differences greater than 1 cm-1 will be printed.
     ============================================================
    I   I   K   K      F(IIKK)       F(KKII)       Difference
     ------------------------------------------------------------
     ------------------------------------------------------------
   Largest absolute difference is    0.41293 cm-1.
   Largest relative difference is .68662D+00.
VPT2 vibrational analysis


 Thresholds for removing resonance denominators:
 Delta_omega = 50 cm-1; Phi(ijk) = 80 cm-1

  -------------------------------
   ANHARMONICITY CONSTANTS X(ij)
               (cm-1)
  -------------------------------
   (*) Near-zero denominators were removed
  -------------------------------
        I  J        X(IJ)
  -------------------------------
        7   7       -3.3714
        7   8       -3.7428
        7   9       -3.8168
        7  10       -1.4736
        7  11       -5.5934
        7  12       -0.9366
        7  13        0.1323
        7  14        1.0575
        7  15        2.2810
        8   8       -0.4962
        8   9       -1.0456
        8  10       -3.9938
```

```
            8 11         -0.3185
            8 12         -3.5968
            8 13         -3.9226
            8 14         -2.8244
            8 15          0.0167
            9  9         -1.8702
            9 10         -1.6960
            9 11         -7.7535
            9 12         -4.5592
            9 13          4.4334
            9 14         -3.1958
            9 15         -3.3331
           10 10         -5.1564
           10 11         -1.9978
           10 12          3.1020
           10 13          2.5136
           10 14        -17.1781
           10 15         -1.0941
           11 11         -5.2326
           11 12          1.1040
           11 13          0.7485
           11 14         -2.4503
           11 15        -17.9321
           12 12         -5.5073
           12 13         -6.0815
           12 14        -11.3931
           12 15        -21.5609
           13 13        -14.8594
           13 14        -61.9914
           13 15         -0.1682
           14 14        -19.1777
           14 15          1.1359
           15 15        -60.9723
```

  HARMONIC AND FUNDAMENTAL FREQUENCIES (cm-1) AND INTENSITIES (km/mol)

Mode	Harmonic Frequency	Fundamental Frequency	Anharmonic Contribution	Harmonic Intensity	Fundamental Intensity	Anharm Contrib
7	699.8107	687.0217	-12.7889	16.9459	17.8522	0.9063
8	776.8756	766.1692	-10.7064	0.3148	0.3167	0.0019
9	872.3265	858.1028	-14.2238	5.3103	5.1470	-0.1633
10	1066.8127	1045.5910	-21.2217	5.7162	5.3460	-0.3702
11	1274.7179	1247.1561	-27.5618	5.7411	5.1214	-0.6197
12	1329.0379	1296.0622	-32.9757	5.7553	5.8177	0.0624
13	2245.5771	2183.6904	-61.8866	11.5267	10.9388	-0.5879
14	2346.6814	2259.9061	-86.7753	2.5570	2.7142	0.1571
15	3143.5898	3001.3178	-142.2720	9.1337	10.9616	1.8278

                      ZERO-POINT VIBRATIONAL ENERGIES
----

	kcal/mol	kJ/mol	Hartree	cm-1
Harmonic contribution :	19.6643	82.2756	0.03133717	6877.715
VPT2-correction :	-0.2308	-0.9655	-0.00036774	-80.710
Harm+VPT2 :	19.4336	81.3101	0.03096943	6797.004

  MAXLEVEL set to   3

                    All levels with up to three quanta

MODE I	MODE J	MODE K	MODE L	MODE M	NI	NJ	NK	NL	NM	Anharmonic Frequency	Anharm Intensity	Harmonic Transition
7	0	0	0	0	1	0	0	0	0	687.021	17.851838	699.810666
8	0	0	0	0	1	0	0	0	0	766.169	0.316657	776.875573
9	0	0	0	0	1	0	0	0	0	858.102	5.146865	872.326546
10	0	0	0	0	1	0	0	0	0	1045.590	5.345863	1066.812671
11	0	0	0	0	1	0	0	0	0	1247.156	5.121331	1274.717879
12	0	0	0	0	1	0	0	0	0	1296.062	5.817536	1329.037884
7	0	0	0	0	2	0	0	0	0	1367.300	0.122705	1399.621332
8	7	0	0	0	1	1	0	0	0	1449.448	0.013096	1476.686239
8	0	0	0	0	2	0	0	0	0	1531.346	0.001854	1553.751146
9	7	0	0	0	1	1	0	0	0	1541.307	0.003677	1572.137212
9	8	0	0	0	1	1	0	0	0	1623.226	0.021214	1649.202119

9	0	0	0	0	2	0	0	0	0	1712.465	0.043109	1744.653092
10	7	0	0	0	1	1	0	0	0	1731.139	0.038765	1766.623337
10	8	0	0	0	1	1	0	0	0	1807.766	0.062566	1843.688244
10	9	0	0	0	1	1	0	0	0	1901.997	0.045577	1939.139217
11	7	0	0	0	1	1	0	0	0	1928.584	0.055823	1974.528545
12	7	0	0	0	1	1	0	0	0	1982.147	0.002558	2028.848550
11	8	0	0	0	1	1	0	0	0	2013.006	0.003929	2051.593453
7	0	0	0	0	3	0	0	0	0	2040.836	0.000000	2099.431998
12	8	0	0	0	1	1	0	0	0	2058.634	0.076742	2105.913457
10	0	0	0	0	2	0	0	0	0	2080.869	0.619114	2133.625342
11	9	0	0	0	1	1	0	0	0	2097.505	0.438577	2147.044425
8	7	0	0	0	1	2	0	0	0	2125.984	0.000000	2176.496905
12	9	0	0	0	1	1	0	0	0	2149.605	0.000194	2201.364430
13	0	0	0	0	1	0	0	0	0	2183.690	10.938549	2245.577064
8	7	0	0	0	2	1	0	0	0	2210.882	0.000000	2253.561812
9	7	0	0	0	1	2	0	0	0	2217.769	0.000000	2271.947878
14	0	0	0	0	1	0	0	0	0	2259.906	2.714097	2346.681387
11	10	0	0	0	1	1	0	0	0	2290.749	0.196357	2341.530550
8	0	0	0	0	3	0	0	0	0	2295.530	0.000000	2330.626720
9	8	7	0	0	1	1	1	0	0	2302.688	0.000000	2349.012785
12	10	0	0	0	1	1	0	0	0	2344.755	0.611399	2395.850555
9	8	0	0	0	1	2	0	0	0	2387.357	0.000000	2426.077693
9	7	0	0	0	2	1	0	0	0	2391.853	0.000000	2444.463758
10	7	0	0	0	1	2	0	0	0	2409.944	0.000000	2466.434003
9	8	0	0	0	2	1	0	0	0	2476.543	0.000000	2521.528665
11	0	0	0	0	2	0	0	0	0	2483.846	0.138774	2549.435759
10	8	7	0	0	1	1	1	0	0	2489.571	0.000000	2543.498910
12	11	0	0	0	1	1	0	0	0	2544.322	0.044133	2603.755763
9	0	0	0	0	3	0	0	0	0	2563.086	0.000000	2616.979638
10	8	0	0	0	1	2	0	0	0	2568.949	0.000000	2620.563817
12	0	0	0	0	2	0	0	0	0	2581.109	0.146811	2658.075768
10	9	7	0	0	1	1	1	0	0	2583.728	0.000000	2638.949883
11	7	0	0	0	1	2	0	0	0	2603.270	0.000000	2674.339211
12	7	0	0	0	1	2	0	0	0	2661.489	0.000000	2728.659216
10	9	8	0	0	1	1	1	0	0	2663.127	0.000000	2716.014790
11	8	7	0	0	1	1	1	0	0	2690.692	0.000000	2751.404118
12	8	7	0	0	1	1	1	0	0	2740.976	0.000000	2805.724123
10	9	0	0	0	1	2	0	0	0	2754.663	0.000000	2811.465763
10	7	0	0	0	2	1	0	0	0	2764.943	0.000000	2833.436008
11	9	7	0	0	1	1	1	0	0	2775.116	0.000000	2846.855091
11	8	0	0	0	1	2	0	0	0	2777.865	0.000000	2828.469026
12	8	0	0	0	1	2	0	0	0	2820.214	0.000000	2882.789031
12	9	7	0	0	1	1	1	0	0	2831.874	0.000000	2901.175096
10	8	0	0	0	2	1	0	0	0	2839.050	0.000000	2910.500915
11	9	8	0	0	1	1	1	0	0	2862.310	0.000000	2923.919999
13	7	0	0	0	1	1	0	0	0	2870.844	0.091567	2945.387730
12	9	8	0	0	1	1	1	0	0	2911.132	0.000000	2978.240003
10	9	0	0	0	2	1	0	0	0	2935.579	0.000000	3005.951888
11	9	0	0	0	1	2	0	0	0	2944.114	0.000000	3019.370971
13	8	0	0	0	1	1	0	0	0	2945.937	0.003908	3022.452638
14	7	0	0	0	1	1	0	0	0	2947.985	0.019956	3046.492053
11	10	7	0	0	1	1	1	0	0	2970.703	0.000000	3041.341216
12	9	0	0	0	1	2	0	0	0	2999.408	0.000000	3073.690976
15	0	0	0	0	1	0	0	0	0	3001.317	10.961334	3143.589841
14	8	0	0	0	1	1	0	0	0	3023.250	0.043478	3123.556960
12	10	7	0	0	1	1	1	0	0	3029.366	0.000000	3095.661221
13	9	0	0	0	1	1	0	0	0	3046.226	0.313656	3117.903610
11	10	8	0	0	1	1	1	0	0	3052.606	0.000000	3118.406123
12	10	8	0	0	1	1	1	0	0	3103.333	0.000000	3172.726128
10	0	0	0	0	3	0	0	0	0	3105.834	0.000000	3200.438013
14	9	0	0	0	1	1	0	0	0	3114.813	0.009377	3219.007933
11	10	9	0	0	1	1	1	0	0	3139.402	0.000000	3213.857096
11	7	0	0	0	2	1	0	0	0	3159.682	0.000000	3249.246425
12	10	9	0	0	1	1	1	0	0	3196.602	0.000000	3268.177101
12	11	7	0	0	1	1	1	0	0	3224.814	0.000000	3303.566429
13	10	0	0	0	1	1	0	0	0	3231.794	0.054309	3312.389735
11	8	0	0	0	2	1	0	0	0	3249.379	0.000000	3326.311332
12	7	0	0	0	2	1	0	0	0	3266.258	0.000000	3357.886434
14	10	0	0	0	1	1	0	0	0	3288.318	0.311454	3413.494058
12	11	8	0	0	1	1	1	0	0	3306.576	0.000000	3380.631337
11	10	0	0	0	1	2	0	0	0	3324.029	0.000000	3408.343221
11	9	0	0	0	2	1	0	0	0	3326.442	0.000000	3421.762305
12	8	0	0	0	2	1	0	0	0	3340.085	0.000000	3434.951341
12	10	0	0	0	1	2	0	0	0	3383.135	0.000000	3462.663226
12	11	9	0	0	1	1	1	0	0	3390.112	0.000000	3476.082309
12	9	0	0	0	2	1	0	0	0	3430.094	0.000000	3530.402314
13	11	0	0	0	1	1	0	0	0	3431.595	0.064443	3520.294944
13	12	0	0	0	1	1	0	0	0	3473.671	0.274985	3574.614948

14	11	0	0	0	1	1	0	0	0	3504.611	0.016774	3621.399266
11	10	0	0	0	2	1	0	0	0	3525.442	0.000000	3616.248430
14	12	0	0	0	1	1	0	0	0	3544.575	0.216256	3675.719271
13	7	0	0	0	1	2	0	0	0	3551.255	0.000000	3645.198396
12	11	10	0	0	1	1	1	0	0	3591.017	0.000000	3670.568434
14	7	0	0	0	1	2	0	0	0	3629.321	0.000000	3746.302719
13	8	7	0	0	1	1	1	0	0	3629.348	0.000000	3722.263303
12	10	0	0	0	2	1	0	0	0	3632.904	0.000000	3724.888439
15	7	0	0	0	1	1	0	0	0	3690.620	0.057330	3843.400507
13	8	0	0	0	1	2	0	0	0	3707.191	0.000000	3799.328211
14	8	7	0	0	1	1	1	0	0	3707.587	0.000000	3823.367626
11	0	0	0	0	3	0	0	0	0	3710.072	0.000000	3824.153638
13	9	7	0	0	1	1	1	0	0	3729.563	0.000000	3817.714276
15	8	0	0	0	1	1	0	0	0	3767.503	0.003355	3920.465414
12	11	0	0	0	1	2	0	0	0	3782.117	0.000000	3878.473643
14	8	0	0	0	1	2	0	0	0	3785.603	0.000000	3900.432533
14	9	7	0	0	1	1	1	0	0	3799.075	0.000000	3918.818599
13	9	8	0	0	1	1	1	0	0	3807.427	0.000000	3894.779184
12	11	0	0	0	2	1	0	0	0	3830.473	0.000000	3932.793648
12	0	0	0	0	3	0	0	0	0	3855.142	0.000000	3987.113652
15	9	0	0	0	1	1	0	0	0	3856.087	0.296873	4015.916387
14	9	8	0	0	1	1	1	0	0	3877.112	0.000000	3995.883506
13	9	0	0	0	1	2	0	0	0	3905.022	0.000000	3990.230156
13	10	7	0	0	1	1	1	0	0	3917.475	0.000000	4012.200401
14	9	0	0	0	1	2	0	0	0	3965.979	0.000000	4091.334479
14	10	7	0	0	1	1	1	0	0	3974.924	0.000000	4113.304724
13	10	8	0	0	1	1	1	0	0	3990.047	0.000000	4089.265308
15	10	0	0	0	1	1	0	0	0	4045.814	0.064879	4210.402512
14	10	8	0	0	1	1	1	0	0	4047.669	0.000000	4190.369631
13	10	9	0	0	1	1	1	0	0	4092.635	0.000000	4184.716281
13	11	7	0	0	1	1	1	0	0	4113.155	0.000000	4220.105609
14	10	9	0	0	1	1	1	0	0	4141.529	0.000000	4285.820604
13	12	7	0	0	1	1	1	0	0	4159.888	0.000000	4274.425614
14	11	7	0	0	1	1	1	0	0	4187.097	0.000000	4321.209932
13	11	8	0	0	1	1	1	0	0	4193.523	0.000000	4297.170517
15	11	0	0	0	1	1	0	0	0	4230.541	0.569197	4418.307720
14	12	7	0	0	1	1	1	0	0	4231.717	0.000000	4375.529937
13	12	8	0	0	1	1	1	0	0	4232.320	0.000000	4351.490522
14	11	8	0	0	1	1	1	0	0	4267.638	0.000000	4398.274839
13	10	0	0	0	1	2	0	0	0	4269.586	0.000000	4379.202406
15	12	0	0	0	1	1	0	0	0	4275.819	0.054823	4472.627725
13	11	9	0	0	1	1	1	0	0	4286.377	0.000000	4392.621490
14	12	8	0	0	1	1	1	0	0	4304.323	0.000000	4452.594844
14	10	0	0	0	1	2	0	0	0	4306.419	0.000000	4480.306729
13	12	9	0	0	1	1	1	0	0	4331.648	0.000000	4446.941494
13	0	0	0	0	2	0	0	0	0	4337.662	0.031431	4491.154129
14	11	9	0	0	1	1	1	0	0	4351.765	0.000000	4493.725812
15	7	0	0	0	1	2	0	0	0	4373.180	0.000000	4543.211173
14	13	0	0	0	1	1	0	0	0	4381.605	0.261159	4592.258451
14	12	9	0	0	1	1	1	0	0	4394.922	0.000000	4548.045817
15	8	7	0	0	1	1	1	0	0	4453.063	0.000000	4620.276080
13	11	10	0	0	1	1	1	0	0	4477.701	0.000000	4587.107614
14	0	0	0	0	2	0	0	0	0	4481.456	0.186408	4693.362774
13	12	10	0	0	1	1	1	0	0	4524.877	0.000000	4641.427619
14	11	10	0	0	1	1	1	0	0	4531.026	0.000000	4688.211937
15	8	0	0	0	1	2	0	0	0	4532.697	0.000000	4697.340987
15	9	7	0	0	1	1	1	0	0	4541.573	0.000000	4715.727053
14	12	10	0	0	1	1	1	0	0	4576.090	0.000000	4742.531942
15	9	8	0	0	1	1	1	0	0	4621.227	0.000000	4792.791960
13	11	0	0	0	1	2	0	0	0	4669.034	0.000000	4795.012823
15	9	0	0	0	1	2	0	0	0	4707.116	0.000000	4888.242933
13	12	11	0	0	1	1	1	0	0	4722.679	0.000000	4849.332828
15	10	7	0	0	1	1	1	0	0	4733.643	0.000000	4910.213178
14	11	0	0	0	1	2	0	0	0	4738.852	0.000000	4896.117146
13	12	0	0	0	1	2	0	0	0	4752.637	0.000000	4903.652832
14	12	11	0	0	1	1	1	0	0	4790.384	0.000000	4950.437150
15	10	8	0	0	1	1	1	0	0	4808.006	0.000000	4987.278085
14	12	0	0	0	1	2	0	0	0	4818.229	0.000000	5004.757155
15	10	9	0	0	1	1	1	0	0	4898.888	0.000000	5082.729058
15	11	7	0	0	1	1	1	0	0	4914.251	0.000000	5118.118386
15	12	7	0	0	1	1	1	0	0	4964.185	0.000000	5172.438391
15	11	8	0	0	1	1	1	0	0	4996.409	0.000000	5195.183293
13	7	0	0	0	2	1	0	0	0	5024.948	0.000000	5190.964794
15	12	8	0	0	1	1	1	0	0	5038.408	0.000000	5249.503298
14	13	7	0	0	1	1	1	0	0	5069.816	0.000000	5292.069117
15	11	9	0	0	1	1	1	0	0	5077.557	0.000000	5290.634266
15	10	0	0	0	1	2	0	0	0	5079.998	0.000000	5277.215183
13	8	0	0	0	2	1	0	0	0	5095.986	0.000000	5268.029702

```
   15   12    9    0    0    1    1    1    0    0   5126.029   0.000000   5344.954271
   14   13    8    0    0    1    1    1    0    0   5141.027   0.000000   5369.134024
   14    7    0    0    0    2    1    0    0    0   5170.593   0.000000   5393.173440
   15   13    0    0    0    1    1    0    0    0   5184.840   0.041497   5389.166905
   13    9    0    0    0    2    1    0    0    0   5204.631   0.000000   5363.480675
   14   13    9    0    0    1    1    1    0    0   5240.945   0.000000   5464.584997
   14    8    0    0    0    2    1    0    0    0   5241.977   0.000000   5470.238347
   15   14    0    0    0    1    1    0    0    0   5262.359   0.043043   5490.271228
   15   11   10    0    0    1    1    1    0    0   5273.040   0.000000   5485.120391
   15   12   10    0    0    1    1    1    0    0   5323.417   0.000000   5539.440396
   14    9    0    0    0    2    1    0    0    0   5333.167   0.000000   5565.689320
   13   10    0    0    0    2    1    0    0    0   5388.280   0.000000   5557.966799
   14   13   10    0    0    1    1    1    0    0   5412.531   0.000000   5659.071122
   15   11    0    0    0    1    2    0    0    0   5449.300   0.000000   5693.025600
   14   10    0    0    0    2    1    0    0    0   5492.691   0.000000   5760.175445
   15   12   11    0    0    1    1    1    0    0   5506.147   0.000000   5747.345604
   15   12    0    0    0    1    2    0    0    0   5539.305   0.000000   5801.665609
   13   11    0    0    0    2    1    0    0    0   5586.315   0.000000   5765.872008
   13   12    0    0    0    2    1    0    0    0   5621.561   0.000000   5820.192013
   14   13   11    0    0    1    1    1    0    0   5627.059   0.000000   5866.976331
   14   13   12    0    0    1    1    1    0    0   5660.192   0.000000   5921.296335
   14   11    0    0    0    2    1    0    0    0   5723.712   0.000000   5968.080653
   14   12    0    0    0    2    1    0    0    0   5754.732   0.000000   6022.400658
   15   13    7    0    0    1    1    1    0    0   5874.275   0.000000   6088.977571
   15    0    0    0    0    2    0    0    0    0   5880.691   0.500230   6287.179682
   15   13    8    0    0    1    1    1    0    0   5947.103   0.000000   6166.042478
   15   14    7    0    0    1    1    1    0    0   5952.720   0.000000   6190.081894
   15   14    8    0    0    1    1    1    0    0   6025.721   0.000000   6267.146801
   15   13    9    0    0    1    1    1    0    0   6044.043   0.000000   6261.493451
   15   14    9    0    0    1    1    1    0    0   6113.933   0.000000   6362.597774
   15   13   10    0    0    1    1    1    0    0   6231.850   0.000000   6455.979576
   15   14   10    0    0    1    1    1    0    0   6289.678   0.000000   6557.083899
   15   13   11    0    0    1    1    1    0    0   6414.812   0.000000   6663.884785
   15   13   12    0    0    1    1    1    0    0   6453.259   0.000000   6718.204789
   13    0    0    0    0    3    0    0    0    0   6461.914   0.000000   6736.731193
   14   13    0    0    0    1    2    0    0    0   6473.585   0.000000   6837.835516
   15   14   11    0    0    1    1    1    0    0   6489.133   0.000000   6764.989107
   15   14   12    0    0    1    1    1    0    0   6525.468   0.000000   6819.309112
   14   13    0    0    0    2    1    0    0    0   6541.164   0.000000   6938.939838
   15    7    0    0    0    2    1    0    0    0   6572.274   0.000000   6986.990348
   15    8    0    0    0    2    1    0    0    0   6646.893   0.000000   7064.055255
   14    0    0    0    0    3    0    0    0    0   6664.652   0.000000   7040.044161
   15    9    0    0    0    2    1    0    0    0   6732.127   0.000000   7159.506228
   15   10    0    0    0    2    1    0    0    0   6924.093   0.000000   7353.992353
   15   11    0    0    0    2    1    0    0    0   7091.982   0.000000   7561.897561
   15   12    0    0    0    2    1    0    0    0   7133.631   0.000000   7616.217566
   15   13    0    0    0    1    2    0    0    0   7338.643   0.000000   7634.743969
   15   14   13    0    0    1    1    1    0    0   7383.890   0.000000   7735.848292
   15   14    0    0    0    1    2    0    0    0   7485.046   0.000000   7836.952615
   15   13    0    0    0    2    1    0    0    0   8064.045   0.000000   8532.756746
   15   14    0    0    0    2    1    0    0    0   8142.869   0.000000   8633.861069
   15    0    0    0    0    3    0    0    0    0   8638.119   0.000000   9430.769523
--------------------------------------------------------------------------------
 Dipole moment function written to files dipolex(y,z)
  @CHECKOUT-I, Total execution time :        0.0000 seconds.
  --executable xcubic finished with status         0
```

85