
Cl2 + H3+ reaction

REACT *

Chlorine

2

Cl 0.997831 0.000000 0.000000

Cl -0.997831 0.000000 0.000000

H3+

3

H -0.442322 -0.246803 0.000000

H 0.434898 -0.259660 0.000000

H 0.007423 0.506463 0.000000

INTERMEDIATE *

MIN1 - Cl2H3+

5

Cl -1.054184 0.061124 -0.000000

Cl 0.920537 -0.238003 0.000000

H 1.310330 1.051420 0.000000

H 1.663428 2.542912 -0.377966

H 1.663428 2.542912 0.377966

TS1

5

Cl -0.997481 0.088565 0.000000

Cl 0.997481 0.088565 0.000000

H 0.497861 -1.801510 0.000000

H 0.000001 -2.542915 0.000000

H -0.497860 -1.801511 0.000000

Prod *

H2

2

H -0.371111 0.000000 0.000000

H 0.371111 0.000000 0.000000

Cl2H+

3

H 1.216558 1.246597 0.000000

Cl 0.981229 -0.040160 0.000000

Cl -1.016291 0.004233 -0.000000

P2 + H3+ reaction

REACT *

P2

2

P 0.951460 0.000000 0.000000

P -0.951460 0.000000 0.000000
H3+
3
H -0.442322 -0.246803 0.000000
H 0.434898 -0.259660 0.000000
H 0.007423 0.506463 0.000000

INTERMEDIATE *

MIN1

5

P 0.972781 -0.129580 0.000000
P -0.972781 -0.129580 0.000000
H 0.000000 3.408277 -0.372652
H 0.000000 1.148277 0.000000
H 0.000000 3.408277 0.372652

MIN2

5

P 0.774197 -0.000002 0.000000
P -1.113387 0.000001 0.000000
H 4.112614 0.374009 0.000000
H 4.112618 -0.373990 0.000000
H 2.199188 0.000001 0.000000

TS1

5

15 0.958965 -0.122101 0.000000
15 -0.958965 -0.122101 -0.000000
H 0.000000 3.026762 -0.000000
H 0.000000 2.239178 -0.441297
H 0.000000 2.239178 0.441297

TS2

5

H 2.795594 2.472009 -0.373304
H 1.556678 0.852914 -0.000000
H 2.795606 2.472000 0.373305
15 0.811086 -0.371900 -0.000000
15 -1.043664 0.183279 0.000000

Prod *

H2

2

H -0.371111 0.000000 0.000000
H 0.371111 0.000000 0.000000

P2H+ (bent)

3

P 0.000000 0.973802 -0.041068
H 0.000000 0.000000 1.232034
P 0.000000 -0.973802 -0.041068

P2H+ (linear)

3

P -0.906063 0.000000 0.000000

H	-2.318679	0.000000	0.000000
P	0.981509	0.000000	0.000000

CNNC + H3+

REACT *

CNNC

4

N	-0.639138	0.000000	0.000000
C	-1.821313	0.000000	0.000000
N	0.639138	0.000000	0.000000
C	1.821313	0.000000	0.000000

H3+

3

H	-0.442322	-0.246803	0.000000
H	0.434898	-0.259660	0.000000
H	0.007423	0.506463	0.000000

INTERMEDIATE *

MIN1

7

N	0.845625	0.000000	0.000000
C	2.044755	-0.000002	0.000000
N	-0.413836	0.000001	0.000000
C	-1.560094	0.000003	0.000000
H	-4.560066	0.373639	0.000000
H	-2.650068	0.000001	0.000000
H	-4.560060	-0.373661	0.000000

MIN2

7

H	-3.117653	2.145505	-0.372501
H	-2.664556	-0.491237	0.000000
H	-3.117653	2.145505	0.372501
C	1.969535	0.191577	0.000000
C	-1.596236	-0.332078	0.000000
N	0.782986	0.016266	0.000000
N	-0.462348	-0.169339	0.000000

MIN3

7

H	-1.471516	-2.773056	0.376670
H	-1.086098	-1.201396	0.000000
H	-1.471516	-2.773056	0.376670
C	1.822888	0.137076	0.000000
C	-1.449400	0.792151	0.000000
N	0.651445	-0.092460	0.000000
N	-0.681522	-0.218216	0.000000

TS1

7

H	-0.000000	-2.628339	0.000000
H	-0.462444	-1.876071	0.000000

H	0.462444	-1.876071	-0.000000
C	1.826728	0.051469	-0.000000
C	-1.826728	0.051469	0.000000
N	0.640840	0.185501	-0.000000
N	-0.640840	0.185501	0.000000

TS2

H	-1.409478	-2.292354	0.394047
H	-1.211558	-1.266424	0.000000
H	-1.409478	-2.292354	-0.394047
C	1.907104	0.004846	0.000000
C	-1.727544	0.406702	0.000000
N	0.713147	0.045069	0.000000
N	-0.576938	0.023368	0.000000

TS3

7

H	-3.240066	2.081335	-0.372498
H	-2.659648	-0.490896	0.000000
H	-3.240066	2.081335	0.372498
C	1.973882	0.196194	0.000000
C	-1.591226	-0.332193	0.000000
N	0.787532	0.019506	0.000000
N	-0.457645	-0.167224	0.000000

Prod *

H2

2

H	-0.371111	0.000000	0.000000
H	0.371111	0.000000	0.000000

CNNCH+ BENT

5

H	-1.042209	1.418021	0.000000
C	1.705633	-0.291159	0.000000
C	-1.502148	-0.562321	0.000000
N	0.610862	0.193060	0.000000
N	-0.710230	0.436276	0.000000

CNNCH+ LINEAR

N	0.671330	0.000000	0.000000
C	1.871224	0.000000	0.000000
N	-0.587355	0.000000	0.000000
C	-1.732899	0.000000	0.000000
H	-2.813776	0.000000	0.000000
