# Statistical Mechanical Equilibrium Constants- $Cl + H_2 \rightarrow HCl + H$

Kp for atom-diatom reactions

Cl + H2 → HCl + H

A + BC → AB + C

| | | | | | | | | |
|---|---|---|---|---|---|---|---|---|
| Mr(A) (g/mol) | 34.9688 | | | trans | rot | vib | $g_{elec}$ | $e^{-\Delta Eo/RT}$ |
| Mr(B) (g/mol) | 1.0078 | | | | | | | |
| Mr(C) (g/mol) | 1.0078 | | Kp= | 218.3191 | 19.562 | 1 | 2 | 0.16494044 |
| | AB=HCl | BC=H2 | | 591.7355 | 1.7037 | 1 | 4 | |
| ro (nm) | 0.12746 | 0.07417 | | | | | | |
| symm.number | 1 | 2 | | | | | | |
| vo (cm-1) | 2989.74 | 4395.2 | Kp= | 0.34936 | | | | |
| Do (eV) | 4.43 | 4.4763 | | | | | | |
| Do (kJ/mol) | 427.42855 | 431.895806 | | | | | | |
| g (grnd.state) | 1 | 1 | | | | | | |
| | A=Cl | C=H | | | | | | |
| g (grnd.state) | 4 | 2 | | | | | | |

| | | | | | |
|---|---|---|---|---|---|
| reduced mass | 1.6266E-27 | 8.3676E-28 | | | |
| I (kg m2) | 2.6426E-47 | 4.6032E-48 | Data from | Karplus and Porter | Table 7.3 |
| Be (cm-1) | 10.592893 | 60.8130047 | | | |
| qr | 19.5621725 | 1.70374742 | | | |
| qv | 1.00000054 | 1 | | | |

| | |
|---|---|
| T (K) | 298.15 |
| kT/hc (cm-1) | 207.22 |
| R (J/mol/K) | 8.314 |
| Na | 6.0221E+23 |
| h bar (J s) | 1.0546E-34 |
| c (m/sec) | 299792500 |