

DATA AND CALCULATIONS

Constants:

Planck's constant	6.63E-34	kg m ² /s
Avogadro's	6.022E+23	mol ⁻¹
Speed of light	2.998E+10	cm/s
Hartree/kJ conversion	2625.50	kJ/mol

Data from Gaussian

	HF	HCl
Rotational Constant B GHz) =	636.2822356	321.7703541
Fundamental freq (cm ⁻¹) =	4357.1959	2924.7696
Energy (Hartrees) =	-100.002907	-460.0599763

Calculated Quantities:

Reduced Mass (u, kg) =	6.2925E+26	6.1477E+26
re (angstroms) =	9.11E-01	1.27E+00
Energy (kJ/mol) =	-262557.63229	-1207887.46777
Frequency (Hz) =	1.30624E+14	8.76817E+13
k (N m ⁻¹) =	1070.50	493.70

Most Abundant Isotope	Mass (amu)
H	1.00783
Li	7.01600
C	12.00000
N	14.00307
O	15.99491
F	18.99840
Na	22.98977
Cl	34.96885
K	38.96371
Br	78.91834

HBr

252.1209116

2799.7343

-2570.465551

6.0518E+26

1.42E+00

-6748757.30426

8.39332E+13

459.56

Mass (kg)
1.6735E-27
1.1650E-26
1.9927E-26
2.3253E-26
2.6560E-26
3.1548E-26
3.8175E-26
5.8067E-26
6.4701E-26
1.3105E-25