

FeH Energy Levels for Thermochemistry

State	Term value / cm^{-1}
$X^4\Delta_{7/2}$	0
$X_{5/2}$	191
$X_{3/2}$	426
$X_{1/2}$	695
$A^4\Pi_{5/2}$	910
$A_{3/2}$	1068
$A_{1/2}$	1228
$A_{-1/2}$	1388
$a^6\Delta_{9/2}$	1766
$a_{7/2}$	1981
$a_{5/2}$	2177
$a_{3/2}$	2356
$a_{1/2}$	2518
$a_{-1/2}$	2656
$C^4\Phi_{9/2}$	3174
$C_{7/2}$	3375
$C_{5/2}$	3575
$C_{3/2}$	3735
$b^6\Pi_{7/2}$	3889
$b_{5/2}$	3939
$b_{3/2}$	3989
$b_{1/2}$	4039
$b_{-1/2}$	4089
$b_{-3/2}$	4139
$c^6\Sigma^+$	4750
$B^4\Sigma^-$	5089
$D^4\Sigma^+$	7158
$E^4\Pi$	7300
$F^4\Delta$	9995

FeH Constants in cm⁻¹

State	B _e	α _e	D _e	ω _e	ω _e x _e
X ⁴ Δ	6.5906	0.2116	8.5 x 10 ⁻⁵	1826.86	31.96
A ⁴ Π	6.86	0.22	1 x 10 ⁻⁴	1875	34
a ⁶ Δ	6.00	0.2	1.4 x 10 ⁻⁴	1680	30
C ⁴ Φ	6.6	0.2	1 x 10 ⁻⁴	1680	30
b ⁶ Π	5.9	0.2	1 x 10 ⁻⁴	1600	30
c ⁶ Σ ⁺	6.7	0.2	1 x 10 ⁻⁴	1600	30
B ⁴ Σ ⁻	6.9	0.2	1 x 10 ⁻⁴	1875	34
D ⁴ Σ ⁺	6.5	0.2	1 x 10 ⁻⁴	1800	30
E ⁴ Π	6.86	0.22	1 x 10 ⁻⁴	1875	34
F ⁴ Δ	5.936	0.19	1 x 10 ⁻⁴	1498	37

Partition Function for FeH using data above:

T/ K	Internal partition function
1000.000	889.5140380859375
1100.000	1087.088012695313
1200.000	1312.495971679688
1300.000	1567.847045898438
1400.000	1855.204589843750
1500.000	2176.580078125000
1600.000	2533.923095703125
1700.000	2929.119873046875
1800.000	3363.998779296875
1900.000	3840.322509765625
2000.000	4359.800781250000
2100.000	4924.085937500000
2200.000	5534.776367187500
2300.000	6193.430175781250
2400.000	6901.558105468750
2500.000	7660.624511718750