

## H2 singlet states

				epsilon 0	e	h bar	m sub e	a0	c								
				8.85419E-12	1.60219E-19	1.05459E-34	9.10953E-31	5.29177E-11	2.99792E+08								
Singlet States																	
n	m	l		a(a0)	a (m)	b (m)	c' (m)	2c' (m)	eccentricity	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)	Evib (0) (eV)	w (s-1)	EK (eV)
2	4	1		2.73570	1.44767E-10	1.15312E-10	8.75257E-11	1.75051E-10	0.60460	-5.76118	0	2.10592	-0.52648	-4.18174	0.28479	7.30819E+15	4.81038
2	1	1		3.73570	1.97685E-10	1.69169E-10	1.02279E-10	2.04558E-10	0.51739	-4.03193	0	1.07930	-0.26982	-3.22245	0.28479	7.30819E+15	4.81038
2	0	0		4.00000	2.11671E-10	1.83312E-10	1.05835E-10	2.11671E-10	0.50000	-3.73688	0	0.93422	-0.23355	-3.03621	0.28479	7.30819E+15	4.81038
2	-2	0		4.66667	2.46949E-10	2.18897E-10	1.14315E-10	2.28631E-10	0.46291	-3.15548	0	0.67618	-0.16904	-2.64835	0.28479	7.30819E+15	4.81038
3	4	0		4.66667	2.46949E-10	2.03426E-10	1.40007E-10	2.80014E-10	0.56695	-2.20446	0	0.70858	-0.11810	-1.61398	0.28479	3.24809E+15	2.13795
3	4	1		4.73570	2.50603E-10	2.07146E-10	1.41039E-10	2.82078E-10	0.56280	-2.16761	0	0.68657	-0.11443	-1.59546	0.28479	3.24809E+15	2.13795
3	3	0		5.00000	2.64589E-10	2.21371E-10	1.44921E-10	2.89842E-10	0.54772	-2.03734	0	0.61120	-0.10187	-1.52801	0.28479	3.24809E+15	2.13795
3	3	2		5.00562	2.64886E-10	2.21673E-10	1.45003E-10	2.90005E-10	0.54742	-2.03474	0	0.60974	-0.10162	-1.52663	0.28479	3.24809E+15	2.13795
3	3	1		5.06904	2.68242E-10	2.25081E-10	1.45918E-10	2.91836E-10	0.54398	-2.00588	0	0.59357	-0.09893	-1.51124	0.28479	3.24809E+15	2.13795
3	2	0		5.33333	2.82228E-10	2.39270E-10	1.49674E-10	2.99348E-10	0.53033	-1.89402	0	0.53269	-0.08878	-1.45011	0.28479	3.24809E+15	2.13795
3	2	1		5.40237	2.85881E-10	2.42973E-10	1.50639E-10	3.01279E-10	0.52693	-1.86685	0	0.51834	-0.08639	-1.43490	0.28479	3.24809E+15	2.13795
3	1	0		5.66667	2.99867E-10	2.57134E-10	1.54280E-10	3.08561E-10	0.51450	-1.76971	0	0.46845	-0.07808	-1.37933	0.28479	3.24809E+15	2.13795
3	1	1		5.73570	3.03520E-10	2.60830E-10	1.55217E-10	3.10434E-10	0.51139	-1.74599	0	0.45661	-0.07610	-1.36548	0.28479	3.24809E+15	2.13795
3	-3	1		7.06904	3.74077E-10	3.32025E-10	1.72316E-10	3.44633E-10	0.46064	-1.38755	0	0.29443	-0.04907	-1.14219	0.28479	3.24809E+15	2.13795
4	4	1		6.73570	3.56438E-10	2.98872E-10	1.94226E-10	3.88452E-10	0.54491	-1.13268	0	0.33632	-0.04204	-0.83840	0.28479	1.82705E+15	1.20259
4	1	2		7.67229	4.06000E-10	3.49094E-10	2.07290E-10	4.14580E-10	0.51057	-0.97861	0	0.25510	-0.03189	-0.75539	0.28479	1.82705E+15	1.20259
4	1	1		7.73570	4.09356E-10	3.52488E-10	2.08145E-10	4.16290E-10	0.50847	-0.96969	0	0.25070	-0.03134	-0.75032	0.28479	1.82705E+15	1.20259
4	-1	0		8.33333	4.40981E-10	3.84438E-10	2.16036E-10	4.32071E-10	0.48990	-0.89305	0	0.21433	-0.02679	-0.70551	0.28479	1.82705E+15	1.20259
4	-1	1		8.40237	4.44634E-10	3.88126E-10	2.16929E-10	4.33857E-10	0.48788	-0.88497	0	0.21065	-0.02633	-0.70066	0.28479	1.82705E+15	1.20259

## H2 singlet states

EDoppler (eV)	H2 Eocs (eV)	H2 IP 1 (eV)	Cal. Te (eV)	Exp. Te (eV)	State	Exp. Te (cm <sup>-1</sup> )	Relative Error
1.81447E-02	-0.12425	15.424814	11.3673	11.36819	B	91689.9	0.00008
1.39823E-02	-0.12841	15.424814	12.3308	12.40385	C	100043.0	0.00589
1.31742E-02	-0.12922	15.424814	12.5178	12.40631	E	100062.8	-0.00899
1.14913E-02	-0.13091	15.424814	12.9074	12.82999	F	103480	-0.00603
4.66874E-03	-0.13773	15.424814	13.9486	13.96780	K	112657	0.00138
4.61517E-03	-0.13778	15.424814	13.9671	13.98466	G	112793	0.00125
4.42004E-03	-0.13798	15.424814	14.0348	14.01839	I	113065	-0.00117
4.41606E-03	-0.13798	15.424814	14.0362	14.02818	Q	113144	-0.00057
4.37155E-03	-0.13803	15.424814	14.0516	14.06042	J	113404	0.00063
4.19471E-03	-0.13820	15.424814	14.1129	14.12043	D	113888	0.00053
4.15070E-03	-0.13825	15.424814	14.1282	14.12055	H	113889	-0.00054
3.98998E-03	-0.13841	15.424814	14.1839	14.19631	L	114500	0.00087
3.94992E-03	-0.13845	15.424814	14.1978	14.21540	M	114654	0.00124
3.30401E-03	-0.13909	15.424814	14.4217	14.41551	N	116268	-0.00043
1.81892E-03	-0.14058	15.424814	14.7270	14.71581	R	118690	-0.00076
1.63883E-03	-0.14076	15.424814	14.8102	14.81549	T	119494	0.00036
1.62783E-03	-0.14077	15.424814	14.8153	14.81772	P	119512	0.00017
1.53061E-03	-0.14087	15.424814	14.8602	14.85591	S	119820	-0.00029
1.52008E-03	-0.14088	15.424814	14.8650	14.85975	O	119851	-0.00036
						Avg. Rel. Error	-0.00035