

F2 parameters.xls

pi	nu 0	e	h bar	m sub e	a0	c	mp
3.1415927E+00	1.2566371E-06	1.6021892E-19	1.0545888E-34	9.1095345E-31	5.2917706E-11	2.9979246E+08	1.6726486E-27
	epsilon 0	uB	eV/cm^-1		aH		md
	8.85E-12	9.27E-24	0.000123985		5.29465E-11		3.3435860E-27
					aD		
			1.41193E-10	(crc)	5.29321E-11		
a (m)	b (m)	c' (m)	2c' (m)	eccentricity	r 2p (r8)		
1.88152E-10	1.74421E-10	7.05569E-11	1.41114E-10	0.37500	0.73318		
3.55556	3.29609	1.33333	2.66667				
				a-c'			
				2.22222			
1				F r1	F r9		
0.5				0.11297	0.78069		
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)	E of H(a0)	
Evib F2 (cm^-1)	-16.09139	10.20435	2.26285	-1.13143	-4.75562	13.60580	
916.64							
Evib F2 (eV)					-36.37915	0.08301	
0.11365						-31.62353	
	w (s-1)	EK (eV)					
	6.16629E+15	4.05876					
cm-1/eV							
1.239810E-04							
kcal/mole/eV							
4.336340E-02							
kJ/mole/eV							
1.036410E-02					-34.84564		
	EDoppler (eV)	F2 Eocs (eV)	F2 ET (eV)	F2 ED (eV)	ED (kcal/mole)	Rel. Error	
	0.14499	0.08817	36.46732	1.62168	37.39738	-0.00976	
	1.606	jchemphys					
Z	r3	denom	1st term	2nd term	num	3 rd term	r8
9	0.51382	2.280910761	0.343500352	0.117992492	2.606639361	1.142806376	0.73318