

CO2 parameters

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			aH		md	
	8.85E-12	9.27E-24			5.29465E-11		3.3435860E-27	
			r C-O					
			1.1600 Å	crc	aD			E C
					5.29321E-11			11.26030
a (m)	b (m)	c' (m)	2c' (m)	eccentricity	O r 2p (r6)	O r8 (initial)		E C+ AO
9.56239E-11	7.59636E-11	5.80815E-11	1.16163E-10	0.60740	0.74776	1		24.38332
1.80703	1.43550	1.09758	2.19516					
				a-c'				E O
				0.709447809				13.61806
				O r1				E O+ AO
3				0.12739				35.11730
0.666666667								
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)		E of H(a0)	
	-104.83940	49.58464	14.50438	-14.50438	-55.25476		13.60580	
					-55.25423			
					match 2X(2XH2+C+C+)		delta 1/r (a0^-1)	
							0.33733	
					Et (eV) sum of MO & AOs		delta E O AO	
					-55.26841		-32.12759	
	w (s-1)	EK (eV)						
	4.16331E+16	27.40365						
	3x				-27.63421			
eV/cm^-1								
0.000123985								
				Emag				
				0.11441				
Evib (0) (cm-1)								
2349	crc							
Evib (0) (eV)	EDoppler (eV)	CO2 Eocs (eV)	CO2 ET (eV)	CO2 ED (eV)	ED (kcal/mole)	rel. error		
0.29124	0.28619	-0.00505	55.26336	5.49557	126.73289	0.00366		
kcal/mole/ev				49.65338				
4.33634E-02								
Do C-O2			angle of intersection with C				angle of intersection with O	
532.2	298K (CRC)		0.580299542				0.8644166	
127.19885			0.951699878				0.526807472	
5.51577			54.53				30.18	
		theta C	125.47				149.82	
ET CO2			2.189892775				2.614785181	
-55.16915			0.478354948				0.261897662	
ET CO			0.498780475				0.264987974	
-36.03532		theta H2 MO	28.58				15.18	
		dH2 MO	1.58687	8.39737E-11			1.74396	9.22862E-11
		dC AO	0.48929	2.58922E-11			0.64637	3.42047E-11
Z	r3	denom	1st term	2nd term	num	3 rd term	r6	
	8	0.59020	3.122278522	0.320278922	0.102578588	3.992159514	1.278604547	0.74776
								C r6 (initial)
								1.20654
								C r3=r4 (final)
								0.84317
								C r1=r2
								0.17113