

CnH2n+2(propene)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	eV/cm^-1			aH		md				
	8.85E-12	0.000123985			5.29465E-11		3.3435860E-27				
			re	r C	aD						
			1.532E-10	1.20654	5.29321E-11						
a (m)	b (m)	c' (m)	2c' (m)	eccentricity	R of Csp3 initial	R of Csp3 methylene fina	E coul sp3	E of H(a0)	Hybridization Factor		
1.12450E-10	8.18192E-11	7.71400E-11	1.54280E-10	0.68600	0.91771	0.81549	14.82575	13.605804	0.91771432		
2.12499	1.54616	1.45774	2.91547								
number of carbons	number of bonds										
3	2										
1.83543											
1											
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)	E initial of Csp3	E initial of Csp3	E initial of Csp3			
E vib CH3 (cm^-1)	-57.58428	18.66704	13.54928	-6.77464	-63.27075	-14.63489	-14.63489	-14.63489			
993											
E vib CH3 (eV)					-63.27074	E final of Csp3 C-C	E final of Csp3 C=C	E final of Csp3			
0.12312					match (n-1)XH2	-15.35946	-15.76868	-15.56407			
cm-1/eV	w (s-1)	EK (eV)			Et (eV) sum of MO & AOs	E(eV) delta Csp3 C-C	E(eV) delta Csp3 C=C	E(eV) delta Csp3			
1.239810E-04	9.43699E+15	6.21159			-66.98746	-0.72457	-1.13379	-0.92918			
kcal/mole/eV											
4.336340E-02					-3.71673		Total E(eV) delta Csp3 C-C + C=2X E(eV) delta Csp3				
							-1.85837	-1.85836			
kJ/mole/eV							Avg E final of Csp3	Avg E(eV) delta Csp3			
0.010364101							-15.56407	-0.929183619			
	EDoppler (eV)	Cn Eocs (eV)	Cn ET (eV)	Cn total bond E (eV)	Cn total bond E (kcal/mole)			Total Bond Energy CH3 (eV)			
	0.16515	0.10359	67.19464	8.65508	199.59409			12.49186			
								Total Bond Energy CH2 (eV)			
								7.83016			
								Total Bond Energy Cn (eV)			
								8.65508			
			angle of intersection								
			0.55324574								
			0.984540746								
			56.41								
		theta C	123.59								
			2.157051907								
			0.439360926								
			0.454887132								
		theta H2 MO	26.06								
		dH2 MO	1.90890	1.01015E-10							
		dC AO	0.45117	2.38748E-11							
	r6	E ele	exp								
	1.20654	11.27671	11.2603								
	Exp		r sp3	E sp3							
C3+	64.4939	10	0.919153831	14.80253							
C2+	47.8878			14.61166867							
C+	24.38332			r3							

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C	11.2603			0.84317					
total	148.02532								
			Emag (a0)	Emag (r3)					
			0.114411043	0.19086					
			Initial Parameters			Final Parameters			
	Theory		r sp3	E sp3		Theory	r sp3	E sp3	
C3+	64.3921	10	0.91771	14.82575100	C3+	64.3921	9.75	0.87495	15.55033
C2+	48.3125			14.63489	C2+	48.3125			15.35946
C+	24.2762				C+	24.2762			
C	11.27671				C2sp3	14.63489			
total	148.25751				total	151.61569			
							Final Parameters		
						Theory	r sp3	E sp3	
					C3+	64.3921	9.5	0.85252	15.95955
					C2+	48.3125			15.76868
					C+	24.2762			
					C2sp3	14.63489			
					total	151.61569	150.68651	r sp3	E sp3
								0.86359	15.75493
									15.56407