C2H6											
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 C-C	r C	aD						
			1.5351E-10	1.20654	5.29321E-11						
a (m)	b (m)	c' (m)	2c' (m)	eccentricity	R of Csp3 initial	R of Csp3 final	E coul sp3				
1.11511E-10	8.08317E-11	7.68173E-11	1.53635E-10	0.68888	0.91771	0.87495	14.82575				
2.10725	1.52750	1.45164	2.90327								
							E of H(a0)				
0.91771					Et -E final of Csp3		13.605804				
1					-16.27589						
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)	E initial of Csp3	Hybridization Factor			E of H(a0)	
Evib CH3 (cm^-1)	-29.10112	9.37273	6.90500	-3.45250	-31.63535	-14.63489	0.91771432			13.60580	
993											
Evib CH3 (eV)					-31.63537	E final of Csp3				delta 1/r (a0^-1)	
0.12312					match H2	-15.35946				0.05325	
										delta E sp3 HO	
cm-1/eV	w (s-1)	EK (eV)			Et (eV) sum of MO &AO	E(eV) delta Csp3				-0.72458	
1.239810E-04	9.55643E+15	6.29021			-33.08452	-1.44915				-1.44915231	
kcal/mole/eV											
4.336340E-02											
kJ/mole/eV											
0.010364101											
					Delta ET CH3, CH3 (eV)						
			Et+osc(C-C) (eV)		0.01487						
			33.18712								
	EDoppler (eV)	CH3CH3 Eocs (e	CH3CH3 ET (eV	CH3CH3 ED (eV	ED (kcal/mole)	Rel. Error					
Do H3C-CH3	0.16416	0.10260	33.17225	3.90247	89.99446	-0.00143					
376											
89.86615679											
3.89690											
Do H-CH2											
108.95			angle of intersection								
455.8468			0.385404801								
4.72444			1.175149854								
			67.33								
ET CH3		theta C	112.67								
-67.95529			1.9664428								
			0.528550795								
			0.556892503								
Do H-CH		theta H2 MO	31.91								
		dH2 MO	1.78885	9.46617E-11							
417.85		dC AO	0.33721	1.78444E-11							
4.33064											
ET CH2											
-49.63241											
Do H-C											
3.47											
ET CH											
-31.70333											
	r6	E ele	exp								
	1.20654	11.27671	11.2603								
	Exp		r sp3	E sp3							
C3+	64.4939	10	0.919153831	14.802532							
C2+	47.8878			14.61166867							
C+	24.38332			r3							
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	14.82575	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					