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	
					aD			
					5.29321E-11			
a (m)	b (m)	c' (m)	2c' (m)	eccentricity				
3.1962E-10	3.0611E-10	9.1961E-11	1.8392E-10	0.2877		R of Csp3 final		
6.0400	5.7846	1.7378	3.4756			0.85252		
0.879746798							E coul ethane	
0.5							15.95955	
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)			
	-8.1572141E+00	7.8292604E+00	6.7526614E-01	-3.3763307E-01	0.009679385		E of H(a0)	
							13.605804	
							Hybridization Factor	
							0.85252	
Evib (0) (eV)	w (s-1)	EK (eV)						
0.022705258	2.4119E+15	1.587557458						
	EDoppler (eV)	H2 Eocs (eV)	H2 ET (eV)					
	-2.41277E-05	-0.011376757	-0.021056142					
					C-C-H Bond angle °			
					121.85			
	-0.44318	2.029934032	C-H bond angle radians					
		116.31	C-H bond angle °					
H2 MO vibration	w(0) (s-1)							
	2.6496374E+00							
	1.654486456							
k(0)	0.995150935	Evib(0) (eV)						
		3.44951E+13	0.022705258					