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				
3.1042E-10	2.9689E-10	9.0627E-11	1.8125E-10	0.2920		R of Csp3 final		
5.8660	5.6104	1.7126	3.4252			0.87495		
0.86846742							E coul alkane	
0.5							15.75493	
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)			
	-8.2988153E+00	7.9445294E+00	7.0736586E-01	-3.5368293E-01	-0.000602959		E of H(a0)	
							13.605804	
							Hybridization Factor	
							0.86359	
Evib (0) (eV)	w (s-1)	EK (eV)						
0.023915512	2.52001E+15	1.658715002						
	EDoppler (eV)	H2 Eocs (eV)	H2 ET (eV)					
	1.5363E-06	-0.01195622	-0.011353261					
					C-C-C Bond angle °			
					C-C-H Bond angle °			
					109.44			
					C-H angle from the verticle			
	-0.33383	1.911157327	C-H bond angle radians		1.97754	H distance from center of base		
		109.50	C-H bond angle °		0.69800	verticle height		
					1.2314838	angle radians		
					70.56	angle °		
H2 MO vibration	w(0) (s-1)							
	2.8924848E+00							
	1.788417774							
k(0)	1.104067015	Evib(0) (eV)						
		3.63338E+13	0.023915512					