pi	nu 0	e	h bar	m sub e	a0	c	mp	D/C m			
3.1415927E+00	1.2566371E-06	1.6021892E-19	1.0545888E-34	9.1095345E-31	5.2917706E-11	2.9979246E+08	1.6726486E-27	2.9979246E+29			
	epsilon 0	eV/cm^-1			aH		md	q/e	graphite van der Waals dipole moment	u (bond moment) D	1.07647
	8.85E-12	0.000123985			5.29465E-11		3.3435860E-27	0.36101	8.04790E-30	2.41270	1.15880
											0.15880
					aD						0.42346
					5.29321E-11						
a (m)	b (m)	c' (m)	2c' (m)	eccentricity			Aromatic Hybridization Factor	E sp3	E sp3		
5.82486E-10	5.55398E-10	1.75567E-10	3.51134E-10	0.30141			0.85252	14.82575	15.95955	2c' (m) graphite	
11.00740	10.49550	3.31774	6.63548					14.63489	15.76868	1.39140E-10	
0.85252											
1											
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)						
Evib C-C (cm^-1)	-4.35014	4.10093	0.19760	-0.09880	-0.15042						
993	ethane			delta Et(H2 MO) and E final of Csp3							
Evib C-C (eV)				31.63537							
0.00317											
cm-1/eV	w (s-1)	EK (eV)		dipole to dipole distance							
1.239810E-04	8.00466E+14	0.52688		3.77697E-10							
kcal/mole/eV											
4.336340E-02				dipole angle (radians)							
kJ/mole/eV				1.19352							
0.010364101											
				dipole angle (°)							
				68.38365							
	EDoppler (eV)	Cn Eocs (eV)	Cn ET (eV)	Cal. ECoulomb (eV)	Cal. E/C graphite (eV)	Expl. E/C graphite (eV)					
	0.00022	-0.00137	0.14905	0.14905	0.04968	0.052					
CC MO vibration	w(0) (s-1)										
u C-C	4.9760578E-01										
6.00000	2.6481303E-01										
k(0)	2.3279275E-01	Evib(0) (eV)									
	4.81622E+12	0.00317									