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	uB			aH		md					
	8.85E-12	9.27E-24			5.29465E-11		3.3435860E-27					
			CH3Cl2- (Tucker)	r C	aD			E of H(a0)				
			curve fit >1.80 Å	1.20654	5.29321E-11			13.605804				
a (m)	b (m)	c' (m)	2c' (m)	eccentricity	R of Csp3 initial	r of Cla- final	E coul sp3	E Cl	Hybridization Factor			
1.40991E-10	1.03457E-10	9.57869E-11	1.91574E-10	0.67938	0.91771	0.86923	14.82575	-12.96764	0.91771432			
2.66434	1.95505	1.81011	3.62022		r (Cl) initial	R of Ca sp3 final		E Cl-	C HO to Cl hybridization factor			
					1.05158	0.83078		-3.612724	0.81317			
								E tolal Cl-				
1.00000								-16.58036				
1.229761809												
	Ve (eV)	Vp (eV)	T (eV)	Vm (eV)	Et (eV)	E initial of Csp3	E initial of Csp3	E initial of Csp3	delta E Cla- (Cla(-)-C)			
Evib C-Cl (cm^-1)	-24.89394	7.51656	4.67169	-2.33584	-31.63539	-14.63489	-14.63489	-14.63489	-0.82688			
225	NIST Cl3-			delta Et(H2 MO) and E final of Csp3						r sp3	E sp3 Final	
Evib C-Cl (eV)				16.07130	-31.63537	E final of Csp3 C-C	E final of Csp3 C=C	E final of Csp3		0.86923	15.65263	
0.02790					matchH2	-15.35946	-15.76868	-15.56407				
									delta E C (Cla(-)-C)	delta E C (C-Clb)		
eV/cm^-1	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	-0.82688	-0.72457		
0.000123985	6.06143E+15	3.98974			-33.28913	-0.72457	-1.13379	-0.92918		r sp3	E sp3 Final	
kcal/mole/eV							Total E(eV) delta Csp3 C-C + C=C	2X E(eV) delta Csp3		0.83078	16.37720	
4.336340E-02							-1.85837	-1.85836			16.18634	
kJ/mole/eV						Avg E final of Csp3	Avg E(eV) delta Csp3					
0.010364101						-15.56407	-0.92918					
							Et (eV) sum of AOs					
							-1.65376					
	EDoppler (eV)	C-Cl Eocs (eV)	C-Cl ET (eV)	C-Cl total bond E (eV)	C-Cl total bond E (kcal/mole)			Et (eV) Cla- AO to Cla(-)-C bond	Et (eV) C HO to Cla(-)-C bond			
	0.13155	0.11760	33.40672	0.52422	12.08900			-0.82688	-0.82688			
					Cla(-)-C bond intercept parameters							
			angle of intersection with Cla-			angle of intersection with C		CH3Cl	C of C-Cl	Cl-	Sum of radii	Cl-.C-Cl bod distance
			0.957326307			1.069778289		1.785E-10				
			0.293191753			#NUM!		2c' (m)	R of Ca sp3 final	r18		
		theta prime	16.80		theta prime	#NUM!		1.79005E-10	4.63005E-11	1.42201E-10	1.88501E-10	1.91574E-10
		theta Cla-	163.20		theta C	#NUM!		3.382711468	0.87495	2.68720	3.56216	3.62022
			2.848400901			#NUM!						
			0.128496625			#NUM!						
			0.128852888			#NUM!						
		theta H2 MO	7.38		theta H2 MO	#NUM!						
		dH2 MO	2.64225	1.39822E-10	dH2 MO	#NUM!	#NUM!					
		dCla- AO	0.83214	4.40350E-11	dC AO	#NUM!	#NUM!					
	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								
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	14.825751	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		r sp3	E sp3			
								0.86359	15.75493			
									15.56407			