

Supporting Information

To

From unsuccessful H₂-Activation with FLPs containing B(Ohfp)₃ to a systematic evaluation of the Lewis Acidity of 33 Lewis Acids based on Fluoride, Chloride, Hydride and Methyl Ion Affinities.

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Techniques and Instruments: All reactions were carried out under an inert atmosphere by using standard vacuum and Schlenk techniques or a glovebox with an argon atmosphere (H₂O and O₂ < 1 ppm), Special J. Young NMR tubes sealed with Teflon valves were used to exclude air and moisture. All solvents were dried over CaH₂ or P₄O₁₀ and distilled afterwards. NMR data were recorded from solutions in d⁸-toluene or d³-acetonitrile at room temperature or 313 K on a BRUKER AVANCE II⁺ 400MHz WB spectrometer. ¹H and ¹³C chemical shifts are given with respect to TMS, ¹⁹F NMR spectra to fluorotrichloromethane, ¹¹B NMR spectra to the boron-trifluoride-diethyl-ether-complex, ³¹P NMR spectra to a 85 % phosphoric(V) acid solution and ⁷Li NMR spectra to 9.7 M LiCl in D₂O. IR spectra were recorded on a Diamond ATR unit (200-30000 cm⁻¹) on a BRUKER alpha Fourier transform-infrared (FT-IR) spectrometer with a resolution of 4 cm⁻¹. Raman spectra were obtained on a BRUKER VERTEX 70 spectrometer with a BRUKER RAM II Raman unit in sealed melting-point capillaries. Data collections for X-ray structure determinations were performed on a Rigaku Spider image plate system or a BRUKER APEX II Quazar CCD diffractometer at 100 and 110 K, respectively, with Mo radiation. The single crystals were mounted in perfluoroether oil on a MiTeGen MicromountTM. 1,3-dimethyl-4,5-diphenyl imidazol-2-ylidene was synthesized from the thiourea precursor according to the literature.^[1]

Preparation of compound 1: Compound **1** was synthesized according to the literature,^[2] but the reaction was executed in CH₂Cl₂ instead of pentane and further purified by sublimation and crystals suitable for X-ray diffraction were obtained. ¹H NMR (400.17 MHz, CD₃CN): δ = 1.96 (quint., 1H, CHD₂CN), 5.48 (sept., 3H, B(Ohfip)₃). ¹⁹F NMR (376.54 MHz, CD₃CN): δ = -75.8 (d, 18F, B(Ohfip)₃). ¹¹B NMR (376.54 MHz, CD₃CN): δ = 17.3 (br, 1B, B(Ohfip)₃). IR (Diamond ATR, corrected): $\tilde{\nu}$ = 650 (cw), 690 (w), 745 (w), 874 (w), 908 (w), 1078 (w), 1109 (vs), 1200 (s), 1230 (m), 1279 (s), 1383 (m), 1406 (m), 1454 (w), 2985 (vw) cm⁻¹. Raman: $\tilde{\nu}$ = 210, 277, 299, 335, 367, 391, 431, 543, 568, 649, 692, 731, 746, 860, 902, 1112, 1209, 1253, 1280, 1309, 1385, 2739, 2757, 2937, 2985 cm⁻¹.

Preparation of compound 1•NMe: The crystals of **1•NMe** were obtained by dissolving **1** in acetonitrile, cooling the solution slowly down to -40°C and keeping these conditions for two weeks.

Analysis of the system 1/PPh₃: Compound **1** (165 mg, 0.3 mmol, 1 eq.) and PPh₃ (85 mg, 0.3 mmol, 1 eq.) were mixed in a J. Young NMR tube and dissolved in d³-acetonitrile. The reaction mixture was characterized by NMR spectroscopy. Subsequently the reaction mixture was evacuated, exposed to hydrogen pressure of one bar, and was then again NMR spectroscopically analyzed.

In a second approach an identically prepared reaction mixture was stirred 20 days, NMR spectroscopically characterized, evacuated, and exposed to hydrogen pressure of one bar for 30 minutes and NMR spectroscopically analyzed. All four different solutions (before and after adding hydrogen) were NMR spectroscopically identical. ¹H NMR (400.17 MHz, CD₃CN): δ = 1.96 (quint., 1H, CHD₂CN), 5.48 (sept., 3H, B(Ohfip)₃), 7.38 (m, 15H, PPh₃). ¹⁹F NMR (376.54 MHz, CD₃CN): δ = -75.8 (d, 18F, B(Ohfip)₃). ¹¹B NMR (376.54 MHz, CD₃CN): δ = 17.3 (br, 1B, B(Ohfip)₃). ³¹P NMR (376.54 MHz, CD₃CN): δ = -5.4 (m, 1P, PPh₃).

Analysis of the system 1/PtBu₃: Compound **1** (165 mg, 0.3 mmol, 1 eq.) and PtBu₃ (63 mg, 0.3 mmol, 1 eq.) were mixed in a J. Young NMR tube and dissolved in d³-acetonitrile. The reaction mixture was characterized by NMR spectroscopy. Subsequently the reaction mixture was evacuated, exposed to hydrogen pressure of one bar, and was then again NMR spectroscopically analyzed. The two solutions (before and after adding hydrogen) were NMR spectroscopically identical. ¹H NMR

(400.17 MHz, CD₃CN): δ = 1.32 (d, 27H, PtBu₃), 1.96 (quint., 1H, CHD₂CN), 5.48 (sept., 3H, B(Ohfip)₃). ¹⁹F NMR (376.54 MHz, CD₃CN): δ = -75.8 (d, 18F, B(Ohfip)₃). ¹¹B NMR (376.54 MHz, CD₃CN): δ = 17.2 (br, 1B, B(Ohfip)₃). ³¹P NMR (376.54 MHz, CD₃CN): δ = 62 (m, 1P, PtBu₃).

Analysis of the system 1/PMePh₂: Compound **1** (131 mg, 0.25 mmol, 1 eq.) and PMePh₂ (50 mg, 0.25 mmol, 1 eq.) were mixed in a J. Young NMR tube and dissolved in d³-acetonitrile. The reaction mixture was characterized by NMR spectroscopy. Subsequently the reaction mixture was evacuated, exposed to hydrogen pressure of one bar, and was then again NMR spectroscopically analyzed. The two solutions (before and after adding hydrogen) were NMR spectroscopically identical. ¹H NMR (400.17 MHz, CD₃CN): δ = 1.64 (s, 3H, PMePh₂), 1.96 (quint., 1H, CHD₂CN), 5.48 (sept., 3H, B(Ohfip)₃), 7.38 (m, 6H, PMe(o/p)Ph₂), 7.45 (m, 4H PMe(m)Ph₂). ¹⁹F NMR (376.54 MHz, CD₃CN): δ = -75.8 (d, 18F, B(Ohfip)₃). ¹¹B NMR (376.54 MHz, CD₃CN): δ = 17.3 (br, 1B, B(Ohfip)₃). ³¹P NMR (376.54 MHz, CD₃CN): δ = 27 (br, 1P, PMePh₂).

Analysis of the system 1/NEt₃: Compound **1** (250 mg, 0.5 mmol, 1 eq.) and NEt₃ (50 mg, 0.5 mmol, 1 eq.) were mixed in a J. Young NMR tube. The reaction mixture turned immediately yellow. Afterwards the reaction mixture was dissolved in d³-acetonitrile and characterized by NMR spectroscopy. Subsequently the reaction mixture was evacuated, exposed to hydrogen pressure of one bar, and was then again NMR spectroscopically analyzed. The two solutions (before and after adding hydrogen) were NMR spectroscopically identical. ¹H NMR (400.17 MHz, CD₃CN): δ = 1.11 (t, 9H, N(CH₂CH₃)₃), 1.96 (quint., 1H, CHD₂CN), 2.76 (q, 6H, N(CH₂CH₃)₃), 4.74 (sept. 3H, B(Ohfip)₃ adduct), 5.38 (sept. 3H, [XB(Ohfip)₃]⁻). ¹⁹F NMR (376.54 MHz, CD₃CN): δ = -76.0 (d, 18F, B(Ohfip)₃ adduct), -75.4 (d, 18F, [XB(Ohfip)₃]⁻). ¹¹B NMR (376.54 MHz, CD₃CN): δ = 3.2 (br, 1B, [XB(Ohfip)₃]⁻), 16.2 (br, 1B, B(Ohfip)₃ adduct).

Analysis of the system 1/2,6-lutidine: Compound **1** (240 mg, 0.5 mmol, 1 eq.) and 2,6-lutidine (50 mg, 0.5 mmol, 1 eq.) were mixed in a J. Young NMR tube and dissolved in d³-acetonitrile. The reaction mixture was characterized by NMR spectroscopy. Subsequently the reaction mixture was evacuated, exposed to hydrogen pressure of one bar, and was then again NMR spectroscopically analyzed. The two solutions (before and after adding hydrogen) were NMR spectroscopically identical. ¹H NMR (400.17 MHz, CD₃CN): δ = 1.96 (quint., 1H, CHD₂CN), 2.47 (s, 6H,

N(C₆H₃(2,6-CH₃))), 5.47 (sept. 3H, B(Ohfip)₃), 7.00 and 7.52 (m, 3H, N(C₆H₃(2,6-CH₃))). ¹⁹F NMR (376.54 MHz, CD₃CN): δ = -76.0 (d, 18F, B(Ohfip)₃). ¹¹B NMR (376.54 MHz, CD₃CN): δ = 17.4 (br, 1B, B(Ohfip)₃).

Analysis of the system 1/NHPh₂: Compound **1** (150 mg, 0.3 mmol, 1 eq.) and NHPh₂ (50 mg, 0.3 mmol, 1 eq.) were mixed in a J. Young NMR tube and dissolved in d³-acetonitrile. The reaction mixture was characterized by NMR spectroscopy. Subsequently the reaction mixture was evacuated, exposed to hydrogen pressure of one bar, and was then again NMR spectroscopically analyzed. The two solutions (before and after adding hydrogen) were NMR spectroscopically identical. ¹H NMR (400.17 MHz, CD₃CN): δ = 1.96 (quint., 1H, CHD₂CN), 5.50 (sept. 3H, B(Ohfip)₃), 6.80 (s, 1H, NHPh₂), 6.94 (m, 2H, NH(*p*)Ph₂), 7.14 (m, 4H, NH(*m*)Ph₂), 7.23 (m, 4H, NH(*o*)Ph₂). ¹⁹F NMR (376.54 MHz, CD₃CN): δ = -75.9 (d, 18F, B(Ohfip)₃). ¹¹B NMR (376.54 MHz, CD₃CN): δ = 17.4 (br, 1B, B(Ohfip)₃).

Analysis of the system 1/1,3-dimethyl-4,5-diphenyl imidazole-2-ylidene: Compound **1** (110 mg, 0.2 mmol, 1 eq.) and 1,3-dimethyl-4,5-diphenyl imidazole-2-ylidene (45 mg, 0.2 mmol, 1 eq.) were mixed in a J. Young NMR tube and dissolved in d⁸-toluene. Subsequently the yellow reaction mixture was evacuated, exposed to hydrogen pressure of one bar, and NMR spectroscopically analyzed. ¹H NMR (400.17 MHz, d⁸-toluene): δ = 2.09 (m, 1H, C₆D₅CHD₂), 3.45 (s, 6H, 2xCH₃ of the NHC compound) 5.12 (sept. 3H, B(Ohfip)₃ adduct), 6.70 (m, 6H, *m/p* protons of the NHC compound), 6.90 (m, 4H, *o* protons of the NHC compound), 7.0 - 7.1 (m, aromatic proton of d⁸-toluene). ¹⁹F NMR (376.54 MHz, d⁸-toluene): δ = -73.6 (d, 18F, B(Ohfip)₃ adduct). ¹¹B NMR (376.54 MHz, CD₃CN): δ = 1.5 (br, 1B, B(Ohfip)₃ adduct).

Analysis of the system 1/1,3-bis(2,6-diisopropylphenyl)imidazol-2-yliden: Compound **1** (60 mg, 0.1 mmol, 1 eq.) and 1,3-bis(2,6-diisopropylphenyl)imidazol-2-yliden (45 mg, 0.1 mmol, 1 eq.) were mixed in a J. Young NMR tube and dissolved in toluene. The brown reaction mixture was characterized by NMR spectroscopy. Subsequently the reaction mixture was evacuated, exposed to hydrogen pressure of one bar, and was then again NMR spectroscopically analyzed. The two solutions (before and after adding hydrogen) were NMR spectroscopically identical. ¹¹B NMR (376.54 MHz, no lock in toluene): δ = 1.9 (br, 1B, B(Ohfip)₃ adduct).

Theoretical Methods: All geometries were optimized at the (RI-)BP86/SV(P) level^[3-6] using TURBOMOLE 6.4.^[7, 8] Vibrational frequencies were calculated with the AOFORCE module and all structures represented true minima without imaginary frequencies. Solvation enthalpies in dichloromethane, *ortho*-difluorobenzene and acetonitrile were calculated with the COSMO module^[9, 10] using the default options and standard optimized COSMO radii (single points on optimized structures). Permittivity values (CH₂Cl₂: ϵ_r = 8.93, *o*-difluorobenzene: ϵ_r = 14.3, H₃CCN: ϵ_r = 36.6) were taken from the literature.^[11] Highly correlated calculations were done according to the method of Klopper *et al.*^[12, 13] RI-MP2 structure re-optimizations were carried out with TURBOMOLE 6.4^[7, 8] and def2-QZVPP basis sets^[14] and corresponding RI-C auxiliary bases^[15] for all atoms. MP2 and ccSD(t) single point calculations with correlation-consistent basis sets were done with Gaussian 09.^[16] The reference values for the Lewis acidity scale were calculated with the G3 method.^[17]

Legend to the following tables and calculations herein.

BP86	BP86 density functional
h	Hartree, 1H = 2625.5 kJ mol ⁻¹
<i>E</i> _{vrt}	Sum of vibrational, rotational and translational energy including ZPE (= FreeH energy)
ZPE	Zero point vibrational energy
<i>S</i>	Entropy
<i>H</i>	Enthalpy
<i>G</i>	<i>Gibbs</i> Energy

Validation Study:

$$\Delta E_{\text{extrapol}} = \Delta E_{\text{CCSD(T)/AVDZ}} - \Delta E_{\text{MP2/AVDZ}} + \Delta E_{\text{MP2/AVQZ}}$$

S-Table 1: Overview of frozen core and basis sets for all used elements of the extrapolation calculations.

element	fc for MP2/def2-QZVPP	AVXZ (X = D, Q)	fc for AVXZ
H	0	aug-cc-pVXZ ^[18]	0
B	1	aug-cc-pVXZ ^[18]	1
C	1	aug-cc-pVXZ ^[18]	1
N	1	aug-cc-pVXZ ^[18]	1
O	1	aug-cc-pVXZ ^[18]	1
F	1	aug-cc-pVXZ ^[18]	1
Al	5	aug-cc-pV(X+d)Z ^[19]	5
P	5	aug-cc-pV(X+d)Z ^[19]	5
Cl	5	aug-cc-pV(X+d)Z ^[19]	5
Ga	14	aug-cc-pwCVXZ-PP ^{[a][20, 21]}	0
As	9	aug-cc-pwCVXZ-PP ^{[a][20, 21]}	0
Br	14	aug-cc-pVXZ-PP ^[22]	9
Sb	4	aug-cc-pwCVXZ-PP ^{[a][20, 21]}	0

[a] Constructed by combining cc-pWCVQZ-PP^[21] with aug-cc-pVQZ-PP Diffuse.^[20]

Thermal contributions to the enthalpy were calculated with BP86/def-TZVP at 1 bar, 298.15 K.

$$\Delta U^0 = \Delta E_{\text{extrapol}} + \Delta E_{\text{vrt}}$$

(ΔE_{vrt} = sum of translation, rotational, vibrational energy inclusive zero point vibrational energy)

$$\Delta H^0 = \Delta U^0 + RT$$

S-Table 2: Energetic data of the FLP screening. The thermal energy corrections are calculated at 298.15 K. NHC = 1,3-dimethyl-4,5-diphenyl imidazole-2-ylidene, IDipp = 1,3-bis(2,6-diisopropylphenyl)imidazol-2-yliden. Permittivity values are given in parenthesis.

Compound	(RI-) BP86/SV(P) energy [h]	EVRT [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]	Tot. En. OC corr. (8.93) [h]	$\Delta_{\text{Solv}}G^0$ (8.93) [kJ mol ⁻¹]	Tot. En. OC corr. (14.3) [h]	$\Delta_{\text{Solv}}G^0$ (14.3) [kJ mol ⁻¹]	Tot. En. OC corr. (36.64) [h]	$\Delta_{\text{Solv}}G^0$ (36.64) [kJ mol ⁻¹]
1	-2390.95955	496.66	0.87631	-6276989.1	-6277250.4	-2390.96505	-6.5	-2390.96545	-7.5	-2390.96589	-8.7
B(C ₆ F ₅) ₃	-2206.75293	471.63	0.82219	-5793377.8	-5793622.9	-2206.75759	-4.3	-2206.75793	-5.2	-2206.75829	-6.1
H ₂	-1.16996	31.70	0.13689	-3037.6	-3078.4	-1.17015	7.4	-1.17017	7.4	-1.17018	7.4
[HB(Ohfip) ₃] ⁻	-2391.59560	513.08	0.85226	-6278642.6	-6278896.7	-2391.65060	-136.4	-2391.65449	-146.6	-2391.65861	-157.5
[HB(C ₆ F ₅) ₃] ⁻	-2207.45157	492.68	0.83844	-5795191.0	-5795441.0	-2207.49784	-113.5	-2207.50108	-122.0	-2207.50452	-131.1
PPh ₃	-1035.73393	741.32	0.56281	-2718586.0	-2718753.8	-1035.74220	-13.7	-1035.74286	-15.5	-1035.74357	-17.3
[HPPH ₃] ⁺	-1036.11240	769.91	0.57343	-2719551.1	-2719722.0	-1036.16659	-134.3	-1036.17041	-144.4	-1036.17447	-155.0
PrBu ₃	-814.40529	983.86	0.53982	-2137242.9	-2137403.8	-814.40883	-1.3	-814.40912	-2.1	-814.40944	-2.9
[HPtBu ₃] ⁺	-814.80160	1013.94	0.54805	-2138253.3	-2138416.7	-814.85664	-136.5	-814.86045	-146.5	-814.86447	-157.1
NEt ₃	-292.17060	547.89	0.39098	-766546.5	-766663.0	-292.17248	3.0	-292.17262	2.7	-292.17277	2.3
[HNEt ₃] ⁺	-292.55037	588.17	0.39266	-767503.3	-767620.4	-292.61891	-172.0	-292.62368	-184.5	-292.62873	-197.8
2,6-lutidine	-326.68165	386.07	0.37027	-857317.4	-857427.8	-326.68679	-5.5	-326.68720	-6.6	-326.68765	-7.8
[2,6-lutidineH]	-327.06021	422.08	0.37479	-858275.3	-858387.0	-327.12863	-171.7	-327.13338	-184.2	-327.13841	-197.4
NHPh ₂	-518.28400	533.52	0.42554	-1360223.8	-1360350.7	-518.29259	-14.6	-518.29326	-16.4	-518.29399	-18.3
[HNHPh ₂] ⁺	-518.63119	569.39	0.43935	-1361099.5	-1361230.5	-518.70241	-179.0	-518.70757	-192.6	-518.71307	-207.0
NHC	-766.36360	780.61	0.54762	-2011312.2	-2011475.5	-766.37643	-25.7	-766.37747	-28.5	-766.37861	-31.4
[HNHC] ⁺	-766.80363	816.09	0.55535	-2012432.0	-2012597.6	-766.86254	-146.7	-766.86680	-157.9	-766.87135	-169.8
IDipp	-1159.13877	1532.87	0.79523	-3041795.1	-3042032.2	-1159.14887	-18.6	-1159.14973	-20.8	-1159.15066	-23.3
[HIDipp] ⁺	-1159.57973	1566.16	0.79153	-3042919.5	-3043155.5	-1159.62947	-122.6	-1159.63299	-131.9	-1159.63671	-141.7

S-Table 3: Part 1 of the energetic data of the validation study. The thermal energy corrections are calculated at 298.15 K.

Compound	CCSD(T)/AVDZ energy [h]	MP2/AVDZ energy [h]	MP2/AVQZ energy [h]	BP86/def-TZVP energy [h]	EVRT (BP86/def-TZVP) [kJ mol ⁻¹]
Cl ⁻	-459.74380	-459.72656	-459.80308	-460.32339	3.72
H ⁻	-0.52403	-0.51196	-0.51709	-0.51016	3.72
F ⁻	-99.66863	-99.66595	-99.77441	-99.87911	3.72
BF ₃	-323.92630	-323.90489	-324.27979	-324.70276	40.86
[BF ₃ Cl] ⁻	-783.73105	-783.69171	-784.13919	-785.08739	45.51
[BF ₃ H] ⁻	-324.57583	-324.54755	-324.92064	-325.35264	61.19
[BF ₃ F] ⁻	-423.72669	-423.69914	-424.18275	-424.72498	47.76
BCl ₃	-1403.92243	-1403.86501	-1404.12135	-1405.75626	31.04
[BCl ₃ Cl] ⁻	-1863.73645	-1863.66506	-1864.00194	-1866.15534	37.12
[BCl ₃ H] ⁻	-1404.60198	-1404.53974	-1404.80295	-1406.44347	54.70
[BCl ₃ F] ⁻	-1503.73570	-1503.67417	-1504.04666	-1505.80099	53.50

BBr ₃	-1271.76505	-1271.71898	-1271.95235	-7748.28799	28.48
[BBr ₃ Cl] ⁻	-1731.58766	-1731.52786	-1731.84258	-8208.69430	34.98
[BBr ₃ H] ⁻	-1272.45777	-1272.40631	-1272.65045	-7748.98759	52.47
[BBr ₃ F] ⁻	-1371.58573	-1371.53548	-1371.88830	-7848.34143	38.06
AlF ₃	-541.21627	-541.19893	-541.55605	-542.33712	31.10
[AlF ₃ Cl] ⁻	-1001.07365	-1001.03787	-1001.47532	-1002.78145	37.90
[AlF ₃ H] ⁻	-541.89719	-541.87139	-542.22845	-543.02669	47.83
[AlF ₃ F] ⁻	-641.06636	-641.04300	-641.51147	-642.40837	39.10
AlCl ₃	-1621.22805	-1621.17230	-1621.43538	-1623.44505	26.33
[AlCl ₃ Cl] ⁻	-2081.08910	-2081.01786	-2081.36279	-2083.89330	33.90
[AlCl ₃ H] ⁻	-1621.91982	-1621.85769	-1622.12563	-1624.14546	44.29
[AlCl ₃ F] ⁻	-1721.08473	-1721.02497	-1721.40059	-1723.52361	35.23

S-Table 4:: Part 2 of the energetic data of the validation study. The thermal energy corrections are calculated at 298.15 K.

Compound	CCSD(T)/AVDZ energy [h]	MP2/AVDZ energy [h]	MP2/AVQZ energy [h]	BP86/def-TZVP energy [h]	Evrt (BP86/def-TZVP) [kJ mol ⁻¹]
AlBr ₃	-1489.08371	-1489.03864	-1489.29605	-7965.99036	24.82
[AlBr ₃ Cl] ⁻	-1948.94503	-1948.88480	-1949.22499	-8426.43807	32.48
[AlBr ₃ H] ⁻	-1489.77765	-1489.72620	-1489.98537	-7966.69272	43.01
[AlBr ₃ F] ⁻	-1588.94082	-1588.89187	-1589.26271	-8066.06903	33.88
GaF ₃	-558.44397	-558.47027	-558.78456	-2224.91244	28.44
[GaF ₃ Cl] ⁻	-1018.31462	-1018.32170	-1018.70754	-2225.62007	35.47
[GaF ₃ H] ⁻	-559.14399	-559.16445	-559.48106	-2324.97033	45.77
[GaF ₃ F] ⁻	-658.28543	-658.30518	-658.72602	-2324.97033	36.47
GaCl ₃	-1638.53793	-1638.52675	-1638.73494	-3306.07616	24.87
[GaCl ₃ Cl] ⁻	-2098.39939	-2098.37088	-2098.65226	-3766.51500	32.36
[GaCl ₃ H] ⁻	-1639.23295	-1639.21693	-1639.43356	-3306.78232	43.18
[GaCl ₃ F] ⁻	-1738.37154	-1738.35446	-1738.67054	-3406.13003	33.41
GaBr ₃	-1506.00214	-1505.98457	-1506.23389	-9648.63444	23.68
[GaBr ₃ Cl] ⁻	-1965.86085	-1965.82640	-1966.15032	-10109.07026	31.31
[GaBr ₃ H] ⁻	-1506.69587	-1506.67316	-1506.93225	-9649.33927	42.11
[GaBr ₃ F] ⁻	-1605.83307	-1605.80988	-1606.16841	-9748.68578	32.36
PF ₅	-839.33115	-839.29605	-839.93790	-840.96036	55.75
[PF ₅ Cl] ⁻	-1299.14595	-1299.09337	-1299.80322	-1301.35977	60.99
[PF ₅ H] ⁻	-840.02963	-839.98853	-840.61981	-841.66526	79.23
[PF ₅ F] ⁻	-939.15165	-939.11028	-939.85401	-941.00075	63.25

S-Table 5: Part 3 of the energetic data of the validation study. The thermal energy corrections are calculated at 298.15 K.

Compound	CCSD(T)/AVDZ energy [h]	MP2/AVDZ energy [h]	MP2/AVQZ energy [h]	BP86/def-TZVP energy [h]	EVRT (BP86/def-TZVP) [kJ mol ⁻¹]
PCl ₅	-2639.30190	-2639.21138	-2639.67582	-2642.74701	42.67
[PCl ₅ Cl] ⁻	-3099.11408	-3099.01083	-3099.55194	-3103.14468	49.53
[PCl ₅ H] ⁻	-2640.01841	-2639.92389	-2640.38628	-2643.47134	66.97
[PCl ₅ F] ⁻	-2739.11992	-2739.02599	-2739.60030	-2742.78836	51.66
AsF ₅	-829.99443	-829.96364	-830.51661	-2735.65774	49.49
[AsF ₅ Cl] ⁻	-1289.82762	-1289.77642	-1290.40684	-3196.08450	55.69
[AsF ₅ H] ⁻	-830.70791	-830.67175	-831.22162	-2736.38634	70.83
[AsF ₅ F] ⁻	-929.83166	-929.79451	-930.45322	-2835.71345	57.30
B(OH) ₃	-251.94592	-251.91094	-252.20599	-252.59931	135.64
[B(OH) ₃ H] ⁻	-252.53693	-252.49575	-252.79510	-253.19643	152.71
[B(OH) ₃ F] ⁻	-351.68837	-351.64777	-352.05589	-352.56773	140.10
SbF ₅	-738.69619	-738.67462	-739.20825	-504.96124	46.33
[SbF ₅ Cl] ⁻	-1198.57085	-1198.53137	-1199.13783	-965.41970	53.39
[SbF ₅ H] ⁻	-739.42544	-739.39885	-739.93919	-505.71266	65.59
[SbF ₅ F] ⁻	-838.55453	-838.52653	-839.16811	-605.04171	54.62
[SbF ₄] ⁻	-639.15362	-639.14524	-639.57548	-405.23423	34.55
HF	-100.26360	-100.25575	-100.36976	-100.49251	29.93

S-Table 6: Energetic data of the reference systems. The thermal energy corrections are calculated at 298.15 K.

Compound	(RI-)BP86/SV(P) energy [h]	EVRT [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]	G3 Enthalpy H [h]
MeSi ₃ ⁺	-408.80757	297.89	0.36	-1073028.00	-1073136.05	-408.67945
MeSi ₃ Cl	-869.25828	309.46	0.36	-2281934.36	-2282042.36	-869.08993
MeSi ₃ H	-409.68913	322.45	0.33	-1075317.98	-1075416.84	-409.56127
MeSi ₃ F	-508.92757	311.07	0.35	-1335880.88	-1335985.90	-508.85133
MeSi ₃ Me	-448.98131	399.76	0.36	-1178402.69	-1178508.71	-448.84834
Cl ⁻						-460.12124
H ⁻						-0.51636
F ⁻						-99.80683
Me ⁻						-39.78805

S-Table 7: Part 1 of the energetic data to determine the affinity values. The thermal energy corrections are calculated at 298.15 K. Thermal-energy-corrected enthalpies (*H*) were used to calculate the affinity values.

Compound	(RI-)BP86/SV(P) energy [h]	EVRT [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]
BF ₃	-324.31769	41.36	0.26	-851455.49	-851531.69
[BF ₃ Cl] ⁻	-784.53230	46.60	0.30	-2059748.31	-2059836.54
[BF ₃ H] ⁻	-324.94632	62.26	0.27	-853085.06	-853164.20
[BF ₃ F] ⁻	-424.20099	49.21	0.27	-1113692.26	-1113772.75
[BF ₃ Me] ⁻	-364.24312	136.67	0.30	-956184.81	-956273.81
BCl ₃	-1405.27457	31.32	0.29	-3689528.65	-3689615.38
[BCl ₃ Cl] ⁻	-1865.50372	37.75	0.32	-4897858.45	-4897954.10
[BCl ₃ H] ⁻	-1405.93901	54.79	0.30	-3691249.66	-3691340.48
[BCl ₃ F] ⁻	-1505.18222	40.74	0.32	-3951827.76	-3951923.42
[BCl ₃ Me] ⁻	-1445.23236	129.98	0.33	-3794339.55	-3794439.29
BBr ₃	-7747.33631	28.68	0.33	-20340677.81	-20340774.90
[BBr ₃ Cl] ⁻	-8207.57694	35.40	0.37	-21549037.46	-21549147.68
[BBr ₃ H] ⁻	-7748.01880	52.50	0.34	-20342445.85	-20342547.76
[BBr ₃ F] ⁻	-8064.92779	34.35	0.39	-21174511.73	-21174626.78
[BBr ₃ Me] ⁻	-8004.96231	121.67	0.41	-21016984.43	-21017105.99
Bi ₃	-59.27797	26.95	0.35	-155605.47	-155710.23
[Bi ₃ Cl] ⁻	-519.53720	34.45	0.40	-1364013.19	-1364131.35
[Bi ₃ H] ⁻	-59.98640	51.22	0.37	-157441.19	-157550.69
[Bi ₃ F] ⁻	-159.21958	37.55	0.39	-417992.56	-418107.67
[Bi ₃ Me] ⁻	-99.27605	127.33	0.40	-260520.46	-260638.71
AlF ₃	-541.88983	31.84	0.28	-1422702.84	-1422786.10
[AlF ₃ Cl] ⁻	-1002.16640	39.20	0.32	-2631156.24	-2631251.75

S-Table 8: Part 2 of the energetic data to determine the affinity values. The thermal energy corrections are calculated at 298.15 K. Thermal-energy-corrected enthalpies (*H*) were used to calculate the affinity values.

Compound	(RI-)BP86/SV(P) energy [h]	EVRT [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]
[AlF ₃ H] ⁻	-542.56444	49.17	0.29	-1424456.72	-1424542.53
[AlF ₃ F] ⁻	-641.82254	40.73	0.30	-1685068.30	-1685156.52
[AlF ₃ Me] ⁻	-581.85677	126.79	0.33	-1527541.49	-1527640.78
AlCl ₃	-1622.90465	26.53	0.31	-4260923.39	-4261017.25
[AlCl ₃ Cl] ⁻	-2083.18568	34.24	0.35	-5469388.11	-5469491.74
[AlCl ₃ H] ⁻	-1623.58970	44.67	0.33	-4262703.86	-4262801.44
[AlCl ₃ F] ⁻	-1722.84767	35.87	0.35	-4523315.44	-4523418.76
[AlCl ₃ Me] ⁻	-1662.88217	122.80	0.37	-4365788.48	-4365898.83
AlBr ₃	-7964.98011	24.94	0.35	-20912107.52	-20912211.62

[AlBr ₃ Cl] ⁻	-8425.26423	32.77	0.41	-22120580.25	-22120701.18
[AlBr ₃ H] ⁻	-7965.67055	43.18	0.37	-20913902.03	-20914011.23
[AlBr ₃ F] ⁻	-8004.96231	34.35	0.39	-21174511.73	-21174626.78
[AlBr ₃ Me] ⁻	-8064.92779	121.67	0.41	-21016984.43	-21017105.99
AlI ₃	-276.93301	24.13	0.38	-727063.77	-727175.64
[AlI ₃ Cl] ⁻	-737.22532	32.15	0.42	-1935557.82	-1935683.90
[AlI ₃ H] ⁻	-277.63619	42.44	0.39	-728891.68	-729008.42
[AlI ₃ F] ⁻	-376.89045	33.87	0.41	-989493.31	-989615.57
[AlI ₃ Me] ⁻	-316.92785	121.31	0.43	-831973.45	-832102.32
GaF ₃	-2224.30029	29.01	0.29	-5839891.16	-5839978.55
[GaF ₃ Cl] ⁻	-2684.57647	36.21	0.34	-7048343.68	-7048444.36
[GaF ₃ H] ⁻	-2224.98949	46.42	0.30	-5841683.27	-5841773.85
[GaF ₃ F] ⁻	-2324.21882	37.40	0.31	-6102219.87	-6102313.54

S-Table 9: Part 3 of the energetic data to determine the affinity values. The thermal energy corrections are calculated at 298.15 K. Thermal-energy-corrected enthalpies (*H*) were used to calculate the affinity values.

Compound	(RI-)BP86/SV(P) energy [h]	E _{vrt} [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]
[GaF ₃ Me] ⁻	-2264.27778	125.00	0.35	-5944756.47	-5944861.69
GaCl ₃	-3305.36839	24.94	0.33	-8678250.35	-8678348.11
[GaCl ₃ Cl] ⁻	-3765.64032	32.51	0.36	-9886691.33	-9886799.41
[GaCl ₃ H] ⁻	-3306.05889	43.35	0.34	-8680044.84	-8680146.49
[GaCl ₃ F] ⁻	-3405.28715	33.76	0.36	-8940579.23	-8940687.11
[GaF ₃ Me] ⁻	-3345.34742	122.10	0.39	-8783118.53	-8783235.71
GaBr ₃	-9647.45623	23.70	0.36	-25329466.62	-25329574.65
[GaBr ₃ Cl] ⁻	-10107.72841	31.36	0.41	-26537908.17	-26538031.29
[GaBr ₃ H] ⁻	-9648.14898	42.11	0.38	-25331267.04	-25331380.42
[GaBr ₃ F] ⁻	-9747.37651	32.60	0.40	-25591799.42	-25591918.95
[GaBr ₃ Me] ⁻	-9687.43727	121.25	0.43	-25434339.69	-25434469.31
Gal ₃	-1959.42418	23.20	0.39	-5144462.09	-5144577.66
[Gal ₃ Cl] ⁻	-2419.70219	31.05	0.44	-6352918.77	-6353049.13
[Gal ₃ H] ⁻	-1960.12637	41.65	0.40	-5146287.25	-5146407.92
[Gal ₃ F] ⁻	-2059.35144	32.29	0.43	-5406813.02	-5406939.94
[Gal ₃ Me] ⁻	-1999.41466	121.12	0.45	-5249359.59	-5249492.62
PF ₅	-840.24920	57.03	0.31	-2206023.18	-2206115.23
[PF ₅ Cl] ⁻	-1300.47676	63.16	0.33	-3414349.10	-3414448.92
[PF ₅ H] ⁻	-840.92368	80.76	0.31	-2207770.29	-2207862.21
[PF ₅ F] ⁻	-940.15393	65.88	0.30	-2468315.19	-2468405.78
[PF ₅ Me] ⁻	-880.21459	155.35	0.36	-2310854.38	-2310961.56
PCl ₅	-2641.86516	43.04	0.38	-6936197.89	-6936309.79

S-Table 10:Part 4 of the energetic data to determine the affinity values. The thermal energy corrections are calculated at 298.15 K. Thermal-energy-corrected enthalpies (*H*) were used to calculate the affinity values.

Compound	(RI-)BP86/SV(P) energy [h]	EVRT [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]
[PCl ₅ Cl] ⁻	-3102.09251	49.86	0.42	-8144522.57	-8144648.16
[PCl ₅ H] ⁻	-2642.56490	66.94	0.40	-6938011.16	-6938129.56
[PCl ₅ F] ⁻	-2741.76810	52.36	0.41	-7198484.71	-7198606.02
[PCl ₅ Me] ⁻	-2681.85046	143.36	0.44	-7041079.36	-7041210.43
AsF ₅	-2734.77740	50.42	0.33	-7180132.50	-7180230.72
[AsF ₅ Cl] ⁻	-3195.03263	57.06	0.36	-8388530.58	-8388637.57
[AsF ₅ H] ⁻	-2735.47713	72.02	0.33	-7181948.05	-7182046.65
[AsF ₅ F] ⁻	-2834.69432	58.86	0.33	-7442456.95	-7442555.10
[AsF ₅ Me] ⁻	-2774.76975	148.93	0.39	-7285034.32	-7285149.74
SbF ₅	-504.34073	47.06	0.35	-1324102.08	-1324207.90
[SbF ₅ Cl] ⁻	-964.63043	54.24	0.39	-2532590.12	-2532705.74
[SbF ₅ H] ⁻	-505.06879	66.27	0.36	-1325994.40	-1326100.42
[SbF ₅ F] ⁻	-604.28148	55.55	0.36	-1586489.03	-1586596.20
[SbF ₅ Me] ⁻	-544.36348	145.04	0.42	-1429084.23	-1429209.53
[SbF ₄] ⁻	-404.71210	35.45	0.35	-1062537.73	-1062642.09
HF	-100.34485	28.63	0.17	-263425.30	-263477.25
MeF	-139.62734	107.38	0.22	-366483.12	-366549.63
B(OH) ₃	-252.27649	133.32	0.28	-662218.64	-662475.47
[B(OH) ₃ H] ⁻	-252.85454	150.85	0.29	-663718.80	-663718.80
[B(OH) ₃ F] ⁻	-352.10612	138.48	0.31	-924317.18	-924317.18
[B(OH) ₃ Me] ⁻	-292.14938	225.69	0.32	-766812.95	-766897.76
B(Ohfip) ₃	-2390.95983	496.86	0.88	-6276989.59	-6277251.89

S-Table 11:Part 5 of the energetic data to determine the affinity values. The thermal energy corrections are calculated at 298.15 K. Thermal-energy-corrected enthalpies (*H*) were used to calculate the affinity values.

Compound	(RI-)BP86/SV(P) energy [h]	EVRT [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]
[B(Ohfip) ₃ Cl] ⁻	-2851.17065	496.54	0.87	-7485278.03	-7485537.36
[B(Ohfip) ₃ H] ⁻	-2391.60549	513.18	0.87	-6278668.47	-6278927.43
[B(Ohfip) ₃ F] ⁻	-2490.85720	500.15	0.89	-6539267.86	-6539531.90
[B(Ohfip) ₃ Me] ⁻	-2430.89606	587.97	0.88	-6381751.46	-6382013.04
Al(OC(CF ₃) ₃) ₃	-3618.91753	540.66	1.06	-9500961.01	-9501277.13
[Al(OC(CF ₃) ₃) ₃ Cl] ⁻	-4079.21138	548.19	1.13	-10709459.60	-10709797.32
[Al(OC(CF ₃) ₃) ₃ H] ⁻	-3619.61749	558.40	1.11	-9502781.03	-9503112.16
[Al(OC(CF ₃) ₃) ₃ F] ⁻	-3718.87763	549.80	1.12	-9763398.12	-9763732.36
[Al(OC(CF ₃) ₃) ₃ Me] ⁻	-3658.91005	636.25	1.14	-9605866.20	-9606207.05

B(OTeF ₅) ₃	-1771.19399	206.58	0.78	-4650078.46	-4650312.34
[B(OTeF ₅) ₃ Cl] ⁻	-2231.47676	211.90	0.85	-5858550.17	-5858803.31
[B(OTeF ₅) ₃ H] ⁻	-1771.92090	228.68	0.83	-4651964.89	-4652213.21
[B(OTeF ₅) ₃ F] ⁻	-1871.15773	215.61	0.83	-4912525.24	-4912772.12
[B(OTeF ₅) ₃ Me] ⁻	-1811.21457	304.14	0.85	-4755055.33	-4755307.57
As(OTeF ₅) ₃	-5146.23685	329.24	1.24	-13511164.60	-13511534.16
[As(OTeF ₅) ₃ Cl] ⁻	-5606.54953	335.27	1.24	-14719714.10	-14720083.44
[As(OTeF ₅) ₃ H] ⁻	-5147.02237	350.71	1.22	-13513205.50	-13513570.11
[As(OTeF ₅) ₃ F] ⁻	-5246.21827	337.96	1.22	-13773658.10	-13774022.65
[As(OTeF ₅) ₃ Me] ⁻	-5186.31577	428.80	1.25	-13616292.65	-13616665.75
Sb(OTeF ₅) ₃	-2915.82616	326.64	1.27	-7655201.63	-7655580.10
[Sb(OTeF ₅) ₃ Cl] ⁻	-3376.16324	334.10	1.29	-8863813.77	-8864197.49
[Sb(OTeF ₅) ₃ H] ⁻	-2916.62459	346.36	1.26	-7657278.19	-7657654.19

S-Table 12:Part 6 of the energetic data to determine the affinity values. The thermal energy corrections are calculated at 298.15 K. Thermal-energy-corrected enthalpies (*H*) were used to calculate the affinity values.

Compound	(RI-)BP86/SV(P) energy [h]	E _{vrt} [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]
[Sb(OTeF ₅) ₃ F] ⁻	-3015.81754	335.75	1.29	-7917720.88	-7918106.00
[Sb(OTeF ₅) ₃ Me] ⁻	-2955.92663	426.83	1.31	-7760385.61	-7760777.44
B(CF ₃) ₃	-1037.00986	152.98	0.50	-2722524.30	-2722672.16
[B(CF ₃) ₃ Cl] ⁻	-1497.30582	160.10	0.50	-3931028.83	-3931178.10
[B(CF ₃) ₃ H] ⁻	-1037.74761	176.43	0.46	-2724437.81	-2724575.21
[B(CF ₃) ₃ F] ⁻	-1136.97516	162.34	0.48	-2984974.84	-2985119.13
[B(CF ₃) ₃ Me] ⁻	-1077.03536	251.85	0.49	-2827512.78	-2827659.65
B(C ₆ F ₅) ₃	-2206.75271	471.95	0.81	-5793376.89	-5793618.43
[B(C ₆ F ₅) ₃ Cl] ⁻	-2667.00121	476.04	0.85	-7001759.82	-7002011.93
[B(C ₆ F ₅) ₃ H] ⁻	-2207.45155	492.67	0.84	-5795190.96	-5795442.86
[B(C ₆ F ₅) ₃ F] ⁻	-2306.67696	477.88	0.85	-6055723.05	-6055975.83
[B(C ₆ F ₅) ₃ Me] ⁻	-2246.72740	568.12	0.85	-5898234.66	-5898489.38
Al(C ₆ F ₅) ₃	-2424.31626	462.17	0.88	-6364601.94	-6364863.97
[Al(C ₆ F ₅) ₃ Cl] ⁻	-2884.60755	466.90	0.91	-7573096.59	-7573368.66
[Al(C ₆ F ₅) ₃ H] ⁻	-2425.01252	477.22	0.89	-6366414.92	-6366679.22
[Al(C ₆ F ₅) ₃ F] ⁻	-2524.27281	468.18	0.90	-6627032.84	-6627300.52
[Al(C ₆ F ₅) ₃ Me] ⁻	-2464.30313	555.74	0.93	-6469494.28	-6469772.08
Ga(C ₆ F ₅) ₃	-4106.80716	461.49	0.89	-10781999.30	-10782265.18
[Ga(C ₆ F ₅) ₃ Cl] ⁻	-4567.08293	466.51	0.91	-11990452.92	-11990724.71
[Ga(C ₆ F ₅) ₃ H] ⁻	-4107.50218	476.60	0.89	-10783808.97	-10784075.12
[Ga(C ₆ F ₅) ₃ F] ⁻	-4206.73211	467.52	0.91	-11044347.22	-11044617.21
[Ga(C ₆ F ₅) ₃ Me] ⁻	-4146.78826	555.62	0.92	-10886875.95	-10887150.01

S-Table 13: Part 7 of the energetic data to determine the affinity values. The thermal energy corrections are calculated at 298.15 K. Thermal-energy-corrected enthalpies (H) were used to calculate the affinity values.

Compound	(RI-)BP86/SV(P) energy [h]	EVRT [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]
B(C ₁₂ F ₉) ₃	-4089.39616	909.52	1.34	-10735838.51	-10736237.10
[B(C ₁₂ F ₉) ₃ Cl] ⁻	-4549.62632	911.86	1.38	-11944175.06	-11944585.04
[B(C ₁₂ F ₉) ₃ H] ⁻	-4090.08244	929.20	1.34	-10737620.66	-10738021.05
[B(C ₁₂ F ₉) ₃ F] ⁻	-4189.31221	914.55	1.37	-10998164.07	-10998571.88
[B(C ₁₂ F ₉) ₃ Me] ⁻	-4129.34508	1005.86	1.36	-10840628.46	-10841033.83
B(C ₆ H ₃ -3,5-(CF ₃) ₂) ₃	-2740.16520	879.48	1.05	-7193449.18	-7193762.90
[B(C ₆ H ₃ -3,5-(CF ₃) ₂) ₃ Cl] ⁻	-3200.43072	883.35	1.09	-8401877.03	-8402203.18
[B(C ₆ H ₃ -3,5-(CF ₃) ₂) ₃ H] ⁻	-2740.86442	898.74	1.06	-7195265.73	-7195582.83
[B(C ₆ H ₃ -3,5-(CF ₃) ₂) ₃ F] ⁻	-2840.10065	884.94	1.09	-7455825.25	-7456150.07
[B(C ₆ H ₃ -3,5-(CF ₃) ₂) ₃ Me] ⁻	-2780.14741	974.12	1.09	-7298328.22	-7298652.37
B(C ₁₀ F ₇) ₃	-3262.34797	741.74	1.10	-8564583.00	-8564909.79
[B(C ₁₀ F ₇) ₃ Cl] ⁻	-3722.60767	745.92	1.12	-9772995.25	-9773329.56
[B(C ₁₀ F ₇) ₃ H] ⁻	-3263.06000	762.19	1.11	-8566432.00	-8566764.12
[B(C ₁₀ F ₇) ₃ F] ⁻	-3362.28421	747.82	1.12	-8826960.51	-8827294.29
[B(C ₁₀ F ₇) ₃ Me] ⁻	-3302.33656	838.17	1.12	-8669477.01	-8669810.85
F ₄ C ₆ (1,2-(B(C ₆ F ₅) ₂) ₂)	-3586.44641	784.90	1.20	-9415463.52	-9415820.57
[F ₄ C ₆ (1,2-(B(C ₆ F ₅) ₂) ₂)Cl] ⁻	-4046.72254	789.20	1.23	-10623918.81	-10624286.18
[F ₄ C ₆ (1,2-(B(C ₆ F ₅) ₂) ₂)H] ⁻	-3587.16490	805.00	1.21	-9417329.83	-9417689.56
[F ₄ C ₆ (1,2-(B(C ₆ F ₅) ₂) ₂)F] ⁻	-3686.39808	791.83	1.23	-9677880.70	-9678247.15
[F ₄ C ₆ (1,2-(B(C ₆ F ₅) ₂) ₂)Me] ⁻	-3626.42419	879.05	1.22	-9520331.44	-9520695.13
B ₂ (C ₆ F ₅) ₂ (C ₆ F ₄) ₂	-2759.39574	620.04	0.99	-7244198.58	-7244494.68
[B ₂ (C ₆ F ₅) ₂ (C ₆ F ₄) ₂ Cl] ⁻	-3219.65734	623.98	1.02	-8452616.07	-8452920.01

S-Table 14: Part 8 of the energetic data to determine the affinity values. The thermal energy corrections are calculated at 298.15 K. Thermal-energy-corrected enthalpies (H) were used to calculate the affinity values.

Compound	(RI-)BP86/SV(P) energy [h]	EVRT [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]
[B ₂ (C ₆ F ₅) ₂ (C ₆ F ₄) ₂ H] ⁻	-2760.10557	639.65	1.00	-7246042.64	-7246339.39
[B ₂ (C ₆ F ₅) ₂ (C ₆ F ₄) ₂ F] ⁻	-2859.32945	625.80	1.01	-7506569.78	-7506872.16
[B ₂ (C ₆ F ₅) ₂ (C ₆ F ₄) ₂ Me] ⁻	-2799.38597	716.35	1.01	-7349097.03	-7349397.63
PF ₂ (C ₂ F ₅) ₃	-2265.88419	287.78	0.70	-5948811.34	-5949021.39
[PF ₂ (C ₂ F ₅) ₃ Cl] ⁻	-2726.10290	292.57	0.69	-7157115.37	-7157322.52
[PF ₂ (C ₂ F ₅) ₃ H] ⁻	-2266.56226	309.87	0.68	-5950569.54	-5950773.36
[PF ₂ (C ₂ F ₅) ₃ F] ⁻	-2365.78476	294.99	0.69	-6211094.08	-6211299.02
[PF ₂ (C ₂ F ₅) ₃ Me] ⁻	-2305.83768	385.36	0.71	-6053612.04	-6053823.61
B(CN) ₃	-303.16014	92.44	0.35	-795855.06	-795959.01

[B(CN) ₃ Cl] ⁻	-763.45377	100.38	0.38	-2004352.65	-2004465.61
[B(CN) ₃ H] ⁻	-303.89945	116.56	0.35	-797772.02	-797875.46
[B(CN) ₃ F] ⁻	-403.12354	102.33	0.37	-1058300.09	-1058410.04
[B(CN) ₃ Me] ⁻	-343.18480	192.85	0.38	-900839.80	-900953.04
B ₁₁ Cl ₁₁ CH ₂ TMS	-5781.55702	534.11	0.81	-15178999.18	-15179241.68
[B ₁₁ Cl ₁₁ CH ₂ TMSCl] ⁻	-6241.86871	543.36	0.85	-16387542.89	-16387796.79
[B ₁₁ Cl ₁₁ CH ₂ TMSH] ⁻	-5782.29716	556.44	0.82	-15180920.08	-15181165.16
[B ₁₁ Cl ₁₁ CH ₂ TMSF] ⁻	-5881.53834	544.90	0.84	-15441490.36	-15441744.27
[B ₁₁ Cl ₁₁ CH ₂ TMSMe] ⁻	-5821.58782	633.59	0.86	-15284000.97	-15284257.79
TMS-F-Al(OC(CF ₃) ₃) ₃	-4127.88010	861.40	1.28	-10836926.59	-10837308.52
[FAl(OC(CF ₃) ₃) ₃] ⁻	-3718.87761	549.78	1.13	-9763398.10	-9763733.57
TMSCl	-869.25828	309.46	0.36	-2281934.36	-2282042.36
TMSH	-409.68913	322.45	0.33	-1075317.98	-1075416.84

S-Table 15: Part 9 of the energetic data to determine the affinity values. The thermal energy corrections are calculated at 298.15 K. Thermal-energy-corrected enthalpies (*H*) were used to calculate the affinity values.

Compound	(RI-)BP86/SV(P) energy [h]	E _{vrt} [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]
TMSF	-508.92757	311.07	0.35	-1335880.88	-1335985.90
TMSMe	-448.98131	399.76	0.36	-1178402.69	-1178508.71
[ClAl(OC(CF ₃) ₃) ₃] ⁻	-4079.21128	547.89	1.14	-10709459.64	-10709798.23
[HAl(OC(CF ₃) ₃) ₃] ⁻	-3619.61838	558.38	1.11	-9502783.39	-9503114.66
[MeAl(OC(CF ₃) ₃) ₃] ⁻	-3658.91052	636.28	1.15	-9605867.39	-9606210.06

S-Table 16: Part 1 of the energetic data to determine the decomposition values of WCAs. The thermal energy corrections are calculated at 298.15 K. The energetic data of [BX₄]⁻, [AlX₄]⁻, GaX₄⁻, [AsF₆]⁻ and [SbF₆]⁻ (X = F, Cl, Br, I) and all underlying Lewis acids were already shown in the tables above.

Compound	(RI-)BP86/SV(P) energy [h]	E _{vrt} [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]
H ⁺	0	6.20	0.11	8.68	-23.78
Cu ⁺	-1640.21528	6.20	0.16	-4306392.95	-4306440.82
[B(Ohfp) ₄] ⁻	-3179.74703	650.70	1.07	-8347804.45	-8348124.72
[Al(OC(CF ₃) ₃) ₄] ⁻	-4744.54973	719.65	1.37	-12456140.63	-12456548.10
[B(OTeF ₅) ₄] ⁻	-2353.44290	270.92	0.97	-6178714.47	-6179002.48
[As(OTeF ₅) ₆] ⁻	-5728.50557	393.29	1.40	-15039852.88	-15040269.02
[Sb(OTeF ₅) ₆] ⁻	-3498.11286	391.67	1.45	-9183936.14	-9184368.77
[B(CN) ₄] ⁻	-396.10083	121.24	0.37	-1039842.97	-1039953.51
[B(CF ₃) ₄] ⁻	-1374.57309	200.53	0.54	-3608752.38	-3608913.48

S-Table 17: Part 2 of the energetic data to determine the decomposition values of WCAs. The thermal energy corrections are calculated at 298.15 K.

Compound	(RI-)BP86/SV(P) energy [h]	E _{vrt} [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G [kJ mol ⁻¹]
[B(C ₆ F ₅) ₄] ⁻	-2934.16744	622.30	0.99	-7703061.17	-7703356.33
[Al(C ₆ F ₅) ₄] ⁻	-3151.74555	612.02	1.06	-8274324.95	-8274641.47
[Ga(C ₆ F ₅) ₄] ⁻	-4834.22867	611.18	1.07	-12691702.06	-12692020.36
[B(C ₁₂ F ₉) ₄] ⁻	-5444.37581	1206.18	1.69	-14293054.48	-14293558.79
[B(C ₆ H ₃ (CF ₃) ₂) ₄] ⁻	-3645.38949	1164.52	1.33	-9569839.56	-9570236.12
[B(C ₁₀ F ₇) ₄] ⁻	-4341.64150	981.78	1.36	-11398038.93	-11398444.87
[F ₄ C ₆ (1,2- (B(C ₆ F ₅) ₂) ₂)(C ₆ F ₅) ₂)] ⁻	-4313.83839	934.56	1.37	-11325088.80	-11325497.31
[B ₂ (C ₆ F ₅) ₃ (C ₆ F ₄) ₂] ⁻	-3486.81296	770.04	1.16	-9153889.78	-9154236.66
HF	-100.34485	28.62	0.17	-263425.31	-263477.26
HCl	-460.69877	22.83	0.19	-1209543.93	-1209599.79
HBr	-2574.72899	21.24	0.20	-6759953.00	-6760012.37
HI	-12.05201	19.44	0.21	-31620.75	-31682.48
HOHfip	-789.24620	183.27	0.40	-2071988.04	-2072108.29
HOC(CF ₃) ₃	-1126.04299	202.27	0.47	-2956232.37	-2956372.04
HOTeF ₅	-582.66184	86.41	0.39	-1529695.59	-1529811.43
HCN	-93.35344	48.13	0.20	-245049.78	-245110.04
HCF ₃	-337.99423	74.06	0.26	-887330.69	-887408.36
HC ₆ F ₅	-727.89270	176.03	0.38	-1910911.04	-1911025.17
HC ₁₂ F ₉	-1355.44401	322.06	0.57	-3558407.25	-3558576.64
HC ₆ (H) ₃ (CF ₃) ₂	-905.70077	312.23	0.46	-2377611.72	-2377747.49
HC ₁₀ F ₇	-1079.75991	266.17	0.48	-2834651.80	-2834795.35

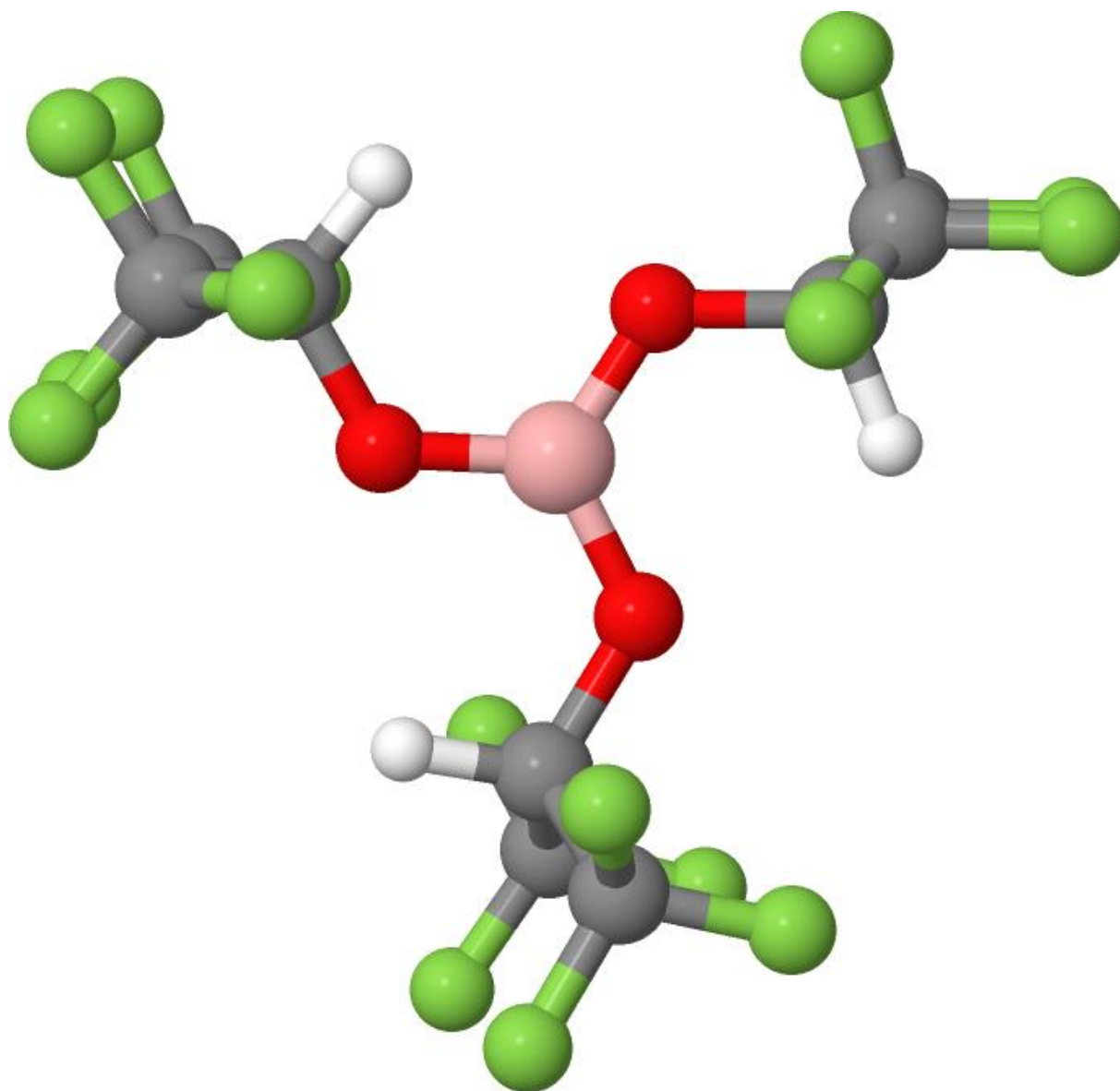
S-Table 18: Part 3 of the energetic data to determine the decomposition values of WCAs. The thermal energy corrections are calculated at 298.15 K.

Compound	(RI-)BP86/SV(P) energy [h]	E _{vrt} [kJ mol ⁻¹]	Entropy S [kJ mol ⁻¹]	Enthalpy H [kJ mol ⁻¹]	Gibbs Energy G[kJ mol ⁻¹]
CuF	-1740.29714	10.31	0.23	-4569154.76	-4569222.28
CuCl	-2100.67728	9.45	0.24	-5515337.28	-5515408.07
CuBr	-4214.71358	9.08	0.25	-11065761.08	-11065835.30
CuI	-1652.04406	8.98	0.26	-4337446.73	-4337523.14
CuOhfip	-2429.19188	158.60	0.45	-6377706.49	-6377839.64
CuOC(CF ₃) ₃	-2765.99722	178.06	0.51	-7261972.82	-7262125.20
CuOTeF ₅	-2222.64055	64.00	0.43	-5835498.52	-5835627.42
CuCN	-1733.31229	28.33	0.25	-4550797.93	-4550872.82

CuCF ₃	-1977.92109	46.83	0.31	-5193002.29	-5193093.45
CuC ₆ F ₅	-2367.83452	152.82	0.43	-6216617.91	-6216746.21
CuC ₁₂ F ₉	-2995.38543	298.74	0.62	-7864113.17	-7864296.66
CuC ₆ H ₃ (CF ₃) ₂	-2545.63221	288.37	0.50	-6683291.97	-6683440.99
CuC ₁₀ F ₇	-2719.70140	242.77	0.53	-7140357.96	-7140515.62

FLP Screening Data:

BOhfp₃ 1



Total energy = -2390.9595546440 H = -65061.3568252 eV

HOMO-LUMO Separation

HOMO: 124. 124 a -0.30865066 H = -8.39882 eV

LUMO: 125. 125 a -0.01537712 H = -0.41843 eV

Gap : +0.29327354 H = +7.98038 eV

Number of MOs= 440, Electrons= 248.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -2390.9650462780

COSMO(14.3): Total energy + OC corr. [a.u.] = -2390.9654538338

COSMO(36.64): Total energy + OC corr. [a.u.] = -2390.965889080

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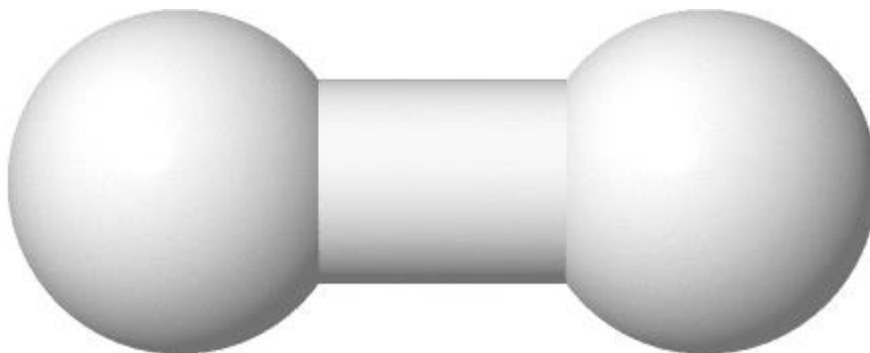
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13	a	36.17	0.15802	YES	YES
14	a	37.73	0.38290	YES	YES
15	a	38.48	0.28804	YES	YES
16	a	49.69	0.00479	YES	YES
17	a	50.84	0.04194	YES	YES
18	a	61.70	0.00049	YES	YES
19	a	71.10	0.05482	YES	YES
20	a	71.55	0.04572	YES	YES
21	a	99.28	0.00110	YES	YES
22	a	144.36	4.34619	YES	YES
23	a	145.69	4.49035	YES	YES
24	a	165.99	0.03093	YES	YES
25	a	196.25	0.05063	YES	YES
26	a	196.38	0.11339	YES	YES
27	a	197.83	0.12439	YES	YES
28	a	246.38	1.38066	YES	YES
29	a	264.58	0.01174	YES	YES
30	a	265.07	0.02364	YES	YES
31	a	286.69	0.09693	YES	YES
32	a	287.22	0.13131	YES	YES
33	a	288.27	0.13786	YES	YES
34	a	316.51	1.50226	YES	YES
35	a	316.79	1.60897	YES	YES
36	a	321.54	0.00065	YES	YES
37	a	333.23	0.11479	YES	YES
38	a	351.22	0.01809	YES	YES
39	a	353.62	0.03228	YES	YES
40	a	373.27	0.43555	YES	YES
41	a	378.98	0.62404	YES	YES
42	a	414.84	0.02776	YES	YES
43	a	493.50	0.06252	YES	YES
44	a	494.12	0.11841	YES	YES
45	a	511.49	0.05624	YES	YES
46	a	522.46	0.95995	YES	YES
47	a	522.70	1.75527	YES	YES
48	a	523.08	3.11081	YES	YES
49	a	527.27	17.18843	YES	YES
50	a	528.14	16.35557	YES	YES
51	a	536.35	0.44078	YES	YES
52	a	536.65	1.20184	YES	YES
53	a	536.68	1.19110	YES	YES
54	a	552.61	0.00949	YES	YES
55	a	608.81	7.84482	YES	YES
56	a	633.87	23.75242	YES	YES
57	a	634.78	24.01476	YES	YES
58	a	674.32	1.85772	YES	YES
59	a	674.67	1.88367	YES	YES
60	a	676.51	125.13073	YES	YES

61	a	712.09	0.19351	YES	YES
62	a	727.68	21.25969	YES	YES
63	a	728.07	20.05575	YES	YES
64	a	847.72	0.08540	YES	YES
65	a	862.06	57.77530	YES	YES
66	a	862.11	62.09851	YES	YES
67	a	887.42	3.61127	YES	YES
68	a	894.59	4.63391	YES	YES
69	a	895.49	47.64725	YES	YES
70	a	896.69	43.35624	YES	YES
71	a	1094.74	0.35419	YES	YES
72	a	1095.64	21.36566	YES	YES
73	a	1101.53	205.00156	YES	YES
74	a	1102.15	171.37313	YES	YES
75	a	1104.04	358.74417	YES	YES
76	a	1163.62	0.38979	YES	YES
77	a	1164.50	2.32727	YES	YES
78	a	1169.53	10.66518	YES	YES
79	a	1172.15	1.36564	YES	YES
80	a	1200.40	141.01893	YES	YES
81	a	1201.16	136.77388	YES	YES
82	a	1206.90	10.33836	YES	YES
83	a	1216.20	598.47191	YES	YES
84	a	1216.67	654.30543	YES	YES
85	a	1237.35	0.64706	YES	YES
86	a	1244.74	292.49004	YES	YES
87	a	1245.43	46.44403	YES	YES
88	a	1245.93	27.54562	YES	YES
89	a	1274.05	683.46856	YES	YES
90	a	1274.66	692.38946	YES	YES
91	a	1280.82	6.85330	YES	YES
92	a	1349.46	17.53770	YES	YES
93	a	1355.51	19.24196	YES	YES
94	a	1357.43	62.65277	YES	YES
95	a	1358.69	12.40603	YES	YES
96	a	1360.55	106.38810	YES	YES
97	a	1363.10	99.95219	YES	YES
98	a	1421.81	716.43937	YES	YES
99	a	1424.55	727.81715	YES	YES
100	a	3007.87	0.15612	YES	YES
101	a	3008.09	12.89519	YES	YES
102	a	3008.14	13.12355	YES	YES

H₂



Total energy = -1.1699588238 H = -31.8362175 eV

HOMO-LUMO Separation

HOMO: 1. 1 a -0.37841649 H = -10.29724 eV

LUMO: 2. 2 a +0.05080754 H = +1.38254 eV

Gap : +0.42922402 H = +11.67979 eV

Number of MOs= 4, Electrons= 2.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -1.1701534789

COSMO(14.3): Total energy + OC corr. [a.u.] = -1.1701668390

COSMO(36.64): Total energy + OC corr. [a.u.] = -1.1701809509

\$coord

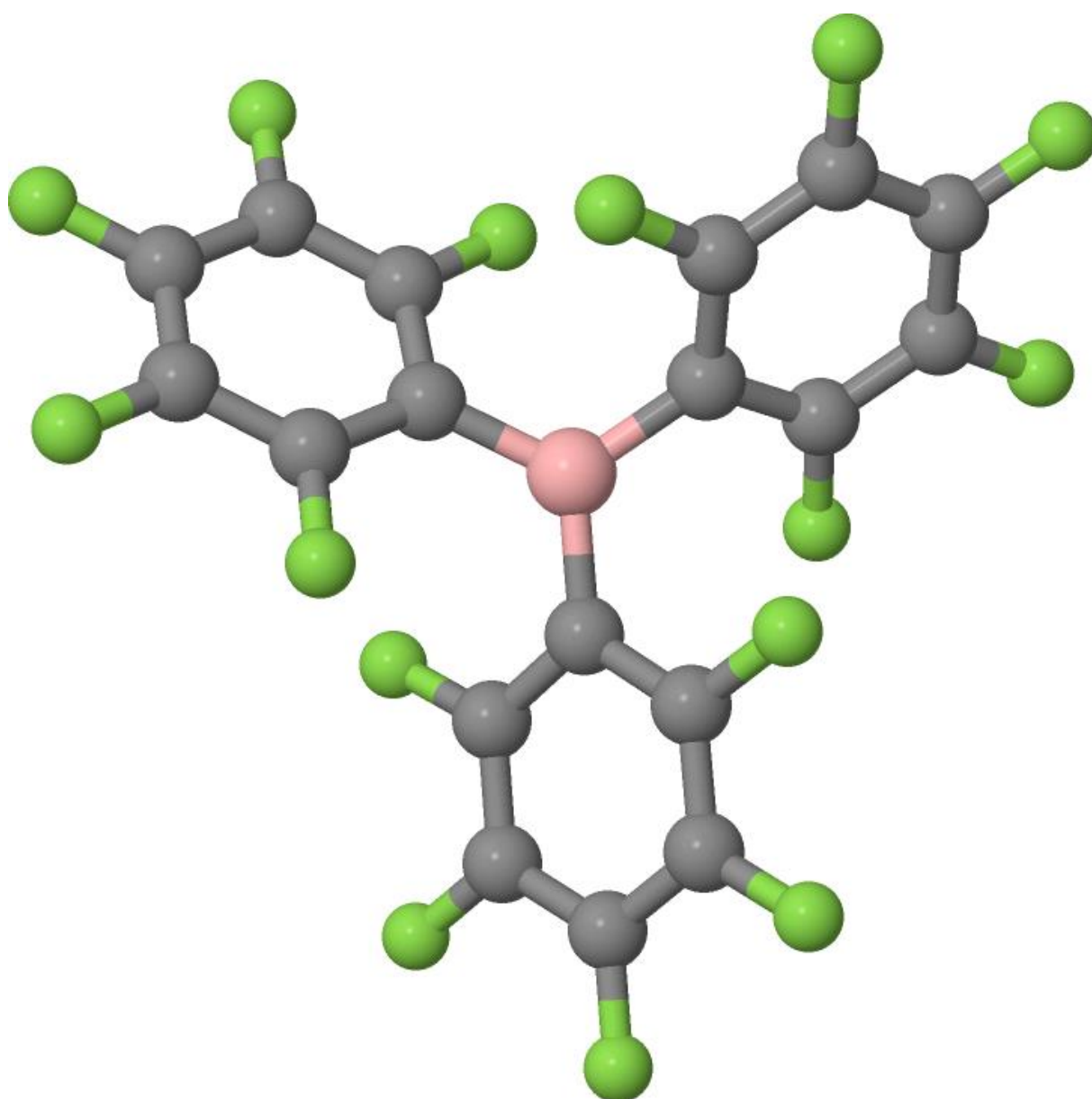
-0.72776464481994	0.0000000000000000	0.0000000000000000	h
0.72776464481994	0.0000000000000000	0.0000000000000000	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-

5		0.00	0.00000	-	-
6	a	4263.72	0.00000	YES	YES

B(C₆F₅)₃



Total energy = -2206.7529283410 H = -60048.8366343 eV

HOMO-LUMO Separation

HOMO: 124. 124 a -0.23809910 H = -6.47901 eV

LUMO: 125. 125 a -0.14440408 H = -3.92944 eV

Gap : +0.09369502 H = +2.54957 eV

Number of MOs= 476, Electrons= 248.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -2206.7575865826

COSMO(14.3): Total energy + OC corr. [a.u.] = -2206.7579289873

COSMO(36.64): Total energy + OC corr. [a.u.] = -2206.7582941436

\$coord

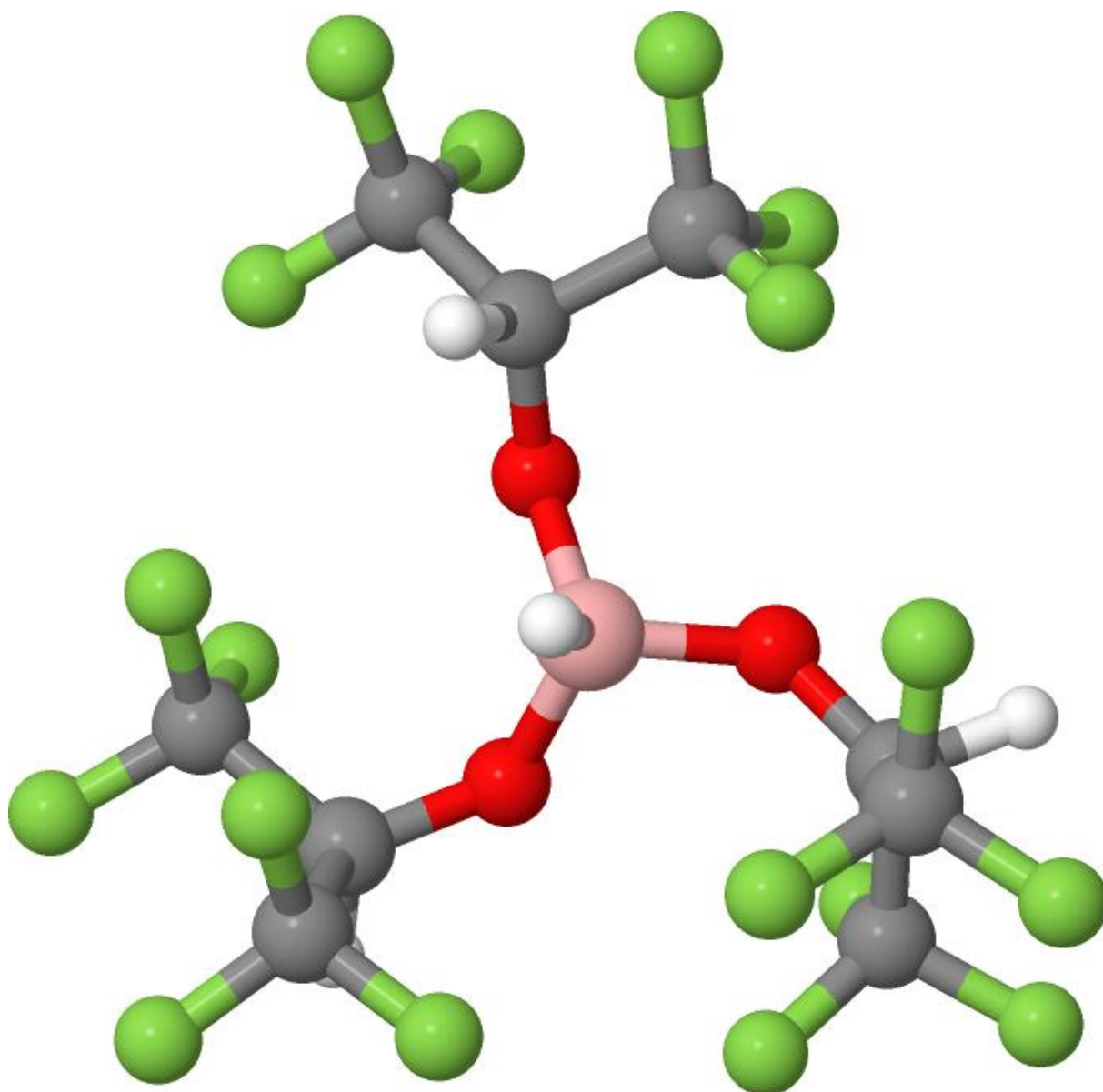
-0.26451905424150	-1.43884158503356	0.82446402653022	b
-2.08542052005186	-2.70221538807131	2.81148547847521	c
2.09325244817007	-2.95960038307846	-0.16164245206234	c
-0.79534262480554	1.32370730700955	-0.13263989961920	c
-1.81352451844043	3.20733602563265	1.46847250115075	c
-2.28244758265257	5.68896969280020	0.66120747986976	c
-1.75994667279504	6.35114421784595	-1.86011361146679	c
-0.76148727201302	4.54029368602900	-3.53179154708505	c
-0.28575893148654	2.08782144676495	-2.64346552756236	c
1.96828383766160	-5.58286347523750	-0.65214697701635	c
4.05024697201732	-6.99528868402013	-1.48887412416319	c
6.38771098227472	-5.77421917473886	-1.82075051993551	c
6.60892599081564	-3.16621027642892	-1.35480418355463	c
4.47260222354212	-1.81243901808062	-0.55849094537566	c
-4.73951237510455	-2.45103029100991	2.67419631992407	c
-6.38352332731117	-3.56784359407378	4.42831583227465	c
-5.36502946910896	-4.97435726970984	6.44189586861882	c
-2.73228659016513	-5.26688262471144	6.66685539752285	c
-1.15383862541411	-4.15385476901425	4.84963749339653	c
0.63934490718098	0.42757669136419	-4.32239115325805	f
-0.28070226142876	5.16959624532165	-5.92782358388675	f
-2.20842189965435	8.69223406577486	-2.66376986588868	f
-3.21065045791062	7.41550189734265	2.25050238687293	f
-2.31710315300749	2.68961193318038	3.89990780193180	f
-5.80126254147039	-1.14598391550597	0.77257395073162	f
-8.88552371968846	-3.31479683573031	4.21190169344966	f
-6.89895421721491	-6.02583605421851	8.13765603644423	f
-1.76940394961438	-6.58815742019572	8.59074865340883	f
1.34730066072010	-4.46249438330942	5.15937677098649	f
4.78882974560720	0.66493853756973	-0.10517130703137	f
8.83705113019342	-2.02131764897203	-1.66379180854108	f
8.39440746445542	-7.08912019504003	-2.57866215057156	f
3.84369002310659	-9.46619287149917	-1.96144025563266	f
-0.22654775071126	-6.82890762503777	-0.38064054252662	f

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	17.41	0.46210	YES	YES
8		a	19.32	0.48199	YES	YES
9		a	32.51	0.00905	YES	YES
10		a	33.23	0.02915	YES	YES
11		a	34.32	0.00736	YES	YES
12		a	35.48	0.00783	YES	YES
13		a	99.86	0.07171	YES	YES
14		a	103.60	0.12700	YES	YES
15		a	104.66	0.08296	YES	YES
16		a	124.10	0.35083	YES	YES
17		a	125.13	0.33513	YES	YES
18		a	126.96	0.16055	YES	YES
19		a	139.02	0.02895	YES	YES
20		a	142.18	0.00874	YES	YES
21		a	148.62	0.00997	YES	YES
22		a	153.32	0.01708	YES	YES
23		a	154.42	0.13322	YES	YES
24		a	154.99	0.17893	YES	YES
25		a	219.72	3.64831	YES	YES
26		a	225.44	3.80632	YES	YES
27		a	225.81	3.65805	YES	YES
28		a	261.44	0.09964	YES	YES
29		a	262.18	0.19956	YES	YES
30		a	263.23	0.19139	YES	YES
31		a	267.82	0.08450	YES	YES
32		a	269.90	0.13364	YES	YES
33		a	271.71	0.06533	YES	YES
34		a	305.37	0.49502	YES	YES
35		a	306.40	0.55544	YES	YES
36		a	308.19	0.60777	YES	YES
37		a	338.55	2.79148	YES	YES
38		a	339.89	2.66338	YES	YES
39		a	346.14	0.10129	YES	YES
40		a	348.94	0.06395	YES	YES
41		a	377.21	6.02492	YES	YES
42		a	379.11	6.52030	YES	YES
43		a	390.01	1.25602	YES	YES
44		a	392.03	1.08963	YES	YES
45		a	393.18	0.64592	YES	YES
46		a	429.39	0.48295	YES	YES
47		a	430.31	0.27469	YES	YES
48		a	430.80	0.31750	YES	YES
49		a	458.87	4.85726	YES	YES
50		a	459.38	4.47827	YES	YES
51		a	484.62	0.00046	YES	YES
52		a	499.62	0.05835	YES	YES
53		a	510.72	0.02398	YES	YES
54		a	516.20	0.00953	YES	YES
55		a	535.90	1.97458	YES	YES
56		a	562.42	2.73554	YES	YES

57	a	562.99	2.91729	YES	YES
58	a	565.68	0.31850	YES	YES
59	a	617.30	29.89937	YES	YES
60	a	617.65	31.05210	YES	YES
61	a	631.98	1.33901	YES	YES
62	a	633.14	1.58151	YES	YES
63	a	636.36	0.71406	YES	YES
64	a	664.27	21.28018	YES	YES
65	a	667.26	22.88787	YES	YES
66	a	675.64	6.75216	YES	YES
67	a	768.86	23.58916	YES	YES
68	a	770.12	23.58629	YES	YES
69	a	774.44	3.10689	YES	YES
70	a	851.40	0.02799	YES	YES
71	a	983.28	105.92850	YES	YES
72	a	983.83	70.53714	YES	YES
73	a	984.63	125.31295	YES	YES
74	a	1020.58	120.04256	YES	YES
75	a	1021.40	103.48645	YES	YES
76	a	1116.33	0.25534	YES	YES
77	a	1153.43	8.83680	YES	YES
78	a	1155.40	18.96615	YES	YES
79	a	1157.87	22.83198	YES	YES
80	a	1176.88	201.59971	YES	YES
81	a	1181.17	223.74645	YES	YES
82	a	1302.58	2.66863	YES	YES
83	a	1313.89	154.71954	YES	YES
84	a	1318.56	178.64096	YES	YES
85	a	1345.01	0.08515	YES	YES
86	a	1348.08	8.13690	YES	YES
87	a	1348.81	6.74998	YES	YES
88	a	1378.31	305.85459	YES	YES
89	a	1379.53	275.64653	YES	YES
90	a	1396.14	0.20842	YES	YES
91	a	1471.98	478.31285	YES	YES
92	a	1479.36	557.02889	YES	YES
93	a	1480.99	630.53979	YES	YES
94	a	1519.74	247.38239	YES	YES
95	a	1520.61	266.61947	YES	YES
96	a	1522.68	11.94812	YES	YES
97	a	1608.45	21.33935	YES	YES
98	a	1610.34	8.63559	YES	YES
99	a	1611.34	7.55547	YES	YES
100	a	1630.44	208.49685	YES	YES
101	a	1630.57	187.06657	YES	YES
102	a	1632.14	2.34112	YES	YES

[HB(Ohfip)₃]⁻



Total energy = -2391.5956026500 H = -65078.6645820 eV

HOMO-LUMO Separation

HOMO: 125. 125 a -0.08594225 H = -2.33861 eV

LUMO: 126. 126 a +0.14785970 H = +4.02347 eV

Gap : +0.23380195 H = +6.36208 eV

Number of MOs= 442, Electrons= 250.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -2391.6506035342

COSMO(14.3): Total energy + OC corr. [a.u.] = -2391.6544885563

COSMO(36.64): Total energy + OC corr. [a.u.] = -2391.6586106952

\$scoord

-0.33135413993766	0.80533362431511	0.23698662211117	b
-0.99369739055051	-1.49309585880956	-1.25140661847219	o
-2.75987210842980	1.82537458733247	1.22899348188800	o
0.68057749119320	2.60579398378054	-1.68144218013812	o
3.22668333786322	2.86314625034753	-2.04378984582731	c
-3.09544886368004	3.53175534597149	3.13621120473664	c
-1.89784973235223	-3.76942958693512	-0.46040264923778	c
-0.36684685685419	-5.07431639151080	1.68524755411957	c
2.11055485834145	-5.13158903328483	1.08310153639753	f
-1.12224205237631	-7.53354672430270	1.96475481835867	f
-0.59123956676409	-3.97579943084782	3.96879413343539	f
-4.79463898689363	-3.80858101591236	0.10937440964851	c
-5.69186128833608	-6.23674700290665	0.00481465535402	f
-5.45565351956138	-2.89191477960755	2.39190145074694	f
-6.04902847081021	-2.48920430773581	-1.66947145289416	f
-2.20116419081391	2.64909709225750	5.80663420807999	c
0.31892509901961	2.76023041746800	6.18755745326171	f
-3.28591484797924	4.11743246064679	7.63999369528495	f
-2.95449851335488	0.25847342340001	6.24172274876749	f
-2.11877444193234	6.24420490973719	2.54907258449841	c
-2.93454675541662	7.00424069150990	0.26569750219110	f
0.42087338527204	6.45936483780910	2.61276315245101	f
-3.04633585951265	7.93576952269202	4.27355376456899	f
3.73995875265100	5.45734882493258	-3.31032082545016	c
2.48237316750747	7.32296221509175	-2.12840820621936	f
6.23899145613382	6.07494281766189	-3.22311596891334	f
3.04231106049624	5.50613917232199	-5.77572242755667	f
4.39529497099053	0.68793882743373	-3.65220789864606	c
6.81208867538347	1.24288288330921	-4.39250794985134	f
3.05768378499198	0.19630301280836	-5.75936376519935	f
4.53930525393306	-1.46442607252614	-2.29403327427883	f
1.26611655522797	0.41336678185489	1.91911352766236	h
4.34061713248587	2.86355375129515	-0.23999120712873	h
-5.17384319134359	3.80705791873361	3.40524023191120	h
-1.72293718243299	-5.13770956235811	-2.06463914777952	h

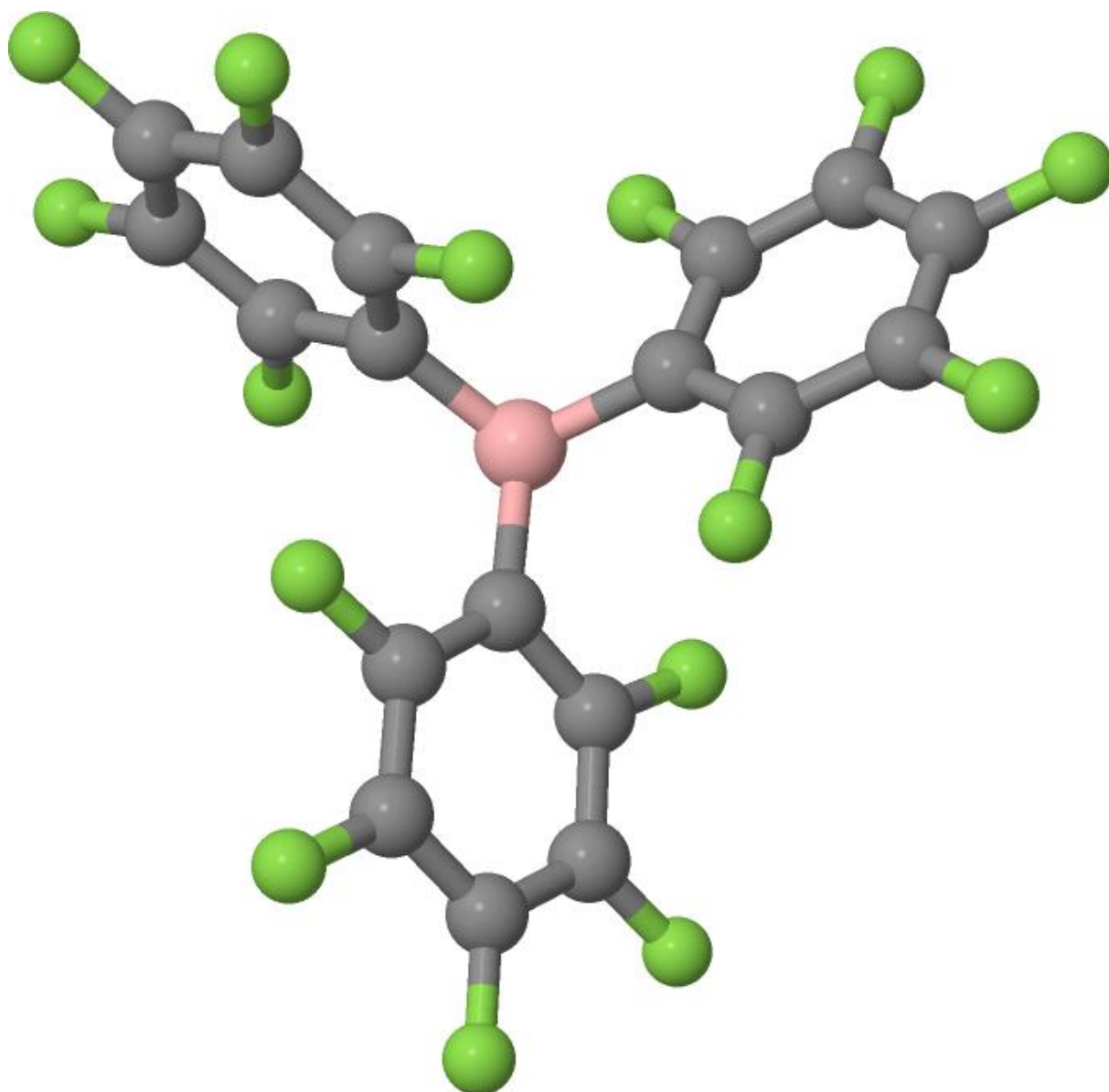
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	11.32	0.02889	YES	YES
8		a	17.63	0.12731	YES	YES
9		a	29.75	0.02560	YES	YES

10	a	31.14	0.19854	YES	YES
11	a	33.21	0.10547	YES	YES
12	a	43.16	0.10456	YES	YES
13	a	43.94	0.14175	YES	YES
14	a	51.73	0.23558	YES	YES
15	a	54.76	0.11590	YES	YES
16	a	69.73	0.06319	YES	YES
17	a	74.71	0.20118	YES	YES
18	a	83.19	0.09201	YES	YES
19	a	87.10	0.06484	YES	YES
20	a	96.32	0.02409	YES	YES
21	a	120.11	0.23347	YES	YES
22	a	141.65	0.54406	YES	YES
23	a	158.78	0.91217	YES	YES
24	a	168.21	0.34564	YES	YES
25	a	176.90	0.58192	YES	YES
26	a	189.51	0.24959	YES	YES
27	a	219.18	0.23755	YES	YES
28	a	233.93	3.82268	YES	YES
29	a	251.24	2.64709	YES	YES
30	a	264.86	4.29555	YES	YES
31	a	279.42	1.05852	YES	YES
32	a	279.48	0.55835	YES	YES
33	a	282.85	0.30749	YES	YES
34	a	294.10	0.33417	YES	YES
35	a	303.12	0.31803	YES	YES
36	a	313.40	0.70417	YES	YES
37	a	316.72	0.73114	YES	YES
38	a	319.16	1.42688	YES	YES
39	a	328.04	0.69377	YES	YES
40	a	371.67	0.71399	YES	YES
41	a	374.58	0.92833	YES	YES
42	a	387.58	1.99186	YES	YES
43	a	478.46	7.13542	YES	YES
44	a	491.31	4.84814	YES	YES
45	a	502.32	2.62758	YES	YES
46	a	507.03	5.82117	YES	YES
47	a	510.37	9.76557	YES	YES
48	a	516.33	3.51044	YES	YES
49	a	516.92	2.72421	YES	YES
50	a	518.24	4.81911	YES	YES
51	a	520.47	3.17964	YES	YES
52	a	529.39	0.02351	YES	YES
53	a	530.09	0.12979	YES	YES
54	a	535.32	0.34063	YES	YES
55	a	592.16	19.55643	YES	YES
56	a	609.25	20.05851	YES	YES
57	a	646.90	3.21704	YES	YES
58	a	668.88	18.84007	YES	YES
59	a	669.89	34.94070	YES	YES
60	a	672.46	51.65654	YES	YES
61	a	717.91	12.43535	YES	YES
62	a	726.75	8.58599	YES	YES
63	a	730.27	3.81901	YES	YES
64	a	807.13	15.87754	YES	YES
65	a	813.11	7.46024	YES	YES
66	a	830.52	27.06038	YES	YES
67	a	853.93	55.09381	YES	YES
68	a	863.08	16.68966	YES	YES

69	a	864.39	28.37000	YES	YES
70	a	872.65	81.29412	YES	YES
71	a	887.92	138.91936	YES	YES
72	a	929.12	160.23565	YES	YES
73	a	1066.19	53.47523	YES	YES
74	a	1067.06	75.32265	YES	YES
75	a	1086.54	34.50510	YES	YES
76	a	1098.67	115.26443	YES	YES
77	a	1106.95	558.22755	YES	YES
78	a	1117.17	376.35901	YES	YES
79	a	1123.89	248.65091	YES	YES
80	a	1127.06	729.22415	YES	YES
81	a	1140.28	235.92968	YES	YES
82	a	1148.58	324.36661	YES	YES
83	a	1167.91	252.42404	YES	YES
84	a	1193.28	81.22707	YES	YES
85	a	1214.76	40.70795	YES	YES
86	a	1216.95	390.02805	YES	YES
87	a	1218.38	255.65523	YES	YES
88	a	1224.78	100.94704	YES	YES
89	a	1229.89	54.03935	YES	YES
90	a	1232.11	354.01052	YES	YES
91	a	1235.61	224.86977	YES	YES
92	a	1243.25	98.91236	YES	YES
93	a	1265.49	264.56334	YES	YES
94	a	1288.88	215.68030	YES	YES
95	a	1302.67	85.06741	YES	YES
96	a	1334.68	66.29073	YES	YES
97	a	1336.25	39.00493	YES	YES
98	a	1338.03	60.06467	YES	YES
99	a	1347.19	38.09423	YES	YES
100	a	1376.67	31.57715	YES	YES
101	a	1378.41	40.99514	YES	YES
102	a	2370.94	176.39734	YES	YES
103	a	2876.64	46.09197	YES	YES
104	a	2902.26	58.01360	YES	YES
105	a	2915.70	45.43099	YES	YES

[HB(C₆F₅)₃]⁻



Total energy = -2207.4515685000 H = -60067.8476111 eV

HOMO-LUMO Separation

HOMO: 125. 125 a -0.09857444 H = -2.68235 eV

LUMO: 126. 126 a +0.05506562 H = +1.49841 eV

Gap : +0.15364006 H = +4.18076 eV

Number of MOs= 478, Electrons= 250.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -2207.4978355941

COSMO(14.3): Total energy + OC corr. [a.u.] = -2207.5010809738

COSMO(36.64): Total energy + OC corr. [a.u.] = -2207.5045221322

\$scoord

-1.18445428037276	1.71775746280263	0.66685612010888	b
-2.06940507695410	0.40702004787438	3.33866535339641	c
-2.69795287268692	0.60376036448449	-1.81365253275775	c
1.88045645749049	1.75399137078324	0.16746523383964	c
3.21091236413480	-0.20271728605044	-1.03829663051360	c
5.80701370453558	-0.10117285861768	-1.59303563749429	c
7.19338268836519	2.05056562005338	-0.89904208531026	c
5.96133513718666	4.04828215441624	0.33264002728616	c
3.35683118853511	3.85911950850599	0.83969017285322	c
-3.96941421578174	-1.72373497258344	-1.95669120438432	c
-5.32324151815761	-2.53457086966173	-4.09825725578308	c
-5.39701955146102	-0.98984360335202	-6.25108159195385	c
-4.12695303942911	1.33846828483331	-6.21950502703658	c
-2.81979644856165	2.07500283459320	-4.02694038182700	c
-4.54771440602938	0.83831280328879	4.20835267116882	c
-5.50550961463772	-0.10487268182160	6.49691845122397	c
-3.93636058004550	-1.58265639794532	8.04324480869342	c
-1.45202292283654	-2.07471336693861	7.26561435990813	c
-0.58224670170177	-1.08931487572430	4.95073088691327	c
2.31059875481060	5.85348784859901	2.03774739731132	f
7.28941433829322	6.11713703609804	1.00609439669639	f
9.68518961162519	2.19160874649112	-1.40395465937507	f
6.98655437843643	-2.03288823313813	-2.76262823586050	f
2.00469905340906	-2.35139056744380	-1.71224635118095	f
-6.16459346402745	2.22773027299415	2.80320435948959	f
-7.90055122064439	0.37684242405685	7.22302961582681	f
-4.80712325376502	-2.51216893137624	10.24767500492518	f
0.06406109340471	-3.50456828802834	8.73226995492229	f
1.82631989452686	-1.69141655298544	4.34290767406216	f
-1.64948122112211	4.34131372751975	-4.12972088922178	f
-4.17745860270173	2.82798636777460	-8.28654740577213	f
-6.67589629795002	-1.72755837961362	-8.32581550487384	f
-6.52778263015575	-4.78051716969818	-4.12001454051221	f
-3.94986445634606	-3.34554408461458	0.01718075597304	f
-1.84695583877209	3.95297866436356	0.84163270662014	h

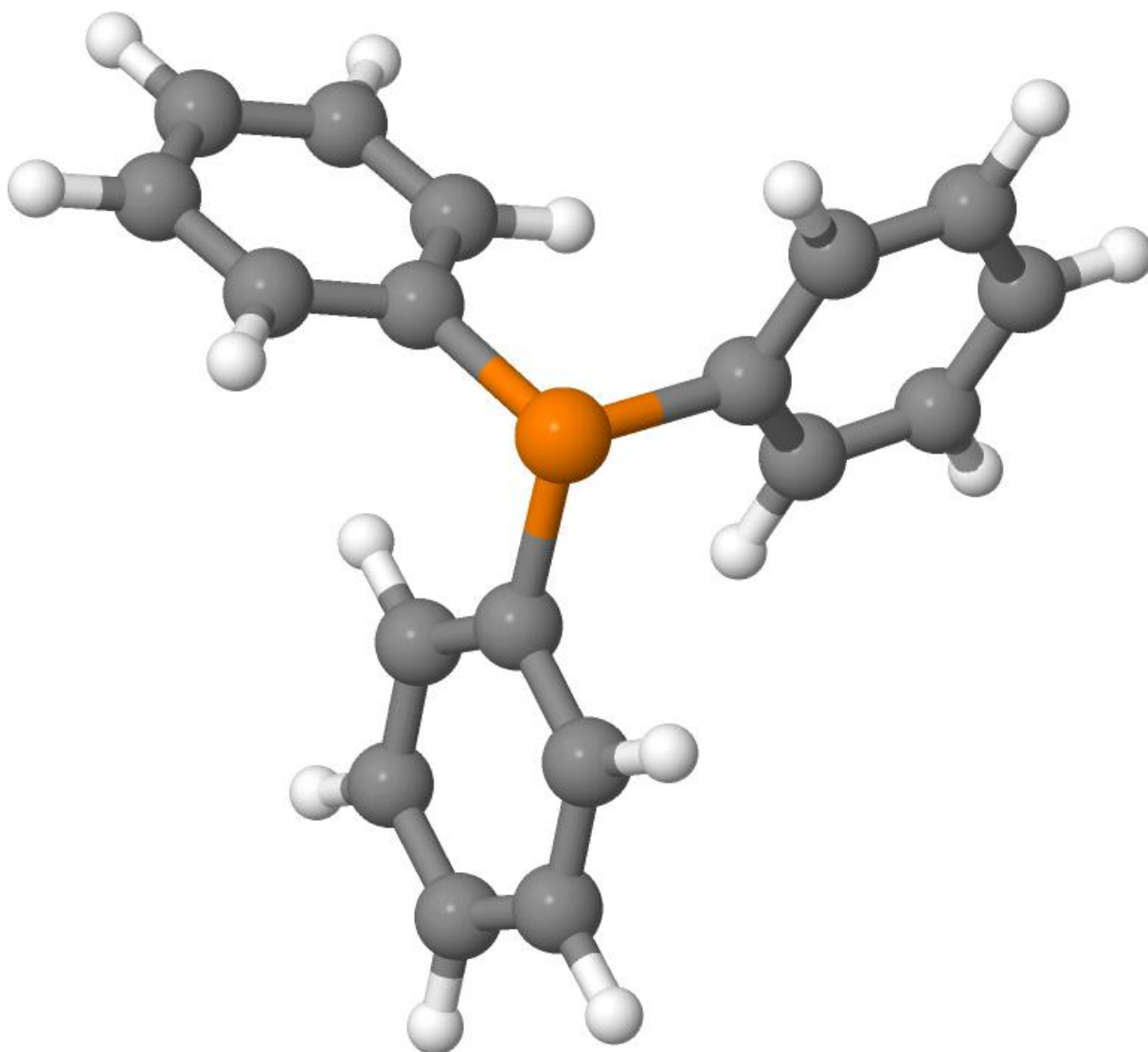
\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	7.22	0.00833	YES	YES
8		a	17.48	0.00523	YES	YES
9		a	21.58	0.01506	YES	YES

10	a	29.29	0.01660	YES	YES
11	a	32.43	0.02052	YES	YES
12	a	39.72	0.09880	YES	YES
13	a	94.74	0.17557	YES	YES
14	a	100.98	0.16746	YES	YES
15	a	106.91	0.11725	YES	YES
16	a	123.15	0.00233	YES	YES
17	a	124.53	0.01094	YES	YES
18	a	126.93	0.00217	YES	YES
19	a	135.35	0.01466	YES	YES
20	a	141.09	0.05820	YES	YES
21	a	143.36	0.06045	YES	YES
22	a	157.62	0.01234	YES	YES
23	a	160.76	0.04323	YES	YES
24	a	162.63	0.03945	YES	YES
25	a	218.73	1.28817	YES	YES
26	a	222.11	1.35070	YES	YES
27	a	228.59	1.73673	YES	YES
28	a	261.86	0.03761	YES	YES
29	a	262.13	0.02376	YES	YES
30	a	262.48	0.04699	YES	YES
31	a	270.10	0.03552	YES	YES
32	a	270.31	0.05000	YES	YES
33	a	270.98	0.06285	YES	YES
34	a	304.33	0.51158	YES	YES
35	a	304.97	0.61203	YES	YES
36	a	306.82	0.43864	YES	YES
37	a	335.39	1.04911	YES	YES
38	a	336.80	1.91997	YES	YES
39	a	340.39	0.84534	YES	YES
40	a	349.44	0.05486	YES	YES
41	a	363.38	0.70477	YES	YES
42	a	373.51	0.16708	YES	YES
43	a	387.44	0.05446	YES	YES
44	a	388.39	0.21629	YES	YES
45	a	390.91	0.02922	YES	YES
46	a	432.37	0.01435	YES	YES
47	a	433.02	0.05664	YES	YES
48	a	433.35	0.16706	YES	YES
49	a	453.66	1.79279	YES	YES
50	a	454.94	1.88929	YES	YES
51	a	470.16	0.03298	YES	YES
52	a	493.55	0.03705	YES	YES
53	a	498.23	0.02056	YES	YES
54	a	506.71	0.03696	YES	YES
55	a	527.57	0.34243	YES	YES
56	a	558.69	5.84117	YES	YES
57	a	559.48	4.95805	YES	YES
58	a	563.50	0.04048	YES	YES
59	a	584.12	9.26419	YES	YES
60	a	590.76	12.76159	YES	YES
61	a	626.13	0.20216	YES	YES
62	a	627.10	0.44076	YES	YES
63	a	632.13	0.06543	YES	YES
64	a	654.30	29.64993	YES	YES
65	a	663.65	5.79162	YES	YES
66	a	678.58	32.11388	YES	YES
67	a	743.94	13.02323	YES	YES
68	a	751.89	13.75663	YES	YES

69	a	769.34	1.07744	YES	YES
70	a	827.59	2.20645	YES	YES
71	a	891.62	67.56132	YES	YES
72	a	901.46	76.02817	YES	YES
73	a	964.99	103.93427	YES	YES
74	a	971.10	172.68898	YES	YES
75	a	976.96	270.84964	YES	YES
76	a	1038.28	15.18410	YES	YES
77	a	1040.34	32.26619	YES	YES
78	a	1080.46	13.94733	YES	YES
79	a	1095.51	214.54221	YES	YES
80	a	1102.23	246.11195	YES	YES
81	a	1126.94	3.21475	YES	YES
82	a	1128.88	0.64028	YES	YES
83	a	1130.49	6.05109	YES	YES
84	a	1263.13	31.15131	YES	YES
85	a	1264.08	8.15529	YES	YES
86	a	1265.16	35.48821	YES	YES
87	a	1348.45	10.26315	YES	YES
88	a	1349.97	8.78581	YES	YES
89	a	1351.21	3.48610	YES	YES
90	a	1372.88	11.13291	YES	YES
91	a	1376.64	6.93067	YES	YES
92	a	1379.92	1.39026	YES	YES
93	a	1460.14	295.13961	YES	YES
94	a	1464.23	334.79226	YES	YES
95	a	1465.63	498.48110	YES	YES
96	a	1502.85	248.69346	YES	YES
97	a	1504.24	295.87231	YES	YES
98	a	1507.78	19.15430	YES	YES
99	a	1613.50	6.92572	YES	YES
100	a	1614.97	0.76475	YES	YES
101	a	1616.19	9.04283	YES	YES
102	a	1619.63	29.07196	YES	YES
103	a	1620.67	29.25174	YES	YES
104	a	1622.81	5.72002	YES	YES
105	a	2400.82	74.46801	YES	YES

PPh₃



Total energy = -1035.7339343770 H = -28183.7703819 eV

HOMO-LUMO Separation

HOMO: 69. 69 a -0.19274302 H = -5.24481 eV

LUMO: 70. 70 a -0.05923774 H = -1.61194 eV

Gap : +0.13350527 H = +3.63287 eV

Number of MOs= 300, Electrons= 138.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -1035.7422025693

COSMO(14.3): Total energy + OC corr. [a.u.] = -1035.7428578125

COSMO(36.64): Total energy + OC corr. [a.u.] = -1035.7435656059

\$scoord

1.51543674810686	-2.24457523699999	4.33094326346248	p
1.09049449571686	1.23239738533235	4.07144127655271	c
3.98078621337314	-2.87941008145485	1.91108563093387	c
-1.38725518819096	-3.47224865158985	2.77981801377691	c
2.13782026082710	2.74087231765613	2.13544099182255	c
1.77766997708811	5.37387615780415	2.13263788581790	c
0.35684423651483	6.53468321692152	4.05232538470651	c
-0.69309295116642	5.05042054755994	5.99120930252602	c
-0.31055952389868	2.42500141581637	6.01101916876093	c
6.52639173639814	-2.66775832809221	2.69910948040449	c
8.51469187672710	-3.14437321956242	1.00827959512538	c
7.98928119077842	-3.88278263713091	-1.49001877173191	c
5.46731974648800	-4.12759949692497	-2.28511370514266	c
3.47475975756121	-3.62451764122588	-0.60058467317832	c
-3.12895772604989	-1.96865903644775	1.42887626518951	c
-5.31856539782558	-3.05152212505455	0.38195308489238	c
-5.79203178082620	-5.64994219132404	0.65666705823096	c
-4.06998249563201	-7.16514959029076	1.99987437348200	c
-1.89826361216989	-6.08040521467441	3.06996370325478	c
3.24839611077868	1.84984266889922	0.61533830348613	h
2.61348892543675	6.52631262903801	0.60983733164484	h
0.07569684489733	8.59955914077709	4.04535883205869	h
-1.79907308886538	5.94687120859853	7.51364263202985	h
-1.10676112904635	1.27686421452799	7.56069334826260	h
6.95134707104027	-2.12829721906504	4.66930483581209	h
10.48832081808107	-2.96049804648187	1.65257573878358	h
9.54837195064464	-4.28009432636819	-2.81461739008268	h
5.04142806089794	-4.71323525825699	-4.24004622652665	h
1.50396800922658	-3.81839609505654	-1.24655369350328	h
-2.77423079751702	0.07056643295169	1.19559080757194	h
-6.66390329238889	-1.84972012985812	-0.66270355750042	h
-7.51038943600922	-6.49467662666735	-0.16585905733774	h
-4.43279165322376	-9.20397426777599	2.23636590535936	h
-0.57577539126600	-7.27352629722765	4.15655803374579	h

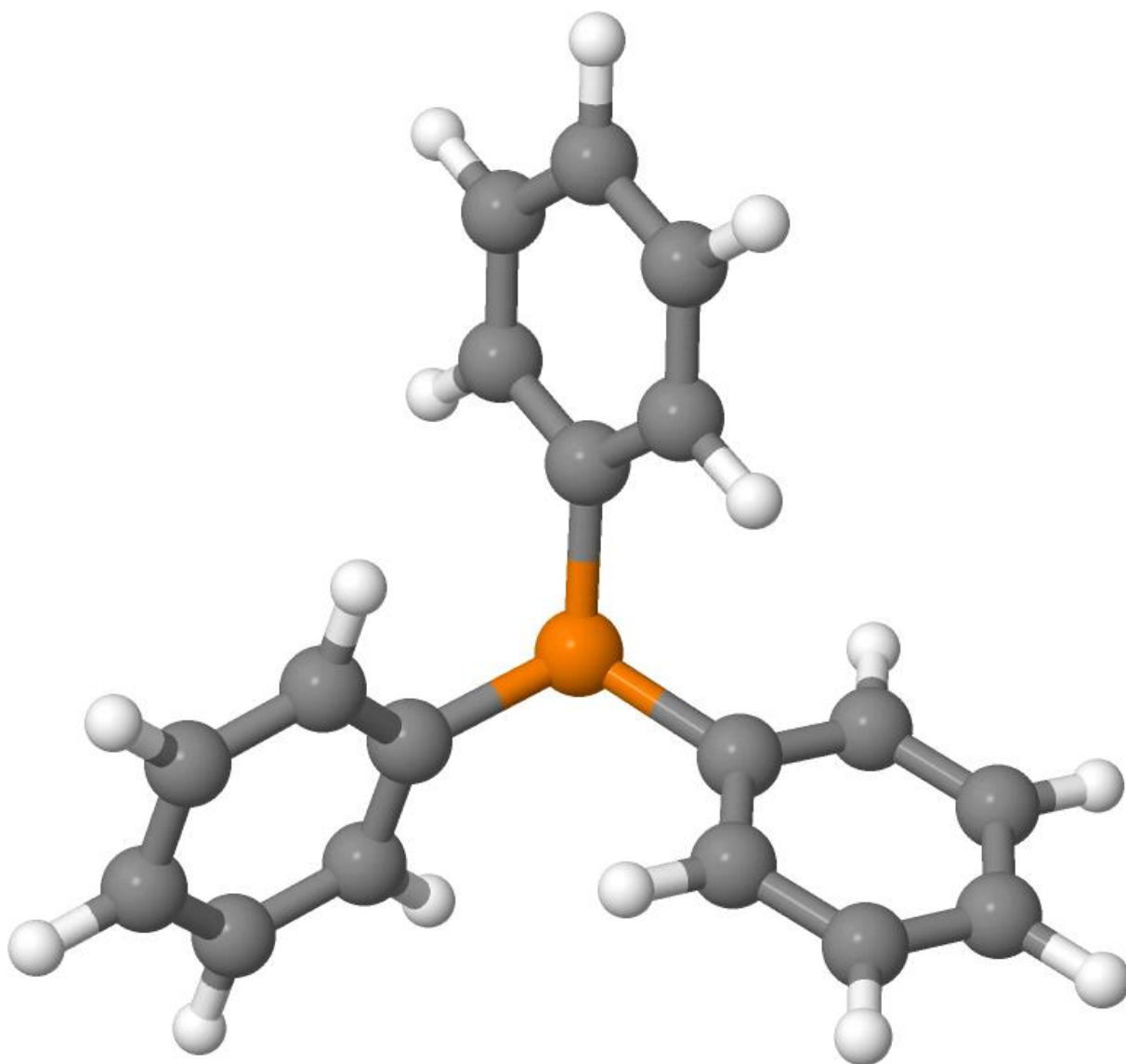
\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	24.29	0.33650	YES	YES
8		a	26.01	0.33478	YES	YES
9		a	42.53	0.00142	YES	YES
10		a	51.61	0.09378	YES	YES

11	a	52.18	0.09506	YES	YES
12	a	65.37	0.40219	YES	YES
13	a	178.50	0.35352	YES	YES
14	a	193.71	1.24059	YES	YES
15	a	194.76	1.26362	YES	YES
16	a	237.91	0.58721	YES	YES
17	a	253.02	0.31882	YES	YES
18	a	254.07	0.31938	YES	YES
19	a	393.68	0.24093	YES	YES
20	a	394.80	1.48019	YES	YES
21	a	394.90	1.44624	YES	YES
22	a	401.18	0.10400	YES	YES
23	a	419.00	6.01280	YES	YES
24	a	419.70	6.22332	YES	YES
25	a	495.04	25.70064	YES	YES
26	a	495.89	25.88253	YES	YES
27	a	503.64	12.89763	YES	YES
28	a	610.23	0.22156	YES	YES
29	a	610.51	0.24216	YES	YES
30	a	610.70	0.08564	YES	YES
31	a	670.05	0.48063	YES	YES
32	a	684.52	1.48287	YES	YES
33	a	684.60	1.36486	YES	YES
34	a	698.60	33.96889	YES	YES
35	a	698.78	35.04075	YES	YES
36	a	699.38	31.00345	YES	YES
37	a	743.24	15.55028	YES	YES
38	a	744.20	15.26881	YES	YES
39	a	744.35	15.42622	YES	YES
40	a	835.64	0.10522	YES	YES
41	a	836.03	0.13597	YES	YES
42	a	838.55	0.16584	YES	YES
43	a	904.36	0.79094	YES	YES
44	a	904.64	0.56597	YES	YES
45	a	905.27	0.50212	YES	YES
46	a	957.11	0.00738	YES	YES
47	a	957.31	0.00696	YES	YES
48	a	958.39	0.12007	YES	YES
49	a	982.54	0.48556	YES	YES
50	a	982.62	0.37249	YES	YES
51	a	982.65	0.35557	YES	YES
52	a	983.17	3.32886	YES	YES
53	a	983.39	3.28362	YES	YES
54	a	983.90	0.82061	YES	YES
55	a	1022.82	4.32995	YES	YES
56	a	1022.90	4.20950	YES	YES
57	a	1023.16	0.30282	YES	YES
58	a	1070.07	1.34535	YES	YES
59	a	1070.52	4.07719	YES	YES
60	a	1070.89	2.37661	YES	YES
61	a	1074.67	10.95945	YES	YES
62	a	1074.90	9.95686	YES	YES
63	a	1082.76	1.07016	YES	YES
64	a	1140.72	0.01116	YES	YES
65	a	1140.88	0.05868	YES	YES
66	a	1141.02	0.04789	YES	YES
67	a	1164.00	5.33668	YES	YES
68	a	1164.30	5.43085	YES	YES
69	a	1165.66	0.89945	YES	YES

70	a	1288.22	5.00947	YES	YES
71	a	1290.57	1.73670	YES	YES
72	a	1291.06	1.77821	YES	YES
73	a	1356.43	0.00856	YES	YES
74	a	1358.68	0.89204	YES	YES
75	a	1358.85	0.91348	YES	YES
76	a	1428.05	13.85945	YES	YES
77	a	1429.54	7.05527	YES	YES
78	a	1429.76	7.24025	YES	YES
79	a	1470.22	4.82848	YES	YES
80	a	1470.44	11.75456	YES	YES
81	a	1470.59	9.25648	YES	YES
82	a	1585.25	0.41630	YES	YES
83	a	1586.40	0.05160	YES	YES
84	a	1586.54	0.03783	YES	YES
85	a	1599.24	5.87560	YES	YES
86	a	1599.25	6.14357	YES	YES
87	a	1601.44	0.16429	YES	YES
88	a	3079.66	2.52583	YES	YES
89	a	3079.75	1.99771	YES	YES
90	a	3080.03	2.10517	YES	YES
91	a	3087.83	0.28228	YES	YES
92	a	3088.08	0.20968	YES	YES
93	a	3088.32	0.18643	YES	YES
94	a	3097.96	7.49011	YES	YES
95	a	3098.01	7.77625	YES	YES
96	a	3098.22	25.30890	YES	YES
97	a	3106.19	12.49403	YES	YES
98	a	3106.42	12.87640	YES	YES
99	a	3106.88	10.41223	YES	YES
100	a	3113.04	34.75538	YES	YES
101	a	3113.21	32.77792	YES	YES
102	a	3113.75	8.78259	YES	YES

HPPh₃⁺



Total energy = -1036.1123997070 H = -28194.0689534 eV

HOMO-LUMO Separation

HOMO: 69. 69 a -0.36577483 H = -9.95325 eV

LUMO: 70. 70 a -0.20743970 H = -5.64472 eV

Gap : +0.15833512 H = +4.30852 eV

Number of MOs= 302, Electrons= 138.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -1036.1665923737

COSMO(14.3): Total energy + OC corr. [a.u.] = -1036.1704137180

COSMO(36.64): Total energy + OC corr. [a.u.] = -1036.1744694508

\$coord

-7.53441103940189	-1.58852540370860	-1.30263283834699	c
-7.49898293490824	-3.74655149350215	0.25171933531058	c
-5.37515621411700	-4.28777477175503	1.75225199669322	c
-3.26903869303350	-2.67327786776251	1.71293686164961	c
-3.30968199818059	-0.51139574950133	0.14750283880464	c
-5.44358738032183	0.03783199361294	-1.36690982585161	c
1.15172242414564	1.19736050058226	-2.91523981533504	c
2.71975345064623	3.19733257814804	-3.74672344554371	c
4.12153780498232	2.90748174317847	-5.97717250924200	c
3.96951376657624	0.64263783745266	-7.36413128605155	c
2.41194642754688	-1.34197493331530	-6.53141272866615	c
0.99133729151843	-1.07677451826256	-4.30504710924587	c
5.23812103765894	-0.22925421181011	4.77716316897320	c
3.74617235354216	0.01959410072101	2.59618393415381	c
1.39956154247483	1.28174307097695	2.75579761485302	c
0.54951486143971	2.29565039250502	5.07925242785070	c
2.06351253245351	2.03910185930223	7.23878643740372	c
4.40010176471250	0.77691054221814	7.08815234673962	c
-0.59796301713955	1.56372272111822	-0.00240863782443	p
-1.56068087368618	4.08463293542123	-0.00279532425351	h
-9.20656022676117	-1.16297141501869	-2.46759285803051	h
-9.15086995815649	-5.01375014699468	0.29811004777481	h
-5.35767859271935	-5.97374110538399	2.97366289338281	h
-1.61519269784323	-3.08950827627457	2.90893246963199	h
-5.48638330079065	1.72762075056240	-2.58688802963131	h
2.84669381348642	4.97840051970254	-2.67144337015383	h
5.33358017786485	4.46420031303693	-6.64178367890398	h
5.07114584395688	0.42917207293045	-9.11831510300734	h
2.28983805283285	-3.10846822831162	-7.62616477712707	h
-0.24543545054395	-2.62697947390760	-3.66791587952939	h
7.07225263319942	-1.20787879405974	4.66393391987363	h
4.41733127455687	-0.75101836982734	0.78116265344146	h
-1.27857746952993	3.28854901713567	5.21139506944387	h
1.41832978495599	2.83732522578322	9.05008672112829	h
5.58313813211452	0.58578392529476	8.79121968988862	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.11	0.03973	YES	YES
8	a	21.24	0.04034	YES	YES
9	a	40.83	0.02134	YES	YES
10	a	48.40	0.04581	YES	YES
11	a	49.31	0.04560	YES	YES
12	a	61.49	0.03650	YES	YES
13	a	171.29	1.78476	YES	YES
14	a	173.42	1.73759	YES	YES
15	a	173.83	1.69103	YES	YES
16	a	236.16	0.16962	YES	YES
17	a	253.33	0.84649	YES	YES
18	a	254.46	0.85087	YES	YES
19	a	389.19	0.25955	YES	YES
20	a	390.04	0.28539	YES	YES
21	a	393.06	0.62912	YES	YES
22	a	396.09	0.45866	YES	YES
23	a	428.04	6.82523	YES	YES
24	a	428.43	6.91207	YES	YES
25	a	488.49	57.39422	YES	YES
26	a	489.47	57.75209	YES	YES
27	a	495.37	22.40608	YES	YES
28	a	605.10	0.07195	YES	YES
29	a	605.30	0.06662	YES	YES
30	a	605.86	0.00348	YES	YES
31	a	679.91	2.56765	YES	YES
32	a	691.66	25.05296	YES	YES
33	a	691.77	25.60299	YES	YES
34	a	692.43	25.41123	YES	YES
35	a	710.66	13.54613	YES	YES
36	a	710.96	14.08475	YES	YES
37	a	737.65	31.97105	YES	YES
38	a	737.87	32.76231	YES	YES
39	a	740.02	32.01094	YES	YES
40	a	832.21	0.31239	YES	YES
41	a	833.13	0.26119	YES	YES
42	a	835.20	0.04865	YES	YES
43	a	872.25	104.12437	YES	YES
44	a	875.22	105.42824	YES	YES
45	a	919.57	0.53740	YES	YES
46	a	920.91	1.93837	YES	YES
47	a	921.33	1.91924	YES	YES
48	a	966.84	0.06502	YES	YES
49	a	967.29	0.07056	YES	YES
50	a	967.90	0.02781	YES	YES
51	a	982.53	2.20572	YES	YES
52	a	982.93	4.23883	YES	YES
53	a	983.39	4.43119	YES	YES
54	a	1005.08	0.07648	YES	YES
55	a	1005.11	0.06050	YES	YES
56	a	1005.42	0.06371	YES	YES
57	a	1021.12	0.06889	YES	YES
58	a	1022.25	0.05449	YES	YES
59	a	1022.37	0.05224	YES	YES
60	a	1079.21	8.18615	YES	YES
61	a	1080.50	4.05661	YES	YES
62	a	1080.72	4.65048	YES	YES

63	a	1089.72	3.54528	YES	YES
64	a	1093.57	83.31447	YES	YES
65	a	1093.80	82.95199	YES	YES
66	a	1153.02	0.13646	YES	YES
67	a	1153.17	0.16034	YES	YES
68	a	1154.27	0.13281	YES	YES
69	a	1168.84	3.08659	YES	YES
70	a	1169.46	2.97224	YES	YES
71	a	1171.19	0.58430	YES	YES
72	a	1294.50	7.36535	YES	YES
73	a	1298.25	4.73280	YES	YES
74	a	1299.59	4.83940	YES	YES
75	a	1367.50	1.74524	YES	YES
76	a	1370.04	0.34237	YES	YES
77	a	1370.85	0.35446	YES	YES
78	a	1432.56	29.94404	YES	YES
79	a	1435.39	24.02598	YES	YES
80	a	1435.55	23.51896	YES	YES
81	a	1470.76	1.44674	YES	YES
82	a	1471.22	2.59996	YES	YES
83	a	1471.45	2.98292	YES	YES
84	a	1587.24	0.46934	YES	YES
85	a	1588.82	1.54657	YES	YES
86	a	1589.28	1.80243	YES	YES
87	a	1596.01	6.74823	YES	YES
88	a	1596.54	6.22770	YES	YES
89	a	1596.95	4.74697	YES	YES
90	a	2403.20	4.95768	YES	YES
91	a	3097.93	0.49003	YES	YES
92	a	3098.09	0.54369	YES	YES
93	a	3099.11	0.51762	YES	YES
94	a	3107.11	0.04183	YES	YES
95	a	3107.51	0.05166	YES	YES
96	a	3107.78	0.03967	YES	YES
97	a	3116.14	0.02868	YES	YES
98	a	3116.35	0.04041	YES	YES
99	a	3116.91	0.05325	YES	YES
100	a	3124.91	0.92801	YES	YES
101	a	3125.08	0.90717	YES	YES
102	a	3125.78	0.86832	YES	YES
103	a	3132.19	1.44330	YES	YES
104	a	3132.31	1.04864	YES	YES
105	a	3132.92	1.06647	YES	YES

PtBu₃

Total energy = -814.4052924748 H = -22161.1081756 eV

HOMO-LUMO Separation

HOMO: 57. 57 a -0.17684406 H = -4.81217 eV

LUMO: 58. 58 a +0.02273946 H = +0.61877 eV

Gap : +0.19958352 H = +5.43095 eV

Number of MOs= 240, Electrons= 114.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -814.4088345698

COSMO(14.3): Total energy + OC corr. [a.u.] = -814.4091237759

COSMO(36.64): Total energy + OC corr. [a.u.] = -814.4094383820

\$coord

0.93300482445971	0.11698026946867	1.11814594524139	p
-1.20168928361680	3.08861596996926	0.50821192898968	c
-2.22479193267287	3.89922427140035	3.13368990321550	c
-3.41839850760687	2.79485353349837	-1.36045696534119	c
0.48176633900918	5.30354976046939	-0.38736668209390	c
3.09402954585591	-0.33318937009606	-1.86242291292435	c
4.26777861906904	-3.00842196636102	-1.78764075596888	c
5.34299448556994	1.51572911675430	-1.51574232546685	c
1.88353010066545	0.07860224912688	-4.48138441956387	c
-1.30328233762954	-2.83547354698855	1.32644229146315	c
-2.43637936439042	-3.84410682546524	-1.16237183326772	c
-3.48974607459470	-2.24424897940478	3.17346854315002	c
0.26243676277908	-4.94681677886939	2.62433568258892	c
-3.22312135954540	5.74788645981494	2.95074511954114	h
-0.65905846664655	4.14722513232714	4.51349243667968	h
-3.58917981038441	2.53998386172927	3.95125183369153	h
-4.42569119543292	4.63893755530163	-1.55790558134914	h
-4.83893332546964	1.39444796258279	-0.71062935230043	h
-2.77934265626467	2.22475221178772	-3.27470111111546	h
-0.65435157674051	7.07897446131540	-0.34217085653558	h
1.17247867208188	5.07185359765355	-2.35354665398068	h
2.13733768729840	5.59122659716801	0.87468720111869	h
5.79357651161512	-3.11993558912776	-3.23850669344293	h
2.89021723731812	-4.52439431672392	-2.23198899172562	h
5.14922907764059	-3.42669486949046	0.07435021238339	h

6.79229137929361	1.13101124705732	-2.99809157193566	h
6.25600549652251	1.25692849887929	0.35976362804790	h
4.79995026716060	3.52875181238942	-1.69083963895248	h
3.31381073872262	-0.29151377920629	-5.98836818535446	h
1.21033340694623	2.04682071113393	-4.75487522569875	h
0.26579624684159	-1.20998528694131	-4.82650058053310	h
-3.70586540999347	-5.47800466748409	-0.74960434543533	h
-0.96813520208847	-4.53435192360261	-2.49152877159981	h
-3.58394110619984	-2.40091302346921	-2.16261899712919	h
-4.52217477863800	-4.03336418146288	3.59545554633720	h
-4.89492775326848	-0.90115337020666	2.38674113649146	h
-2.78740530400674	-1.48374204010489	5.00219308125131	h
-1.00126939348531	-6.57590424294589	3.06618833904723	h
1.09695126347125	-4.26915673440217	4.43020719182223	h
1.82016428971859	-5.68083477838033	1.43518958248007	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	91.17	0.01011	YES	YES
8		a	94.99	0.00958	YES	YES
9		a	122.66	0.00066	YES	YES
10		a	166.86	0.05592	YES	YES
11		a	177.42	0.02030	YES	YES
12		a	182.01	0.01345	YES	YES
13		a	198.93	0.00285	YES	YES
14		a	202.44	0.04801	YES	YES
15		a	206.18	0.02214	YES	YES
16		a	236.68	0.04832	YES	YES
17		a	243.35	0.13284	YES	YES
18		a	248.56	0.09329	YES	YES
19		a	257.07	0.38263	YES	YES
20		a	259.61	0.34496	YES	YES
21		a	270.98	0.01096	YES	YES
22		a	280.76	0.04432	YES	YES
23		a	282.90	0.07874	YES	YES
24		a	295.99	0.02197	YES	YES
25		a	331.54	0.23686	YES	YES
26		a	340.47	0.28963	YES	YES
27		a	344.70	0.25131	YES	YES
28		a	354.05	0.01572	YES	YES
29		a	367.94	0.17307	YES	YES
30		a	368.64	0.23202	YES	YES
31		a	397.91	0.14011	YES	YES
32		a	399.34	0.37335	YES	YES
33		a	401.67	0.29659	YES	YES
34		a	452.49	3.68756	YES	YES
35		a	454.21	3.76223	YES	YES
36		a	473.68	0.66650	YES	YES
37		a	532.76	0.11547	YES	YES
38		a	557.86	4.84055	YES	YES
39		a	559.91	4.71571	YES	YES

40	a	793.94	11.57775	YES	YES
41	a	794.31	11.16116	YES	YES
42	a	797.27	1.12847	YES	YES
43	a	909.54	1.49114	YES	YES
44	a	912.15	1.66322	YES	YES
45	a	913.17	1.51443	YES	YES
46	a	919.19	0.71615	YES	YES
47	a	920.14	1.28085	YES	YES
48	a	923.17	1.37452	YES	YES
49	a	927.99	0.27662	YES	YES
50	a	930.76	0.93381	YES	YES
51	a	932.59	0.70862	YES	YES
52	a	988.82	0.08254	YES	YES
53	a	998.44	0.58649	YES	YES
54	a	998.73	1.19480	YES	YES
55	a	1004.60	2.49136	YES	YES
56	a	1006.34	2.71936	YES	YES
57	a	1010.94	2.80326	YES	YES
58	a	1146.61	38.45106	YES	YES
59	a	1147.74	38.32682	YES	YES
60	a	1157.36	0.42612	YES	YES
61	a	1170.14	0.26795	YES	YES
62	a	1178.52	1.76477	YES	YES
63	a	1179.30	1.56308	YES	YES
64	a	1195.48	0.68490	YES	YES
65	a	1196.05	0.59642	YES	YES
66	a	1197.52	1.96532	YES	YES
67	a	1336.65	0.71744	YES	YES
68	a	1339.83	3.97281	YES	YES
69	a	1342.21	3.73109	YES	YES
70	a	1343.27	3.69042	YES	YES
71	a	1345.92	0.92608	YES	YES
72	a	1348.98	21.82227	YES	YES
73	a	1369.32	15.07979	YES	YES
74	a	1371.39	15.32699	YES	YES
75	a	1380.07	0.30666	YES	YES
76	a	1409.02	1.40136	YES	YES
77	a	1409.98	2.01974	YES	YES
78	a	1414.92	0.32365	YES	YES
79	a	1422.12	3.56595	YES	YES
80	a	1422.24	0.88618	YES	YES
81	a	1425.09	0.99036	YES	YES
82	a	1425.76	1.56922	YES	YES
83	a	1428.04	0.12778	YES	YES
84	a	1431.03	0.39956	YES	YES
85	a	1439.93	5.33586	YES	YES
86	a	1440.65	2.33542	YES	YES
87	a	1441.36	1.40195	YES	YES
88	a	1447.74	6.93609	YES	YES
89	a	1450.29	8.01214	YES	YES
90	a	1452.64	6.48890	YES	YES
91	a	1462.02	16.84767	YES	YES
92	a	1462.71	8.56850	YES	YES
93	a	1463.87	11.78510	YES	YES
94	a	2922.09	31.26609	YES	YES
95	a	2923.02	27.94869	YES	YES
96	a	2924.81	25.29875	YES	YES
97	a	2926.15	31.22392	YES	YES
98	a	2927.30	14.68006	YES	YES

99	a	2927.97	14.67952	YES	YES
100	a	2931.35	121.46261	YES	YES
101	a	2931.94	138.14367	YES	YES
102	a	2934.52	2.06122	YES	YES
103	a	3002.63	13.71768	YES	YES
104	a	3005.08	17.86811	YES	YES
105	a	3005.94	27.36728	YES	YES
106	a	3011.05	4.86882	YES	YES
107	a	3011.47	5.22297	YES	YES
108	a	3012.50	31.60653	YES	YES
109	a	3014.07	49.92558	YES	YES
110	a	3014.99	41.25034	YES	YES
111	a	3017.51	2.71995	YES	YES
112	a	3049.08	10.67978	YES	YES
113	a	3049.20	18.87541	YES	YES
114	a	3049.90	23.24196	YES	YES
115	a	3053.34	4.61692	YES	YES
116	a	3056.70	16.73449	YES	YES
117	a	3059.70	14.91660	YES	YES
118	a	3070.35	11.43597	YES	YES
119	a	3074.23	9.41096	YES	YES
120	a	3074.66	14.82728	YES	YES

HPtBu₃⁺

Total energy = -814.8016025984 H = -22171.8923289 eV

HOMO-LUMO Separation

HOMO: 57. 57 a -0.41792493 H = -11.37232 eV

LUMO: 58. 58 a -0.17970953 H = -4.89015 eV

Gap : +0.23821539 H = +6.48217 eV

Number of MOs= 242, Electrons= 114.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -814.8566406220

COSMO(14.3): Total energy + OC corr. [a.u.] = -814.8604460106

COSMO(36.64): Total energy + OC corr. [a.u.] = -814.8644705603

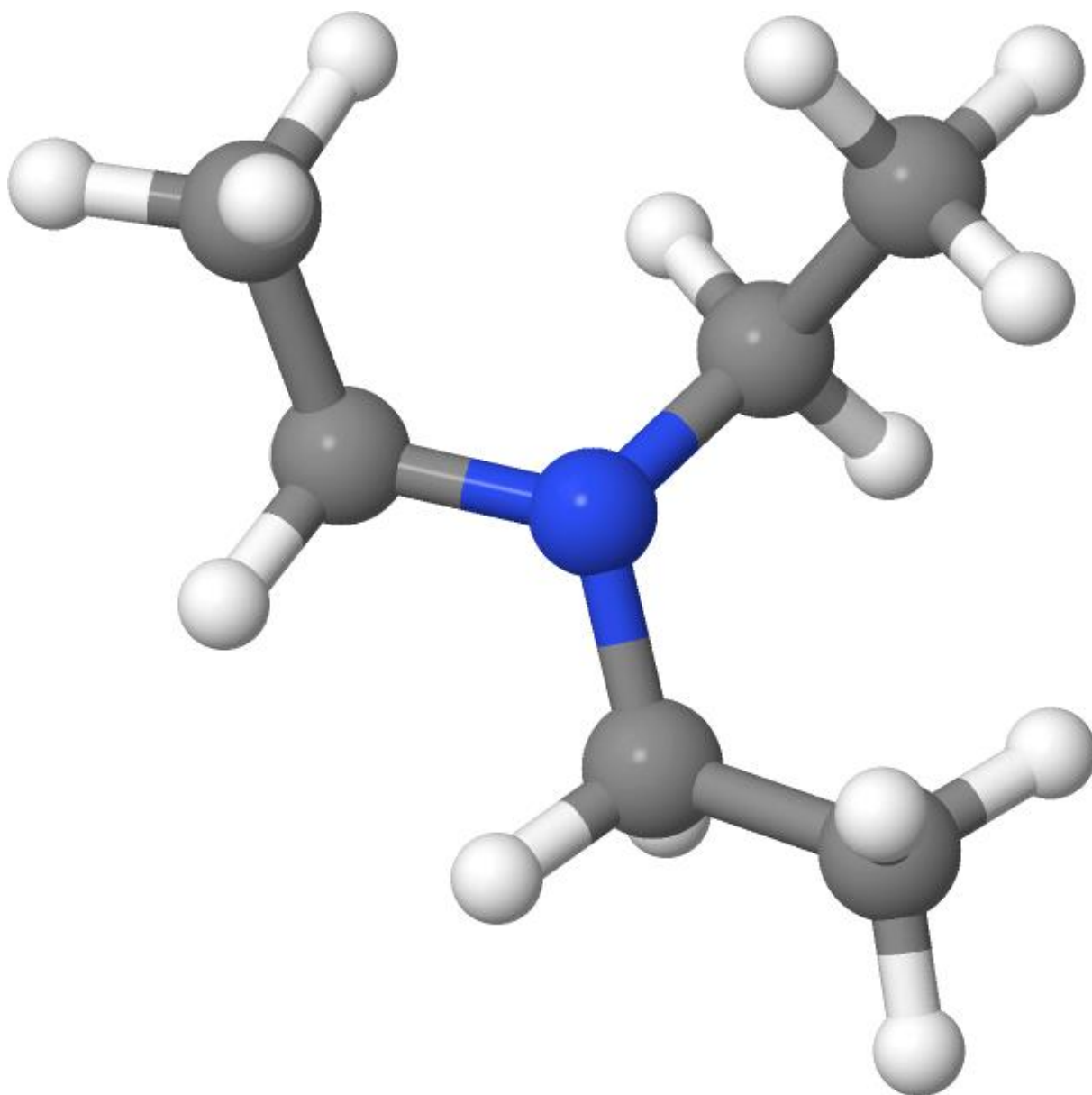
\$coord			
0.19870121339021	-0.30109001024857	1.08104396474156	p
-0.13674902449690	3.30156625589388	0.76173153655907	c
-2.18161758703821	4.19514054565772	2.65874344410947	c
-0.85253645498812	4.01910971947172	-1.97750426906080	c
2.35716757444737	4.63432019447955	1.49945397952720	c
3.46719786960489	-1.62748790564369	0.20653511623911	c
3.42439531420672	-4.54957966866700	0.21558373976816	c
5.36858571002537	-0.79021364708712	2.27126095078716	c
4.28225974936376	-0.67062788773815	-2.42981624966458	c
-2.62446906388179	-2.22628697058474	-0.15225634985269	c
-2.35727852876424	-2.70524810605421	-3.02059939800058	c
-5.13357269708956	-0.82239019659010	0.37367822253862	c
-2.72437696181713	-4.74630204247200	1.33731089004419	c
0.07911567470305	-0.68865040564831	3.75011843381375	h
-2.24712629384356	6.29578935532687	2.58390895514551	h
-1.71236250355624	3.66455096418707	4.63687206202710	h
-4.10580864855744	3.51040149560893	2.21849415361642	h
-0.97005757565829	6.11479893224037	-2.10049498994074	h
-2.72080447886803	3.26699959327091	-2.55924222534363	h
0.58254348609382	3.39714134636827	-3.37673210839968	h
2.00520817313708	6.70589006388624	1.41651728153763	h
3.93706792489967	4.23427024387671	0.18440083609044	h
2.95774027118524	4.19766745304224	3.46235583846461	h
5.38775752573176	-5.20249295436684	-0.16187154804028	h
2.21490600199626	-5.37064641140554	-1.28419142401254	h
2.86399927827450	-5.34590868560580	2.07481558086686	h
7.21558047336867	-1.70304796079901	1.84665938412067	h
4.79183023501405	-1.43391170096239	4.18658486142705	h
5.70747928268882	1.27023397644338	2.32813057402597	h
6.14830407965194	-1.52173127649922	-2.89423677671110	h
4.52498660357232	1.41034182404883	-2.50485230965178	h
2.94728699514982	-1.24209141803948	-3.94453439406114	h
-4.04875063179592	-3.77135969182564	-3.67126876835736	h
-0.68035909497326	-3.86691524495126	-3.50332287701714	h
-2.28146342338648	-0.92732236398345	-4.13131772035759	h
-6.69614142550354	-2.08581116857583	-0.24670970288936	h
-5.33177045611794	0.96203135436598	-0.70387412515303	h
-5.43574394944018	-0.44083778418606	2.41545658723511	h
-4.45529670002946	-5.77681703304359	0.73277596481816	h
-2.88748101764571	-4.43410037074453	3.40831959219524	h
-1.10354956491153	-6.01188695630945	0.97330047880027	h

\$vibrational spectrum						
#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		73.08	0.00177	YES	YES
8	a		81.37	0.00138	YES	YES
9	a		112.62	0.00097	YES	YES
10	a		149.62	0.07162	YES	YES
11	a		173.05	0.24534	YES	YES
12	a		178.67	0.56076	YES	YES

13	a	192.81	0.55540	YES	YES
14	a	198.87	0.25020	YES	YES
15	a	200.28	0.10036	YES	YES
16	a	222.99	0.19958	YES	YES
17	a	235.84	0.19485	YES	YES
18	a	240.62	0.19548	YES	YES
19	a	252.51	0.10538	YES	YES
20	a	253.83	0.14720	YES	YES
21	a	255.53	0.11611	YES	YES
22	a	275.73	0.19988	YES	YES
23	a	280.82	0.18148	YES	YES
24	a	289.19	0.10634	YES	YES
25	a	341.31	0.47764	YES	YES
26	a	352.39	1.04914	YES	YES
27	a	353.11	0.44507	YES	YES
28	a	356.29	0.45381	YES	YES
29	a	367.51	0.37305	YES	YES
30	a	373.41	0.34575	YES	YES
31	a	391.38	0.17500	YES	YES
32	a	396.77	0.81365	YES	YES
33	a	398.93	1.18840	YES	YES
34	a	455.09	9.34888	YES	YES
35	a	456.90	9.51730	YES	YES
36	a	475.24	0.96689	YES	YES
37	a	538.34	0.06556	YES	YES
38	a	575.19	1.07334	YES	YES
39	a	576.04	1.06461	YES	YES
40	a	786.81	5.49019	YES	YES
41	a	787.76	4.85557	YES	YES
42	a	788.97	0.90568	YES	YES
43	a	834.94	25.08353	YES	YES
44	a	861.16	24.54615	YES	YES
45	a	908.26	1.37232	YES	YES
46	a	909.59	3.48614	YES	YES
47	a	912.53	3.93892	YES	YES
48	a	920.33	1.65893	YES	YES
49	a	923.24	1.85535	YES	YES
50	a	924.19	0.78729	YES	YES
51	a	932.29	0.05139	YES	YES
52	a	937.16	0.05781	YES	YES
53	a	939.21	0.02777	YES	YES
54	a	991.42	0.38546	YES	YES
55	a	1006.41	8.96867	YES	YES
56	a	1007.31	2.53180	YES	YES
57	a	1009.54	9.65747	YES	YES
58	a	1012.25	2.91376	YES	YES
59	a	1014.31	11.73356	YES	YES
60	a	1140.73	71.78146	YES	YES
61	a	1142.37	72.15328	YES	YES
62	a	1154.45	0.98261	YES	YES
63	a	1173.71	0.19499	YES	YES
64	a	1188.19	1.27009	YES	YES
65	a	1189.64	1.29039	YES	YES
66	a	1198.44	2.17150	YES	YES
67	a	1199.78	1.89347	YES	YES
68	a	1200.35	1.80034	YES	YES
69	a	1345.96	0.66899	YES	YES
70	a	1348.44	3.61725	YES	YES
71	a	1351.85	0.48909	YES	YES

72	a	1354.44	9.16634	YES	YES
73	a	1356.08	32.79566	YES	YES
74	a	1359.31	4.90022	YES	YES
75	a	1379.40	19.67749	YES	YES
76	a	1382.46	20.27665	YES	YES
77	a	1392.67	0.09333	YES	YES
78	a	1411.57	2.56127	YES	YES
79	a	1412.75	1.97316	YES	YES
80	a	1417.51	0.13234	YES	YES
81	a	1421.24	1.43580	YES	YES
82	a	1422.55	4.39202	YES	YES
83	a	1424.57	0.60082	YES	YES
84	a	1425.39	1.57218	YES	YES
85	a	1429.61	0.76120	YES	YES
86	a	1430.90	1.81563	YES	YES
87	a	1440.99	9.54233	YES	YES
88	a	1443.25	3.83063	YES	YES
89	a	1444.90	8.64302	YES	YES
90	a	1449.92	16.65585	YES	YES
91	a	1450.19	22.86171	YES	YES
92	a	1453.36	27.19466	YES	YES
93	a	1463.60	10.17857	YES	YES
94	a	1464.39	21.30040	YES	YES
95	a	1465.70	22.32787	YES	YES
96	a	2407.61	9.59305	YES	YES
97	a	2957.26	1.62094	YES	YES
98	a	2957.51	3.82560	YES	YES
99	a	2958.23	4.13204	YES	YES
100	a	2959.28	5.92809	YES	YES
101	a	2959.77	6.85437	YES	YES
102	a	2960.09	13.48552	YES	YES
103	a	2961.66	6.37366	YES	YES
104	a	2962.06	6.75961	YES	YES
105	a	2963.78	3.06777	YES	YES
106	a	3029.81	2.28132	YES	YES
107	a	3031.52	1.90860	YES	YES
108	a	3031.94	1.35277	YES	YES
109	a	3035.12	8.82845	YES	YES
110	a	3035.65	8.57201	YES	YES
111	a	3036.34	8.73017	YES	YES
112	a	3040.49	8.34813	YES	YES
113	a	3040.98	7.96193	YES	YES
114	a	3043.69	2.56872	YES	YES
115	a	3062.89	1.40112	YES	YES
116	a	3065.58	9.71512	YES	YES
117	a	3066.17	9.54948	YES	YES
118	a	3073.20	7.71310	YES	YES
119	a	3074.15	7.25885	YES	YES
120	a	3074.76	6.99766	YES	YES
121	a	3099.75	3.92146	YES	YES
122	a	3102.27	3.74220	YES	YES
123	a	3102.71	4.74247	YES	YES

NEt₃



Total energy = -292.1706007889 H = -7950.3710863 eV

HOMO-LUMO Separation

HOMO: 29. 29 a -0.16755204 H = -4.55933 eV

LUMO: 30. 30 a +0.03673767 H = +0.99968 eV

Gap : +0.20428971 H = +5.55901 eV

Number of MOs= 128, Electrons= 58.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -292.1724771131

COSMO(14.3): Total energy + OC corr. [a.u.] = -292.1726179965

COSMO(36.64): Total energy + OC corr. [a.u.] = -292.1727688972

\$coord

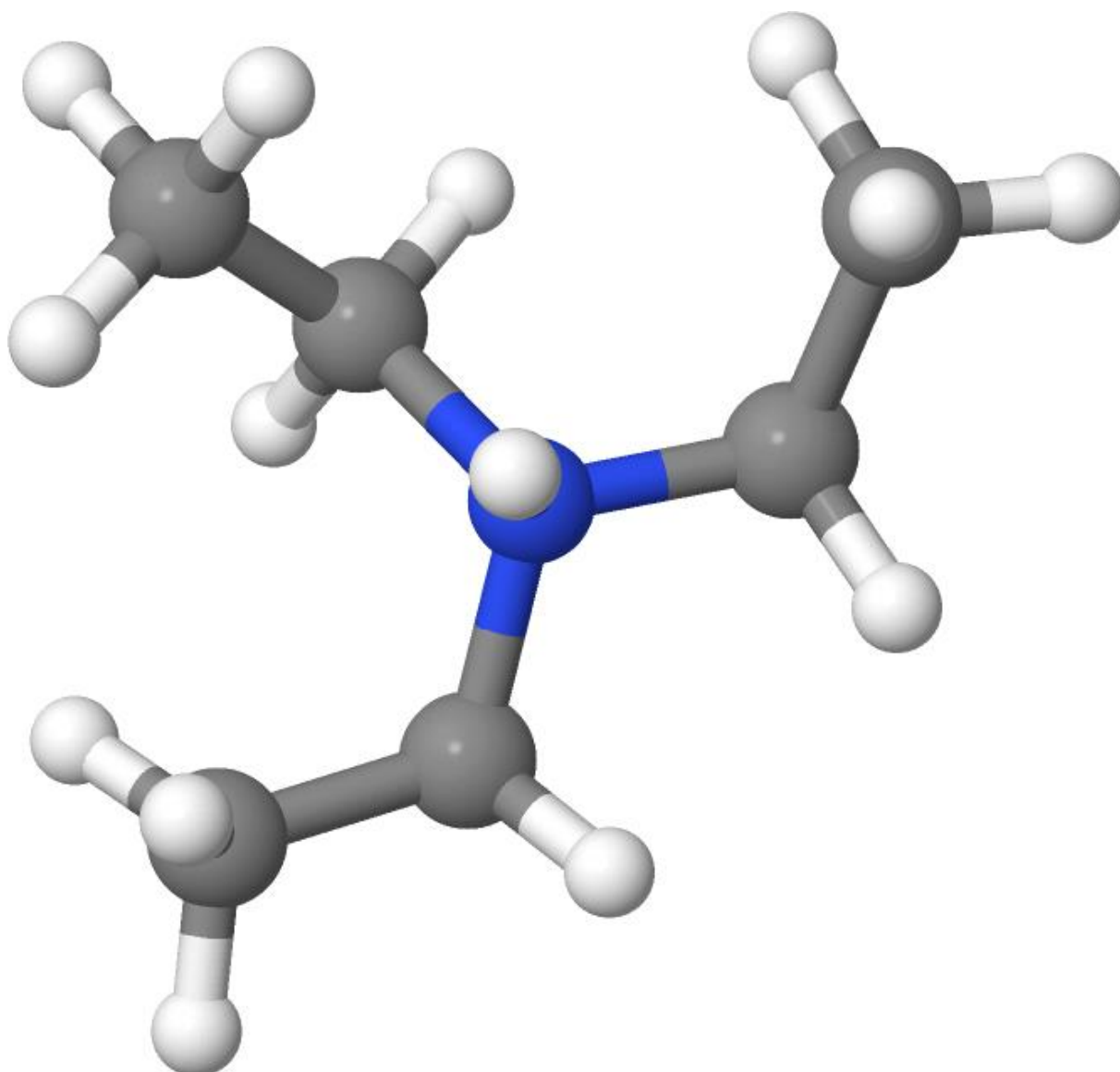
0.41574617817505	0.94862325206455	0.71092631126776	n
-2.19770318648912	1.72765029611391	1.15347337461830	c
-4.01202145918664	-0.48805056989691	1.59070091486836	c
2.26222633541571	2.95846462309127	1.14246577942637	c
0.79504357554358	-0.44517265662591	-1.66528471691089	c
1.55286203033020	-3.21949174943303	-1.28404218562240	c
4.95394185117195	1.98562897599441	1.58945288973159	c
-2.95006091714865	2.94083997693748	-0.43202356825726	h
-2.21037819361043	2.94394810274107	2.86925925973940	h
-5.94316355309014	0.22639266954640	2.01685092951785	h
-3.36222786701634	-1.66773599785581	3.20423494604729	h
-4.16695176667186	-1.73079627884640	-0.09795249487584	h
1.64864620844283	4.02212411332916	2.85025537404983	h
2.28960950320443	4.37560239406858	-0.45231129350532	h
2.26545495641923	0.52522535410753	-2.82863369735363	h
-0.96531511542011	-0.35683746340301	-2.82684689261738	h
1.81172610080760	-4.18990614938943	-3.13489564453196	h
0.08381365832250	-4.25689441617770	-0.19866739449988	h
3.35062518783504	-3.36513293991117	-0.20724287047745	h
6.24924964256908	3.58911346431286	2.00519007602601	h
5.72280663563723	0.98427866213159	-0.09115373444936	h
4.99599255730376	0.65196374482278	3.21343284891502	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	58.93	0.00090	YES	YES
8		a	87.01	0.02353	YES	YES
9		a	148.21	0.92861	YES	YES
10		a	178.52	0.81790	YES	YES
11		a	229.78	0.00677	YES	YES
12		a	243.84	0.29563	YES	YES
13		a	281.04	0.02360	YES	YES

14	a	332.33	1.49819	YES	YES
15	a	336.98	0.39454	YES	YES
16	a	394.23	2.00555	YES	YES
17	a	449.35	1.40780	YES	YES
18	a	494.83	0.18522	YES	YES
19	a	739.37	8.96889	YES	YES
20	a	755.76	7.79790	YES	YES
21	a	788.18	1.76174	YES	YES
22	a	794.90	2.20318	YES	YES
23	a	917.48	0.56939	YES	YES
24	a	920.26	1.15976	YES	YES
25	a	1012.33	6.53430	YES	YES
26	a	1057.82	0.72215	YES	YES
27	a	1068.98	10.23936	YES	YES
28	a	1072.15	28.74153	YES	YES
29	a	1074.51	2.10787	YES	YES
30	a	1092.95	22.86908	YES	YES
31	a	1126.34	15.14269	YES	YES
32	a	1209.29	25.12547	YES	YES
33	a	1216.64	43.85427	YES	YES
34	a	1263.59	5.57942	YES	YES
35	a	1297.95	34.54913	YES	YES
36	a	1309.78	5.65725	YES	YES
37	a	1335.99	5.97919	YES	YES
38	a	1346.36	33.20846	YES	YES
39	a	1351.96	6.53191	YES	YES
40	a	1361.02	46.80237	YES	YES
41	a	1365.73	14.00547	YES	YES
42	a	1392.09	5.07953	YES	YES
43	a	1418.33	2.79555	YES	YES
44	a	1424.09	0.32327	YES	YES
45	a	1429.20	2.84994	YES	YES
46	a	1430.51	5.08749	YES	YES
47	a	1435.46	0.03489	YES	YES
48	a	1441.32	9.02597	YES	YES
49	a	1449.74	10.02603	YES	YES
50	a	1450.92	0.50372	YES	YES
51	a	1462.40	11.41158	YES	YES
52	a	2780.02	44.74658	YES	YES
53	a	2791.97	197.75186	YES	YES
54	a	2899.72	53.21623	YES	YES
55	a	2940.62	25.00253	YES	YES
56	a	2942.87	33.81472	YES	YES
57	a	2943.77	14.36637	YES	YES
58	a	2944.96	34.97487	YES	YES
59	a	2970.42	2.49106	YES	YES
60	a	2977.20	40.37172	YES	YES
61	a	3025.41	47.92467	YES	YES
62	a	3027.01	15.30637	YES	YES
63	a	3028.63	37.26995	YES	YES
64	a	3034.98	10.14356	YES	YES
65	a	3035.38	40.82059	YES	YES
66	a	3041.65	20.77065	YES	YES

HNEt₃⁺



Total energy = -292.5503737555 H = -7960.7052404 eV

HOMO-LUMO Separation

HOMO: 29. 29 a -0.47573295 H = -12.94536 eV

LUMO: 30. 30 a -0.15293086 H = -4.16146 eV

Gap : +0.32280209 H = +8.78390 eV

Number of MOs= 130, Electrons= 58.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -292.6189093735

COSMO(14.3): Total energy + OC corr. [a.u.] = -292.6236789359

COSMO(36.64): Total energy + OC corr. [a.u.] = -292.6287280005

\$scoord

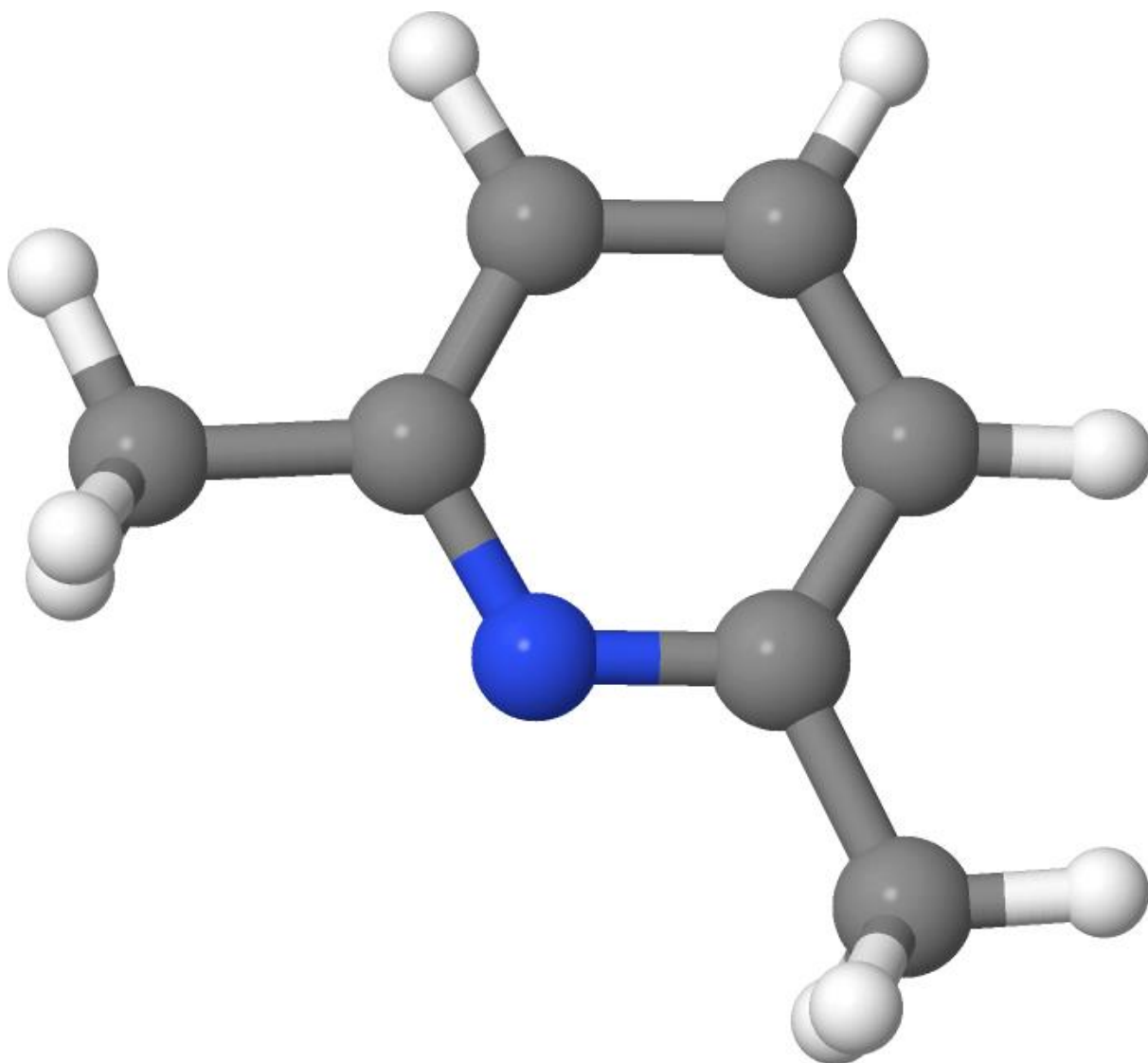
0.63228476171542	0.16377358514572	0.93120327222698	n
-1.70153855047430	0.08254913267778	2.62868942367573	c
-3.32215283466870	-2.26009245951710	2.21105604867070	c
2.58351719080444	2.03376712533280	1.94081768730692	c
-0.04063725280725	0.61037344184175	-1.86093129026331	c
1.18560221552357	-1.30793480918921	-3.62381784220939	c
5.10598336393830	1.97320932335907	0.55625398759344	c
1.45430485872301	-1.61821656060465	1.03098847784842	h
-2.74917019913631	1.86250325224936	2.25993200972021	h
-0.99049719129602	0.15151089757259	4.59978284343231	h
-4.93958421813111	-2.19181278753635	3.54734326799875	h
-2.26125441704935	-4.02969840529585	2.61497786458428	h
-4.12845965288405	-2.37679677104274	0.27680645309808	h
2.83843186132410	1.54914106726228	3.96534863345096	h
1.67053144061474	3.92053819224015	1.84289072151859	h
0.53261895273429	2.57619785445090	-2.30431154469721	h
-2.12755766265102	0.52021979999164	-2.00077593609165	h
0.60996689140968	-0.87888622132529	-5.59677817041206	h
0.54840952122318	-3.26790509215914	-3.20770702752654	h
3.28205731382913	-1.24342142911831	-3.55629402995551	h
6.40712956049727	3.30706217062163	1.52343302772673	h
4.96492983335430	2.59366094716725	-1.44230264286171	h
6.00546707182902	0.07487443714321	0.62665759054180	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	selection rules RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	46.58	0.65610	YES	YES
8		a	108.05	0.72904	YES	YES
9		a	147.38	0.01223	YES	YES
10		a	196.73	0.35899	YES	YES
11		a	226.66	0.08717	YES	YES
12		a	235.96	0.08194	YES	YES
13		a	281.61	0.19252	YES	YES
14		a	315.84	0.41157	YES	YES
15		a	332.44	0.53671	YES	YES
16		a	387.19	0.84327	YES	YES
17		a	460.22	0.09990	YES	YES

18	a	471.83	1.53117	YES	YES
19	a	740.56	7.37806	YES	YES
20	a	765.63	15.39144	YES	YES
21	a	781.88	0.42466	YES	YES
22	a	825.60	7.08587	YES	YES
23	a	874.68	2.99507	YES	YES
24	a	878.75	3.51441	YES	YES
25	a	985.81	46.36437	YES	YES
26	a	995.89	18.69679	YES	YES
27	a	1027.44	15.77537	YES	YES
28	a	1039.03	2.87550	YES	YES
29	a	1056.35	1.06127	YES	YES
30	a	1079.49	0.49291	YES	YES
31	a	1130.80	15.05936	YES	YES
32	a	1153.70	6.22307	YES	YES
33	a	1167.28	2.96036	YES	YES
34	a	1252.59	1.14894	YES	YES
35	a	1272.30	1.73057	YES	YES
36	a	1303.46	1.92596	YES	YES
37	a	1315.68	1.48165	YES	YES
38	a	1348.26	0.45053	YES	YES
39	a	1364.28	7.21516	YES	YES
40	a	1374.59	27.13885	YES	YES
41	a	1376.40	14.38550	YES	YES
42	a	1382.51	33.05250	YES	YES
43	a	1391.20	9.09007	YES	YES
44	a	1399.26	22.33170	YES	YES
45	a	1427.06	5.76289	YES	YES
46	a	1431.34	2.01173	YES	YES
47	a	1434.90	19.77286	YES	YES
48	a	1436.63	0.12313	YES	YES
49	a	1440.70	1.19804	YES	YES
50	a	1443.32	5.14006	YES	YES
51	a	1447.82	6.37304	YES	YES
52	a	1452.36	35.39254	YES	YES
53	a	1458.53	40.27641	YES	YES
54	a	2960.51	1.99470	YES	YES
55	a	2960.95	2.49460	YES	YES
56	a	2963.92	3.36495	YES	YES
57	a	2994.51	2.39224	YES	YES
58	a	3000.65	5.91757	YES	YES
59	a	3014.07	3.10494	YES	YES
60	a	3043.60	1.18412	YES	YES
61	a	3045.77	1.41525	YES	YES
62	a	3046.28	1.18992	YES	YES
63	a	3056.70	0.51030	YES	YES
64	a	3058.27	0.80111	YES	YES
65	a	3060.50	0.98540	YES	YES
66	a	3066.13	0.83303	YES	YES
67	a	3069.55	8.05517	YES	YES
68	a	3076.28	3.37228	YES	YES
69	a	3254.13	19.70859	YES	YES

2,6-lutidine



Total energy = -326.6816516110 H = -8889.4650946 eV

HOMO-LUMO Separation

HOMO: 29. 29 a -0.20518745 H = -5.58344 eV

LUMO: 30. 30 a -0.05822093 H = -1.58427 eV

Gap : +0.14696651 H = +3.99916 eV

Number of MOs= 130, Electrons= 58.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -326.6867910217

COSMO(14.3): Total energy + OC corr. [a.u.] = -326,6872047573

COSMO(36.64): Total energy + OC corr. [a.u.] = -326.6876527215

\$scoord

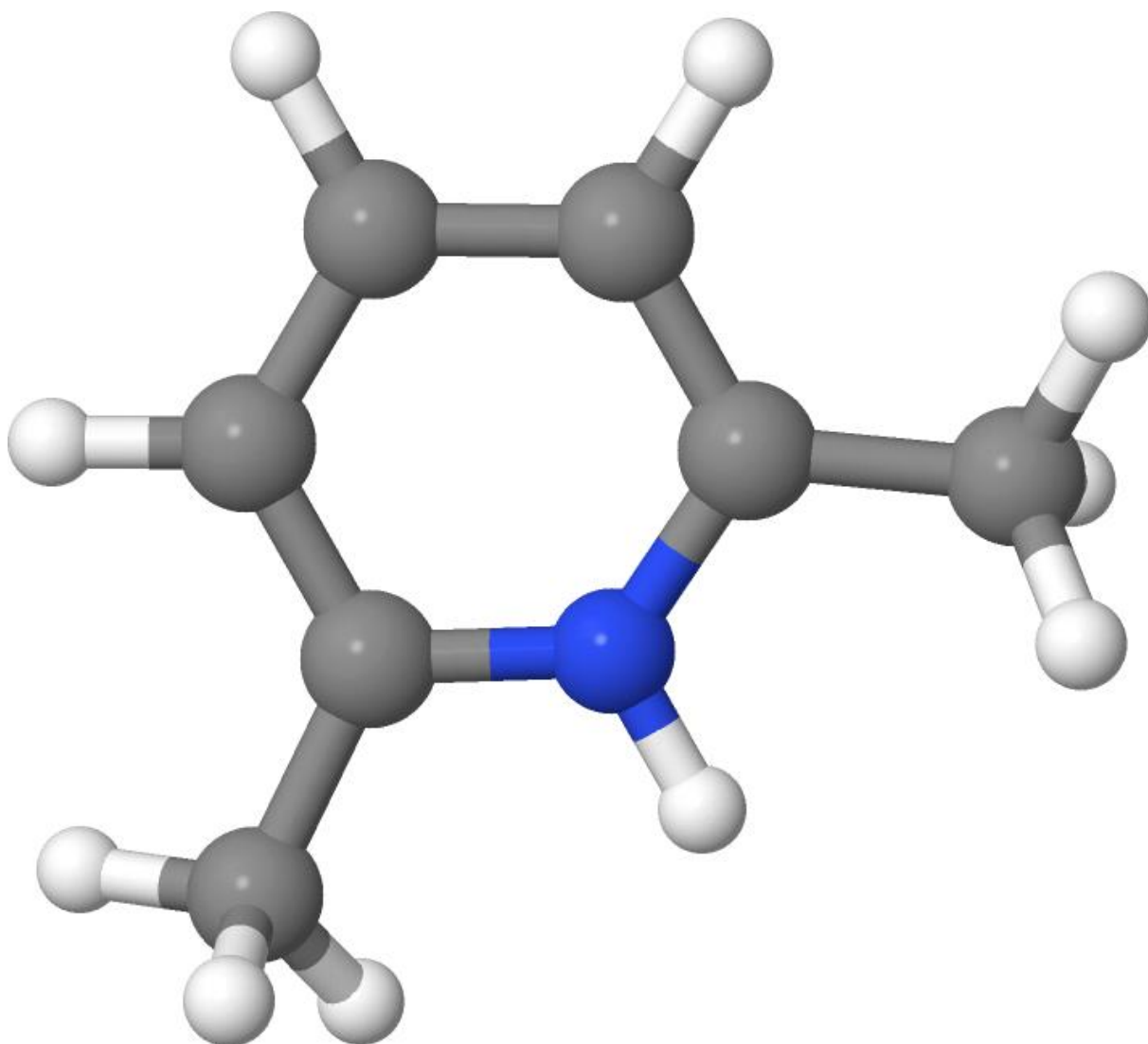
-2.24083169109270	1.59444268312055	0.08322744042329	c
-2.32163963049325	-1.06687585333177	-0.10027737694246	c
-0.04841377567277	-2.39208955902705	-0.41419139001358	c
2.22443762603987	-1.03485869214410	-0.53315737419470	c
2.14277018474572	1.62490451216705	-0.33251953123155	c
-0.04919464807220	2.88800478781860	-0.03131854372288	n
4.51511143356340	3.21544021508289	-0.44549513033826	c
-4.61544413679560	3.15221114607672	0.40884433561209	c
-4.14101151039010	-2.07633379031708	0.00351617192769	h
-0.04786414933915	-4.47147426067070	-0.56241116569494	h
4.04459525056577	-2.01848293902240	-0.77637219103331	h
4.42151842832900	4.54919267947620	-2.06911683203122	h
6.24515192229725	2.04453213246298	-0.63908932292295	h
4.68497972156636	4.39328402690932	1.28753809090090	h
-4.43455997634410	4.41076540172427	2.08232073364108	h
-6.32253818837898	1.95459053463373	0.63939997589830	h
-4.89931779443795	4.40618334253171	-1.25615206850585	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	56.98	0.23146	YES	YES
8		a	62.32	1.72123	YES	YES
9		a	184.61	0.00944	YES	YES
10		a	202.18	7.45786	YES	YES
11		a	275.70	1.22695	YES	YES
12		a	410.70	2.39437	YES	YES
13		a	426.36	0.00146	YES	YES
14		a	530.15	1.68696	YES	YES
15		a	545.27	1.66599	YES	YES
16		a	550.72	0.05317	YES	YES
17		a	711.39	0.75492	YES	YES
18		a	731.14	1.78883	YES	YES
19		a	760.14	24.56685	YES	YES
20		a	878.10	0.00712	YES	YES
21		a	898.06	2.59664	YES	YES
22		a	953.64	0.26397	YES	YES
23		a	970.65	0.01452	YES	YES

24	a	988.43	3.83620	YES	YES
25	a	1021.42	0.67676	YES	YES
26	a	1022.07	12.81749	YES	YES
27	a	1027.04	0.31757	YES	YES
28	a	1086.73	6.19158	YES	YES
29	a	1141.97	2.25517	YES	YES
30	a	1214.16	11.30984	YES	YES
31	a	1260.25	10.64299	YES	YES
32	a	1320.58	0.29528	YES	YES
33	a	1354.65	3.99794	YES	YES
34	a	1357.02	10.37003	YES	YES
35	a	1401.38	3.59834	YES	YES
36	a	1414.04	17.36632	YES	YES
37	a	1414.40	0.38782	YES	YES
38	a	1418.19	1.66459	YES	YES
39	a	1443.95	13.00049	YES	YES
40	a	1459.27	81.33171	YES	YES
41	a	1595.01	67.06657	YES	YES
42	a	1596.58	47.60680	YES	YES
43	a	2946.83	23.75283	YES	YES
44	a	2947.43	7.41816	YES	YES
45	a	3023.57	3.90415	YES	YES
46	a	3023.81	9.87172	YES	YES
47	a	3050.22	14.74275	YES	YES
48	a	3050.78	9.70017	YES	YES
49	a	3088.64	2.58687	YES	YES
50	a	3101.98	22.04481	YES	YES
51	a	3111.23	14.22217	YES	YES

2,6-lutidineH⁺



Total energy = -327.0602070095 H = -8899.7661170 eV

HOMO-LUMO Separation

HOMO: 29. 29 a -0.41895293 H = -11.40030 eV

LUMO: 30. 30 a -0.27146501 H = -7.38694 eV

Gap : +0.14748792 H = +4.01335 eV

Number of MOs= 132, Electrons= 58.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -327.1286344499

COSMO(14.3): Total energy + OC corr. [a.u.] = -327.1333833595

COSMO(36.64): Total energy + OC corr. [a.u.] = -327,1384088041

\$scoord

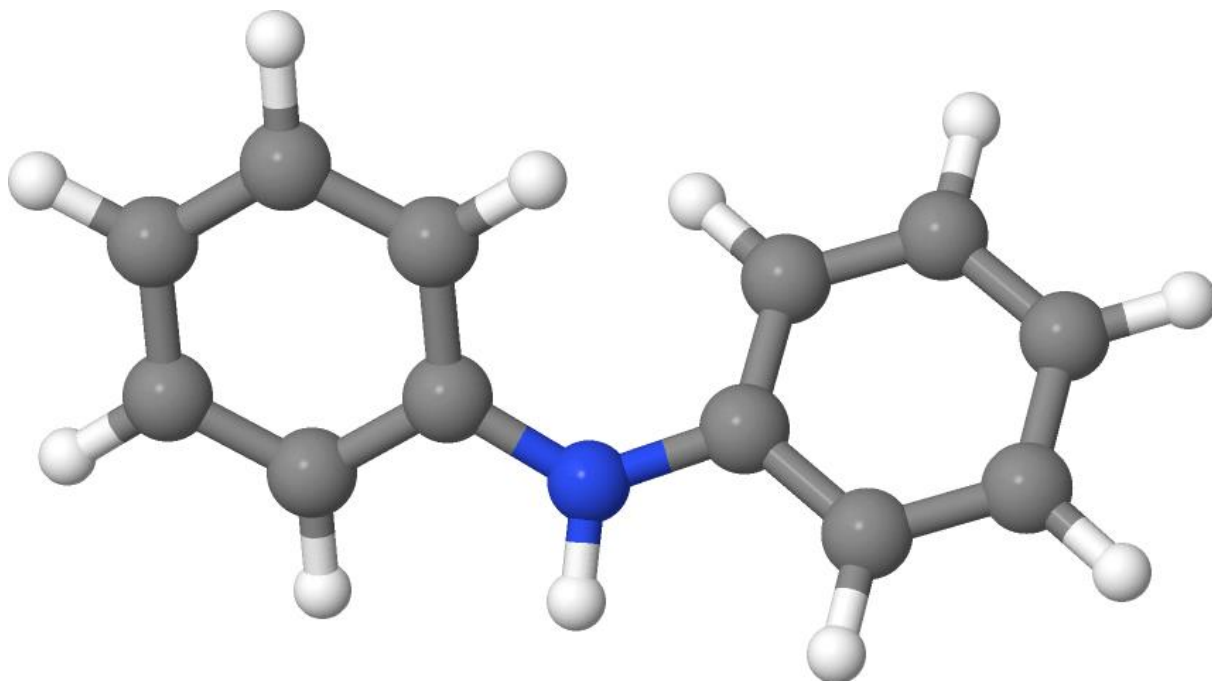
-2.32407498233858	1.32767573868668	0.00794153221230	c
-2.32391409668981	-1.31937083492848	0.01388884001991	c
-0.02072912155153	-2.63879593861693	-0.00484948144284	c
2.28335662210690	-1.32125680533659	-0.02144638411399	c
2.28564003749818	1.32564807148609	-0.01052898661661	c
-0.01858532823378	2.50428544151413	0.00029044605771	n
4.61326601482837	2.93924220129929	0.05462012228288	c
-4.65029575712504	2.94373120411236	-0.05463777789459	c
-4.13949357855971	-2.33266664684578	0.02718228997513	h
-0.02152340378153	-4.72158635230726	-0.00646840364432	h
4.09799996761268	-2.33587754863888	-0.03681723236013	h
-0.01762571694017	4.45246574162870	0.00257525346116	h
5.03826582278099	3.53957355163991	2.02925279356809	h
4.40348973637714	4.67309420698670	-1.11289984018557	h
6.27156941169009	1.87003312172787	-0.64687504330554	h
-4.44311429898261	4.66927582841429	1.12577727121348	h
-6.31209862305656	1.87119998009321	0.63351636901822	h
-5.06761243580638	3.55842860336084	-2.02656408397382	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	47.31	1.61139	YES	YES
8		a	52.49	0.55939	YES	YES
9		a	195.06	1.98026	YES	YES
10		a	198.18	0.00608	YES	YES
11		a	271.26	0.02312	YES	YES
12		a	399.92	5.10678	YES	YES
13		a	409.40	2.42163	YES	YES
14		a	517.63	0.02130	YES	YES
15		a	533.26	0.01760	YES	YES
16		a	553.80	0.00192	YES	YES
17		a	704.27	3.66196	YES	YES
18		a	710.84	0.09851	YES	YES
19		a	773.36	68.97136	YES	YES
20		a	819.48	8.82863	YES	YES
21		a	902.75	0.10796	YES	YES
22		a	915.05	0.95780	YES	YES
23		a	958.47	0.49678	YES	YES
24		a	1001.63	1.13343	YES	YES

25	a	1007.61	0.14180	YES	YES
26	a	1016.62	14.39057	YES	YES
27	a	1023.69	4.12297	YES	YES
28	a	1024.48	23.30493	YES	YES
29	a	1092.14	3.54619	YES	YES
30	a	1162.87	6.80170	YES	YES
31	a	1201.88	0.45824	YES	YES
32	a	1278.80	0.00586	YES	YES
33	a	1322.67	4.49176	YES	YES
34	a	1359.97	6.70620	YES	YES
35	a	1364.16	15.56217	YES	YES
36	a	1368.47	19.03033	YES	YES
37	a	1384.78	4.19494	YES	YES
38	a	1415.25	26.31855	YES	YES
39	a	1422.13	0.01157	YES	YES
40	a	1426.05	30.82325	YES	YES
41	a	1446.35	29.03033	YES	YES
42	a	1533.08	33.65511	YES	YES
43	a	1624.03	150.14478	YES	YES
44	a	1629.93	61.60719	YES	YES
45	a	2949.96	3.84784	YES	YES
46	a	2950.32	2.46598	YES	YES
47	a	3030.15	1.91077	YES	YES
48	a	3030.59	2.04104	YES	YES
49	a	3079.31	0.65525	YES	YES
50	a	3079.53	0.58376	YES	YES
51	a	3127.36	0.04511	YES	YES
52	a	3143.97	3.04648	YES	YES
53	a	3146.57	5.83022	YES	YES
54	a	3380.92	70.55916	YES	YES

NHPh₂



Total energy = -518.2839976124 H = -14103.2331726 eV

HOMO-LUMO Separation

HOMO: 45. 45 a -0.17323023 H = -4.71384 eV

LUMO: 46. 46 a -0.04732360 H = -1.28774 eV

Gap : +0.12590663 H = +3.42610 eV

Number of MOs= 204, Electrons= 90.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -518.2925885447

COSMO(14.3): Total energy + OC corr. [a.u.] = -518.2932649556

COSMO(36.64): Total energy + OC corr. [a.u.] = -518.2939938299

\$coord

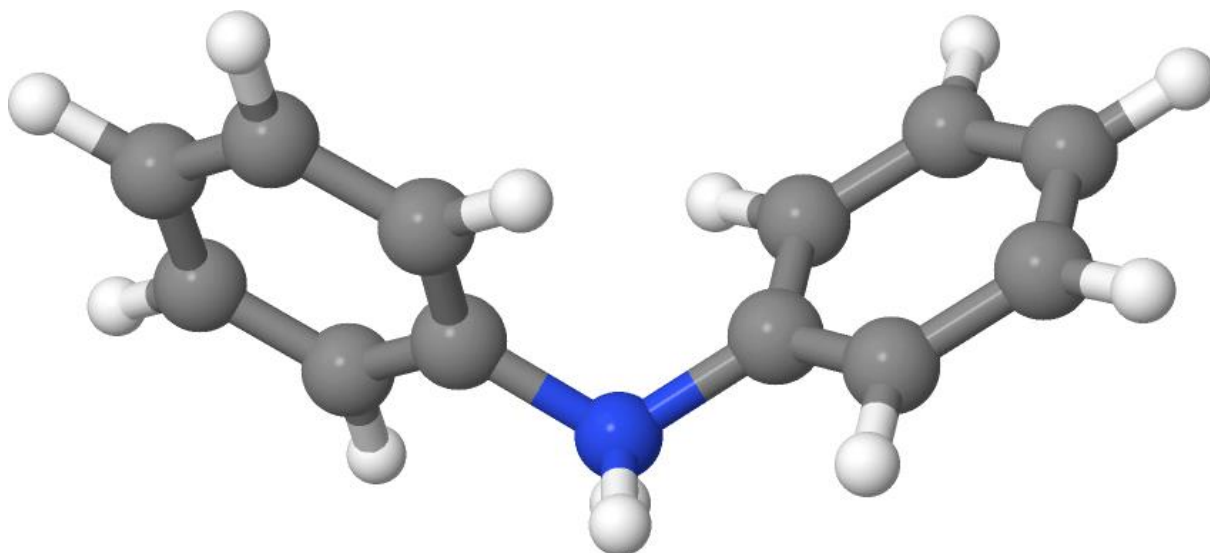
-0.60833367217688	0.94561047446946	-2.11688748957764	n
-0.37839462524717	-1.65065539869512	-2.57777040643245	c
0.87775284085260	2.55585149011599	-0.63198804570914	c
2.35101556878331	1.69753595248425	1.43358538091674	c
3.75129993924243	3.42079422134621	2.88282859034669	c
3.70539946298361	6.02203448998846	2.34677356863497	c
2.21442811902402	6.88844081070823	0.32489485969433	c
0.82977222770010	5.18470131079593	-1.15463715527713	c
-2.54235779446958	-2.99913990794119	-3.40582925472759	c
-2.39749982296848	-5.58004698013861	-3.97739797886093	c
-0.10419203077057	-6.89663389573799	-3.71453012028415	c
2.04997631840318	-5.56936731047825	-2.90600980879111	c
1.93718252469073	-2.97836437116168	-2.35396638002496	c
-2.09111548418089	1.80234319889090	-3.01207940322150	h
2.35094867162688	-0.31763623840517	1.94382581724487	h
4.87827187887303	2.70774307420381	4.48506872126378	h
4.80974846464171	7.36017787039111	3.49795691621844	h
2.13872614792567	8.92220368543651	-0.12478126377472	h
-0.30823591419965	5.88392939695417	-2.75698601085434	h
-4.36038342269962	-1.99271151277319	-3.58973295403308	h
-4.11109002427129	-6.57779345559386	-4.61948345563176	h
0.00443385543317	-8.93076137619196	-4.14536548061745	h
3.87557864366787	-6.55960293658687	-2.72526894372192	h
3.66828826389687	-1.96614450749835	-1.80602570575773	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	43.00	1.11036	YES	YES
8		a	53.70	0.00771	YES	YES
9		a	105.38	0.02819	YES	YES
10		a	216.37	6.10843	YES	YES
11		a	220.73	0.40905	YES	YES
12		a	302.78	0.12924	YES	YES
13		a	332.84	3.96043	YES	YES
14		a	405.90	0.87063	YES	YES
15		a	412.50	0.42910	YES	YES
16		a	426.68	135.47432	YES	YES
17		a	492.13	2.01721	YES	YES
18		a	507.57	10.67167	YES	YES
19		a	562.35	3.42521	YES	YES
20		a	607.13	0.23915	YES	YES
21		a	611.37	1.43553	YES	YES
22		a	635.94	1.30488	YES	YES
23		a	689.27	58.83768	YES	YES
24		a	697.79	7.17776	YES	YES
25		a	743.93	3.87516	YES	YES
26		a	746.12	63.35511	YES	YES
27		a	800.80	0.10373	YES	YES
28		a	802.61	1.75263	YES	YES
29		a	819.10	0.00473	YES	YES
30		a	867.55	6.41774	YES	YES
31		a	875.79	3.09540	YES	YES
32		a	881.29	0.91612	YES	YES
33		a	938.59	0.21825	YES	YES
34		a	944.29	0.04005	YES	YES
35		a	964.17	0.63660	YES	YES
36		a	968.61	0.18934	YES	YES
37		a	977.09	3.33843	YES	YES
38		a	978.49	0.29285	YES	YES
39		a	1026.10	8.39685	YES	YES
40		a	1027.92	0.32966	YES	YES
41		a	1072.83	3.14676	YES	YES
42		a	1084.66	10.76778	YES	YES
43		a	1137.97	0.41495	YES	YES
44		a	1138.69	1.22371	YES	YES
45		a	1158.25	11.71054	YES	YES
46		a	1164.56	1.78734	YES	YES
47		a	1230.50	3.52008	YES	YES
48		a	1252.04	11.30609	YES	YES
49		a	1310.29	0.59198	YES	YES
50		a	1316.66	100.26918	YES	YES
51		a	1370.30	91.34436	YES	YES
52		a	1374.66	4.40765	YES	YES
53		a	1423.43	9.77043	YES	YES
54		a	1458.56	2.78316	YES	YES
55		a	1489.14	122.53874	YES	YES
56		a	1494.38	4.33164	YES	YES
57		a	1524.36	342.58669	YES	YES

58	a	1594.42	8.83101	YES	YES
59	a	1600.86	16.54090	YES	YES
60	a	1615.67	317.76399	YES	YES
61	a	1628.32	5.80388	YES	YES
62	a	3077.28	12.51819	YES	YES
63	a	3077.85	11.86136	YES	YES
64	a	3090.79	2.19969	YES	YES
65	a	3091.36	1.09602	YES	YES
66	a	3099.70	9.39872	YES	YES
67	a	3099.95	34.39118	YES	YES
68	a	3115.65	45.65906	YES	YES
69	a	3116.66	1.03993	YES	YES
70	a	3122.99	1.05900	YES	YES
71	a	3129.26	3.09120	YES	YES
72	a	3461.98	18.24412	YES	YES

H₂NPh₂⁺



Total energy = -518.6311872843 H = -14112.6806897 eV

HOMO-LUMO Separation

HOMO: 45. 45 a -0.37796117 H = -10.28485 eV

LUMO: 46. 46 a -0.20554651 H = -5.59321 eV

Gap : +0.17241466 H = +4.69164 eV

Number of MOs= 206, Electrons= 90.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -518.7024134406

COSMO(14.3): Total energy + OC corr. [a.u.] = -518.707573322

COSMO(36.64): Total energy + OC corr. [a.u.] = -518.7130746692

\$coord

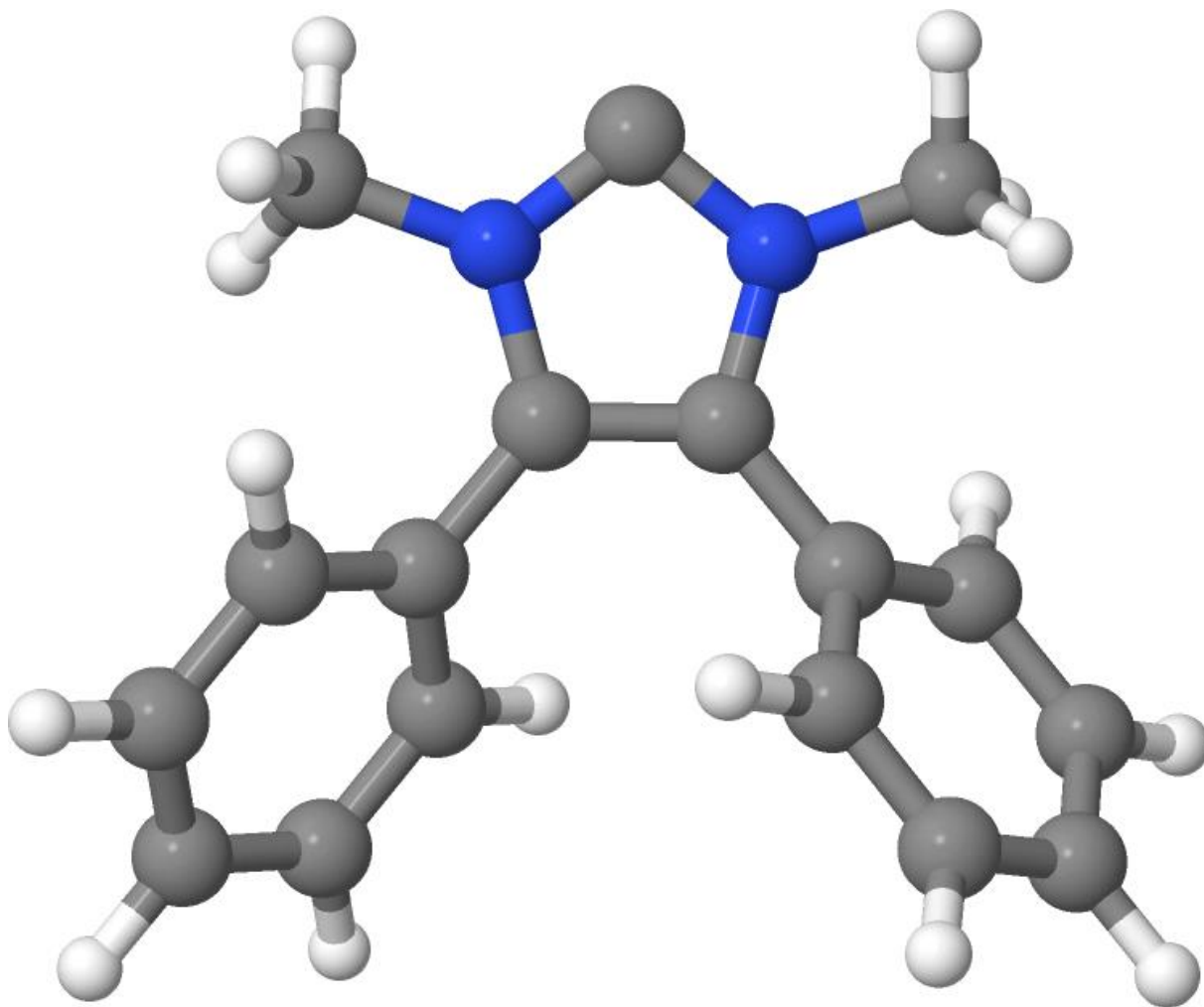
-0.57379732842554	2.71743192721442	0.42084300237543	c
-3.24499435697218	1.82550495109452	0.77186515417426	n
-3.75522104872347	-0.90638137178385	0.22104108630111	c
1.38021570744966	1.41174667829921	1.64038701728888	c
3.86042885084142	2.30498384367605	1.33838854898700	c
4.34434639800966	4.44775938319276	-0.15981887773953	c
2.35109729766644	5.71587738850679	-1.37036695000391	c
-0.14554536300430	4.85192529270873	-1.08353401764249	c
-4.69162056651711	-2.43431624052671	2.16773738034286	c
-5.18842686884008	-4.99111608004575	1.64026184964061	c
-4.74819743478734	-5.95656064085028	-0.79284602858799	c
-3.80468095306762	-4.37895653521446	-2.71447850026919	c
-3.29037521954767	-1.82382235259318	-2.21946693198841	c
-4.40766878271970	2.94592964529263	-0.35350150657722	h
-3.81473906625871	2.18508076300887	2.62162391737799	h
0.99476588374064	-0.27902116238940	2.79238910073354	h
5.42666488684753	1.30989969424548	2.28118503793623	h
6.29687304982073	5.13223439304167	-0.38775839689717	h
2.72621507054261	7.39058972433127	-2.54751339790937	h
-1.71444402974527	5.85322672990514	-2.02528788378033	h
-5.04549876432583	-1.67041339227560	4.07587687614145	h
-5.92631262222092	-6.22348910095061	3.14633781979065	h
-5.14280258784247	-7.95961100921520	-1.19892846900602	h
-3.45976181083420	-5.14001363975916	-4.62064945783843	h
-2.52927388317058	-0.58693400334526	-3.71162754073731	h

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	24.53	0.90418	YES	YES
8		a	28.71	0.58195	YES	YES
9		a	66.19	0.10313	YES	YES
10		a	194.46	6.55372	YES	YES
11		a	225.71	1.69189	YES	YES
12		a	283.33	0.17078	YES	YES
13		a	345.06	7.43792	YES	YES
14		a	402.37	0.19183	YES	YES
15		a	403.35	0.00591	YES	YES
16		a	442.14	1.15532	YES	YES
17		a	461.25	14.67459	YES	YES
18		a	547.05	8.95769	YES	YES
19		a	597.97	10.05043	YES	YES

20	a	607.44	2.17046	YES	YES
21	a	608.84	8.62970	YES	YES
22	a	688.29	21.60539	YES	YES
23	a	690.95	29.18576	YES	YES
24	a	730.13	29.13891	YES	YES
25	a	734.10	38.01664	YES	YES
26	a	792.87	3.48054	YES	YES
27	a	797.91	4.00364	YES	YES
28	a	809.34	0.09791	YES	YES
29	a	810.46	0.01416	YES	YES
30	a	884.12	2.71954	YES	YES
31	a	904.54	0.08636	YES	YES
32	a	918.31	2.71270	YES	YES
33	a	960.30	0.00374	YES	YES
34	a	960.73	0.00295	YES	YES
35	a	981.55	18.98534	YES	YES
36	a	986.24	0.72061	YES	YES
37	a	1002.44	0.01365	YES	YES
38	a	1002.59	0.01094	YES	YES
39	a	1021.07	0.25974	YES	YES
40	a	1021.75	3.12470	YES	YES
41	a	1078.30	4.62451	YES	YES
42	a	1083.92	14.86033	YES	YES
43	a	1125.26	3.84556	YES	YES
44	a	1142.26	0.11690	YES	YES
45	a	1153.15	0.06428	YES	YES
46	a	1153.69	0.15773	YES	YES
47	a	1161.73	2.00891	YES	YES
48	a	1163.46	0.87040	YES	YES
49	a	1211.95	2.34763	YES	YES
50	a	1291.32	6.70329	YES	YES
51	a	1322.00	2.41307	YES	YES
52	a	1342.97	32.45082	YES	YES
53	a	1385.68	10.07080	YES	YES
54	a	1387.87	1.36571	YES	YES
55	a	1464.87	15.26029	YES	YES
56	a	1469.14	6.50316	YES	YES
57	a	1479.71	32.29869	YES	YES
58	a	1482.05	11.20428	YES	YES
59	a	1576.12	55.21517	YES	YES
60	a	1598.80	2.92327	YES	YES
61	a	1605.46	2.46845	YES	YES
62	a	1623.57	8.25148	YES	YES
63	a	1631.85	0.47994	YES	YES
64	a	3089.88	2.31299	YES	YES
65	a	3091.69	2.42128	YES	YES
66	a	3111.54	0.50315	YES	YES
67	a	3112.83	0.40971	YES	YES
68	a	3121.87	0.22814	YES	YES
69	a	3122.03	0.22414	YES	YES
70	a	3130.61	0.00601	YES	YES
71	a	3130.78	0.00233	YES	YES
72	a	3137.75	0.01588	YES	YES
73	a	3137.84	0.01903	YES	YES
74	a	3223.62	40.59925	YES	YES
75	a	3263.93	50.27334	YES	YES

NHC



Total energy = -766.3636041728 H = -20853.8265786 eV

HOMO-LUMO Separation

HOMO: 66. 66 a -0.16699696 H = -4.54422 eV

LUMO: 67. 67 a -0.06695452 H = -1.82193 eV

Gap : +0.10004244 H = +2.72229 eV

Number of MOs= 298, Electrons= 132.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -766.3764278717

COSMO(14.3): Total energy + OC corr. [a.u.] = -766.377472578

COSMO(36.64): Total energy + OC corr. [a.u.] = -766.3786085406

\$scoord

1.10680996834233	1.37085618806531	-1.31275917751558	c
1.41908289674881	-1.15765254658460	-0.67057807992238	c
3.88712056456037	-1.78392111520448	-1.43511717972638	n
5.15241861599859	0.19495064601792	-2.53904544062607	c
3.39863899245174	2.10558556441561	-2.44140776307015	n
-1.13404011013115	3.00794234385970	-1.02880298999570	c
-0.34089027563668	-2.88109848883659	0.63780708525602	c
-1.57387712796242	-2.09450603575963	2.88121566368699	c
-3.26521393852897	-3.70087376512767	4.14008681356658	c
-3.75411737663987	-6.13714469553886	3.19858873876891	c
-2.54344026260988	-6.94667562939799	0.97748885916034	c
-0.86184458316809	-5.33667696475942	-0.29404318622457	c
-0.96571289013400	5.44388291356654	0.07014612384756	c
-3.11757866174466	6.97446602377847	0.32370334320308	c
-5.48687306641464	6.10189865503672	-0.50084416668087	c
-5.68610740215105	3.68321101687594	-1.58334851860979	c
-3.53589404101163	2.15644035151821	-1.85223004775905	c
5.11009831761182	-4.21835164298186	-1.03847352175511	c
3.91754146740224	4.58056790360019	-3.53064567421278	c
-1.17404890102676	-0.19916903717819	3.64414064958651	h
-4.19906840981518	-3.04739861709969	5.88476097594692	h
-5.07731728340829	-7.40196726235892	4.19398980503569	h
-2.92494426333593	-8.84782860370006	0.21351674383080	h
0.02772347866771	-5.97776992179319	-2.06371930855779	h
0.86877668632572	6.13054274916614	0.77628955598872	h
-2.94305728976386	8.86131214508142	1.19142018200122	h
-7.17634474735898	7.30447730476044	-0.29889088574868	h
-7.53511569159751	2.98207261494719	-2.24097334319776	h
-3.69621915528327	0.27529599372526	-2.72940188332350	h
7.16742080633865	-3.92026229003150	-1.27812006228849	h
4.46991151796690	-5.64955360094967	-2.43869289704028	h
4.71223543837379	-4.94122766787124	0.89152209063862	h
5.59275851650123	4.36926209191498	-4.76678030106858	h
4.34831286164026	6.00848678612084	-2.05009707416528	h
2.27844786897600	5.25329521821408	-4.65569984416441	h

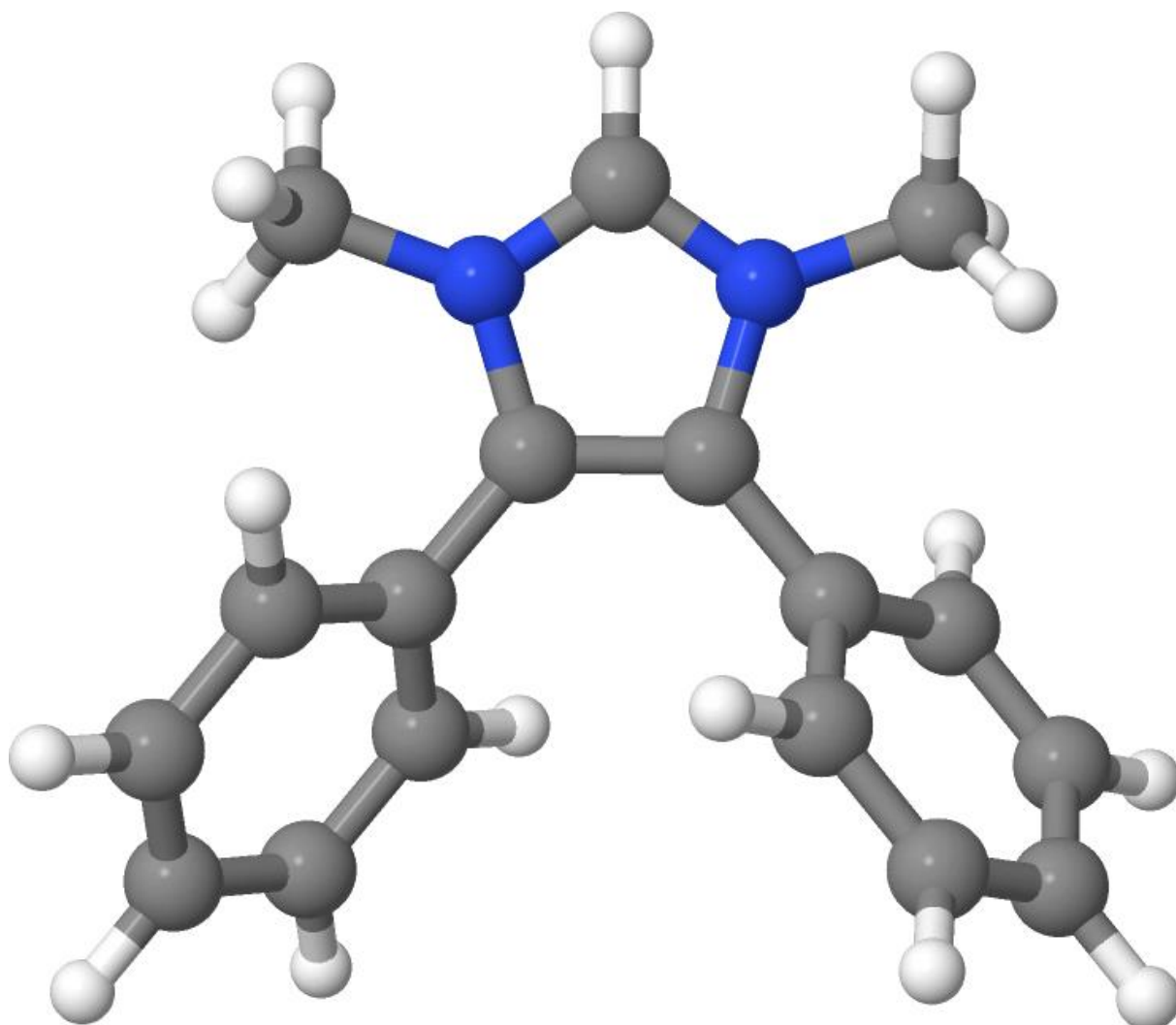
\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	42.26	0.37026	YES	YES

8	a	51.06	0.05882	YES	YES
9	a	53.04	0.05808	YES	YES
10	a	66.29	0.24554	YES	YES
11	a	90.75	0.29741	YES	YES
12	a	124.41	0.03403	YES	YES
13	a	144.94	2.19131	YES	YES
14	a	157.03	0.90685	YES	YES
15	a	196.33	6.08889	YES	YES
16	a	204.23	0.28730	YES	YES
17	a	248.96	1.10500	YES	YES
18	a	249.78	0.00909	YES	YES
19	a	273.96	2.46016	YES	YES
20	a	309.91	0.36396	YES	YES
21	a	350.61	1.58372	YES	YES
22	a	391.24	0.95964	YES	YES
23	a	399.88	0.95778	YES	YES
24	a	404.54	0.00623	YES	YES
25	a	405.84	0.00637	YES	YES
26	a	495.79	5.49778	YES	YES
27	a	503.60	5.09233	YES	YES
28	a	604.69	12.19803	YES	YES
29	a	605.62	0.46212	YES	YES
30	a	609.79	0.01786	YES	YES
31	a	620.81	5.43964	YES	YES
32	a	621.66	6.31254	YES	YES
33	a	644.29	4.05409	YES	YES
34	a	687.99	5.99179	YES	YES
35	a	697.58	23.63350	YES	YES
36	a	699.51	51.49263	YES	YES
37	a	706.76	0.77156	YES	YES
38	a	755.71	24.63165	YES	YES
39	a	766.17	8.30275	YES	YES
40	a	832.36	0.07033	YES	YES
41	a	834.32	0.10197	YES	YES
42	a	851.39	7.52287	YES	YES
43	a	906.36	1.64877	YES	YES
44	a	909.41	5.55781	YES	YES
45	a	955.62	0.13601	YES	YES
46	a	957.11	0.16701	YES	YES
47	a	979.31	0.31115	YES	YES
48	a	980.06	0.41679	YES	YES
49	a	983.45	1.13983	YES	YES
50	a	984.49	1.32554	YES	YES
51	a	993.32	11.09396	YES	YES
52	a	1018.88	16.99643	YES	YES
53	a	1030.91	0.38691	YES	YES
54	a	1040.51	3.20480	YES	YES
55	a	1041.79	4.13930	YES	YES
56	a	1053.18	1.27441	YES	YES
57	a	1072.77	0.92449	YES	YES
58	a	1076.38	13.80035	YES	YES
59	a	1113.42	2.15240	YES	YES
60	a	1115.00	2.34592	YES	YES
61	a	1141.11	0.01534	YES	YES
62	a	1141.27	0.00981	YES	YES
63	a	1161.52	0.18108	YES	YES
64	a	1162.99	0.18758	YES	YES
65	a	1189.73	0.32998	YES	YES
66	a	1253.28	13.31689	YES	YES

67	a	1286.84	0.11172	YES	YES
68	a	1291.62	1.00962	YES	YES
69	a	1293.44	0.65688	YES	YES
70	a	1346.77	22.48913	YES	YES
71	a	1357.74	0.41959	YES	YES
72	a	1358.24	0.25351	YES	YES
73	a	1366.37	24.27417	YES	YES
74	a	1375.27	7.84451	YES	YES
75	a	1395.14	15.65886	YES	YES
76	a	1401.48	22.48078	YES	YES
77	a	1432.38	3.18699	YES	YES
78	a	1433.88	11.66275	YES	YES
79	a	1436.56	0.32007	YES	YES
80	a	1441.95	12.98310	YES	YES
81	a	1447.69	33.32080	YES	YES
82	a	1449.56	10.88150	YES	YES
83	a	1481.15	9.88198	YES	YES
84	a	1496.57	29.75135	YES	YES
85	a	1578.32	3.16351	YES	YES
86	a	1585.95	3.49511	YES	YES
87	a	1603.01	0.61788	YES	YES
88	a	1615.89	21.87441	YES	YES
89	a	1620.71	17.56090	YES	YES
90	a	2953.42	68.40990	YES	YES
91	a	2955.41	32.52443	YES	YES
92	a	3033.97	11.23102	YES	YES
93	a	3035.62	12.23757	YES	YES
94	a	3084.14	5.62205	YES	YES
95	a	3084.43	0.10724	YES	YES
96	a	3088.10	2.08603	YES	YES
97	a	3088.18	1.56475	YES	YES
98	a	3096.15	4.30578	YES	YES
99	a	3096.36	2.50899	YES	YES
100	a	3106.11	18.35306	YES	YES
101	a	3106.65	17.61790	YES	YES
102	a	3112.59	33.64209	YES	YES
103	a	3112.82	8.96608	YES	YES
104	a	3118.28	7.29053	YES	YES
105	a	3118.47	6.31411	YES	YES

HNHC⁺



Total energy = -766.8036260825 H = -20865.8001908 eV

HOMO-LUMO Separation

HOMO: 66. 66 a -0.33339426 H = -9.07212 eV

LUMO: 67. 67 a -0.20249783 H = -5.51025 eV

Gap : +0.13089643 H = +3.56188 eV

Number of MOs= 300, Electrons= 132.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -766.8625397058

COSMO(14.3): Total energy + OC corr. [a.u.] = -766.8668014243

COSMO(36.64): Total energy + OC corr. [a.u.] = -766.8713450863

\$coord

1.10452409258215	1.37327930701446	-1.33389396063332	c
1.43213487334020	-1.15748011869954	-0.65195986777971	c
3.88655006461725	-1.82286465826094	-1.39017395830943	n
4.99823321016267	0.19162206085769	-2.47604460465017	c
3.36809503664847	2.14498494607473	-2.47116181932105	n
-1.13496506273073	3.01531142694891	-1.07619565482882	c
-0.30869689623500	-2.88658929121516	0.67292406271501	c
-1.43429334805890	-2.11722741762284	2.97411728348660	c
-3.10633843165448	-3.73213228790007	4.24687145186380	c
-3.67717329449376	-6.12531641947613	3.24346358594068	c
-2.57571205346264	-6.90160301826205	0.95400706275210	c
-0.90313999165488	-5.29455527716459	-0.33094835497985	c
-0.97028012698357	5.40629100747438	0.11383543635178	c
-3.12595689034794	6.93244216684226	0.35005843151276	c
-5.46421862786343	6.09045250043205	-0.58836984435881	c
-5.64672201655892	3.71284069444987	-1.76055460821507	c
-3.49960136497205	2.17849047238813	-2.00527553835626	c
5.12977047966836	-4.26868215281928	-0.99226022936657	c
3.90119435224515	4.63109472506344	-3.57719564976348	c
6.92322824798860	0.23453011392026	-3.24180305091454	h
-0.97762822729378	-0.24998990551749	3.77325666614008	h
-3.96368640220903	-3.11863751439041	6.04234956198931	h
-4.99132961815838	-7.39027742269854	4.24821565944246	h
-3.03564223190065	-8.76725955067479	0.151744402657708	h
-0.09914783151625	-5.90051130295751	-2.15446837812683	h
0.84045180719764	6.06049269368946	0.90974078085551	h
-2.98134525868032	8.78475515978631	1.29020200332812	h
-7.15462754416104	7.29189068537698	-0.40016374331903	h
-7.47652557193423	3.04933533288285	-2.49999050718120	h
-3.64416571143059	0.32404222003686	-2.94011909740494	h
7.20104908049585	-3.97528482430867	-0.91892966009103	h
4.66636914683315	-5.59672542966015	-2.54657581860760	h
4.47412292692726	-5.07565725627077	0.82396161921105	h
5.37268658431303	4.41823051461357	-5.05091092792629	h
4.57097046320398	5.96708057276022	-2.10757081962770	h
2.14886787309758	5.37949259767709	-4.44258807490323	h

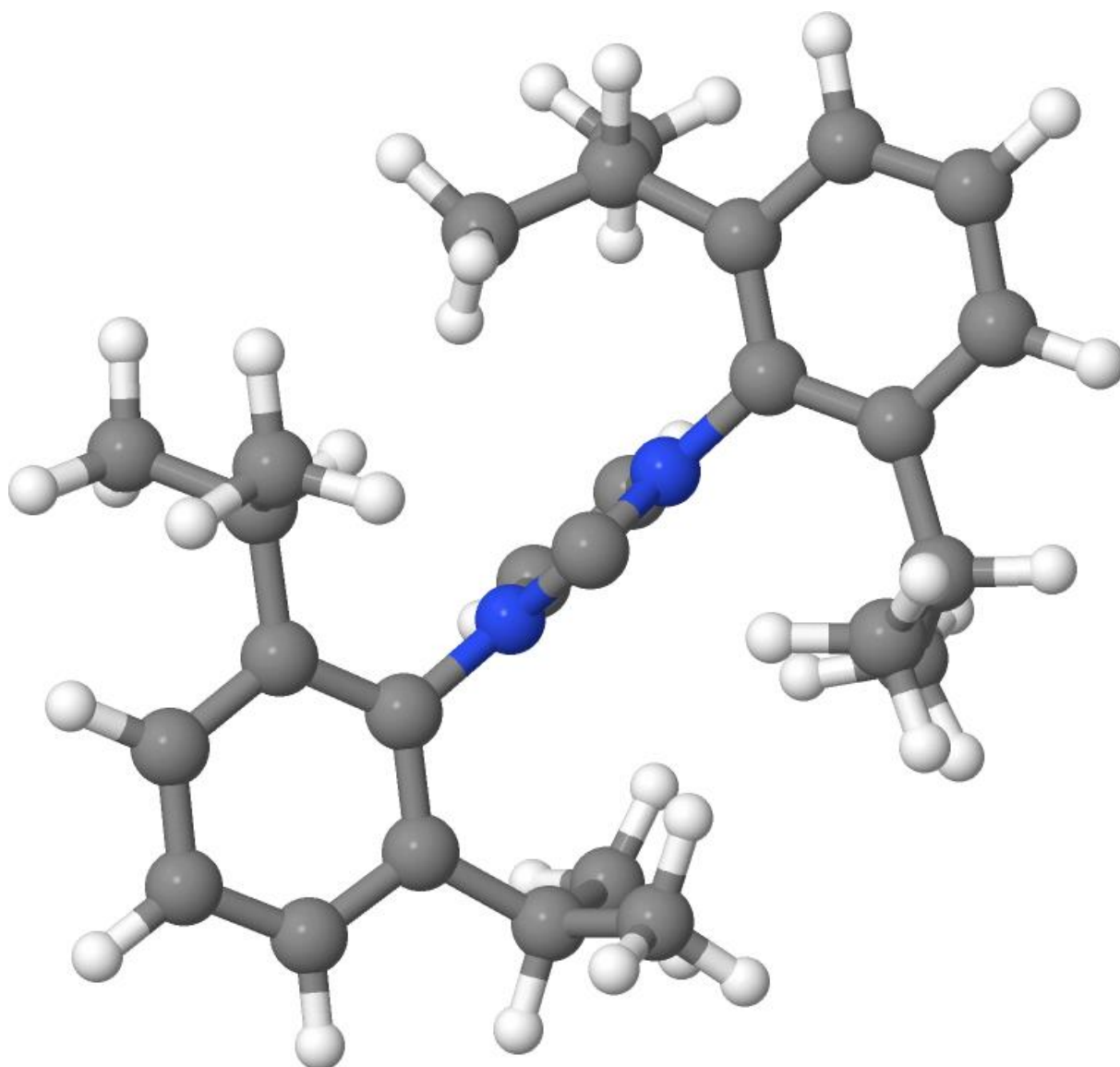
\$vibrational spectrum

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3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	39.76	0.13943	YES	YES
8		a	46.29	0.00069	YES	YES

9	a	51.13	0.06764	YES	YES
10	a	63.89	0.00612	YES	YES
11	a	91.74	4.30647	YES	YES
12	a	108.52	0.13045	YES	YES
13	a	121.56	1.25595	YES	YES
14	a	139.85	0.07615	YES	YES
15	a	187.83	1.41109	YES	YES
16	a	198.75	0.00891	YES	YES
17	a	245.84	0.02906	YES	YES
18	a	246.51	0.54856	YES	YES
19	a	265.78	5.80445	YES	YES
20	a	309.07	2.07859	YES	YES
21	a	351.88	0.08184	YES	YES
22	a	395.08	1.64398	YES	YES
23	a	396.90	0.12916	YES	YES
24	a	399.84	0.40089	YES	YES
25	a	400.67	0.30479	YES	YES
26	a	485.82	2.75694	YES	YES
27	a	498.65	7.05145	YES	YES
28	a	590.36	4.38119	YES	YES
29	a	606.62	4.53098	YES	YES
30	a	607.46	2.73574	YES	YES
31	a	607.92	1.42599	YES	YES
32	a	625.70	13.04050	YES	YES
33	a	646.16	3.59273	YES	YES
34	a	691.92	7.43317	YES	YES
35	a	698.50	43.85970	YES	YES
36	a	699.52	20.77776	YES	YES
37	a	720.33	6.84688	YES	YES
38	a	725.21	5.33510	YES	YES
39	a	754.23	30.79347	YES	YES
40	a	770.16	8.57085	YES	YES
41	a	834.01	0.30173	YES	YES
42	a	835.35	0.32441	YES	YES
43	a	842.00	7.11590	YES	YES
44	a	918.63	1.17473	YES	YES
45	a	920.25	2.42213	YES	YES
46	a	963.96	0.31781	YES	YES
47	a	964.62	0.43777	YES	YES
48	a	983.99	6.67127	YES	YES
49	a	984.74	5.52505	YES	YES
50	a	997.61	0.06059	YES	YES
51	a	997.82	0.02959	YES	YES
52	a	1005.91	1.33845	YES	YES
53	a	1017.58	4.52401	YES	YES
54	a	1032.55	0.35215	YES	YES
55	a	1043.54	0.26894	YES	YES
56	a	1063.75	0.53524	YES	YES
57	a	1074.44	4.88870	YES	YES
58	a	1077.49	1.57610	YES	YES
59	a	1082.40	14.00224	YES	YES
60	a	1107.20	1.06648	YES	YES
61	a	1112.72	1.50012	YES	YES
62	a	1150.02	0.05897	YES	YES
63	a	1150.11	0.03700	YES	YES
64	a	1163.49	0.96003	YES	YES
65	a	1165.85	0.63969	YES	YES
66	a	1177.54	33.38330	YES	YES
67	a	1185.93	1.00090	YES	YES

68	a	1288.24	6.51006	YES	YES
69	a	1291.23	0.32439	YES	YES
70	a	1297.48	2.78971	YES	YES
71	a	1321.46	0.26689	YES	YES
72	a	1362.89	1.54258	YES	YES
73	a	1364.70	0.14507	YES	YES
74	a	1390.16	4.38984	YES	YES
75	a	1392.46	30.87411	YES	YES
76	a	1407.89	16.67958	YES	YES
77	a	1420.11	24.70261	YES	YES
78	a	1423.13	35.33258	YES	YES
79	a	1429.13	22.08859	YES	YES
80	a	1437.84	13.92168	YES	YES
81	a	1438.92	8.65937	YES	YES
82	a	1454.77	4.59195	YES	YES
83	a	1456.35	3.69333	YES	YES
84	a	1485.87	4.10777	YES	YES
85	a	1499.57	0.23644	YES	YES
86	a	1570.18	50.91383	YES	YES
87	a	1576.74	10.03884	YES	YES
88	a	1590.45	4.05038	YES	YES
89	a	1599.47	9.61703	YES	YES
90	a	1614.40	4.66540	YES	YES
91	a	1615.62	14.95594	YES	YES
92	a	2987.28	5.64599	YES	YES
93	a	2987.42	5.88624	YES	YES
94	a	3082.82	3.67720	YES	YES
95	a	3082.95	0.20290	YES	YES
96	a	3097.71	3.38637	YES	YES
97	a	3098.39	3.05734	YES	YES
98	a	3100.87	0.80057	YES	YES
99	a	3101.78	0.63796	YES	YES
100	a	3107.39	1.09796	YES	YES
101	a	3107.54	0.24232	YES	YES
102	a	3114.55	2.16846	YES	YES
103	a	3114.66	0.73009	YES	YES
104	a	3121.98	6.41459	YES	YES
105	a	3122.07	3.38930	YES	YES
106	a	3129.74	2.14243	YES	YES
107	a	3129.76	2.04754	YES	YES
108	a	3202.02	36.20969	YES	YES

Idipp



Total energy = -1159.1387699340 H = -31541.7887242 eV

HOMO-LUMO Separation

HOMO: 106. 106 a -0.17440807 H = -4.74589 eV

LUMO: 107. 107 a -0.04879343 H = -1.32774 eV

Gap : +0.12561464 H = +3.41815 eV

Number of MOs= 478, Electrons= 212.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -1159.1488723597

COSMO(14.3): Total energy + OC corr. [a.u.] = -1159.1497271125

COSMO(36.64): Total energy + OC corr. [a.u.] = -1159.1506612741

\$coord

1.60706910264073	-1.90005155643397	2.22291748887186	n
0.25588467608966	-3.95921434476391	3.18941097439821	c
-2.22347506896786	-3.23036024661690	3.27272369728183	c
-2.29109124852033	-0.73194860708935	2.39678802589189	n
0.06866815982113	0.15139617812400	1.68887633044378	c
4.31973761011986	-1.97309414923109	1.80145511840536	c
-4.64193259293179	0.65405882921753	2.06984800773213	c
5.31825762618128	-3.47560901316666	-0.20482170281777	c
7.96980727707297	-3.52373703339617	-0.52991440904758	c
9.60234491768462	-2.16390118802273	1.03388242143205	c
8.58406681333800	-0.71643101976377	2.99441896578190	c
5.95787984001409	-0.58789928193574	3.44028392326507	c
-5.90448977985081	1.76140269463738	4.17920628341105	c
-8.24714554290836	2.95787885105802	3.72138516262297	c
-9.30662121305271	3.10769388643179	1.30393952733633	c
-8.01382281845782	2.04945633699873	-0.74167559063754	c
-5.68511989737795	0.79936097732126	-0.40805377754083	c
5.15103744194473	1.08913552013936	5.66367927302171	c
3.34154717203863	-0.16391041009074	7.57012138596715	c
4.24465428700914	3.71311649863283	4.75496747223439	c
3.85900801628475	-5.14370722580184	-2.09011376575979	c
1.31450255732414	-4.15322327267389	-3.07675951845513	c
3.62965515587381	-7.90422043654048	-1.15334817486173	c
-4.33568763445636	-0.27029712091814	-2.72095446243973	c
-2.92757724580459	1.85660215541443	-4.14129628020930	c
-6.09880881873935	-1.76271588394754	-4.49785328643349	c
-4.90061757645363	1.96879830154891	6.89475385955591	c
-2.66917648932482	3.83970196945482	7.04679341055677	c
-4.34811250140585	-0.53210861877432	8.28365686515218	c
1.16596925464105	-5.72149209588920	3.78135142931728	h
-3.91881636483452	-4.25207766129571	3.87960077134337	h
8.75651118694391	-4.66549606476712	-2.08770255218059	h
11.66189212179228	-2.23161435522561	0.72690415500189	h
9.85567922421812	0.35650129979051	4.25050819424164	h
-9.24829507173519	3.82234009179800	5.33287076813598	h
-11.13577770735752	4.06367713560354	1.01723590836382	h
-8.83089674503301	2.18508299844892	-2.65185922809148	h
6.93103212820133	1.42487377303134	6.73668220594961	h
3.14505469679039	1.06339726577553	9.26654807124597	h
4.09081228049255	-2.02150708850702	8.21022941297506	h
1.42254643792827	-0.47302813801571	6.79458307017701	h
3.78164518251802	4.93954925298521	6.40076532332449	h
2.55179668313007	3.53175495291060	3.52152003960310	h
5.75274584265739	4.66507168968506	3.64120712847480	h
5.12523750865941	-5.22130671655003	-3.76871773972522	h

0.77238214769199	-5.22516547165242	-4.80392489763792	h
1.41641434448275	-2.11861871948375	-3.57615087817506	h
-0.22513352223485	-4.41622812620186	-1.67771329771758	h
2.88019140456370	-9.13183048334993	-2.68934208462493	h
2.31514823631104	-8.06536509401509	0.47674981016642	h
5.49344461054419	-8.67187813718653	-0.55997467838146	h
-2.88123725042525	-1.60598708039364	-2.03273851030743	h
-1.91824765210322	1.08193844343274	-5.81718997281604	h
-1.51422932903285	2.76313735385725	-2.87941047671590	h
-4.26736394546204	3.33269669890871	-4.81738866269352	h
-4.96931146819996	-2.70762105384101	-5.99879766615433	h
-7.49496851518329	-0.52637492206934	-5.47120975773615	h
-7.16753740597475	-3.24686876312361	-3.46143251491949	h
-6.48048487671042	2.85332258563077	7.96501822708505	h
-2.05181909383754	4.08496261620416	9.04332165131928	h
-3.22385200609890	5.72437586322190	6.30138839249470	h
-1.02566415428530	3.17666886491784	5.92705803067709	h
-4.07887834726588	-0.15075679040869	10.33510773521547	h
-2.61165887912562	-1.47772351532075	7.58938029556263	h
-5.94951200082743	-1.88150637223321	8.09389714117023	h

\$vibrational spectrum

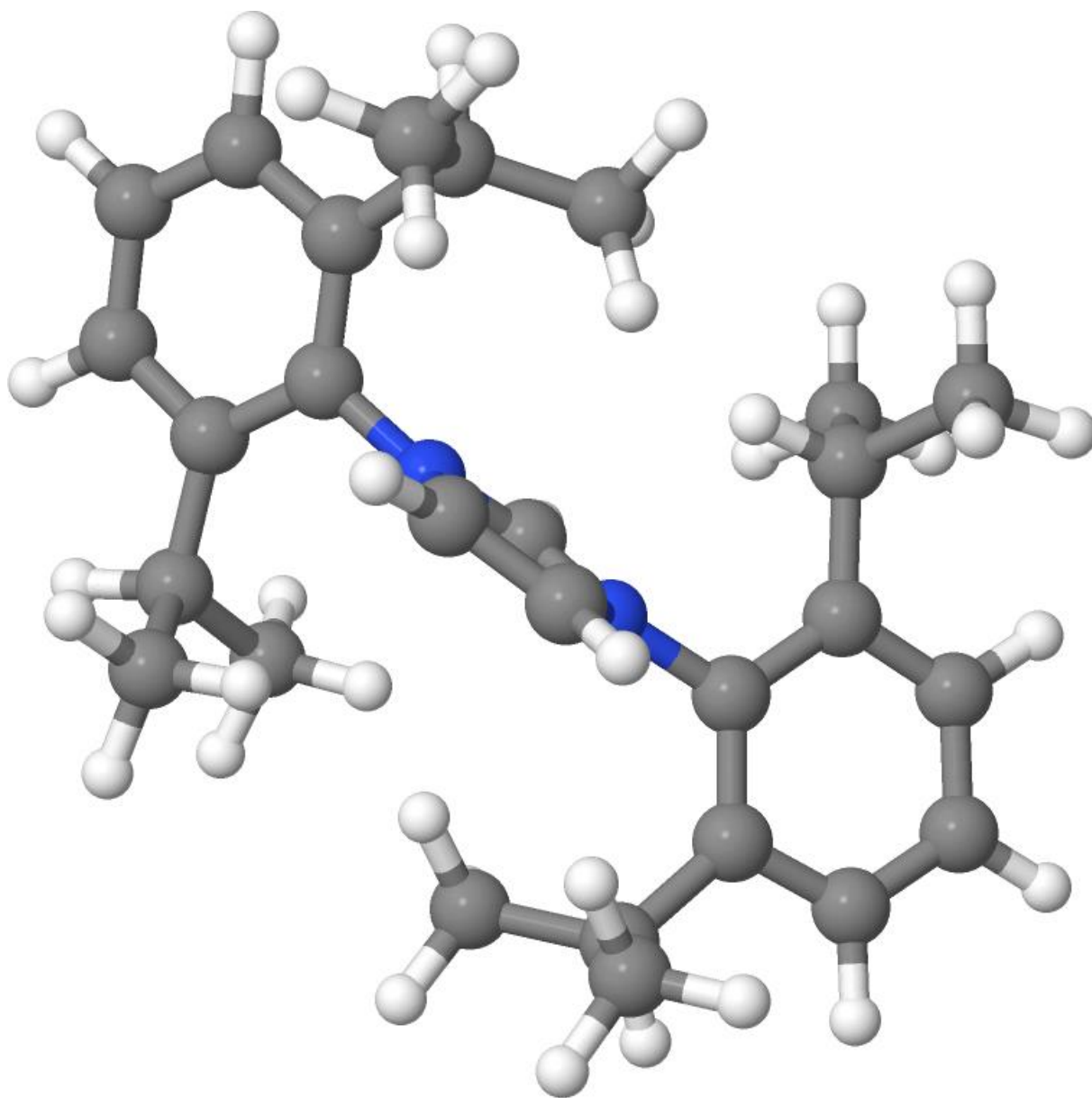
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3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	28.55	0.05749	YES	YES
8		a	37.16	0.00771	YES	YES
9		a	44.97	0.04139	YES	YES
10		a	53.24	0.01136	YES	YES
11		a	66.66	0.08318	YES	YES
12		a	70.30	0.04709	YES	YES
13		a	78.18	0.06436	YES	YES
14		a	85.31	0.05403	YES	YES
15		a	95.14	0.70878	YES	YES
16		a	96.92	0.14759	YES	YES
17		a	114.96	2.40407	YES	YES
18		a	133.59	0.25318	YES	YES
19		a	144.20	0.87665	YES	YES
20		a	145.91	1.46894	YES	YES
21		a	151.45	2.32085	YES	YES
22		a	184.79	1.05505	YES	YES
23		a	193.68	1.39446	YES	YES
24		a	211.57	1.90917	YES	YES
25		a	230.06	0.39680	YES	YES
26		a	232.92	0.06313	YES	YES
27		a	237.71	0.48657	YES	YES
28		a	247.68	0.04516	YES	YES
29		a	252.99	2.55828	YES	YES
30		a	264.15	2.01386	YES	YES
31		a	272.27	0.26858	YES	YES
32		a	274.82	2.34556	YES	YES
33		a	276.48	0.14160	YES	YES
34		a	285.13	1.58707	YES	YES

35	a	288.49	0.32773	YES	YES
36	a	293.91	1.03816	YES	YES
37	a	297.28	0.90456	YES	YES
38	a	299.59	0.93845	YES	YES
39	a	306.11	0.79804	YES	YES
40	a	316.54	0.56537	YES	YES
41	a	335.36	0.44348	YES	YES
42	a	376.03	1.88294	YES	YES
43	a	389.80	0.03869	YES	YES
44	a	407.33	0.81380	YES	YES
45	a	435.85	7.86824	YES	YES
46	a	456.51	0.15290	YES	YES
47	a	458.83	0.27567	YES	YES
48	a	481.31	1.84668	YES	YES
49	a	486.45	0.66330	YES	YES
50	a	508.56	2.73161	YES	YES
51	a	531.12	0.13055	YES	YES
52	a	548.87	0.52163	YES	YES
53	a	557.65	0.10464	YES	YES
54	a	575.52	2.82823	YES	YES
55	a	581.71	0.72745	YES	YES
56	a	600.97	3.72347	YES	YES
57	a	627.72	0.82856	YES	YES
58	a	629.48	1.04636	YES	YES
59	a	657.63	0.52993	YES	YES
60	a	663.53	2.76116	YES	YES
61	a	716.04	45.94234	YES	YES
62	a	721.31	0.43652	YES	YES
63	a	739.12	11.99322	YES	YES
64	a	753.44	34.06223	YES	YES
65	a	757.82	10.90348	YES	YES
66	a	796.94	0.52775	YES	YES
67	a	803.49	7.71359	YES	YES
68	a	804.69	3.98407	YES	YES
69	a	810.49	2.76790	YES	YES
70	a	812.22	8.88412	YES	YES
71	a	883.51	0.34104	YES	YES
72	a	884.50	1.33740	YES	YES
73	a	892.40	0.31803	YES	YES
74	a	893.42	0.00727	YES	YES
75	a	908.76	1.69309	YES	YES
76	a	910.61	3.89180	YES	YES
77	a	913.80	1.92207	YES	YES
78	a	917.09	0.51008	YES	YES
79	a	920.23	21.93056	YES	YES
80	a	922.97	4.69981	YES	YES
81	a	924.35	7.24744	YES	YES
82	a	927.37	14.14644	YES	YES
83	a	943.48	2.54786	YES	YES
84	a	948.86	0.84384	YES	YES
85	a	949.54	0.14790	YES	YES
86	a	950.21	0.75622	YES	YES
87	a	963.47	0.24106	YES	YES
88	a	964.44	0.17429	YES	YES
89	a	1035.86	0.81512	YES	YES
90	a	1040.75	3.09840	YES	YES
91	a	1050.24	4.93911	YES	YES
92	a	1053.06	9.16502	YES	YES
93	a	1062.20	3.96849	YES	YES

94	a	1078.04	9.08142	YES	YES
95	a	1094.14	8.20629	YES	YES
96	a	1099.05	8.68188	YES	YES
97	a	1104.77	1.99861	YES	YES
98	a	1107.59	6.64409	YES	YES
99	a	1113.14	6.74332	YES	YES
100	a	1114.21	1.94889	YES	YES
101	a	1119.51	3.02610	YES	YES
102	a	1131.24	1.53628	YES	YES
103	a	1135.10	3.09071	YES	YES
104	a	1148.09	2.85949	YES	YES
105	a	1151.09	1.07753	YES	YES
106	a	1172.05	6.28238	YES	YES
107	a	1176.60	9.98419	YES	YES
108	a	1188.13	4.44954	YES	YES
109	a	1217.71	18.14342	YES	YES
110	a	1218.40	3.15554	YES	YES
111	a	1225.48	24.50636	YES	YES
112	a	1231.19	3.19213	YES	YES
113	a	1237.67	1.60843	YES	YES
114	a	1246.27	1.28294	YES	YES
115	a	1293.71	3.17777	YES	YES
116	a	1294.56	2.60704	YES	YES
117	a	1298.65	10.48573	YES	YES
118	a	1304.05	0.58343	YES	YES
119	a	1306.58	2.77171	YES	YES
120	a	1315.90	3.66889	YES	YES
121	a	1321.78	7.97214	YES	YES
122	a	1330.65	3.82850	YES	YES
123	a	1344.19	2.30258	YES	YES
124	a	1346.37	12.99714	YES	YES
125	a	1349.34	4.38464	YES	YES
126	a	1352.79	8.41415	YES	YES
127	a	1354.68	6.36802	YES	YES
128	a	1363.53	3.39028	YES	YES
129	a	1365.89	4.55223	YES	YES
130	a	1368.16	54.43059	YES	YES
131	a	1369.97	3.23854	YES	YES
132	a	1371.53	1.60284	YES	YES
133	a	1373.90	1.22188	YES	YES
134	a	1379.98	1.17812	YES	YES
135	a	1421.61	2.38013	YES	YES
136	a	1423.20	0.18409	YES	YES
137	a	1424.97	10.90997	YES	YES
138	a	1425.20	3.38292	YES	YES
139	a	1428.16	4.80837	YES	YES
140	a	1431.31	7.78632	YES	YES
141	a	1434.37	13.54389	YES	YES
142	a	1435.48	6.26653	YES	YES
143	a	1439.96	13.12146	YES	YES
144	a	1441.59	2.34230	YES	YES
145	a	1443.74	5.30654	YES	YES
146	a	1444.52	10.56526	YES	YES
147	a	1444.78	6.32139	YES	YES
148	a	1446.46	1.82513	YES	YES
149	a	1451.00	70.39088	YES	YES
150	a	1453.34	12.52544	YES	YES
151	a	1455.78	3.64423	YES	YES
152	a	1456.92	4.89714	YES	YES

153	a	1462.74	4.43893	YES	YES
154	a	1465.34	12.14341	YES	YES
155	a	1556.36	0.19914	YES	YES
156	a	1595.30	0.75268	YES	YES
157	a	1597.75	2.89450	YES	YES
158	a	1598.44	1.32515	YES	YES
159	a	1599.90	1.13174	YES	YES
160	a	2926.97	44.30399	YES	YES
161	a	2931.83	26.50943	YES	YES
162	a	2931.92	26.25471	YES	YES
163	a	2937.78	34.15685	YES	YES
164	a	2940.00	17.69816	YES	YES
165	a	2941.10	18.05953	YES	YES
166	a	2941.56	28.23818	YES	YES
167	a	2943.25	29.17960	YES	YES
168	a	2947.22	16.97837	YES	YES
169	a	2949.51	57.63129	YES	YES
170	a	2950.43	22.54934	YES	YES
171	a	3010.18	31.12299	YES	YES
172	a	3013.94	2.51980	YES	YES
173	a	3016.35	16.18714	YES	YES
174	a	3016.59	21.56006	YES	YES
175	a	3019.34	30.11409	YES	YES
176	a	3023.30	17.67588	YES	YES
177	a	3023.84	24.52617	YES	YES
178	a	3024.46	1.67349	YES	YES
179	a	3026.09	20.66254	YES	YES
180	a	3028.98	24.08430	YES	YES
181	a	3037.03	7.27904	YES	YES
182	a	3038.42	27.46390	YES	YES
183	a	3046.42	12.44745	YES	YES
184	a	3056.55	13.21374	YES	YES
185	a	3058.03	7.90287	YES	YES
186	a	3063.10	6.98511	YES	YES
187	a	3078.30	11.62475	YES	YES
188	a	3080.51	2.46786	YES	YES
189	a	3083.69	4.52493	YES	YES
190	a	3088.27	17.29158	YES	YES
191	a	3098.34	15.66275	YES	YES
192	a	3109.07	27.16017	YES	YES
193	a	3112.58	24.21675	YES	YES
194	a	3184.49	1.33250	YES	YES
195	a	3205.24	0.21248	YES	YES

Hldipp⁺



Total energy = -1159.5796702410 H = -31553.7862388 eV

HOMO-LUMO Separation

HOMO: 106. 106 a -0.33222716 H = -9.04037 eV

LUMO: 107. 107 a -0.20015996 H = -5.44663 eV

Gap : +0.13206720 H = +3.59373 eV

Number of MOs= 480, Electrons= 212.00, Symmetry: c1

COSMO(8.93): Total energy + OC corr. [a.u.] = -1159.6294746431

COSMO(14.3): Total energy + OC corr. [a.u.] = -1159.6329874263

COSMO(36.64): Total energy + OC corr. [a.u.] = -1159.6367147203

\$coord

2.20011458681112	0.32822655853087	0.73089457208629	n
1.43080120152951	0.63552509610522	3.22384912330682	c
-1.16555350251969	0.52385004762193	3.25760253438872	c
-1.97484477708571	0.20431779614434	0.77727359002047	n
0.10233524403753	0.07100585686982	-0.70880497873193	c
4.82006928065354	0.19700582541390	-0.17452756170385	c
-4.60048919751570	-0.07378891205653	-0.06052994516287	c
6.22493654700390	-2.06336949388954	0.25838726486218	c
8.70628269306918	-2.14254098411869	-0.72587449641586	c
9.76185441137180	-0.11532374966748	-2.04562276619684	c
8.35210510714649	2.09504709425689	-2.37160270219261	c
5.86529654265319	2.33674003985364	-1.44003323654428	c
-6.31316836664219	1.99999488766243	0.15323043906636	c
-8.81313713609680	1.56094606892512	-0.67243934050875	c
-9.59604986565640	-0.76125064484206	-1.66285714397254	c
-7.86819655993158	-2.74940786397096	-1.84222988761065	c
-5.34508857951269	-2.47207630772279	-1.03626724114757	c
4.61871726683258	4.93307262634549	-1.81155213986832	c
3.92711200831114	6.26153606206446	0.68942178356112	c
2.46496958190603	4.98955874919815	-3.77821400147698	c
5.44032839140472	-4.41254677794944	1.78164492909684	c
2.76899932941594	-5.46699986455876	1.35229633560580	c
6.03530662934695	-4.10608389970796	4.62858013373991	c
-3.60113807704105	-4.76538353947706	-1.22735695445002	c
-3.10802689203808	-5.51300344750014	-4.00639224957383	c
-4.61847705124841	-7.02607730962183	0.31507783590015	c
-5.80879399735327	4.66994238331208	1.18827461131120	c
-3.37128959916897	5.96791290198803	0.29165149847648	c
-6.15342554761364	4.85786905910571	4.08630290467938	c
2.79401605227535	0.92050147593888	4.75270071368025	h
-2.50508163480980	0.61763201645540	4.82900522153392	h
0.08901088451893	-0.24116219012481	-2.75356255994864	h
9.83164355025314	-3.87167766286321	-0.43604981144011	h
11.69642039701713	-0.24814987484904	-2.80332134340251	h
9.20122913292595	3.71686378154081	-3.36526704360599	h
-10.18161552408182	3.12617416539354	-0.54327952082523	h
-11.56100934570945	-1.01454695904447	-2.30304258452223	h
-8.48985099182808	-4.57990180683959	-2.61424142345530	h
6.14651149499065	6.10241917100503	-2.65360500503266	h
3.32761055933245	8.23939076100261	0.30823957144238	h
5.57953781043744	6.33775653047372	1.98434100112693	h
2.34760720749255	5.32389955164437	1.70471346449839	h
2.02526711860117	6.97903043400485	-4.29338946198065	h

0.68283329616180	4.14846207775858	-3.05962855661026	h
3.01469563164781	3.98737358455036	-5.54177334149530	h
6.74430372093512	-5.90910057344908	1.09346796586595	h
2.64894697281607	-7.40325021728150	2.15930631647830	h
2.31561029228694	-5.61600141928913	-0.69301008586163	h
1.28210397458353	-4.33508819939847	2.30939681979072	h
5.80535134625545	-5.94854835494666	5.61311754500208	h
4.75065730547469	-2.73548684415201	5.56933130451913	h
8.00820670629171	-3.45630612615316	4.93478191476683	h
-1.75321173222576	-4.26173405328073	-0.38379253674363	h
-1.75581394554472	-7.11947676238475	-4.10605143525235	h
-2.30978409234584	-3.91952692052857	-5.12343273946794	h
-4.87574250927255	-6.12081624669041	-4.96743101371997	h
-3.23518464025636	-8.60853692483212	0.27865245954399	h
-6.42587894280213	-7.75836434310588	-0.46639977423449	h
-4.95438298404900	-6.50326385274571	2.32190168457627	h
-7.37529602558249	5.81145583155724	0.37775932188457	h
-3.42262126480197	7.99944111449752	0.82634558236220	h
-3.17541089338440	5.87514747559716	-1.79715441589850	h
-1.64319353235958	5.16011000509558	1.16203988641627	h
-6.25729383949542	6.87687194290171	4.65938416078836	h
-4.55554902831286	4.00570009741883	5.15045342260135	h
-7.92651143787003	3.92350423422676	4.71365734687878	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	19.06	0.04045	YES	YES
8		a	22.00	0.01416	YES	YES
9		a	38.33	0.02851	YES	YES
10		a	42.07	0.02750	YES	YES
11		a	51.51	0.03567	YES	YES
12		a	69.20	0.00249	YES	YES
13		a	74.91	0.03981	YES	YES
14		a	79.14	0.01996	YES	YES
15		a	87.61	0.09580	YES	YES
16		a	100.28	0.02654	YES	YES
17		a	114.06	0.22042	YES	YES
18		a	127.90	0.01498	YES	YES
19		a	138.82	0.02307	YES	YES
20		a	145.13	0.10799	YES	YES
21		a	148.92	0.12311	YES	YES
22		a	183.52	0.24471	YES	YES
23		a	197.45	0.60744	YES	YES
24		a	215.71	0.03938	YES	YES
25		a	218.13	0.56367	YES	YES
26		a	226.05	0.14987	YES	YES
27		a	232.04	0.12560	YES	YES
28		a	232.55	0.30689	YES	YES
29		a	237.58	0.32576	YES	YES
30		a	241.13	0.18522	YES	YES
31		a	254.93	0.60221	YES	YES

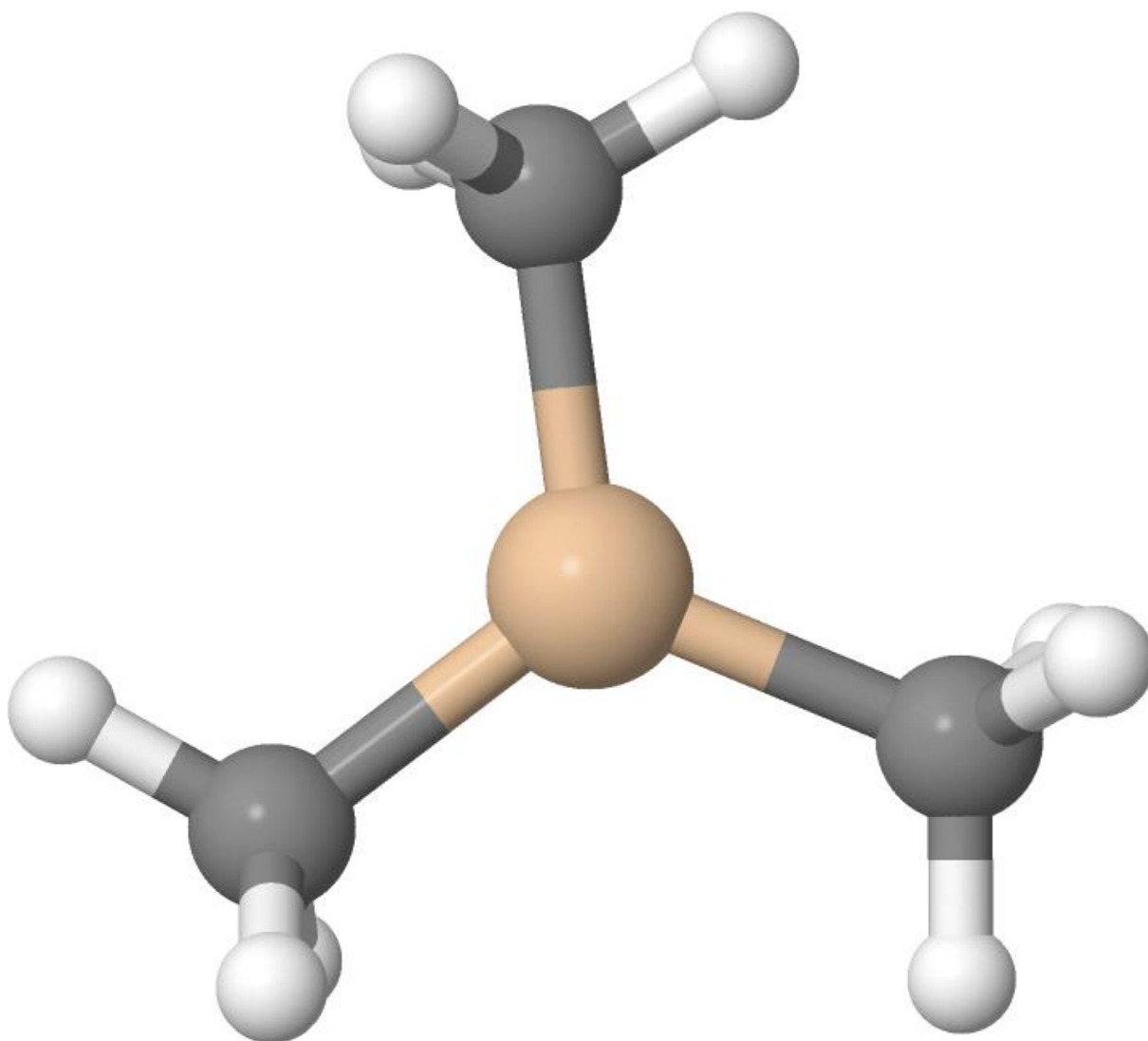
32	a	257.14	0.08430	YES	YES
33	a	263.03	0.06014	YES	YES
34	a	276.85	0.36129	YES	YES
35	a	279.32	0.27300	YES	YES
36	a	287.20	0.14054	YES	YES
37	a	291.91	0.47041	YES	YES
38	a	298.46	0.02499	YES	YES
39	a	299.14	0.07494	YES	YES
40	a	308.04	0.12975	YES	YES
41	a	328.81	0.07220	YES	YES
42	a	369.87	0.96409	YES	YES
43	a	380.19	1.42780	YES	YES
44	a	402.56	0.92677	YES	YES
45	a	426.79	10.03851	YES	YES
46	a	448.05	3.66015	YES	YES
47	a	459.10	0.67836	YES	YES
48	a	477.78	1.10234	YES	YES
49	a	484.54	0.33936	YES	YES
50	a	501.66	0.93057	YES	YES
51	a	526.97	0.09507	YES	YES
52	a	536.28	1.31154	YES	YES
53	a	553.28	1.40821	YES	YES
54	a	566.72	0.21841	YES	YES
55	a	577.98	0.35748	YES	YES
56	a	599.66	1.28519	YES	YES
57	a	624.48	0.10661	YES	YES
58	a	625.02	0.33323	YES	YES
59	a	660.21	0.48222	YES	YES
60	a	676.44	24.98168	YES	YES
61	a	719.09	3.93143	YES	YES
62	a	719.99	22.92065	YES	YES
63	a	732.82	2.00445	YES	YES
64	a	750.44	19.90248	YES	YES
65	a	753.49	10.94303	YES	YES
66	a	797.32	25.02604	YES	YES
67	a	801.73	8.71459	YES	YES
68	a	805.93	18.44537	YES	YES
69	a	806.48	7.67376	YES	YES
70	a	813.87	0.10218	YES	YES
71	a	830.02	0.34203	YES	YES
72	a	880.93	0.72585	YES	YES
73	a	885.69	2.16852	YES	YES
74	a	902.32	0.72460	YES	YES
75	a	902.89	0.49899	YES	YES
76	a	904.81	0.39255	YES	YES
77	a	910.11	0.88572	YES	YES
78	a	911.63	1.03106	YES	YES
79	a	915.13	4.28011	YES	YES
80	a	918.24	2.09020	YES	YES
81	a	920.35	14.12254	YES	YES
82	a	931.29	5.62876	YES	YES
83	a	937.61	1.04207	YES	YES
84	a	939.11	0.08772	YES	YES
85	a	947.42	0.26311	YES	YES
86	a	948.87	0.46905	YES	YES
87	a	949.80	1.23005	YES	YES
88	a	984.88	0.14886	YES	YES
89	a	985.85	0.17704	YES	YES
90	a	1033.70	13.47681	YES	YES

91	a	1043.24	12.17469	YES	YES
92	a	1050.14	3.66819	YES	YES
93	a	1059.76	7.60739	YES	YES
94	a	1076.82	13.08548	YES	YES
95	a	1083.26	8.98209	YES	YES
96	a	1093.16	3.61663	YES	YES
97	a	1097.97	1.99278	YES	YES
98	a	1098.51	9.32063	YES	YES
99	a	1102.42	3.36836	YES	YES
100	a	1109.21	2.12754	YES	YES
101	a	1112.29	2.53515	YES	YES
102	a	1114.60	1.61357	YES	YES
103	a	1128.83	16.18875	YES	YES
104	a	1135.58	3.97466	YES	YES
105	a	1146.86	6.74514	YES	YES
106	a	1150.58	0.78307	YES	YES
107	a	1170.82	18.84145	YES	YES
108	a	1179.72	8.80290	YES	YES
109	a	1184.26	26.87320	YES	YES
110	a	1212.59	1.12942	YES	YES
111	a	1223.30	0.82271	YES	YES
112	a	1225.61	0.44490	YES	YES
113	a	1238.16	4.60337	YES	YES
114	a	1242.69	1.98493	YES	YES
115	a	1286.53	6.44852	YES	YES
116	a	1295.75	2.40429	YES	YES
117	a	1297.57	3.14423	YES	YES
118	a	1301.06	3.23731	YES	YES
119	a	1315.76	0.48927	YES	YES
120	a	1317.45	5.79179	YES	YES
121	a	1319.92	5.07071	YES	YES
122	a	1325.89	18.83322	YES	YES
123	a	1332.05	0.99450	YES	YES
124	a	1347.08	4.04134	YES	YES
125	a	1350.21	9.18138	YES	YES
126	a	1351.12	7.18401	YES	YES
127	a	1353.18	0.22842	YES	YES
128	a	1353.36	14.88808	YES	YES
129	a	1360.97	1.01580	YES	YES
130	a	1369.64	2.80453	YES	YES
131	a	1371.81	0.85890	YES	YES
132	a	1372.73	3.19828	YES	YES
133	a	1373.87	2.06226	YES	YES
134	a	1378.73	4.15386	YES	YES
135	a	1382.59	0.45413	YES	YES
136	a	1421.55	0.41502	YES	YES
137	a	1423.00	3.70312	YES	YES
138	a	1424.63	1.75744	YES	YES
139	a	1426.73	5.66935	YES	YES
140	a	1427.97	0.20274	YES	YES
141	a	1429.64	6.77127	YES	YES
142	a	1432.86	7.97568	YES	YES
143	a	1433.64	4.08819	YES	YES
144	a	1438.56	1.98591	YES	YES
145	a	1439.38	39.11210	YES	YES
146	a	1441.22	10.56240	YES	YES
147	a	1441.81	23.45832	YES	YES
148	a	1443.40	12.68008	YES	YES
149	a	1444.93	4.66800	YES	YES

150	a	1447.48	5.04235	YES	YES
151	a	1448.76	3.74669	YES	YES
152	a	1451.70	1.49238	YES	YES
153	a	1453.25	5.36193	YES	YES
154	a	1459.56	6.94389	YES	YES
155	a	1462.24	12.19282	YES	YES
156	a	1511.74	72.96510	YES	YES
157	a	1544.08	8.14255	YES	YES
158	a	1591.18	5.64613	YES	YES
159	a	1594.87	9.10152	YES	YES
160	a	1598.60	2.11015	YES	YES
161	a	1599.00	3.28189	YES	YES
162	a	2942.05	15.17431	YES	YES
163	a	2949.06	12.27076	YES	YES
164	a	2950.09	25.47114	YES	YES
165	a	2952.72	16.74715	YES	YES
166	a	2953.03	14.62062	YES	YES
167	a	2954.06	12.41276	YES	YES
168	a	2955.40	16.85982	YES	YES
169	a	2958.14	12.02079	YES	YES
170	a	2963.28	7.40175	YES	YES
171	a	2963.83	7.45092	YES	YES
172	a	2966.87	6.11562	YES	YES
173	a	3016.86	0.47468	YES	YES
174	a	3025.81	19.44505	YES	YES
175	a	3031.60	13.06795	YES	YES
176	a	3033.18	3.66334	YES	YES
177	a	3033.60	6.68227	YES	YES
178	a	3035.81	6.14226	YES	YES
179	a	3037.11	5.25003	YES	YES
180	a	3037.25	14.52310	YES	YES
181	a	3037.98	37.67620	YES	YES
182	a	3038.48	15.98161	YES	YES
183	a	3042.35	12.25086	YES	YES
184	a	3044.10	12.36771	YES	YES
185	a	3045.55	34.83209	YES	YES
186	a	3046.13	16.91896	YES	YES
187	a	3046.30	16.41198	YES	YES
188	a	3052.22	40.54114	YES	YES
189	a	3057.07	18.63892	YES	YES
190	a	3100.54	0.12022	YES	YES
191	a	3101.28	0.96868	YES	YES
192	a	3105.87	4.80763	YES	YES
193	a	3110.97	3.76709	YES	YES
194	a	3124.93	3.98825	YES	YES
195	a	3125.26	4.15053	YES	YES
196	a	3215.71	15.43015	YES	YES
197	a	3226.39	23.87840	YES	YES
198	a	3233.30	5.87474	YES	YES

Reference Systems:

Me₃Si⁺



Total energy = -408.8075732993 H = -11124.2264001 eV

HOMO-LUMO Separation

HOMO: 20. 10 e' -0.49435447 H = -13.45208 eV

LUMO: 21. 3 a'' -0.31257354 H = -8.50556 eV

Gap : +0.18178093 H = +4.94651 eV

Number of MOs= 78, Electrons= 40.00, Symmetry: c3h

\$coord

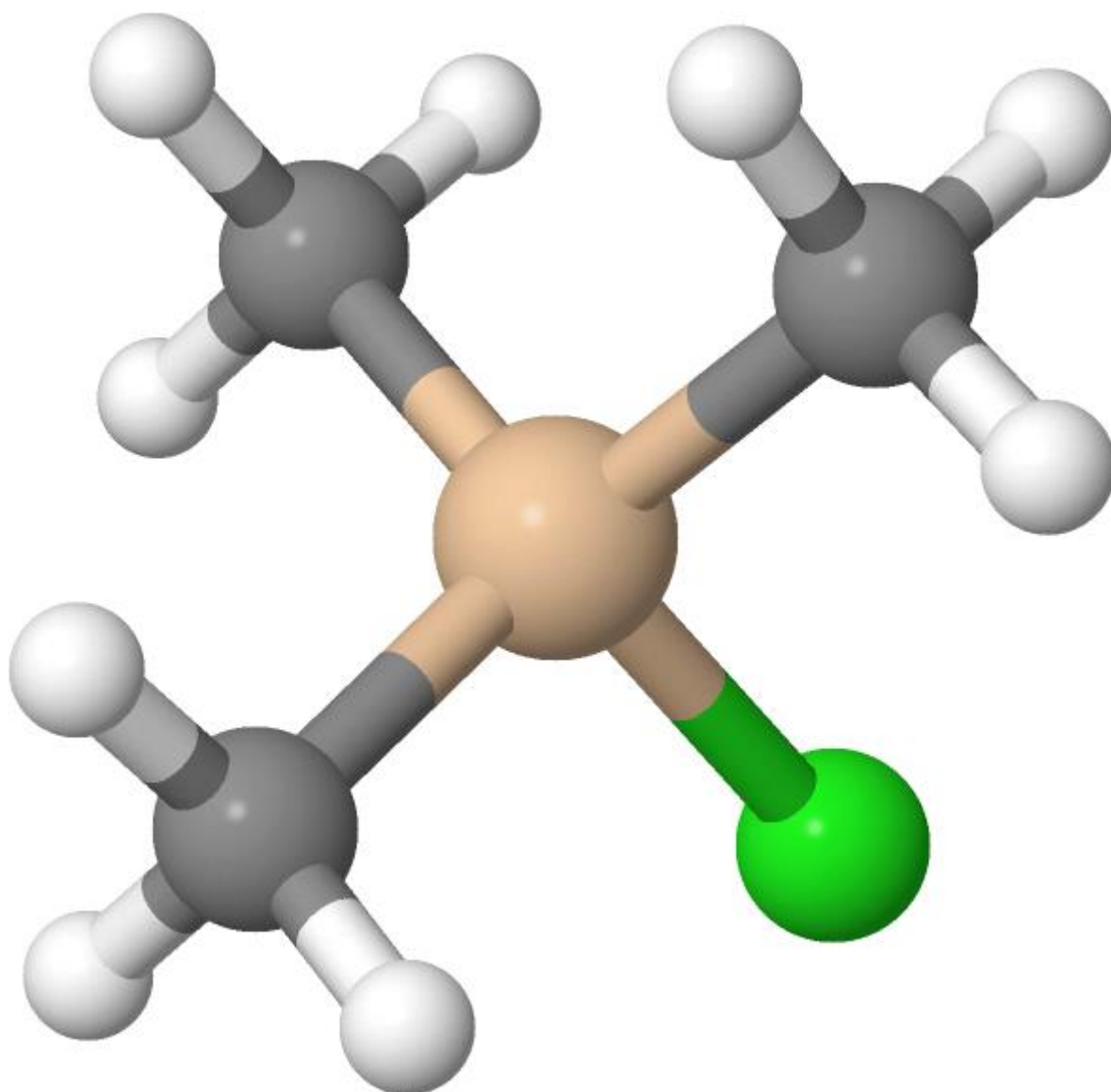
0.000000000000000	0.000000000000000	0.000000000000000	si
3.49007261768953	-0.05102198119062	0.000000000000000	c
4.21598361588840	0.99907538329754	-1.68185518476710	h
4.29188449121501	-1.98982393331792	0.000000000000000	h
4.21598361588840	0.99907538329754	1.68185518476710	h
-1.70084997698227	3.04800253856691	0.000000000000000	c
-1.78922264070727	-2.99698055737629	0.000000000000000	c
-2.97321647017555	3.15161122164956	-1.68185518476710	h
-1.24276714571285	-4.15068660494709	-1.68185518476710	h
-2.97321647017555	3.15161122164956	1.68185518476710	h
-1.24276714571285	-4.15068660494709	1.68185518476710	h
-0.42270417029591	4.71179296615961	0.000000000000000	h
-3.86918032091909	-2.72196903284169	0.000000000000000	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e"	34.18	0.00000	NO	YES
8		e"	34.18	0.00000	NO	YES
9		a"	68.79	2.71782	YES	NO
10		e'	210.69	2.16108	YES	YES
11		e'	210.69	2.16108	YES	YES
12		a"	216.17	1.22128	YES	NO
13		a'	591.03	0.00000	NO	YES
14		e"	622.46	0.00000	NO	YES
15		e"	622.46	0.00000	NO	YES
16		a'	696.56	0.00000	NO	YES
17		e'	741.46	8.39008	YES	YES
18		e'	741.46	8.39008	YES	YES
19		a"	817.30	83.59584	YES	NO
20		e'	882.59	132.69329	YES	YES
21		e'	882.59	132.69329	YES	YES
22		e'	1240.98	77.01039	YES	YES
23		e'	1240.98	77.01039	YES	YES
24		a'	1247.07	0.00000	NO	YES
25		e'	1361.01	11.70102	YES	YES
26		e'	1361.01	11.70102	YES	YES
27		e"	1362.38	0.00000	NO	YES
28		e"	1362.38	0.00000	NO	YES
29		a"	1369.23	47.43940	YES	NO
30		a'	1370.15	0.00000	NO	YES
31		e'	2925.46	46.05912	YES	YES
32		e'	2925.46	46.05912	YES	YES
33		a'	2930.55	0.00000	NO	YES
34		a"	3000.29	44.56238	YES	NO
35		e"	3000.67	0.00000	NO	YES
36		e"	3000.67	0.00000	NO	YES

37	e'	3067.31	14.37619	YES	YES
38	e'	3067.31	14.37619	YES	YES
39	a'	3067.97	0.00000	NO	YES

Me₃SiCl



Total energy = -869.2582785558 H = -23653.7347211 eV

HOMO-LUMO Separation

HOMO: 21. 8 e -0.25291432 H = -6.88215 eV

LUMO: 22. 13 a1 +0.01863263 H = +0.50702 eV

Gap : +0.27154694 H = +7.38917 eV

Number of MOs= 66, Electrons= 58.00, Symmetry: c3v

\$coord

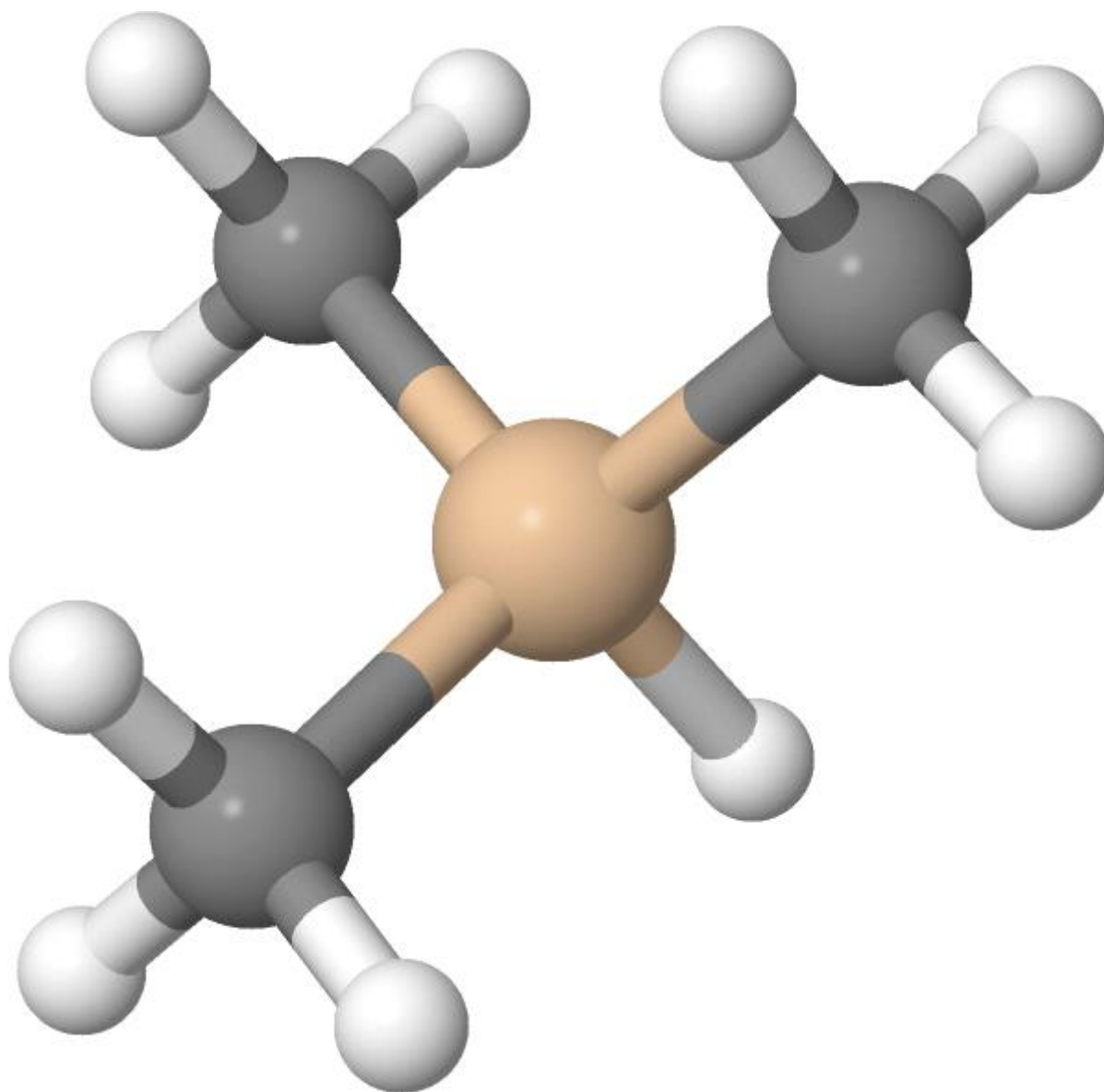
0.0000000000000000	0.0000000000000000	0.76987551794057	si
-1.70338096319108	2.95034237289256	-0.29809384695722	c
-1.70338096319108	-2.95034237289256	-0.29809384695722	c
3.40676192638215	0.0000000000000000	-0.29809384695722	c
0.0000000000000000	0.0000000000000000	4.76420043309599	cl
-0.73834152132835	4.67737617383226	0.41154189212120	h
-3.68155582893062	2.97811060105534	0.41154189212120	h
-1.76201891937934	3.05190629226267	-2.39987870142035	h
-0.73834152132835	-4.67737617383226	0.41154189212120	h
-1.76201891937934	-3.05190629226267	-2.39987870142035	h
-3.68155582893062	-2.97811060105534	0.41154189212120	h
4.41989735025896	-1.69926557277691	0.41154189212120	h
4.41989735025896	1.69926557277691	0.41154189212120	h
3.52403783875872	0.0000000000000000	-2.39987870142035	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a2	167.59	0.00000	NO	NO
8		e	169.75	0.56506	YES	YES
9		e	169.75	0.56506	YES	YES
10		e	181.86	0.03874	YES	YES
11		e	181.86	0.03874	YES	YES
12		a1	215.25	0.45808	YES	YES
13		e	225.98	4.85775	YES	YES
14		e	225.98	4.85775	YES	YES
15		a1	466.25	40.64007	YES	YES
16		a1	612.98	28.15153	YES	YES
17		e	677.71	6.20935	YES	YES
18		e	677.71	6.20935	YES	YES
19		a2	677.97	0.00000	NO	NO
20		e	756.41	22.38776	YES	YES
21		e	756.41	22.38776	YES	YES
22		e	852.84	96.11182	YES	YES
23		e	852.84	96.11182	YES	YES
24		a1	858.55	145.93862	YES	YES
25		e	1241.56	36.03086	YES	YES
26		e	1241.56	36.03086	YES	YES
27		a1	1250.43	7.07521	YES	YES
28		a2	1391.12	0.00000	NO	NO
29		e	1399.13	0.01460	YES	YES
30		e	1399.13	0.01460	YES	YES

31	e	1404.83	6.86986	YES	YES
32	e	1404.83	6.86986	YES	YES
33	a1	1416.12	11.72855	YES	YES
34	e	2941.81	3.32593	YES	YES
35	e	2941.81	3.32593	YES	YES
36	a1	2943.97	4.20141	YES	YES
37	e	3032.45	0.58492	YES	YES
38	e	3032.45	0.58492	YES	YES
39	a1	3034.48	15.25008	YES	YES
40	a2	3044.70	0.00000	NO	NO
41	e	3045.23	5.79433	YES	YES
42	e	3045.23	5.79433	YES	YES

Me3SiH



Total energy = -409.6891298663 H = -11148.2147884 eV

HOMO-LUMO Separation

HOMO: 15. 6 e -0.26679090 H = -7.25975 eV

LUMO: 16. 9 a1 +0.03241712 H = +0.88212 eV

Gap : +0.29920802 H = +8.14187 eV

Number of MOs= 55, Electrons= 42.00, Symmetry: c3v

\$scoord

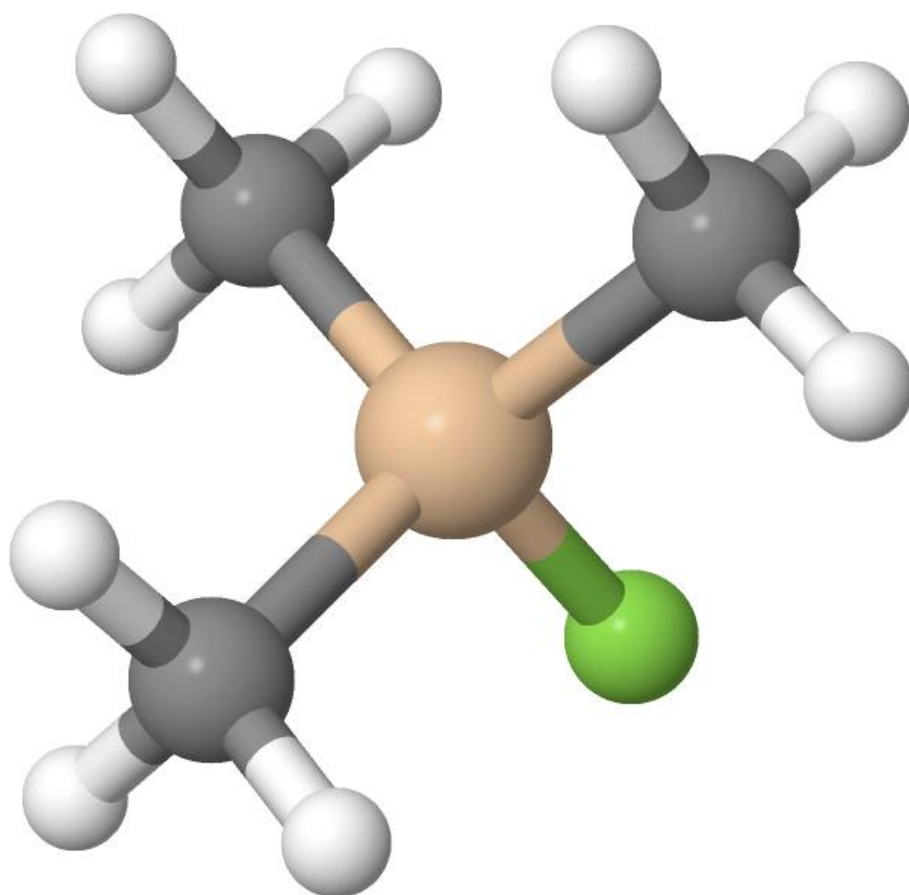
0.000000000000000	0.000000000000000	0.91349788552103	si
-1.70389413050220	2.95123120474819	-0.21945234505776	c
-1.70389413050220	-2.95123120474819	-0.21945234505776	c
3.40778826100438	0.000000000000000	-0.21945234505776	c
0.000000000000000	0.000000000000000	3.77587450047056	h
-0.74878831958580	4.69286519733812	0.47249253277433	h
-3.68974631763778	2.99490230548743	0.47249253277433	h
-1.75489133275006	3.03956095008537	-2.32117774767042	h
-0.74878831958580	-4.69286519733812	0.47249253277433	h
-1.75489133275006	-3.03956095008537	-2.32117774767042	h
-3.68974631763778	-2.99490230548743	0.47249253277433	h
4.43853463722359	-1.69796289185070	0.47249253277433	h
4.43853463722359	1.69796289185070	0.47249253277433	h
3.50978266550014	0.000000000000000	-2.32117774767042	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a2		165.26	0.00000	NO	NO
8	e		175.75	0.00201	YES	YES
9	e		175.75	0.00201	YES	YES
10	e		198.36	0.59466	YES	YES
11	e		198.36	0.59466	YES	YES
12	a1		232.64	0.93581	YES	YES
13	a1		594.45	1.51266	YES	YES
14	e		605.14	7.10460	YES	YES
15	e		605.14	7.10460	YES	YES
16	a2		670.21	0.00000	NO	NO
17	e		685.16	12.17947	YES	YES
18	e		685.16	12.17947	YES	YES
19	e		835.10	16.79420	YES	YES
20	e		835.10	16.79420	YES	YES
21	a1		857.85	69.13100	YES	YES

22	e	889.59	161.56294	YES	YES
23	e	889.59	161.56294	YES	YES
24	e	1238.71	30.57305	YES	YES
25	e	1238.71	30.57305	YES	YES
26	a1	1248.84	5.63688	YES	YES
27	a2	1397.02	0.00000	NO	NO
28	e	1401.66	0.31651	YES	YES
29	e	1401.66	0.31651	YES	YES
30	e	1410.54	5.00856	YES	YES
31	e	1410.54	5.00856	YES	YES
32	a1	1417.52	14.17313	YES	YES
33	a1	2137.51	161.56304	YES	YES
34	e	2938.50	8.45536	YES	YES
35	e	2938.50	8.45536	YES	YES
36	a1	2939.51	2.46195	YES	YES
37	e	3029.10	0.48297	YES	YES
38	e	3029.10	0.48297	YES	YES
39	a1	3030.55	22.13846	YES	YES
40	a2	3032.88	0.00000	NO	NO
41	e	3033.33	12.42138	YES	YES
42	e	3033.33	12.42138	YES	YES

Me₃SiF



Total energy = -508.9275711884 H = -13848.6317106 eV

HOMO-LUMO Separation

HOMO: 18. 7 e -0.26548305 H = -7.22417 eV

LUMO: 19. 11 a1 +0.02663142 H = +0.72468 eV

Gap : +0.29211447 H = +7.94884 eV

Number of MOs= 63, Electrons= 50.00, Symmetry: c3v

\$scoord

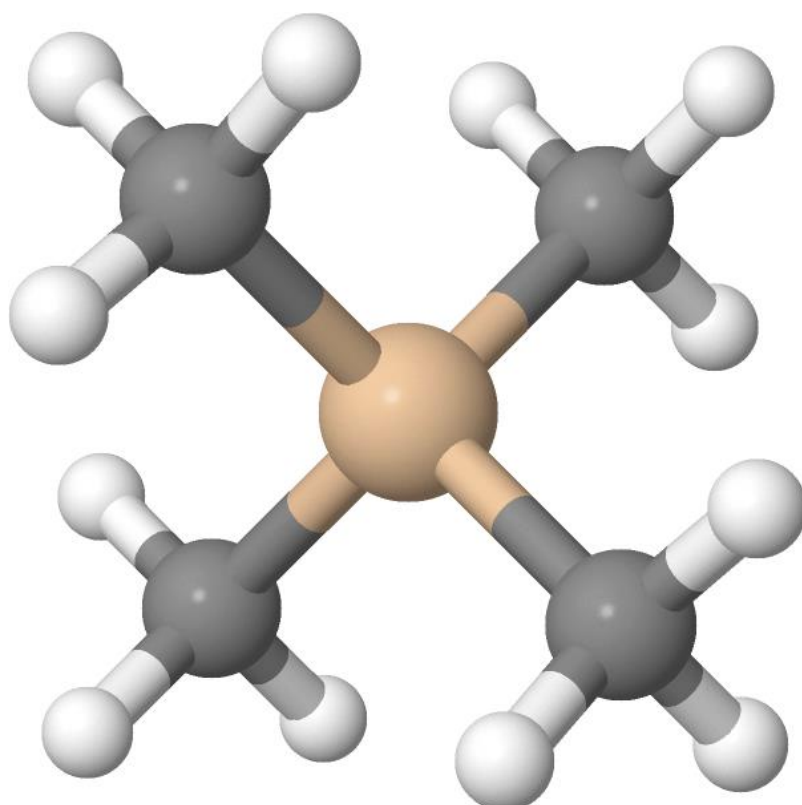
0.000000000000000	0.000000000000000	0.80170237140333	si
-1.70407079611717	-2.95153719856927	-0.23906941923149	c
-1.70407079611717	2.95153719856927	-0.23906941923149	c
3.40814159223432	0.000000000000000	-0.23906941923149	c
0.000000000000000	0.000000000000000	3.93047173780635	f
-0.73842105846497	-4.67607142834268	0.47943585164706	h
-1.78138127455104	-3.08544287517417	-2.33745402199301	h
-3.68038611762287	-2.97752710949138	0.47943585164706	h
-0.73842105846497	4.67607142834268	0.47943585164706	h
-3.68038611762287	2.97752710949138	0.47943585164706	h
-1.78138127455104	3.08544287517417	-2.33745402199301	h
4.41880717608783	1.69854431885129	0.47943585164706	h
3.56276254910205	0.000000000000000	-2.33745402199301	h
4.41880717608783	-1.69854431885129	0.47943585164706	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a2		149.85	0.00000	NO	NO
8	e		166.53	0.00055	YES	YES
9	e		166.53	0.00055	YES	YES
10	e		187.10	0.03229	YES	YES
11	e		187.10	0.03229	YES	YES
12	a1		227.98	0.11541	YES	YES
13	e		269.12	11.96812	YES	YES
14	e		269.12	11.96812	YES	YES
15	a1		585.17	0.01850	YES	YES
16	a2		667.52	0.00000	NO	NO
17	e		676.00	3.90793	YES	YES
18	e		676.00	3.90793	YES	YES
19	e		754.37	29.70240	YES	YES
20	e		754.37	29.70240	YES	YES
21	a1		770.96	4.25989	YES	YES

22	e	852.18	136.51484	YES	YES
23	e	852.18	136.51484	YES	YES
24	a1	909.00	166.80255	YES	YES
25	e	1246.64	46.39760	YES	YES
26	e	1246.64	46.39760	YES	YES
27	a1	1253.80	15.04985	YES	YES
28	a2	1391.91	0.00000	NO	NO
29	e	1399.66	0.03409	YES	YES
30	e	1399.66	0.03409	YES	YES
31	e	1405.49	4.81520	YES	YES
32	e	1405.49	4.81520	YES	YES
33	a1	1416.74	16.47970	YES	YES
34	e	2941.58	3.57362	YES	YES
35	e	2941.58	3.57362	YES	YES
36	a1	2943.79	1.09387	YES	YES
37	e	3032.50	0.46593	YES	YES
38	e	3032.50	0.46593	YES	YES
39	a1	3034.93	16.83549	YES	YES
40	a2	3037.19	0.00000	NO	NO
41	e	3037.88	8.86774	YES	YES
42	e	3037.88	8.86774	YES	YES

Me₃SiMe



Total energy = -448.9813133214 H = -12217.4101093 eV

HOMO-LUMO Separation

HOMO: 12. 5 t2 -0.25792252 H = -7.01843 eV

LUMO: 13. 6 a1 +0.02724223 H = +0.74130 eV

Gap : +0.28516475 H = +7.75973 eV

Number of MOs= 43, Electrons= 50.00, Symmetry: td

\$coord

0.0000000000000000	0.0000000000000000	0.0000000000000000	si
2.07667375478765	-2.07667375478765	2.07667375478765	c
-2.07667375478765	2.07667375478765	2.07667375478765	c
2.07667375478765	2.07667375478765	-2.07667375478765	c
-2.07667375478765	-2.07667375478765	-2.07667375478765	c
3.31775967033017	-3.31775967033017	0.91622601920978	h
0.91622601920978	-3.31775967033017	3.31775967033017	h
3.31775967033017	-0.91622601920978	3.31775967033017	h
-3.31775967033017	3.31775967033017	0.91622601920978	h
-0.91622601920978	3.31775967033017	3.31775967033017	h
-3.31775967033017	0.91622601920978	3.31775967033017	h
0.91622601920978	3.31775967033017	-3.31775967033017	h
3.31775967033017	0.91622601920978	-3.31775967033017	h
3.31775967033017	3.31775967033017	-0.91622601920978	h
-3.31775967033017	-0.91622601920978	-3.31775967033017	h
-3.31775967033017	-3.31775967033017	-0.91622601920978	h
-0.91622601920978	-3.31775967033017	-3.31775967033017	h

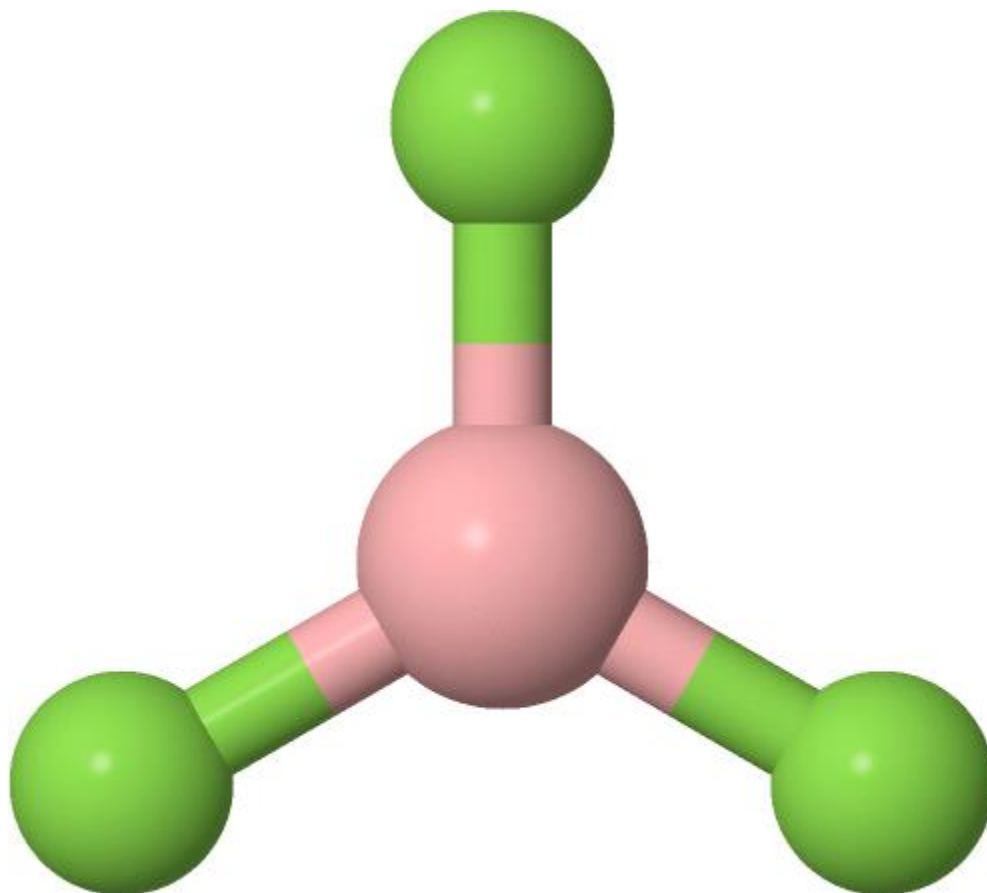
\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a2	163.78	0.00000	NO	NO
8		t1	179.09	0.00000	NO	NO
9		t1	179.09	0.00000	NO	NO
10		t1	179.09	0.00000	NO	NO
11		e	180.46	0.00000	NO	YES
12		e	180.46	0.00000	NO	YES
13		t2	224.92	2.15460	YES	YES
14		t2	224.92	2.15460	YES	YES
15		t2	224.92	2.15460	YES	YES
16		a1	562.22	0.00000	NO	YES
17		t1	669.66	0.00000	NO	NO
18		t1	669.66	0.00000	NO	NO
19		t1	669.66	0.00000	NO	NO
20		t2	672.44	12.08215	YES	YES
21		t2	672.44	12.08215	YES	YES
22		t2	672.44	12.08215	YES	YES
23		e	812.31	0.00000	NO	YES

24	e	812.31	0.00000	NO	YES
25	t2	864.33	132.35779	YES	YES
26	t2	864.33	132.35779	YES	YES
27	t2	864.33	132.35779	YES	YES
28	t2	1237.34	31.53159	YES	YES
29	t2	1237.34	31.53159	YES	YES
30	t2	1237.34	31.53159	YES	YES
31	a1	1250.59	0.00000	NO	YES
32	t1	1399.17	0.00000	NO	NO
33	t1	1399.17	0.00000	NO	NO
34	t1	1399.17	0.00000	NO	NO
35	e	1404.15	0.00000	NO	YES
36	e	1404.15	0.00000	NO	YES
37	t2	1417.64	9.47506	YES	YES
38	t2	1417.64	9.47506	YES	YES
39	t2	1417.64	9.47506	YES	YES
40	t2	2934.96	10.65240	YES	YES
41	t2	2934.96	10.65240	YES	YES
42	t2	2934.96	10.65240	YES	YES
43	a1	2937.33	0.00000	NO	YES
44	e	3025.93	0.00000	NO	YES
45	e	3025.93	0.00000	NO	YES
46	t1	3026.72	0.00000	NO	NO
47	t1	3026.72	0.00000	NO	NO
48	t1	3026.72	0.00000	NO	NO
49	t2	3028.30	26.91845	YES	YES
50	t2	3028.30	26.91845	YES	YES
51	t2	3028.30	26.91845	YES	YES

Ion Affinity Scale:

BF₃



Total energy = -324.3176879974 H = -8825.1383352 eV

HOMO-LUMO Separation

HOMO: 11. 1 a2' -0.36038084 H = -9.80647 eV

LUMO: 12. 2 a2" -0.01048005 H = -0.28518 eV

Gap : +0.34990079 H = +9.52129 eV

Number of MOs= 38, Electrons= 32.00, Symmetry: d3h

```

$coord
  0.0000000000000000  0.0000000000000000  0.0000000000000000  b
  2.50094344537878   0.0000000000000000  0.0000000000000000  f
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 -1.25047172268939  -2.16588055712621    0.0000000000000000  f

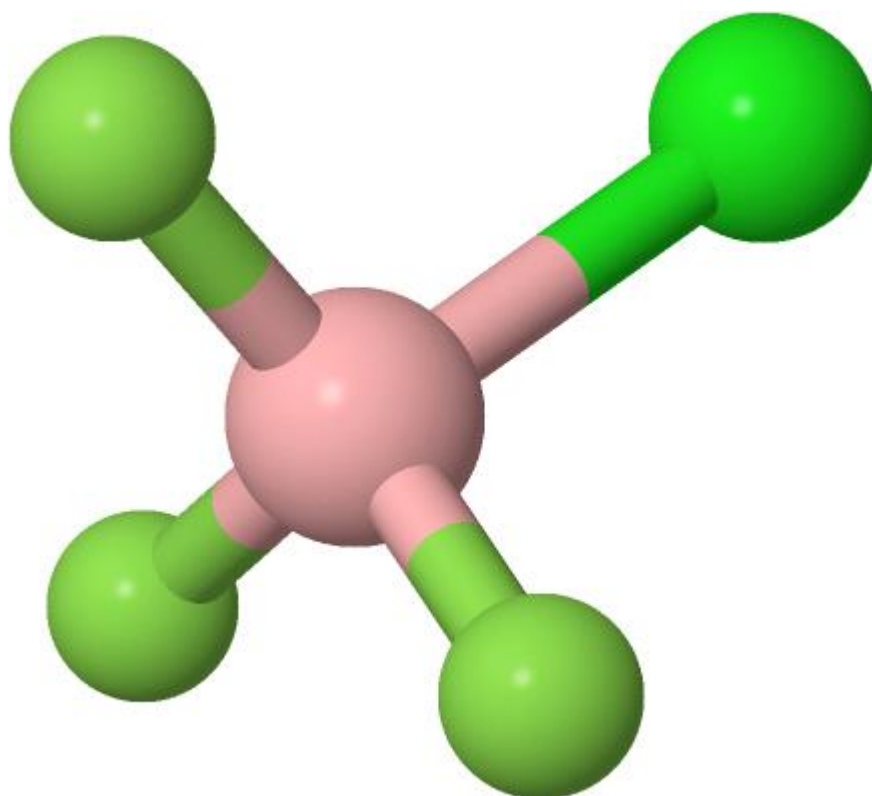
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```

$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#                               cm** (-1)          km/mol            IR      RAMAN
  1              0.00          0.00000          -        -
  2              0.00          0.00000          -        -
  3              0.00          0.00000          -        -
  4              0.00          0.00000          -        -
  5              0.00          0.00000          -        -
  6              0.00          0.00000          -        -
  7             e'          462.40          10.31323        YES      YES
  8             e'          462.40          10.31323        YES      YES
  9             a2''         656.08          82.00580        YES      NO
 10             a1'          862.52           0.00000        NO       YES
 11             e'         1457.76          387.73541       YES      YES
 12             e'         1457.76          387.73541       YES      YES

```

BF₃Cl⁻



Total energy = -784.5322969364 H = -21348.2221449 eV

HOMO-LUMO Separation

HOMO: 18. 7 e -0.04255314 H = -1.15793 eV

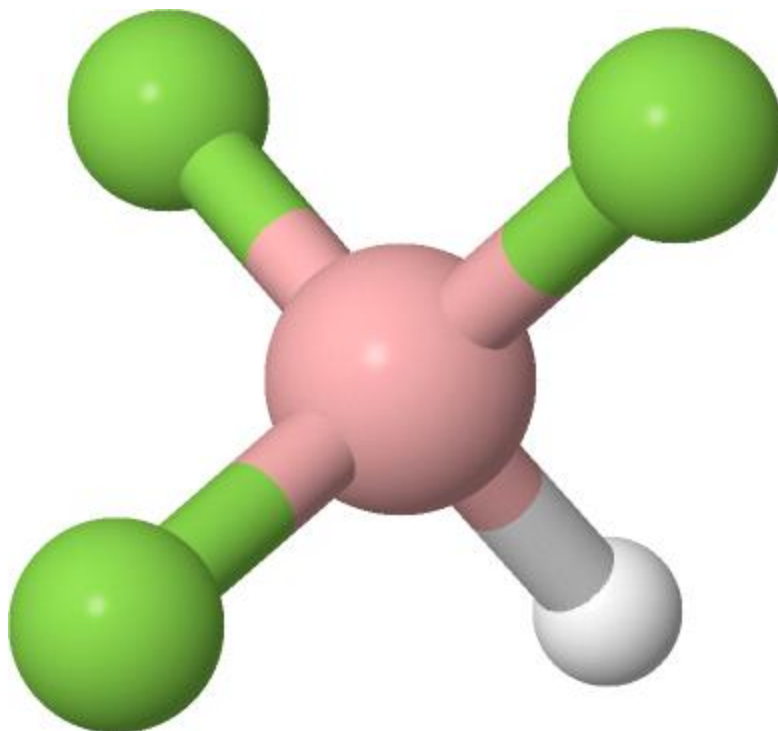
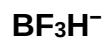
LUMO: 19. 11 a1 +0.30557457 H = +8.31511 eV

Gap : +0.34812771 H = +9.47304 eV

Number of MOs= 51, Electrons= 50.00, Symmetry: c3v

```
$coord
  0.0000000000000000  0.0000000000000000  -0.82601821080417  b
  0.0000000000000000  0.0000000000000000   2.88558955471781  cl
 -1.25601173739481    2.17547614407066    -1.63825591640009  f
 -1.25601173739481   -2.17547614407066    -1.63825591640009  f
  2.51202347478961    0.0000000000000000    -1.63825591640009  f
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#          #          cm** (-1)      km/mol          IR          RAMAN
  1          0.00          0.00000          -          -
  2          0.00          0.00000          -          -
  3          0.00          0.00000          -          -
  4          0.00          0.00000          -          -
  5          0.00          0.00000          -          -
  6          0.00          0.00000          -          -
  7          e          269.08          0.01315        YES          YES
  8          e          269.08          0.01315        YES          YES
  9          a1         341.81         12.63300        YES          YES
 10          e          463.68          1.66177        YES          YES
 11          e          463.68          1.66177        YES          YES
 12          a1         642.04          91.50421        YES          YES
 13          a1         879.75         397.61113        YES          YES
 14          e         1163.85         287.21938        YES          YES
 15          e         1163.85         287.21938        YES          YES
```

Total energy = -324.9463150558 H = -8842.2441575 eV

HOMO-LUMO Separation

HOMO: 12. 6 a1 -0.01829212 H = -0.49775 eV

LUMO: 13. 6 e +0.35993995 H = +9.79447 eV

Gap : +0.37823207 H = +10.29222 eV

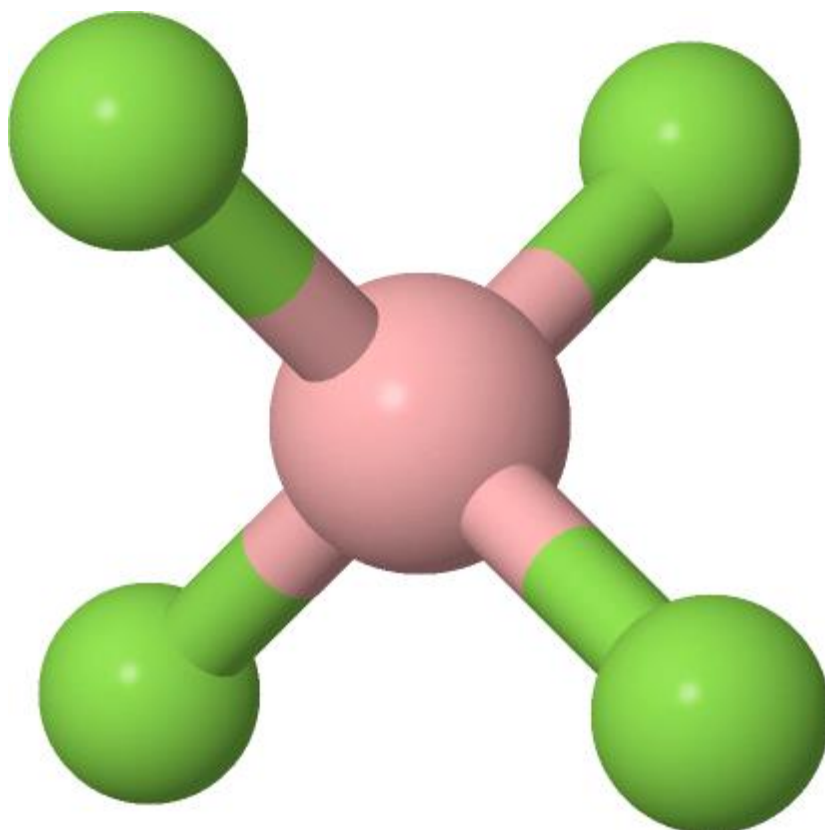
Number of MOs= 40, Electrons= 34.00, Symmetry: c3v

\$coord			
0.0000000000000000	0.0000000000000000	0.73483833733775	b
0.0000000000000000	0.0000000000000000	3.15033549352848	h
-1.26363028527391	2.18867185607716	-0.19510030550591	f
-1.26363028527391	-2.18867185607716	-0.19510030550591	f
2.52726057054781	0.0000000000000000	-0.19510030550591	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	412.34	0.05108	YES	YES
8		e	412.34	0.05108	YES	YES
9		a1	587.42	3.09589	YES	YES
10		e	934.59	31.88910	YES	YES
11		e	934.59	31.88910	YES	YES
12		a1	940.29	119.23729	YES	YES
13		e	1184.68	323.62855	YES	YES
14		e	1184.68	323.62855	YES	YES
15		a1	2162.61	596.29201	YES	YES

BF₃F⁻



Total energy = -424.2009934024 H = -11543.1029119 eV

HOMO-LUMO Separation

HOMO: 10. 1 t1 -0.06610077 H = -1.79869 eV

LUMO: 11. 5 a1 +0.33153072 H = +9.02141 eV

Gap : +0.39763149 H = +10.82011 eV

Number of MOs= 31, Electrons= 42.00, Symmetry: td

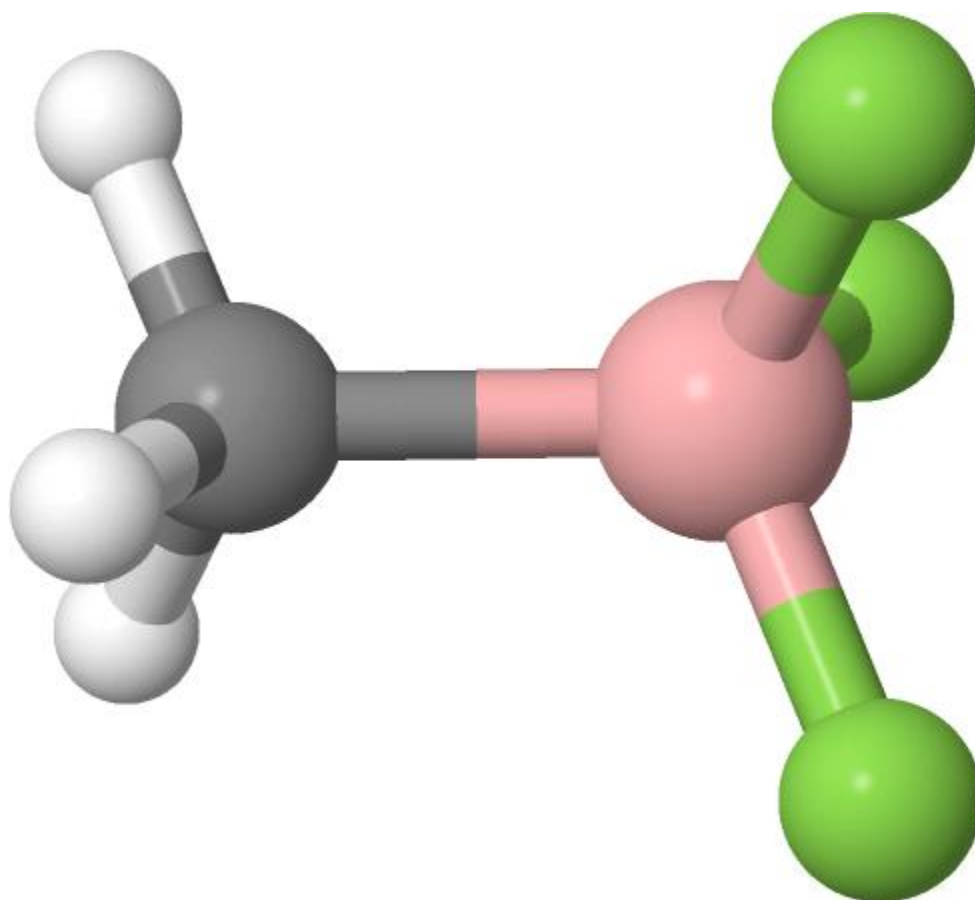
\$coord

0.0000000000000000	0.0000000000000000	0.0000000000000000	b
1.54603262616822	-1.54603262616822	1.54603262616822	f
-1.54603262616822	1.54603262616822	1.54603262616822	f
1.54603262616822	1.54603262616822	-1.54603262616822	f
-1.54603262616822	-1.54603262616822	-1.54603262616822	f

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	346.19	0.00000	NO	YES
8		e	346.19	0.00000	NO	YES
9		t2	508.82	1.61185	YES	YES
10		t2	508.82	1.61185	YES	YES
11		t2	508.82	1.61185	YES	YES
12		a1	738.15	0.00000	NO	YES
13		t2	1114.88	336.91610	YES	YES
14		t2	1114.88	336.91610	YES	YES
15		t2	1114.88	336.91610	YES	YES

BF₃Me⁻



Total energy = -364.2431200453 H = -9911.5652368 eV

HOMO-LUMO Separation

HOMO: 15. 8 a1 -0.03167340 H = -0.86188 eV

LUMO: 16. 9 a1 +0.22826992 H = +6.21154 eV

Gap : +0.25994332 H = +7.07342 eV

Number of MOs= 52, Electrons= 42.00, Symmetry: c3v

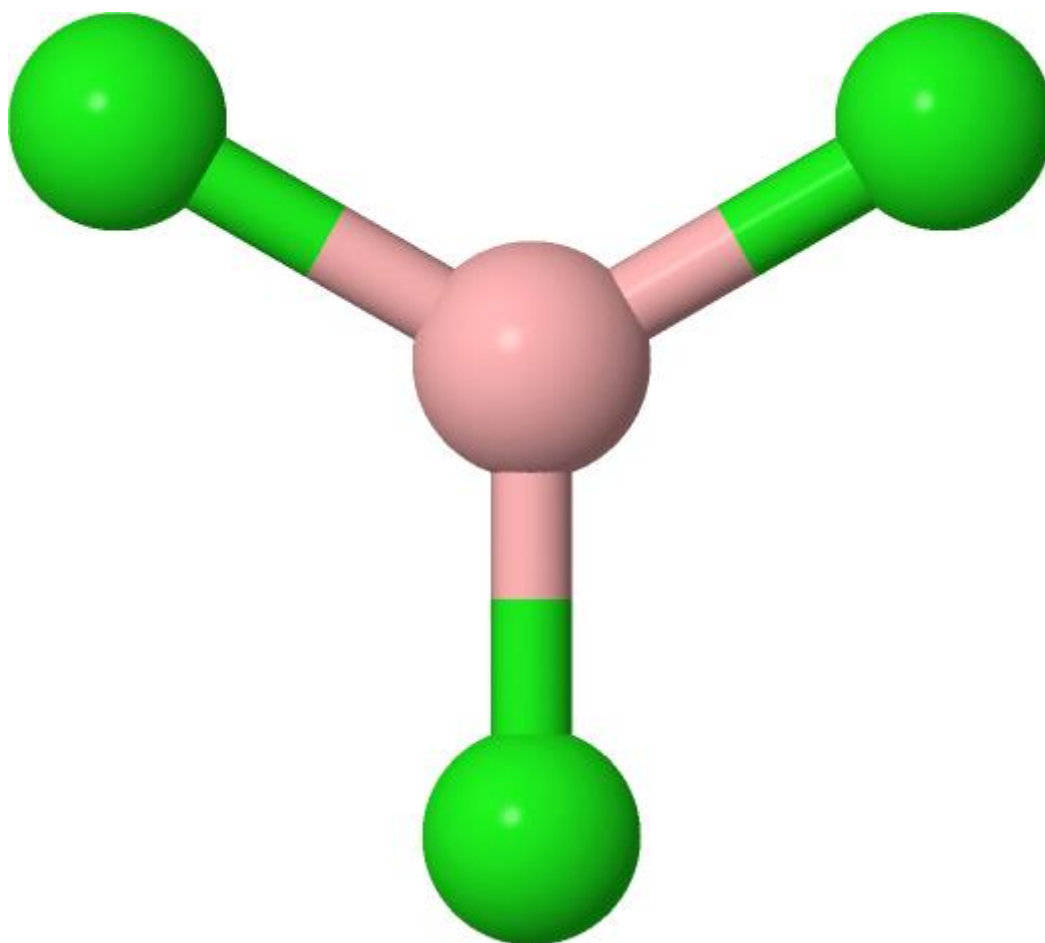
\$coord
0.0000000000000000 0.0000000000000000 0.06254924012410 b

-1.26548685065042	2.19188752163685	-0.89085721831631	f
-1.26548685065042	-2.19188752163685	-0.89085721831631	f
2.53097370130084	0.00000000000000	-0.89085721831631	f
0.00000000000000	0.00000000000000	3.17450456426312	c
-1.96258799257971	0.00000000000000	3.95809233652828	h
0.98129399628986	1.69965105873634	3.95809233652828	h
0.98129399628986	-1.69965105873634	3.95809233652828	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a2		202.55	0.00000	NO	NO
8	e		273.84	0.25058	YES	YES
9	e		273.84	0.25058	YES	YES
10	e		434.00	0.05043	YES	YES
11	e		434.00	0.05043	YES	YES
12	a1		490.14	5.31864	YES	YES
13	a1		681.17	0.01141	YES	YES
14	e		777.54	10.48869	YES	YES
15	e		777.54	10.48869	YES	YES
16	a1		1030.20	255.67239	YES	YES
17	e		1093.80	235.56836	YES	YES
18	e		1093.80	235.56836	YES	YES
19	a1		1251.60	84.88700	YES	YES
20	e		1414.67	0.80018	YES	YES
21	e		1414.67	0.80018	YES	YES
22	a1		2881.63	34.87763	YES	YES
23	e		2958.41	102.17431	YES	YES
24	e		2958.41	102.17431	YES	YES

BCl₃



Total energy = -1405.2745738590 H = -38239.4885391 eV

HOMO-LUMO Separation

HOMO: 19. 2 a2' -0.27827700 H = -7.57231 eV

LUMO: 20. 3 a2'' -0.08752924 H = -2.38179 eV

Gap : +0.19074777 H = +5.19051 eV

Number of MOs= 46, Electrons= 56.00, Symmetry: d3h

```

$coord
  0.000000000000000  0.000000000000000  0.000000000000000  b
  1.65942438441921 -2.87420734513278  0.000000000000000  cl
  1.65942438441921  2.87420734513278  0.000000000000000  cl
 -3.31884876883843  0.000000000000000  0.000000000000000  cl

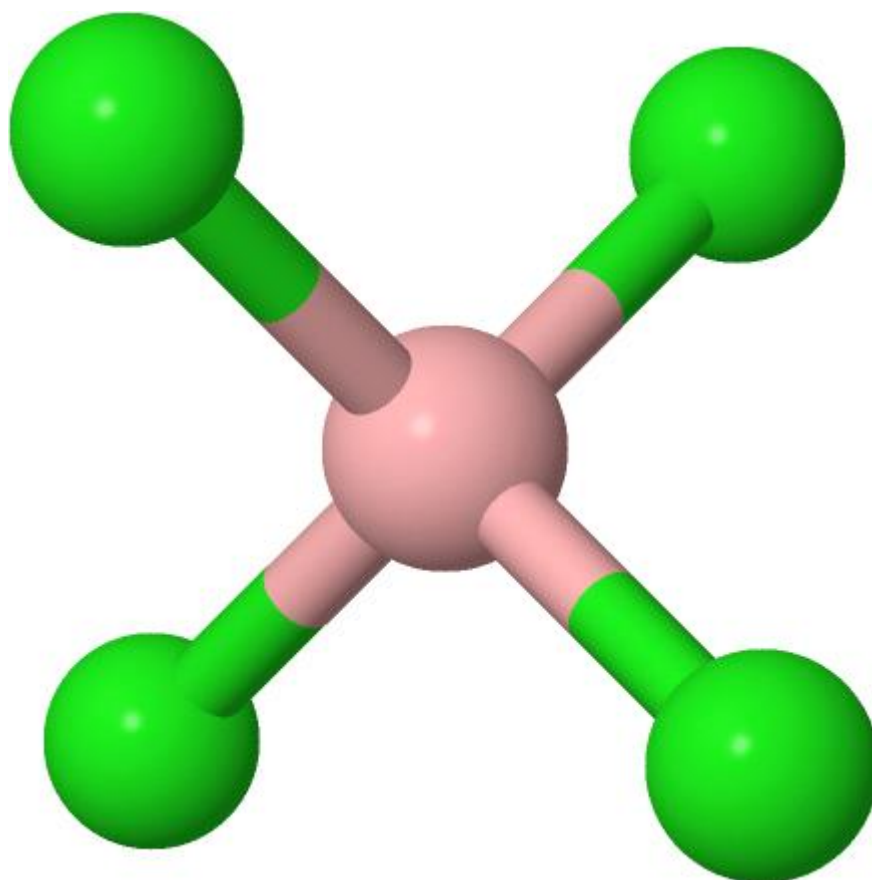
```

```

$vibrational spectrum
# mode      symmetry    wave number    IR intensity    selection rules
#                               cm** (-1)      km/mol          IR      RAMAN
  1              0.00      0.00000
  2              0.00      0.00000
  3              0.00      0.00000
  4              0.00      0.00000
  5              0.00      0.00000
  6              0.00      0.00000
  7             e'      247.27      0.48750      YES      YES
  8             e'      247.27      0.48750      YES      YES
  9            a2"      438.45      4.33720      YES      NO
 10            a1'      456.39      0.00000      NO      YES
 11            e'      950.43     332.93191     YES      YES
 12            e'      950.43     332.93191     YES      YES

```

BCl₄⁻



Total energy = -1865.5037220420 H = -50762.9679820 eV

HOMO-LUMO Separation

HOMO: 17. 2 t1 -0.06276488 H = -1.70792 eV

LUMO: 18. 7 a1 +0.23031721 H = +6.26725 eV

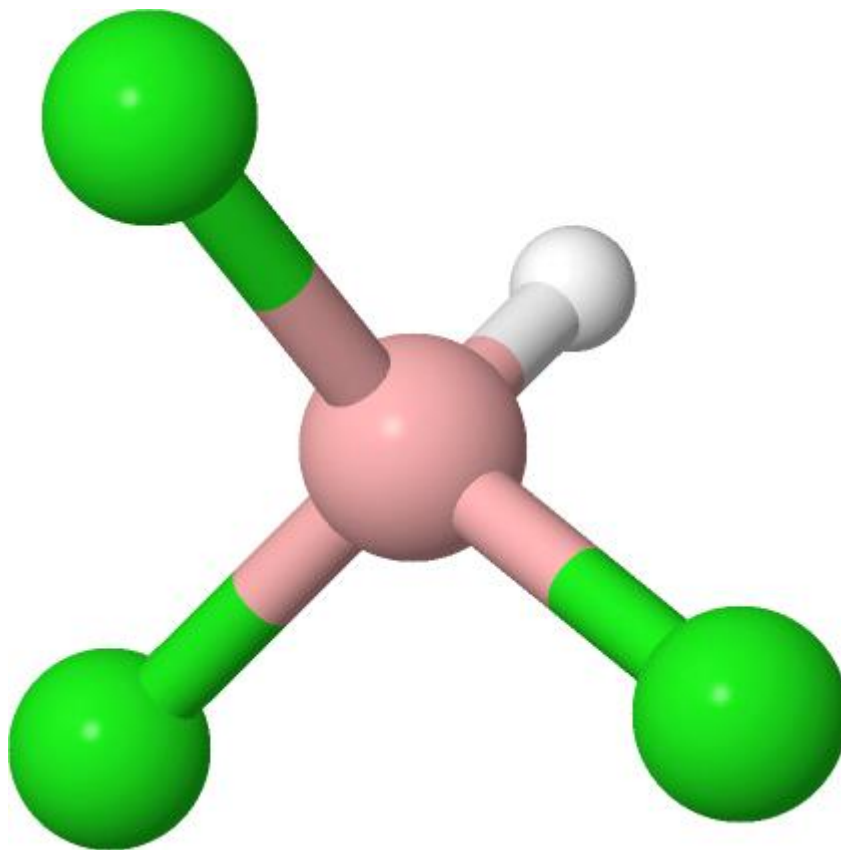
Gap : +0.29308209 H = +7.97517 eV

Number of MOs= 38, Electrons= 74.00, Symmetry: td

```
$coord
0.0000000000000000 0.0000000000000000 0.0000000000000000 b
2.05303091810228 -2.05303091810228 2.05303091810228 cl
-2.05303091810228 2.05303091810228 2.05303091810228 cl
-2.05303091810228 -2.05303091810228 -2.05303091810228 cl
2.05303091810228 2.05303091810228 -2.05303091810228 cl
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 176.18 0.00000 NO YES
8 e 176.18 0.00000 NO YES
9 t2 259.68 0.34696 YES YES
10 t2 259.68 0.34696 YES YES
11 t2 259.68 0.34696 YES YES
12 a1 388.07 0.00000 NO YES
13 t2 704.25 260.67773 YES YES
14 t2 704.25 260.67773 YES YES
15 t2 704.25 260.67773 YES YES
```


BCl₃H⁻



Total energy = -1405.9390102490 H = -38257.5687835 eV

HOMO-LUMO Separation

HOMO: 20. 9 a1 -0.04564264 H = -1.24200 eV

LUMO: 21. 10 a1 +0.25218932 H = +6.86242 eV

Gap : +0.29783196 H = +8.10442 eV

Number of MOs= 48, Electrons= 58.00, Symmetry: c3v

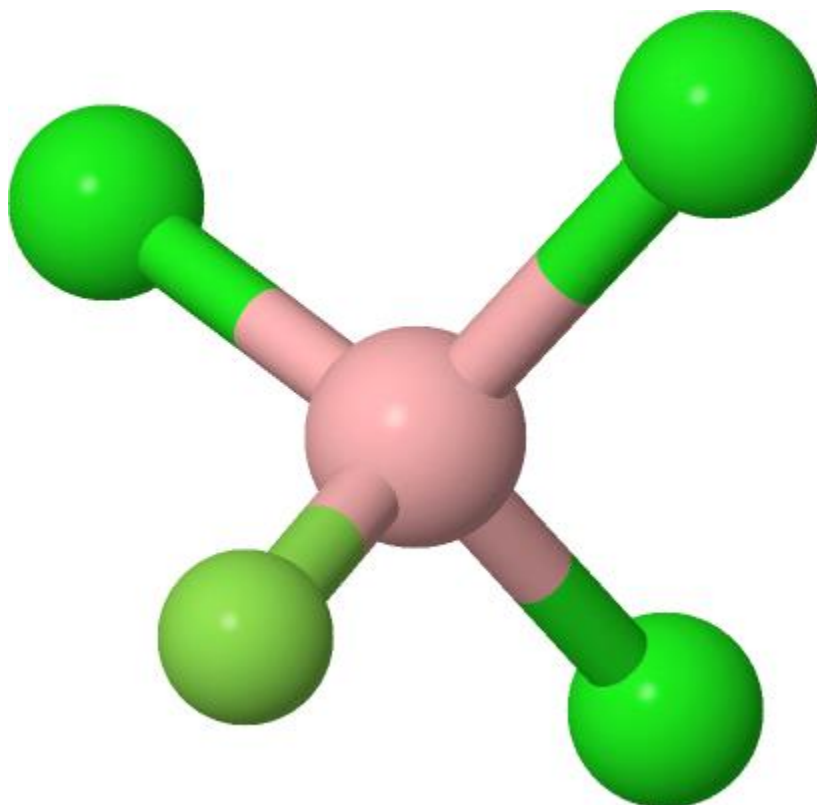
\$coord

0.0000000000000000	0.0000000000000000	1.04694169379341	b
0.0000000000000000	0.0000000000000000	3.36986220364630	h
-1.69242820591811	2.93137164081281	-0.13835412759625	cl
-1.69242820591811	-2.93137164081281	-0.13835412759625	cl
3.38485641183622	0.0000000000000000	-0.13835412759625	cl

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	207.44	0.60504	YES	YES
8		e	207.44	0.60504	YES	YES
9		a1	298.78	0.19446	YES	YES
10		a1	589.54	10.01637	YES	YES
11		e	632.19	172.07252	YES	YES
12		e	632.19	172.07252	YES	YES
13		e	996.78	148.12291	YES	YES
14		e	996.78	148.12291	YES	YES
15		a1	2458.11	271.80582	YES	YES

BCl₃F⁻



Total energy = -1505.1822233410 H = -40958.115522 eV

HOMO-LUMO Separation

HOMO: 23. 2 a2 -0.05379410 H = -1.46381 eV

LUMO: 24. 12 a1 +0.24202929 H = +6.58596 eV

Gap : +0.29582338 H = +8.04977 eV

Number of MOs= 56, Electrons= 66.00, Symmetry: c3v

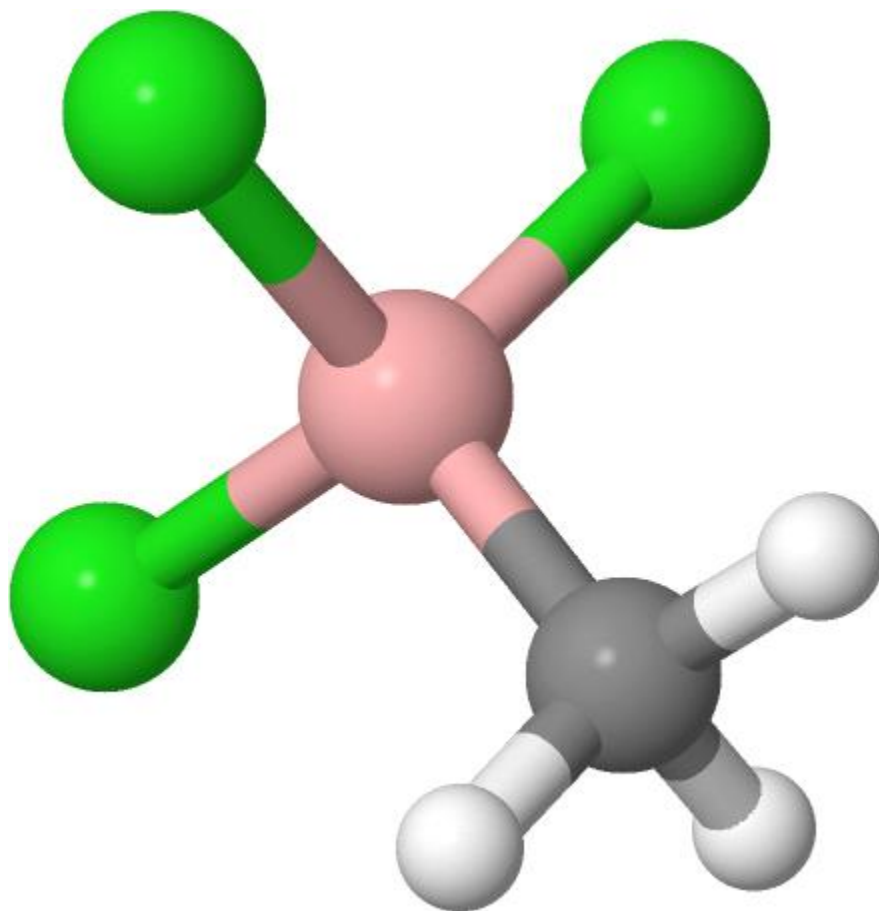
\$coord

0.0000000000000000	0.0000000000000000	-0.20689776130708	b
-1.68894091314195	-2.92533147254360	1.00610637336944	c1
-1.68894091314195	2.92533147254360	1.00610637336944	c1
0.0000000000000000	0.0000000000000000	-2.81135785470600	f
3.37788182628387	0.0000000000000000	1.00610637336944	c1

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	192.55	0.04792	YES	YES
8		e	192.55	0.04792	YES	YES
9		a1	281.01	0.03768	YES	YES
10		e	329.43	1.75719	YES	YES
11		e	329.43	1.75719	YES	YES
12		a1	450.00	4.45842	YES	YES
13		e	710.04	348.07327	YES	YES
14		e	710.04	348.07327	YES	YES
15		a1	1115.99	230.42740	YES	YES

BCl₃Me⁻



Total energy = -1445.2323594340 H = -39326.7958255 eV

HOMO-LUMO Separation

HOMO: 23. 2 a2 -0.04928126 H = -1.34101 eV

LUMO: 24. 12 a1 +0.21654995 H = +5.89263 eV

Gap : +0.26583121 H = +7.23364 eV

Number of MOs= 60, Electrons= 66.00, Symmetry: c3v

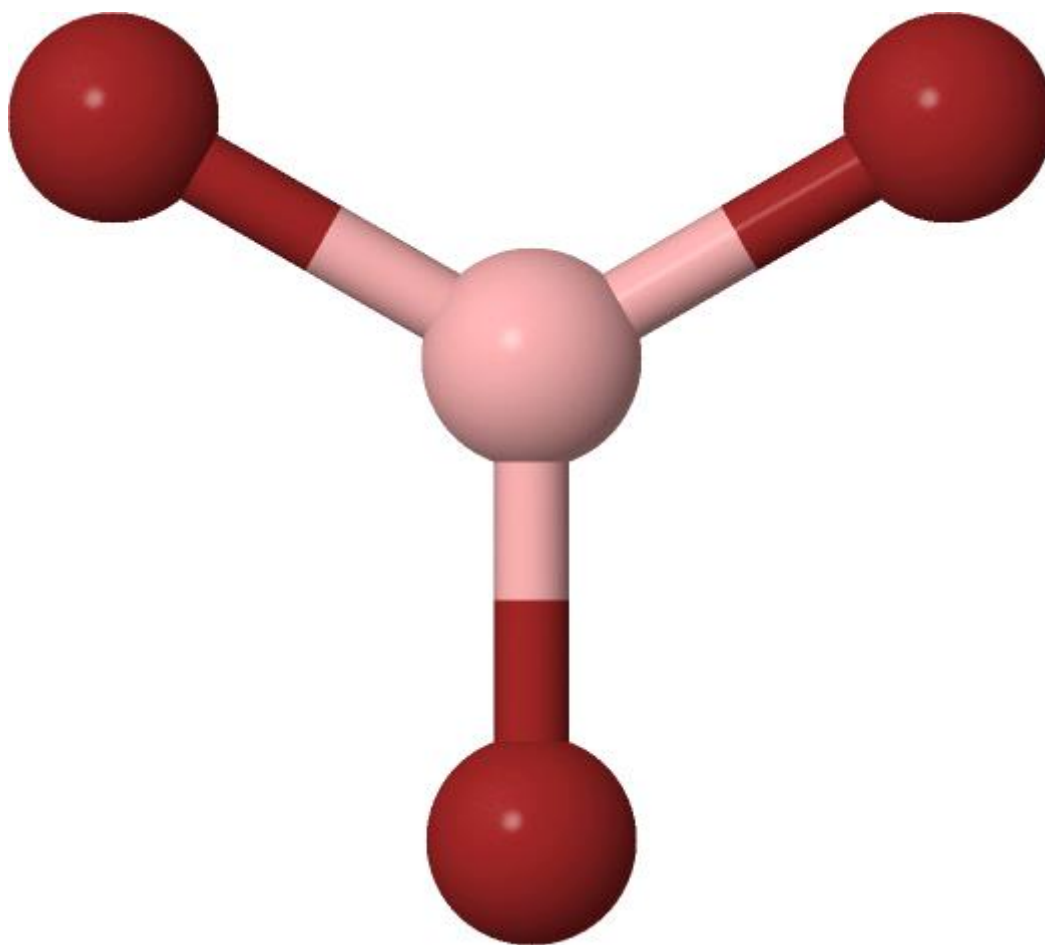
\$coord

0.0000000000000000	0.0000000000000000	0.64290271060174	b
-1.69241460356382	2.93134808084408	-0.60889407140311	cl
-1.69241460356382	-2.93134808084408	-0.60889407140311	cl
3.38482920712764	0.0000000000000000	-0.60889407140311	cl
0.0000000000000000	0.0000000000000000	3.69263406197627	c
-1.96732404917026	0.0000000000000000	4.45058276289375	h
0.98366202458513	1.70375260405751	4.45058276289375	h
0.98366202458513	-1.70375260405751	4.45058276289375	h

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	e		187.83	0.07223	YES	YES
8	e		187.83	0.07223	YES	YES
9	a2		248.78	0.00000	NO	NO
10	e		269.49	0.99052	YES	YES
11	e		269.49	0.99052	YES	YES
12	a1		278.87	0.11626	YES	YES
13	a1		439.56	10.49684	YES	YES
14	e		596.29	143.41959	YES	YES
15	e		596.29	143.41959	YES	YES
16	e		908.47	110.29874	YES	YES
17	e		908.47	110.29874	YES	YES
18	a1		957.44	87.93890	YES	YES
19	a1		1272.45	33.12994	YES	YES
20	e		1409.71	0.09524	YES	YES
21	e		1409.71	0.09524	YES	YES
22	a1		2906.24	34.94854	YES	YES
23	e		2989.83	55.27737	YES	YES
24	e		2989.83	55.27737	YES	YES

BBr₃



Total energy = -7747.3363149320 H = -210815.8674001 eV

HOMO-LUMO Separation

HOMO: 37. 4 a₂' -0.25684390 H = -6.98908 eV

LUMO: 38. 5 a₂" -0.10599162 H = -2.88418 eV

Gap : +0.15085228 H = +4.10490 eV

Number of MOs= 74, Electrons= 110.00, Symmetry: d_{3h}

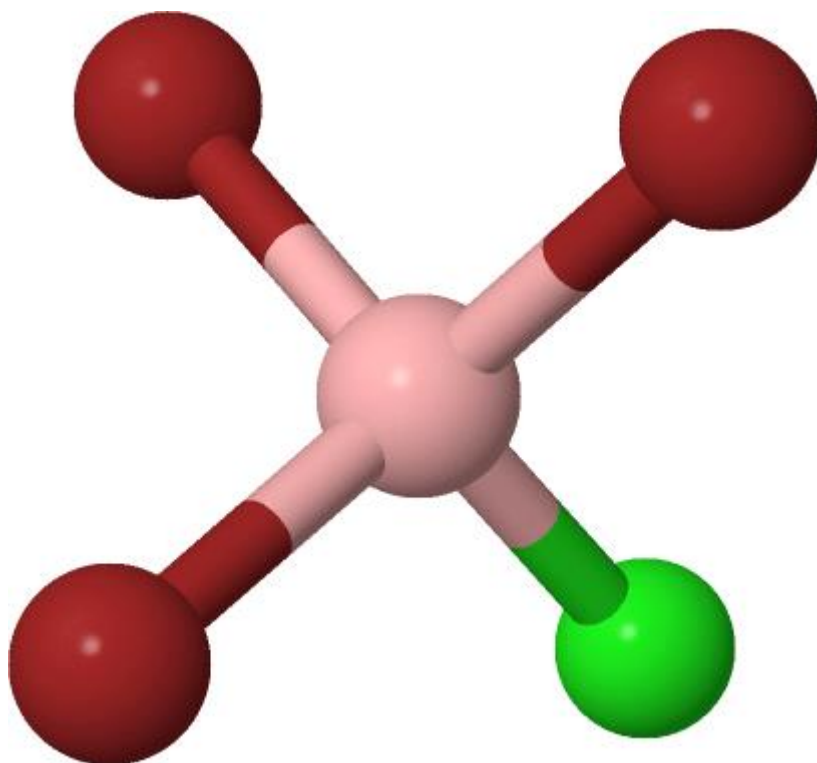
```
$coord
0.0000000000000000 0.0000000000000000 0.0000000000000000 b
1.80973934650694 -3.13456049660651 0.0000000000000000 br
```

1.80973934650694	3.13456049660651	0.000000000000000	br
-3.61947869301387	0.000000000000000	0.000000000000000	br

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e'	147.24	0.04859	YES	YES
8		e'	147.24	0.04859	YES	YES
9		a1'	273.58	0.00000	NO	YES
10		a2''	375.17	0.21867	YES	NO
11		e'	814.06	276.69566	YES	YES
12		e'	814.06	276.69566	YES	YES

BBr₃Cl⁻



Total energy = -8207.5769422720 H = -223339.6592069 eV

HOMO-LUMO Separation

HOMO: 44. 5 a2 -0.06066766 H = -1.65085 eV

LUMO: 45. 20 a1 +0.15931163 H = +4.33509 eV

Gap : +0.21997930 H = +5.98594 eV

Number of MOs= 87, Electrons= 128.00, Symmetry: c3v

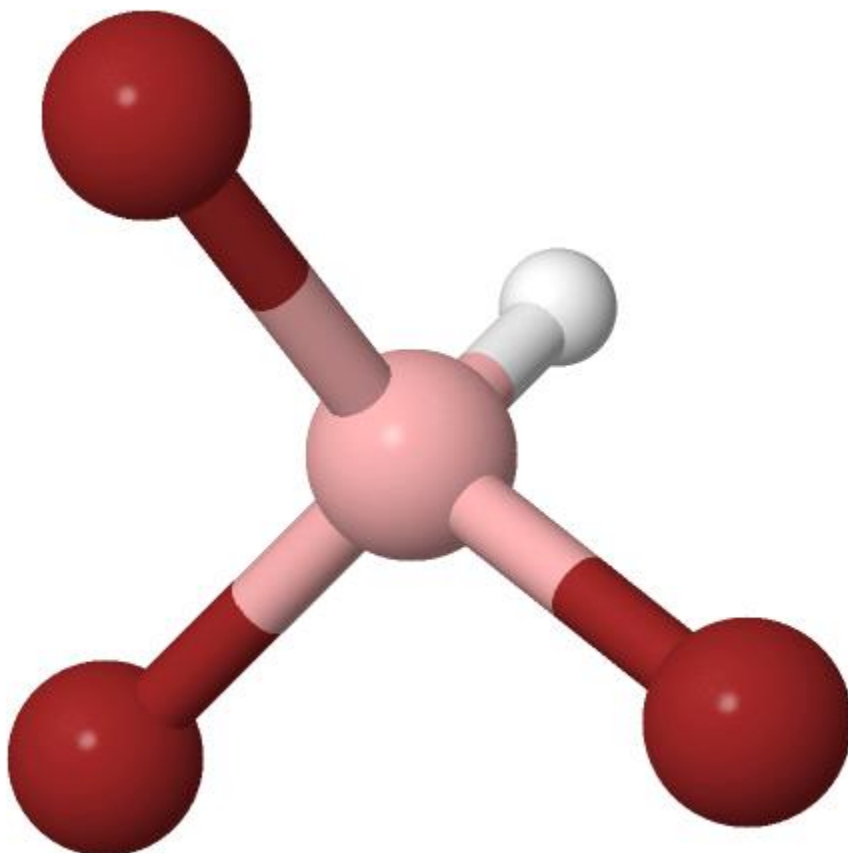
\$coord

0.0000000000000000	0.0000000000000000	0.67866976213241	b
-1.83098833670155	3.17136482723311	-0.65010516739832	br
-1.83098833670155	-3.17136482723311	-0.65010516739832	br
3.66197667340310	0.0000000000000000	-0.65010516739832	br
0.0000000000000000	0.0000000000000000	4.18894487536972	cl

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	113.46	0.15307	YES	YES
8		e	113.46	0.15307	YES	YES
9		a1	173.50	0.70912	YES	YES
10		e	178.52	0.53806	YES	YES
11		e	178.52	0.53806	YES	YES
12		a1	278.86	0.01932	YES	YES
13		e	566.42	228.81354	YES	YES
14		e	566.42	228.81354	YES	YES
15		a1	690.36	208.84816	YES	YES

BBr₃H⁻



Total energy = -7748.0187968920 H = -210834.4386897 eV

HOMO-LUMO Separation

HOMO: 38. 5 a2 -0.05195918 H = -1.41388 eV

LUMO: 39. 16 a1 +0.17493499 H = +4.76023 eV

Gap : +0.22689417 H = +6.17411 eV

Number of MOs= 76, Electrons= 112.00, Symmetry: c3v

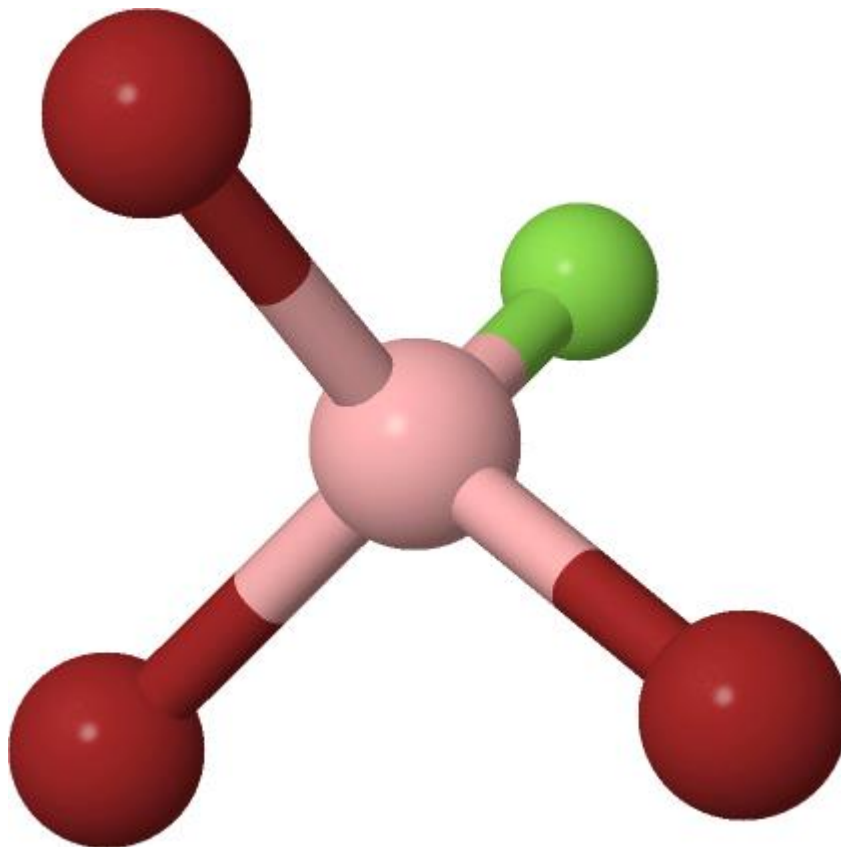
\$coord				
	0.0000000000000000	0.0000000000000000	1.18003489175432	b
	0.0000000000000000	0.0000000000000000	3.48933306077356	h

-1.84917655020902	3.20286773712696	-0.06788763994053	br
-1.84917655020902	-3.20286773712696	-0.06788763994053	br
3.69835310041804	0.000000000000000	-0.06788763994053	br

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	119.94	0.52294	YES	YES
8		e	119.94	0.52294	YES	YES
9		a1	178.63	0.33432	YES	YES
10		a1	471.08	0.69577	YES	YES
11		e	517.54	157.91793	YES	YES
12		e	517.54	157.91793	YES	YES
13		e	940.49	131.77619	YES	YES
14		e	940.49	131.77619	YES	YES
15		a1	2520.57	166.35838	YES	YES

BBr₃F⁻



Total energy = -7847.2579748030 H = -213534.8756556 eV

HOMO-LUMO Separation

HOMO: 41. 5 a2 -0.05596532 H = -1.52289 eV

LUMO: 42. 18 a1 +0.16367035 H = +4.45370 eV

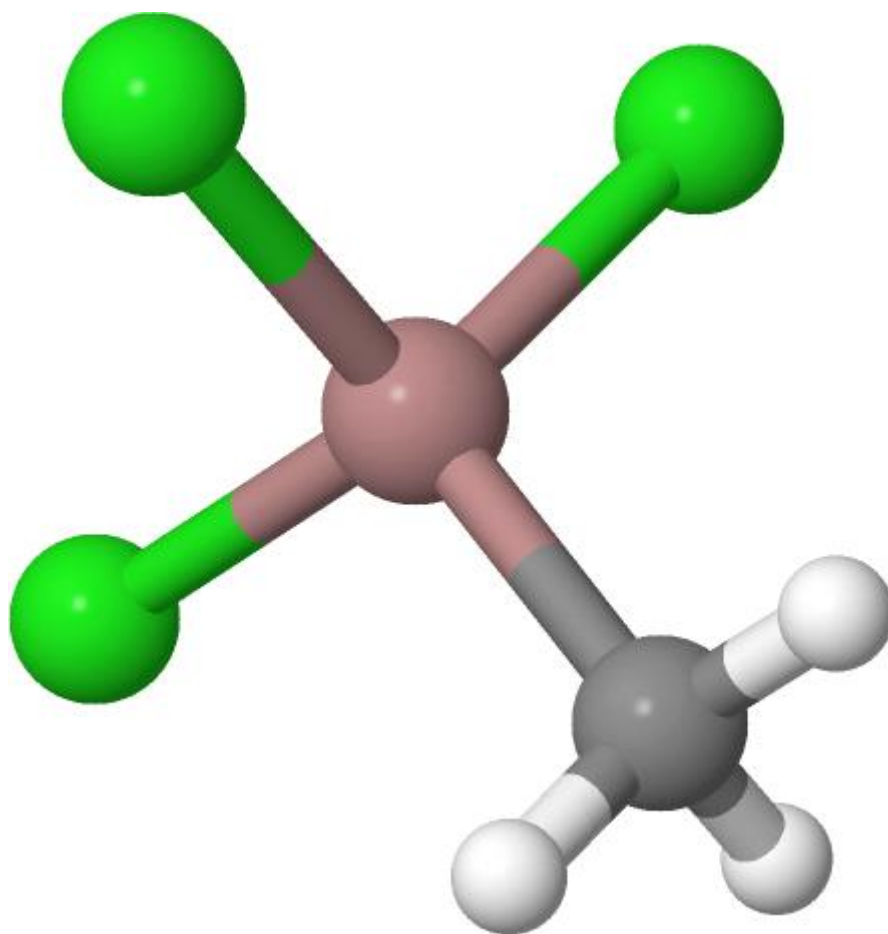
Gap : +0.21963568 H = +5.97659 eV

Number of MOs= 84, Electrons= 120.00, Symmetry: c3v

```
$coord
0.0000000000000000 0.0000000000000000 0.27601605386019 b
-1.84603815201412 3.19743187199899 -1.04543316059289 br
-1.84603815201412 -3.19743187199899 -1.04543316059289 br
3.69207630402822 0.0000000000000000 -1.04543316059289 br
0.0000000000000000 0.0000000000000000 2.86028342791850 f
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 116.58 0.23343 YES YES
8 e 116.58 0.23343 YES YES
9 a1 174.58 0.43789 YES YES
10 e 255.01 2.74272 YES YES
11 e 255.01 2.74272 YES YES
12 a1 340.53 0.63476 YES YES
13 e 598.71 326.36126 YES YES
14 e 598.71 326.36126 YES YES
15 a1 1127.47 199.83686 YES YES
```

BBr₃Me⁻



Total energy = -3345.3474532630 H = -91031.5876897 eV

HOMO-LUMO Separation

HOMO: 32. 16 a1 -0.07413194 H = -2.01723 eV

LUMO: 33. 17 a1 +0.14423742 H = +3.92490 eV

Gap : +0.21836937 H = +5.94214 eV

Number of MOs= 72, Electrons= 92.00, Symmetry: c3v

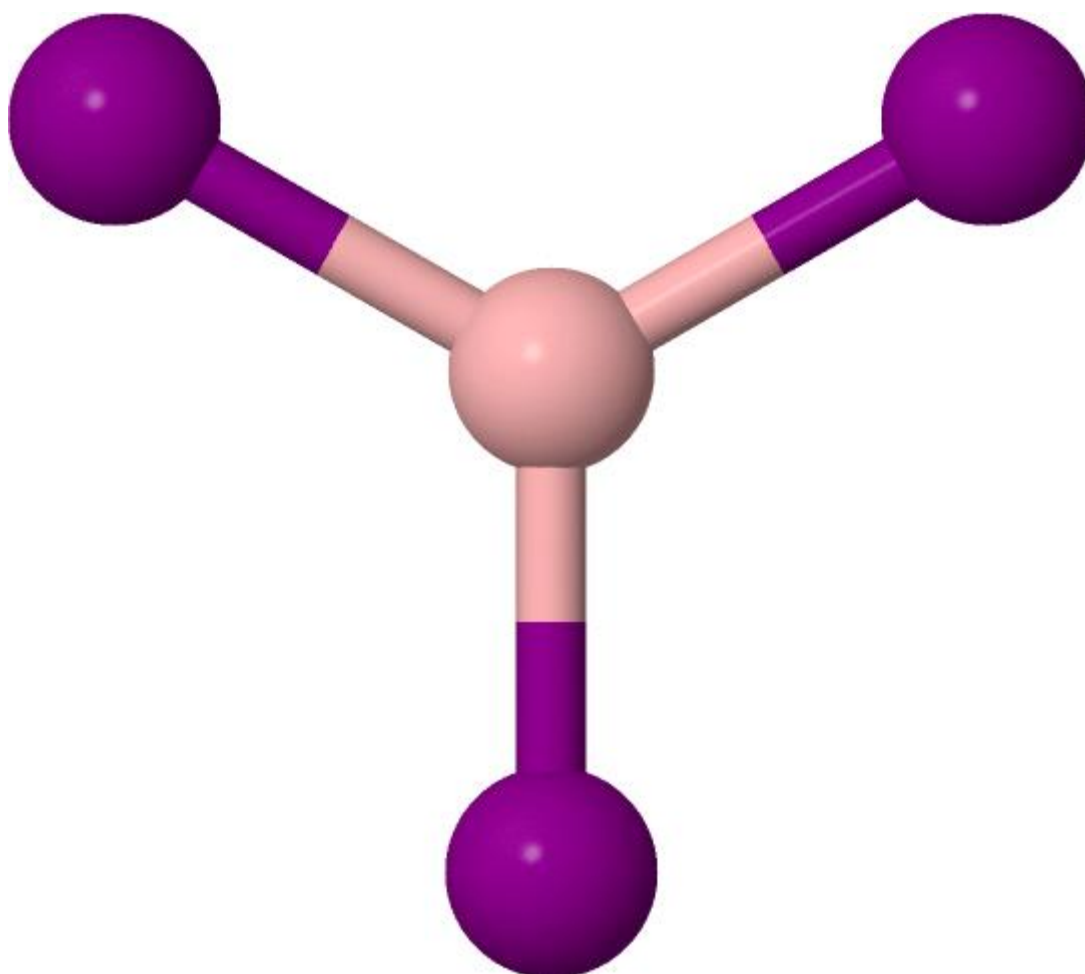
\$coord

0.0000000000000000	0.0000000000000000	0.54652101416919	ga
-1.99139921727666	3.44920462247607	-0.98989009274557	cl
-1.99139921727666	-3.44920462247607	-0.98989009274557	cl
3.98279843455332	0.0000000000000000	-0.98989009274557	cl
0.0000000000000000	0.0000000000000000	4.32279180593536	c
-1.97414829018557	0.0000000000000000	5.04597506757467	h
0.98707414509278	1.70966257013832	5.04597506757467	h
0.98707414509278	-1.70966257013832	5.04597506757467	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a2		94.31	0.00000	NO	NO
8	e		106.18	0.09273	YES	YES
9	e		106.18	0.09273	YES	YES
10	e		144.02	5.05102	YES	YES
11	e		144.02	5.05102	YES	YES
12	a1		146.68	9.65598	YES	YES
13	a1		320.06	20.49978	YES	YES
14	e		345.74	75.70034	YES	YES
15	e		345.74	75.70034	YES	YES
16	a1		530.18	39.33343	YES	YES
17	e		710.18	44.34009	YES	YES
18	e		710.18	44.34009	YES	YES
19	a1		1157.74	6.46364	YES	YES
20	e		1401.01	0.67677	YES	YES
21	e		1401.01	0.67677	YES	YES
22	a1		2933.91	24.91279	YES	YES
23	e		3034.55	25.49023	YES	YES
24	e		3034.55	25.49023	YES	YES

BI₃



Total energy = -59.2779668041 H = -1613.0364659 eV

HOMO-LUMO Separation

HOMO: 9. 1 a2' -0.23761662 H = -6.46588 eV

LUMO: 10. 2 a2" -0.12548651 H = -3.41466 eV

Gap : +0.11213011 H = +3.05122 eV

Number of MOs= 36, Electrons= 26.00, Symmetry: d3h

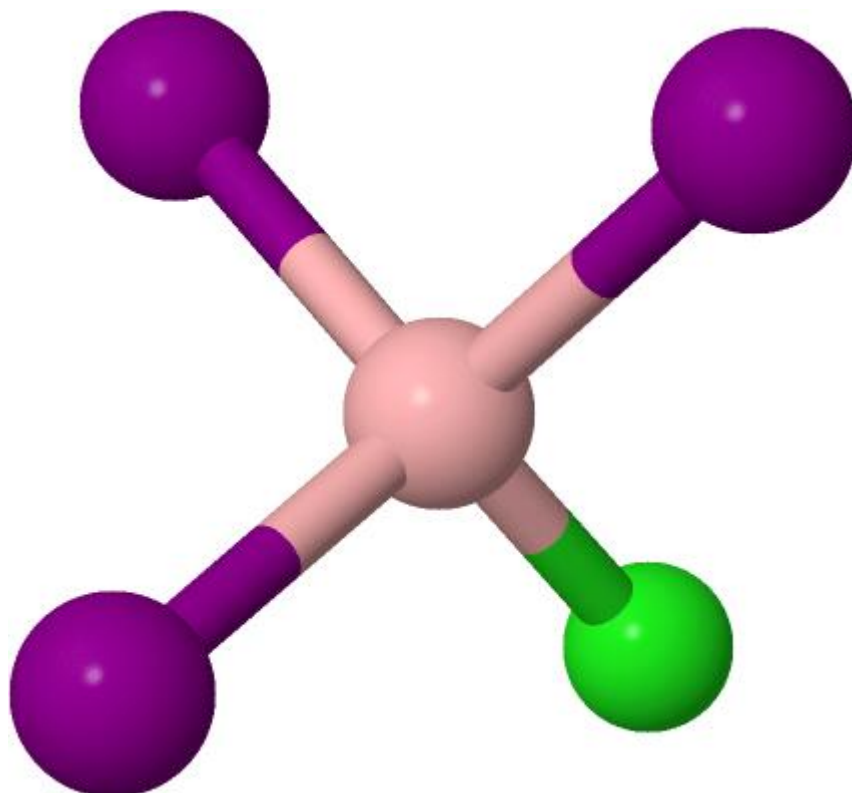
\$coord
0.0000000000000000 0.0000000000000000 0.0000000000000000 b
122

2.02804453821179	-3.51267618019538	0.000000000000000	i
2.02804453821179	3.51267618019538	0.000000000000000	i
-4.05608907642358	0.000000000000000	0.000000000000000	i

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e'	98.92	0.00034	YES	YES
8		e'	98.92	0.00034	YES	YES
9		a1'	187.43	0.00000	NO	YES
10		a2''	309.05	1.11033	YES	NO
11		e'	692.60	256.56526	YES	YES
12		e'	692.60	256.56526	YES	YES

BI₃Cl⁻



Total energy = -519.5372026164 H = -14137.3346353 eV
123

HOMO-LUMO Separation

HOMO: 16. 1 a2 -0.06978504 H = -1.89895 eV

LUMO: 17. 10 a1 +0.07106726 H = +1.93384 eV

Gap : +0.14085230 H = +3.83279 eV

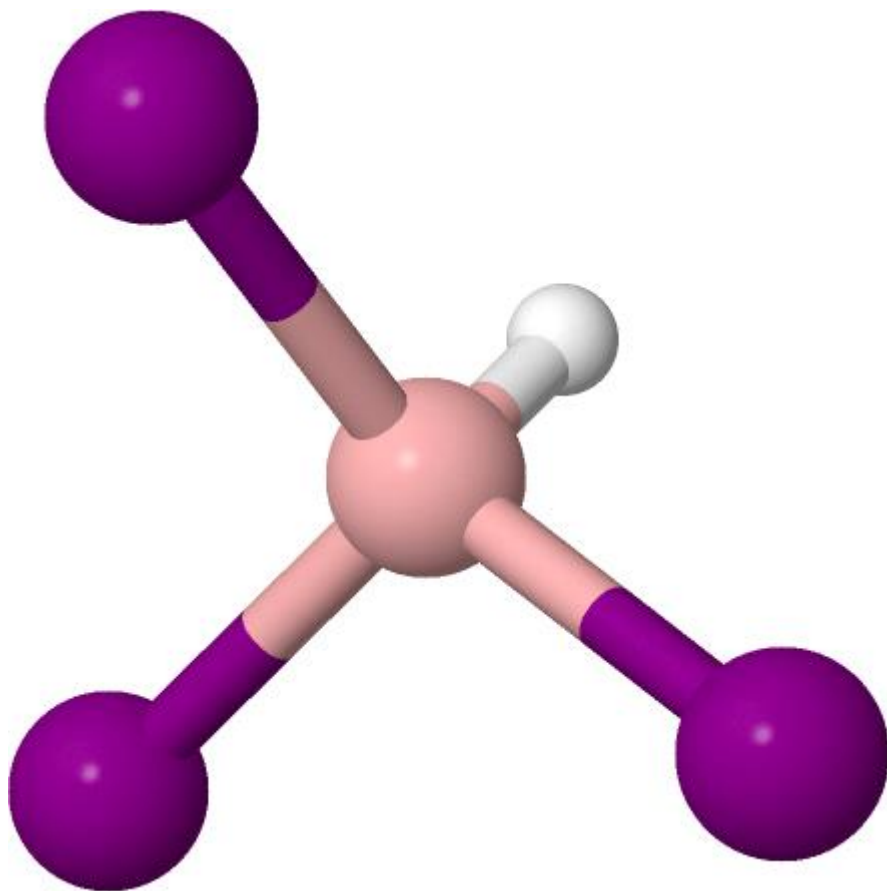
Number of MOs= 49, Electrons= 44.00, Symmetry: c3v

\$coord

0.0000000000000000	0.0000000000000000	1.07609484471088	b
0.0000000000000000	0.0000000000000000	4.52654856755802	cl
-2.04737631945617	3.54615980751146	-0.45208290711037	i
-2.04737631945617	-3.54615980751146	-0.45208290711037	i
4.09475263891234	0.0000000000000000	-0.45208290711037	i

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	80.82	0.26606	YES	YES
8		e	80.82	0.26606	YES	YES
9		a1	121.09	0.70287	YES	YES
10		e	147.86	0.66494	YES	YES
11		e	147.86	0.66494	YES	YES
12		a1	231.65	0.00208	YES	YES
13		e	482.50	249.05472	YES	YES
14		e	482.50	249.05472	YES	YES
15		a1	709.15	197.04180	YES	YES



Total energy = -59.9863990779 H = -1632.3138999 eV

HOMO-LUMO Separation

HOMO: 10. 1 a2 -0.06633932 H = -1.80519 eV

LUMO: 11. 6 a1 +0.08335888 H = +2.26831 eV

Gap : +0.14969821 H = +4.07350 eV

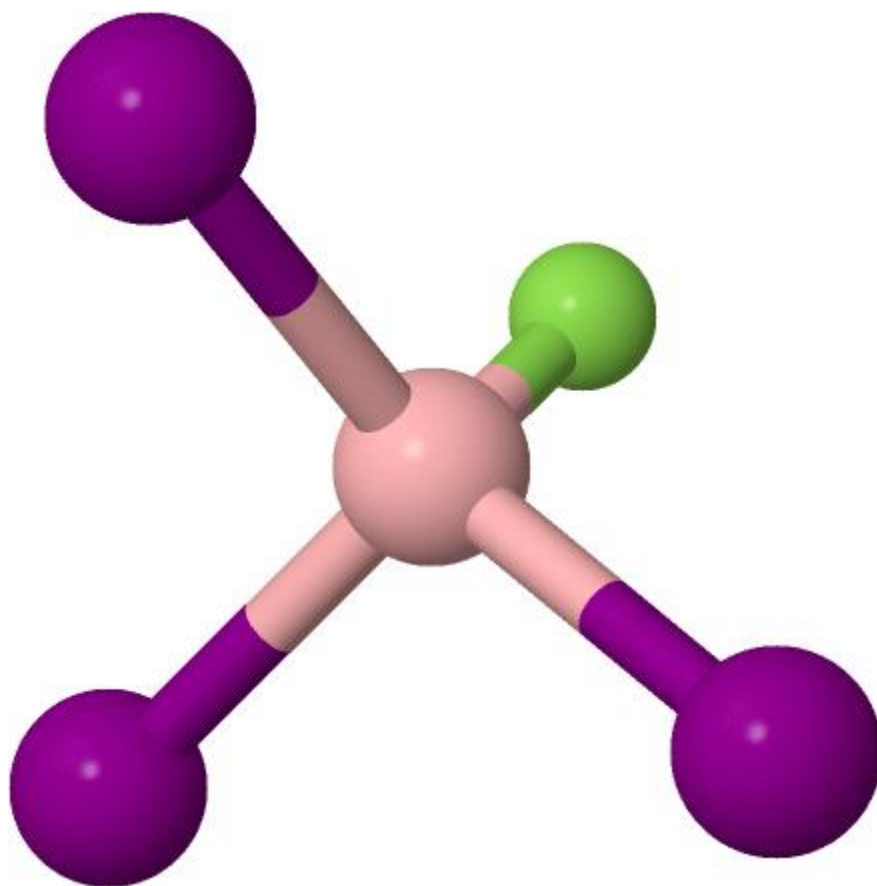
Number of MOs= 38, Electrons= 28.00, Symmetry: c3v

\$coord
0.0000000000000000 0.0000000000000000 1.28994335781693 b

0.0000000000000000	0.0000000000000000	3.58757006152407	h
-2.06419522629213	3.57529100867910	-0.04612867636500	i
-2.06419522629213	-3.57529100867910	-0.04612867636500	i
4.12839045258425	0.0000000000000000	-0.04612867636500	i

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm ⁻¹	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	83.29	0.42940	YES	YES
8		e	83.29	0.42940	YES	YES
9		a1	125.37	0.27808	YES	YES
10		a1	388.99	0.53568	YES	YES
11		e	460.02	164.69338	YES	YES
12		e	460.02	164.69338	YES	YES
13		e	873.38	175.97369	YES	YES
14		e	873.38	175.97369	YES	YES
15		a1	2579.64	78.45532	YES	YES

BI₃F⁻



Total energy = -159.2195762940 H = -4332.5875784 eV

HOMO-LUMO Separation

HOMO: 13. 1 a2 -0.06896751 H = -1.87670 eV

LUMO: 14. 8 a1 +0.07173331 H = +1.95196 eV

Gap : +0.14070082 H = +3.82867 eV

Number of MOs= 46, Electrons= 36.00, Symmetry: c3v

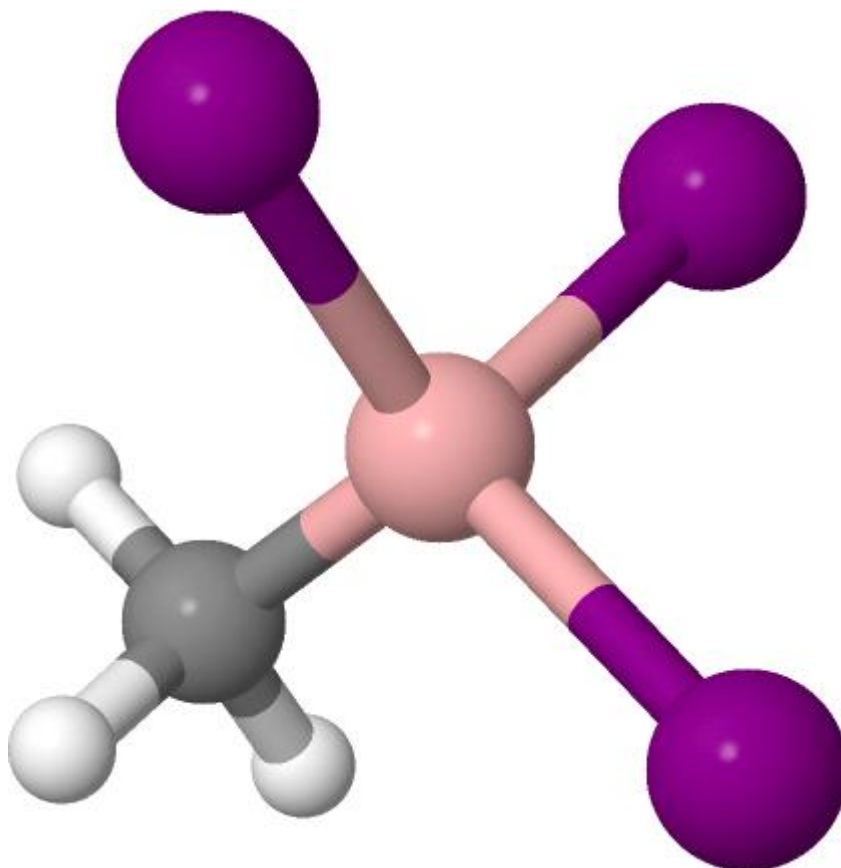
\$coord

0.0000000000000000	0.0000000000000000	0.37793919537401	b
0.0000000000000000	0.0000000000000000	2.92887706900028	f
-2.06826177647938	3.58233448021494	-1.10227208812476	i
-2.06826177647938	-3.58233448021494	-1.10227208812476	i
4.13652355295874	0.0000000000000000	-1.10227208812476	i

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	80.78	0.36348	YES	YES
8		e	80.78	0.36348	YES	YES
9		a1	118.79	0.42329	YES	YES
10		e	216.66	4.04528	YES	YES
11		e	216.66	4.04528	YES	YES
12		a1	278.16	0.02584	YES	YES
13		e	513.38	376.47767	YES	YES
14		e	513.38	376.47767	YES	YES
15		a1	1168.33	194.42355	YES	YES

BI₃Me⁻



Total energy = -99.2760535958 H = -2701.4404048 eV

HOMO-LUMO Separation

HOMO: 13. 1 a2 -0.06447315 H = -1.75440 eV

LUMO: 14. 8 a1 +0.08289598 H = +2.25572 eV

Gap : +0.14736913 H = +4.01012 eV

Number of MOs= 50, Electrons= 36.00, Symmetry: c3v

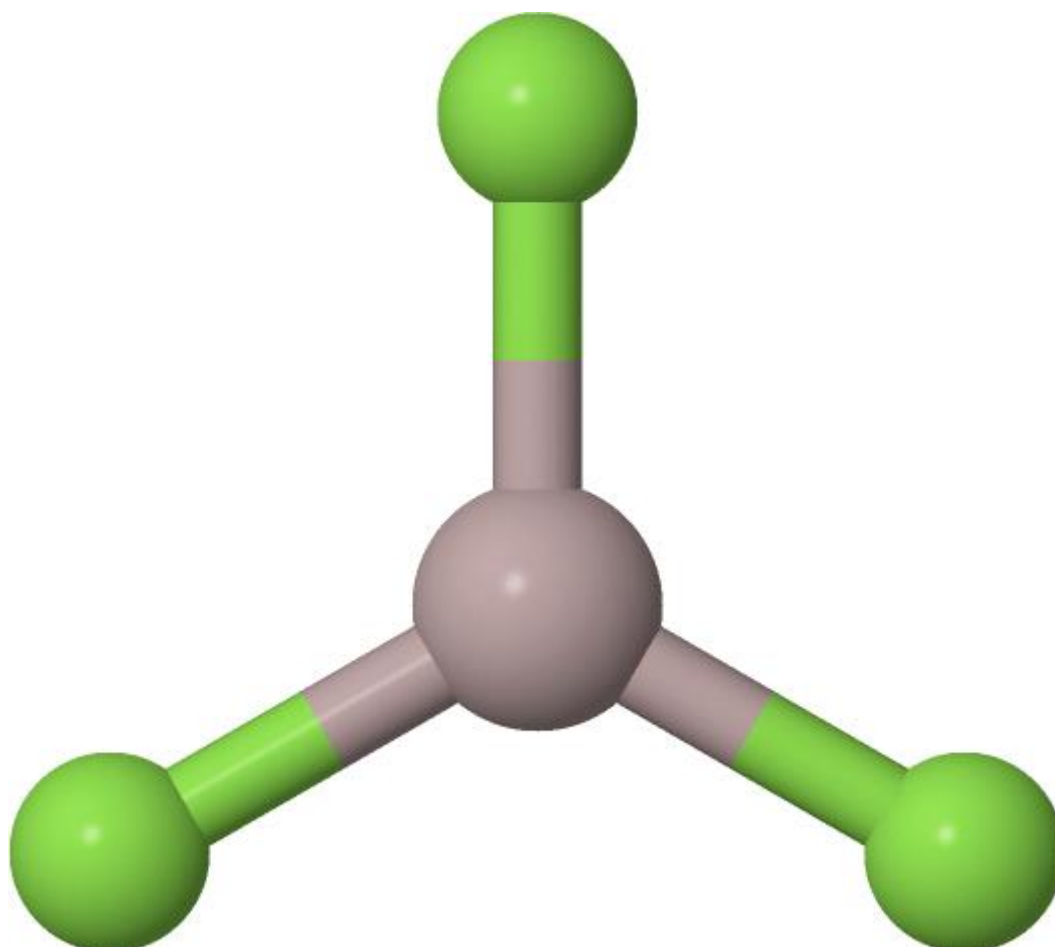
```
$coord
0.0000000000000000 0.0000000000000000 1.31194685180342 b
-2.05739073026128 3.56350527583377 -0.21447716928197 i
-2.05739073026128 -3.56350527583377 -0.21447716928197 i
4.11478146052256 0.0000000000000000 -0.21447716928197 i
```

0.0000000000000000	0.0000000000000000	4.33639098337007	c
-1.96703218388142	0.0000000000000000	5.08795966048097	h
0.98351609194071	1.70349984130289	5.08795966048097	h
0.98351609194071	-1.70349984130289	5.08795966048097	h

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	81.79	0.39280	YES	YES
8		e	81.79	0.39280	YES	YES
9		a1	120.78	0.32471	YES	YES
10		e	200.08	1.31606	YES	YES
11		e	200.08	1.31606	YES	YES
12		a2	276.06	0.00000	NO	NO
13		a1	290.54	0.94154	YES	YES
14		e	436.81	171.90198	YES	YES
15		e	436.81	171.90198	YES	YES
16		e	882.08	125.75521	YES	YES
17		e	882.08	125.75521	YES	YES
18		a1	947.64	44.63740	YES	YES
19		a1	1283.84	18.58349	YES	YES
20		e	1404.68	0.49993	YES	YES
21		e	1404.68	0.49993	YES	YES
22		a1	2919.06	22.54961	YES	YES
23		e	3005.96	22.77039	YES	YES
24		e	3005.96	22.77039	YES	YES

AlF₃



Total energy = -541.8898279751 H = -14745.5808650 eV

HOMO-LUMO Separation

HOMO: 14. 1 a2' -0.34035667 H = -9.26158 eV

LUMO: 15. 6 a1' -0.08218627 H = -2.23640 eV

Gap : +0.25817040 H = +7.02518 eV

Number of MOs= 41, Electrons= 40.00, Symmetry: d3h

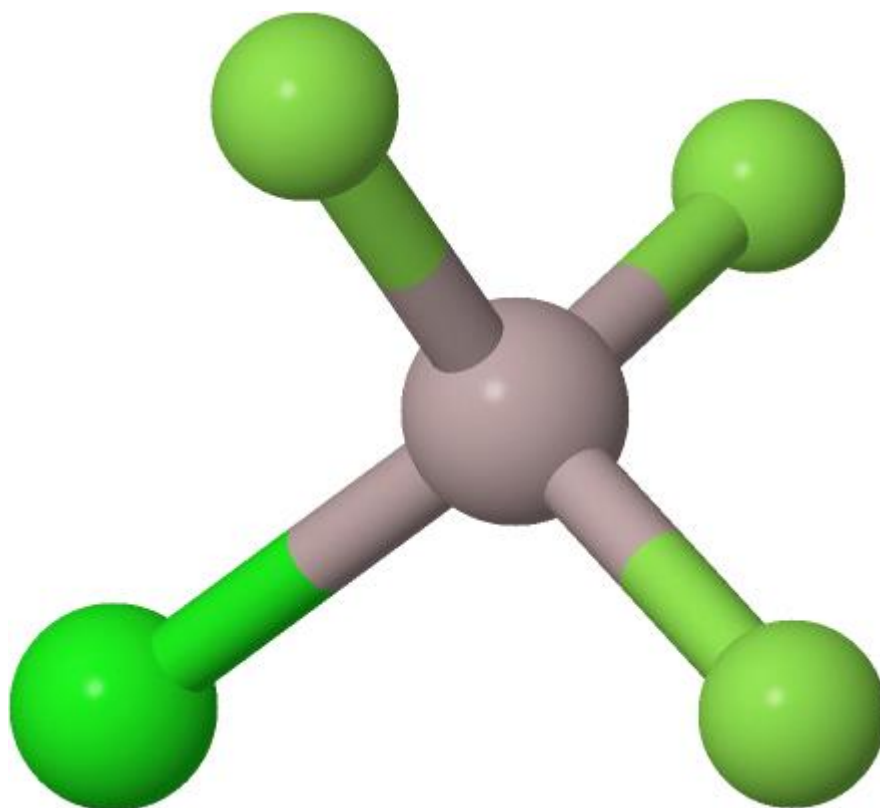
\$coord
0.0000000000000000 0.0000000000000000 0.0000000000000000 a1

3.13298906347820	0.000000000000000	0.000000000000000	f
-1.56649453173910	2.71324811875093	0.000000000000000	f
-1.56649453173910	-2.71324811875093	0.000000000000000	f

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e'	234.30	31.87985	YES	YES
8		e'	234.30	31.87985	YES	YES
9		a2''	285.44	120.37391	YES	NO
10		a1'	677.43	0.00000	NO	YES
11		e'	958.97	134.33459	YES	YES
12		e'	958.97	134.33459	YES	YES

AlF₃Cl⁻



Total energy = -1002.1664046250 H = -27270.3509028 eV

HOMO-LUMO Separation

HOMO: 21. 8 e -0.08115677 H = -2.20839 eV

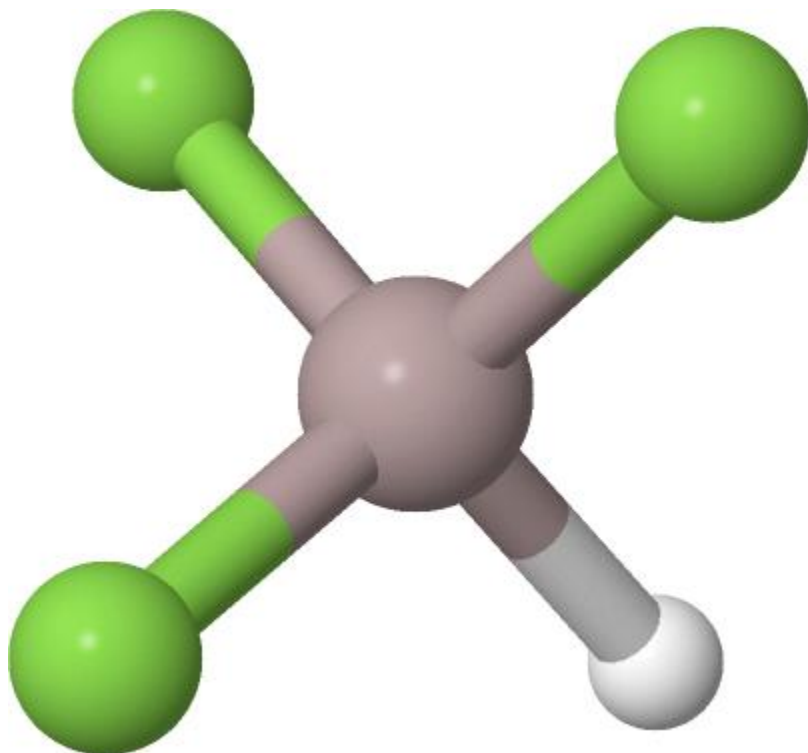
LUMO: 22. 13 a1 +0.19343491 H = +5.26363 eV

Gap : +0.27459167 H = +7.47202 eV

Number of MOs= 54, Electrons= 58.00, Symmetry: c3v

```
$coord
0.0000000000000000 0.0000000000000000 -0.72742219667529 al
0.0000000000000000 0.0000000000000000 3.41987007572844 cl
-1.52273504045382 2.63745445653147 -1.78291701398023 f
-1.52273504045382 -2.63745445653147 -1.78291701398023 f
3.04547008090764 0.0000000000000000 -1.78291701398023 f
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm**(-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 173.80 0.27105 YES YES
8 e 173.80 0.27105 YES YES
9 a1 273.70 16.76362 YES YES
10 e 278.80 21.63772 YES YES
11 e 278.80 21.63772 YES YES
12 a1 453.46 94.62783 YES YES
13 a1 686.51 133.81356 YES YES
14 e 819.95 128.81368 YES YES
15 e 819.95 128.81368 YES YES
```

Total energy = -542.5644407140 H = -14763.9380220 eV

HOMO-LUMO Separation

HOMO: 15. 8 a1 -0.05669287 H = -1.54269 eV

LUMO: 16. 9 a1 +0.22650657 H = +6.16356 eV

Gap : +0.28319943 H = +7.70625 eV

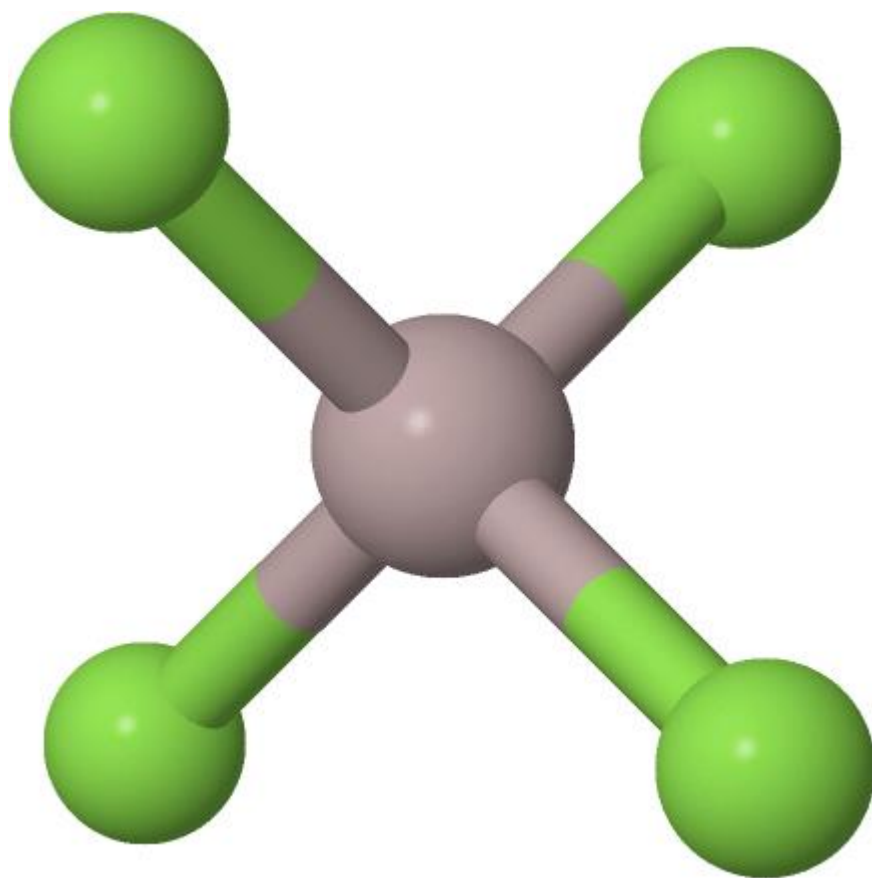
Number of MOs= 43, Electrons= 42.00, Symmetry: c3v

\$coord			
0.0000000000000000	0.0000000000000000	0.72922352282946	a1
0.0000000000000000	0.0000000000000000	3.83461720900048	h
-1.52134394708293	2.63504501213502	-0.41302993215883	f
-1.52134394708293	-2.63504501213502	-0.41302993215883	f
3.04268789416587	0.0000000000000000	-0.41302993215883	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	241.06	3.35578	YES	YES
8		e	241.06	3.35578	YES	YES
9		a1	339.93	45.72797	YES	YES
10		a1	653.69	57.09612	YES	YES
11		e	664.04	69.71804	YES	YES
12		e	664.04	69.71804	YES	YES
13		e	803.33	255.74186	YES	YES
14		e	803.33	255.74186	YES	YES
15		a1	1726.42	369.07363	YES	YES

AlF₄⁻



Total energy = -641.8225449096 H = -17464.8899986 eV

HOMO-LUMO Separation

HOMO: 12. 1 t1 -0.09224600 H = -2.51014 eV

LUMO: 13. 6 a1 +0.20234716 H = +5.50615 eV

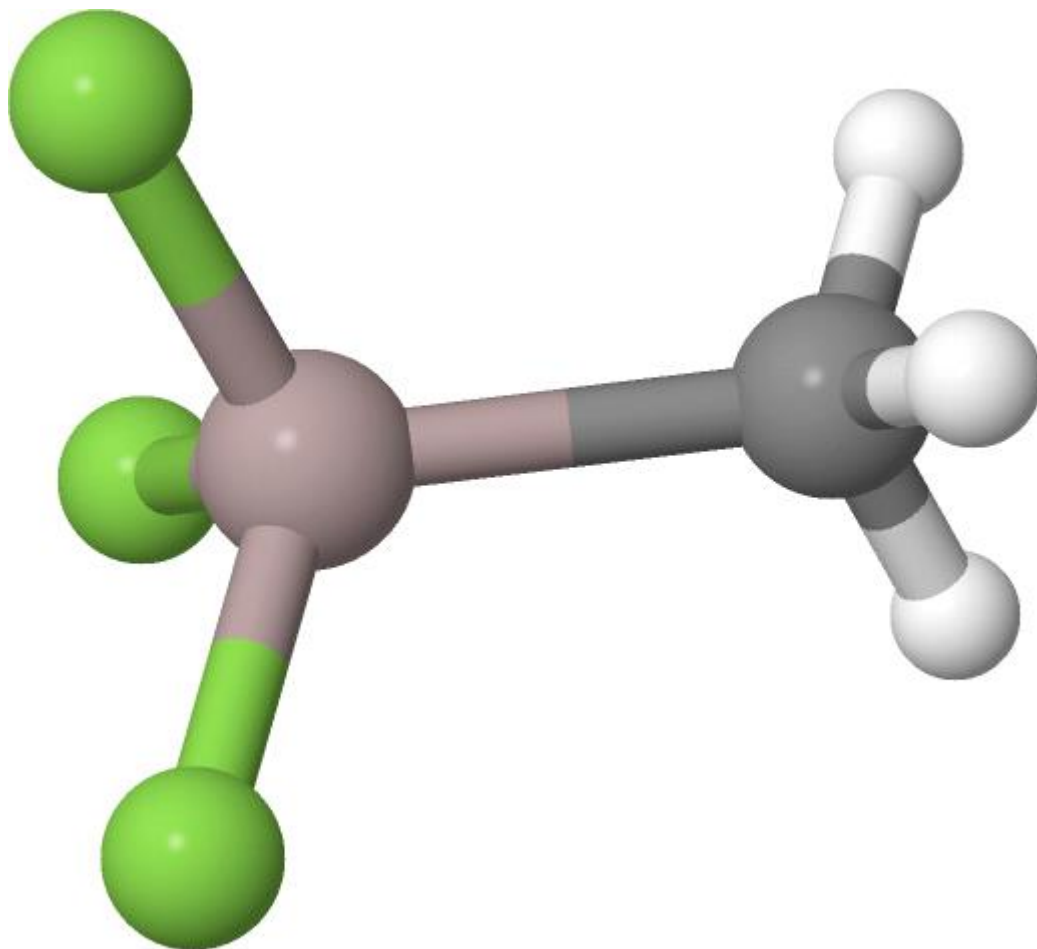
Gap : +0.29459316 H = +8.01629 eV

Number of MOs= 33, Electrons= 50.00, Symmetry: td

```
$coord
0.0000000000000000 0.0000000000000000 0.0000000000000000 a1
1.86618241082356 -1.86618241082356 1.86618241082356 f
-1.86618241082356 1.86618241082356 1.86618241082356 f
-1.86618241082356 -1.86618241082356 -1.86618241082356 f
1.86618241082356 1.86618241082356 -1.86618241082356 f
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm**(-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 205.04 0.00000 NO YES
8 e 205.04 0.00000 NO YES
9 t2 310.98 34.16335 YES YES
10 t2 310.98 34.16335 YES YES
11 t2 310.98 34.16335 YES YES
12 a1 609.80 0.00000 NO YES
13 t2 808.35 152.06903 YES YES
14 t2 808.35 152.06903 YES YES
15 t2 808.35 152.06903 YES YES
```

AlF₃Me⁻



Total energy = -581.8567669610 H = -15833.1372285 eV

HOMO-LUMO Separation

HOMO: 18. 10 a1 -0.05325723 H = -1.44920 eV

LUMO: 19. 11 a1 +0.19098017 H = +5.19684 eV

Gap : +0.24423739 H = +6.64604 eV

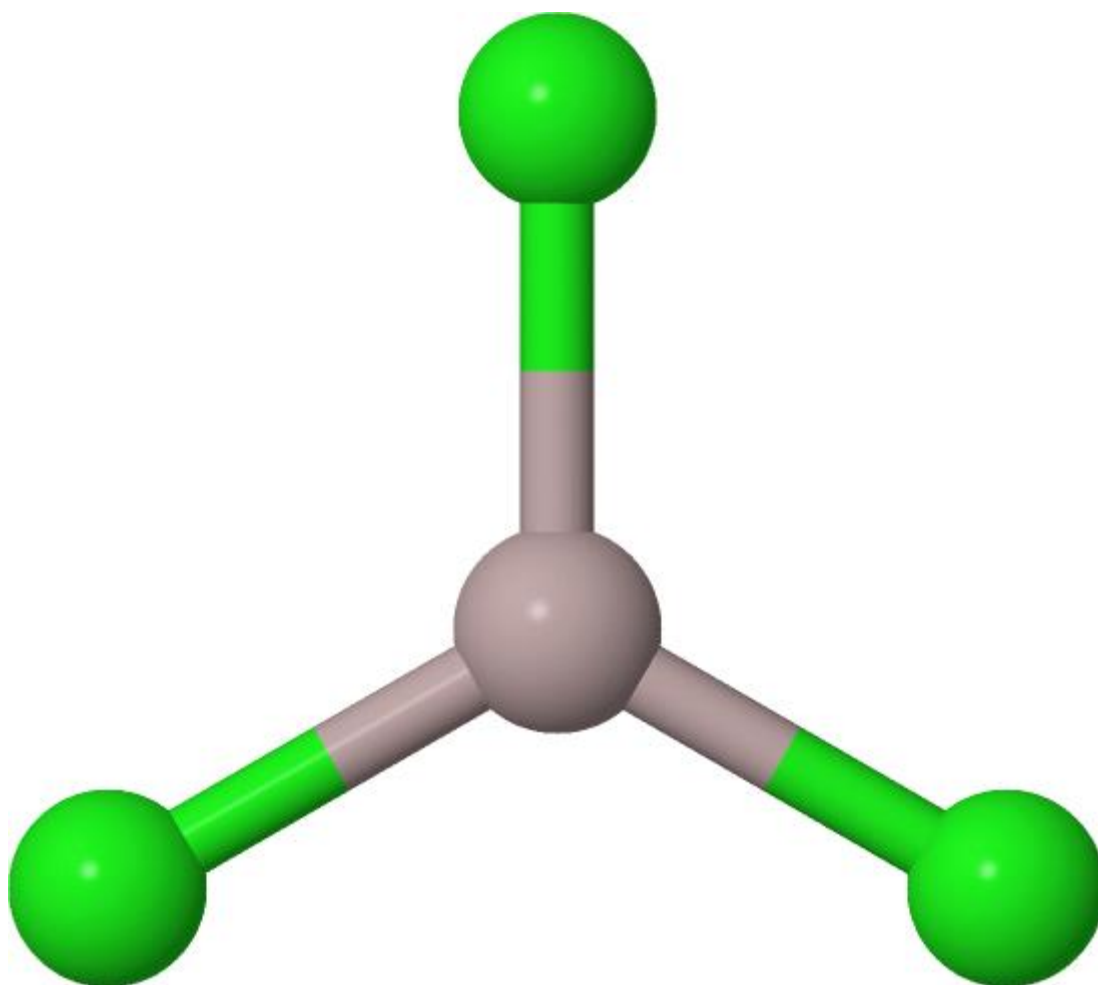
Number of MOs= 55, Electrons= 50.00, Symmetry: c3v

\$coord	0.000000000000000	0.000000000000000	0.06322768467727	al
	-1.52162197217187	2.63552656571483	-1.08971991940731	f
	-1.52162197217187	-2.63552656571483	-1.08971991940731	f
	3.04324394434374	0.000000000000000	-1.08971991940731	f
	0.000000000000000	0.000000000000000	3.85820539054666	c
	0.97890067260722	-1.69550570051906	4.65005350682376	h
	-1.95780134521445	0.000000000000000	4.65005350682376	h
	0.97890067260722	1.69550570051906	4.65005350682376	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a2		107.72	0.00000	NO	NO
8	e		160.69	0.03016	YES	YES
9	e		160.69	0.03016	YES	YES
10	e		259.82	10.50210	YES	YES
11	e		259.82	10.50210	YES	YES
12	a1		303.90	41.52434	YES	YES
13	a1		535.58	14.48599	YES	YES
14	e		636.68	9.77803	YES	YES
15	e		636.68	9.77803	YES	YES
16	a1		681.94	146.08058	YES	YES
17	e		792.84	163.57792	YES	YES
18	e		792.84	163.57792	YES	YES
19	a1		1160.30	31.10901	YES	YES
20	e		1406.50	0.00057	YES	YES
21	e		1406.50	0.00057	YES	YES
22	a1		2890.78	30.43773	YES	YES
23	e		2974.61	64.69738	YES	YES
24	e		2974.61	64.69738	YES	YES

AlCl₃



Total energy = -1622.9046540400 H = -44161.5077029 eV

HOMO-LUMO Separation

HOMO: 22. 2 a2' -0.28928407 H = -7.87182 eV

LUMO: 23. 8 a1' -0.08019004 H = -2.18208 eV

Gap : +0.20909403 H = +5.68974 eV

Number of MOs= 49, Electrons= 64.00, Symmetry: d3h

```

$coord
  0.0000000000000000  0.0000000000000000  0.0000000000000000  al
  3.96057383511402   0.0000000000000000  0.0000000000000000  cl
 -1.98028691755701   3.42995755477270   0.0000000000000000  cl
 -1.98028691755701  -3.42995755477270   0.0000000000000000  cl

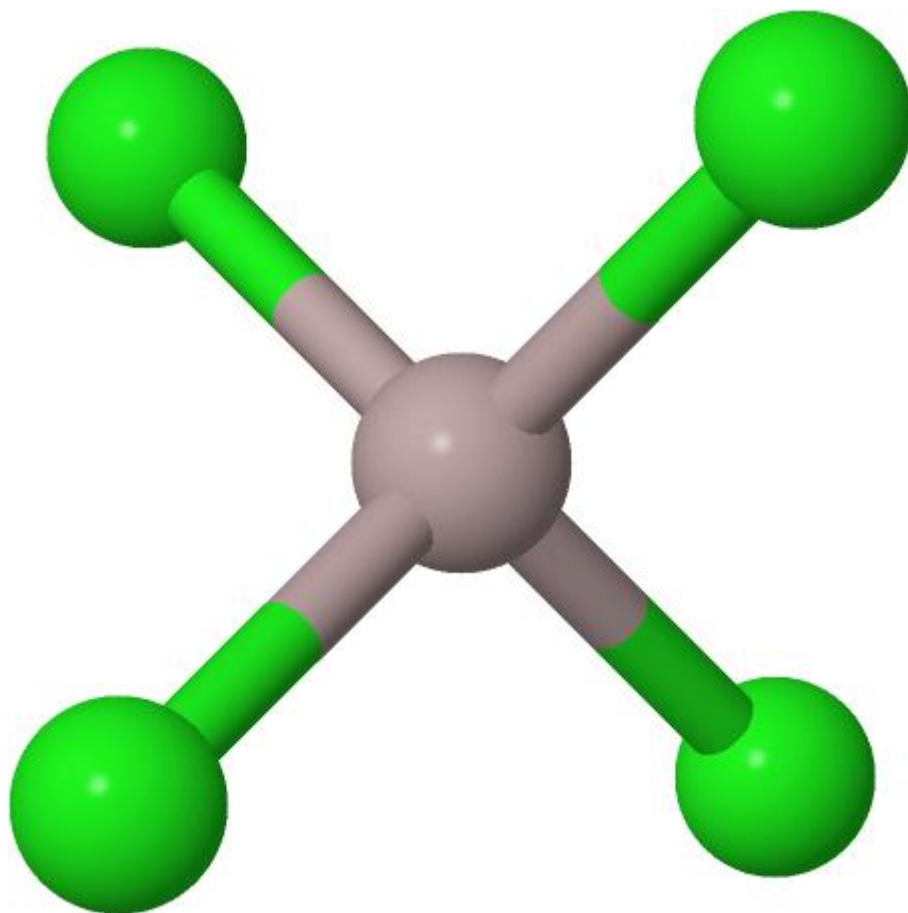
```

```

$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#                               cm** (-1)          km/mol            IR      RAMAN
  1              0.00          0.00000          -        -
  2              0.00          0.00000          -        -
  3              0.00          0.00000          -        -
  4              0.00          0.00000          -        -
  5              0.00          0.00000          -        -
  6              0.00          0.00000          -        -
  7             e'          142.97          6.63031        YES      YES
  8             e'          142.97          6.63031        YES      YES
  9            a2''         196.76         32.68906        YES      NO
 10            a1'          370.72          0.00000        NO       YES
 11            e'          616.53         149.58914       YES      YES
 12            e'          616.53         149.58914       YES      YES

```

AlCl₄⁻



Total energy = -2083.1856780740 H = -56686.3987603 eV

HOMO-LUMO Separation

HOMO: 19. 2 t1 -0.09356637 H = -2.54607 eV

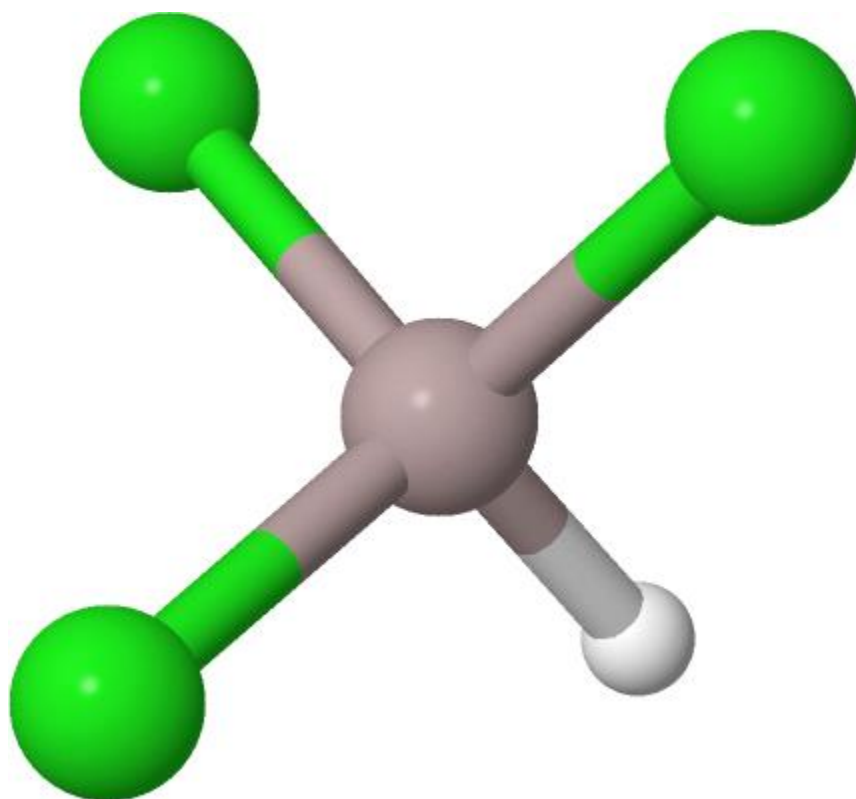
LUMO: 20. 8 a1 +0.16565845 H = +4.50780 eV

Gap : +0.25922482 H = +7.05387 eV

Number of MOs= 40, Electrons= 82.00, Symmetry: td

```
$coord
  0.0000000000000000  0.0000000000000000  0.0000000000000000  a1
  2.37663889125521    2.37663889125521    2.37663889125521    cl
 -2.37663889125521    2.37663889125521   -2.37663889125521    cl
 -2.37663889125521   -2.37663889125521    2.37663889125521    cl
  2.37663889125521   -2.37663889125521   -2.37663889125521    cl
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#              #              cm** (-1)          km/mol            IR      RAMAN
  1              0.00          0.00000          -          -
  2              0.00          0.00000          -          -
  3              0.00          0.00000          -          -
  4              0.00          0.00000          -          -
  5              0.00          0.00000          -          -
  6              0.00          0.00000          -          -
  7              e          110.62          0.00000          NO      YES
  8              e          110.62          0.00000          NO      YES
  9              t2          172.88          5.49967          YES     YES
 10              t2          172.88          5.49967          YES     YES
 11              t2          172.88          5.49967          YES     YES
 12              a1          333.46          0.00000          NO      YES
 13              t2          511.49          148.76144         YES     YES
 14              t2          511.49          148.76144         YES     YES
 15              t2          511.49          148.76144         YES     YES
```

Total energy = -1623.5897043640 H = -44180.1488813 eV

HOMO-LUMO Separation

HOMO: 23. 11 a1 -0.07663057 H = -2.08523 eV

LUMO: 24. 12 a1 +0.19199368 H = +5.22442 eV

Gap : +0.26862425 H = +7.30964 eV

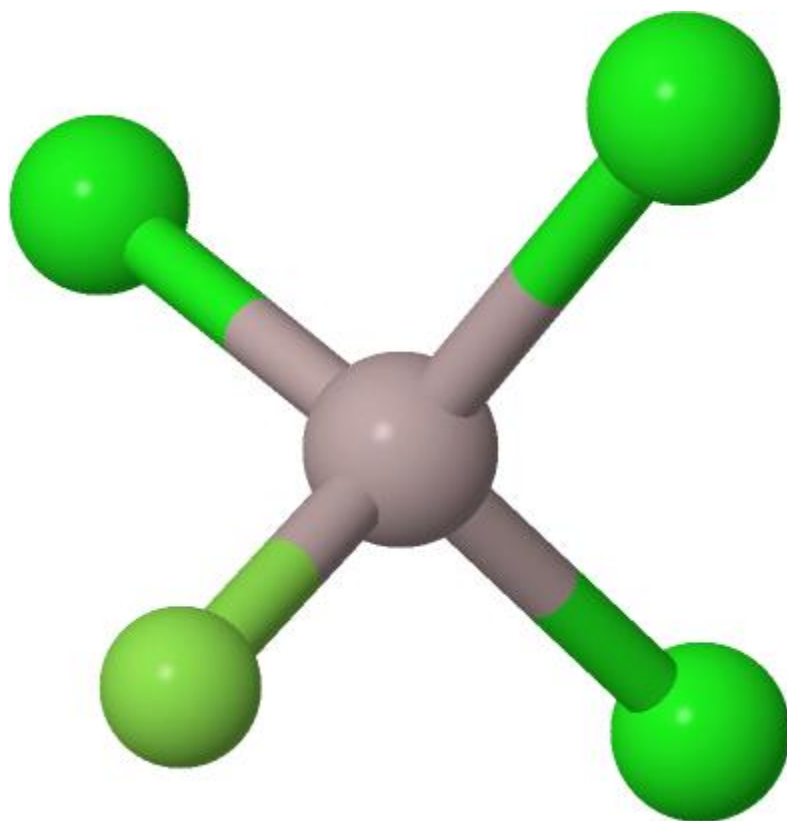
Number of MOs= 51, Electrons= 66.00, Symmetry: c3v

\$coord			
0.0000000000000000	0.0000000000000000	1.12435376403097	a1
0.0000000000000000	0.0000000000000000	4.18307112737825	h
3.89776533115663	0.0000000000000000	-0.32487294247281	cl
-1.94888266557832	3.37556379477191	-0.32487294247281	cl
-1.94888266557832	-3.37556379477191	-0.32487294247281	cl

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm ⁻¹ (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	133.13	0.34048	YES	YES
8		e	133.13	0.34048	YES	YES
9		a1	199.34	5.15386	YES	YES
10		a1	392.62	29.08191	YES	YES
11		e	466.63	66.52602	YES	YES
12		e	466.63	66.52602	YES	YES
13		e	658.33	263.33898	YES	YES
14		e	658.33	263.33898	YES	YES
15		a1	1806.32	330.03883	YES	YES

AlCl₃F⁻



Total energy = -1722.8476694180 H = -46881.0970716 eV

HOMO-LUMO Separation

HOMO: 26. 2 a2 -0.08755016 H = -2.38236 eV

LUMO: 27. 14 a1 +0.17571894 H = +4.78156 eV

Gap : +0.26326910 H = +7.16392 eV

Number of MOs= 59, Electrons= 74.00, Symmetry: c3v

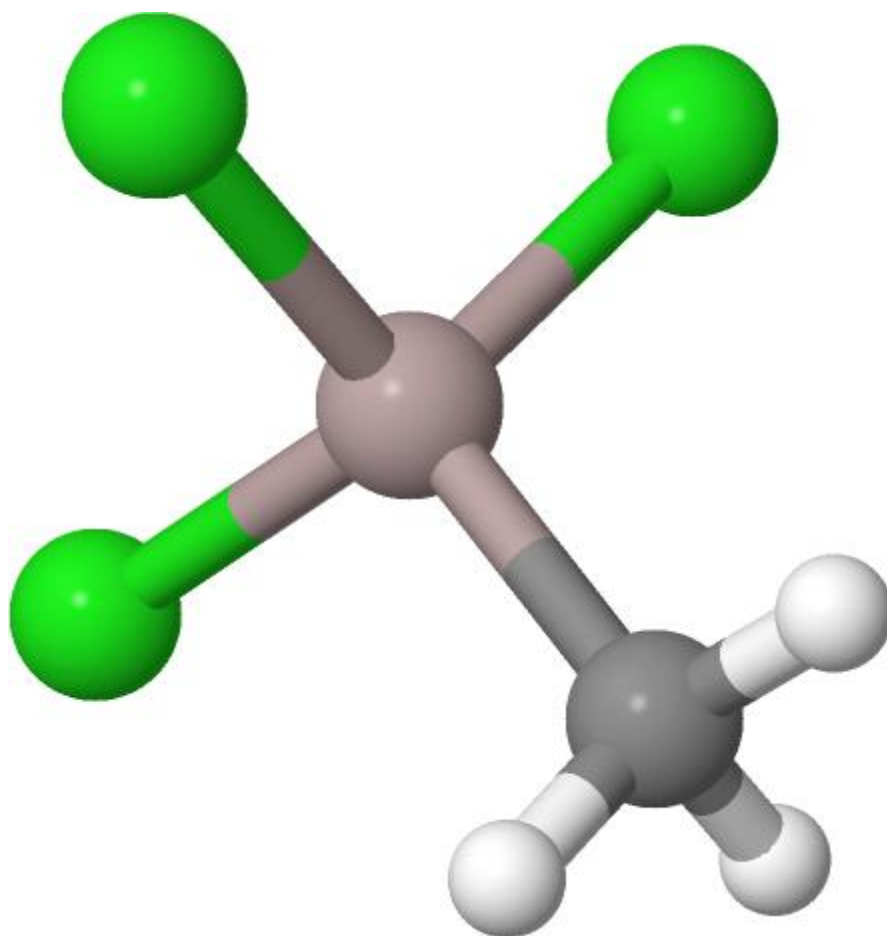
\$coord

0.0000000000000000	0.0000000000000000	0.16954733902068	a1
1.94716919592779	3.37259597827996	-1.18494994700156	cl
1.94716919592779	-3.37259597827996	-1.18494994700156	cl
-3.89433839185558	0.0000000000000000	-1.18494994700156	cl
0.0000000000000000	0.0000000000000000	3.38530250198397	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	123.06	0.19118	YES	YES
8		e	123.06	0.19118	YES	YES
9		a1	184.80	5.52163	YES	YES
10		e	224.81	10.70646	YES	YES
11		e	224.81	10.70646	YES	YES
12		a1	363.94	6.64279	YES	YES
13		e	509.81	180.51127	YES	YES
14		e	509.81	180.51127	YES	YES
15		a1	788.49	103.41447	YES	YES

AlCl₃Me⁻



Total energy = -1662.8821684580 H = -45249.3518388 eV

HOMO-LUMO Separation

HOMO: 26. 13 a1 -0.07333128 H = -1.99545 eV

LUMO: 27. 14 a1 +0.17645992 H = +4.80172 eV

Gap : +0.24979121 H = +6.79717 eV

Number of MOs= 63, Electrons= 74.00, Symmetry: c3v

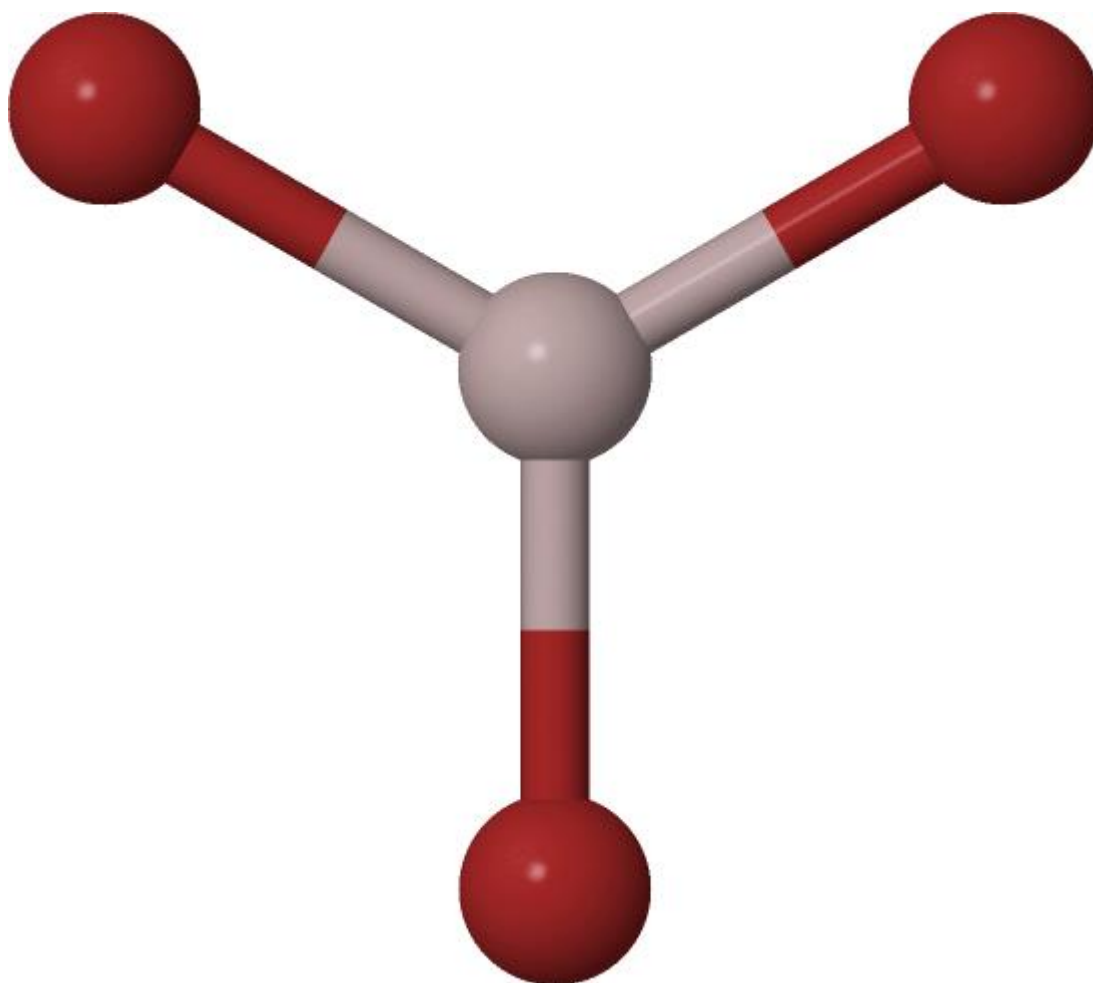
\$coord

0.0000000000000000	0.0000000000000000	0.64769790148050	a1
-1.95186307080471	3.38072600805117	-0.80891078135591	cl
-1.95186307080471	-3.38072600805117	-0.80891078135591	cl
3.90372614160943	0.0000000000000000	-0.80891078135591	cl
0.0000000000000000	0.0000000000000000	4.40538739432422	c
0.98163746635444	-1.70024596633907	5.17386829108654	h
-1.96327493270888	0.0000000000000000	5.17386829108654	h
0.98163746635444	1.70024596633907	5.17386829108654	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	e		114.90	0.01101	YES	YES
8	e		114.90	0.01101	YES	YES
9	a2		128.72	0.00000	NO	NO
10	e		167.00	2.90757	YES	YES
11	e		167.00	2.90757	YES	YES
12	a1		182.91	7.44405	YES	YES
13	a1		352.75	16.67997	YES	YES
14	e		464.05	99.59615	YES	YES
15	e		464.05	99.59615	YES	YES
16	a1		609.00	88.04717	YES	YES
17	e		680.01	94.98356	YES	YES
18	e		680.01	94.98356	YES	YES
19	a1		1167.59	23.84851	YES	YES
20	e		1401.67	0.21673	YES	YES
21	e		1401.67	0.21673	YES	YES
22	a1		2908.77	24.87398	YES	YES
23	e		2999.14	38.38991	YES	YES
24	e		2999.14	38.38991	YES	YES

AlBr₃



Total energy = -7964.9801139490 H = -216738.2598727 eV

HOMO-LUMO Separation

HOMO: 40. 4 a2' -0.26980030 H = -7.34164 eV

LUMO: 41. 12 a1' -0.09118868 H = -2.48137 eV

Gap : +0.17861162 H = +4.86027 eV

Number of MOs= 77, Electrons= 118.00, Symmetry: d3h

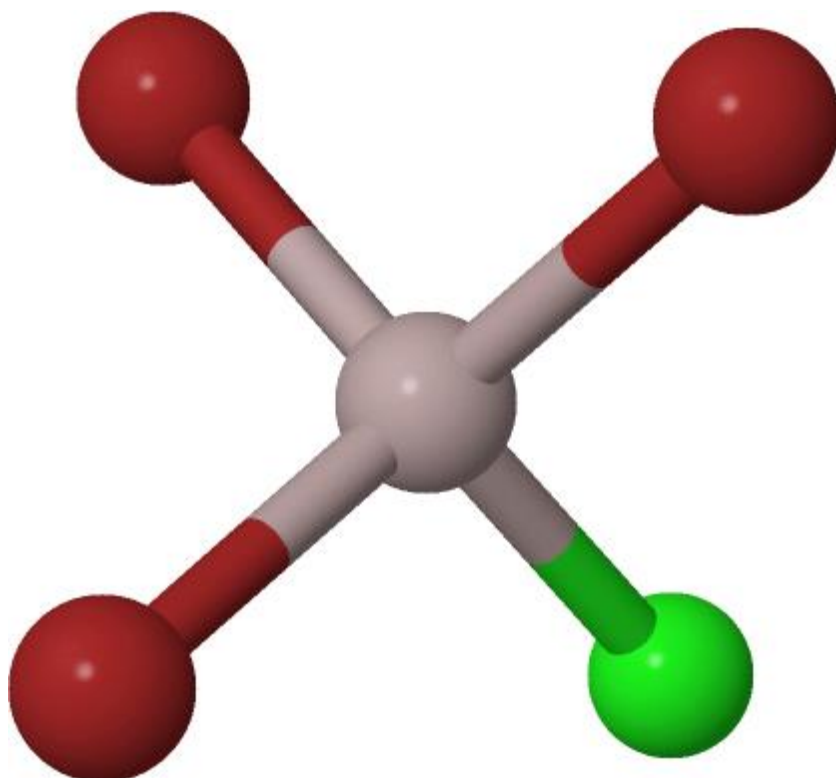
\$coord

0.0000000000000000	0.0000000000000000	0.0000000000000000	al
2.12853759229810	-3.68673525568063	0.0000000000000000	br
2.12853759229810	3.68673525568063	0.0000000000000000	br
-4.25707518459619	0.0000000000000000	0.0000000000000000	br

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e'	92.44	1.76951	YES	YES
8		e'	92.44	1.76951	YES	YES
9		a2''	171.88	15.86962	YES	NO
10		a1'	222.20	0.00000	NO	YES
11		e'	497.29	132.88804	YES	YES
12		e'	497.29	132.88804	YES	YES

AlBr₃Cl⁻



Total energy = -8425.2642336210 H = -229263.2351668 eV

HOMO-LUMO Separation

HOMO: 68. 68 a -0.08895094 H = -2.42048 eV

LUMO: 69. 69 a +0.12807685 H = +3.48515 eV

Gap : +0.21702779 H = +5.90563 eV

Number of MOs= 132, Electrons= 136.00, Symmetry: c1

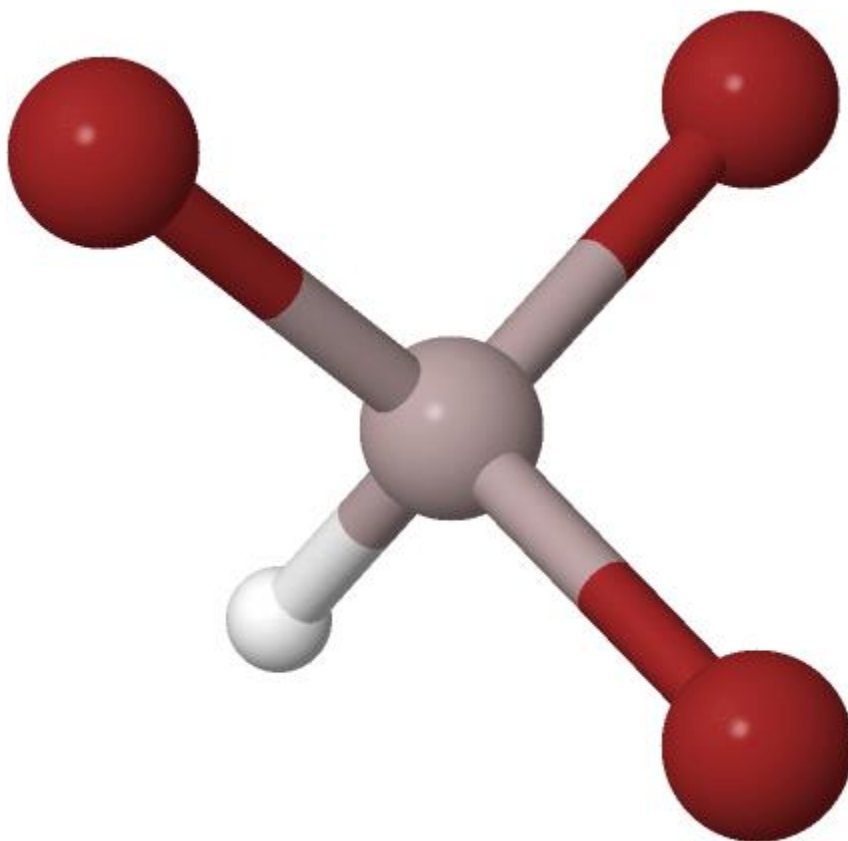
\$coord

-0.00158534693949	0.00000545564121	0.70619861627652	al
-0.00735010523899	0.00003519071155	4.81437007040518	cl
4.17963727369548	-0.00596780180754	-0.78843133096337	br
-2.08276162288932	3.62462577934916	-0.79300699606998	br
-2.09307935352443	-3.61867543261777	-0.79298958560652	br

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	72.95	0.00641	YES	YES
8		a	73.64	0.01803	YES	YES
9		a	121.74	0.59310	YES	YES
10		a	122.62	2.35093	YES	YES
11		a	123.48	2.27997	YES	YES
12		a	228.98	1.17655	YES	YES
13		a	399.17	133.05031	YES	YES
14		a	399.30	133.21617	YES	YES
15		a	490.33	122.56896	YES	YES

AlBr₃H⁻



Total energy = -7965.6705517250 H = -216757.0476512 eV

HOMO-LUMO Separation

HOMO: 41. 5 a2 -0.08035430 H = -2.18655 eV

LUMO: 42. 18 a1 +0.14647372 H = +3.98576 eV

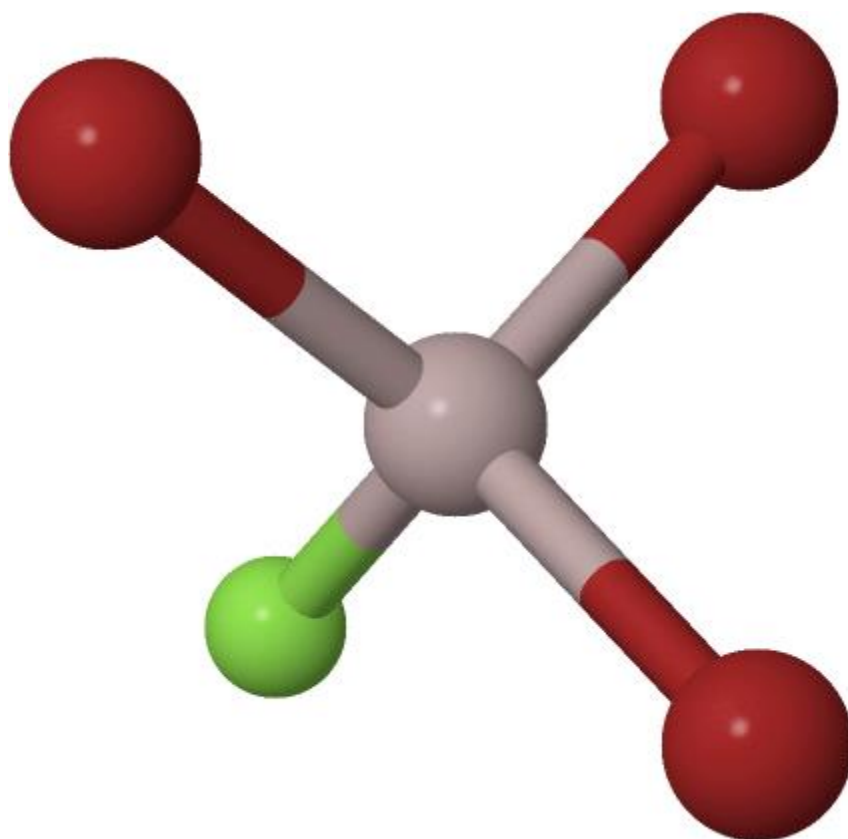
Gap : +0.22682802 H = +6.17231 eV

Number of MOs= 79, Electrons= 120.00, Symmetry: c3v

```
$coord
0.000000000000000 0.000000000000000 1.37276083778793 al
0.000000000000000 0.000000000000000 4.41919293984503 h
-2.10422263270652 3.64462051028403 -0.17308672136368 br
-2.10422263270652 -3.64462051028403 -0.17308672136368 br
4.20844526541303 0.000000000000000 -0.17308672136368 br
```

\$vibrational spectrum						
#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm ⁻¹	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	75.29	0.02383	YES	YES
8		e	75.29	0.02383	YES	YES
9		a1	123.08	0.47302	YES	YES
10		a1	290.77	13.36413	YES	YES
11		e	362.12	68.38405	YES	YES
12		e	362.12	68.38405	YES	YES
13		e	622.05	239.54619	YES	YES
14		e	622.05	239.54619	YES	YES
15		a1	1825.97	286.04077	YES	YES

AlBr₃F⁻



Total energy = -8064.9277902200 H = -219457.9760708 eV

HOMO-LUMO Separation

HOMO: 44. 5 a2 -0.08520724 H = -2.31861 eV

LUMO: 45. 20 a1 +0.13760203 H = +3.74434 eV

Gap : +0.22280927 H = +6.06295 eV

Number of MOs= 87, Electrons= 128.00, Symmetry: c3v

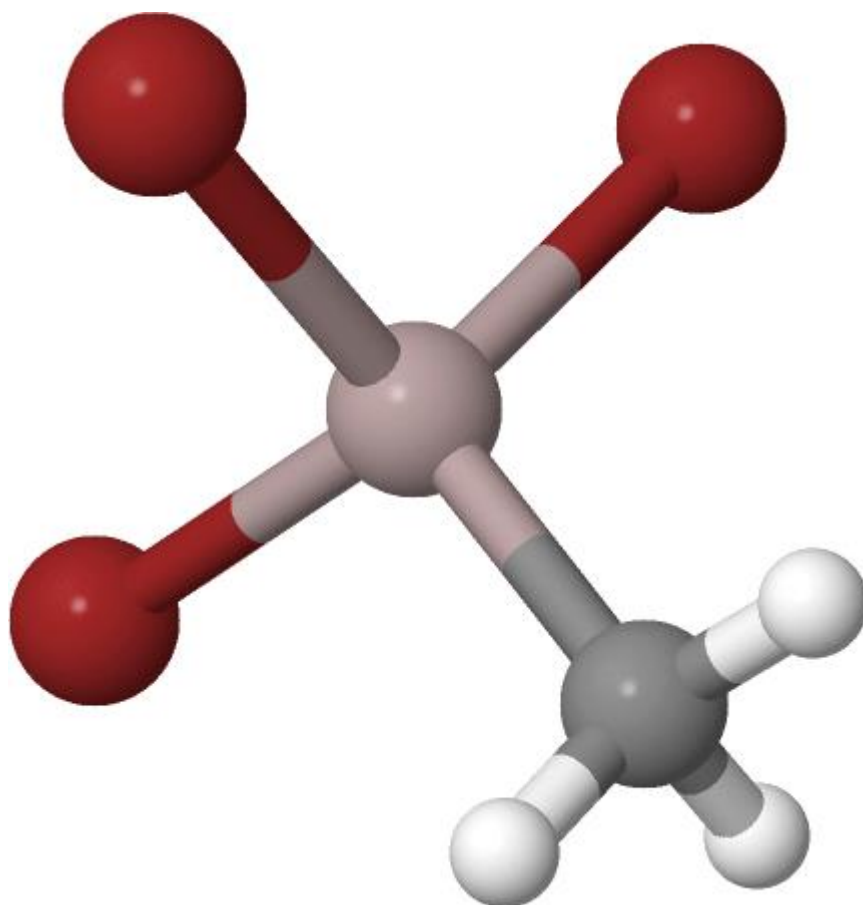
\$coord

0.0000000000000000	0.0000000000000000	0.23531306680164	al
0.0000000000000000	0.0000000000000000	3.44741549686142	f
-2.09832273443766	3.63440158672288	-1.22943294207618	br
-2.09832273443766	-3.63440158672288	-1.22943294207618	br
4.19664546887530	0.0000000000000000	-1.22943294207618	br

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	e		71.87	0.06370	YES	YES
8	e		71.87	0.06370	YES	YES
9	a1		120.38	0.60418	YES	YES
10	e		182.29	3.84661	YES	YES
11	e		182.29	3.84661	YES	YES
12	a1		246.01	3.46042	YES	YES
13	e		398.57	169.59697	YES	YES
14	e		398.57	169.59697	YES	YES
15	a1		786.15	89.88451	YES	YES

AlBr₃Me⁻



Total energy = -8004.9623052830 H = -217826.2312740 eV

HOMO-LUMO Separation

HOMO: 44. 5 a2 -0.07834465 H = -2.13187 eV

LUMO: 45. 20 a1 +0.14832746 H = +4.03620 eV

Gap : +0.22667211 H = +6.16807 eV

Number of MOs= 91, Electrons= 128.00, Symmetry: c3v

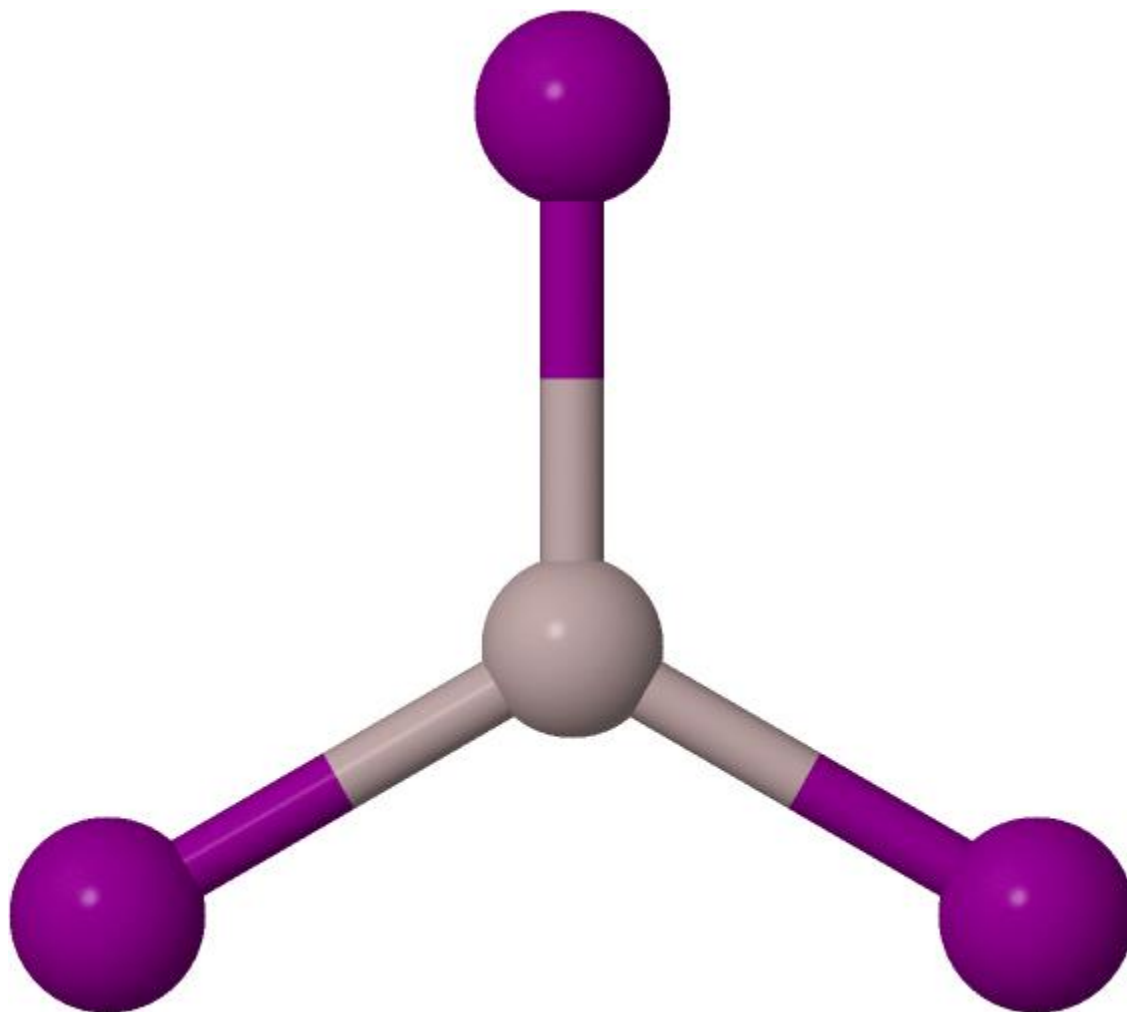
\$coord
0.0000000000000000 0.0000000000000000 1.12972090093669 a1
152

0.0000000000000000	0.0000000000000000	4.88365030903506	c
0.98298817481571	-1.70258546202020	5.64139555119278	h
-1.96597634963141	0.0000000000000000	5.64139555119278	h
0.98298817481571	1.70258546202020	5.64139555119278	h
-2.10537846798639	3.64662247571394	-0.44299930053435	br
-2.10537846798639	-3.64662247571394	-0.44299930053435	br
4.21075693597277	0.0000000000000000	-0.44299930053435	br

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	e		72.16	0.01138	YES	YES
8	e		72.16	0.01138	YES	YES
9	a1		117.13	0.93575	YES	YES
10	e		134.31	1.47239	YES	YES
11	e		134.31	1.47239	YES	YES
12	a2		138.40	0.00000	NO	NO
13	a1		254.58	10.65663	YES	YES
14	e		364.74	97.28201	YES	YES
15	e		364.74	97.28201	YES	YES
16	a1		603.98	67.12807	YES	YES
17	e		679.36	86.72261	YES	YES
18	e		679.36	86.72261	YES	YES
19	a1		1165.34	17.77889	YES	YES
20	e		1399.09	0.37040	YES	YES
21	e		1399.09	0.37040	YES	YES
22	a1		2915.51	22.50943	YES	YES
23	e		3008.93	27.53425	YES	YES
24	e		3008.93	27.53425	YES	YES

AlI₃



Total energy = -276.9330064407 H = -7535.7348115 eV

HOMO-LUMO Separation

HOMO: 12. 1 a2' -0.24951186 H = -6.78957 eV

LUMO: 13. 5 a1' -0.11044668 H = -3.00541 eV

Gap : +0.13906518 H = +3.78416 eV

Number of MOs= 39, Electrons= 34.00, Symmetry: d3h

```

$coord
  0.0000000000000000  0.0000000000000000  0.0000000000000000  al
  4.69669627075877  0.0000000000000000  0.0000000000000000  i
 -2.34834813537938  4.06745828433673  0.0000000000000000  i
 -2.34834813537938 -4.06745828433673  0.0000000000000000  i

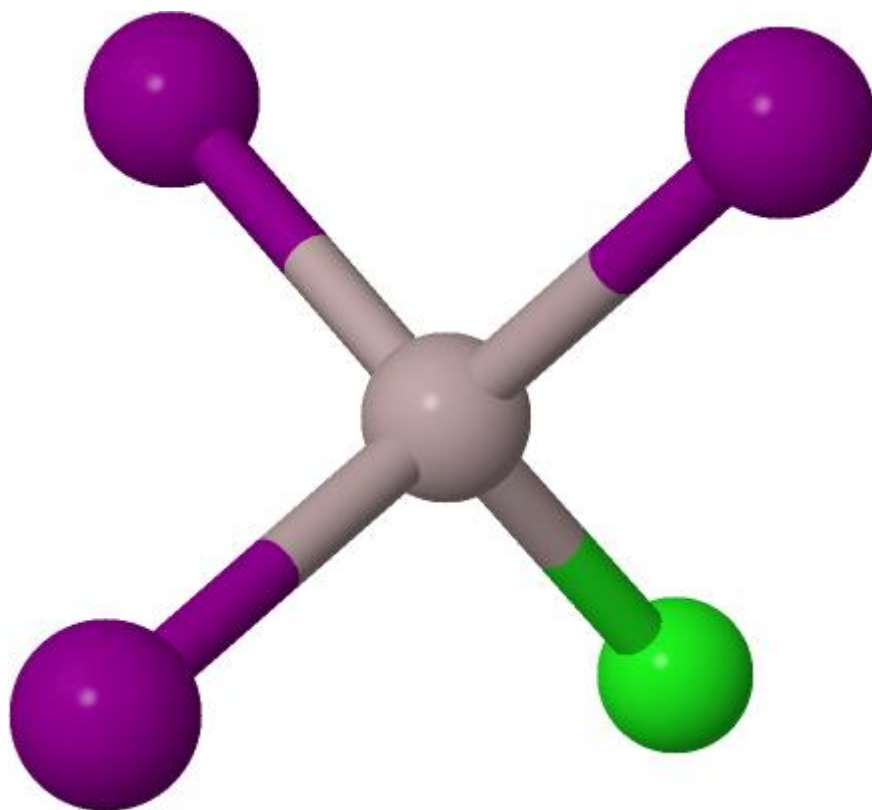
```

```

$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#                               cm** (-1)          km/mol           IR      RAMAN
  1              0.00          0.00000          -      -
  2              0.00          0.00000          -      -
  3              0.00          0.00000          -      -
  4              0.00          0.00000          -      -
  5              0.00          0.00000          -      -
  6              0.00          0.00000          -      -
  7             e'          63.32          0.74209        YES     YES
  8             e'          63.32          0.74209        YES     YES
  9            a2''         140.95          6.15831        YES     NO
 10            a1'          154.92          0.00000        NO      YES
 11            e'          417.93         135.59245       YES     YES
 12            e'          417.93         135.59245       YES     YES

```

Al₃Cl⁻



Total energy = -737.2253177722 H = -20060.9330120 eV

HOMO-LUMO Separation

HOMO: 19. 1 a2 -0.09189657 H = -2.50063 eV

LUMO: 20. 12 a1 +0.06526130 H = +1.77585 eV

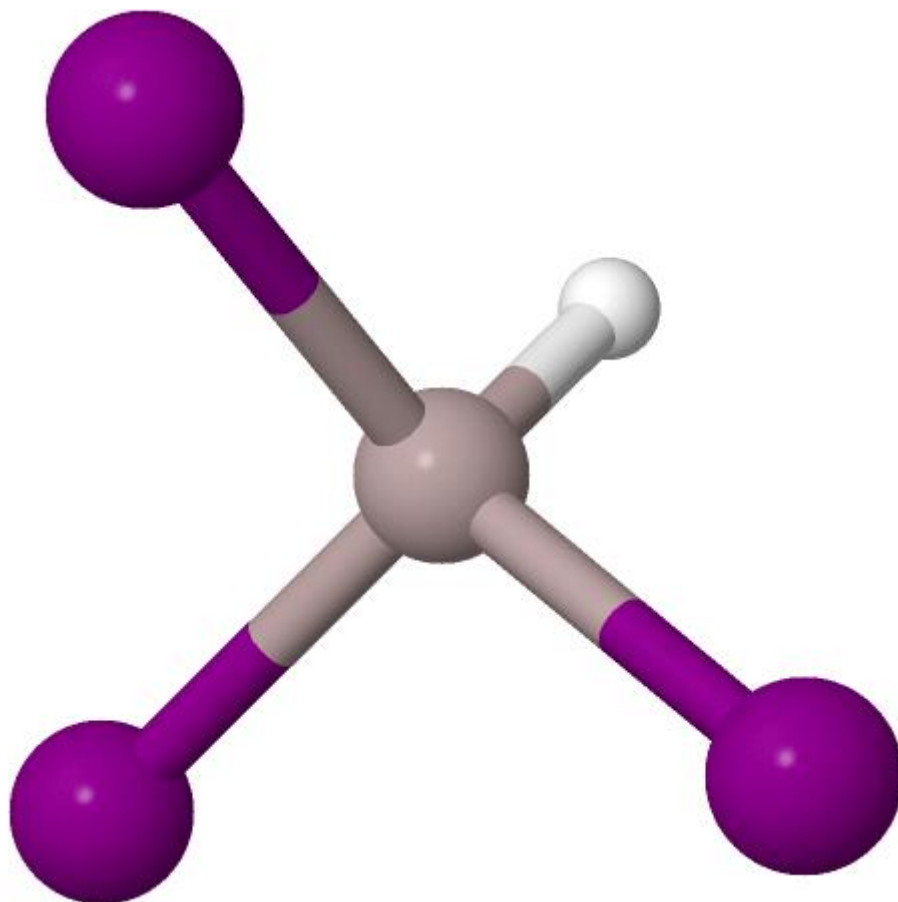
Gap : +0.15715787 H = +4.27649 eV

Number of MOs= 52, Electrons= 52.00, Symmetry: c3v

```
$coord
0.0000000000000000 0.0000000000000000 1.10364672828044 al
4.62127894448158 0.0000000000000000 -0.56145725403827 i
0.0000000000000000 0.0000000000000000 5.18927791443086 cl
-2.31063947224079 4.00214496389518 -0.56145725403827 i
-2.31063947224079 -4.00214496389518 -0.56145725403827 i
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 53.89 0.01231 YES YES
8 e 53.89 0.01231 YES YES
9 a1 88.93 0.05554 YES YES
10 e 104.93 1.43451 YES YES
11 e 104.93 1.43451 YES YES
12 a1 178.64 1.01078 YES YES
13 e 329.10 148.91083 YES YES
14 e 329.10 148.91083 YES YES
15 a1 494.38 110.94495 YES YES
```


AlH_3H^-



Total energy = -277.6361915397 H = -7554.8694625 eV

HOMO-LUMO Separation

HOMO: 13. 1 a2 -0.08712193 H = -2.37071 eV

LUMO: 14. 8 a1 +0.07715438 H = +2.09948 eV

Gap : +0.16427631 H = +4.47019 eV

Number of MOs= 41, Electrons= 36.00, Symmetry: c3v

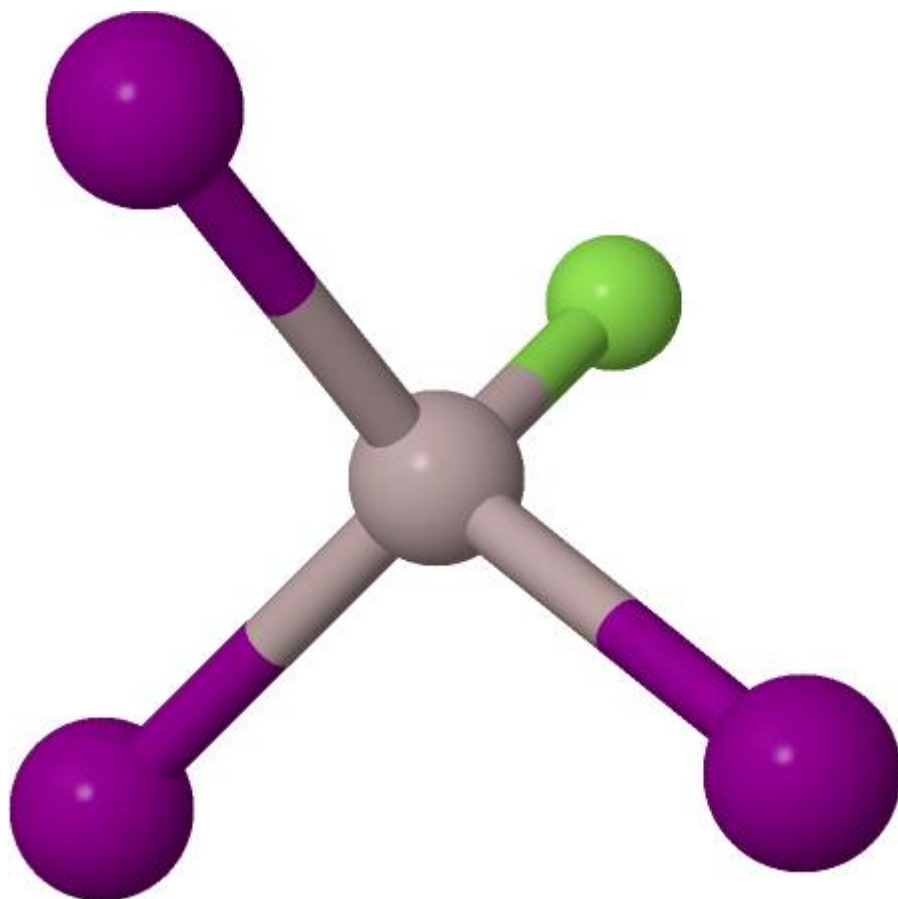
\$coord			
0.0000000000000000	0.0000000000000000	1.55660705505121	al
0.0000000000000000	0.0000000000000000	4.59041268171559	h
-2.32700220376250	4.03048604624140	-0.12247208264161	i

-2.32700220376250	-4.03048604624140	-0.12247208264161	i
4.65400440752500	0.00000000000000	-0.12247208264161	i

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	55.81	0.00525	YES	YES
8		e	55.81	0.00525	YES	YES
9		a1	91.25	0.01812	YES	YES
10		a1	236.73	5.50196	YES	YES
11		e	302.04	88.04078	YES	YES
12		e	302.04	88.04078	YES	YES
13		e	583.40	261.74540	YES	YES
14		e	583.40	261.74540	YES	YES
15		a1	1852.34	223.99936	YES	YES

Al₃F⁻



Total energy = -376.8904544645 H = -10255.7169126 eV

HOMO-LUMO Separation

HOMO: 16. 1 a2 -0.09064897 H = -2.46669 eV

LUMO: 17. 10 a1 +0.07078461 H = +1.92615 eV

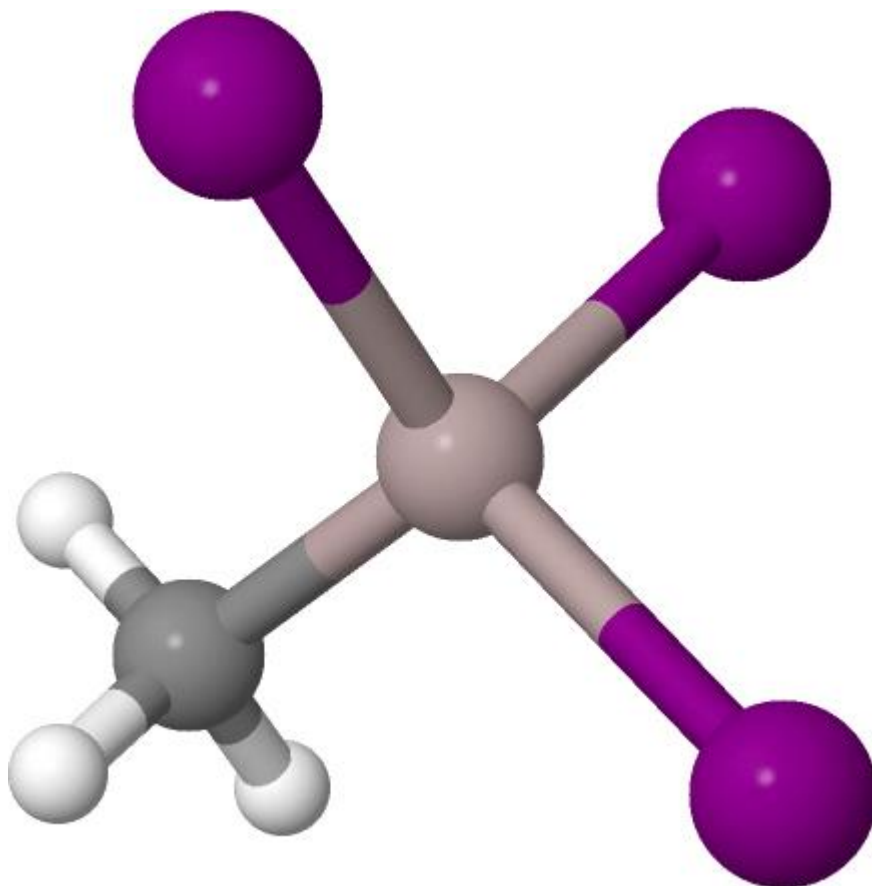
Gap : +0.16143358 H = +4.39283 eV

Number of MOs= 49, Electrons= 44.00, Symmetry: c3v

```
$coord
0.0000000000000000 0.0000000000000000 0.31997018060201 al
-2.31881576047436 4.01630671053304 -1.28028643162997 i
0.0000000000000000 0.0000000000000000 3.52088911428787 f
-2.31881576047436 -4.01630671053304 -1.28028643162997 i
4.63763152094869 0.0000000000000000 -1.28028643162997 i
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 56.05 0.00003 YES YES
8 e 56.05 0.00003 YES YES
9 a1 91.94 0.04420 YES YES
10 e 161.56 1.82643 YES YES
11 e 161.56 1.82643 YES YES
12 a1 199.18 1.45717 YES YES
13 e 346.41 191.28417 YES YES
14 e 346.41 191.28417 YES YES
15 a1 799.15 81.56196 YES YES
```

All₃Me⁻



Total energy = -316.9278507686 H = -8624.0505184 eV

HOMO-LUMO Separation

HOMO: 16. 1 a2 -0.08466834 H = -2.30394 eV

LUMO: 17. 10 a1 +0.08024312 H = +2.18353 eV

Gap : +0.16491146 H = +4.48747 eV

Number of MOs= 53, Electrons= 44.00, Symmetry: c3v

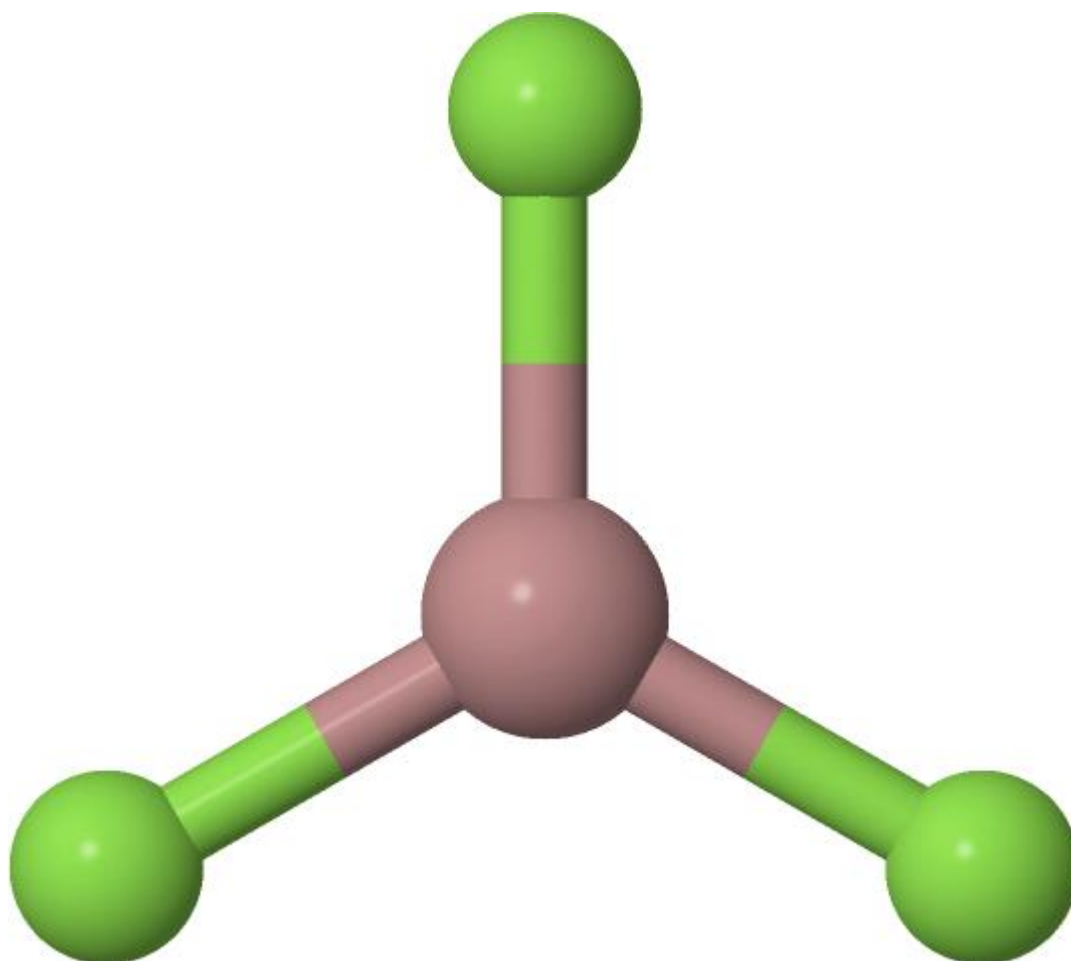
\$coord
0.0000000000000000 0.0000000000000000 1.42598633053008 a1

-2.32568861982005	4.02821085211306	-0.31121149710286	i
-2.32568861982005	-4.02821085211306	-0.31121149710286	i
4.65137723964010	0.00000000000000	-0.31121149710286	i
0.00000000000000	0.00000000000000	5.17175425560311	c
0.98476068819286	-1.70565554524652	5.91551507175825	h
-1.96952137638571	0.00000000000000	5.91551507175825	h
0.98476068819286	1.70565554524652	5.91551507175825	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	e		54.00	0.00285	YES	YES
8	e		54.00	0.00285	YES	YES
9	a1		87.63	0.08467	YES	YES
10	e		123.47	1.03954	YES	YES
11	e		123.47	1.03954	YES	YES
12	a2		156.22	0.00000	NO	NO
13	a1		201.88	6.08700	YES	YES
14	e		300.17	116.84533	YES	YES
15	e		300.17	116.84533	YES	YES
16	a1		604.63	53.12154	YES	YES
17	e		681.85	101.75758	YES	YES
18	e		681.85	101.75758	YES	YES
19	a1		1164.27	10.75961	YES	YES
20	e		1396.29	0.55127	YES	YES
21	e		1396.29	0.55127	YES	YES
22	a1		2923.87	17.62688	YES	YES
23	e		3021.68	15.18390	YES	YES
24	e		3021.68	15.18390	YES	YES

GaF₃



Total energy = -2224.3002868750 H = -60526.3248263 eV

HOMO-LUMO Separation

HOMO: 20. 1 a2' -0.34478234 H = -9.38201 eV

LUMO: 21. 8 a1' -0.12666794 H = -3.44681 eV

Gap : +0.21811440 H = +5.93520 eV

Number of MOs= 50, Electrons= 58.00, Symmetry: d3h

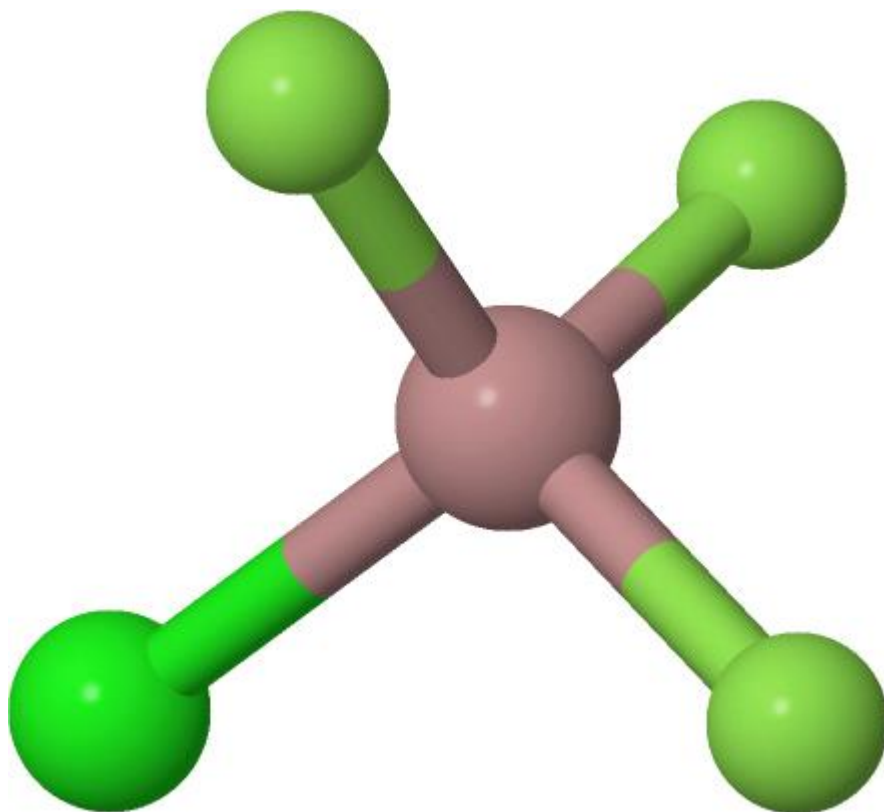
\$coord
0.0000000000000000 0.0000000000000000 0.0000000000000000 ga

3.29683317468794	0.000000000000000	0.000000000000000	f
-1.64841658734397	2.85514128131905	0.000000000000000	f
-1.64841658734397	-2.85514128131905	0.000000000000000	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e'	185.56	25.16335	YES	YES
8		e'	185.56	25.16335	YES	YES
9		a2''	204.47	44.32325	YES	NO
10		a1'	646.34	0.00000	NO	YES
11		e'	742.34	69.68490	YES	YES
12		e'	742.34	69.68490	YES	YES

GaF₃Cl⁻



Total energy = -2684.5764718860 H = -73051.0842071 eV

HOMO-LUMO Separation

HOMO: 27. 11 e -0.08911821 H = -2.42503 eV

LUMO: 28. 16 a1 +0.14745417 H = +4.01243 eV

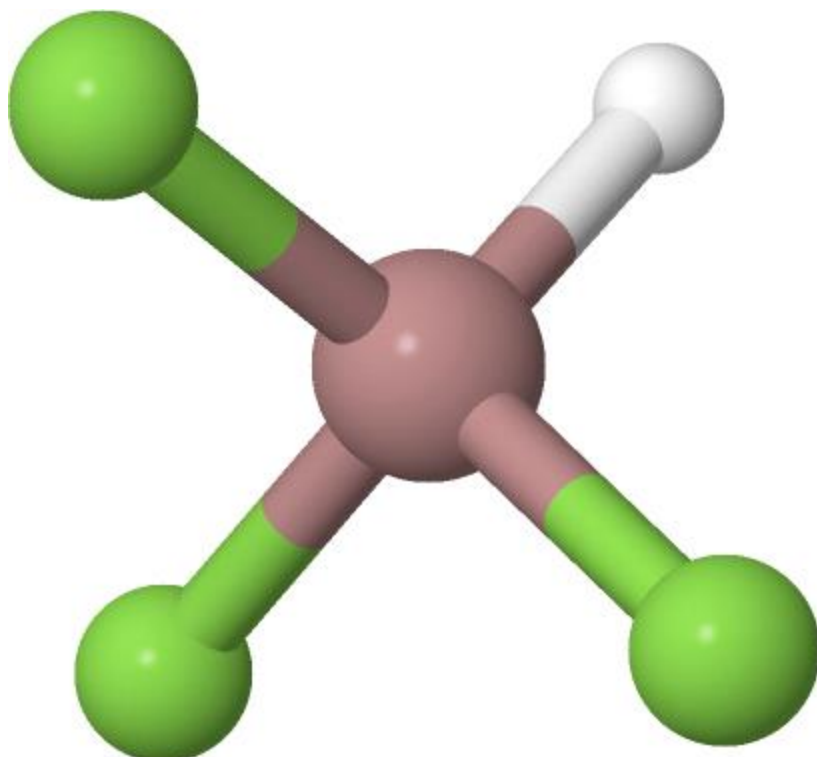
Gap : +0.23657237 H = +6.43747 eV

Number of MOs= 63, Electrons= 76.00, Symmetry: c3v

```
$coord
0.0000000000000000 0.0000000000000000 -0.51528094579166 ga
0.0000000000000000 0.0000000000000000 3.70248813617967 cl
-1.59635995620197 2.76497655131024 -1.67275357137765 f
-1.59635995620197 -2.76497655131024 -1.67275357137765 f
3.19271991240394 0.0000000000000000 -1.67275357137765 f
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 143.44 0.65468 YES YES
8 e 143.44 0.65468 YES YES
9 e 207.81 22.33876 YES YES
10 e 207.81 22.33876 YES YES
11 a1 223.39 36.71473 YES YES
12 a1 357.59 60.86265 YES YES
13 a1 607.75 46.42649 YES YES
14 e 644.84 78.60036 YES YES
15 e 644.84 78.60036 YES YES
```


GaF₃H⁻



Total energy = -2224.9894937810 H = -60545.0791111 eV

HOMO-LUMO Separation

HOMO: 21. 11 a1 -0.06528686 H = -1.77655 eV

LUMO: 22. 12 a1 +0.19781664 H = +5.38287 eV

Gap : +0.26310350 H = +7.15941 eV

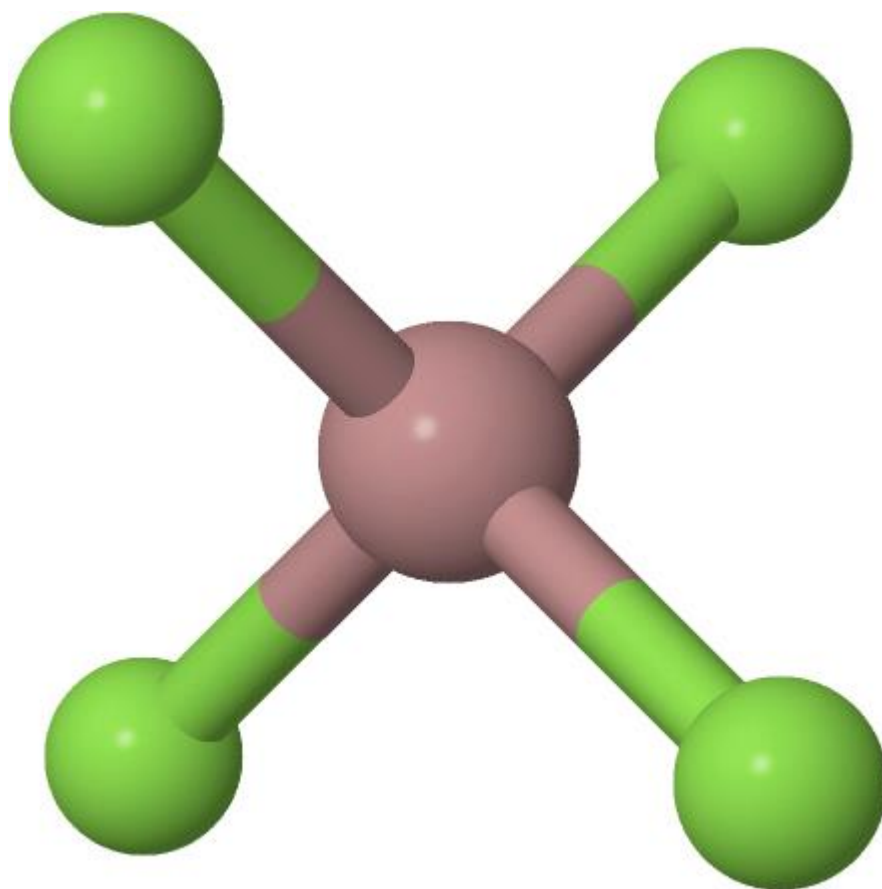
Number of MOs= 52, Electrons= 60.00, Symmetry: c3v

\$coord			
0.0000000000000000	0.0000000000000000	-0.55717986172024	ga
0.0000000000000000	0.0000000000000000	-3.60423967110573	h
-1.58858423308381	-2.75150860380400	0.74531794643092	f
-1.58858423308381	2.75150860380400	0.74531794643092	f
3.17716846616762	0.0000000000000000	0.74531794643092	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	191.18	6.40207	YES	YES
8		e	191.18	6.40207	YES	YES
9		a1	229.26	41.33868	YES	YES
10		a1	589.00	38.08318	YES	YES
11		e	606.87	101.29894	YES	YES
12		e	606.87	101.29894	YES	YES
13		e	619.82	102.02990	YES	YES
14		e	619.82	102.02990	YES	YES
15		a1	1790.68	299.65695	YES	YES

GaF₃F⁻



Total energy = -2324.2188187970 H = -63245.2479658 eV

HOMO-LUMO Separation

HOMO: 16. 1 t1 -0.09836630 H = -2.67668 eV

LUMO: 17. 7 a1 +0.16064039 H = +4.37125 eV

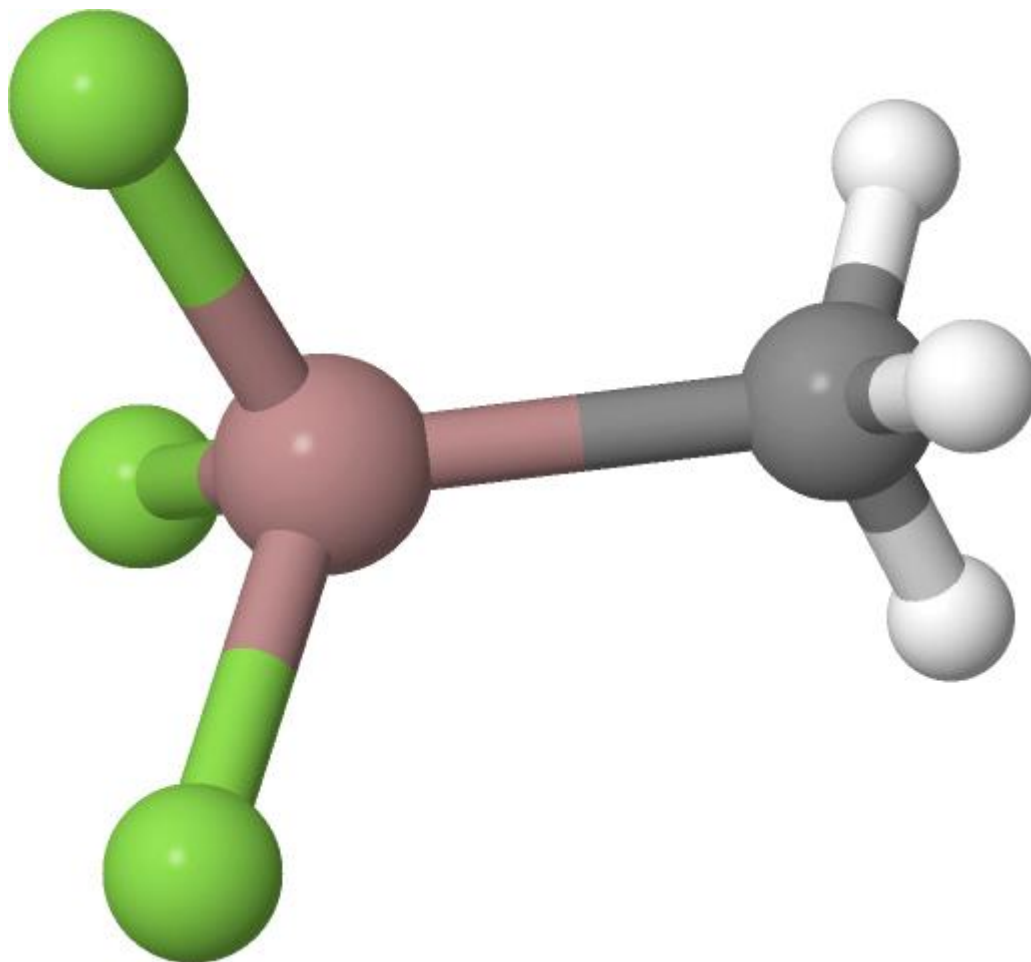
Gap : +0.25900669 H = +7.04793 eV

Number of MOs= 39, Electrons= 68.00, Symmetry: td

```
$coord
0.0000000000000000 0.0000000000000000 0.0000000000000000 ga
1.96370818051068 -1.96370818051068 1.96370818051068 f
-1.96370818051068 1.96370818051068 1.96370818051068 f
-1.96370818051068 -1.96370818051068 -1.96370818051068 f
1.96370818051068 1.96370818051068 -1.96370818051068 f
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm**(-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 164.01 0.00000 NO YES
8 e 164.01 0.00000 NO YES
9 t2 227.61 36.66840 YES YES
10 t2 227.61 36.66840 YES YES
11 t2 227.61 36.66840 YES YES
12 a1 593.36 0.00000 NO YES
13 t2 641.44 86.11490 YES YES
14 t2 641.44 86.11490 YES YES
15 t2 641.44 86.11490 YES YES
```

GaF₃Me⁻



Total energy = -2264.2777785150 H = -61614.1683423 eV

HOMO-LUMO Separation

HOMO: 24. 13 a1 -0.06009089 H = -1.63516 eV

LUMO: 25. 14 a1 +0.17640423 H = +4.80021 eV

Gap : +0.23649512 H = +6.43536 eV

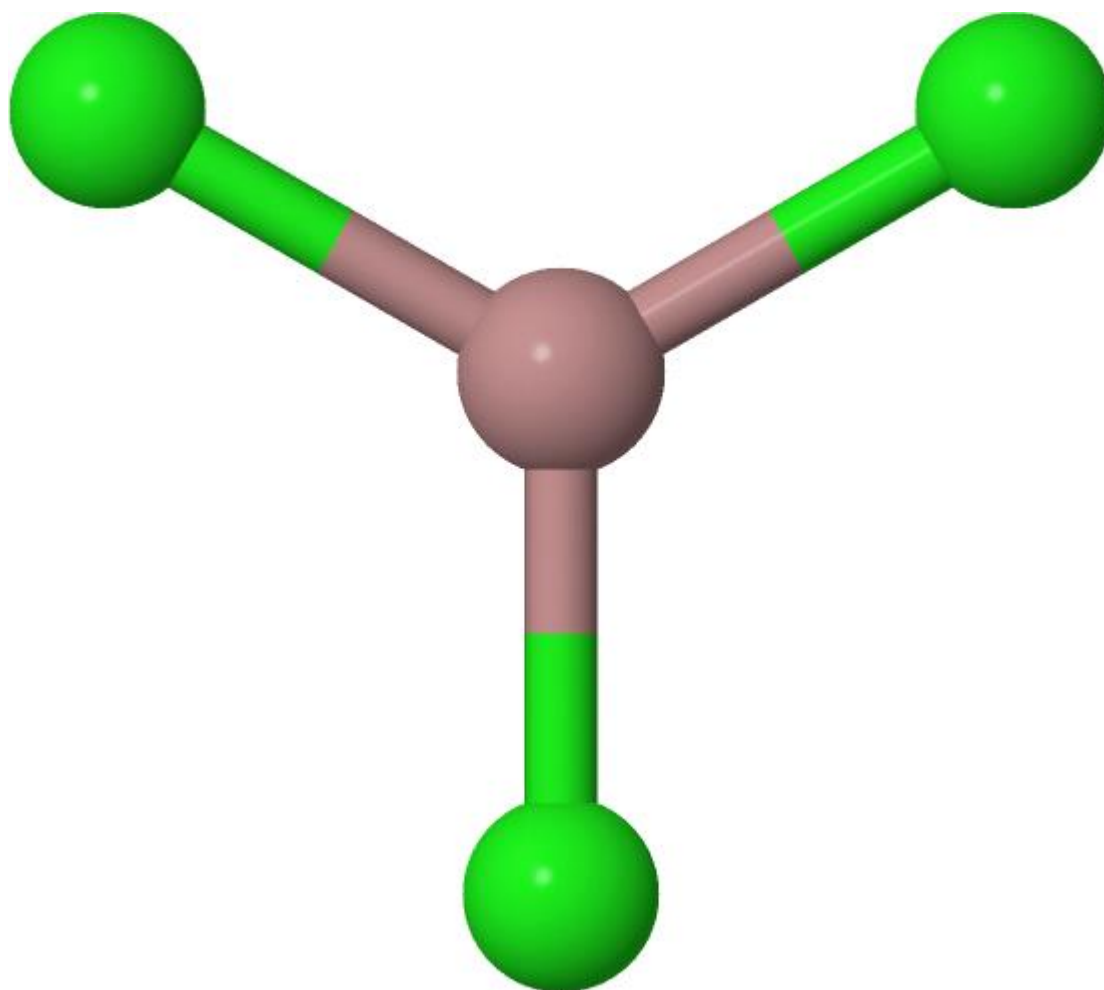
Number of MOs= 64, Electrons= 68.00, Symmetry: c3v

\$coord	0.000000000000000	0.000000000000000	0.10972436250527	ga
	-1.58833350652399	2.75107433266358	-1.20467410897707	f
	-1.58833350652399	-2.75107433266358	-1.20467410897707	f
	3.17666701304798	0.000000000000000	-1.20467410897707	f
	0.000000000000000	0.000000000000000	3.90788704118369	c
	-1.96840928602393	0.000000000000000	4.65372375083535	h
	0.98420464301197	1.70469244674191	4.65372375083535	h
	0.98420464301197	-1.70469244674191	4.65372375083535	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a2		60.49	0.00000	NO	NO
8	e		142.25	0.26634	YES	YES
9	e		142.25	0.26634	YES	YES
10	e		204.34	13.52492	YES	YES
11	e		204.34	13.52492	YES	YES
12	a1		230.06	46.24215	YES	YES
13	a1		510.57	17.94755	YES	YES
14	a1		588.26	67.55368	YES	YES
15	e		604.29	64.15073	YES	YES
16	e		604.29	64.15073	YES	YES
17	e		688.74	54.03429	YES	YES
18	e		688.74	54.03429	YES	YES
19	a1		1152.35	12.86317	YES	YES
20	e		1405.54	0.39807	YES	YES
21	e		1405.54	0.39807	YES	YES
22	a1		2921.54	28.34417	YES	YES
23	e		3015.52	41.95484	YES	YES
24	e		3015.52	41.95484	YES	YES

GaCl₃



Total energy = -3305.3683914220 H = -89943.7014463 eV

HOMO-LUMO Separation

HOMO: 28. 2 a2' -0.29091862 H = -7.91630 eV

LUMO: 29. 10 a1' -0.11514092 H = -3.13315 eV

Gap : +0.17577769 H = +4.78316 eV

Number of MOs= 58, Electrons= 82.00, Symmetry: d3h

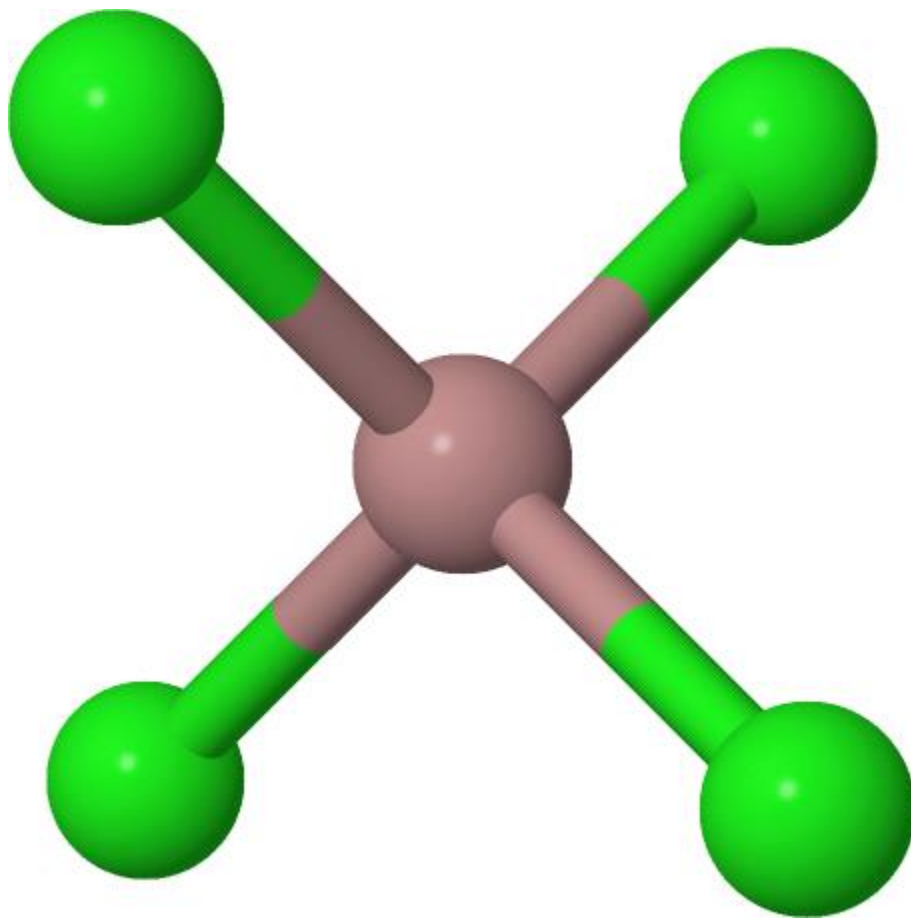
\$coord

0.0000000000000000	0.0000000000000000	0.0000000000000000	ga
2.02365768857463	-3.50507793373866	0.0000000000000000	cl
2.02365768857463	3.50507793373866	0.0000000000000000	cl
-4.04731537714927	0.0000000000000000	0.0000000000000000	cl

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e'	121.66	6.07092	YES	YES
8		e'	121.66	6.07092	YES	YES
9		a2''	131.72	9.98504	YES	NO
10		a1'	355.99	0.00000	NO	YES
11		e'	452.30	71.52306	YES	YES
12		e'	452.30	71.52306	YES	YES

GaCl₃Cl⁻



Total energy = -3765.6403204790 H = -102468.3450167 eV

HOMO-LUMO Separation

HOMO: 23. 2 t1 -0.09571171 H = -2.60445 eV

LUMO: 24. 9 a1 +0.10646039 H = +2.89694 eV

Gap : +0.20217210 H = +5.50139 eV

Number of MOs= 46, Electrons= 100.00, Symmetry: td

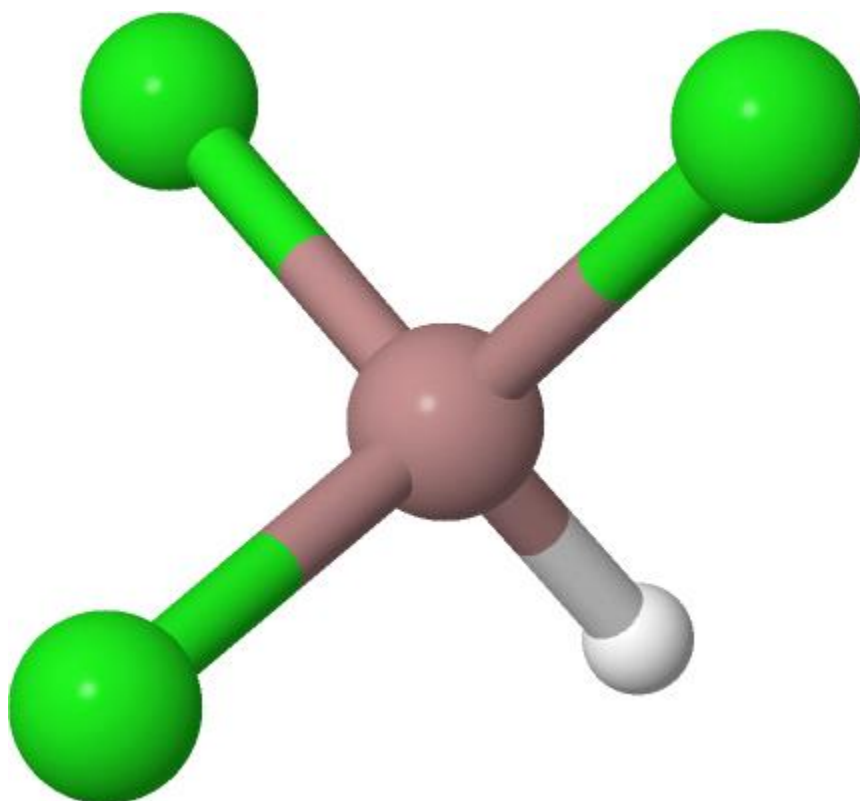
\$coord

0.0000000000000000	0.0000000000000000	0.0000000000000000	ga
2.43003282227266	-2.43003282227266	2.43003282227266	cl
-2.43003282227266	2.43003282227266	2.43003282227266	cl
-2.43003282227266	-2.43003282227266	-2.43003282227266	cl
2.43003282227266	2.43003282227266	-2.43003282227266	cl

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	101.43	0.00000	NO	YES
8		e	101.43	0.00000	NO	YES
9		t2	144.32	8.04872	YES	YES
10		t2	144.32	8.04872	YES	YES
11		t2	144.32	8.04872	YES	YES
12		a1	318.59	0.00000	NO	YES
13		t2	371.75	79.94657	YES	YES
14		t2	371.75	79.94657	YES	YES
15		t2	371.75	79.94657	YES	YES

GaCl₃H⁻



Total energy = -3306.0588873420 H = -89962.4908070 eV

HOMO-LUMO Separation

HOMO: 29. 14 a1 -0.07788261 H = -2.11929 eV

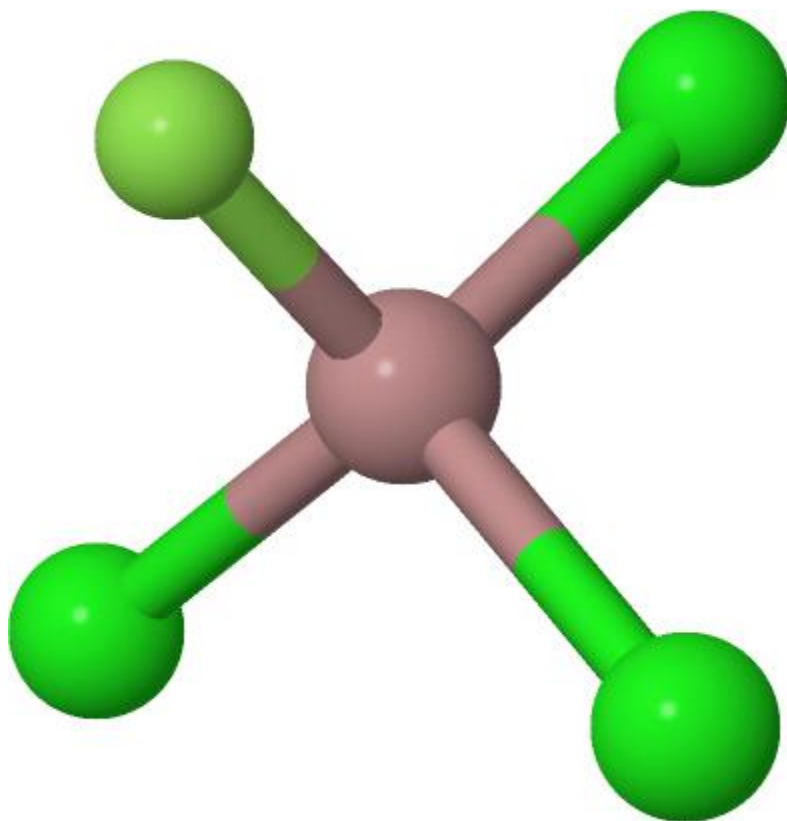
LUMO: 30. 15 a1 +0.14143615 H = +3.84868 eV

Gap : +0.21931876 H = +5.96797 eV

Number of MOs= 60, Electrons= 84.00, Symmetry: c3v

```
$coord
0.0000000000000000 0.0000000000000000 0.90337649734177 ga
0.0000000000000000 0.0000000000000000 3.91827037590957 h
-1.98720409625508 3.44193845972278 -0.62931118556468 cl
-1.98720409625508 -3.44193845972278 -0.62931118556468 cl
3.97440819251015 0.0000000000000000 -0.62931118556468 cl
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm**(-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 117.88 1.22282 YES YES
8 e 117.88 1.22282 YES YES
9 a1 153.43 7.78300 YES YES
10 a1 330.20 17.28411 YES YES
11 e 349.30 81.82929 YES YES
12 e 349.30 81.82929 YES YES
13 e 612.62 120.19452 YES YES
14 e 612.62 120.19452 YES YES
15 a1 1844.93 288.58613 YES YES
```



Total energy = -3405.2871498980 H = -92662.6307507 eV

HOMO-LUMO Separation

HOMO: 32. 2 a2 -0.09176001 H = -2.49692 eV

LUMO: 33. 17 a1 +0.11991700 H = +3.26311 eV

Gap : +0.21167700 H = +5.76003 eV

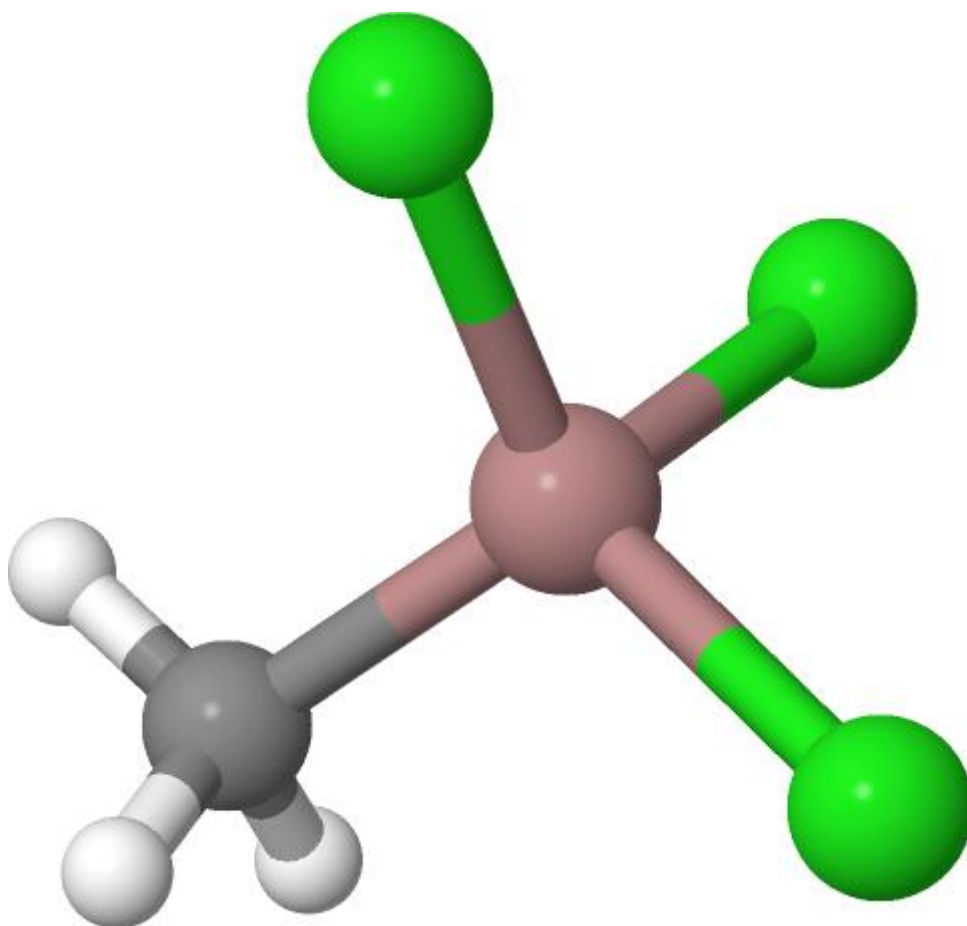
Number of MOs= 68, Electrons= 92.00, Symmetry: c3v

```
$coord
0.0000000000000000 0.0000000000000000 -0.12969107547806 ga
0.0000000000000000 0.0000000000000000 -3.52091186558897 f
1.99425070287695 3.45414354041283 1.21686764702233 cl
1.99425070287695 -3.45414354041283 1.21686764702233 cl
-3.98850140575390 0.0000000000000000 1.21686764702233 cl
```

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	110.12	0.38696	YES	YES
8		e	110.12	0.38696	YES	YES
9		a1	148.36	6.85298	YES	YES
10		e	185.26	17.21616	YES	YES
11		e	185.26	17.21616	YES	YES
12		a1	331.45	6.70644	YES	YES
13		e	372.33	89.76198	YES	YES
14		e	372.33	89.76198	YES	YES
15		a1	634.90	65.94203	YES	YES

GaCl₃Me⁻



Total energy = -3345.3474204160 H = -91031.5867959 eV

HOMO-LUMO Separation

HOMO: 46. 18 a -0.07430836 H = -2.02203 eV

LUMO: 47. 19 a +0.14429030 H = +3.92634 eV

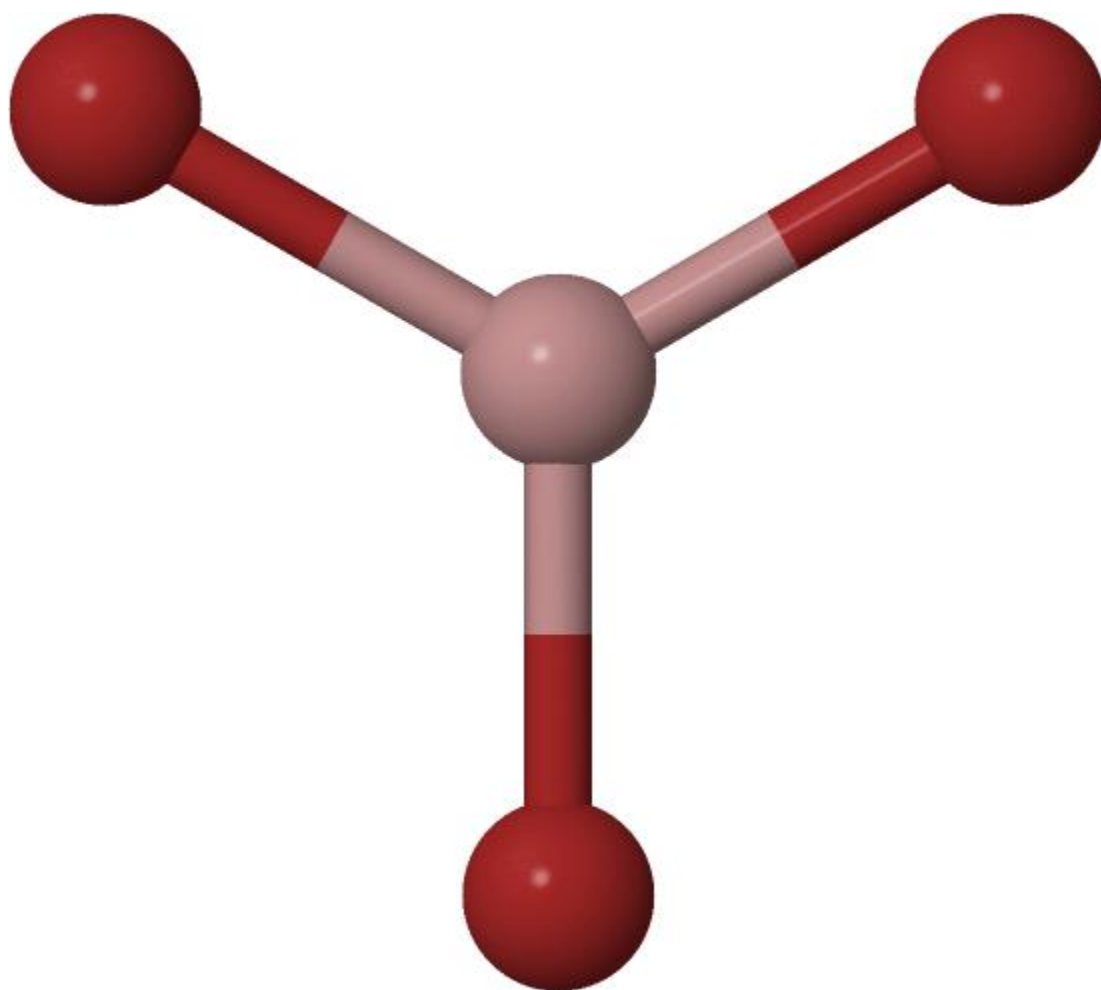
Gap : +0.21859867 H = +5.94838 eV

Number of MOs= 106, Electrons= 92.00, Symmetry: c3

```
$coord
0.0000000000000000 0.0000000000000000 0.55067745221224 ga
0.53428541739349 3.94499191430454 -0.99351744652133 cl
-3.68360592420868 -1.50979121281793 -0.99351744652133 cl
3.14932050681519 -2.43520070148661 -0.99351744652133 cl
0.0000000000000000 0.0000000000000000 4.32892230185130 c
-1.23581414279239 1.53902001468815 5.05337626465192 h
1.95073750104884 0.30073643467022 5.05337626465192 h
-0.71492335825644 -1.83975644935838 5.05337626465192 h
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 a 41.37 0.00046 YES YES
8 e 106.60 0.11951 YES YES
9 e 106.60 0.11951 YES YES
10 e 144.43 5.01397 YES YES
11 e 144.43 5.01397 YES YES
12 a 147.38 9.59614 YES YES
13 a 319.98 20.67443 YES YES
14 e 345.11 75.46338 YES YES
15 e 345.11 75.46338 YES YES
16 a 529.63 39.23322 YES YES
17 e 707.44 44.10082 YES YES
18 e 707.44 44.10082 YES YES
19 a 1158.65 6.41948 YES YES
20 e 1400.51 0.71108 YES YES
21 e 1400.51 0.71108 YES YES
22 a 2933.92 24.77368 YES YES
23 e 3034.24 25.08883 YES YES
24 e 3034.24 25.08883 YES YES
```

GaBr₃



Total energy = -9647.4562270050 H = -262520.7903755 eV

HOMO-LUMO Separation

HOMO: 46. 4 a2' -0.27055509 H = -7.36218 eV

LUMO: 47. 14 a1' -0.12283129 H = -3.34241 eV

Gap : +0.14772380 H = +4.01977 eV

Number of MOs= 86, Electrons= 136.00, Symmetry: d3h

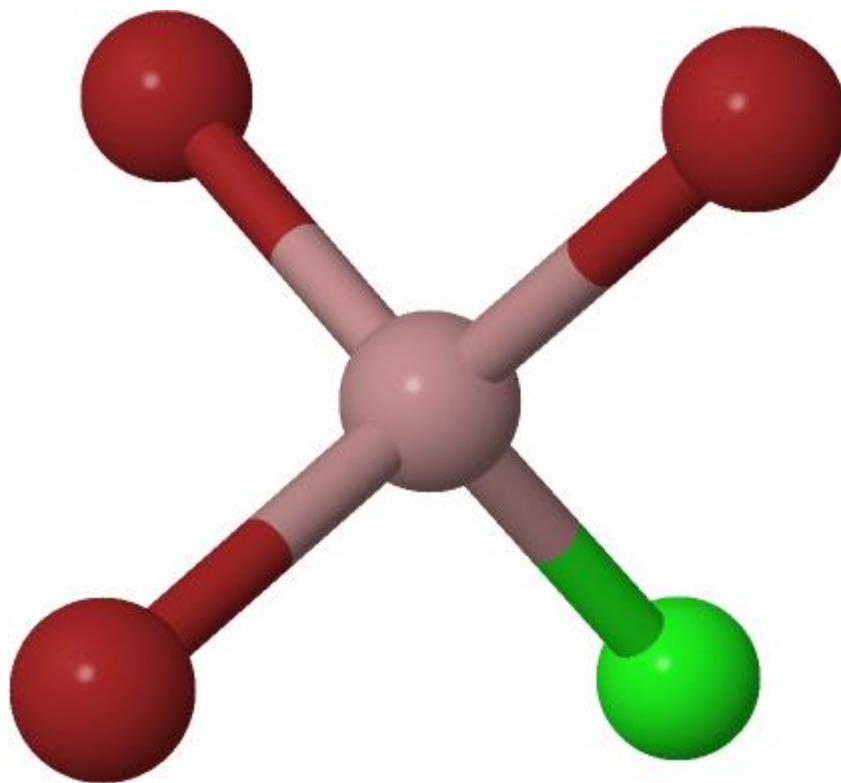
\$coord

0.0000000000000000	0.0000000000000000	0.0000000000000000	ga
2.16257643211860	-3.74569225568044	0.0000000000000000	br
2.16257643211860	3.74569225568044	0.0000000000000000	br
-4.32515286423719	0.0000000000000000	0.0000000000000000	br

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e'	80.60	1.76733	YES	YES
8		e'	80.60	1.76733	YES	YES
9		a2''	107.12	3.93380	YES	NO
10		a1'	215.16	0.00000	NO	YES
11		e'	337.84	58.67186	YES	YES
12		e'	337.84	58.67186	YES	YES

GaBr₃Cl⁻



Total energy = -10107.7284083800 H = -275045.4408118 eV

HOMO-LUMO Separation

HOMO: 53. 5 a2 -0.09069682 H = -2.46799 eV

LUMO: 54. 25 a1 +0.07596451 H = +2.06710 eV

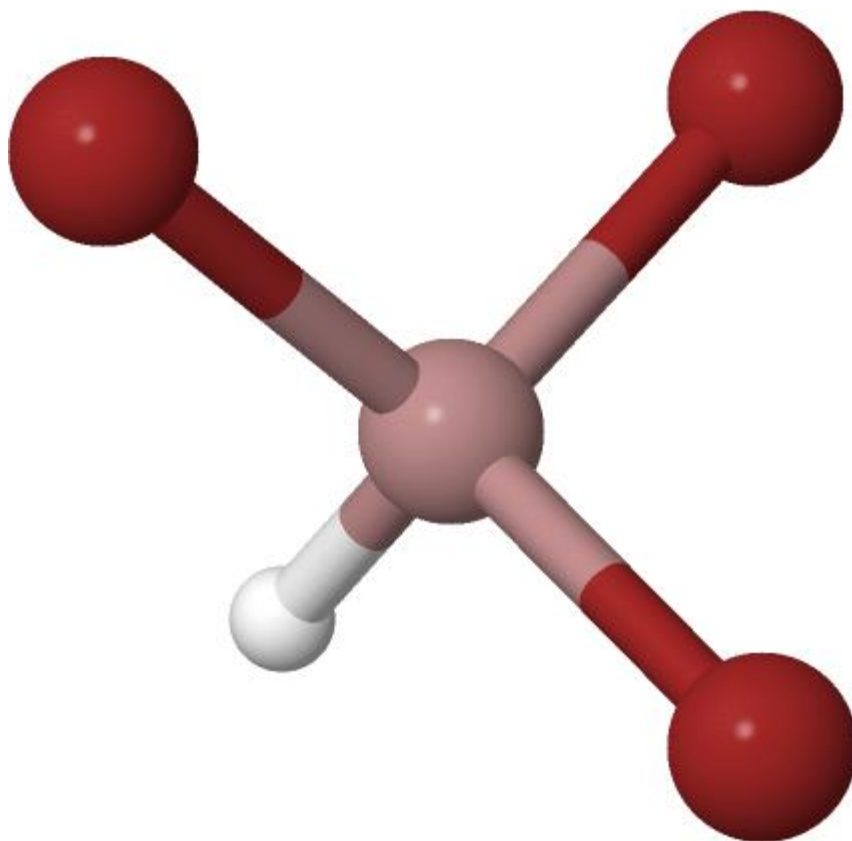
Gap : +0.16666133 H = +4.53509 eV

Number of MOs= 99, Electrons= 154.00, Symmetry: c3v

```
$coord
0.0000000000000000 0.0000000000000000 0.61403684337475 ga
-2.12671757550345 3.68358289412167 -0.89114389532616 br
-2.12671757550345 -3.68358289412167 -0.89114389532616 br
4.25343515100689 0.0000000000000000 -0.89114389532616 br
0.0000000000000000 0.0000000000000000 4.81822705764719 cl
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 65.03 0.01917 YES YES
8 e 65.03 0.01917 YES YES
9 a1 97.92 1.39335 YES YES
10 e 110.12 3.21221 YES YES
11 e 110.12 3.21221 YES YES
12 a1 200.01 3.62010 YES YES
13 e 257.19 63.62558 YES YES
14 e 257.19 63.62558 YES YES
15 a1 362.58 65.35432 YES YES
```


GaBr₃H⁻



Total energy = -9648.1489813970 H = -262539.6411924 eV

HOMO-LUMO Separation

HOMO: 47. 5 a2 -0.07810363 H = -2.12531 eV

LUMO: 48. 21 a1 +0.10428520 H = +2.83775 eV

Gap : +0.18238884 H = +4.96306 eV

Number of MOs= 88, Electrons= 138.00, Symmetry: c3v

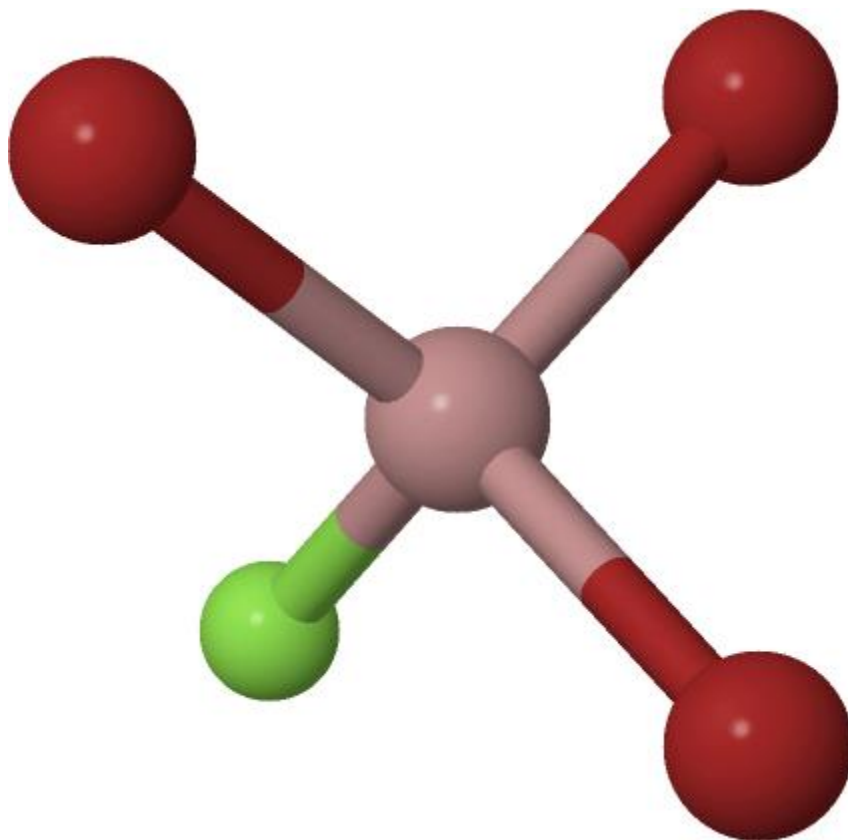
```
$coord
  0.0000000000000000  0.0000000000000000  1.23873990445645  ga
  0.0000000000000000  0.0000000000000000  4.24745832061676  h
 -2.13310334344654   3.69464336864445  -0.37812285100191  br
```

-2.13310334344654	-3.69464336864445	-0.37812285100191	br
4.26620668689308	0.00000000000000	-0.37812285100191	br

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	69.02	0.12872	YES	YES
8		e	69.02	0.12872	YES	YES
9		a1	101.27	1.16374	YES	YES
10		a1	213.63	7.74465	YES	YES
11		e	240.92	55.24792	YES	YES
12		e	240.92	55.24792	YES	YES
13		e	583.92	129.45844	YES	YES
14		e	583.92	129.45844	YES	YES
15		a1	1850.99	256.75156	YES	YES

GaBr₃F⁻



Total energy = -9747.3765093580 H = -265239.7611467 eV

HOMO-LUMO Separation

HOMO: 50. 5 a2 -0.08836676 H = -2.40458 eV

LUMO: 51. 23 a1 +0.08633076 H = +2.34918 eV

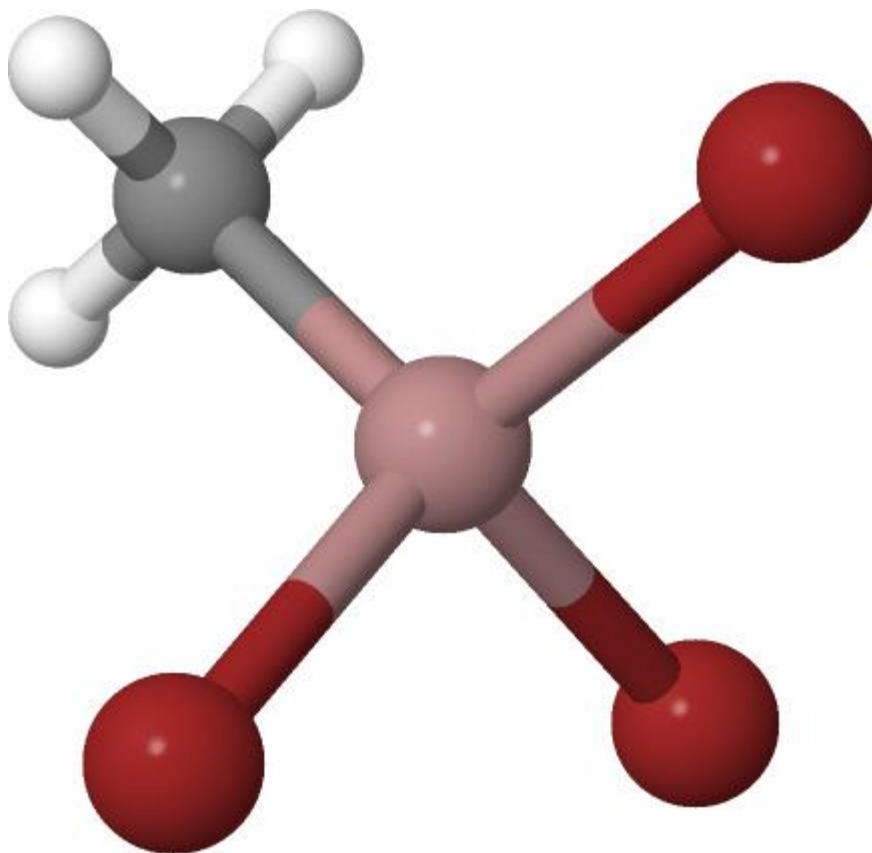
Gap : +0.17469752 H = +4.75376 eV

Number of MOs= 96, Electrons= 146.00, Symmetry: c3v

```
$coord
0.0000000000000000 0.0000000000000000 0.18587458226830 ga
-2.13689113931496 3.70120402353725 -1.25355465418831 br
-2.13689113931496 -3.70120402353725 -1.25355465418831 br
4.27378227862991 0.0000000000000000 -1.25355465418831 br
0.0000000000000000 0.0000000000000000 3.57478938029661 f
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 66.87 0.08506 YES YES
8 e 66.87 0.08506 YES YES
9 a1 100.47 0.90392 YES YES
10 e 157.76 7.17600 YES YES
11 e 157.76 7.17600 YES YES
12 a1 206.36 3.03588 YES YES
13 e 261.23 78.70517 YES YES
14 e 261.23 78.70517 YES YES
15 a1 634.25 63.19927 YES YES
```

GaBr₃Me⁻



Total energy = -9687.4372660070 H = -263608.7304202 eV

HOMO-LUMO Separation

HOMO: 73. 73 a -0.07592005 H = -2.06589 eV

LUMO: 74. 74 a +0.10896953 H = +2.96521 eV

Gap : +0.18488957 H = +5.03110 eV

Number of MOs= 148, Electrons= 146.00, Symmetry: c1

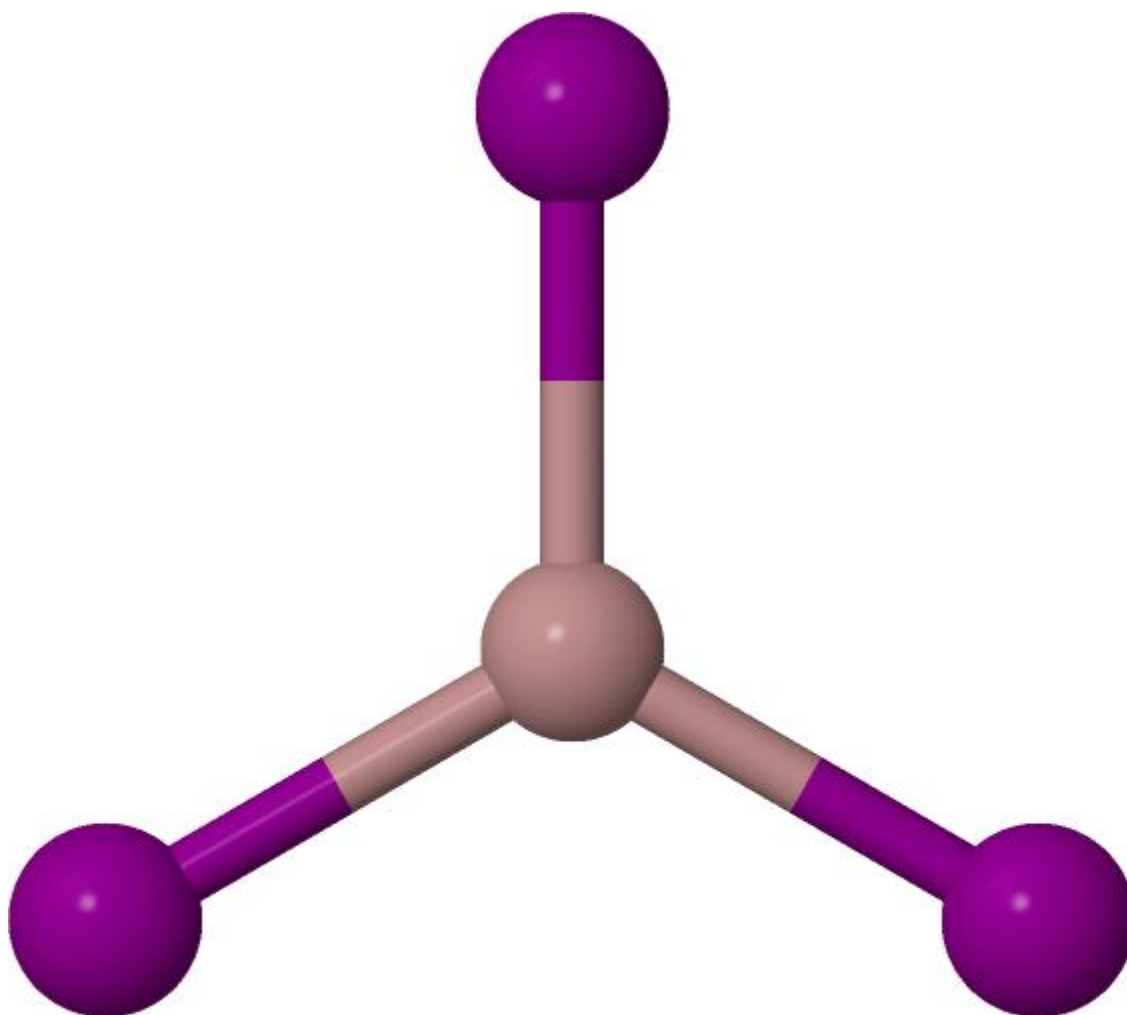
```
$coord
-0.00170986962314    0.00174446845937    1.03144777540605    ga
 3.89540743372798   -1.74788675738294   -0.61139533085899    br
```

-0.43563149492147	4.24916718842059	-0.61093407414662	br
-3.45997630172645	-2.50284807173805	-0.60953282320044	br
0.00833720065232	0.00022218610984	4.80954543530703	c
1.67237001852861	1.07175644079928	5.51359839237791	h
0.10920961302721	-1.97310566925844	5.52411615801707	h
-1.74677349339745	0.90231706385932	5.53179469801450	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		68.46	0.06274	YES	YES
8	a		69.62	0.05125	YES	YES
9	a		76.76	0.00115	YES	YES
10	a		101.46	1.65219	YES	YES
11	a		121.27	1.97112	YES	YES
12	a		122.39	2.05014	YES	YES
13	a		208.38	10.74084	YES	YES
14	a		242.87	56.51096	YES	YES
15	a		247.26	56.60762	YES	YES
16	a		527.59	33.43101	YES	YES
17	a		708.57	50.71636	YES	YES
18	a		710.55	50.52869	YES	YES
19	a		1154.64	2.72673	YES	YES
20	a		1396.50	0.71616	YES	YES
21	a		1396.87	0.74396	YES	YES
22	a		2940.70	22.31390	YES	YES
23	a		3043.05	17.65625	YES	YES
24	a		3045.39	17.45572	YES	YES

Gal₃



Total energy = -1959.4241759030 H = -53318.6750202 eV

HOMO-LUMO Separation

HOMO: 18. 1 a2' -0.25004009 H = -6.80394 eV

LUMO: 19. 7 a1' -0.13744527 H = -3.74008 eV

Gap : +0.11259483 H = +3.06386 eV

Number of MOs= 48, Electrons= 52.00, Symmetry: d3h

```

$coord
  0.0000000000000000  0.0000000000000000  0.0000000000000000  ga
  4.74513012952716   0.0000000000000000  0.0000000000000000  i
 -2.37256506476358   4.10940323643347   0.0000000000000000  i
 -2.37256506476358  -4.10940323643347   0.0000000000000000  i

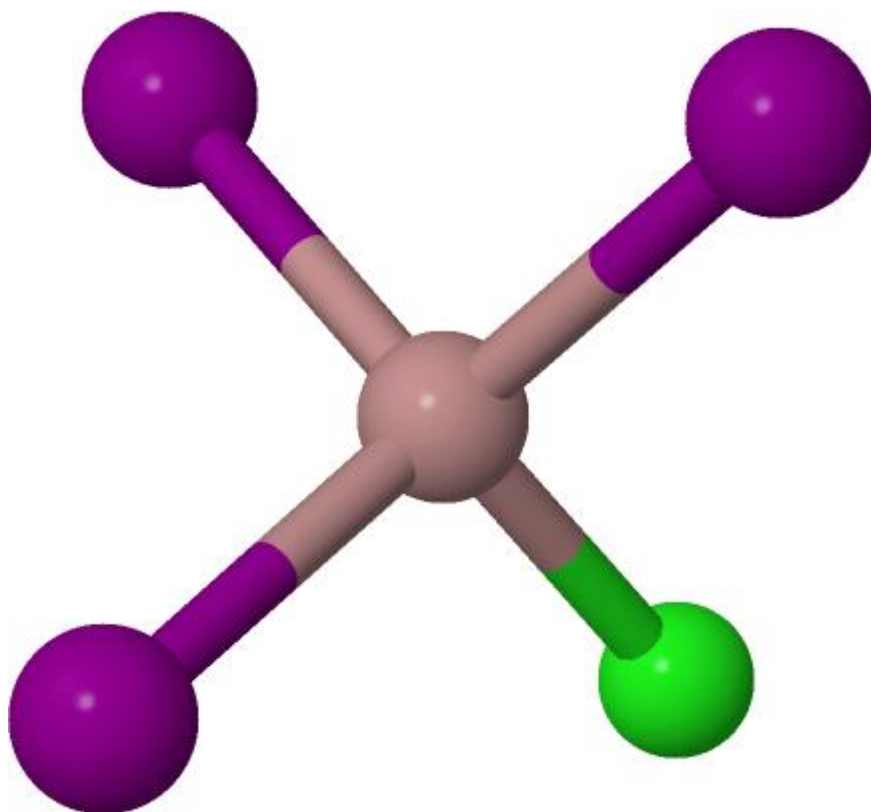
```

```

$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#                               cm** (-1)          km/mol            IR      RAMAN
  1              0.00          0.00000          -        -
  2              0.00          0.00000          -        -
  3              0.00          0.00000          -        -
  4              0.00          0.00000          -        -
  5              0.00          0.00000          -        -
  6              0.00          0.00000          -        -
  7              e'          58.17          0.69905        YES      YES
  8              e'          58.17          0.69905        YES      YES
  9              a2''         88.46          1.32121        YES      NO
 10              a1'         150.18          0.00000        NO       YES
 11              e'          276.94          57.28796       YES      YES
 12              e'          276.94          57.28796       YES      YES

```

Gal₃Cl⁻



Total energy = -2419.7021901080 H = -65843.4841759 eV

HOMO-LUMO Separation

HOMO: 25. 1 a2 -0.09337679 H = -2.54091 eV

LUMO: 26. 15 a1 +0.02907108 H = +0.79106 eV

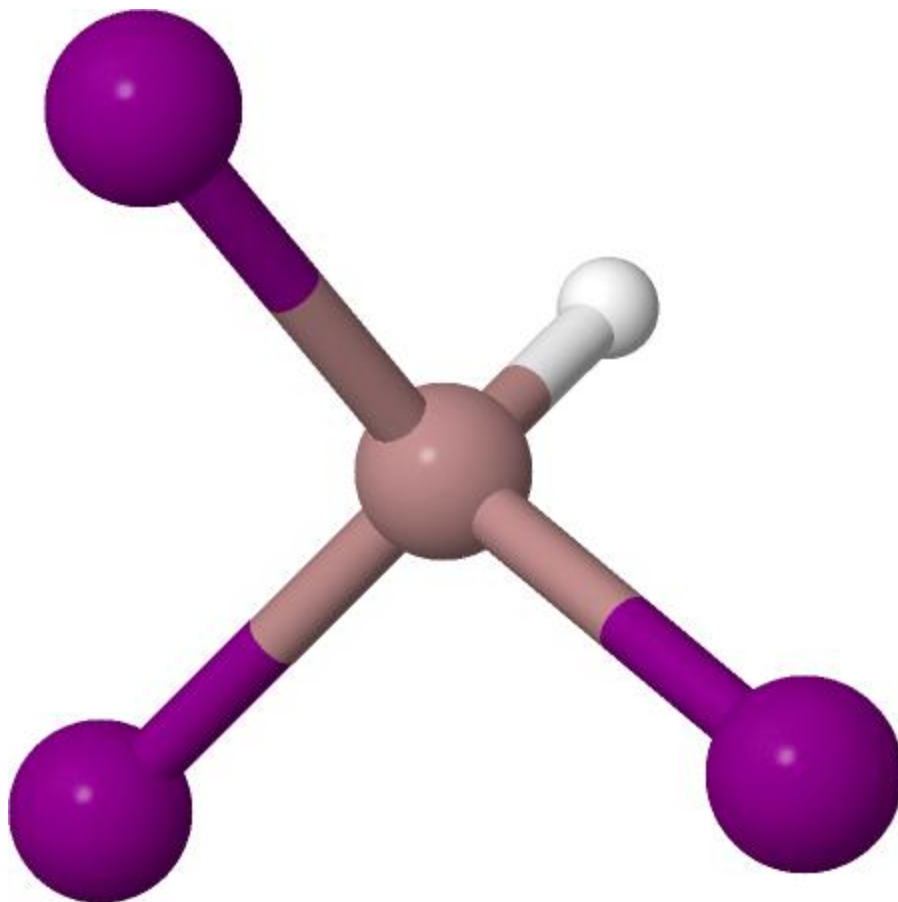
Gap : +0.12244787 H = +3.33198 eV

Number of MOs= 61, Electrons= 70.00, Symmetry: c3v

```
$coord
0.0000000000000000 0.0000000000000000 0.98956262329625 ga
0.0000000000000000 0.0000000000000000 5.18103643663510 cl
4.67418563735289 0.0000000000000000 -0.66369221585933 i
-2.33709281867645 4.04796350395196 -0.66369221585933 i
-2.33709281867645 -4.04796350395196 -0.66369221585933 i
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 50.32 0.00003 YES YES
8 e 50.32 0.00003 YES YES
9 a1 77.40 0.21344 YES YES
10 e 96.57 2.09594 YES YES
11 e 96.57 2.09594 YES YES
12 a1 153.26 1.82920 YES YES
13 e 214.00 67.08536 YES YES
14 e 214.00 67.08536 YES YES
15 a1 365.59 63.75455 YES YES
```


Gal₃H⁻



Total energy = -1960.1263674600 H = -53337.7826355 eV

HOMO-LUMO Separation

HOMO: 19. 1 a2 -0.08548133 H = -2.32607 eV

LUMO: 20. 11 a1 +0.04960785 H = +1.34990 eV

Gap : +0.13508918 H = +3.67597 eV

Number of MOs= 50, Electrons= 54.00, Symmetry: c3v

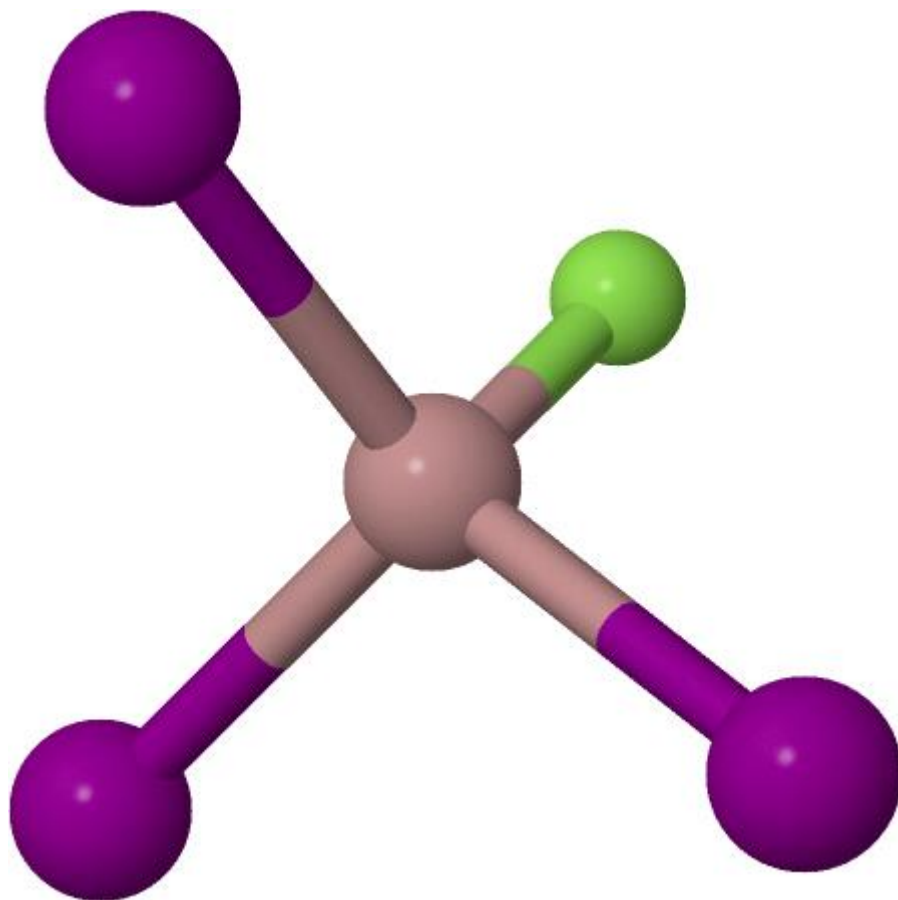
\$coord
0.0000000000000000 0.0000000000000000 1.45461303674547 ga
189

0.0000000000000000	0.0000000000000000	4.45578283342057	h
-2.34282237892904	4.05788739341448	-0.27818118773376	i
-2.34282237892904	-4.05788739341448	-0.27818118773376	i
4.68564475785807	0.0000000000000000	-0.27818118773376	i

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	52.07	0.00949	YES	YES
8		e	52.07	0.00949	YES	YES
9		a1	78.31	0.17940	YES	YES
10		a1	168.57	3.29159	YES	YES
11		e	200.20	56.30507	YES	YES
12		e	200.20	56.30507	YES	YES
13		e	554.05	157.67961	YES	YES
14		e	554.05	157.67961	YES	YES
15		a1	1865.27	212.11276	YES	YES

Gal₃F⁻



Total energy = -2059.3514372520 H = -56037.8356996 eV

HOMO-LUMO Separation

HOMO: 22. 1 a2 -0.09282692 H = -2.52595 eV

LUMO: 23. 13 a1 +0.03529436 H = +0.96041 eV

Gap : +0.12812128 H = +3.48636 eV

Number of MOs= 58, Electrons= 62.00, Symmetry: c3v

```
$coord
0.000000000000000 0.000000000000000 0.25267631164178 ga
0.000000000000000 0.000000000000000 3.63272646608656 f
-2.35055247712255 4.07127631623312 -1.29513425924277 i
```

```

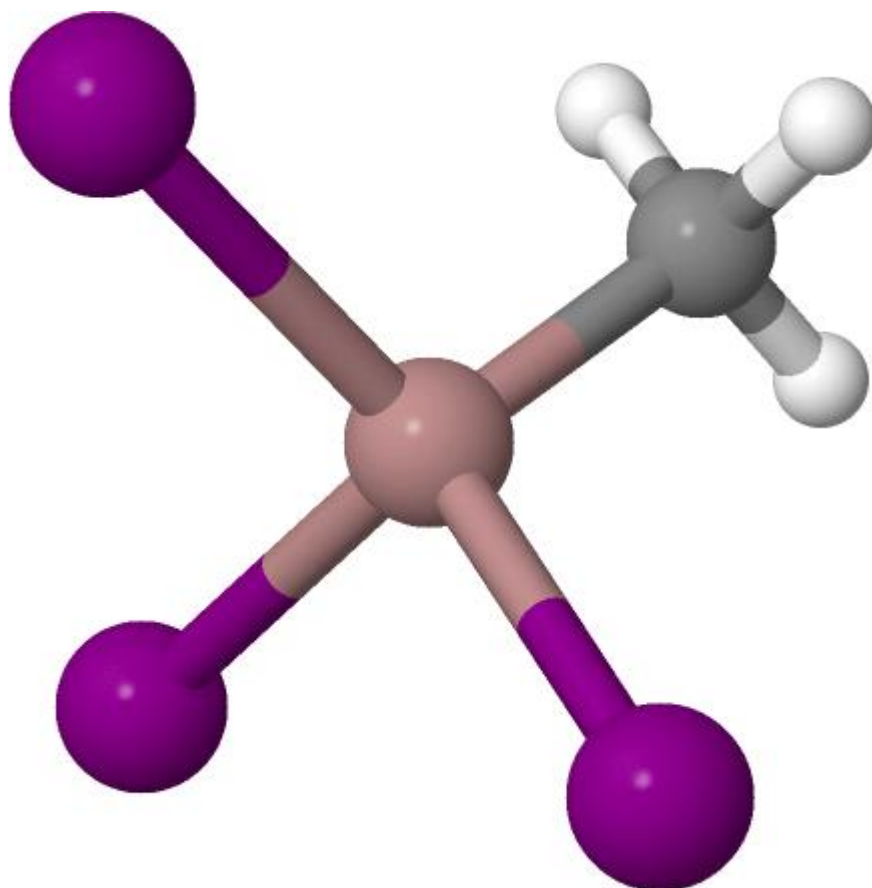
-2.35055247712255      -4.07127631623312      -1.29513425924277      i
  4.70110495424508      0.000000000000000      -1.29513425924277      i

```

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	51.36	0.00383	YES	YES
8		e	51.36	0.00383	YES	YES
9		a1	79.03	0.12548	YES	YES
10		e	139.78	3.81651	YES	YES
11		e	139.78	3.81651	YES	YES
12		a1	157.69	1.24201	YES	YES
13		e	221.31	86.55067	YES	YES
14		e	221.31	86.55067	YES	YES
15		a1	640.40	61.26901	YES	YES

Gal₃Me⁻



Total energy = -1999.4146608670 H = -54406.8721027 eV

HOMO-LUMO Separation

HOMO: 22. 1 a2 -0.08311231 H = -2.26160 eV

LUMO: 23. 13 a1 +0.05319529 H = +1.44752 eV

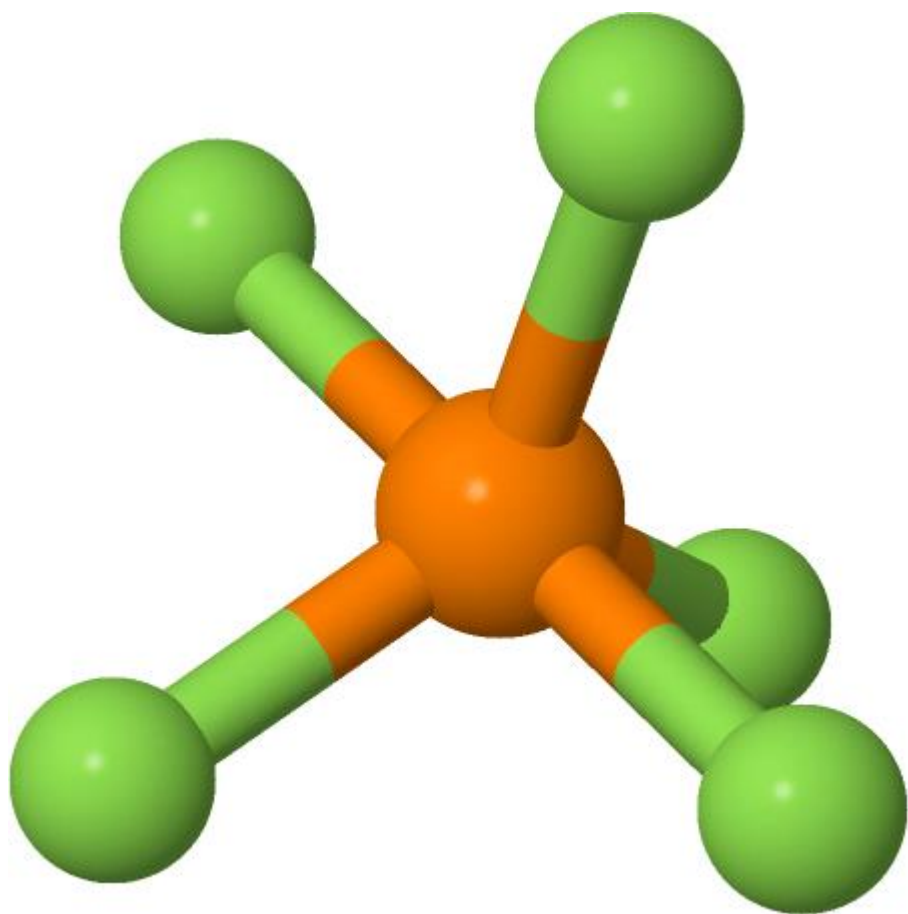
Gap : +0.13630760 H = +3.70912 eV

Number of MOs= 62, Electrons= 62.00, Symmetry: c3v

```
$coord
0.0000000000000000 0.0000000000000000 1.32852745786750 ga
2.34636474921823 -4.06402295873459 -0.45049351757167 i
2.34636474921823 4.06402295873459 -0.45049351757167 i
-4.69272949843647 0.0000000000000000 -0.45049351757167 i
0.0000000000000000 0.0000000000000000 5.10579272887771 c
1.98052042812081 0.0000000000000000 5.80602973096550 h
-0.99026021406041 -1.71518100346666 5.80602973096550 h
-0.99026021406041 1.71518100346666 5.80602973096550 h
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 50.54 0.01076 YES YES
8 e 50.54 0.01076 YES YES
9 a1 76.25 0.32028 YES YES
10 e 117.14 1.61542 YES YES
11 e 117.14 1.61542 YES YES
12 a2 139.34 0.00000 NO NO
13 a1 159.84 5.64941 YES YES
14 e 196.24 59.63570 YES YES
15 e 196.24 59.63570 YES YES
16 a1 526.52 28.35428 YES YES
17 e 717.52 68.46099 YES YES
18 e 717.52 68.46099 YES YES
19 a1 1153.99 0.20549 YES YES
20 e 1394.79 0.74523 YES YES
21 e 1394.79 0.74523 YES YES
22 a1 2943.41 17.19174 YES YES
23 e 3051.09 8.63174 YES YES
24 e 3051.09 8.63174 YES YES
```

PF₅



Total energy = -840.2492032425 H = -22864.3571691 eV

HOMO-LUMO Separation

HOMO: 22. 2 e" -0.35747201 H = -9.72731 eV

LUMO: 23. 9 a1' -0.05622513 H = -1.52996 eV

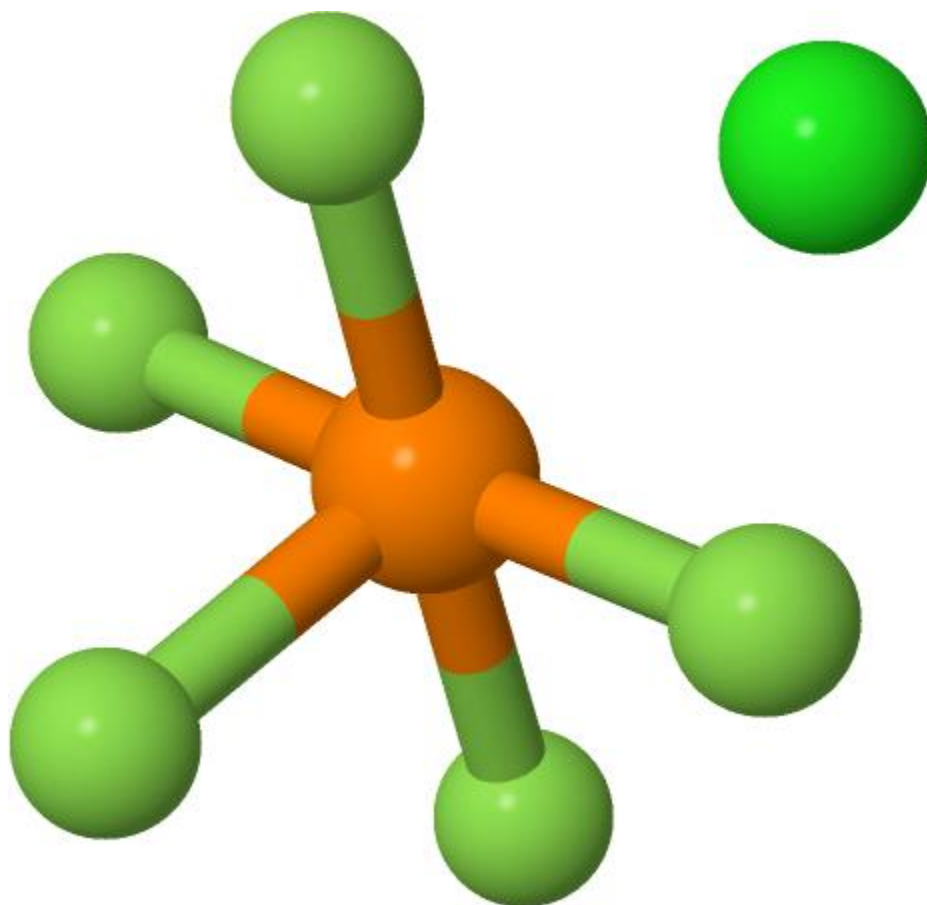
Gap : +0.30124687 H = +8.19735 eV

Number of MOs= 61, Electrons= 60.00, Symmetry: d3h

\$coord				
0.0000000000000000	0.0000000000000000	0.0000000000000000		p
0.0000000000000000	0.0000000000000000	3.04636865560241		f
0.0000000000000000	0.0000000000000000	-3.04636865560241		f
3.00850745438720	0.0000000000000000	0.0000000000000000		f
-1.50425372719360	2.60544388297417	0.0000000000000000		f
-1.50425372719360	-2.60544388297417	0.0000000000000000		f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e'	136.48	0.60081	YES	YES
8		e'	136.48	0.60081	YES	YES
9		e"	461.96	0.00000	NO	YES
10		e"	461.96	0.00000	NO	YES
11		e'	491.80	35.23189	YES	YES
12		e'	491.80	35.23189	YES	YES
13		a2"	520.93	50.21885	YES	NO
14		a1'	647.92	0.00000	NO	YES
15		a1'	753.45	0.00000	NO	YES
16		e'	975.05	255.36250	YES	YES
17		e'	975.05	255.36250	YES	YES
18		a2"	982.74	363.13418	YES	NO



Total energy = -1300.4767612970 H = -35387.7933424 eV

HOMO-LUMO Separation

HOMO: 30. 9 e -0.06891287 H = -1.87522 eV

LUMO: 31. 16 a1 +0.15096542 H = +4.10798 eV

Gap : +0.21987830 H = +5.98320 eV

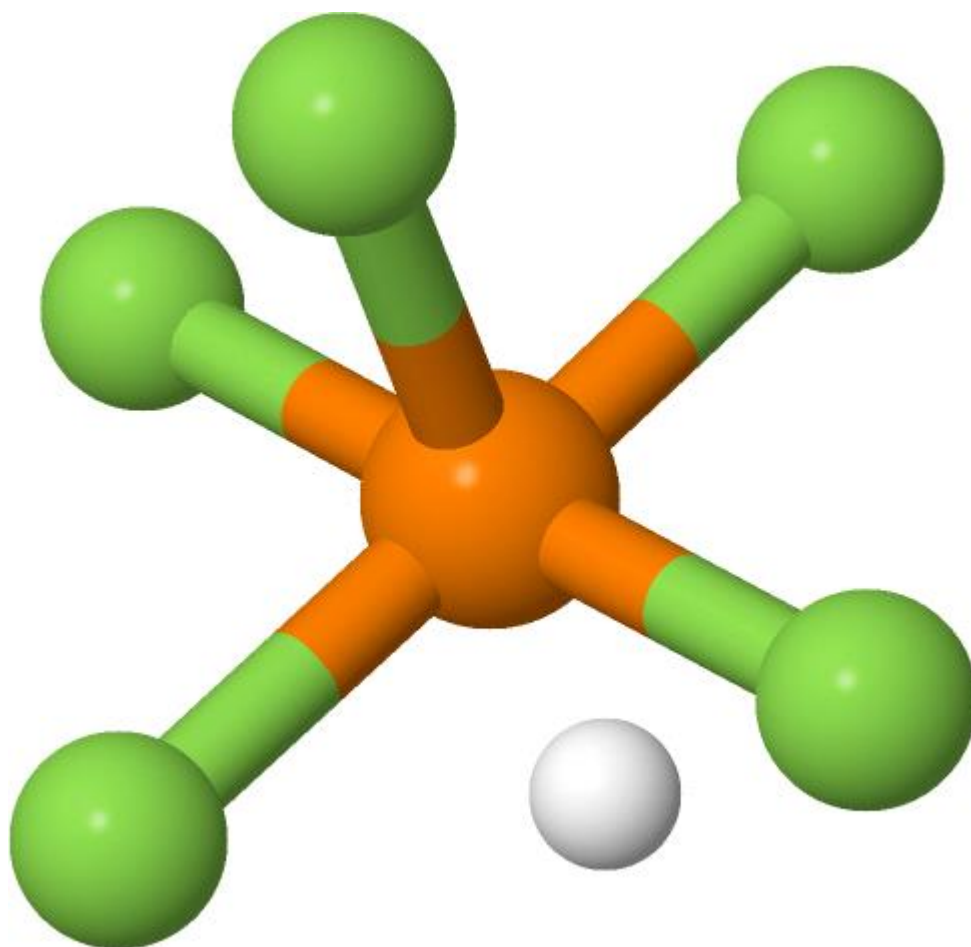
Number of MOs= 81, Electrons= 78.00, Symmetry: c4v

\$coord
0.0000000000000000 0.0000000000000000 0.56651612350433 p
196

-2.20211177352107	2.20211177352107	0.53287693083336	f
-2.20211177352107	-2.20211177352107	0.53287693083336	f
2.20211177352107	-2.20211177352107	0.53287693083336	f
2.20211177352107	2.20211177352107	0.53287693083336	f
0.000000000000000	0.000000000000000	3.68660998398681	f
0.000000000000000	0.000000000000000	-3.61272909364374	cl

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	e		218.20	0.24862	YES	YES
8	e		218.20	0.24862	YES	YES
9	b2		270.70	0.00000	NO	YES
10	a1		301.69	29.90658	YES	YES
11	e		369.57	0.36077	YES	YES
12	e		369.57	0.36077	YES	YES
13	b1		435.08	0.00000	NO	YES
14	e		495.76	21.41887	YES	YES
15	e		495.76	21.41887	YES	YES
16	a1		507.70	95.61353	YES	YES
17	b2		587.62	0.00000	NO	YES
18	a1		665.44	7.64245	YES	YES
19	a1		794.38	418.36906	YES	YES
20	e		903.89	349.56529	YES	YES
21	e		903.89	349.56529	YES	YES



Total energy = -840.9236781914 H = -22882.7105767 eV

HOMO-LUMO Separation

HOMO: 24. 11 a1 -0.06895026 H = -1.87623 eV

LUMO: 25. 12 a1 +0.22311404 H = +6.07125 eV

Gap : +0.29206430 H = +7.94748 eV

Number of MOs= 69, Electrons= 62.00, Symmetry: c4v

Total energy = -840.9236781914 H = -22882.7105767 eV

HOMO-LUMO Separation

HOMO: 24. 11 a1 -0.06895026 H = -1.87623 eV

LUMO: 25. 12 a1 +0.22311404 H = +6.07125 eV

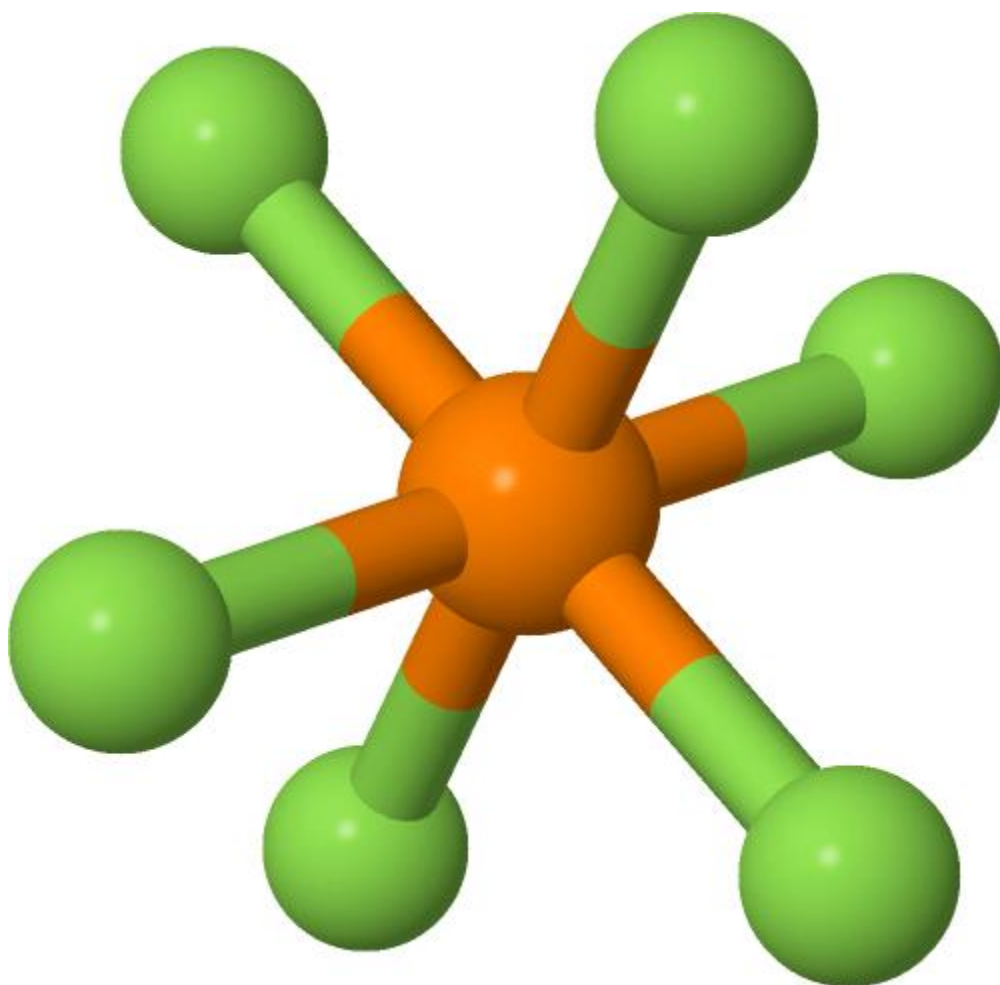
Gap : +0.29206430 H = +7.94748 eV

Number of MOs= 69, Electrons= 62.00, Symmetry: c4v

```
$coord
0.0000000000000000 0.0000000000000000 0.46364145783169 p
0.0000000000000000 0.0000000000000000 -2.67436422528472 f
0.0000000000000000 3.16159440965303 0.43754886873233 f
0.0000000000000000 -3.16159440965303 0.43754886873233 f
-3.16159440965303 0.0000000000000000 0.43754886873233 f
3.16159440965303 0.0000000000000000 0.43754886873233 f
0.0000000000000000 0.0000000000000000 3.17171126141158 h
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 b1 260.72 0.00000 NO YES
8 e 310.07 0.32035 YES YES
9 e 310.07 0.32035 YES YES
10 b2 406.25 0.00000 NO YES
11 e 469.82 10.53701 YES YES
12 e 469.82 10.53701 YES YES
13 a1 526.54 26.46732 YES YES
14 b1 553.80 0.00000 NO YES
15 a1 610.68 11.19539 YES YES
16 a1 790.53 215.60575 YES YES
17 e 844.23 383.17277 YES YES
18 e 844.23 383.17277 YES YES
19 e 1160.55 93.14417 YES YES
20 e 1160.55 93.14417 YES YES
21 a1 2274.47 291.33995 YES YES
```

PF₅F⁻



Total energy = -940.1540447847 H = -25582.9077743 eV

HOMO-LUMO Separation

HOMO: 27. 1 a_{2g} -0.09824182 H = -2.67330 eV

LUMO: 28. 9 a_{1g} +0.22526865 H = +6.12988 eV

Gap : +0.32351047 H = +8.80317 eV

Number of MOs= 78, Electrons= 70.00, Symmetry: d_{4h}

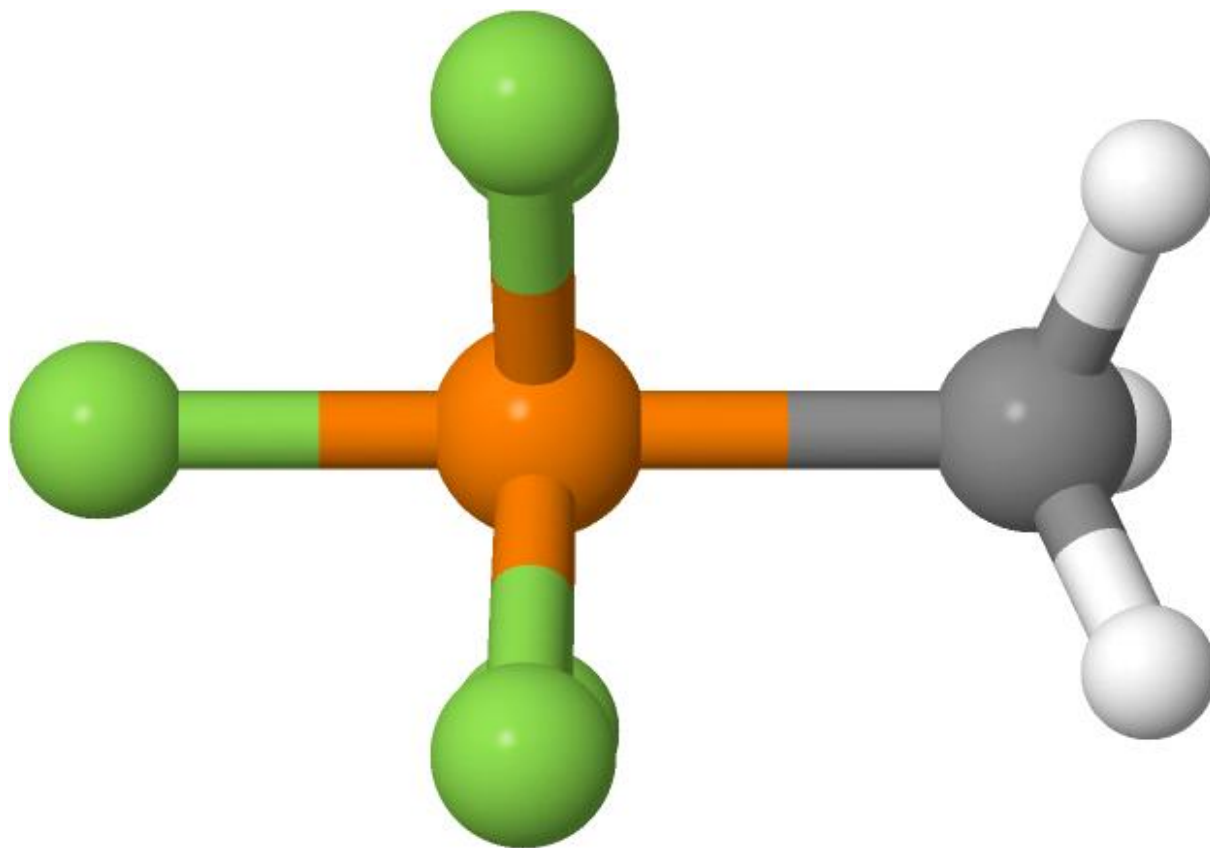
\$coord

0.0000000000000000	0.0000000000000000	0.0000000000000000	p
2.20910111969793	2.20910111969793	0.0000000000000000	f
-2.20910111969793	2.20910111969793	0.0000000000000000	f
-2.20910111969793	-2.20910111969793	0.0000000000000000	f
2.20910111969793	-2.20910111969793	0.0000000000000000	f
0.0000000000000000	0.0000000000000000	3.12429285766013	f
0.0000000000000000	0.0000000000000000	-3.12429285766013	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	b1u		288.91	0.00000	NO	NO
8	eu		290.65	0.00706	YES	NO
9	eu		290.65	0.00706	YES	NO
10	eg		430.42	0.00000	NO	YES
11	eg		430.42	0.00000	NO	YES
12	b1g		433.02	0.00000	NO	YES
13	a2u		525.01	26.56235	YES	NO
14	eu		526.54	26.20983	YES	NO
15	eu		526.54	26.20983	YES	NO
16	alg		581.99	0.00000	NO	YES
17	b2g		583.10	0.00000	NO	YES
18	alg		698.91	0.00000	NO	YES
19	a2u		900.90	405.80812	YES	NO
20	eu		904.16	406.25961	YES	NO
21	eu		904.16	406.25961	YES	NO

PF₅Me⁻



Total energy = -880.2145902005 H = -23951.8712998 eV

HOMO-LUMO Separation

HOMO: 35. 22 a' -0.07669243 H = -2.08691 eV

LUMO: 36. 23 a' +0.21327140 H = +5.80341 eV

Gap : +0.28996383 H = +7.89032 eV

Number of MOs= 108, Electrons= 70.00, Symmetry: cs

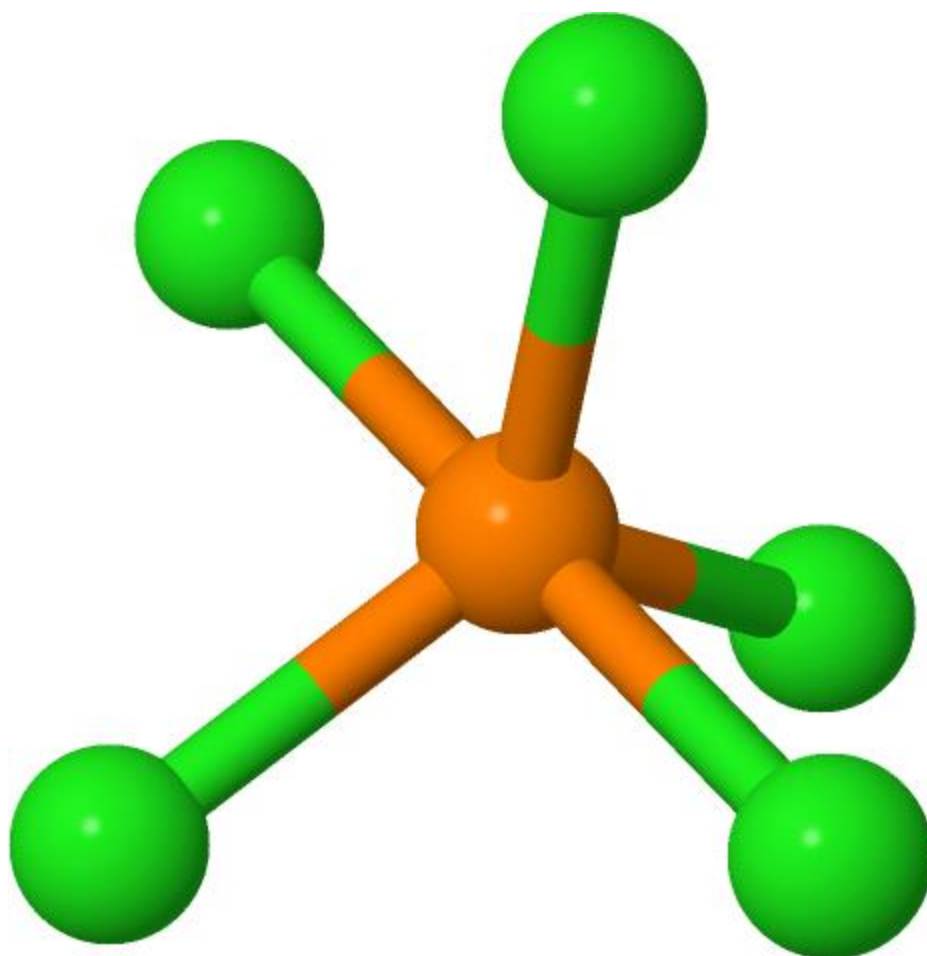
\$coord			
-0.05692567033972	-0.03931965283828	0.00000000000000	p
2.67425917289532	1.52265065467711	0.00000000000000	f

-1.10250718239643	1.93614331932020	-2.25244463818262	f
1.12091062742787	-1.95774524406887	2.23059398010503	f
1.12091062742787	-1.95774524406887	-2.23059398010503	f
-1.10250718239643	1.93614331932020	2.25244463818262	f
-3.18017762683984	-1.72140284636978	0.00000000000000	c
-3.36014445170875	-2.92675759626374	-1.70908049961057	h
-4.73354668684704	-0.31057235201314	0.00000000000000	h
-3.36014445170875	-2.92675759626374	1.70908049961057	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a''	41.19	0.02041	YES	YES
8		a'	258.68	0.10331	YES	YES
9		a''	268.37	0.09107	YES	YES
10		a''	285.51	0.00002	YES	YES
11		a'	378.36	0.65968	YES	YES
12		a''	381.88	0.76604	YES	YES
13		a'	402.94	0.03396	YES	YES
14		a'	477.49	11.07577	YES	YES
15		a''	477.70	11.49418	YES	YES
16		a'	517.42	41.49991	YES	YES
17		a'	542.51	4.15213	YES	YES
18		a''	548.30	0.03524	YES	YES
19		a'	648.32	0.13115	YES	YES
20		a''	798.17	193.59853	YES	YES
21		a'	798.91	185.86026	YES	YES
22		a'	838.46	370.25152	YES	YES
23		a'	922.93	174.95250	YES	YES
24		a''	923.09	165.95171	YES	YES
25		a'	1251.55	21.14059	YES	YES
26		a''	1410.19	0.40105	YES	YES
27		a'	1417.20	0.29691	YES	YES
28		a'	2950.33	20.05216	YES	YES
29		a''	3049.81	38.21894	YES	YES
30		a'	3051.31	36.50564	YES	YES

PCl₅



Total energy = -2641.8651644240 H = -71888.8497352 eV

HOMO-LUMO Separation

HOMO: 36. 4 e" -0.26535683 H = -7.22073 eV

LUMO: 37. 13 a1' -0.17403995 H = -4.73587 eV

Gap : +0.09131688 H = +2.48486 eV

Number of MOs= 75, Electrons= 100.00, Symmetry: d3h


```

$coord
  0.0000000000000000  0.0000000000000000 -4.08790281089642 c1
  0.0000000000000000  0.0000000000000000  0.0000000000000000 p
-1.96569823765703    3.40468921997058    0.0000000000000000 c1
  0.0000000000000000  0.0000000000000000  4.08790281089642 c1
-1.96569823765703   -3.40468921997058    0.0000000000000000 c1
  3.93139647531407    0.0000000000000000  0.0000000000000000 c1

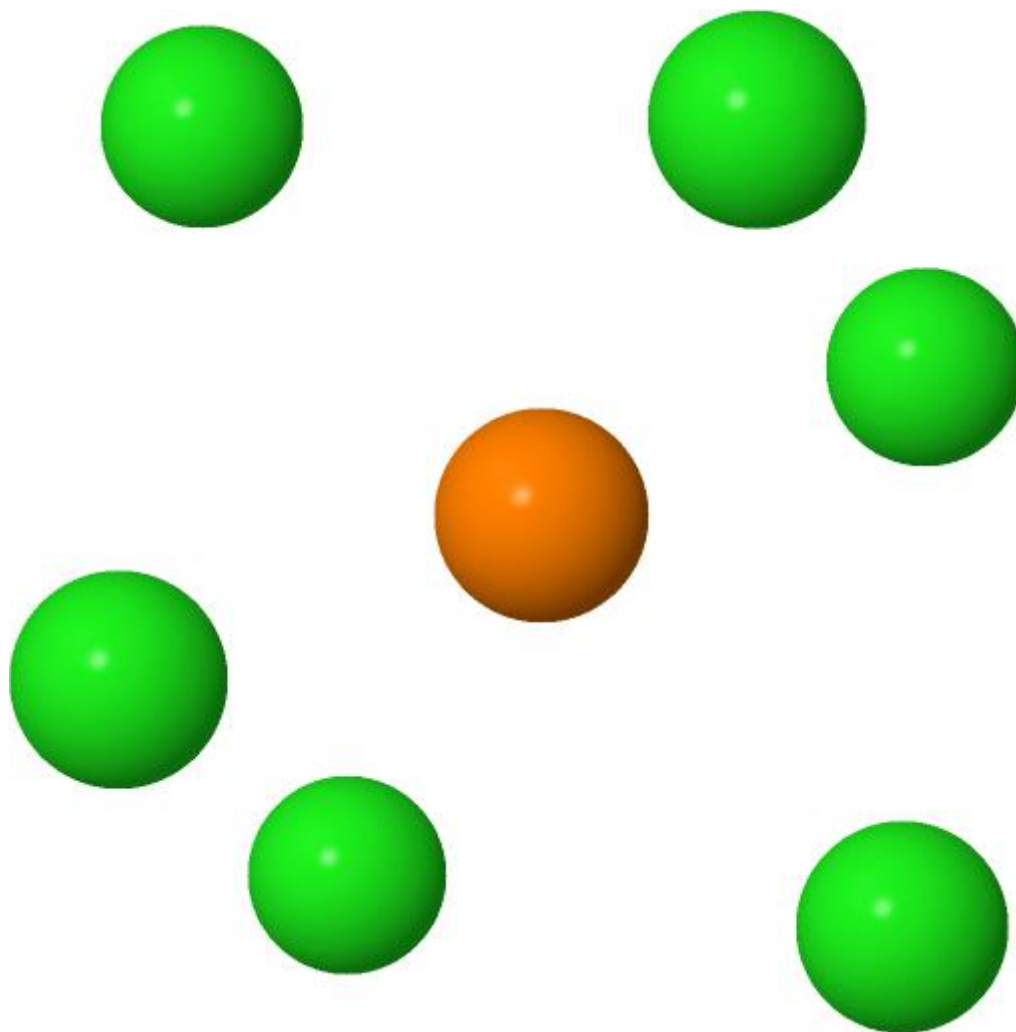
```

```

$vibrational spectrum
# mode      symmetry  wave number  IR intensity  selection rules
#                               cm** (-1)      km/mol        IR      RAMAN
  1              0.00      0.00000
  2              0.00      0.00000
  3              0.00      0.00000
  4              0.00      0.00000
  5              0.00      0.00000
  6              0.00      0.00000
  7             e'      80.58      0.49728      YES      YES
  8             e'      80.58      0.49728      YES      YES
  9             e"     240.91      0.00000      NO       YES
 10             e"     240.91      0.00000      NO       YES
 11             e'     252.79      2.39185      YES      YES
 12             e'     252.79      2.39185      YES      YES
 13            a1'     267.63      0.00000      NO       YES
 14            a2"     280.24      5.67370      YES      NO
 15            a1'     356.71      0.00000      NO       YES
 16            a2"     446.90     296.45732      YES      NO
 17             e'     532.67     168.27394      YES      YES
 18             e'     532.67     168.27394      YES      YES
$end

```

PCl₅Cl⁻



Total energy = -3102.0925130020 H = -84412.2802083 eV

HOMO-LUMO Separation

HOMO: 59. 59 a -0.08256512 H = -2.24671 eV

LUMO: 60. 60 a -0.01150271 H = -0.31300 eV

Gap : +0.07106242 H = +1.93371 eV

Number of MOs= 126, Electrons= 118.00, Symmetry: c1

```

$coord
  0.06440479690209   -2.74788502138460    1.25980020273893   cl
  1.80299207107689    0.57744608718687   -0.55316797604184    p
  4.99928513600603   -1.77980752293030   -1.81487538861234   cl
  3.54117170241422    3.90278477477610   -2.36619456953135   cl
 -0.23058536862153   -0.28602892917969   -4.08557695618660   cl
 -1.39369255773388    2.93474437414330    0.70852713014406   cl
  3.83620425527588    1.44087041874958    2.97924975476482   cl

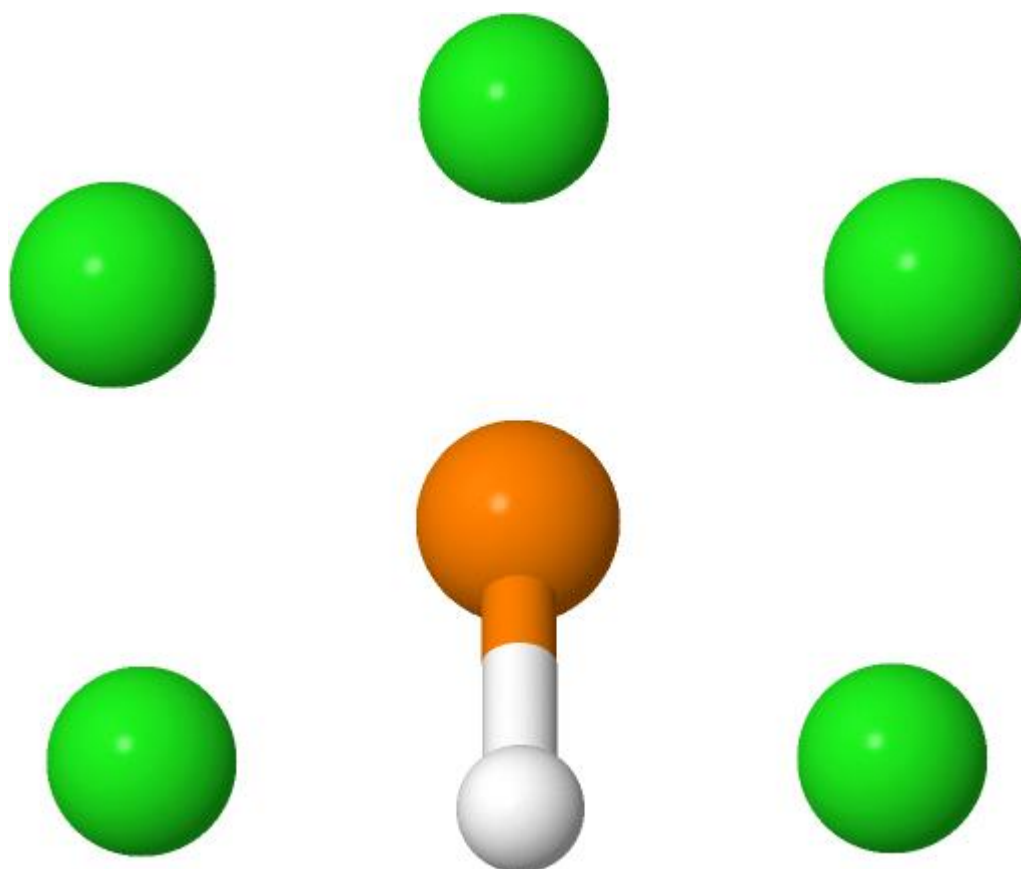
```

```

$vibrational spectrum
#  mode      symmetry  wave number  IR intensity  selection rules
#                               cm** (-1)      km/mol        IR          RAMAN
  1              0.00      0.00000      -          -
  2              0.00      0.00000      -          -
  3              0.00      0.00000      -          -
  4              0.00      0.00000      -          -
  5              0.00      0.00000      -          -
  6              0.00      0.00000      -          -
  7              a      143.55      0.00001     YES        YES
  8              a      143.73      0.00013     YES        YES
  9              a      143.94      0.00035     YES        YES
 10              a      209.91      0.00000     YES        YES
 11              a      210.06      0.00000     YES        YES
 12              a      210.17      0.00000     YES        YES
 13              a      240.09      0.00002     YES        YES
 14              a      240.41      0.00001     YES        YES
 15              a      250.35      0.00023     YES        YES
 16              a      250.46      0.00040     YES        YES
 17              a      250.90      0.00037     YES        YES
 18              a      311.63      0.00003     YES        YES
 19              a      423.93      291.20978   YES        YES
 20              a      424.66      291.00626   YES        YES
 21              a      425.34      291.04102   YES        YES

```

PCl_5H^-



Total energy = -2642.5649034710 H = -71907.8906143 eV

HOMO-LUMO Separation

HOMO: 51. 51 a -0.06965545 H = -1.89542 eV

LUMO: 52. 52 a +0.01720626 H = +0.46821 eV

Gap : +0.08686171 H = +2.36363 eV

Number of MOs= 110, Electrons= 102.00, Symmetry: c1

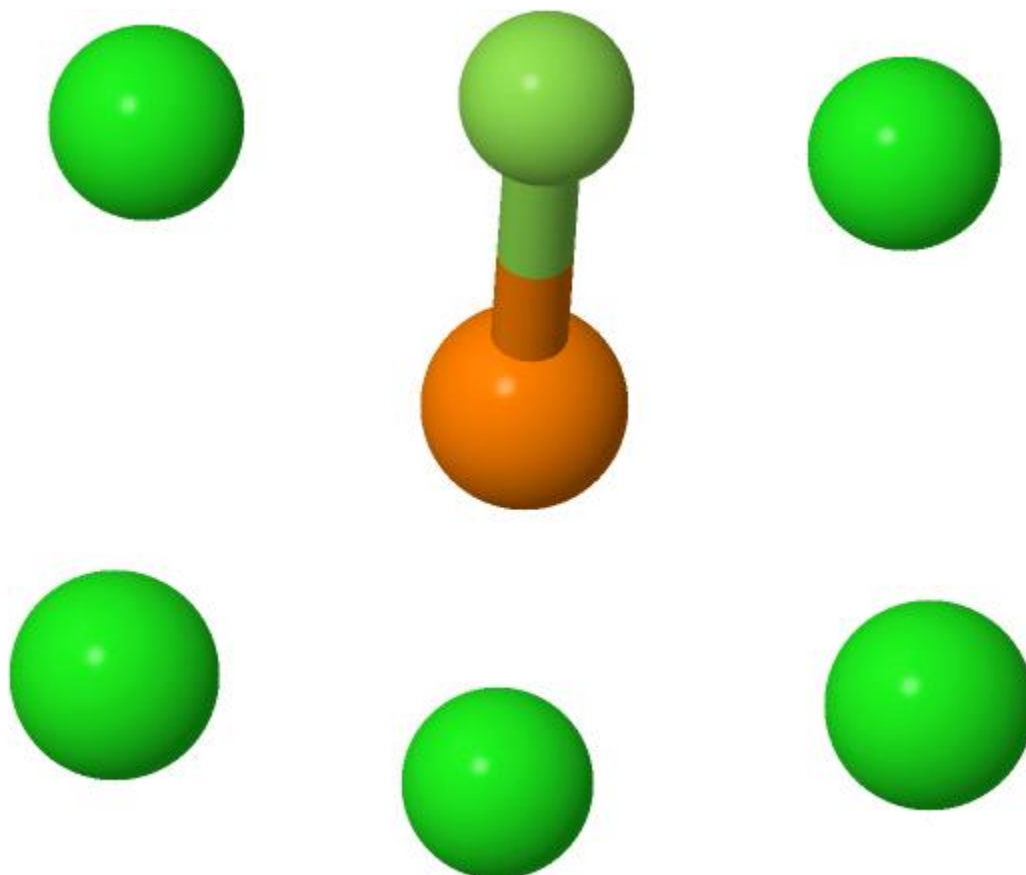
```
$coord
0.34403312354663 -2.63202202566369 1.75566095440838 c1
1.89156876370969 0.61755837234537 -0.42371856518768 p
```

5.07731462780740	-1.78932205236544	-1.74727717627921	c1
3.53135017586054	3.90813723437441	-2.46993342935026	c1
-0.38345836749277	-0.42011393197629	-3.74492942726738	c1
-1.20032615484059	3.06921600239158	1.03559199263656	c1
3.35929786672884	1.28867058225539	1.72236784831526	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	123.16	0.00008	YES	YES
8		a	156.94	0.00326	YES	YES
9		a	157.01	0.00229	YES	YES
10		a	201.61	0.00022	YES	YES
11		a	223.76	0.67750	YES	YES
12		a	223.78	0.67566	YES	YES
13		a	236.03	0.00148	YES	YES
14		a	241.05	1.47494	YES	YES
15		a	279.26	16.24688	YES	YES
16		a	393.18	102.39770	YES	YES
17		a	407.64	335.02364	YES	YES
18		a	408.03	335.29323	YES	YES
19		a	941.83	72.22400	YES	YES
20		a	943.54	72.20404	YES	YES
21		a	2366.71	36.50404	YES	YES

PCl₅F⁻



Total energy = -2741.7680952050 H = -74607.3483459 eV

HOMO-LUMO Separation

HOMO: 55. 55 a -0.07645622 H = -2.08048 eV

LUMO: 56. 56 a +0.00983058 H = +0.26750 eV

Gap : +0.08628680 H = +2.34798 eV

Number of MOs= 122, Electrons= 110.00, Symmetry: c1

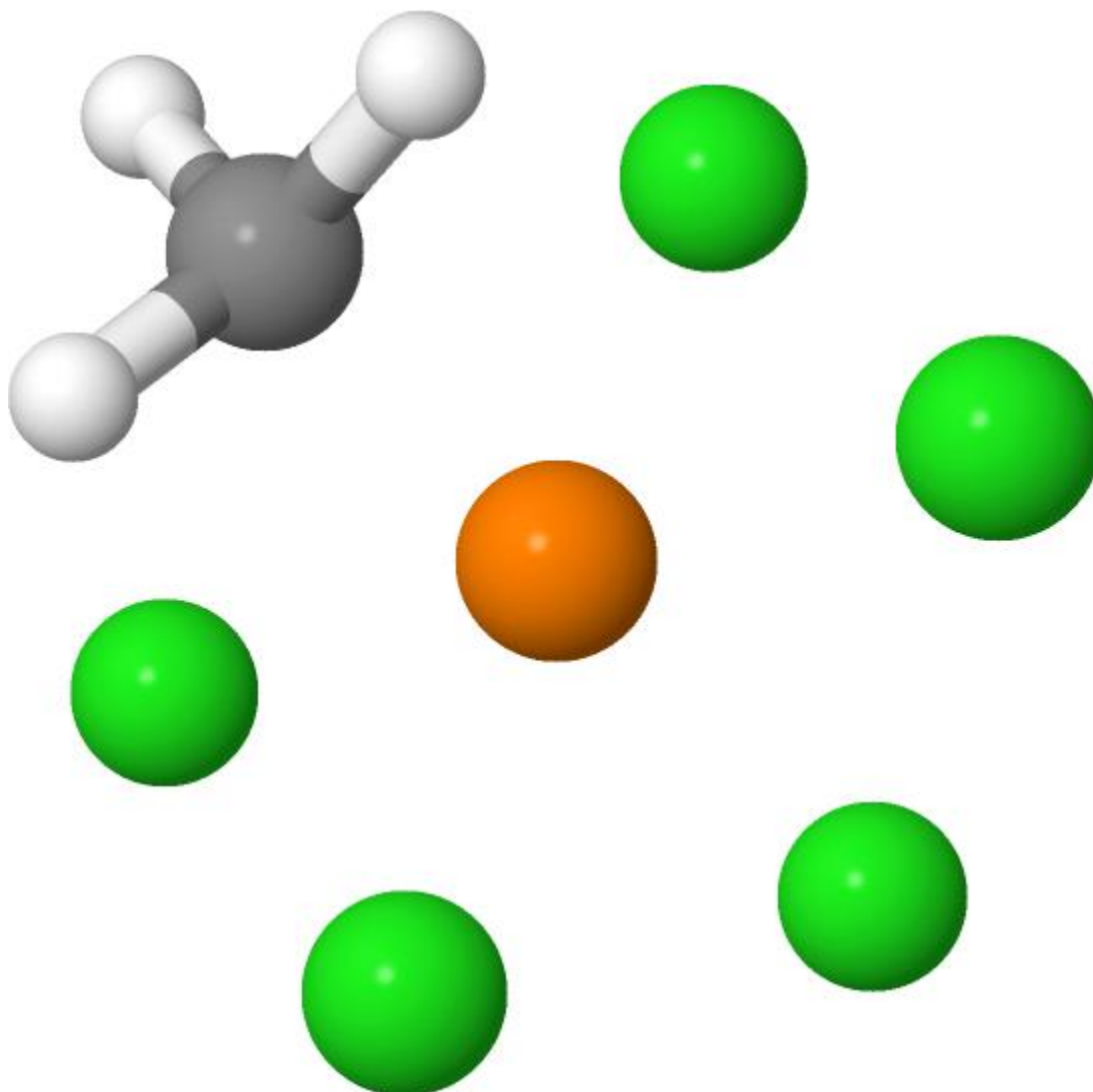
\$coord
0.25638086940060 -2.65341860646472 1.57828164831229 c1

1.87675440568066	0.61052924611194	-0.43992449863714	p
5.02628132009746	-1.77087958378667	-1.76298575201022	cl
3.51932389921359	3.88372681336555	-2.42143856310387	cl
-0.32418015533321	-0.37132937202591	-3.83725160224414	cl
-1.25060346983475	3.00159233127628	0.92050800969887	cl
3.51563419348283	1.34228129810982	2.09057295525988	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	137.72	0.00020	YES	YES
8		a	158.56	0.00550	YES	YES
9		a	158.89	0.01080	YES	YES
10		a	213.29	0.00006	YES	YES
11		a	228.32	0.00266	YES	YES
12		a	228.51	0.00201	YES	YES
13		a	240.81	0.00055	YES	YES
14		a	250.86	2.48122	YES	YES
15		a	281.17	15.26444	YES	YES
16		a	324.10	6.16279	YES	YES
17		a	324.72	6.64053	YES	YES
18		a	351.68	39.82489	YES	YES
19		a	451.75	358.30327	YES	YES
20		a	452.27	357.87473	YES	YES
21		a	777.24	199.25072	YES	YES

PCl₅Me⁻



Total energy = -2681.8504609100 H = -72976.9056320 eV

HOMO-LUMO Separation

HOMO: 55. 55 a -0.07081913 H = -1.92709 eV

LUMO: 56. 56 a +0.01614507 H = +0.43933 eV

Gap : +0.08696421 H = +2.36642 eV

Number of MOs= 128, Electrons= 110.00, Symmetry: c1

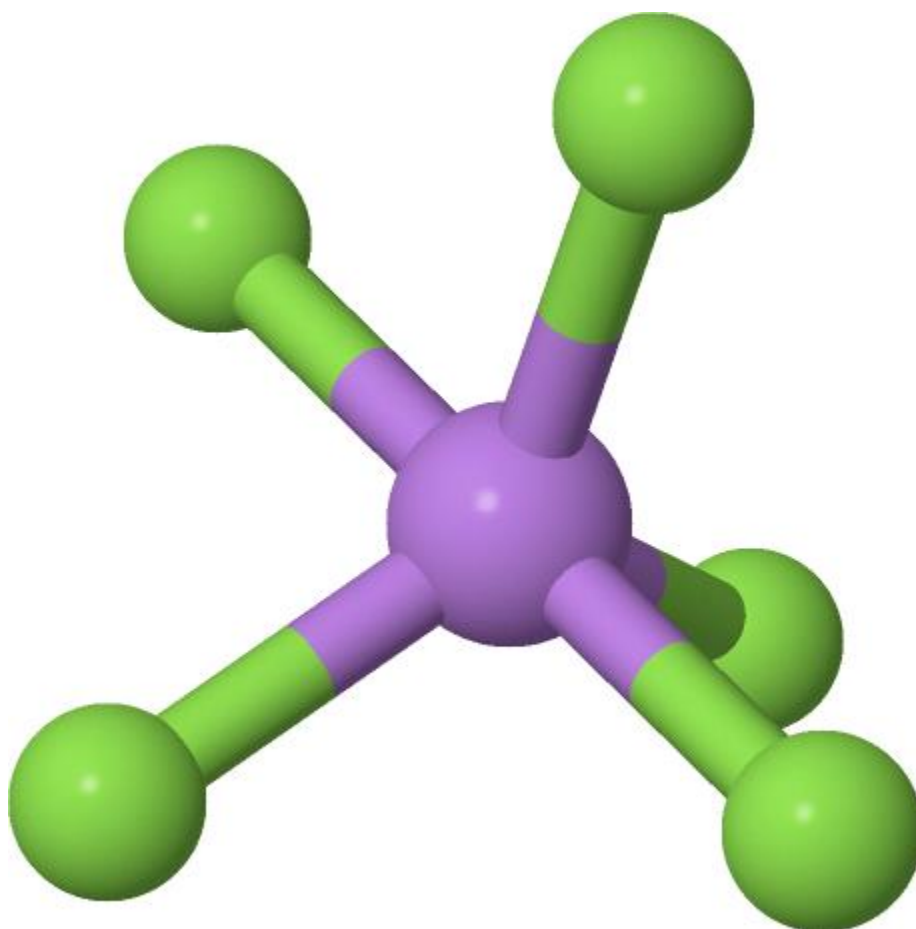
\$coord

-0.45210463257213	-3.08302839922531	0.99991008823729	c1
1.48657081263979	0.43847925332003	-0.35527222294802	p
4.89493876996422	-1.85672140665580	-1.43743639427207	c1
3.41668160870716	3.90604258396688	-1.88407525827468	c1
-0.09409506486164	-0.25900116907733	-4.18307832734102	c1
-1.94706851197921	2.75809014178864	0.55255507162945	c1
2.73923825292605	1.01039054175447	2.94897645606858	c
4.26532962751741	-0.37721241308816	3.30300995582270	h
1.14248472684311	0.73587571779508	4.27092243207293	h
3.46153730542611	2.97319691036284	3.02648562781777	h

\$vibrational spectrum

#	mode	symmetry	wave number cm**(-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	27.92	1.04855	YES	YES
8		a	142.74	0.00167	YES	YES
9		a	146.15	0.03696	YES	YES
10		a	154.77	0.20524	YES	YES
11		a	192.15	0.00985	YES	YES
12		a	222.75	1.11091	YES	YES
13		a	225.96	1.38821	YES	YES
14		a	231.31	0.75924	YES	YES
15		a	237.72	10.29745	YES	YES
16		a	265.25	6.71931	YES	YES
17		a	302.83	0.50957	YES	YES
18		a	316.88	0.11693	YES	YES
19		a	358.78	69.13546	YES	YES
20		a	379.99	281.98794	YES	YES
21		a	381.67	282.81127	YES	YES
22		a	649.97	61.65910	YES	YES
23		a	886.91	53.43409	YES	YES
24		a	890.68	50.65751	YES	YES
25		a	1214.35	6.99116	YES	YES
26		a	1380.75	1.94222	YES	YES
27		a	1401.88	1.63693	YES	YES
28		a	2978.33	8.84647	YES	YES
29		a	3102.71	4.51860	YES	YES
30		a	3107.87	3.92755	YES	YES

AsF₅



Total energy = -2734.7773956860 H = -74417.1216250 eV

HOMO-LUMO Separation

HOMO: 28. 3 e" -0.36401497 H = -9.90536 eV

LUMO: 29. 11 a1' -0.15521427 H = -4.22360 eV

Gap : +0.20880070 H = +5.68176 eV

Number of MOs= 70, Electrons= 78.00, Symmetry: d3h

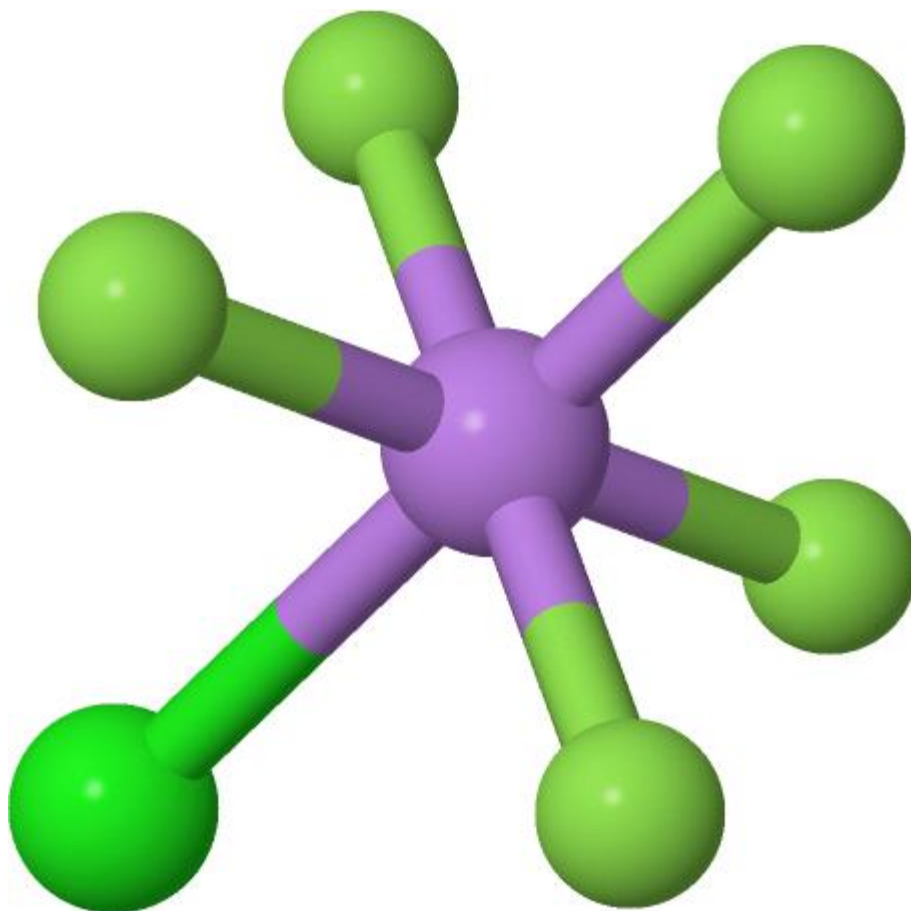
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$coord
0.0000000000000000 0.0000000000000000 0.0000000000000000 as
0.0000000000000000 0.0000000000000000 3.28211704458301 f
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3.25162921666207	0.000000000000000	0.000000000000000	f
0.000000000000000	0.000000000000000	-3.28211704458301	f
-1.62581460833104	2.81599350531705	0.000000000000000	f
-1.62581460833104	-2.81599350531705	0.000000000000000	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e'	114.76	0.69959	YES	YES
8		e'	114.76	0.69959	YES	YES
9		e'	338.10	38.32508	YES	YES
10		e'	338.10	38.32508	YES	YES
11		e''	351.13	0.00000	NO	YES
12		e''	351.13	0.00000	NO	YES
13		a2''	371.53	47.62463	YES	NO
14		a1'	622.66	0.00000	NO	YES
15		a1'	666.85	0.00000	NO	YES
16		a2''	749.02	131.35908	YES	NO
17		e'	756.21	103.11295	YES	YES
18		e'	756.21	103.11295	YES	YES

AsF₅Cl⁻



Total energy = -3195.0326299880 H = -86941.3109077 eV

HOMO-LUMO Separation

HOMO: 37. 11 e -0.09027890 H = -2.45662 eV

LUMO: 38. 19 a1 +0.07708499 H = +2.09759 eV

Gap : +0.16736389 H = +4.55421 eV

Number of MOs= 92, Electrons= 96.00, Symmetry: c4v

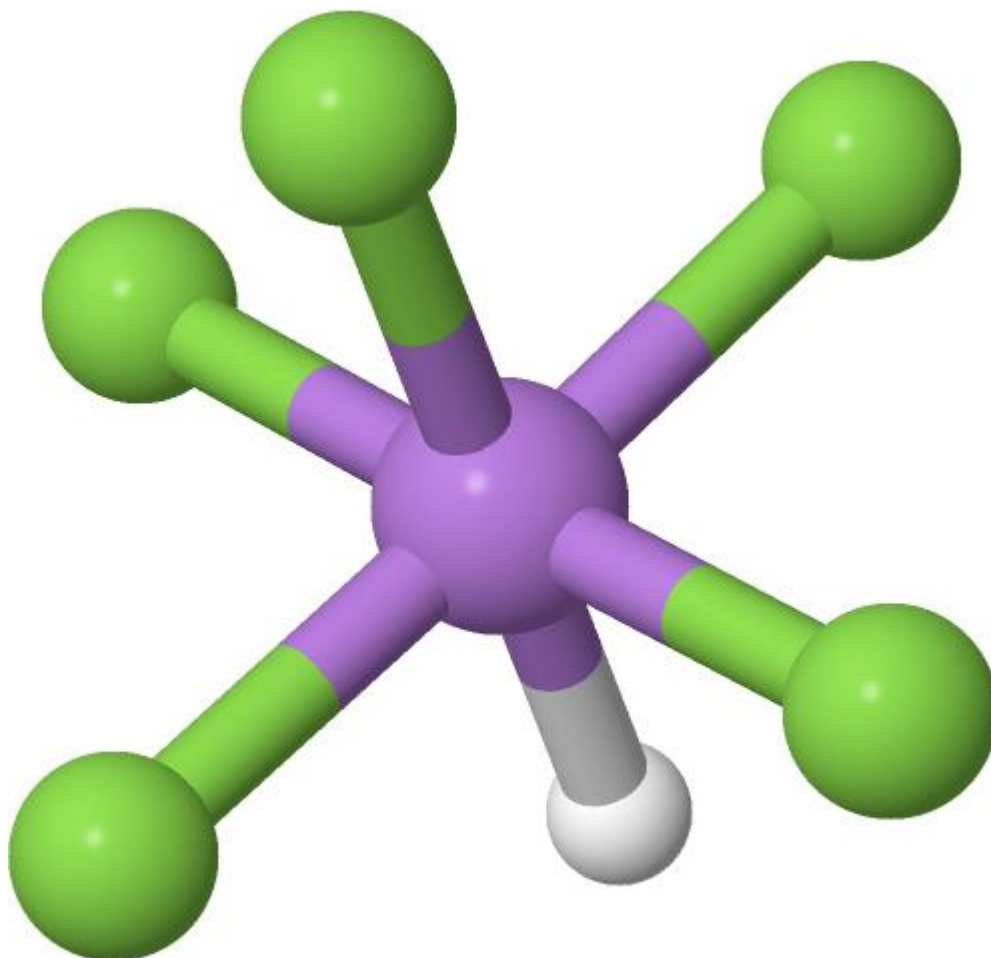
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$coord
0.0000000000000000 0.0000000000000000 -0.43331751884795 as
0.0000000000000000 0.0000000000000000 -3.77272286076037 f
3.35555921940014 0.0000000000000000 -0.43808145311548 f
```

0.0000000000000000	0.0000000000000000	3.87645408099356	c1
0.0000000000000000	3.3555921940014	-0.43808145311548	f
-3.3555921940014	0.0000000000000000	-0.43808145311548	f
0.0000000000000000	-3.3555921940014	-0.43808145311548	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	171.36	0.19812	YES	YES
8		e	171.36	0.19812	YES	YES
9		b1	208.61	0.00000	NO	YES
10		e	283.33	3.50802	YES	YES
11		e	283.33	3.50802	YES	YES
12		a1	309.08	11.39395	YES	YES
13		b2	329.94	0.00000	NO	YES
14		e	360.01	30.50176	YES	YES
15		e	360.01	30.50176	YES	YES
16		a1	368.11	123.10493	YES	YES
17		b1	562.21	0.00000	NO	YES
18		a1	592.78	3.51338	YES	YES
19		a1	653.72	131.31476	YES	YES
20		e	680.17	158.47829	YES	YES
21		e	680.17	158.47829	YES	YES

AsF₅H⁻



Total energy = -2735.4771268630 H = -74436.1622899 eV

HOMO-LUMO Separation

HOMO: 31. 14 a1 -0.08997266 H = -2.44828 eV

LUMO: 32. 15 a1 +0.13753991 H = +3.74265 eV

Gap : +0.22751257 H = +6.19094 eV

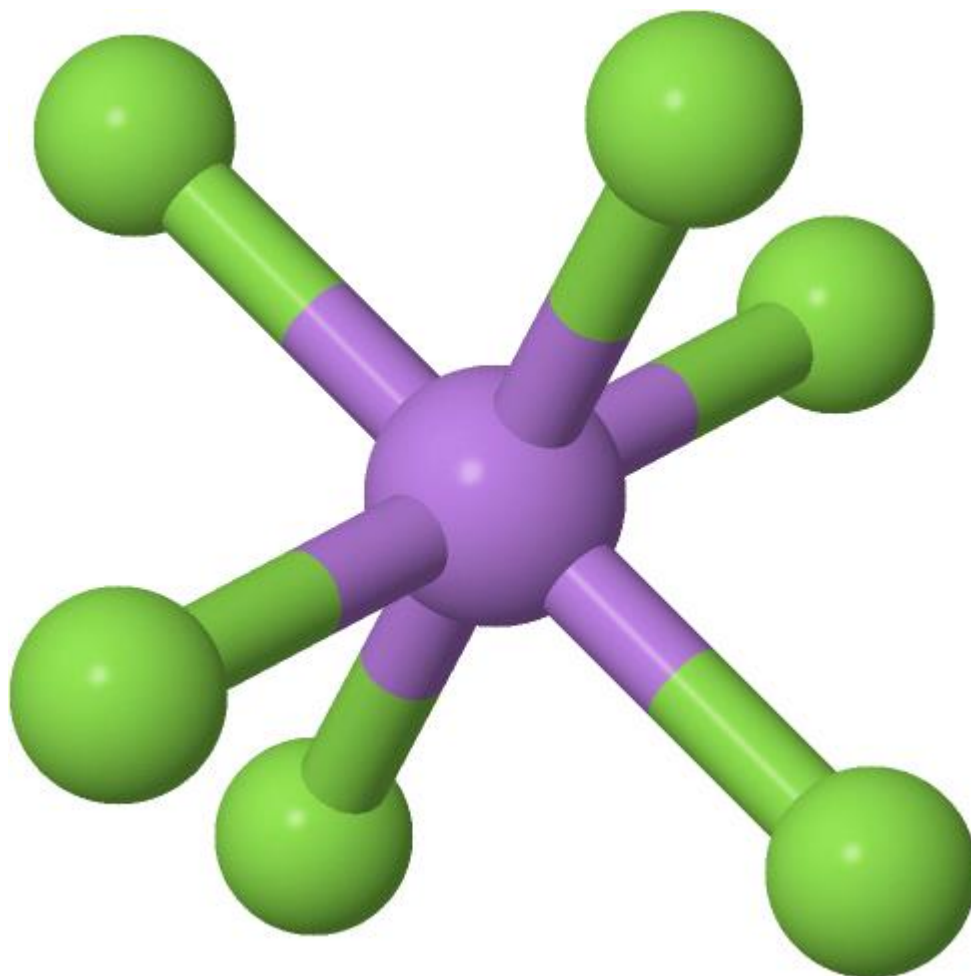
Number of MOs= 80, Electrons= 80.00, Symmetry: c4v

\$coord
0.0000000000000000 0.0000000000000000 0.38239836163687 as

0.0000000000000000	0.0000000000000000	-2.97547073022714	f
0.0000000000000000	3.39657345858529	0.32313422639753	f
0.0000000000000000	-3.39657345858529	0.32313422639753	f
-3.39657345858529	0.0000000000000000	0.32313422639753	f
3.39657345858529	0.0000000000000000	0.32313422639753	f
0.0000000000000000	0.0000000000000000	3.29687677487597	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		b1	199.63	0.00000	NO	YES
8		e	231.97	1.88336	YES	YES
9		e	231.97	1.88336	YES	YES
10		b2	315.49	0.00000	NO	YES
11		e	351.02	20.67164	YES	YES
12		e	351.02	20.67164	YES	YES
13		a1	371.77	58.11589	YES	YES
14		b1	536.84	0.00000	NO	YES
15		a1	564.28	4.28553	YES	YES
16		a1	641.39	83.04114	YES	YES
17		e	645.63	205.79303	YES	YES
18		e	645.63	205.79303	YES	YES
19		e	952.99	53.81997	YES	YES
20		e	952.99	53.81997	YES	YES
21		a1	2082.31	199.31364	YES	YES



Total energy = -2834.6943201780 H = -77136.0010241 eV

HOMO-LUMO Separation

HOMO: 20. 1 t1g -0.11575310 H = -3.14980 eV

LUMO: 21. 7 a1g +0.11511864 H = +3.13254 eV

Gap : +0.23087174 H = +6.28234 eV

Number of MOs= 51, Electrons= 88.00, Symmetry: oh

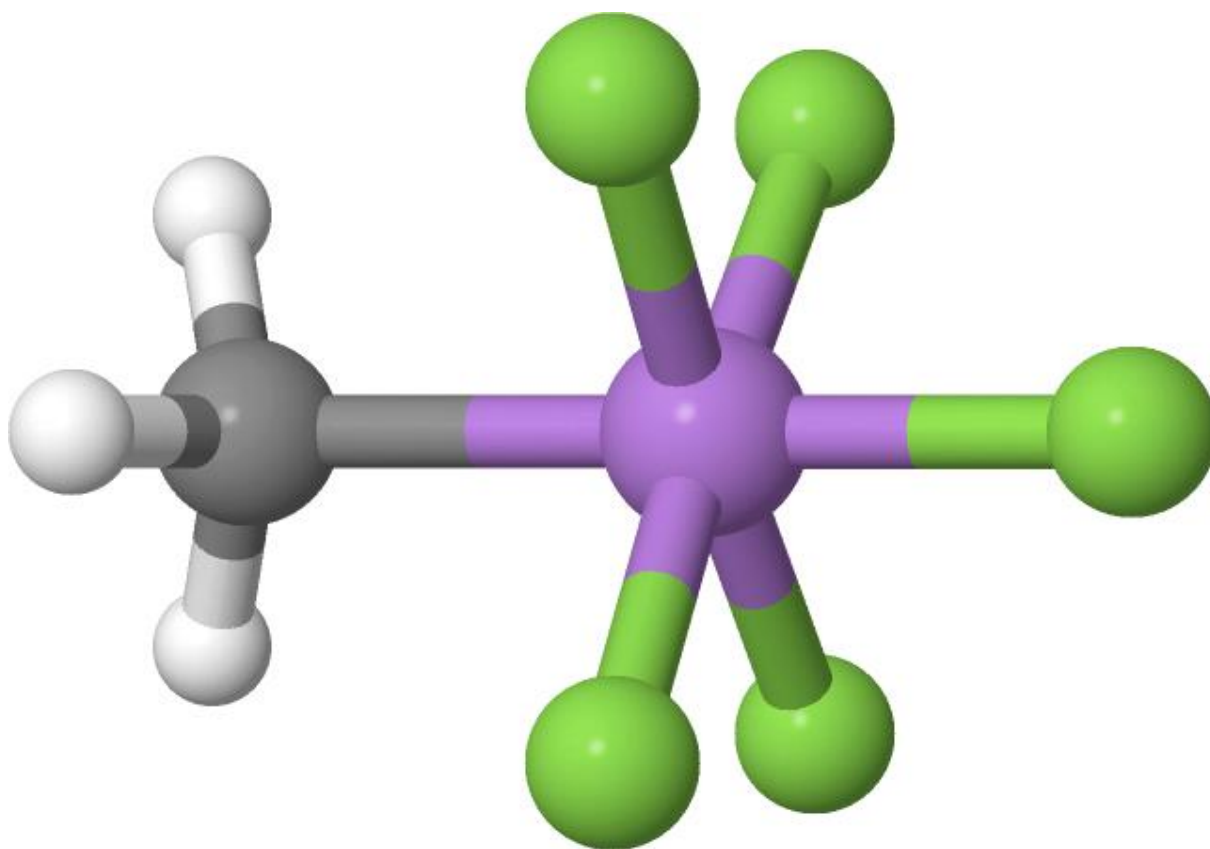
\$coord

0.0000000000000000	0.0000000000000000	0.0000000000000000	as
3.35279407395715	0.0000000000000000	0.0000000000000000	f
0.0000000000000000	0.0000000000000000	-3.35279407395715	f
-3.35279407395715	0.0000000000000000	0.0000000000000000	f
0.0000000000000000	-3.35279407395715	0.0000000000000000	f
0.0000000000000000	0.0000000000000000	3.35279407395715	f
0.0000000000000000	3.35279407395715	0.0000000000000000	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	t2u		214.13	0.00000	NO	NO
8	t2u		214.13	0.00000	NO	NO
9	t2u		214.13	0.00000	NO	NO
10	t2g		331.95	0.00000	NO	YES
11	t2g		331.95	0.00000	NO	YES
12	t2g		331.95	0.00000	NO	YES
13	t1u		373.80	48.80969	YES	NO
14	t1u		373.80	48.80969	YES	NO
15	t1u		373.80	48.80969	YES	NO
16	eg		563.54	0.00000	NO	YES
17	eg		563.54	0.00000	NO	YES
18	alg		623.92	0.00000	NO	YES
19	t1u		684.14	174.15058	YES	NO
20	t1u		684.14	174.15058	YES	NO
21	t1u		684.14	174.15058	YES	NO

AsF₅Me⁻



Total energy = -2774.7697506190 H = -75505.3695920 eV

HOMO-LUMO Separation

HOMO: 44. 28 a' -0.08920779 H = -2.42747 eV

LUMO: 45. 29 a' +0.14185512 H = +3.86008 eV

Gap : +0.23106292 H = +6.28755 eV

Number of MOs= 122, Electrons= 88.00, Symmetry: cs

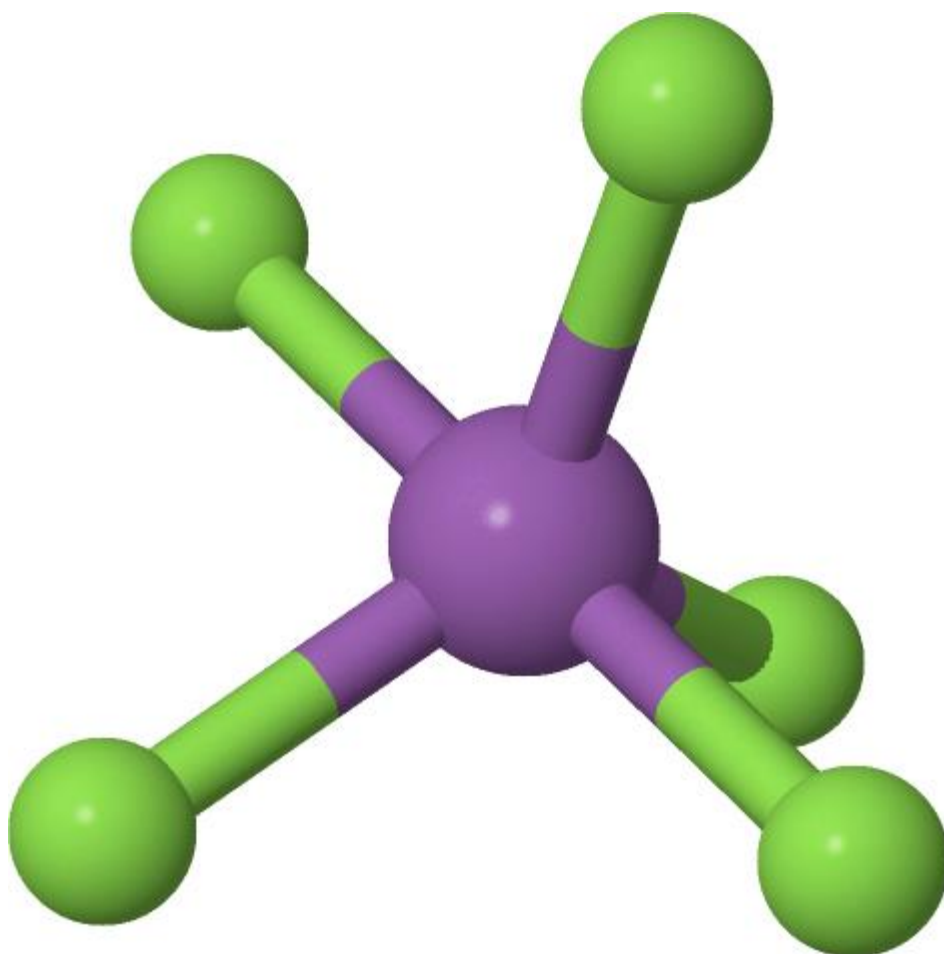
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$coord
  0.03313089187617    0.06363188358114    0.000000000000000    as
 -1.68355466384085   -2.82648405736923    0.000000000000000    f
  2.04327537615389   -1.24882065809653   -2.42071102331427    f
 -2.09570691570980    1.21390141660026    2.39935376103455    f
 -2.09570691570980    1.21390141660026   -2.39935376103455    f
```

2.04327537615389	-1.24882065809653	2.42071102331427	f
2.02299973448659	3.23002913410536	0.00000000000000	c
1.54244743573890	4.32456309957921	-1.72053988474862	h
4.05450705322598	2.72197332541716	0.00000000000000	h
1.54244743573890	4.32456309957921	1.72053988474862	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a''	31.45	0.00368	YES	YES
8		a'	197.98	0.20100	YES	YES
9		a''	206.48	0.34564	YES	YES
10		a''	217.25	0.01143	YES	YES
11		a'	286.20	4.02890	YES	YES
12		a''	288.40	4.60026	YES	YES
13		a'	313.17	0.09167	YES	YES
14		a'	355.49	19.15162	YES	YES
15		a''	356.93	19.92803	YES	YES
16		a'	375.85	74.13606	YES	YES
17		a'	522.77	1.75163	YES	YES
18		a''	531.03	0.00264	YES	YES
19		a'	580.34	0.07565	YES	YES
20		a''	631.96	164.21960	YES	YES
21		a'	633.84	164.27199	YES	YES
22		a'	653.04	137.70793	YES	YES
23		a'	843.92	34.91598	YES	YES
24		a''	845.30	33.09030	YES	YES
25		a'	1200.15	10.07614	YES	YES
26		a''	1398.23	2.27620	YES	YES
27		a'	1408.61	1.87334	YES	YES
28		a'	2969.65	13.41421	YES	YES
29		a''	3083.73	17.39455	YES	YES
30		a'	3087.31	16.11925	YES	YES

SbF₅



Total energy = -504.3407250911 H = -13723.8172067 eV

HOMO-LUMO Separation

HOMO: 18. 2 e" -0.37156128 H = -10.11070 eV

LUMO: 19. 7 a1' -0.21438411 H = -5.83369 eV

Gap : +0.15717717 H = +4.27701 eV

Number of MOs= 57, Electrons= 50.00, Symmetry: d3h

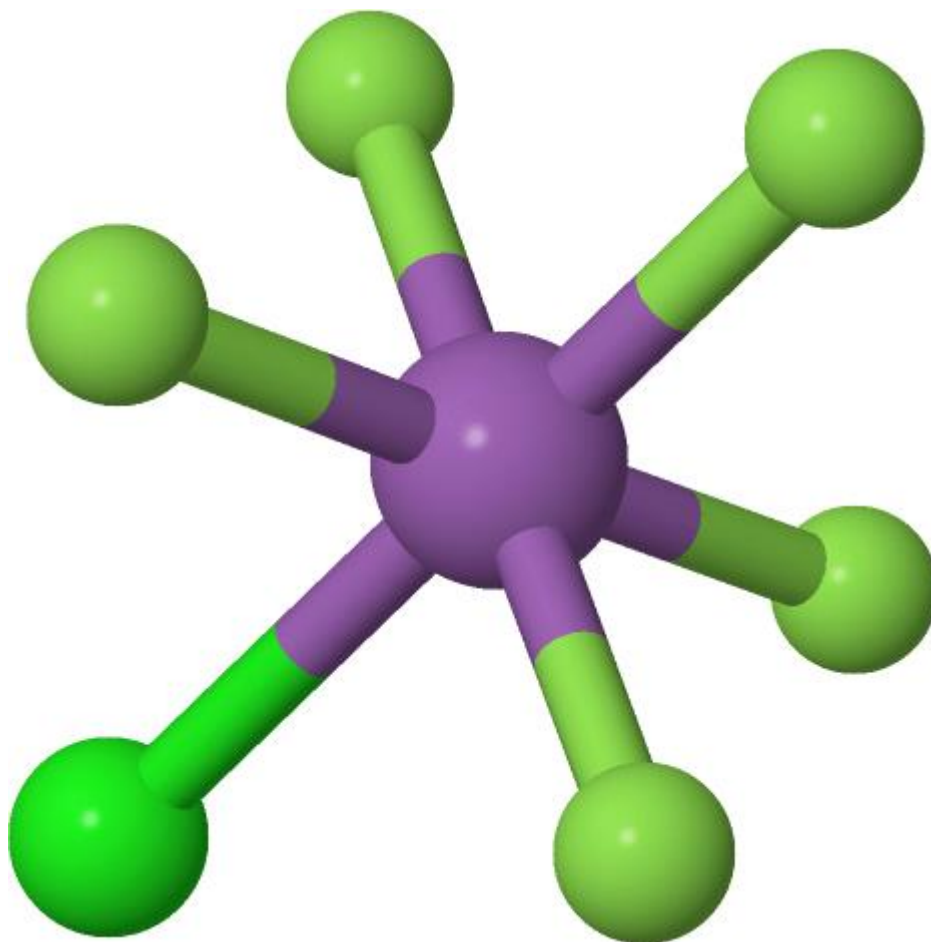
\$coord
0.0000000000000000 0.0000000000000000 0.0000000000000000 sb

0.0000000000000000	0.0000000000000000	3.63912956471427	f
3.61760081427441	0.0000000000000000	0.0000000000000000	f
0.0000000000000000	0.0000000000000000	-3.63912956471427	f
-1.80880040713721	3.13293420591291	0.0000000000000000	f
-1.80880040713721	-3.13293420591291	0.0000000000000000	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e'	88.03	0.00001	YES	YES
8		e'	88.03	0.00001	YES	YES
9		e'	223.98	41.50896	YES	YES
10		e'	223.98	41.50896	YES	YES
11		e''	242.20	0.00000	NO	YES
12		e''	242.20	0.00000	NO	YES
13		a2''	263.46	41.44034	YES	NO
14		a1'	589.48	0.00000	NO	YES
15		a1'	600.83	0.00000	NO	YES
16		a2''	653.83	73.85341	YES	NO
17		e'	663.99	64.29207	YES	YES
18		e'	663.99	64.29207	YES	YES

SbF₅Cl⁻



Total energy = -964.6304288799 H = -26248.9444524 eV

HOMO-LUMO Separation

HOMO: 26. 8 e -0.12045058 H = -3.27763 eV

LUMO: 27. 13 a1 +0.02537861 H = +0.69059 eV

Gap : +0.14582918 H = +3.96822 eV

Number of MOs= 77, Electrons= 68.00, Symmetry: c4v

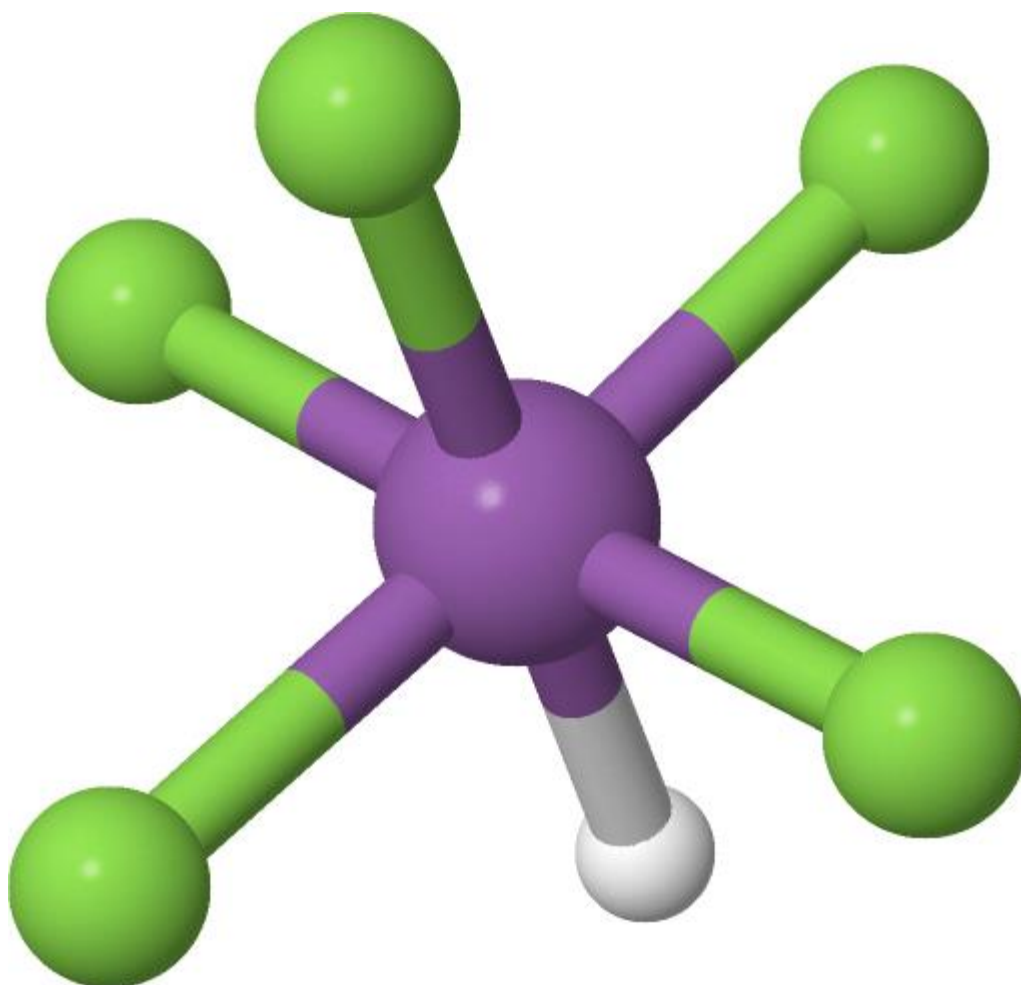
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$coord
0.0000000000000000 0.0000000000000000 -0.36248279471726 sb
0.0000000000000000 0.0000000000000000 -4.04746523165868 f
226
```

0.0000000000000000	3.70395878565940	-0.39057155001440	f
0.0000000000000000	-3.70395878565940	-0.39057155001440	f
-3.70395878565940	0.0000000000000000	-0.39057155001440	f
3.70395878565940	0.0000000000000000	-0.39057155001440	f
0.0000000000000000	0.0000000000000000	4.25094017028587	c1

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	120.28	0.07170	YES	YES
8		e	120.28	0.07170	YES	YES
9		b1	143.20	0.00000	NO	YES
10		e	206.04	6.70514	YES	YES
11		e	206.04	6.70514	YES	YES
12		b2	241.01	0.00000	NO	YES
13		a1	255.36	49.32616	YES	YES
14		e	258.94	31.65782	YES	YES
15		e	258.94	31.65782	YES	YES
16		a1	318.14	67.07648	YES	YES
17		b1	547.71	0.00000	NO	YES
18		a1	553.99	0.12685	YES	YES
19		a1	598.69	80.49741	YES	YES
20		e	610.19	106.37732	YES	YES
21		e	610.19	106.37732	YES	YES

SbF₅H⁻



Total energy = -505.0687852817 H = -13743.6287438 eV

HOMO-LUMO Separation

HOMO: 20. 8 a1 -0.11694385 H = -3.18221 eV

LUMO: 21. 9 a1 +0.07957602 H = +2.16538 eV

Gap : +0.19651987 H = +5.34758 eV

Number of MOs= 65, Electrons= 52.00, Symmetry: c4v

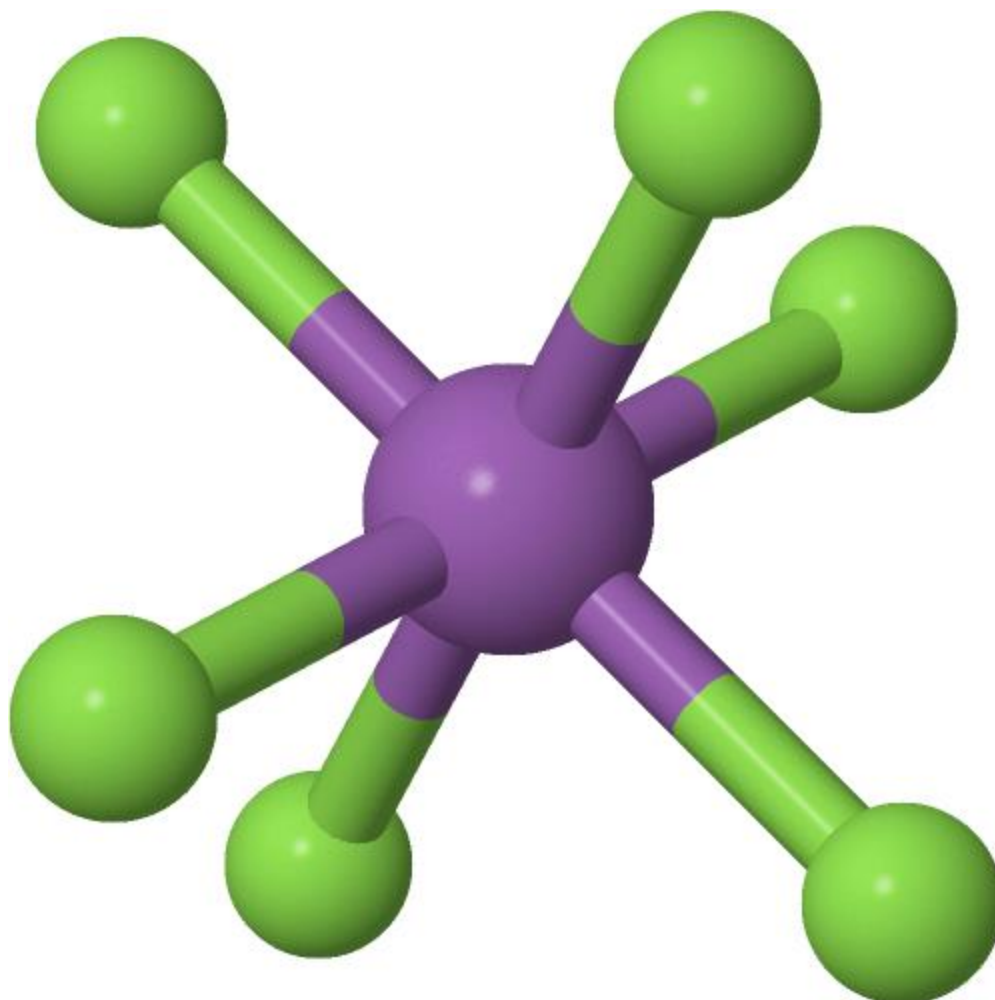
\$coord

0.0000000000000000	0.0000000000000000	0.33927218199449	sb
0.0000000000000000	0.0000000000000000	-3.35919538066339	f
0.0000000000000000	3.73777946305173	0.24792161802656	f
0.0000000000000000	-3.73777946305173	0.24792161802656	f
-3.73777946305173	0.0000000000000000	0.24792161802656	f
3.73777946305173	0.0000000000000000	0.24792161802656	f
0.0000000000000000	0.0000000000000000	3.64345475609674	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	b1		141.18	0.00000	NO	YES
8	e		161.20	3.61402	YES	YES
9	e		161.20	3.61402	YES	YES
10	b2		237.28	0.00000	NO	YES
11	e		257.99	23.67828	YES	YES
12	e		257.99	23.67828	YES	YES
13	a1		266.59	64.75091	YES	YES
14	b1		531.59	0.00000	NO	YES
15	a1		542.28	0.07557	YES	YES
16	a1		590.14	59.61286	YES	YES
17	e		591.53	139.81271	YES	YES
18	e		591.53	139.81271	YES	YES
19	e		756.27	58.28467	YES	YES
20	e		756.27	58.28467	YES	YES
21	a1		1841.89	197.03993	YES	YES

SbF₅F⁻



Total energy = -604.2814774648 H = -16443.3449959 eV

HOMO-LUMO Separation

HOMO: 13. 1 t_{1g} -0.14371093 H = -3.91058 eV

LUMO: 14. 4 a_{1g} +0.04495291 H = +1.22323 eV

Gap : +0.18866384 H = +5.13381 eV

Number of MOs= 42, Electrons= 60.00, Symmetry: oh

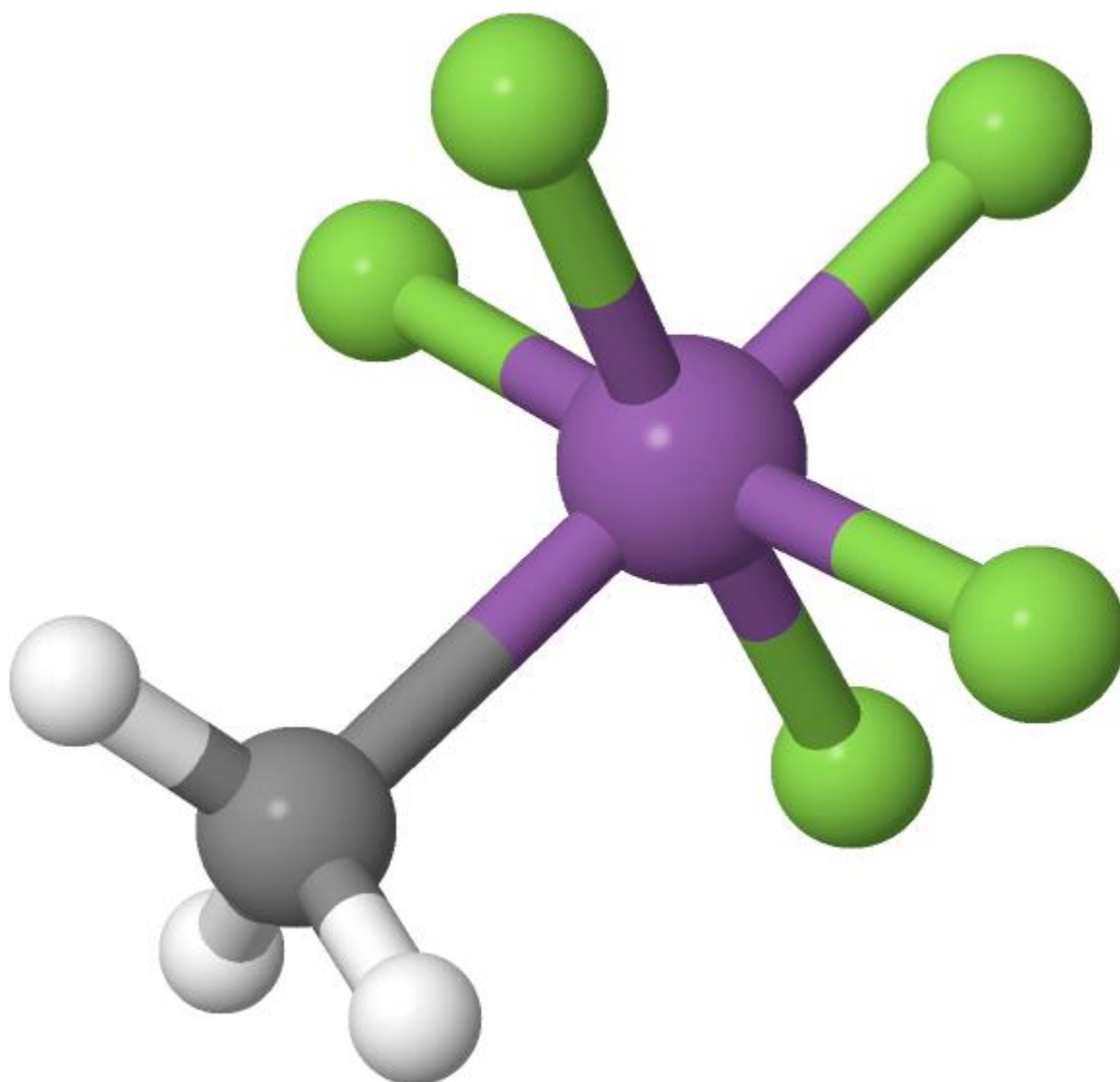
\$coord

0.0000000000000000	0.0000000000000000	0.0000000000000000	sb
0.0000000000000000	-3.69652417408783	0.0000000000000000	f
0.0000000000000000	0.0000000000000000	3.69652417408783	f
0.0000000000000000	0.0000000000000000	-3.69652417408783	f
3.69652417408783	0.0000000000000000	0.0000000000000000	f
-3.69652417408783	0.0000000000000000	0.0000000000000000	f
0.0000000000000000	3.69652417408783	0.0000000000000000	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	t2u		143.37	0.00000	NO	NO
8	t2u		143.37	0.00000	NO	NO
9	t2u		143.37	0.00000	NO	NO
10	t2g		243.10	0.00000	NO	YES
11	t2g		243.10	0.00000	NO	YES
12	t2g		243.10	0.00000	NO	YES
13	t1u		264.72	54.12468	YES	NO
14	t1u		264.72	54.12468	YES	NO
15	t1u		264.72	54.12468	YES	NO
16	eg		550.76	0.00000	NO	YES
17	eg		550.76	0.00000	NO	YES
18	alg		567.62	0.00000	NO	YES
19	t1u		615.93	113.79364	YES	NO
20	t1u		615.93	113.79364	YES	NO
21	t1u		615.93	113.79364	YES	NO

SbF₅Me⁻



Total energy = -544.3636059066 H = -14812.8958258 eV

HOMO-LUMO Separation

HOMO: 30. 30 a -0.10852737 H = -2.95318 eV

LUMO: 31. 31 a +0.08800167 H = +2.39465 eV

Gap : +0.19652904 H = +5.34783 eV

Number of MOs= 103, Electrons= 60.00, Symmetry: c1

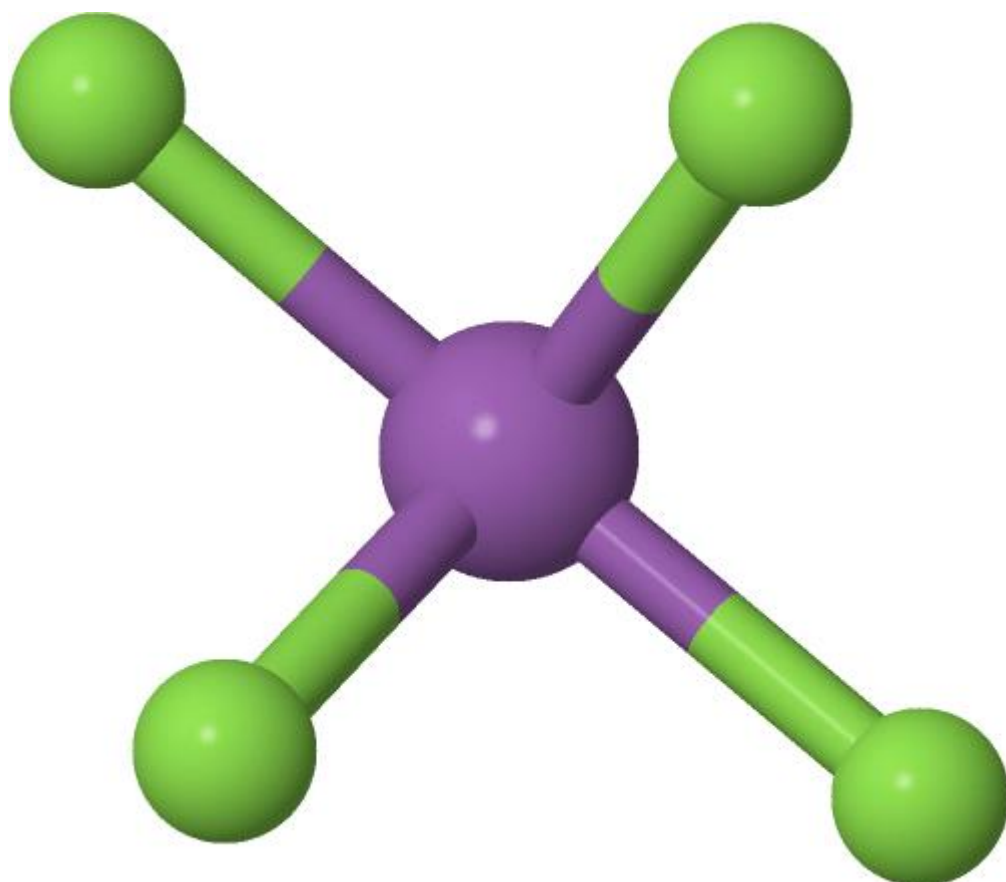
\$coord

0.07584422188046	-0.52758197632087	1.29753640867881	sb
3.73756772843624	0.22487828716325	1.61137428393907	f
-3.57601878008589	-1.36350655604054	1.18790938701201	f
-0.72413139195467	2.80962711675394	2.80545632582177	f
0.91356749749950	-3.94531570265176	0.00067742541952	f
0.17166624831718	-1.93073199046248	4.71006892729998	f
-0.12641625396354	1.01095540804310	-2.47685880241145	c
-0.52666774353961	-0.58997185363729	-3.76483887252990	h
1.72835058449039	1.89079389733974	-2.89140169544362	h
-1.67376211108002	2.42085336981283	-2.47992149806020	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	34.89	0.01233	YES	YES
8		a	139.70	1.07825	YES	YES
9		a	142.15	0.74042	YES	YES
10		a	149.20	0.06401	YES	YES
11		a	203.56	5.45323	YES	YES
12		a	206.00	4.64661	YES	YES
13		a	237.62	0.10943	YES	YES
14		a	260.09	23.84481	YES	YES
15		a	264.15	33.03103	YES	YES
16		a	269.93	67.14428	YES	YES
17		a	487.50	6.39595	YES	YES
18		a	526.69	0.06229	YES	YES
19		a	536.78	1.17050	YES	YES
20		a	582.05	120.12121	YES	YES
21		a	582.56	120.84180	YES	YES
22		a	598.26	82.11915	YES	YES
23		a	768.06	33.71605	YES	YES
24		a	769.96	34.24457	YES	YES
25		a	1132.02	9.21100	YES	YES
26		a	1391.13	4.40228	YES	YES
27		a	1403.78	3.76620	YES	YES
28		a	2974.35	7.64370	YES	YES
29		a	3099.59	5.91376	YES	YES
30		a	3104.21	5.29696	YES	YES

SbF₄⁻



total energy = -404.7120987377 H = -11012.7828036 eV

HOMO-LUMO Separation

HOMO: 21. 21 a -0.04197523 H = -1.14220 eV

LUMO: 22. 22 a +0.12567471 H = +3.41978 eV

Gap : +0.16764994 H = +4.56199 eV

Number of MOs= 69, Electrons= 42.00, Symmetry: c1

```
$coord
-0.64571399823056   -0.21829268248846    0.93420219189074   sb
 3.05683114439228   -0.50039590106422    0.42809130417455    f
-1.65914692650522    0.97713344508454   -2.47171355978610    f
-0.80289995553107   -3.79212667221234   -0.60142588064506    f
```

0.05092973587457

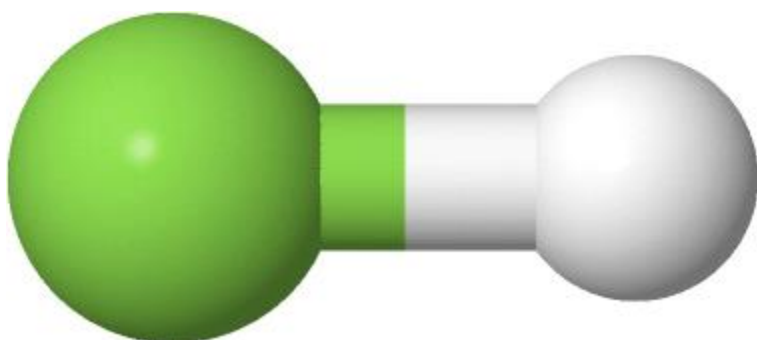
3.53368181068044

1.71084594436592 f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm ⁻¹	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	91.84	1.95854	YES	YES
8		a	131.98	10.69448	YES	YES
9		a	221.42	24.99695	YES	YES
10		a	224.67	1.15773	YES	YES
11		a	245.40	7.92612	YES	YES
12		a	473.57	0.94186	YES	YES
13		a	492.59	195.51295	YES	YES
14		a	560.92	84.54979	YES	YES
15		a	571.37	56.46861	YES	YES

HF



Total energy = -100.3448514265 H = -2730.5238901 eV

HOMO-LUMO Separation

HOMO: 4. 1 e1 -0.31370755 H = -8.53642 eV

LUMO: 5. 4 a1 +0.01933552 H = +0.52615 eV

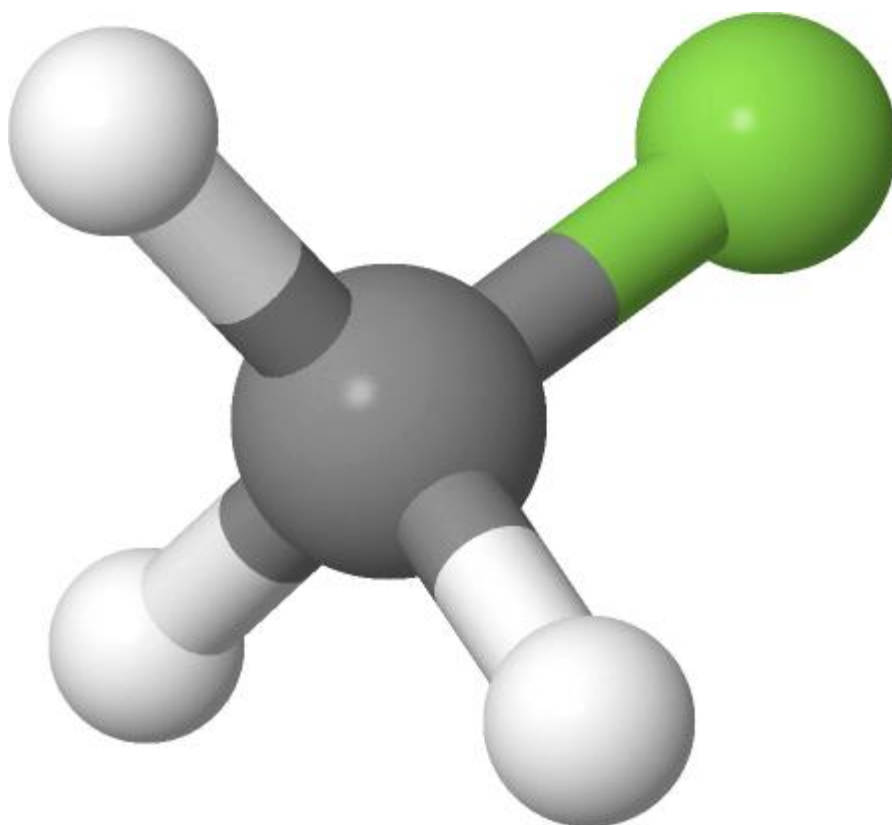
Gap : +0.33304307 H = +9.06257 eV

Number of MOs= 12, Electrons= 10.00, Symmetry: c6v

```
$coord
  0.0000000000000000  0.0000000000000000 -0.89245684630327 h
  0.0000000000000000  0.0000000000000000  0.89245684630327 f
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#                               cm** (-1)          km/mol            IR      RAMAN
  1                0.00          0.00000          -        -
  2                0.00          0.00000          -        -
  3                0.00          0.00000          -        -
  4                0.00          0.00000          -        -
  5                0.00          0.00000          -        -
  6              a1        3750.47        57.45826        YES      YES
```

MeF



Total energy = -139.6273405894 H = -3799.4554157 eV

HOMO-LUMO Separation

HOMO: 7. 2 e -0.28184371 H = -7.66936 eV

LUMO: 8. 6 a1 +0.05286891 H = +1.43864 eV

Gap : +0.33471261 H = +9.10800 eV

Number of MOs= 24, Electrons= 18.00, Symmetry: c3v

\$coord

0.0000000000000000	0.0000000000000000	-0.08946862819212	c
0.0000000000000000	0.0000000000000000	2.51333290530533	f
0.99064253344976	-1.71584320007376	-0.80782680459231	h
0.99064253344976	1.71584320007376	-0.80782680459231	h
-1.98128506689955	0.0000000000000000	-0.80782680459231	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a1	1081.17	96.28322	YES	YES
8		e	1168.05	0.43272	YES	YES
9		e	1168.05	0.43272	YES	YES
10		e	1435.12	2.62560	YES	YES
11		e	1435.12	2.62560	YES	YES
12		a1	1466.06	8.50256	YES	YES
13		a1	2916.55	38.60261	YES	YES
14		e	3001.35	48.67290	YES	YES
15		e	3001.35	48.67290	YES	YES

B(OH)₃

Total energy = -252.2764879713 H = -6864.7964248 eV

HOMO-LUMO Separation

HOMO: 16. 3 a" -0.25975033 H = -7.06817 eV

LUMO: 17. 14 a' -0.00478022 H = -0.13008 eV

Gap : +0.25497011 H = +6.93809 eV

Number of MOs= 62, Electrons= 32.00, Symmetry: cs

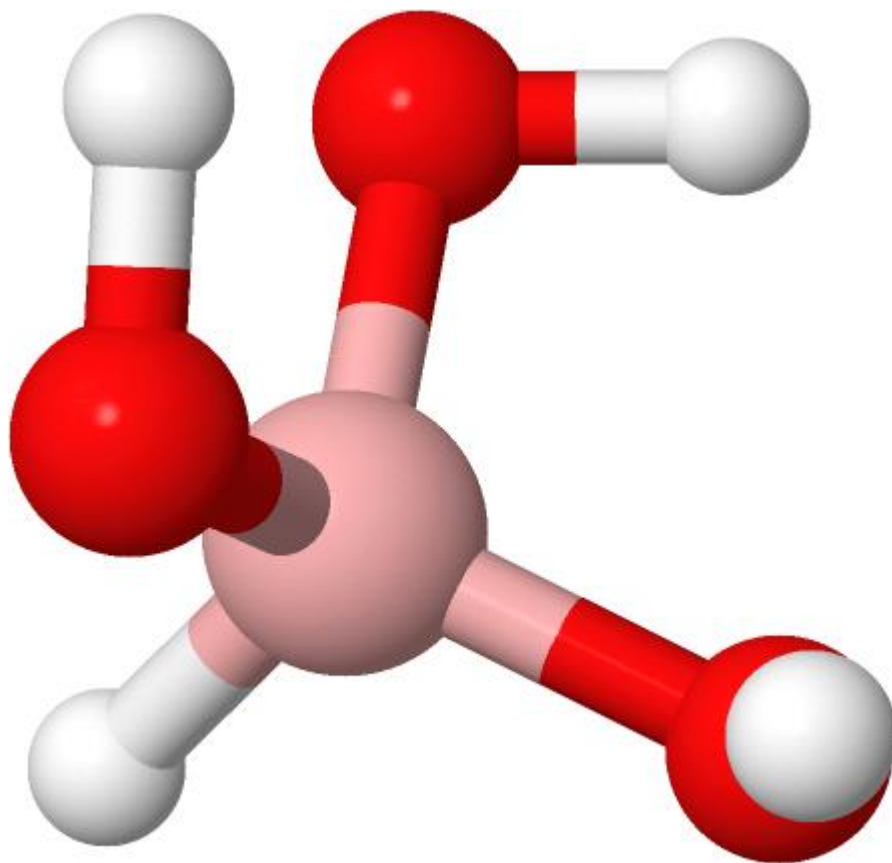
\$coord

-0.43837845044127	-0.10517495111802	0.000000000000000	b
-0.08732991978794	-2.68880113356353	0.000000000000000	o
1.47523540214697	1.69326291989697	0.000000000000000	o
-2.89351300961934	0.72819095864049	0.000000000000000	o
1.68119916173094	-3.21266201448690	0.000000000000000	h
3.18945674863207	1.00740394845515	0.000000000000000	h
-2.92666993266143	2.57778027217583	0.000000000000000	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a"	264.74	8.57192	YES	YES
8		a'	430.51	31.54250	YES	YES
9		a'	442.85	3.68465	YES	YES
10		a"	465.63	197.49268	YES	YES
11		a"	514.16	131.42807	YES	YES
12		a"	648.42	74.55759	YES	YES
13		a'	854.58	4.77132	YES	YES
14		a'	885.01	204.65546	YES	YES
15		a'	990.98	203.10782	YES	YES
16		a'	1005.79	2.16555	YES	YES
17		a'	1405.16	416.87450	YES	YES
18		a'	1457.22	304.26133	YES	YES
19		a'	3613.50	56.65851	YES	YES
20		a'	3622.80	21.95398	YES	YES
21		a'	3643.52	44.31654	YES	YES

B(OH)₃H⁻



Total energy = -252.8545404360 H = -6880.5260416 eV

HOMO-LUMO Separation

HOMO: 17. 7 a +0.02085911 H = +0.56761 eV

LUMO: 18. 8 a +0.22859816 H = +6.22048 eV

Gap : +0.20773904 H = +5.65287 eV

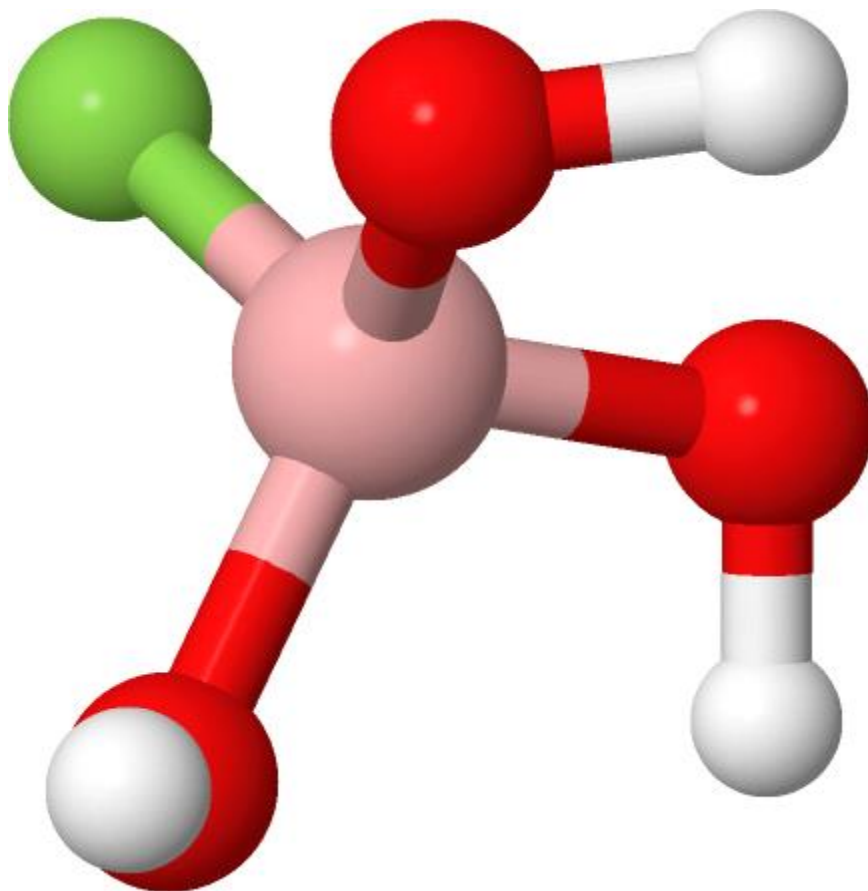
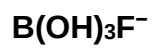
Number of MOs= 64, Electrons= 34.00, Symmetry: c3

```
$coord
  0.0000000000000000  0.0000000000000000 -0.87668974191924 b
 -2.58044428978562 -0.61050890699895  0.12619275819510 o
```

1.81893836759057	-1.92947585450538	0.12619275819510	o
0.76150592219504	2.53998476150432	0.12619275819510	o
0.000000000000000	0.000000000000000	-3.28291841490094	h
-2.80198391610815	0.83942163377839	1.26464715237314	h
0.67403149871575	-2.84630006923426	1.26464715237314	h
2.12795241739239	2.00687843545585	1.26464715237314	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	e		237.92	40.55677	YES	YES
8	e		237.92	40.55677	YES	YES
9	e		380.35	8.46527	YES	YES
10	e		380.35	8.46527	YES	YES
11	a		492.84	22.20531	YES	YES
12	a		529.34	64.00978	YES	YES
13	a		802.00	93.68650	YES	YES
14	e		826.05	142.63647	YES	YES
15	e		826.05	142.63647	YES	YES
16	e		978.83	27.38696	YES	YES
17	e		978.83	27.38696	YES	YES
18	a		1107.89	0.46086	YES	YES
19	e		1187.32	283.03211	YES	YES
20	e		1187.32	283.03211	YES	YES
21	a		2170.70	624.40495	YES	YES
22	a		3518.70	3.55651	YES	YES
23	e		3527.62	6.72722	YES	YES
24	e		3527.62	6.72722	YES	YES



Total energy = -352.1061187249 H = -9581.3004391 eV

HOMO-LUMO Separation

HOMO: 21. 12 e -0.00236809 H = -0.06444 eV

LUMO: 22. 10 a +0.22209608 H = +6.04355 eV

Gap : +0.22446417 H = +6.10798 eV

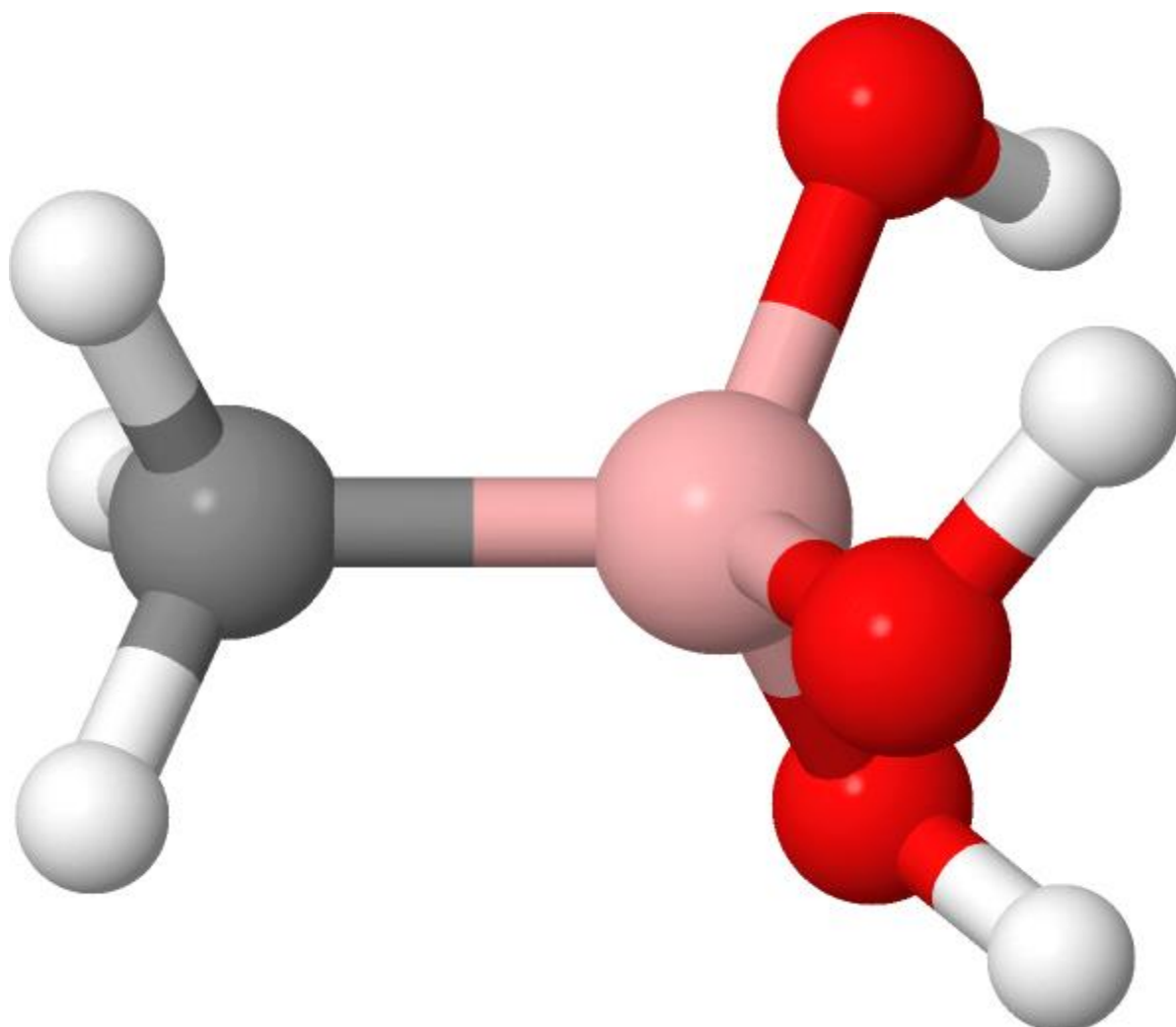
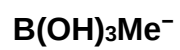
Number of MOs= 76, Electrons= 42.00, Symmetry: c3

```
$coord
  0.0000000000000000  0.0000000000000000 -0.71896641527384 b
 -2.57250396523420 -0.63656285057509  0.23054011649840 o
  1.83753158232055 -1.90957235994147  0.23054011649840 o
```

0.73497238291364	2.54613521051656	0.23054011649840	o
0.000000000000000	0.000000000000000	-3.43407302778137	f
-2.98438528800251	0.91228720888851	1.15380636452000	h
0.70212874555622	-3.04069707853498	1.15380636452000	h
2.28225654244632	2.12840986964647	1.15380636452000	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	200.29	37.61345	YES	YES
8		e	200.29	37.61345	YES	YES
9		e	338.06	1.25572	YES	YES
10		e	338.06	1.25572	YES	YES
11		a	385.09	72.75757	YES	YES
12		e	474.67	13.82796	YES	YES
13		e	474.67	13.82796	YES	YES
14		a	493.02	38.05718	YES	YES
15		a	714.39	1.46734	YES	YES
16		e	862.94	173.30719	YES	YES
17		e	862.94	173.30719	YES	YES
18		a	906.10	284.42005	YES	YES
19		a	1132.26	112.10816	YES	YES
20		e	1171.09	285.69225	YES	YES
21		e	1171.09	285.69225	YES	YES
22		a	3582.81	0.72595	YES	YES
23		e	3586.53	2.07752	YES	YES
24		e	3586.53	2.07752	YES	YES



Total energy = -292.1493788272 H = -7949.7936070 eV

HOMO-LUMO Separation

HOMO: 21. 9 a +0.01092355 H = +0.29724 eV

LUMO: 22. 10 a +0.21619415 H = +5.88295 eV

Gap : +0.20527060 H = +5.58570 eV

Number of MOs= 82, Electrons= 42.00, Symmetry: c3

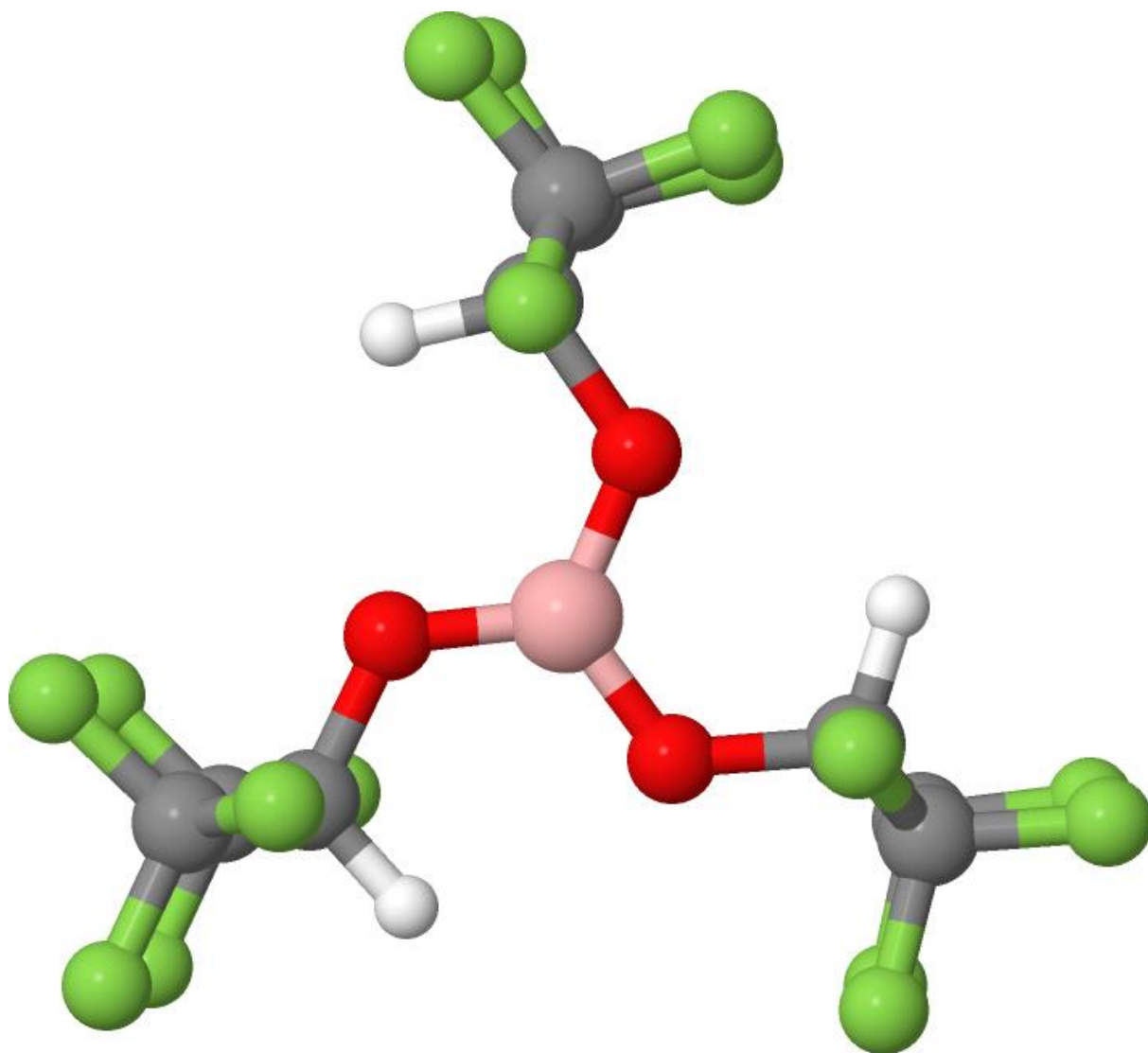
\$coord

0.000000000000000	0.000000000000000	0.46695201688736	b
-2.64475959157524	0.22796200027954	1.49522965030731	o
1.12495891244803	-2.40440999334648	1.49522965030731	o
1.51980067912721	2.17644799306695	1.49522965030731	o
0.000000000000000	0.000000000000000	-2.64613604193990	c
-2.39316225584958	1.64922027665110	2.65932667201492	h
-0.23168552809146	-2.89714944726935	2.65932667201492	h
2.62484778394104	1.24792917061826	2.65932667201492	h
1.91347702842149	-0.44571052543123	-3.42816164730470	h
-0.57074187645320	1.87997497888659	-3.42816164730470	h
-1.34273515196830	-1.43426445345536	-3.42816164730470	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	205.51	0.22246	YES	YES
8		e	223.28	32.56687	YES	YES
9		e	223.28	32.56687	YES	YES
10		e	302.11	15.39756	YES	YES
11		e	302.11	15.39756	YES	YES
12		e	402.88	9.32628	YES	YES
13		e	402.88	9.32628	YES	YES
14		a	443.26	9.68784	YES	YES
15		a	500.22	70.10842	YES	YES
16		a	665.39	4.14944	YES	YES
17		e	751.99	47.56853	YES	YES
18		e	751.99	47.56853	YES	YES
19		a	849.27	209.62032	YES	YES
20		e	874.84	105.00928	YES	YES
21		e	874.84	105.00928	YES	YES
22		e	1138.92	220.64063	YES	YES
23		e	1138.92	220.64063	YES	YES
24		a	1151.01	15.98968	YES	YES
25		a	1250.85	57.26323	YES	YES
26		e	1407.21	1.52911	YES	YES
27		e	1407.21	1.52911	YES	YES
28		a	2871.15	61.15941	YES	YES
29		e	2946.87	107.85061	YES	YES
30		e	2946.87	107.85061	YES	YES
31		a	3542.76	1.56471	YES	YES
32		e	3549.46	5.07572	YES	YES
33		e	3549.46	5.07572	YES	YES

B(OHfip)₃



Total energy = -2390.9598261780 H = -65061.3642141 eV

HOMO-LUMO Separation

HOMO: 124. 124 a -0.30889637 H = -8.40550 eV

LUMO: 125. 125 a -0.01533300 H = -0.41723 eV

Gap : +0.29356337 H = +7.98827 eV

Number of MOs= 440, Electrons= 248.00, Symmetry: c1

\$coord

0.92630451015858	0.31214856818833	-1.05573958815919	b
0.67002097592167	-2.05204580143485	-0.02162499491727	o
-1.17581000870113	1.65016156198183	-1.77267797685470	o
3.28731067506544	1.33438699646573	-1.37308482636274	o
3.65550293689503	3.75344964948577	-2.42311598474485	c
2.77333729841187	-3.45774592148467	0.81411872469336	c
-3.63770521346458	0.68222179538354	-1.45545529357264	c
5.00425506450638	5.41058810676685	-0.43443566125427	c
3.55751310594993	5.50885863950295	1.66604266247442	f
7.27666576688729	4.48015895211671	0.21744786978503	f
5.31564056215733	7.78134323372537	-1.30653834990440	f
5.10158933457562	3.44592766555988	-4.93903432364415	c
7.37429787931046	2.35938692184300	-4.61406462793879	f
5.43349739012485	5.70269334665167	-6.06693629082839	f
3.72844753970490	1.96225574279044	-6.49846272687933	f
2.83883280689141	-5.96182362738498	-0.68445300099665	c
4.80326701284353	-7.40120691300523	0.05860794674463	f
0.69870971392218	-7.30061362540198	-0.40908880210364	f
3.12704605894333	-5.43136180814865	-3.16521992339040	f
2.57455330827398	-3.77404653779368	3.71073690299332	c
0.55936787979582	-5.16413581937456	4.39088880029085	f
2.34005286668591	-1.46563688218505	4.77634824003653	f
4.67228657742542	-4.87272805890396	4.64126194008328	f
-4.87291376215938	0.42435632247987	-4.08765262398255	c
-3.41092246882342	-1.07783275870173	-5.54282878303159	f
-5.11820037014165	2.66403875407475	-5.26104878443316	f
-7.17408559195367	-0.64563790240984	-3.89045566070374	f
-5.07193759584025	2.43184580665076	0.38845588499050	c
-3.82050584000378	2.48461330385737	2.61370963066944	f
-7.42409182737147	1.55521854746257	0.81136970533503	f
-5.23657338815473	4.81348013108020	-0.47929022602109	f
1.83127555758915	4.69278417498600	-2.87259813637454	h
4.57960643187644	-2.45823354816727	0.42837748372460	h
-3.61422492658453	-1.23389439955752	-0.59739276490616	h

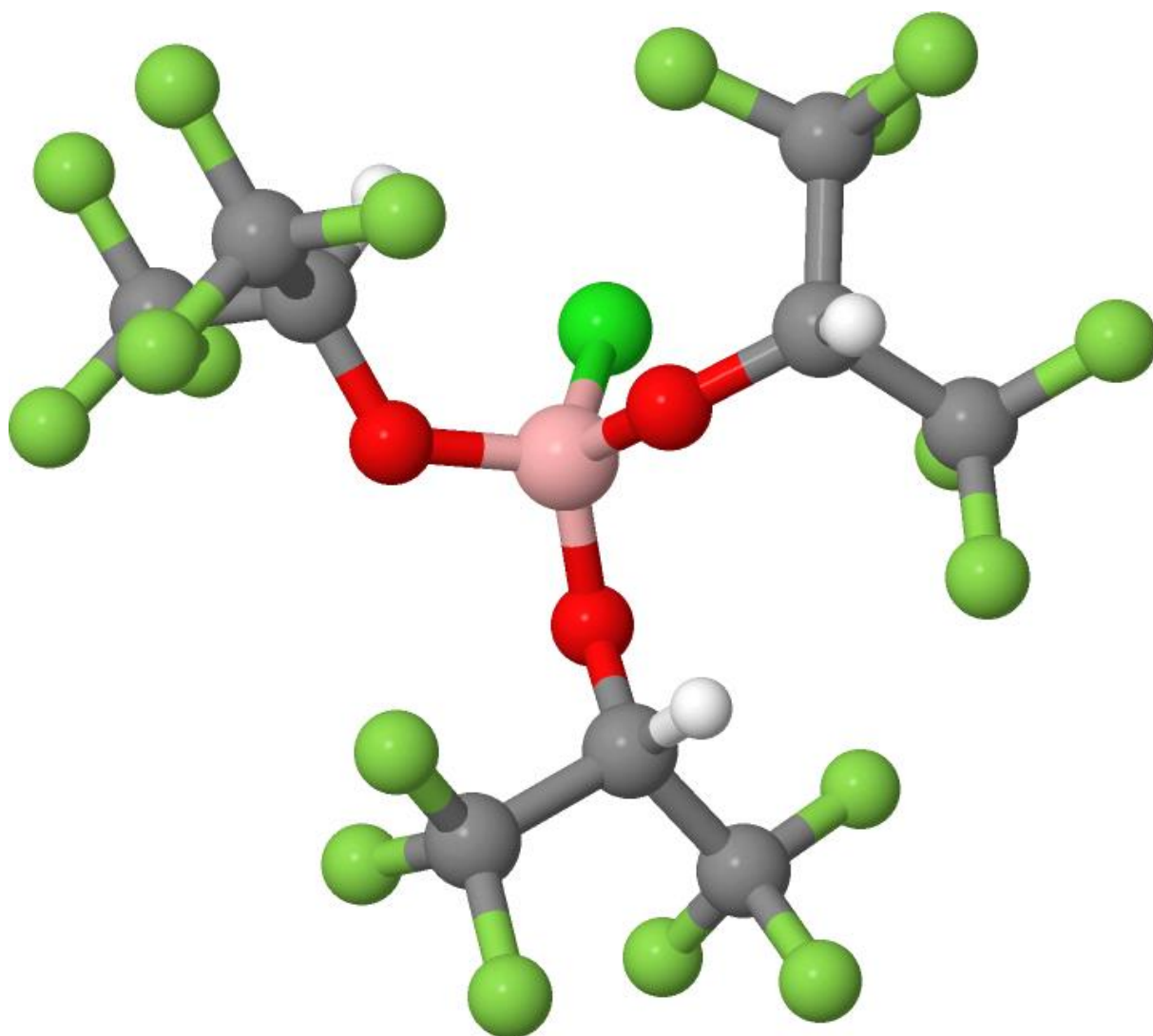
\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
#						
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	13.35	0.10422	YES	YES
8		a	14.74	0.05886	YES	YES
9		a	14.84	0.07706	YES	YES
10		a	18.49	0.00162	YES	YES
11		a	30.64	0.02038	YES	YES
12		a	31.61	0.00971	YES	YES
13		a	37.20	0.42169	YES	YES
14		a	37.71	0.29304	YES	YES
15		a	39.03	0.21121	YES	YES
16		a	48.56	0.00110	YES	YES
17		a	49.48	0.00060	YES	YES
18		a	61.31	0.00654	YES	YES
19		a	70.69	0.04815	YES	YES

20	a	72.36	0.02555	YES	YES
21	a	99.20	0.00067	YES	YES
22	a	145.21	4.42386	YES	YES
23	a	145.49	4.48822	YES	YES
24	a	166.26	0.00636	YES	YES
25	a	196.38	0.08242	YES	YES
26	a	197.55	0.06877	YES	YES
27	a	197.99	0.12688	YES	YES
28	a	246.93	1.33722	YES	YES
29	a	264.71	0.00027	YES	YES
30	a	265.84	0.00481	YES	YES
31	a	287.08	0.05287	YES	YES
32	a	287.34	0.04673	YES	YES
33	a	287.50	0.29886	YES	YES
34	a	317.05	1.56693	YES	YES
35	a	317.35	1.60431	YES	YES
36	a	322.07	0.00209	YES	YES
37	a	334.93	0.02434	YES	YES
38	a	355.17	0.00210	YES	YES
39	a	355.58	0.00606	YES	YES
40	a	373.58	0.39853	YES	YES
41	a	374.49	0.43443	YES	YES
42	a	414.01	0.00325	YES	YES
43	a	493.67	0.07127	YES	YES
44	a	493.91	0.08510	YES	YES
45	a	511.64	0.00944	YES	YES
46	a	521.84	0.91918	YES	YES
47	a	522.00	2.88144	YES	YES
48	a	522.95	2.45046	YES	YES
49	a	527.51	16.77720	YES	YES
50	a	527.94	16.90031	YES	YES
51	a	536.48	0.11314	YES	YES
52	a	536.55	1.58769	YES	YES
53	a	537.30	0.99351	YES	YES
54	a	552.62	0.00782	YES	YES
55	a	607.73	6.42618	YES	YES
56	a	634.52	24.65789	YES	YES
57	a	634.88	24.72586	YES	YES
58	a	673.97	0.85669	YES	YES
59	a	674.25	0.13302	YES	YES
60	a	676.09	126.92371	YES	YES
61	a	712.12	0.00232	YES	YES
62	a	727.78	20.56124	YES	YES
63	a	727.92	20.34745	YES	YES
64	a	848.20	0.02669	YES	YES
65	a	862.44	61.24449	YES	YES
66	a	862.73	61.86513	YES	YES
67	a	888.76	0.27146	YES	YES
68	a	894.47	7.05325	YES	YES
69	a	895.20	30.95722	YES	YES
70	a	896.62	58.48481	YES	YES
71	a	1095.61	9.27780	YES	YES
72	a	1097.99	12.06971	YES	YES
73	a	1102.00	144.68171	YES	YES
74	a	1103.08	141.24284	YES	YES
75	a	1105.58	453.21442	YES	YES
76	a	1163.21	0.26557	YES	YES
77	a	1164.32	0.58341	YES	YES
78	a	1169.32	13.18783	YES	YES
79	a	1172.62	0.28224	YES	YES
80	a	1201.54	143.77738	YES	YES
81	a	1203.10	140.02020	YES	YES

82	a	1208.34	2.42816	YES	YES
83	a	1215.70	626.26866	YES	YES
84	a	1216.85	645.53844	YES	YES
85	a	1237.19	1.13932	YES	YES
86	a	1244.57	299.70387	YES	YES
87	a	1245.30	18.18789	YES	YES
88	a	1246.28	45.99586	YES	YES
89	a	1274.74	685.42603	YES	YES
90	a	1274.78	689.62899	YES	YES
91	a	1281.18	0.43251	YES	YES
92	a	1351.54	6.03977	YES	YES
93	a	1358.30	11.85716	YES	YES
94	a	1358.63	109.69850	YES	YES
95	a	1359.54	18.65540	YES	YES
96	a	1365.66	97.75883	YES	YES
97	a	1366.15	67.70267	YES	YES
98	a	1423.21	716.83719	YES	YES
99	a	1425.28	722.44648	YES	YES
100	a	3006.83	8.04465	YES	YES
101	a	3008.01	9.51376	YES	YES
102	a	3011.30	9.46232	YES	YES

B(OHfip)₃Cl⁻



Total energy = -2851.1706476330 H = -77584.3449610 eV

HOMO-LUMO Separation

HOMO: 133. 133 a -0.10642846 H = -2.89607 eV

LUMO: 134. 134 a +0.13253018 H = +3.60633 eV

Gap : +0.23895864 H = +6.50240 eV

Number of MOs= 458, Electrons= 266.00, Symmetry: c1

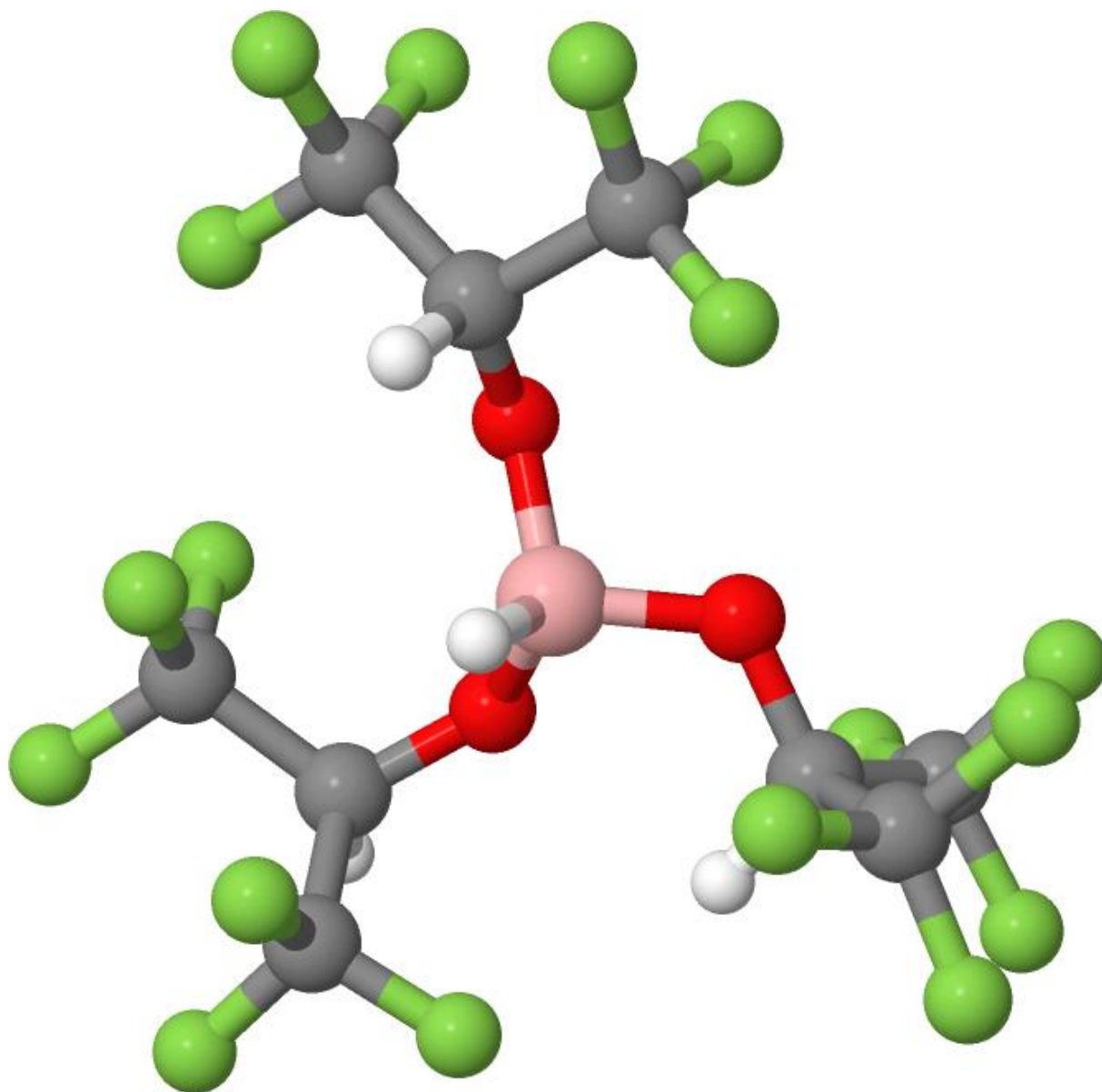
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-0.93767489907783	0.87855616136416	-1.15737311880601	b
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1.11250972693220	2.33855497249704	0.00954331209240	o
0.23306650562922	-1.09280126534868	-2.76734047602716	o
-0.37895207256839	-2.26830447054290	-4.98589539154528	c
2.41632356687920	4.21112144115212	-1.23875455185424	c
-1.82033218617028	-2.43513370896097	2.05945565625645	c
5.17300470610083	3.39178614652616	-1.77766337821118	c
6.46838050532559	5.22823134366617	-3.04005476689807	f
6.48578058659515	2.87435861708501	0.35289688595279	f
5.23404201421546	1.30409581201668	-3.23279987809842	f
2.30012847541532	6.65705060701410	0.36751016968442	c
3.45226469854375	8.63034806362209	-0.82202967600121	f
3.42613719776632	6.39210658536738	2.64691161838491	f
-0.11547602683770	7.33575088508624	0.78149925762168	f
-0.26888497900313	-0.61212903083777	-7.44456426288429	c
0.62004616471741	-2.06929119993250	-9.38908774948012	f
-2.50437739054995	0.32395859673766	-8.22436781474560	f
1.36192388646481	1.31680450021873	-7.16712950574303	f
-2.83028291039417	-3.87778883412798	-4.91923520402719	c
-2.57802174290662	-5.72266313312376	-3.14522057494271	f
-3.17696200520429	-5.07735089809452	-7.17650110110668	f
-4.93847208053674	-2.58677694309504	-4.40090137011440	f
-0.04829621651999	-2.03469124974631	4.37174681497665	c
-0.00654805097813	-4.12139549947801	5.89753274558857	f
2.35573231005664	-1.64703907210722	3.61622268733486	f
-0.75197851786464	-0.05998150756467	5.80652403408247	f
-4.30046573379087	-3.78226261249066	2.84337583325183	c
-3.88036594305010	-6.24051727036095	3.46731767936275	f
-5.97578498612878	-3.77117180043540	0.93016717734065	f
-5.43088091495408	-2.67151553047621	4.85712130304400	f
-3.12116186343347	3.05425363086619	-3.03669171124181	c1
1.11834218112828	-3.70869532751746	-5.35335154290786	h
1.55671024690598	4.70637655052681	-3.10176188704237	h
-0.80519665491967	-3.77350952607098	0.78514275348652	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
	1		0.00	0.00000	-	-
	2		0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	15.77	0.28370	YES	YES
	8	a	23.63	0.20818	YES	YES
	9	a	27.18	0.07362	YES	YES
	10	a	32.45	0.00721	YES	YES
	11	a	36.85	0.11716	YES	YES
	12	a	43.19	0.02396	YES	YES
	13	a	48.79	0.09598	YES	YES
	14	a	55.77	0.08845	YES	YES
	15	a	63.42	0.33249	YES	YES
	16	a	68.86	0.07410	YES	YES
	17	a	71.79	0.08760	YES	YES
	18	a	77.20	0.01651	YES	YES
	19	a	89.57	0.27280	YES	YES
	20	a	103.18	0.29752	YES	YES
	21	a	116.95	0.85211	YES	YES
	22	a	119.60	0.41533	YES	YES
	23	a	131.45	0.59886	YES	YES
	24	a	148.82	0.47663	YES	YES
	25	a	160.15	0.58798	YES	YES
	26	a	171.76	1.52850	YES	YES
	27	a	184.81	0.84612	YES	YES
	28	a	192.44	0.37003	YES	YES
	29	a	204.51	0.79282	YES	YES
	30	a	240.31	4.86986	YES	YES
	31	a	249.32	2.40945	YES	YES
	32	a	279.75	1.58698	YES	YES
	33	a	283.53	0.41424	YES	YES
	34	a	284.22	0.46624	YES	YES
	35	a	286.28	0.38317	YES	YES
	36	a	292.26	0.27685	YES	YES
	37	a	314.69	0.09450	YES	YES
	38	a	317.79	0.80205	YES	YES
	39	a	319.72	1.20057	YES	YES
	40	a	321.21	1.91559	YES	YES
	41	a	352.08	0.29370	YES	YES
	42	a	371.75	0.56612	YES	YES
	43	a	391.70	0.90344	YES	YES
	44	a	427.15	10.69084	YES	YES
	45	a	445.62	4.87071	YES	YES
	46	a	482.49	14.98392	YES	YES
	47	a	496.01	14.30583	YES	YES
	48	a	504.16	5.58486	YES	YES
	49	a	510.95	8.82366	YES	YES
	50	a	517.56	5.77751	YES	YES
	51	a	519.82	2.90564	YES	YES
	52	a	520.05	2.71757	YES	YES
	53	a	522.17	2.79127	YES	YES
	54	a	530.18	0.43082	YES	YES
	55	a	534.26	0.64093	YES	YES
	56	a	534.63	0.21983	YES	YES
	57	a	541.09	0.56164	YES	YES
	58	a	596.38	36.79191	YES	YES
	59	a	607.38	33.39504	YES	YES
	60	a	663.37	11.15986	YES	YES

61	a	669.64	37.68027	YES	YES
62	a	670.28	38.91473	YES	YES
63	a	684.20	42.37253	YES	YES
64	a	719.18	5.53412	YES	YES
65	a	723.98	1.52250	YES	YES
66	a	737.89	28.91326	YES	YES
67	a	800.29	16.36806	YES	YES
68	a	830.98	50.83452	YES	YES
69	a	842.20	26.11939	YES	YES
70	a	866.43	29.80791	YES	YES
71	a	872.25	40.29124	YES	YES
72	a	873.62	34.44947	YES	YES
73	a	888.11	159.17008	YES	YES
74	a	954.01	381.55850	YES	YES
75	a	1001.50	218.23597	YES	YES
76	a	1067.28	110.85918	YES	YES
77	a	1085.21	96.93137	YES	YES
78	a	1091.34	149.18301	YES	YES
79	a	1105.93	2.76236	YES	YES
80	a	1113.06	151.72774	YES	YES
81	a	1127.62	78.55982	YES	YES
82	a	1142.37	565.55805	YES	YES
83	a	1163.73	78.44555	YES	YES
84	a	1167.35	1135.64003	YES	YES
85	a	1172.04	184.36555	YES	YES
86	a	1191.74	97.07758	YES	YES
87	a	1212.20	494.83143	YES	YES
88	a	1218.81	286.94650	YES	YES
89	a	1223.40	34.64102	YES	YES
90	a	1227.92	232.64959	YES	YES
91	a	1232.34	210.07765	YES	YES
92	a	1236.54	160.42402	YES	YES
93	a	1254.77	160.94203	YES	YES
94	a	1269.51	189.45129	YES	YES
95	a	1272.60	159.89138	YES	YES
96	a	1306.78	175.62278	YES	YES
97	a	1329.66	55.46181	YES	YES
98	a	1336.04	9.61908	YES	YES
99	a	1340.46	34.33626	YES	YES
100	a	1348.66	91.37254	YES	YES
101	a	1358.77	54.39529	YES	YES
102	a	1389.21	49.24382	YES	YES
103	a	2931.59	36.13457	YES	YES
104	a	2936.30	22.71687	YES	YES
105	a	2949.29	20.75452	YES	YES



Total energy = -2391.6054905720 H = -65078.9336462 eV

HOMO-LUMO Separation

HOMO: 125. 125 a -0.08628556 H = -2.34795 eV

LUMO: 126. 126 a +0.14128670 H = +3.84461 eV

Gap : +0.22757226 H = +6.19256 eV
252

Number of MOs= 442, Electrons= 250.00, Symmetry: c1

\$scoord

-0.34680371592116	0.23286367765900	-1.12507413001092	b
-1.04948723279632	-0.37044010471627	1.53240421484979	o
1.76438807287220	2.07422452058279	-0.96670065797845	o
0.61325165560721	-2.19431481143342	-2.22477312790777	o
0.48003709939839	-2.94441100163269	-4.69079758297222	c
1.32135492670981	4.60198657370450	-1.30116309647519	c
-2.54884434811812	-2.42153558818127	2.05232573927086	c
3.66902076055426	5.82311931814265	-2.55351211525627	c
3.20093289135576	8.24691540179804	-3.28871887961870	f
5.70244626760622	5.88929848270655	-1.00062213102461	f
4.34900929194913	4.53754200018134	-4.64195385152999	f
0.63966271717232	5.95646823113493	1.21807043303069	c
0.48677886095734	8.52032461771638	0.91562480043422	f
2.34629512589531	5.51926195495798	3.05720913712788	f
-1.63669987173538	5.18647428912012	2.05848131725242	f
2.00648209705666	-1.28068809727318	-6.57058609587226	c
2.08351358847582	-2.38263071183888	-8.90980542339092	f
1.04477410611355	1.05442798906333	-6.88851489807159	f
4.41373763755665	-1.05828772938999	-5.77888441078374	f
-2.24594892465249	-3.46211994347201	-5.69722048610911	c
-3.61226036607513	-4.68985230287043	-3.91133966672469	f
-2.17369753200754	-5.01332855453599	-7.75650047651022	f
-3.55977853481881	-1.39276115559395	-6.38500761126228	f
-1.26980180778736	-4.02783192188729	4.13156840405651	c
-2.68683597828980	-6.08969937881238	4.76576028845750	f
0.98015702245140	-4.90027186805941	3.31273409023216	f
-0.85072761424592	-2.71868527652829	6.28433669028299	f
-5.24853743237084	-1.57711544909599	2.80611425276406	c
-6.82152599203199	-3.58560759001825	3.18830603248271	f
-6.28707039377708	-0.17041852999343	0.94670316858576	f
-5.29062440278159	-0.17626554459655	4.94263359242728	f
-2.12733542372791	1.13918172700193	-2.38001901720020	h
1.40606462040393	-4.83817712758215	-4.85279221448204	h
-0.30431974774206	5.00070967225347	-2.60093538964302	h
-2.78684925970778	-3.72492312523981	0.41194070469915	h

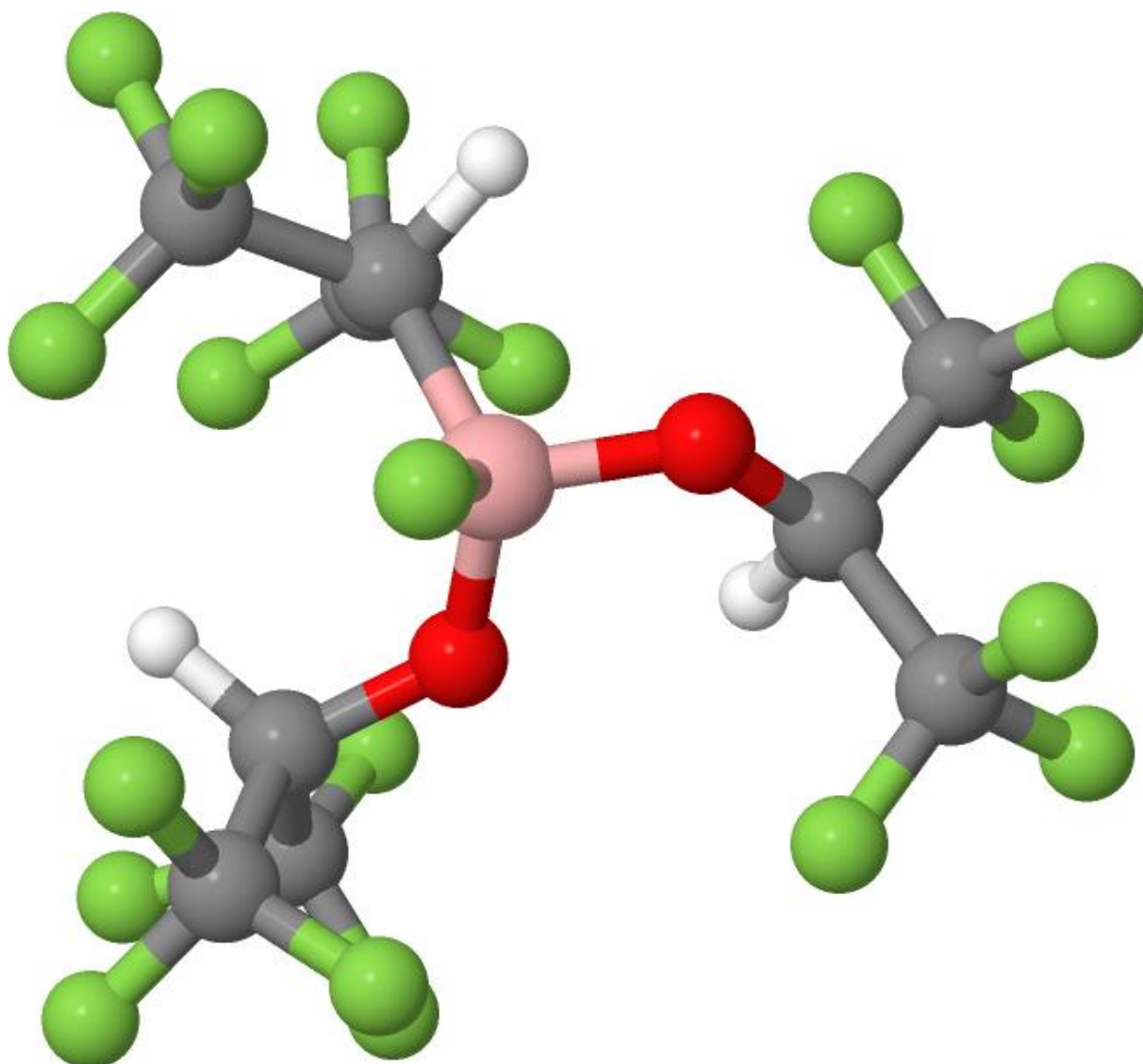
vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
#						
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	7.11	0.09462	YES	YES
8		a	18.42	0.09057	YES	YES
9		a	20.71	0.02820	YES	YES
10		a	26.05	0.08702	YES	YES
11		a	29.37	0.03698	YES	YES
12		a	36.09	0.33267	YES	YES
13		a	37.38	0.14014	YES	YES
14		a	43.46	0.02064	YES	YES

15	a	53.77	0.05210	YES	YES
16	a	57.88	0.18077	YES	YES
17	a	67.68	0.11626	YES	YES
18	a	77.73	0.09643	YES	YES
19	a	85.12	0.04035	YES	YES
20	a	99.70	0.08472	YES	YES
21	a	117.99	0.32142	YES	YES
22	a	145.92	0.58950	YES	YES
23	a	156.98	1.31713	YES	YES
24	a	164.63	0.28156	YES	YES
25	a	178.10	0.23492	YES	YES
26	a	195.90	0.50738	YES	YES
27	a	210.54	0.04884	YES	YES
28	a	237.29	4.57206	YES	YES
29	a	254.79	1.16796	YES	YES
30	a	264.05	3.51609	YES	YES
31	a	282.02	0.79764	YES	YES
32	a	285.61	0.05216	YES	YES
33	a	286.38	0.13284	YES	YES
34	a	291.96	0.08460	YES	YES
35	a	298.42	1.22115	YES	YES
36	a	316.15	0.88118	YES	YES
37	a	319.34	1.49121	YES	YES
38	a	321.08	1.29420	YES	YES
39	a	330.96	1.23204	YES	YES
40	a	365.64	0.70058	YES	YES
41	a	377.97	1.33106	YES	YES
42	a	388.67	3.33933	YES	YES
43	a	473.56	9.36405	YES	YES
44	a	485.89	4.45940	YES	YES
45	a	503.73	4.20873	YES	YES
46	a	509.11	8.05347	YES	YES
47	a	513.84	9.73299	YES	YES
48	a	517.49	4.68584	YES	YES
49	a	517.63	0.90422	YES	YES
50	a	518.75	1.60412	YES	YES
51	a	520.32	4.87236	YES	YES
52	a	528.74	0.02178	YES	YES
53	a	531.92	0.67215	YES	YES
54	a	533.63	0.26957	YES	YES
55	a	589.80	19.11069	YES	YES
56	a	606.00	24.47545	YES	YES
57	a	654.37	4.72952	YES	YES
58	a	668.31	17.94881	YES	YES
59	a	669.82	29.53208	YES	YES
60	a	671.46	56.36836	YES	YES
61	a	717.59	9.51257	YES	YES
62	a	719.85	4.42882	YES	YES
63	a	731.34	5.18544	YES	YES
64	a	799.17	26.17670	YES	YES
65	a	834.46	21.19964	YES	YES
66	a	838.08	24.17458	YES	YES
67	a	864.68	10.90037	YES	YES
68	a	867.31	17.18042	YES	YES
69	a	871.89	45.46743	YES	YES
70	a	888.51	150.63503	YES	YES
71	a	915.08	106.80318	YES	YES
72	a	943.71	154.52291	YES	YES
73	a	1070.36	252.12578	YES	YES
74	a	1074.68	93.89661	YES	YES
75	a	1083.21	89.47648	YES	YES
76	a	1088.35	141.18448	YES	YES

77	a	1106.10	122.10170	YES	YES
78	a	1112.59	297.86642	YES	YES
79	a	1117.43	356.75824	YES	YES
80	a	1119.41	205.73725	YES	YES
81	a	1149.41	482.13606	YES	YES
82	a	1158.89	311.40987	YES	YES
83	a	1164.37	297.25893	YES	YES
84	a	1176.11	594.57294	YES	YES
85	a	1195.25	19.98025	YES	YES
86	a	1212.89	58.16173	YES	YES
87	a	1217.96	416.93510	YES	YES
88	a	1221.81	341.48480	YES	YES
89	a	1230.28	76.93730	YES	YES
90	a	1232.71	147.70653	YES	YES
91	a	1235.97	148.47572	YES	YES
92	a	1239.36	170.45526	YES	YES
93	a	1268.88	170.92915	YES	YES
94	a	1271.21	222.19972	YES	YES
95	a	1290.06	153.02783	YES	YES
96	a	1326.22	30.20008	YES	YES
97	a	1337.51	15.49040	YES	YES
98	a	1340.38	63.83885	YES	YES
99	a	1348.74	55.62346	YES	YES
100	a	1360.31	48.48406	YES	YES
101	a	1375.93	31.10436	YES	YES
102	a	2344.32	184.78323	YES	YES
103	a	2882.43	39.80069	YES	YES
104	a	2913.00	47.80824	YES	YES
105	a	2953.26	20.26982	YES	YES

B(OHfip)₃F⁻



Total energy = -2415.6590249690 H = -65733.4639920 eV

HOMO-LUMO Separation

HOMO: 125. 125 a -0.11025468 H = -3.00018 eV

LUMO: 126. 126 a +0.14850403 H = +4.04100 eV

Gap : +0.25875871 H = +7.04119 eV

Number of MOs= 440, Electrons= 250.00, Symmetry: c1

\$coord

0.76541972441916	-1.41491488871992	-0.82291527616201	b
-1.72989413525305	-2.46963453537751	-1.55428669187346	o
-3.99908544239266	-1.60510823777580	-0.63989168730871	c
0.41589771550184	-0.07263671479410	1.60208038221396	o
2.33543493369974	0.99478221669793	2.99342726038229	c
1.20906781628418	3.21006642007768	4.55273787267077	c
-0.16624226316636	2.40642066495164	6.56171620529279	f
3.05115582933895	4.75506678929604	5.45645754739023	f
-0.32696855006338	4.64014311982384	3.11537403340944	f
3.66785482924302	-0.95201966546918	4.76425291309836	c
2.02694136710731	-2.61139442319210	5.76628979936806	f
4.86817322352826	0.22926539017632	6.72544013459910	f
5.46210527889955	-2.26351229608656	3.52062012846083	f
-5.12962951086342	-3.51276162225856	1.27923767717448	c
-7.52729703114374	-2.84354756988057	1.96976980548293	f
-5.24600951407421	-5.88725118552263	0.35338026731253	f
-3.73332380438905	-3.58635763651030	3.40408483223700	f
-5.84907709228275	-1.14683929517949	-2.87126427553386	c
-4.68721827087554	0.08528062021473	-4.77633519225738	f
-7.85974401648017	0.28440923341440	-2.15572470722545	f
-6.78914161733477	-3.32132980737951	-3.85145976814984	f
1.79753304934926	0.45824529103390	-3.27219856174762	c
2.44979841364729	-3.44696936769023	-0.60160545410076	f
4.59997215873223	0.24483683856533	-3.86397008785945	c
5.39351112457802	1.88199319904760	-5.71860636145056	f
5.20650914218706	-2.09093221099481	-4.70654941764255	f
6.11709062536684	0.73896416459100	-1.83702327902892	f
0.93615086806181	3.19071071627374	-3.19173449207592	c
0.93468557103485	4.34352917984583	-5.50561334037119	f
2.42814078388714	4.65822208743026	-1.67877279134938	f
-1.46383974757877	3.43337961907087	-2.31386288195353	f
-3.84531849196658	0.22209629665922	0.39603017782479	h
3.86965433355291	1.83796037937166	1.82095775091067	h
0.81769269944503	-0.39016276971056	-4.92004252173752	h

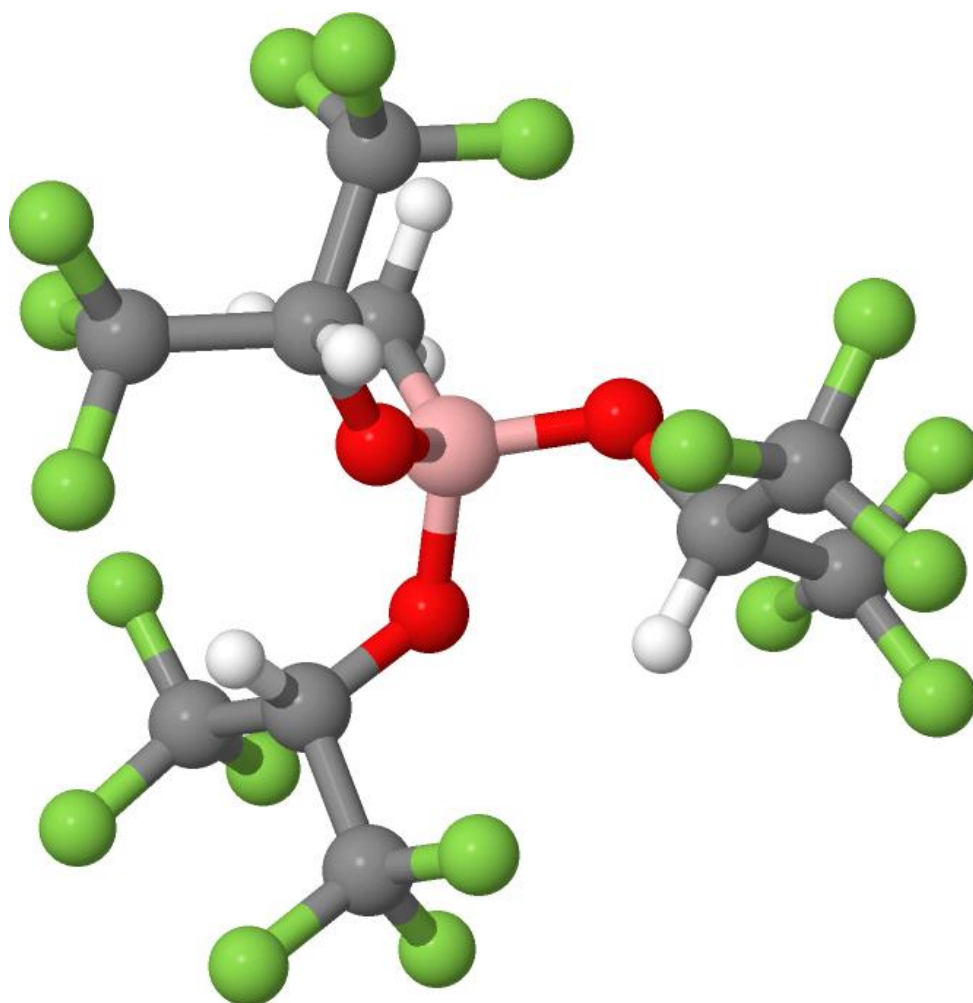
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	18.76	0.16513	YES	YES
8		a	23.92	0.20061	YES	YES
9		a	32.31	0.10270	YES	YES
10		a	39.17	0.17522	YES	YES
11		a	41.89	0.09810	YES	YES
12		a	46.10	0.06566	YES	YES
13		a	48.62	0.14070	YES	YES
14		a	57.34	0.06229	YES	YES
15		a	60.96	0.07198	YES	YES
16		a	71.42	0.20020	YES	YES
17		a	77.42	0.17090	YES	YES
18		a	94.07	0.03783	YES	YES
19		a	101.77	0.08186	YES	YES

20	a	110.09	0.32827	YES	YES
21	a	122.69	0.10518	YES	YES
22	a	152.66	0.59911	YES	YES
23	a	161.37	0.37176	YES	YES
24	a	163.59	1.27645	YES	YES
25	a	182.29	0.13860	YES	YES
26	a	185.83	1.21739	YES	YES
27	a	198.34	0.82895	YES	YES
28	a	210.74	1.61351	YES	YES
29	a	253.41	0.77124	YES	YES
30	a	276.95	0.52796	YES	YES
31	a	283.50	0.29654	YES	YES
32	a	284.93	0.38150	YES	YES
33	a	293.55	0.03672	YES	YES
34	a	301.61	0.49679	YES	YES
35	a	304.02	0.18045	YES	YES
36	a	318.55	0.84269	YES	YES
37	a	321.68	0.90809	YES	YES
38	a	325.53	0.34779	YES	YES
39	a	326.15	0.28595	YES	YES
40	a	335.45	0.14836	YES	YES
41	a	379.55	1.03721	YES	YES
42	a	385.63	1.85524	YES	YES
43	a	482.79	8.85360	YES	YES
44	a	488.19	3.26941	YES	YES
45	a	502.90	1.05912	YES	YES
46	a	511.85	14.88386	YES	YES
47	a	518.44	6.35676	YES	YES
48	a	519.55	1.02161	YES	YES
49	a	520.18	0.78268	YES	YES
50	a	521.87	4.51620	YES	YES
51	a	523.65	1.43591	YES	YES
52	a	534.13	0.69214	YES	YES
53	a	535.17	0.43596	YES	YES
54	a	536.06	0.55676	YES	YES
55	a	551.15	4.47948	YES	YES
56	a	602.74	27.13161	YES	YES
57	a	645.16	87.40491	YES	YES
58	a	666.42	9.49439	YES	YES
59	a	670.65	45.30080	YES	YES
60	a	675.55	60.07558	YES	YES
61	a	705.43	1.86033	YES	YES
62	a	710.50	2.84593	YES	YES
63	a	727.47	8.90723	YES	YES
64	a	757.07	3.80856	YES	YES
65	a	830.58	21.68750	YES	YES
66	a	844.79	38.93824	YES	YES
67	a	854.49	107.87759	YES	YES
68	a	867.65	19.95575	YES	YES
69	a	874.13	13.14953	YES	YES
70	a	886.38	36.58066	YES	YES
71	a	920.92	204.33577	YES	YES
72	a	962.89	73.73508	YES	YES
73	a	1030.05	66.02489	YES	YES
74	a	1058.49	38.28269	YES	YES
75	a	1072.78	304.07564	YES	YES
76	a	1083.87	162.82698	YES	YES
77	a	1087.36	85.66143	YES	YES
78	a	1107.63	57.32964	YES	YES
79	a	1117.72	55.85312	YES	YES
80	a	1126.03	134.86384	YES	YES
81	a	1170.35	289.79663	YES	YES

82	a	1173.76	407.76154	YES	YES
83	a	1178.72	111.14991	YES	YES
84	a	1183.48	906.29833	YES	YES
85	a	1195.49	181.53894	YES	YES
86	a	1207.74	491.24709	YES	YES
87	a	1217.21	324.83787	YES	YES
88	a	1221.35	208.01593	YES	YES
89	a	1223.17	249.73838	YES	YES
90	a	1229.30	135.22971	YES	YES
91	a	1237.57	133.61960	YES	YES
92	a	1264.64	49.66249	YES	YES
93	a	1272.26	256.87369	YES	YES
94	a	1274.22	140.23397	YES	YES
95	a	1329.19	82.45697	YES	YES
96	a	1340.16	116.84047	YES	YES
97	a	1350.97	168.99719	YES	YES
98	a	1357.38	101.82824	YES	YES
99	a	1368.74	6.12387	YES	YES
100	a	2962.91	16.96445	YES	YES
101	a	2964.39	15.93383	YES	YES
102	a	3018.16	0.60648	YES	YES

B(OHfip)₃Me⁻



Total energy = -2430.8960595640 H = -66148.0850352 eV

HOMO-LUMO Separation

HOMO: 129. 129 a -0.09286292 H = -2.52693 eV

LUMO: 130. 130 a +0.14221558 H = +3.86989 eV

Gap : +0.23507850 H = +6.39682 eV

Number of MOs= 460, Electrons= 258.00, Symmetry: c1

\$coord

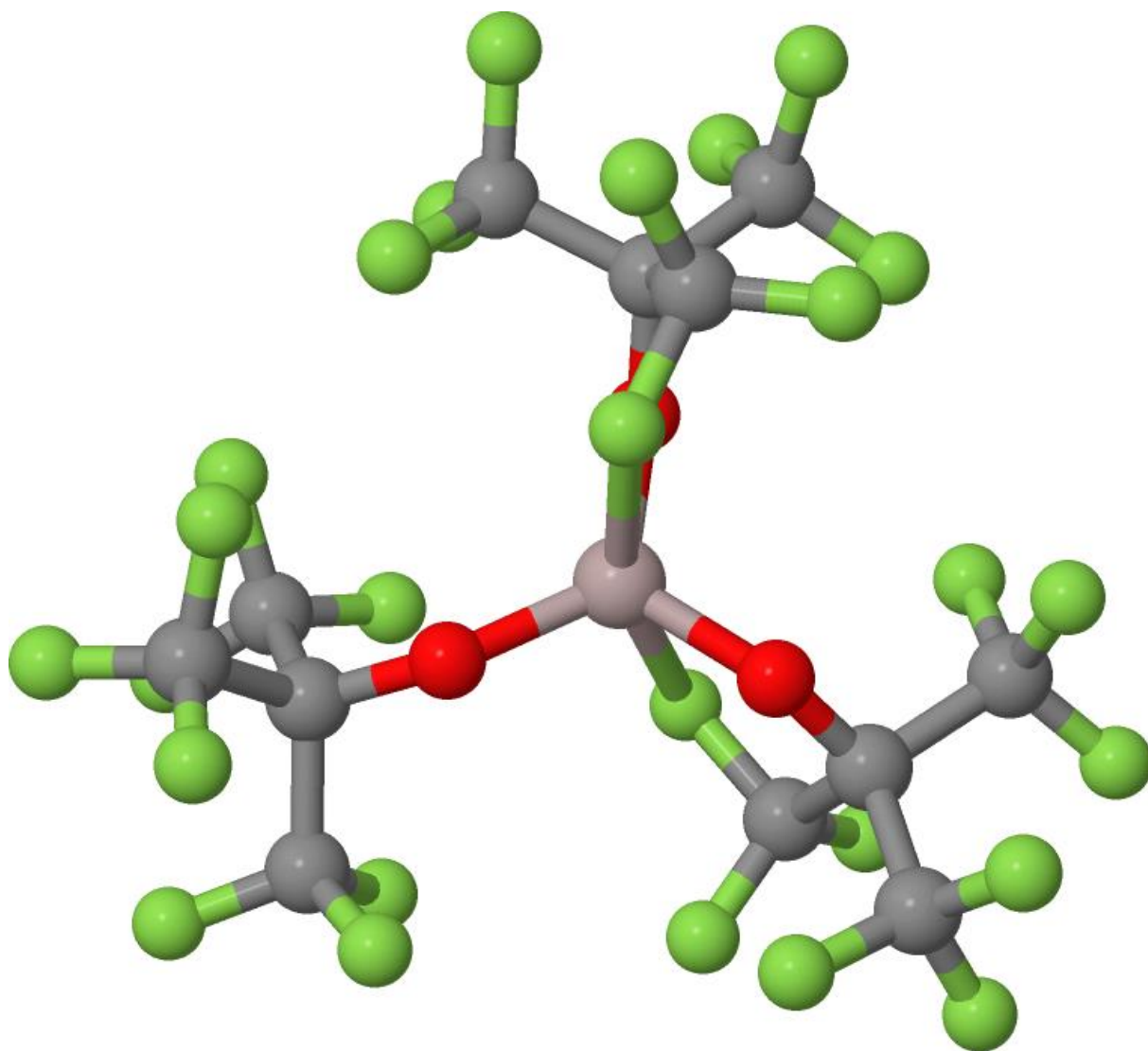
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-1.58063012025892	-1.17665095370602	2.71408072416973	o
-0.86264109230720	2.63277572124408	0.35840389545415	o
0.79189627640036	-1.17762834018103	-1.30325841925582	o
1.31358588406668	-3.27515318079266	-2.70066551598987	c
0.53599666637748	3.94888889869429	-1.38245651193121	c
0.24074748086268	-0.51810730702364	4.45101944868480	c
2.66075960809661	5.44051808130517	-0.03116657507346	c
4.27679470758929	6.54317713789895	-1.70016250244688	f
1.77292296321252	7.28821570849496	1.49849606824374	f
4.07281073548594	3.87143893258019	1.41875418909180	f
-1.17862122897844	5.72472049020095	-2.95950487084097	c
0.18106739182236	7.24007009888751	-4.54160960288473	f
-2.61849537523215	7.24949483446058	-1.50752116569524	f
-2.75607779552810	4.35350736802462	-4.42961901260911	f
1.46823780531435	-2.59234219611145	-5.55505472468467	c
2.13918874024005	-4.61177111600878	-7.00291624699756	f
-0.70456887723625	-1.66310775103412	-6.49762881238403	f
3.27458516177093	-0.80200445840069	-5.90703407125720	f
-0.33009772508678	-5.69411133167842	-2.31375415051850	c
-0.93477785226651	-6.04443044777331	0.12083747937802	f
1.01529311791810	-7.76836450002939	-3.06377218741096	f
-2.49583362892100	-5.70685406261914	-3.67968366699321	f
-1.05435117369654	0.58511074327260	6.83302657199153	c
0.65356930054100	1.56719398335754	8.49267920811061	f
-2.64048357948481	2.46938997411683	6.19690474580285	f
-2.41723614753578	-1.16745264917132	8.11768067006841	f
1.92595468201796	-2.81677721516823	5.10911820523501	c
3.56278473365258	-2.30245099390126	7.03474523844142	f
3.36219864537251	-3.49243582558162	3.10066924244339	f
0.57415645194723	-4.86612274705123	5.80011922191568	f
-4.24036757481563	-0.63279501226708	-1.17148236800002	c
3.26158959321442	-3.96408003627390	-2.23581496897974	h
1.52531290965218	2.69636925923450	-2.76143177554111	h
1.54225293609280	0.98886818208252	3.76288429685129	h
-5.62780455532591	0.66841224403175	-0.26745358253223	h
-4.93906528261165	-2.59046612530081	-0.85399215245576	h
-4.27883978997757	-0.25869360218090	-3.23792619725545	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	16.90	0.03774	YES	YES
8		a	20.82	0.03439	YES	YES
9		a	25.69	0.22360	YES	YES
10		a	31.18	0.00798	YES	YES
11		a	35.36	0.19354	YES	YES
12		a	40.75	0.19493	YES	YES
13		a	45.35	0.02270	YES	YES
14		a	50.19	0.14086	YES	YES
15		a	63.11	0.06930	YES	YES
16		a	64.51	0.15153	YES	YES
17		a	71.87	0.03586	YES	YES
18		a	74.24	0.01793	YES	YES
19		a	94.00	0.27655	YES	YES
20		a	100.44	0.03032	YES	YES
21		a	109.51	0.42084	YES	YES
22		a	128.57	0.80650	YES	YES
23		a	160.06	0.90405	YES	YES
24		a	162.53	0.32142	YES	YES
25		a	168.00	0.73975	YES	YES
26		a	183.12	0.74968	YES	YES
27		a	187.56	0.15705	YES	YES
28		a	205.60	0.13426	YES	YES
29		a	214.05	1.59110	YES	YES
30		a	223.29	0.26661	YES	YES
31		a	243.97	2.05843	YES	YES
32		a	265.23	2.09315	YES	YES
33		a	280.96	0.35860	YES	YES
34		a	283.28	0.68050	YES	YES
35		a	286.07	0.04942	YES	YES
36		a	287.23	0.11716	YES	YES
37		a	302.97	0.86521	YES	YES
38		a	315.39	0.85392	YES	YES
39		a	317.95	0.67391	YES	YES
40		a	318.96	0.92808	YES	YES
41		a	330.67	0.05896	YES	YES
42		a	357.51	1.25165	YES	YES
43		a	362.18	0.55867	YES	YES
44		a	385.63	2.74332	YES	YES
45		a	444.43	5.28369	YES	YES
46		a	475.50	17.18049	YES	YES
47		a	485.09	2.53157	YES	YES
48		a	501.23	2.17368	YES	YES
49		a	502.93	2.61460	YES	YES
50		a	516.64	7.29504	YES	YES
51		a	518.37	3.06165	YES	YES
52		a	520.01	4.60400	YES	YES
53		a	520.43	4.02527	YES	YES
54		a	524.54	4.64984	YES	YES
55		a	532.08	0.25288	YES	YES
56		a	532.43	0.33764	YES	YES
57		a	533.07	0.49250	YES	YES
58		a	547.42	1.58993	YES	YES
59		a	588.06	23.28850	YES	YES

60	a	601.96	33.00956	YES	YES
61	a	664.95	21.35668	YES	YES
62	a	667.75	27.54764	YES	YES
63	a	669.41	53.07013	YES	YES
64	a	684.46	15.80419	YES	YES
65	a	705.98	4.19154	YES	YES
66	a	714.75	6.60639	YES	YES
67	a	725.88	13.91947	YES	YES
68	a	763.61	21.19243	YES	YES
69	a	790.19	8.50875	YES	YES
70	a	820.71	25.74253	YES	YES
71	a	853.53	43.84940	YES	YES
72	a	854.17	70.44078	YES	YES
73	a	867.35	13.57054	YES	YES
74	a	871.20	21.16172	YES	YES
75	a	872.42	32.27306	YES	YES
76	a	946.40	325.37798	YES	YES
77	a	996.84	350.74413	YES	YES
78	a	1036.90	96.97450	YES	YES
79	a	1070.24	135.04267	YES	YES
80	a	1081.10	120.47340	YES	YES
81	a	1086.08	111.82154	YES	YES
82	a	1110.33	104.03658	YES	YES
83	a	1112.21	11.74460	YES	YES
84	a	1117.66	19.63559	YES	YES
85	a	1150.40	308.51062	YES	YES
86	a	1160.14	332.04493	YES	YES
87	a	1162.75	370.14490	YES	YES
88	a	1166.30	542.73033	YES	YES
89	a	1188.91	430.39011	YES	YES
90	a	1204.28	249.42371	YES	YES
91	a	1206.06	409.08281	YES	YES
92	a	1213.71	313.34293	YES	YES
93	a	1221.91	22.33385	YES	YES
94	a	1234.55	111.89010	YES	YES
95	a	1236.56	192.96506	YES	YES
96	a	1242.72	263.22212	YES	YES
97	a	1266.26	149.37908	YES	YES
98	a	1268.44	159.55328	YES	YES
99	a	1285.11	16.47553	YES	YES
100	a	1303.02	221.24887	YES	YES
101	a	1317.80	11.54017	YES	YES
102	a	1326.71	36.02498	YES	YES
103	a	1333.91	54.04748	YES	YES
104	a	1352.18	69.74244	YES	YES
105	a	1363.01	53.58033	YES	YES
106	a	1370.11	15.89237	YES	YES
107	a	1418.10	0.85985	YES	YES
108	a	1423.95	0.30216	YES	YES
109	a	2887.08	54.20901	YES	YES
110	a	2936.61	17.56812	YES	YES
111	a	2948.82	23.83498	YES	YES
112	a	2966.13	18.83626	YES	YES
113	a	3012.78	36.04528	YES	YES
114	a	3034.37	29.70972	YES	YES

Al(OC(CF₃)₃)₃



Total energy = -3618.9175253530 H = -98475.8123494 eV

HOMO-LUMO Separation

HOMO: 176. 176 a -0.28418638 H = -7.73311 eV

LUMO: 177. 177 a -0.05537636 H = -1.50687 eV

Gap : +0.22881002 H = +6.22624 eV

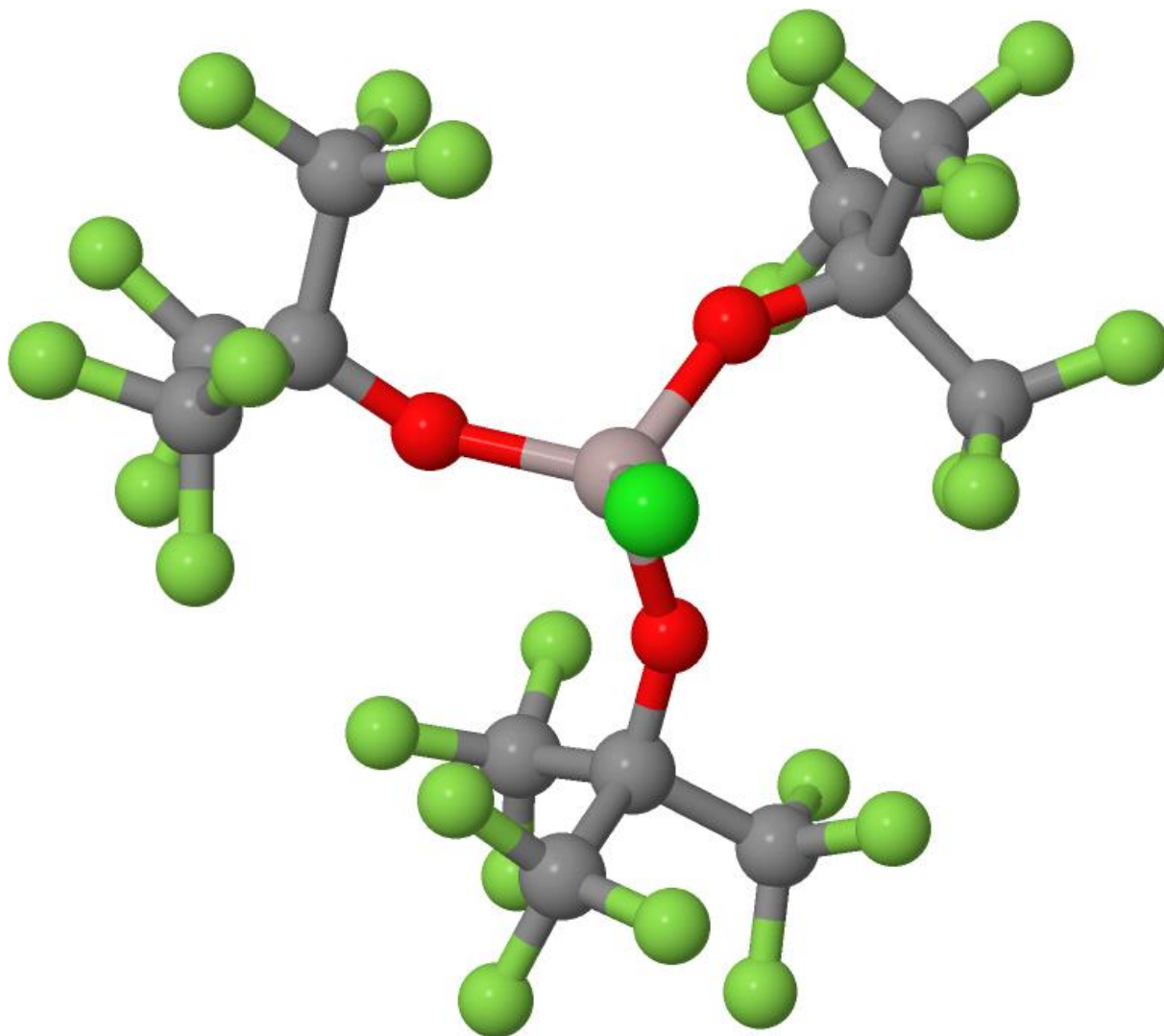
Number of MOs= 606, Electrons= 352.00, Symmetry: c1

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-2.64753350949925	-1.35921034202375	0.87916444376328	o	
2.85296355987990	-1.65781884673847	1.56677620357484	o	
0.78362766312710	5.18845044617551	-0.10062939852082	c	
2.90481497175571	6.82009145221517	-1.40254908898732	c	
4.99239185770606	5.42976941378485	-1.75098214241677	f	
3.50694072074410	8.83869996636515	0.04140359836961	f	
2.12035324023289	7.65875609219474	-3.66379976379074	f	
1.46159467626997	4.79991067002383	2.77721587844819	c	
0.34835066365244	2.44222775207185	3.47570844288105	f	
0.54281950763181	6.50630353933136	4.35648568941833	f	
3.92427591091059	4.51659751684828	3.18121727795555	f	
-1.85188168276756	6.56365491526770	-0.32485825549863	c	
-2.72600387079323	6.39822873931433	-2.68695805155014	f	
-1.70298860983723	9.01777187402965	0.32948307435956	f	
-3.53416535335249	5.42620933569718	1.22819468078006	f	
4.47997152670816	-3.17468393537803	0.24018608296748	c	
5.20595711765587	-5.51529244149035	1.92922632406174	c	
6.81563973024779	-4.82007877569162	3.76314867711961	f	
6.31919232488005	-7.33620705281034	0.52465229254572	f	
3.13402858699396	-6.48385690964403	3.01218143250429	f	
3.13884412195086	-4.12907084541470	-2.24578978300834	c	
1.69726551518734	-6.14980447088383	-1.88394390564298	f	
4.62252233202257	-4.49621557411046	-4.22244253162323	f	
1.42082480090651	-2.14931859339107	-2.94566670747463	f	
6.91966961808408	-1.62123380238161	-0.47974477280758	c	
6.34937243140839	0.03944045765577	-2.33952088716279	f	
8.80144802955068	-3.12185559502789	-1.30214647452749	f	
7.73242500279638	-0.30429289971330	1.51691914450464	f	
-5.02684753024321	-2.02032701220472	0.12539540325345	c	
-6.92330453657122	-1.36599496320453	2.32716497689798	c	
-6.69973230070277	-3.04517944901210	4.22576570165274	f	
-9.33726013316909	-1.39517504223389	1.51611612894346	f	
-6.41550092914186	0.93692410489969	3.26345052846100	f	
-5.07368017382862	-4.95197350167138	-0.40903270845064	c	
-3.87826029045727	-5.45028558302857	-2.61552852447802	f	
-7.44236591387125	-5.85876226837630	-0.56885525448013	f	
-3.84957414241384	-6.19727065826277	1.42391166903146	f	
-5.79810525099702	-0.54934703910731	-2.34594226085290	c	
-6.46295942873425	1.84626888128835	-1.81051523623911	f	
-7.71776237447014	-1.65827581225588	-3.57571416829643	f	
-3.78634609185594	-0.44609013779502	-3.92397827479494	f	

\$vibrational spectrum						
#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		15.53	0.05552	YES	YES
8	a		18.37	0.00392	YES	YES
9	a		25.26	0.07851	YES	YES
10	a		29.55	0.01566	YES	YES

11	a	32.20	0.07016	YES	YES
12	a	36.68	0.01292	YES	YES
13	a	42.30	0.15050	YES	YES
14	a	57.08	0.43287	YES	YES
15	a	62.78	0.02145	YES	YES
16	a	64.64	0.21092	YES	YES
17	a	68.11	0.18027	YES	YES
18	a	70.66	0.11548	YES	YES
19	a	75.11	0.22170	YES	YES
20	a	76.98	0.18019	YES	YES
21	a	78.88	0.62158	YES	YES
22	a	84.84	0.16318	YES	YES
23	a	92.46	0.10732	YES	YES
24	a	94.14	0.49568	YES	YES
25	a	103.33	0.67371	YES	YES
26	a	108.10	0.08442	YES	YES
27	a	121.69	1.25084	YES	YES
28	a	148.34	10.41694	YES	YES
29	a	153.52	2.19437	YES	YES
30	a	154.71	1.09641	YES	YES
31	a	156.40	9.58488	YES	YES
32	a	160.88	3.07525	YES	YES
33	a	165.90	1.14689	YES	YES
34	a	176.48	100.84604	YES	YES
35	a	184.70	8.09223	YES	YES
36	a	190.18	4.59515	YES	YES
37	a	216.60	0.06578	YES	YES
38	a	261.55	0.77952	YES	YES
39	a	269.38	2.92301	YES	YES
40	a	269.87	2.47747	YES	YES
41	a	281.02	13.61305	YES	YES
42	a	282.11	6.38972	YES	YES
43	a	284.67	1.46725	YES	YES
44	a	285.54	0.98230	YES	YES
45	a	296.02	7.24735	YES	YES
46	a	298.25	7.98381	YES	YES
47	a	302.61	13.84405	YES	YES
48	a	305.39	5.58727	YES	YES
49	a	310.77	1.01585	YES	YES
50	a	315.63	3.14267	YES	YES
51	a	317.66	2.85960	YES	YES
52	a	319.65	2.04599	YES	YES
53	a	324.78	0.33971	YES	YES
54	a	333.80	1.76652	YES	YES
55	a	333.98	2.94110	YES	YES
56	a	348.73	0.52813	YES	YES
57	a	357.10	11.34702	YES	YES
58	a	360.55	4.89622	YES	YES
59	a	372.09	19.41691	YES	YES
60	a	399.37	40.31735	YES	YES
61	a	430.87	38.39266	YES	YES
62	a	470.34	4.22788	YES	YES
63	a	474.90	1.78310	YES	YES
64	a	499.24	7.19846	YES	YES
65	a	504.91	6.98029	YES	YES
66	a	515.99	4.11416	YES	YES
67	a	517.10	5.50506	YES	YES
68	a	519.97	5.66286	YES	YES
69	a	522.03	4.29212	YES	YES
70	a	522.42	3.57826	YES	YES
71	a	523.57	1.58592	YES	YES
72	a	524.55	2.44267	YES	YES

73	a	531.52	0.17568	YES	YES
74	a	548.73	1.63700	YES	YES
75	a	550.14	1.65082	YES	YES
76	a	551.31	2.00222	YES	YES
77	a	551.97	0.81091	YES	YES
78	a	555.83	0.34552	YES	YES
79	a	557.18	0.52807	YES	YES
80	a	579.21	35.86739	YES	YES
81	a	598.66	35.15841	YES	YES
82	a	693.35	16.12835	YES	YES
83	a	698.62	49.81940	YES	YES
84	a	707.94	10.24611	YES	YES
85	a	708.95	30.69097	YES	YES
86	a	710.13	18.35747	YES	YES
87	a	711.07	69.05506	YES	YES
88	a	713.11	9.85647	YES	YES
89	a	732.71	6.31108	YES	YES
90	a	740.25	1.24818	YES	YES
91	a	774.07	5.08255	YES	YES
92	a	840.39	39.24893	YES	YES
93	a	879.59	13.16180	YES	YES
94	a	891.74	179.55646	YES	YES
95	a	906.01	283.00308	YES	YES
96	a	962.12	39.18575	YES	YES
97	a	965.89	125.44208	YES	YES
98	a	968.68	176.36218	YES	YES
99	a	970.77	217.88363	YES	YES
100	a	1034.23	29.82878	YES	YES
101	a	1039.99	63.88010	YES	YES
102	a	1111.26	0.85357	YES	YES
103	a	1141.50	6.75377	YES	YES
104	a	1147.56	13.33048	YES	YES
105	a	1160.93	14.62375	YES	YES
106	a	1164.17	29.33129	YES	YES
107	a	1166.88	40.18330	YES	YES
108	a	1173.61	4.42270	YES	YES
109	a	1175.57	328.77703	YES	YES
110	a	1182.52	148.23272	YES	YES
111	a	1189.44	1.38472	YES	YES
112	a	1204.08	111.66247	YES	YES
113	a	1206.05	232.56382	YES	YES
114	a	1207.56	83.51517	YES	YES
115	a	1215.90	70.85381	YES	YES
116	a	1220.06	68.21555	YES	YES
117	a	1224.37	73.58903	YES	YES
118	a	1225.09	802.80150	YES	YES
119	a	1235.26	677.26567	YES	YES
120	a	1246.20	311.23928	YES	YES
121	a	1257.08	249.51965	YES	YES
122	a	1265.92	587.81532	YES	YES
123	a	1268.70	386.54662	YES	YES
124	a	1274.58	828.34975	YES	YES
125	a	1294.38	131.04378	YES	YES
126	a	1296.06	647.16599	YES	YES
127	a	1303.09	52.87901	YES	YES
128	a	1303.84	98.54843	YES	YES
129	a	1339.17	158.32945	YES	YES



Total energy = -4079.2113812690 H = -111001.0525803 eV

HOMO-LUMO Separation

HOMO: 185. 185 a -0.13548798 H = -3.68682 eV

LUMO: 186. 186 a +0.10827916 H = +2.94643 eV

Gap : +0.24376713 H = +6.63324 eV

Number of MOs= 624, Electrons= 370.00, Symmetry: c1

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5.51272677448408	0.10284493644840	-0.32435848495344	cl
1.45832275367388	-0.06399043627064	-0.13155660086138	al
0.20269093077057	-2.57234222889416	-1.95905887434557	o
0.33337081093061	-0.53451746077181	2.99337002842579	o
0.00206405250130	2.73749185409163	-1.24683498604522	o
2.69784298046372	-5.74438458622945	1.20475108439524	f
-4.53129702804643	-4.14560715709790	-1.36535634416667	f
1.43506282572583	-4.44364477440525	-6.44756869647574	f
-0.17253717793116	-5.07209155358540	-2.24350373813280	c
-4.44198896120432	0.81693003438534	3.88889852823569	f
2.78154750081846	3.80207643232885	4.31430555039502	f
1.41031413082710	-3.50877262886748	6.86797032126781	f
-0.13430713403497	0.46420807809674	5.28976046204006	c
2.23297644194857	7.17144008727999	-0.31277723845522	f
-4.69767897082055	4.03961330872356	-2.41446160992033	f
1.91724912141580	1.71777224853377	-5.92118011068968	f
-0.22520237629809	4.51215480160531	-3.05917702990869	c
4.13025575519728	0.86592159551754	6.85235629245910	f
3.93844999331110	-6.31570399650870	-3.78711304312502	f
0.52375309305956	-6.61048771369053	0.22019831826360	c
-3.05244230429100	-5.53065118058887	-2.88584248105504	c
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-2.68402300648967	2.02591200013561	5.25638997897204	c
2.08562114485670	2.23949803626835	6.18985100664007	c
-0.41397030898474	-1.78812342860494	7.23039268056536	c
1.89436783929612	6.60096583134716	-2.75858716388001	c
-2.89942591338173	5.79604197278901	-2.74065405338282	c
-0.03097411419797	3.33909871661488	-5.79435290405292	c
-1.29010041069541	-6.37024825190766	1.99580800711527	f
0.81760384313880	-9.11564647734738	-0.23919021229718	f
-3.73642151994310	-7.98870875179328	-2.62652225368395	f
-3.56742131763646	-4.84775116076803	-5.29344773478402	f
0.72551555911516	-8.35564466451077	-5.37727615647675	f
-3.63696825252678	2.39000242817065	7.61172526284985	f
-2.33690628499436	4.32629582202667	4.21759609424212	f
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-2.65965021891225	-2.96484953084068	6.93290489076218	f
-0.27755548204839	-1.00772473819195	9.66915989157020	f
4.12617123885126	5.78182531202304	-3.68043339825141	f
1.30527640626372	8.77184519942859	-3.99655237752335	f
-2.92501253811626	7.32303390328694	-0.69629587701478	f
-3.55540435836458	7.22119361914769	-4.76951633452886	f
-2.14729668098016	2.04913846925225	-6.39072801473708	f
0.31757601986796	5.12410107663258	-7.60034536152690	f

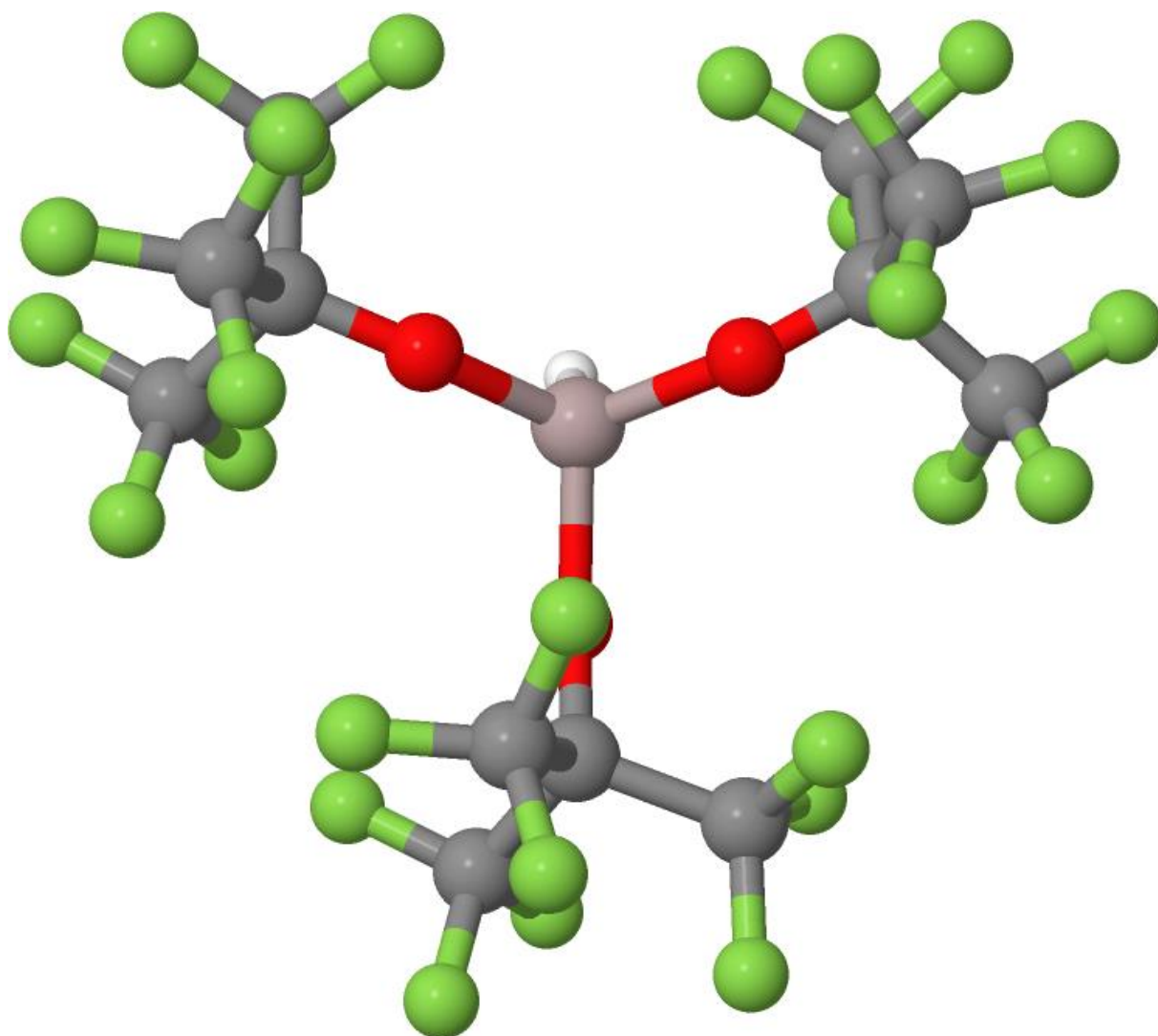
\$vibrational spectrum						
#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	11.96	0.03338	YES	YES
8		a	14.37	0.01599	YES	YES
9		a	15.09	0.09908	YES	YES

10	a	17.83	0.05522	YES	YES
11	a	21.79	0.15420	YES	YES
12	a	25.83	0.15690	YES	YES
13	a	34.14	0.02462	YES	YES
14	a	40.41	0.05954	YES	YES
15	a	49.22	0.04282	YES	YES
16	a	64.81	0.17131	YES	YES
17	a	65.85	0.19068	YES	YES
18	a	68.00	0.08918	YES	YES
19	a	71.02	0.07985	YES	YES
20	a	74.19	0.02722	YES	YES
21	a	74.78	0.10300	YES	YES
22	a	79.61	0.06459	YES	YES
23	a	80.23	0.09282	YES	YES
24	a	82.80	0.03925	YES	YES
25	a	84.75	0.12144	YES	YES
26	a	89.80	0.05701	YES	YES
27	a	96.32	0.52801	YES	YES
28	a	100.74	2.26165	YES	YES
29	a	103.68	2.12415	YES	YES
30	a	146.03	0.27403	YES	YES
31	a	156.73	0.19879	YES	YES
32	a	158.12	0.05098	YES	YES
33	a	158.94	0.26592	YES	YES
34	a	160.03	0.59271	YES	YES
35	a	160.62	1.09529	YES	YES
36	a	181.40	0.53772	YES	YES
37	a	189.82	5.09467	YES	YES
38	a	192.33	4.71998	YES	YES
39	a	222.00	0.31139	YES	YES
40	a	266.53	1.71536	YES	YES
41	a	268.11	0.60357	YES	YES
42	a	272.67	5.55757	YES	YES
43	a	273.86	3.37602	YES	YES
44	a	275.38	2.99735	YES	YES
45	a	282.75	0.47869	YES	YES
46	a	283.11	0.61485	YES	YES
47	a	283.67	1.54211	YES	YES
48	a	284.01	0.91687	YES	YES
49	a	301.70	10.76504	YES	YES
50	a	302.33	10.08420	YES	YES
51	a	307.00	0.35496	YES	YES
52	a	314.43	0.62446	YES	YES
53	a	314.74	0.27253	YES	YES
54	a	316.51	1.39447	YES	YES
55	a	318.60	2.64314	YES	YES
56	a	318.84	2.30745	YES	YES
57	a	323.90	0.09732	YES	YES
58	a	347.22	6.02074	YES	YES
59	a	347.44	2.20896	YES	YES
60	a	349.63	12.04850	YES	YES
61	a	351.59	11.03656	YES	YES
62	a	355.49	6.00451	YES	YES
63	a	379.73	1.10066	YES	YES
64	a	430.86	75.26764	YES	YES
65	a	435.11	70.20334	YES	YES
66	a	490.73	39.68716	YES	YES
67	a	517.40	4.86132	YES	YES
68	a	518.86	2.65198	YES	YES
69	a	519.56	3.43448	YES	YES
70	a	519.84	5.24830	YES	YES
71	a	520.30	6.01949	YES	YES

72	a	520.72	5.37761	YES	YES
73	a	523.25	3.40852	YES	YES
74	a	524.31	2.71389	YES	YES
75	a	525.47	2.93634	YES	YES
76	a	543.69	26.29105	YES	YES
77	a	544.56	27.21904	YES	YES
78	a	547.10	53.67128	YES	YES
79	a	553.01	0.26748	YES	YES
80	a	554.30	0.22868	YES	YES
81	a	554.76	3.97591	YES	YES
82	a	554.87	1.32027	YES	YES
83	a	555.85	8.79787	YES	YES
84	a	556.19	9.00498	YES	YES
85	a	706.65	7.89337	YES	YES
86	a	707.18	13.54449	YES	YES
87	a	707.31	6.21422	YES	YES
88	a	708.33	59.72729	YES	YES
89	a	709.23	53.97229	YES	YES
90	a	709.65	63.00492	YES	YES
91	a	729.06	6.70316	YES	YES
92	a	734.70	4.26015	YES	YES
93	a	735.04	4.09449	YES	YES
94	a	785.20	10.87258	YES	YES
95	a	809.73	24.45019	YES	YES
96	a	812.52	25.24429	YES	YES
97	a	953.36	16.27978	YES	YES
98	a	954.62	20.33037	YES	YES
99	a	954.95	55.82170	YES	YES
100	a	958.77	261.90284	YES	YES
101	a	960.70	224.50323	YES	YES
102	a	961.87	199.10786	YES	YES
103	a	1111.30	6.88201	YES	YES
104	a	1114.04	7.63998	YES	YES
105	a	1118.75	2.83258	YES	YES
106	a	1129.91	5.31402	YES	YES
107	a	1131.14	0.94595	YES	YES
108	a	1132.56	5.02550	YES	YES
109	a	1135.14	22.23266	YES	YES
110	a	1137.86	6.93568	YES	YES
111	a	1138.69	12.63796	YES	YES
112	a	1194.46	11.33500	YES	YES
113	a	1198.01	39.73353	YES	YES
114	a	1200.16	22.64615	YES	YES
115	a	1201.87	36.37715	YES	YES
116	a	1207.48	3.38990	YES	YES
117	a	1208.00	35.60104	YES	YES
118	a	1214.99	811.77493	YES	YES
119	a	1215.62	997.18878	YES	YES
120	a	1231.47	783.54856	YES	YES
121	a	1232.60	528.02107	YES	YES
122	a	1237.07	7.80039	YES	YES
123	a	1238.67	100.78054	YES	YES
124	a	1242.19	39.39403	YES	YES
125	a	1244.72	25.88982	YES	YES
126	a	1250.51	36.26672	YES	YES
127	a	1252.08	572.65387	YES	YES
128	a	1257.26	842.96972	YES	YES
129	a	1261.69	888.42989	YES	YES
130	a	1337.38	281.83666	YES	YES
131	a	1340.49	347.87647	YES	YES
132	a	1358.69	50.66758	YES	YES

\$nmr dft shielding constants

#	NO.	TYPE	MULT.	ISOTROPIC	ANISOTROPIC	dD/dB-CONTRIBUTION
	1	cl	1	998.46924850	137.14998330	-160.07018370
	2	al	1	542.74795381	34.28169431	-273.51212791
	3	o	1	284.27130662	41.87672482	-135.02357429
	4	o	1	284.78958344	38.76282512	-134.52510209
	5	o	1	284.35539936	39.84622405	-136.02549101
	6	f	1	261.48016645	122.14184823	-225.42554925
	7	f	1	263.24505913	120.28123875	-226.98871834
	8	f	1	263.02644908	119.32484761	-218.99632919
	9	c	1	102.03468728	25.53507655	-157.25094365
	10	f	1	263.48587847	120.88937729	-225.00767096
	11	f	1	260.90934477	120.48199108	-227.20311974
	12	f	1	262.02925352	116.03537819	-219.09840552
	13	c	1	102.16822067	25.63385833	-158.25372384
	14	f	1	263.12028895	119.26021077	-220.63729926
	15	f	1	262.55734582	117.96483217	-225.67355157
	16	f	1	262.59700125	120.72268802	-224.48021643
	17	c	1	102.22291707	26.19417168	-157.12804463
	18	f	1	263.49517953	121.58810358	-209.98137641
	19	f	1	263.30649614	120.84589157	-214.79086737
	20	c	1	56.79850551	13.23022581	-201.61106191
	21	c	1	56.31231275	13.01542974	-201.36746839
	22	c	1	56.40511398	12.43120063	-202.55352755
	23	c	1	56.81328124	12.82677219	-200.63088307
	24	c	1	57.06918340	14.20281781	-202.40772463
	25	c	1	56.19125869	11.91584177	-202.29531997
	26	c	1	56.57792007	12.98767734	-202.35518857
	27	c	1	56.25035227	12.61533807	-201.42666043
	28	c	1	56.96100955	13.00413225	-201.40931089
	29	f	1	261.07658658	121.49372598	-221.72765950
	30	f	1	262.80576982	125.52704213	-199.08313972
	31	f	1	262.40528027	128.35703657	-203.23681149
	32	f	1	262.64539458	123.77884260	-211.09685573
	33	f	1	262.43148168	126.67921188	-200.80252595
	34	f	1	262.14764785	127.09934559	-201.23422728
	35	f	1	261.22233334	119.38300024	-221.60632553
	36	f	1	263.53330161	125.25241744	-202.58876575
	37	f	1	262.63362665	123.04918366	-216.39161692
	38	f	1	261.77706274	126.80519255	-201.80681455
	39	f	1	261.34289624	118.97166647	-217.19503594
	40	f	1	261.58317713	126.98407365	-201.41399625
	41	f	1	262.84759310	122.55885241	-212.74397231
	42	f	1	262.06877026	126.60334267	-202.42285065
	43	f	1	263.55523907	121.22175636	-217.56715042
	44	f	1	263.22649989	125.19159330	-199.35684570



Total energy = -3619.6174856330 H = -98494.8592486 eV

HOMO-LUMO Separation

HOMO: 177. 177 a -0.12556432 H = -3.41678 eV

LUMO: 178. 178 a +0.11683005 H = +3.17911 eV

Gap : +0.24239438 H = +6.59589 eV

Number of MOs= 608, Electrons= 354.00, Symmetry: c1

\$scoord

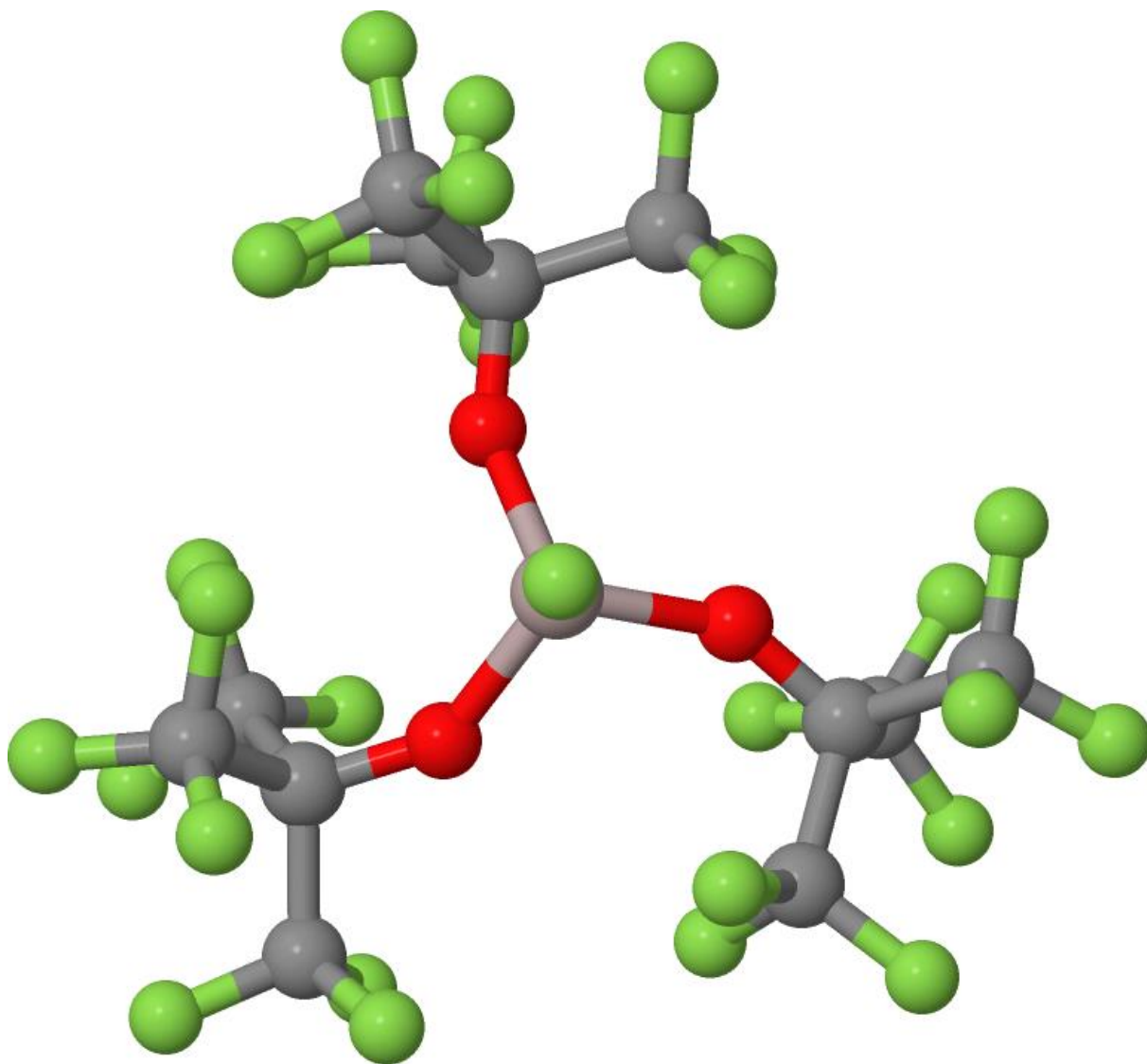
-0.22511210882741	-1.27012386941445	0.93767598478694	al
3.03217926405380	-0.38999630319597	0.54746853120496	o
5.44175095884593	-0.96992400009525	1.12311907998981	c
7.19775784118008	0.06925079984587	-1.05754805569476	c
6.48249600706234	2.39967266187512	-1.74788568475610	f
9.66644178824096	0.18190248086971	-0.36309384490676	f
7.05857455106006	-1.42483163649940	-3.12469651113375	f
5.87159689486081	-3.91876214804070	1.37003243907861	c
8.34759145092260	-4.57205453008366	1.21564423792886	f
4.63365564824187	-5.15052854214321	-0.47136193335415	f
4.99936074805072	-4.78879689093360	3.60520980030373	f
6.23567107312059	0.32142436523246	3.69719547134692	c
8.41533890150194	-0.63193924374741	4.65515892669211	f
4.41967194797731	-0.00212781507415	5.44267393587668	f
6.57515512174807	2.83168429949586	3.39253619179250	f
-2.50401683343371	3.67272584974814	2.78079240405479	c
-5.21429081343048	3.77492638605725	4.03255273269740	c
-6.31404058521140	6.08201073907877	3.81567230776466	f
-6.76271963538711	2.07632813936223	2.96189558434357	f
-5.08545457056642	3.22639283928489	6.52596598999788	f
-0.57517410234401	5.11869457622620	4.54730203846792	c
0.04224149865231	3.68750016792513	6.54753862148778	f
-1.51566580742464	7.33337149257654	5.43851463030293	f
1.57675154070771	5.65817999379107	3.28620435606496	f
-2.60980115293345	5.06585077815828	0.14238138189924	c
-2.66360743436110	7.62032212734784	0.38268949246916	f
-4.68838780969889	4.38426761352937	-1.16800806213408	f
-0.57988980331982	4.46401693957300	-1.25243068292038	f
-1.42379813055616	-1.35422599970091	-2.24450452409471	o
-2.95534447355057	-2.59919781896437	-3.85120250771084	c
-2.02587936428969	-5.40783593417856	-4.28011909694903	c
-2.66072055637340	-6.88467115270287	-2.29456897869284	f
-3.03439930811179	-6.47721327886947	-6.38221011568104	f
0.49863210908223	-5.48118086138526	-4.51198365803290	f
-5.76937872115142	-2.67117137574867	-2.85032656544099	c
-6.90493471967617	-0.40715977980872	-3.14840928990353	f
-5.80747550572714	-3.22810299097692	-0.37099731540057	f
-7.20955341806931	-4.41417064334325	-4.06144311381069	f
-2.90617207591043	-1.16533054060258	-6.46859276519129	c
-0.71825682089527	-1.61912804861267	-7.70852829574967	f
-3.08584888920179	1.33750468351625	-6.12677775144163	f
-4.82460702997305	-1.88375130797549	-8.01582818493353	f
-1.81964060111596	1.23342505423610	2.55447641141454	o
-0.61069707376889	-3.82722727563236	2.49781638796734	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	5.58	0.02652	YES	YES
8		a	12.26	0.00423	YES	YES
9		a	14.90	0.05777	YES	YES

10	a	17.82	0.01622	YES	YES
11	a	25.48	0.16007	YES	YES
12	a	29.94	0.17458	YES	YES
13	a	32.09	0.11871	YES	YES
14	a	47.06	0.01434	YES	YES
15	a	54.61	0.00600	YES	YES
16	a	61.36	0.03964	YES	YES
17	a	63.47	0.07187	YES	YES
18	a	66.25	0.05401	YES	YES
19	a	70.59	0.03307	YES	YES
20	a	71.10	0.11584	YES	YES
21	a	75.29	0.02160	YES	YES
22	a	76.31	0.09707	YES	YES
23	a	79.31	0.04347	YES	YES
24	a	80.28	0.06967	YES	YES
25	a	83.89	0.08393	YES	YES
26	a	85.53	0.24128	YES	YES
27	a	97.06	0.39185	YES	YES
28	a	150.08	0.12043	YES	YES
29	a	153.37	0.01994	YES	YES
30	a	154.38	0.17328	YES	YES
31	a	156.22	0.12597	YES	YES
32	a	159.21	0.01546	YES	YES
33	a	162.21	0.18335	YES	YES
34	a	183.74	3.05869	YES	YES
35	a	187.70	3.24695	YES	YES
36	a	202.45	0.23211	YES	YES
37	a	237.59	0.53635	YES	YES
38	a	256.86	0.00770	YES	YES
39	a	258.62	0.01266	YES	YES
40	a	262.55	3.13369	YES	YES
41	a	272.39	4.26617	YES	YES
42	a	276.31	2.65292	YES	YES
43	a	283.38	0.04612	YES	YES
44	a	283.61	0.14301	YES	YES
45	a	283.79	0.08243	YES	YES
46	a	295.10	4.33035	YES	YES
47	a	298.58	8.02448	YES	YES
48	a	299.86	9.53049	YES	YES
49	a	306.30	0.16040	YES	YES
50	a	307.18	0.73918	YES	YES
51	a	310.02	0.09249	YES	YES
52	a	312.67	0.25975	YES	YES
53	a	317.57	0.86187	YES	YES
54	a	320.02	1.24347	YES	YES
55	a	329.33	1.01206	YES	YES
56	a	333.56	0.71271	YES	YES
57	a	340.29	0.32311	YES	YES
58	a	341.53	1.98163	YES	YES
59	a	354.74	8.41990	YES	YES
60	a	358.81	13.53650	YES	YES
61	a	388.78	15.54287	YES	YES
62	a	425.18	71.86673	YES	YES
63	a	442.78	21.55337	YES	YES
64	a	516.84	3.87927	YES	YES
65	a	517.20	1.37020	YES	YES
66	a	517.52	3.04654	YES	YES
67	a	518.52	7.02546	YES	YES
68	a	518.60	1.40251	YES	YES
69	a	519.16	7.16868	YES	YES
70	a	520.15	7.47300	YES	YES
71	a	521.64	2.48070	YES	YES

72	a	522.72	2.18253	YES	YES
73	a	528.24	2.91049	YES	YES
74	a	535.19	4.38392	YES	YES
75	a	537.86	12.06940	YES	YES
76	a	552.41	0.30827	YES	YES
77	a	552.73	0.96750	YES	YES
78	a	553.39	0.99764	YES	YES
79	a	553.60	2.29679	YES	YES
80	a	553.88	0.07163	YES	YES
81	a	554.85	2.04376	YES	YES
82	a	662.78	215.31700	YES	YES
83	a	689.24	216.29136	YES	YES
84	a	705.64	7.85152	YES	YES
85	a	707.19	10.32462	YES	YES
86	a	707.71	56.32099	YES	YES
87	a	708.89	61.65612	YES	YES
88	a	709.04	75.44830	YES	YES
89	a	709.60	32.53561	YES	YES
90	a	723.34	5.79443	YES	YES
91	a	732.72	17.02207	YES	YES
92	a	733.92	44.68562	YES	YES
93	a	772.23	4.63822	YES	YES
94	a	790.91	71.34598	YES	YES
95	a	796.06	33.64434	YES	YES
96	a	948.02	1.38157	YES	YES
97	a	953.84	191.22071	YES	YES
98	a	955.53	164.67730	YES	YES
99	a	956.34	81.60784	YES	YES
100	a	956.56	8.26144	YES	YES
101	a	960.38	344.97227	YES	YES
102	a	1107.98	5.31128	YES	YES
103	a	1109.05	7.86308	YES	YES
104	a	1113.82	5.11788	YES	YES
105	a	1126.56	3.08646	YES	YES
106	a	1128.43	1.32770	YES	YES
107	a	1129.72	2.86743	YES	YES
108	a	1132.56	10.34364	YES	YES
109	a	1132.99	32.47443	YES	YES
110	a	1135.28	12.92562	YES	YES
111	a	1192.38	8.21299	YES	YES
112	a	1195.53	25.29299	YES	YES
113	a	1198.52	44.73947	YES	YES
114	a	1200.58	18.90819	YES	YES
115	a	1202.89	27.77602	YES	YES
116	a	1206.86	59.19878	YES	YES
117	a	1211.84	1018.65098	YES	YES
118	a	1213.57	910.71966	YES	YES
119	a	1228.71	666.94398	YES	YES
120	a	1230.55	422.17834	YES	YES
121	a	1233.73	46.55933	YES	YES
122	a	1235.75	25.95411	YES	YES
123	a	1238.17	123.49547	YES	YES
124	a	1242.62	44.05698	YES	YES
125	a	1246.93	151.99279	YES	YES
126	a	1251.10	627.59085	YES	YES
127	a	1255.65	488.87601	YES	YES
128	a	1257.04	1000.68841	YES	YES
129	a	1329.16	298.05087	YES	YES
130	a	1331.51	278.93962	YES	YES
131	a	1349.56	37.57090	YES	YES
132	a	1905.21	193.66737	YES	YES



Total energy = -3718.8776285440 H = -101195.8667014 eV

HOMO-LUMO Separation

HOMO: 181. 181 a -0.14308004 H = -3.89341 eV

LUMO: 182. 182 a +0.11135517 H = +3.03013 eV

Gap : +0.25443521 H = +6.92354 eV

Number of MOs= 620, Electrons= 362.00, Symmetry: c1

\$coord

4.75656215040162	0.06425475780692	-0.22222787026356	f
1.56542419801456	-0.05740933615383	-0.10516192524327	al
0.29066039337122	-2.50391094671476	-2.02108903398312	o
0.41753136755074	-0.61779025299462	3.00429705797027	o
0.13462126664955	2.79218870229235	-1.14340442193112	o
2.90006138816457	-5.61244736830489	1.10254468369572	f
-4.39889807971409	-4.18307330450695	-1.37351743784920	f
1.47367676206175	-4.36474378183864	-6.54387476139797	f
-0.03275116271742	-5.01473638160320	-2.30249623495089	c
-4.31442366314188	0.83692707400813	3.97308443929977	f
2.97086629628122	3.68208880680474	4.17048046454250	f
1.53542723151895	-3.52318029922173	6.93499303553861	f
0.01370355691471	0.43244171400280	5.29049992564938	c
2.30156702023404	7.27378484649512	-0.28925785474432	f
-4.53497029316843	4.03345623061348	-2.46341236944217	f
2.20215835775468	1.64307125871590	-5.71996816094550	f
-0.05345697183379	4.50405923043921	-3.01864913198543	c
4.31697095602248	0.79825422376993	6.76620001252460	f
4.09083866465904	-6.11775418609421	-3.91206186535125	f
0.73257856590400	-6.53272892039362	0.15052072951114	c
-2.90880434824010	-5.54716312697340	-2.90176614355882	c
1.63221778902325	-5.97038804399870	-4.58821223449019	c
-2.50905939212708	2.03848822499055	5.28510995060343	c
2.28080611500489	2.18781634156973	6.10485588136824	c
-0.26259354773371	-1.77186616036854	7.28189855783635	c
2.04893834286421	6.60688168553957	-2.72211873754409	c
-2.73905379842312	5.78515054130077	-2.81575152373037	c
0.22541999559764	3.24053506783826	-5.70471359161244	c
-1.06054994255434	-6.32716176180922	1.94803635511251	f
1.08241954042186	-9.03205699107157	-0.30379385761181	f
-3.52924739249610	-8.01994933692398	-2.61196565434166	f
-3.47552558970654	-4.90256645134431	-5.30765099788070	f
0.92089953010226	-8.28990575094201	-5.42250365180876	f
-3.40990536162438	2.45363437106379	7.65414127621110	f
-2.14581499560467	4.31793025709777	4.20406328398495	f
1.69960839478552	3.69552533084566	8.09298599396848	f
-2.52590910433424	-2.92846161764543	7.04368337175053	f
-0.08072962782797	-0.93688416292730	9.70145566865470	f
4.31414781055457	5.75286178952600	-3.52867876714706	f
1.50936185925988	8.72800331113731	-4.06286243772885	f
-2.82539090297013	7.39253921851821	-0.83408805743466	f
-3.35422890326283	7.12614136765744	-4.91462769523488	f
-1.85743053909328	1.90477509724988	-6.30991704542750	f
0.60227606345674	4.96336873254727	-7.56507922458269	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	selection rules RAMAN
#						
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	11.41	0.02389	YES	YES

8	a	13.00	0.01470	YES	YES
9	a	16.78	0.10091	YES	YES
10	a	17.99	0.03581	YES	YES
11	a	23.33	0.12680	YES	YES
12	a	24.89	0.19022	YES	YES
13	a	34.55	0.03112	YES	YES
14	a	39.77	0.03906	YES	YES
15	a	51.80	0.01623	YES	YES
16	a	64.48	0.11964	YES	YES
17	a	66.55	0.25920	YES	YES
18	a	69.28	0.12142	YES	YES
19	a	72.32	0.07834	YES	YES
20	a	73.24	0.06028	YES	YES
21	a	75.77	0.12775	YES	YES
22	a	81.58	0.04535	YES	YES
23	a	83.55	0.00975	YES	YES
24	a	83.69	0.05908	YES	YES
25	a	85.20	0.29779	YES	YES
26	a	89.22	0.30134	YES	YES
27	a	96.98	0.19665	YES	YES
28	a	133.18	1.99898	YES	YES
29	a	136.36	2.00153	YES	YES
30	a	149.81	0.23767	YES	YES
31	a	157.00	0.33409	YES	YES
32	a	157.85	0.14175	YES	YES
33	a	160.01	0.17165	YES	YES
34	a	165.97	1.62871	YES	YES
35	a	167.76	1.36071	YES	YES
36	a	191.76	1.38867	YES	YES
37	a	194.45	7.30085	YES	YES
38	a	196.06	6.69654	YES	YES
39	a	228.89	0.19194	YES	YES
40	a	268.04	1.83759	YES	YES
41	a	269.39	1.04649	YES	YES
42	a	273.70	4.00074	YES	YES
43	a	277.47	2.97210	YES	YES
44	a	278.87	3.61005	YES	YES
45	a	283.00	0.09847	YES	YES
46	a	283.37	0.11735	YES	YES
47	a	284.00	0.13147	YES	YES
48	a	289.19	3.89422	YES	YES
49	a	302.11	11.47712	YES	YES
50	a	303.03	11.05958	YES	YES
51	a	307.43	0.10390	YES	YES
52	a	315.41	0.51576	YES	YES
53	a	315.69	0.10467	YES	YES
54	a	317.81	1.97132	YES	YES
55	a	320.32	3.64940	YES	YES
56	a	320.78	3.10003	YES	YES
57	a	326.28	0.33317	YES	YES
58	a	348.36	2.27057	YES	YES
59	a	350.44	0.82982	YES	YES
60	a	355.82	12.30095	YES	YES
61	a	357.91	25.67765	YES	YES
62	a	359.53	24.65554	YES	YES
63	a	404.17	7.49186	YES	YES
64	a	439.00	84.21402	YES	YES
65	a	443.17	76.26540	YES	YES
66	a	515.54	0.19779	YES	YES
67	a	517.11	5.03775	YES	YES
68	a	518.89	3.21649	YES	YES
69	a	519.30	2.59770	YES	YES

70	a	519.73	5.71731	YES	YES
71	a	519.93	8.23158	YES	YES
72	a	521.00	6.23438	YES	YES
73	a	523.24	3.07612	YES	YES
74	a	524.47	2.37100	YES	YES
75	a	527.59	0.17941	YES	YES
76	a	545.90	33.43144	YES	YES
77	a	546.47	32.02923	YES	YES
78	a	552.85	0.48432	YES	YES
79	a	554.06	0.23743	YES	YES
80	a	554.53	1.58859	YES	YES
81	a	554.76	0.86924	YES	YES
82	a	555.48	6.88878	YES	YES
83	a	557.28	13.22258	YES	YES
84	a	705.86	12.35032	YES	YES
85	a	706.81	7.33782	YES	YES
86	a	707.04	6.18993	YES	YES
87	a	708.15	70.26583	YES	YES
88	a	708.76	49.21528	YES	YES
89	a	709.29	63.14077	YES	YES
90	a	715.86	1.06427	YES	YES
91	a	734.24	7.42833	YES	YES
92	a	734.69	5.94022	YES	YES
93	a	758.50	8.37984	YES	YES
94	a	805.67	33.48755	YES	YES
95	a	808.72	32.45477	YES	YES
96	a	839.58	54.53907	YES	YES
97	a	954.13	18.54873	YES	YES
98	a	954.48	42.65520	YES	YES
99	a	955.70	60.53881	YES	YES
100	a	959.99	251.02350	YES	YES
101	a	961.91	263.65008	YES	YES
102	a	962.55	190.17153	YES	YES
103	a	1111.10	8.06744	YES	YES
104	a	1112.44	7.45118	YES	YES
105	a	1116.93	2.01436	YES	YES
106	a	1128.10	4.22237	YES	YES
107	a	1130.97	14.79205	YES	YES
108	a	1131.95	2.09370	YES	YES
109	a	1134.04	14.55960	YES	YES
110	a	1136.73	15.70889	YES	YES
111	a	1137.52	8.64226	YES	YES
112	a	1193.84	17.43614	YES	YES
113	a	1197.81	54.97016	YES	YES
114	a	1199.47	30.69681	YES	YES
115	a	1202.57	43.05266	YES	YES
116	a	1207.70	49.34032	YES	YES
117	a	1209.05	25.38143	YES	YES
118	a	1214.25	938.48032	YES	YES
119	a	1215.35	910.65933	YES	YES
120	a	1230.74	673.65797	YES	YES
121	a	1231.91	449.31655	YES	YES
122	a	1236.69	16.65653	YES	YES
123	a	1237.90	116.74737	YES	YES
124	a	1242.18	33.34116	YES	YES
125	a	1245.84	40.65169	YES	YES
126	a	1251.20	122.07520	YES	YES
127	a	1253.65	497.01621	YES	YES
128	a	1256.33	782.58610	YES	YES
129	a	1261.83	963.36704	YES	YES
130	a	1333.88	281.84160	YES	YES
131	a	1335.69	292.48951	YES	YES

132

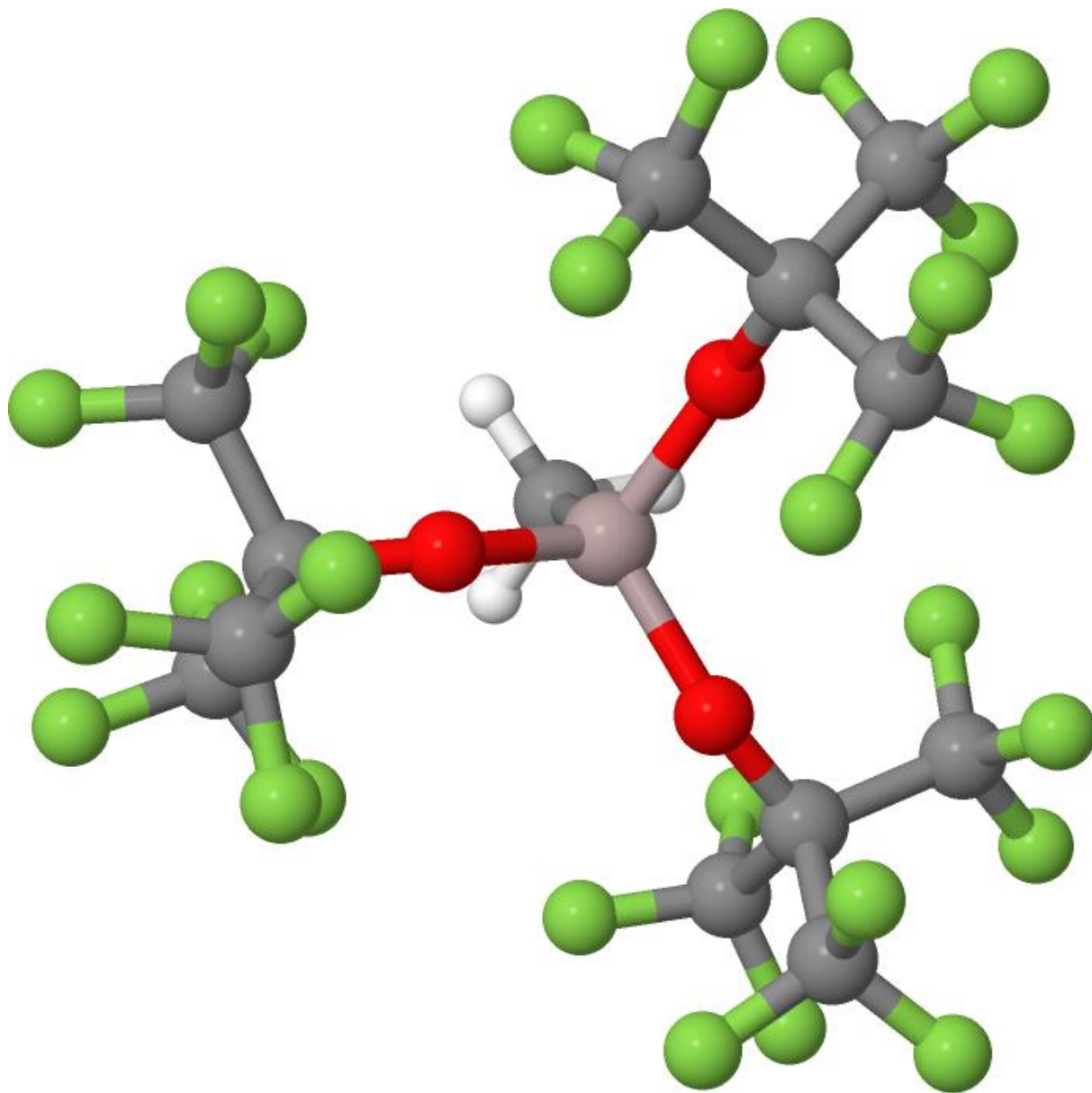
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1354.25

25.10213

YES

YES



Total energy = -3658.9100531590 H = -99564.0650205 eV

HOMO-LUMO Separation

HOMO: 181. 181 a -0.11724796 H = -3.19048 eV

LUMO: 182. 182 a +0.11668146 H = +3.17507 eV

Gap : +0.23392942 H = +6.36555 eV

Number of MOs= 626, Electrons= 362.00, Symmetry: c1

\$coord

-0.23268558088712	-0.30274495276767	-1.29142524918409	al
-1.86648285513644	2.32934247180660	0.10992082907064	o
-3.79498089423787	3.97752842493055	0.02004347612337	c
-4.32071097355186	4.94971748841273	2.79462077230706	c
-2.14991185646258	5.47950421906234	3.98752611475874	f
-5.77403545137776	7.06424931684429	2.84052651415927	f
-5.53376227833501	3.16018090767783	4.15610036335671	f
-6.30194916958896	2.73248483025113	-1.03176403364066	c
-8.40074220791080	4.08576652879981	-0.45358940765771	f
-6.60113287002884	0.40039111504814	-0.07930471097927	f
-6.21982937587240	2.51669727185127	-3.57919305227794	f
-3.10539669156251	6.31134632274718	-1.71428379499728	c
-5.15597945920697	7.72251287686590	-2.33837207413161	f
-2.03130132931464	5.51985646943772	-3.87698504664745	f
-1.44654088474452	7.86149879038132	-0.55081660393217	f
5.13122704721630	1.61773393586027	-0.31781366309783	c
7.43548452511474	0.94913872494562	-2.10189350085104	c
9.71004501554376	1.37030610896052	-0.99441775621620	f
7.35527615664891	-1.49044112350823	-2.78975258566392	f
7.36369858928441	2.34935918088496	-4.23978230821990	f
4.86135943290490	4.59234871605189	-0.18742085710879	c
3.76773466241506	5.47703844838646	-2.30122789369596	f
7.12888304907880	5.77251311764989	0.06367444959053	f
3.41842107463483	5.29286043344583	1.79050701300320	f
5.71411376066939	0.59036803944543	2.42414309933831	c
7.47445464089036	1.99612624625506	3.65453905259646	f
6.59466152045646	-1.80418850603196	2.31745385258431	f
3.61140164610296	0.57814271471386	3.83808890276751	f
-0.67396599580109	-2.79035646969423	0.99664145101500	o
-0.91011611155025	-5.28568362218250	1.41333455692680	c
-3.14987052710007	-6.47586634123083	-0.17874774108025	c
-2.44503179163975	-6.85100511160559	-2.60904829163612	f
-3.92948389897600	-8.73971451455624	0.73926446814755	f
-5.15607266231985	-4.92410914432434	-0.19787421097385	f
1.60610994186738	-6.74151888528340	0.72768251922266	c
3.39674869534473	-6.36114501256820	2.50153974680259	f
2.52711963121610	-5.90331262007323	-1.48820247139407	f
1.26623971462870	-9.27602583610645	0.51967479486334	f
-1.49360479788297	-5.69082661276971	4.31532623376910	c
-3.91811529024677	-5.08185285144258	4.84358599638010	f
-0.00751062759012	-4.21982012199544	5.74258476389874	f
-1.13765354329088	-8.12171637529355	5.06206288909748	f
3.04616282692697	0.54605246735252	-1.29268092416415	o
-1.26114524478148	-1.16538852377618	-4.76734529615140	c
-0.04497989776315	-2.68799839478508	-5.56334911617606	h
-1.09421437255022	0.50551694046199	-6.03682824824119	h
-3.25193529123410	-1.83486708853555	-4.87672302166030	h

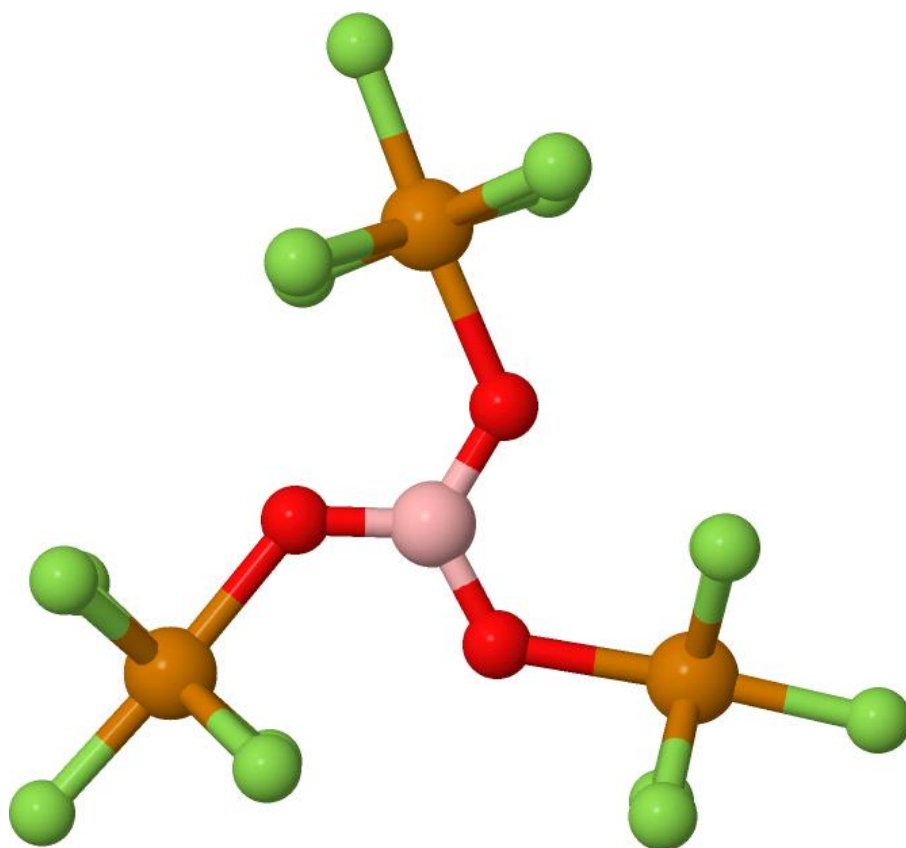
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	7.24	0.00455	YES	YES
8		a	11.82	0.00174	YES	YES
9		a	14.38	0.00510	YES	YES
10		a	22.83	0.01411	YES	YES
11		a	27.26	0.26548	YES	YES
12		a	28.41	0.06381	YES	YES
13		a	34.22	0.08510	YES	YES
14		a	51.29	0.05931	YES	YES
15		a	55.36	0.04875	YES	YES
16		a	64.17	0.06956	YES	YES
17		a	66.01	0.04484	YES	YES
18		a	68.70	0.03569	YES	YES
19		a	71.35	0.14144	YES	YES
20		a	72.92	0.03093	YES	YES
21		a	74.89	0.00671	YES	YES
22		a	77.13	0.00392	YES	YES
23		a	80.53	0.03679	YES	YES
24		a	82.29	0.14115	YES	YES
25		a	84.47	0.17478	YES	YES
26		a	86.50	0.12673	YES	YES
27		a	96.32	0.49358	YES	YES
28		a	117.40	0.24159	YES	YES
29		a	135.41	0.15097	YES	YES
30		a	143.23	0.00418	YES	YES
31		a	151.50	0.32545	YES	YES
32		a	153.04	0.07609	YES	YES
33		a	156.17	0.14117	YES	YES
34		a	157.85	0.25444	YES	YES
35		a	161.51	0.12727	YES	YES
36		a	163.24	0.41140	YES	YES
37		a	188.56	4.29148	YES	YES
38		a	188.95	4.00707	YES	YES
39		a	197.68	0.90270	YES	YES
40		a	234.19	0.04226	YES	YES
41		a	256.28	0.07990	YES	YES
42		a	263.03	3.69798	YES	YES
43		a	266.62	0.28472	YES	YES
44		a	272.41	6.46200	YES	YES
45		a	274.96	3.36778	YES	YES
46		a	281.38	0.05045	YES	YES
47		a	283.21	0.09178	YES	YES
48		a	283.69	0.09706	YES	YES
49		a	288.23	6.72433	YES	YES
50		a	298.63	12.86325	YES	YES
51		a	300.45	10.01737	YES	YES
52		a	306.18	0.41271	YES	YES
53		a	309.28	0.11348	YES	YES
54		a	311.70	0.34398	YES	YES
55		a	312.38	0.50700	YES	YES
56		a	317.14	1.97411	YES	YES
57		a	319.46	1.83235	YES	YES
58		a	326.36	1.52093	YES	YES
59		a	338.55	5.05423	YES	YES

60	a	340.13	3.58061	YES	YES
61	a	340.31	0.90882	YES	YES
62	a	354.30	9.89345	YES	YES
63	a	359.24	13.17285	YES	YES
64	a	383.95	25.57575	YES	YES
65	a	417.54	67.83377	YES	YES
66	a	422.56	35.87188	YES	YES
67	a	510.25	0.18836	YES	YES
68	a	516.77	2.22319	YES	YES
69	a	517.23	5.97133	YES	YES
70	a	518.34	6.66375	YES	YES
71	a	518.69	5.40780	YES	YES
72	a	519.87	0.90698	YES	YES
73	a	520.32	4.21991	YES	YES
74	a	522.05	5.07616	YES	YES
75	a	522.79	4.03920	YES	YES
76	a	526.26	0.07187	YES	YES
77	a	532.72	8.64408	YES	YES
78	a	533.92	9.89052	YES	YES
79	a	552.21	0.19759	YES	YES
80	a	552.55	0.52369	YES	YES
81	a	553.23	0.43098	YES	YES
82	a	553.42	0.98165	YES	YES
83	a	553.81	0.54398	YES	YES
84	a	554.03	1.15093	YES	YES
85	a	624.65	47.31723	YES	YES
86	a	675.09	92.83545	YES	YES
87	a	677.44	77.43491	YES	YES
88	a	705.07	4.61802	YES	YES
89	a	706.84	41.11378	YES	YES
90	a	707.11	33.03890	YES	YES
91	a	707.78	9.47455	YES	YES
92	a	708.10	48.91843	YES	YES
93	a	708.83	76.87013	YES	YES
94	a	726.33	11.21815	YES	YES
95	a	731.79	19.49919	YES	YES
96	a	732.46	17.44425	YES	YES
97	a	775.85	12.14423	YES	YES
98	a	789.53	46.88277	YES	YES
99	a	794.79	35.17923	YES	YES
100	a	946.75	1.00197	YES	YES
101	a	951.83	118.44189	YES	YES
102	a	953.75	104.71500	YES	YES
103	a	954.58	125.97313	YES	YES
104	a	955.20	103.02586	YES	YES
105	a	958.36	333.17896	YES	YES
106	a	1105.68	5.35906	YES	YES
107	a	1107.35	5.35930	YES	YES
108	a	1112.66	7.12344	YES	YES
109	a	1123.65	7.33777	YES	YES
110	a	1128.59	2.92346	YES	YES
111	a	1130.42	1.76945	YES	YES
112	a	1131.52	6.10244	YES	YES
113	a	1132.21	34.03527	YES	YES
114	a	1134.68	12.20824	YES	YES
115	a	1189.65	48.10062	YES	YES
116	a	1191.21	12.58267	YES	YES
117	a	1193.26	46.81988	YES	YES
118	a	1196.77	51.12733	YES	YES
119	a	1198.64	30.52606	YES	YES
120	a	1202.97	32.29786	YES	YES
121	a	1207.02	36.95867	YES	YES

122	a	1212.50	987.54226	YES	YES
123	a	1213.97	891.27070	YES	YES
124	a	1228.70	698.28297	YES	YES
125	a	1230.44	269.88166	YES	YES
126	a	1233.20	92.52735	YES	YES
127	a	1234.34	112.08761	YES	YES
128	a	1237.94	235.51213	YES	YES
129	a	1243.67	94.61648	YES	YES
130	a	1244.53	181.73836	YES	YES
131	a	1250.05	630.84923	YES	YES
132	a	1252.07	469.60697	YES	YES
133	a	1257.83	812.43591	YES	YES
134	a	1332.00	319.59988	YES	YES
135	a	1336.73	309.97958	YES	YES
136	a	1355.86	64.67843	YES	YES
137	a	1405.18	2.21214	YES	YES
138	a	1407.75	1.55330	YES	YES
139	a	2932.28	10.98508	YES	YES
140	a	3019.51	24.35505	YES	YES
141	a	3025.54	19.74539	YES	YES

B(OTeF₅)₃



Total energy = -1771.1939856690 H = -48196.6680216 eV

HOMO-LUMO Separation

HOMO: 91. 91 a -0.36725095 H = -9.99341 eV

LUMO: 92. 92 a -0.24931959 H = -6.78434 eV

Gap : +0.11793135 H = +3.20908 eV

Number of MOs= 305, Electrons= 182.00, Symmetry: c1

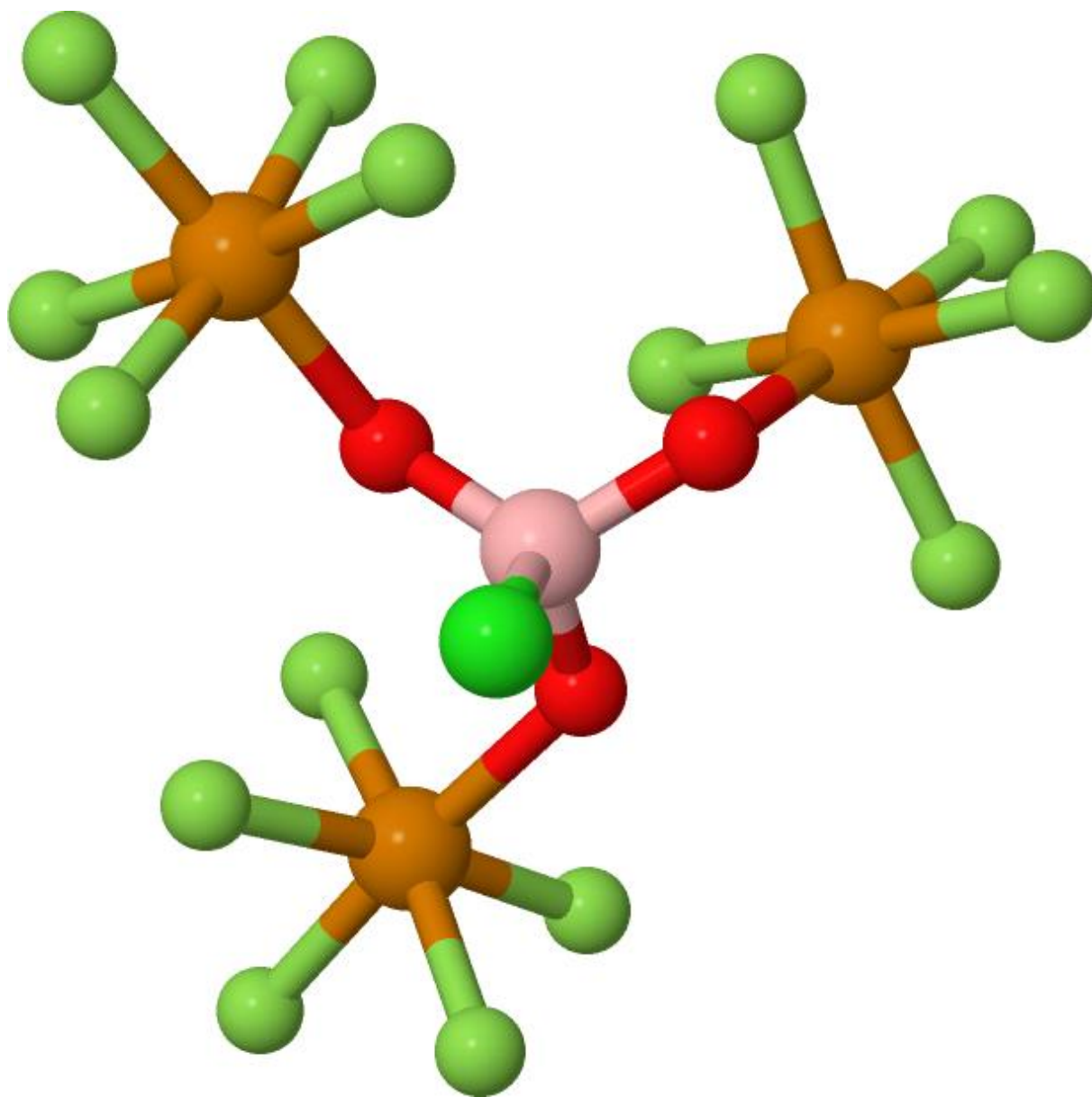
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-0.02564052118565	-0.05424541992051	-0.08454270270845	b
1.62872141175010	5.42293734449591	-0.00061167739023	te
1.55543609497826	9.03265296443863	0.05847669915737	f
4.17003000497895	5.43897722889097	2.56922162066224	f
1.91377428796531	1.68503659946597	-0.06306106382926	o
-0.93645042024892	5.36604050255005	2.56627002682810	f
-0.90103381431168	5.45167362421983	-2.60216645384213	f
4.21039139599854	5.51540696187568	-2.52777602886771	f
3.97686398050800	-4.09144332223974	0.00082653169852	te
7.22600030963748	-5.66489907586187	0.05843115878379	f
5.08224722091444	-1.81243616513308	2.60234751395788	f
0.52587700165617	-2.60299823189215	-0.07165221782988	o
5.16599408025938	-1.85290995363594	-2.59828428900563	f
2.90595319612335	-6.42808564041747	-2.54149832328048	f
2.82647717482859	-6.38307603960375	2.55001444668858	f
-5.60770824325998	-1.33012164014633	-0.00027339529909	te
-8.71384463633304	-3.16662015999105	0.14574493753658	f
-4.39895409722187	-3.64433003596723	-2.52191946073204	f
-2.49820994909348	0.76194336264438	-0.13826077040678	o
-6.97370274176239	0.75829152545404	-2.61598706191209	f
-6.86661311589774	0.96915694943031	2.48913852338700	f
-4.27376728667395	-3.42680190475740	2.64637234616899	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1		a	-2.49	0.00000	YES	YES
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7			0.00	0.00004	-	-
8		a	26.08	0.08729	YES	YES
9		a	31.31	0.09090	YES	YES
10		a	39.35	0.17822	YES	YES
11		a	47.98	0.00952	YES	YES
12		a	56.69	0.00504	YES	YES
13		a	66.84	0.00938	YES	YES
14		a	76.56	0.00327	YES	YES

15	a	80.33	0.03580	YES	YES
16	a	99.41	0.43366	YES	YES
17	a	106.69	0.39638	YES	YES
18	a	116.37	0.07672	YES	YES
19	a	154.20	0.21750	YES	YES
20	a	157.58	0.03700	YES	YES
21	a	162.21	0.05500	YES	YES
22	a	167.31	0.11606	YES	YES
23	a	168.13	0.04786	YES	YES
24	a	174.54	0.00371	YES	YES
25	a	199.76	7.09476	YES	YES
26	a	203.42	5.05641	YES	YES
27	a	212.52	1.60031	YES	YES
28	a	251.01	5.44498	YES	YES
29	a	253.03	4.74119	YES	YES
30	a	254.49	4.99593	YES	YES
31	a	257.04	0.60629	YES	YES
32	a	257.74	5.55691	YES	YES
33	a	259.92	62.72995	YES	YES
34	a	260.82	69.33072	YES	YES
35	a	262.20	23.49809	YES	YES
36	a	266.45	92.24727	YES	YES
37	a	269.42	25.57055	YES	YES
38	a	271.67	16.44272	YES	YES
39	a	273.02	67.88916	YES	YES
40	a	275.64	16.47364	YES	YES
41	a	278.01	7.17292	YES	YES
42	a	287.59	10.92511	YES	YES
43	a	373.47	109.96044	YES	YES
44	a	378.88	107.79430	YES	YES
45	a	451.59	0.24050	YES	YES
46	a	582.08	10.68481	YES	YES
47	a	582.43	10.89280	YES	YES
48	a	583.81	10.66198	YES	YES
49	a	591.17	0.43286	YES	YES
50	a	599.69	0.70768	YES	YES
51	a	599.82	1.21525	YES	YES
52	a	601.88	0.67966	YES	YES
53	a	630.24	29.37755	YES	YES
54	a	631.49	49.40684	YES	YES
55	a	640.99	0.38314	YES	YES
56	a	650.23	168.15782	YES	YES
57	a	653.38	182.78774	YES	YES
58	a	654.64	8.01422	YES	YES
59	a	655.80	0.79111	YES	YES
60	a	657.31	8.68786	YES	YES
61	a	661.43	34.38144	YES	YES
62	a	663.72	33.10829	YES	YES
63	a	664.66	257.23386	YES	YES
64	a	960.52	0.02589	YES	YES
65	a	1310.41	836.53364	YES	YES
66	a	1316.79	868.14417	YES	YES



Total energy = -2231.4767607140 H = -60721.6067265 eV

HOMO-LUMO Separation

HOMO: 100. 100 a -0.16388216 H = -4.45946 eV

LUMO: 101. 101 a -0.10846200 H = -2.95140 eV

Gap : +0.05542016 H = +1.50806 eV

Number of MOs= 323, Electrons= 200.00, Symmetry: c1

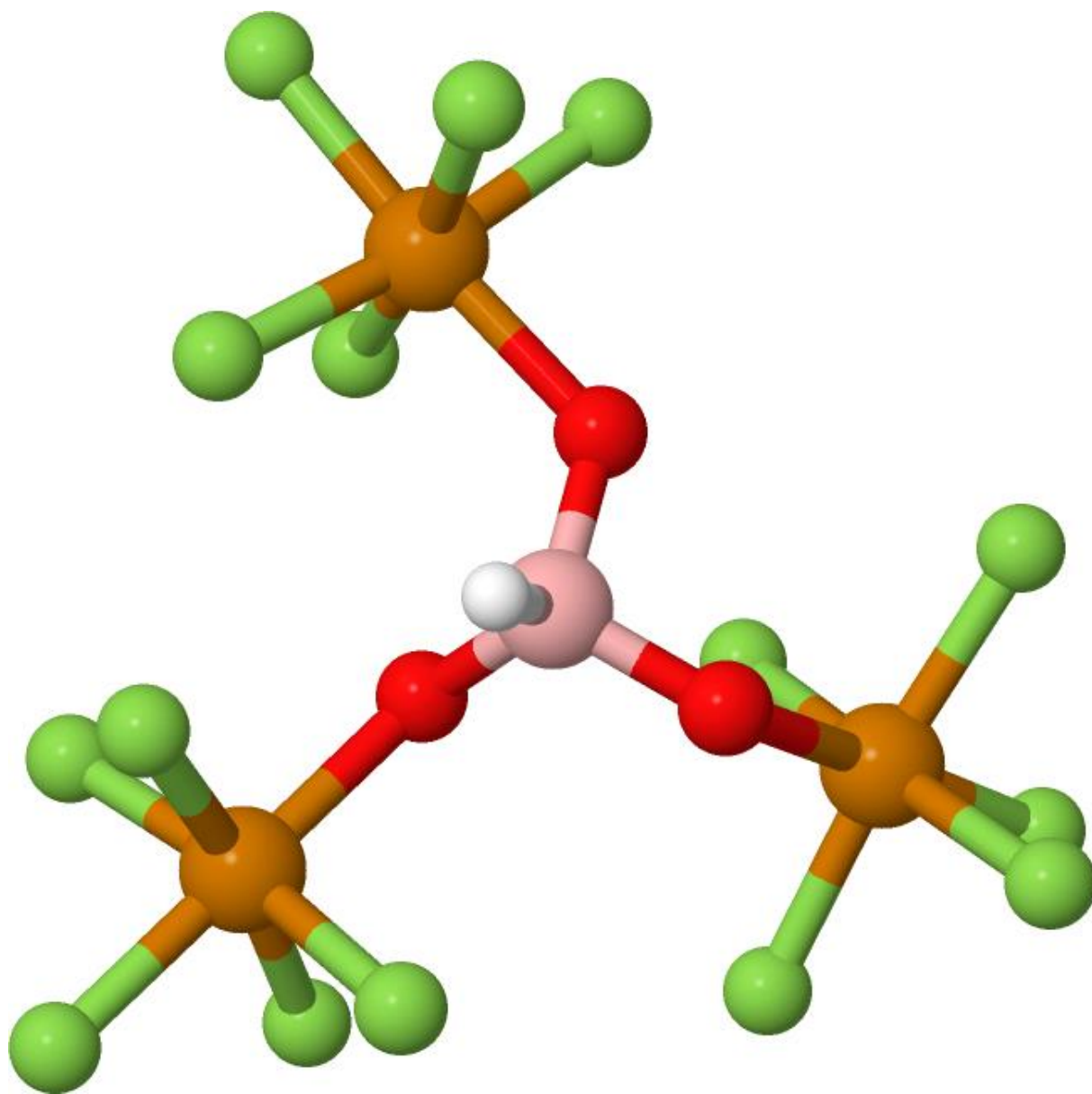
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-0.13709892759021	0.15192816504248	1.80190864151838	b
4.83167626579734	-1.97984580919021	-0.33472294858202	te
7.96264312032242	-3.82170202010918	-0.65430712418574	f
6.60349543809100	0.06913642409084	2.10476358546823	f
1.71736284225010	-0.08614992430073	-0.28015080916909	o
6.04664328016973	0.20202409403614	-2.97825491597309	f
3.54262467633081	-4.22868531891699	-2.89175497536240	f
3.93960235764953	-4.39069535100460	2.25834341078493	f
-4.08569695945727	-3.57520797829664	-0.08787789529809	te
-6.53917489712919	-5.25014436993102	-2.20324048812701	f
-5.36193620389812	-5.61621665277954	2.65486767042733	f
-1.67331665315759	-2.10712598227530	2.30752198748700	o
-1.79950649607762	-6.29184386246928	-0.97414700154271	f
-3.07651478878483	-1.73565773897971	-3.09068338745194	f
-6.70294427189325	-1.11090289177712	0.59139444427837	f
-0.95054928163989	5.44728277997459	-0.28203860253706	te
-0.29371557130040	8.81651164612249	-1.50944160383179	f
-0.09495144423431	4.31013758549902	-3.63661828506285	f
-1.91235941783998	2.14630807910600	0.96947699586623	o
2.56772865723972	5.36406388918266	0.68893007712765	f
-1.77025558288536	7.03199037195502	2.90178389973977	f
-4.39546856289623	5.93689681189310	-1.33973581843446	f
1.28454790157726	0.74594698236754	4.96304321584304	c1

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	15.82	0.02411	YES	YES
8		a	23.54	0.05913	YES	YES
9		a	24.70	0.03537	YES	YES
10		a	30.40	0.06224	YES	YES
11		a	43.25	0.01853	YES	YES
12		a	48.60	0.01420	YES	YES
13		a	65.05	0.14777	YES	YES
14		a	76.55	0.22564	YES	YES
15		a	83.33	0.16834	YES	YES
16		a	103.21	0.17275	YES	YES
17		a	107.32	0.11239	YES	YES
18		a	113.63	0.40005	YES	YES
19		a	121.24	0.14184	YES	YES
20		a	127.23	1.04717	YES	YES
21		a	162.34	0.59129	YES	YES
22		a	166.41	0.04238	YES	YES
23		a	171.88	0.11179	YES	YES
24		a	172.35	0.13051	YES	YES
25		a	182.18	0.63777	YES	YES
26		a	190.39	5.61317	YES	YES

27	a	197.14	2.80651	YES	YES
28	a	199.87	5.21926	YES	YES
29	a	201.01	0.46789	YES	YES
30	a	233.49	6.20447	YES	YES
31	a	242.91	1.61493	YES	YES
32	a	249.13	2.41774	YES	YES
33	a	249.81	1.24124	YES	YES
34	a	255.38	4.32357	YES	YES
35	a	267.26	99.83841	YES	YES
36	a	269.69	113.47373	YES	YES
37	a	274.46	4.27279	YES	YES
38	a	276.41	32.05524	YES	YES
39	a	278.27	32.97557	YES	YES
40	a	279.43	10.86083	YES	YES
41	a	280.21	21.48136	YES	YES
42	a	281.31	42.01114	YES	YES
43	a	287.52	26.68258	YES	YES
44	a	327.58	33.14057	YES	YES
45	a	337.44	55.85113	YES	YES
46	a	401.15	25.14967	YES	YES
47	a	441.76	11.31405	YES	YES
48	a	473.43	10.57105	YES	YES
49	a	543.43	46.55247	YES	YES
50	a	565.19	32.56281	YES	YES
51	a	576.71	4.13657	YES	YES
52	a	578.45	0.31060	YES	YES
53	a	584.45	1.13520	YES	YES
54	a	586.12	0.14113	YES	YES
55	a	590.77	9.88261	YES	YES
56	a	603.14	56.36149	YES	YES
57	a	613.39	30.99550	YES	YES
58	a	620.14	108.62665	YES	YES
59	a	628.55	70.20976	YES	YES
60	a	631.89	71.70853	YES	YES
61	a	638.20	95.19694	YES	YES
62	a	640.15	57.77270	YES	YES
63	a	643.02	143.79282	YES	YES
64	a	645.47	72.20434	YES	YES
65	a	650.67	38.52982	YES	YES
66	a	731.36	59.66882	YES	YES
67	a	849.09	113.26021	YES	YES
68	a	917.73	462.69750	YES	YES
69	a	964.26	517.19370	YES	YES



Total energy = -1771.9209019090 H = -48216.4484302 eV

HOMO-LUMO Separation

HOMO: 92. 92 a -0.17554507 H = -4.77683 eV

LUMO: 93. 93 a -0.10614593 H = -2.88838 eV

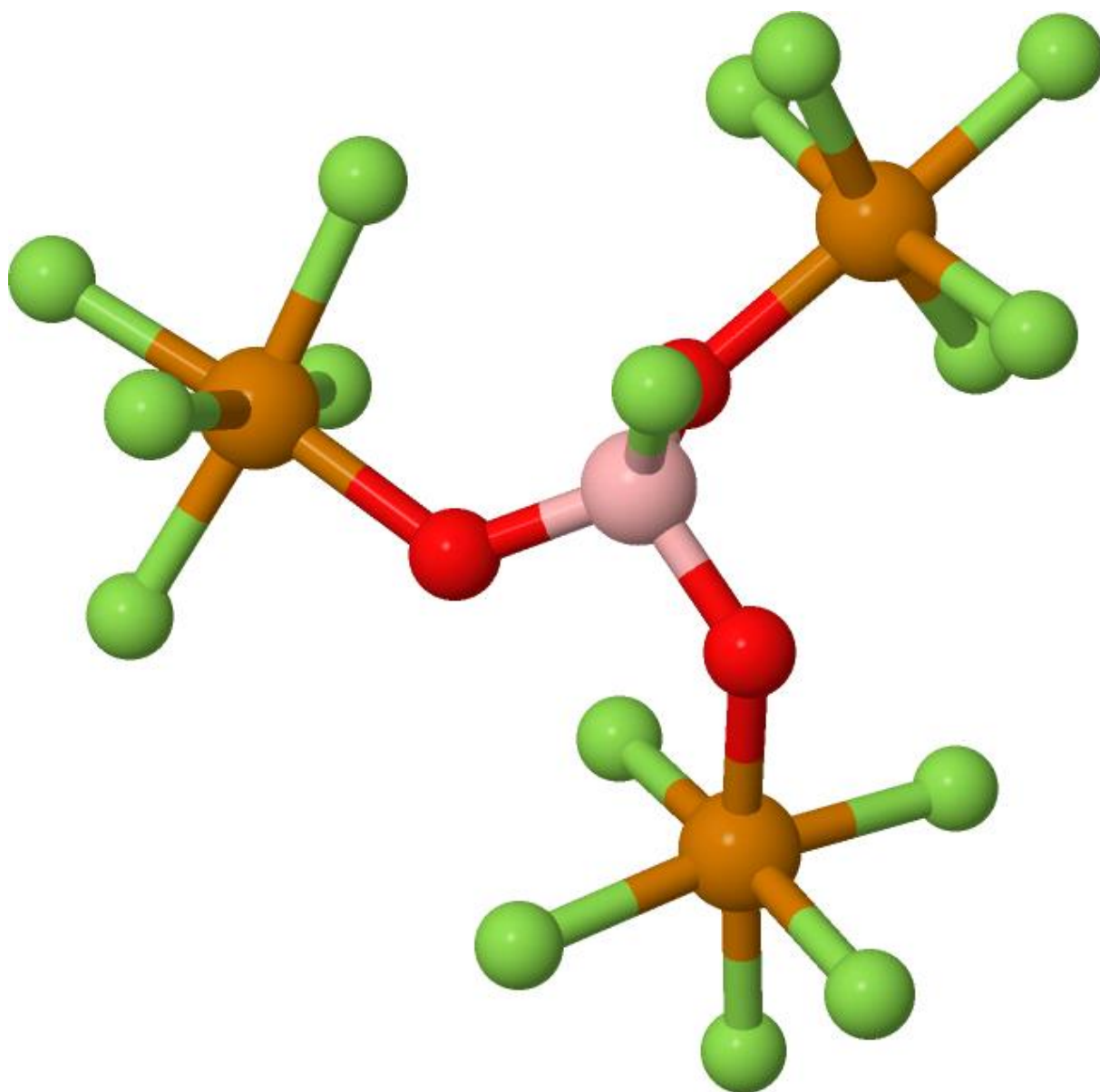
Gap : +0.06939915 H = +1.88845 eV

Number of MOs= 307, Electrons= 184.00, Symmetry: c1

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$coord
-0.18519813741495      0.04670118933361      1.71725860819176      b
-3.11405741770759     -4.53440864658206     -0.00760819361992     te
-3.83544419862201     -8.00146574847576     -0.87560513884863     f
-4.29588851295224     -5.40493532874048      3.34150341883223     f
-2.66223349266791     -1.02839831203615      0.89053892359112     o
 0.22717991189170     -5.69350382668322      0.92931253251464     f
-2.05589085035548     -4.14568308896580     -3.47492940341967     f
-6.53794906271940     -3.79051487717997     -0.98364608185698     f
-2.08894067445024      5.18183585254472      0.01516669108669     te
-3.44803863802133      7.88331731643281     -2.02584717184100     f
-5.55733886901352      4.50289434202721      0.98654168574407     f
-0.66370786811485      2.68780428020389      2.36963484973826     o
-2.47474156988926      3.05843697060457     -2.94724439300339     f
 1.20292425269789      6.24666082816270     -1.19707046155629     f
-1.86629403633193      7.64147844569899      2.71060378512833     f
 5.16771099877244     -0.62568130639318     -0.02750755941961     te
 8.79414961474487     -0.93307522208661      0.20833061294564     f
 5.79802940453425      1.74091065635328     -2.72291041862125     f
 1.56751650000638     -0.32718302496339     -0.47728419122330     o
 5.30845565973888     -3.33130106131608     -2.46116157085973     f
 5.06335966589406     -3.07551627801774      2.68130977426708     f
 5.46714323964631      2.05059300932544      2.44581471517097     f
 0.63290785745512     -0.80762367162073      3.73543072488727     h
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#           #           cm** (-1)        km/mol           IR      RAMAN
 1           1           0.00            0.00000          -        -
 2           2           0.00            0.00000          -        -
 3           3           0.00            0.00000          -        -
 4           4           0.00            0.00000          -        -
 5           5           0.00            0.00000          -        -
 6           6           0.00            0.00000          -        -
 7           7           a              7.35            0.02764          YES       YES
 8           8           a             20.67            0.03526          YES       YES
 9           9           a             26.79            0.00296          YES       YES
10          10           a             31.34            0.14747          YES       YES
11          11           a             35.72            0.00210          YES       YES
12          12           a             39.40            0.01213          YES       YES
13          13           a             69.23            0.20513          YES       YES
14          14           a             79.46            0.40599          YES       YES
15          15           a             91.52            0.09131          YES       YES
16          16           a            103.13            0.30897          YES       YES
17          17           a            104.72            0.12992          YES       YES
18          18           a            111.76            0.04299          YES       YES
19          19           a            162.24            0.68995          YES       YES
20          20           a            164.33            1.53600          YES       YES
21          21           a            168.29            0.41802          YES       YES
22          22           a            170.31            0.33869          YES       YES
23          23           a            174.87            0.45572          YES       YES
```

24	a	176.56	0.75284	YES	YES
25	a	188.81	4.06433	YES	YES
26	a	196.88	5.00432	YES	YES
27	a	198.15	0.00964	YES	YES
28	a	242.91	0.17249	YES	YES
29	a	245.13	2.77127	YES	YES
30	a	245.67	2.11990	YES	YES
31	a	253.70	14.46413	YES	YES
32	a	254.40	19.47101	YES	YES
33	a	264.65	91.62887	YES	YES
34	a	265.35	14.99331	YES	YES
35	a	272.46	49.08508	YES	YES
36	a	275.18	11.04183	YES	YES
37	a	275.46	45.40130	YES	YES
38	a	278.62	28.54175	YES	YES
39	a	278.85	4.15010	YES	YES
40	a	280.86	32.48440	YES	YES
41	a	284.96	19.98895	YES	YES
42	a	289.44	43.46401	YES	YES
43	a	348.57	90.59359	YES	YES
44	a	397.11	37.22181	YES	YES
45	a	463.60	11.30267	YES	YES
46	a	503.42	1.16171	YES	YES
47	a	555.20	77.45137	YES	YES
48	a	563.58	25.75713	YES	YES
49	a	575.18	0.95720	YES	YES
50	a	576.18	0.01313	YES	YES
51	a	581.69	2.52125	YES	YES
52	a	583.31	0.47496	YES	YES
53	a	599.38	45.15339	YES	YES
54	a	609.48	74.02013	YES	YES
55	a	614.06	99.88149	YES	YES
56	a	624.73	68.24153	YES	YES
57	a	628.98	80.36216	YES	YES
58	a	635.54	97.14982	YES	YES
59	a	637.33	78.69054	YES	YES
60	a	640.70	70.83753	YES	YES
61	a	642.03	160.33596	YES	YES
62	a	643.89	44.43145	YES	YES
63	a	679.25	17.31113	YES	YES
64	a	808.89	170.62828	YES	YES
65	a	869.10	298.66790	YES	YES
66	a	920.58	197.21911	YES	YES
67	a	1023.64	205.78905	YES	YES
68	a	1041.21	171.37129	YES	YES
69	a	2417.30	108.35728	YES	YES



Total energy = -1871.1577298640 H = -50916.8214504 eV

HOMO-LUMO Separation

HOMO: 96. 96 a -0.19533229 H = -5.31527 eV

LUMO: 97. 97 a -0.10545689 H = -2.86963 eV

Gap : +0.08987541 H = +2.44564 eV

Number of MOs= 319, Electrons= 192.00, Symmetry: c1

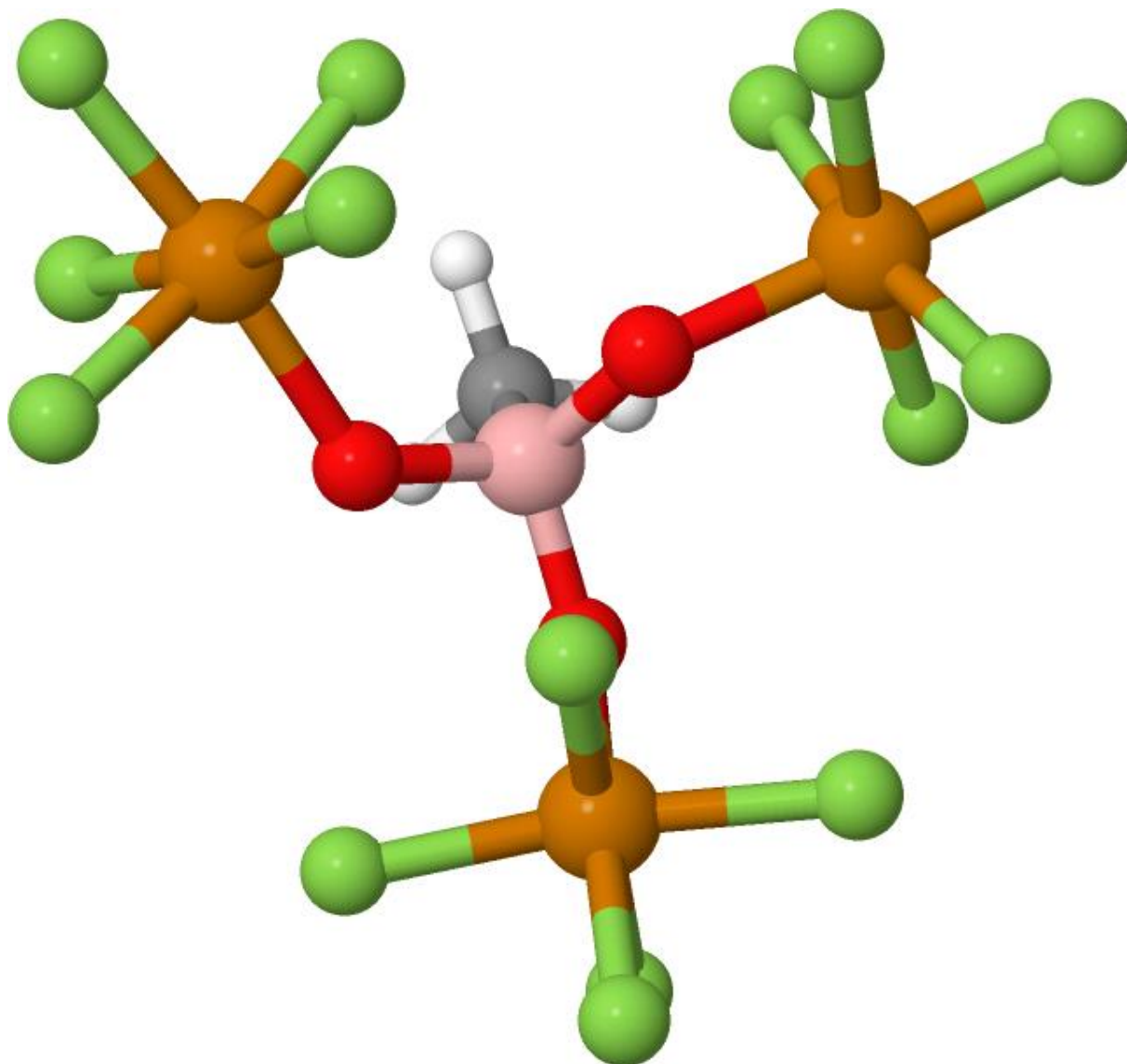
\$scoord

-0.01247064193748	0.04240957012829	1.66424647873926	b
4.98791746285881	-1.91360025900473	-0.30466564068989	te
8.25393042737512	-3.53933489839392	-0.33664080722174	f
6.44392457115112	0.32495432171472	2.17986968875710	f
1.74949631632133	-0.26698332533471	-0.52268274497621	o
6.24812463542550	0.22232330043670	-2.96863310333108	f
4.03066705360858	-4.36860535947288	-2.82300933315297	f
4.08699786354296	-4.28370851235265	2.32776340924097	f
-4.20608553638105	-3.49325140753080	-0.07310965965016	te
-6.89226040664003	-4.96096776051396	-2.05536981616730	f
-5.39447423061581	-5.57604344277071	2.66759691577364	f
-1.58968977098458	-2.25987218894181	2.13688407629326	o
-2.15428811167240	-6.27746653418728	-1.23363637127362	f
-3.32498076629123	-1.62507205383706	-3.07998460157428	f
-6.64875038630914	-0.94849680361377	0.85704856201003	f
-0.94364175457144	5.34750486332064	-0.30303467797272	te
-0.31119855289784	8.75496808166406	-1.43619499445142	f
-0.10097261453071	4.32215077336992	-3.69713060023499	f
-1.85634604075120	2.01532269310903	0.85587898824148	o
2.58266280960739	5.24295806215112	0.64178202786787	f
-1.74477671161676	6.84303678942677	2.92984324086696	f
-4.39636563397026	5.85544884831449	-1.32975165963724	f
1.19258001927907	0.54232524231857	3.90293062254304	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	22.72	0.07304	YES	YES
8		a	25.31	0.05380	YES	YES
9		a	30.42	0.00233	YES	YES
10		a	35.17	0.04852	YES	YES
11		a	38.13	0.00782	YES	YES
12		a	46.89	0.02001	YES	YES
13		a	70.20	0.04935	YES	YES
14		a	83.79	0.08262	YES	YES
15		a	89.56	0.00183	YES	YES
16		a	105.79	0.35046	YES	YES
17		a	108.33	0.10950	YES	YES
18		a	118.69	0.21811	YES	YES
19		a	148.10	0.03488	YES	YES
20		a	153.77	0.46922	YES	YES
21		a	161.14	0.35511	YES	YES
22		a	172.58	0.11111	YES	YES
23		a	175.30	0.04821	YES	YES
24		a	176.54	0.09666	YES	YES
25		a	192.15	5.51631	YES	YES
26		a	198.62	2.58520	YES	YES
27		a	205.82	1.42313	YES	YES

28	a	211.13	2.01679	YES	YES
29	a	217.59	10.02203	YES	YES
30	a	245.63	5.38777	YES	YES
31	a	248.89	0.06203	YES	YES
32	a	249.92	0.03145	YES	YES
33	a	253.81	17.78915	YES	YES
34	a	264.55	33.16071	YES	YES
35	a	272.68	86.12161	YES	YES
36	a	276.93	50.45409	YES	YES
37	a	279.51	22.34445	YES	YES
38	a	281.16	6.74337	YES	YES
39	a	281.50	7.74112	YES	YES
40	a	282.95	51.90320	YES	YES
41	a	284.83	25.59786	YES	YES
42	a	285.93	23.39249	YES	YES
43	a	304.10	96.39729	YES	YES
44	a	349.72	31.55198	YES	YES
45	a	358.77	65.72125	YES	YES
46	a	430.93	10.93210	YES	YES
47	a	513.95	0.71819	YES	YES
48	a	554.36	2.91656	YES	YES
49	a	567.08	28.72978	YES	YES
50	a	569.79	29.42422	YES	YES
51	a	581.74	2.03728	YES	YES
52	a	583.52	0.41446	YES	YES
53	a	584.15	0.68621	YES	YES
54	a	585.10	0.56534	YES	YES
55	a	604.49	76.61753	YES	YES
56	a	606.27	80.70845	YES	YES
57	a	616.44	19.18508	YES	YES
58	a	635.42	5.28345	YES	YES
59	a	637.76	60.51805	YES	YES
60	a	639.80	30.90207	YES	YES
61	a	642.15	150.11510	YES	YES
62	a	643.04	154.13686	YES	YES
63	a	645.59	167.70778	YES	YES
64	a	666.09	22.24827	YES	YES
65	a	673.42	28.57391	YES	YES
66	a	819.13	39.70762	YES	YES
67	a	889.54	509.85038	YES	YES
68	a	910.58	670.13829	YES	YES
69	a	1165.29	200.42065	YES	YES



Total energy = -1811.2145650770 H = -49285.6840161 eV

HOMO-LUMO Separation

HOMO: 96. 96 a -0.17210162 H = -4.68313 eV

LUMO: 97. 97 a -0.10438593 H = -2.84049 eV

Gap : +0.06771568 H = +1.84264 eV

Number of MOs= 325, Electrons= 192.00, Symmetry: c1

\$coord

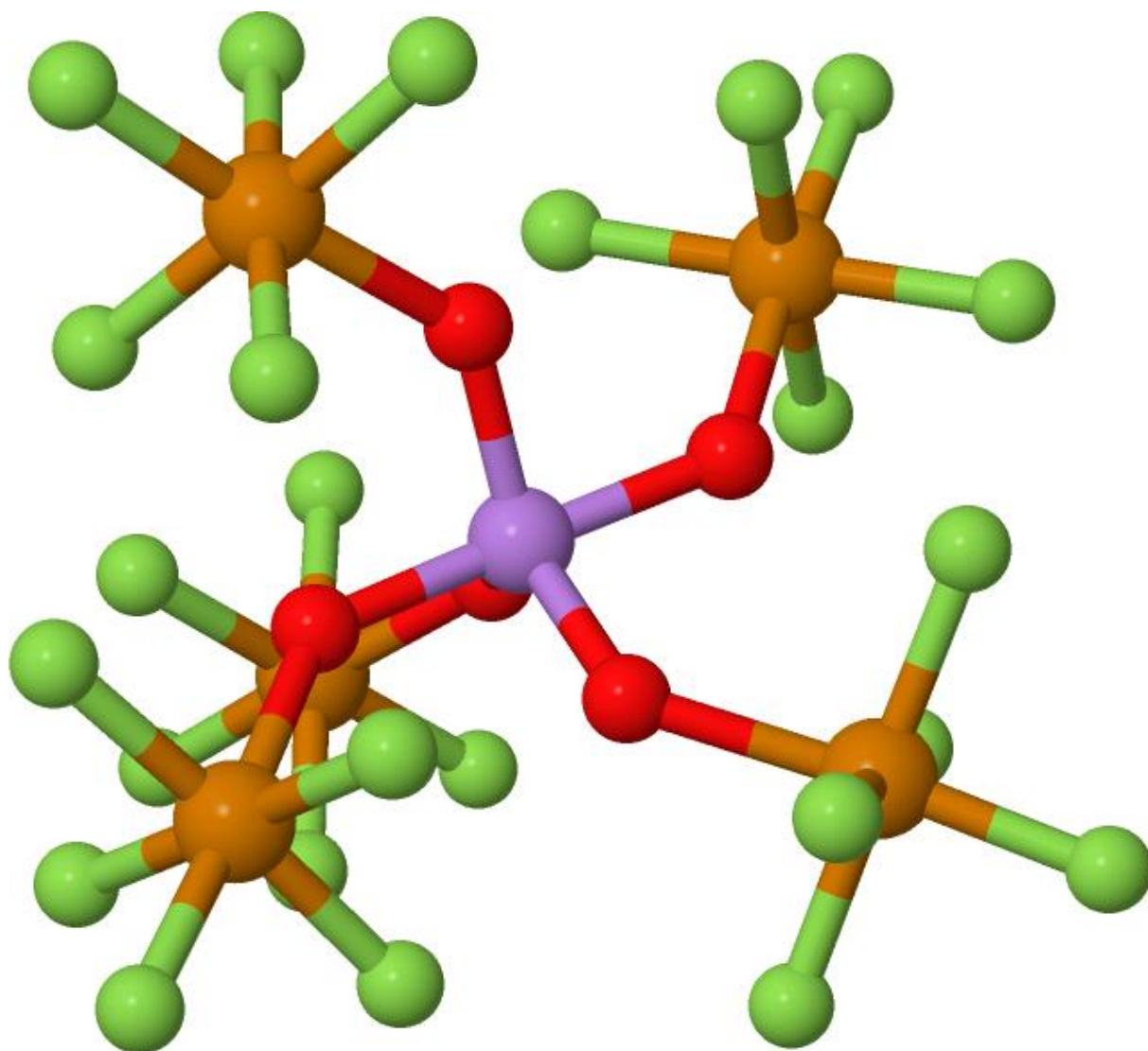
-0.08756254120598	-0.10995736194336	1.97711499515614	b
4.88129394204756	2.02233484163639	-0.14727503204457	te
8.09528353323886	3.74799459272308	-0.28300251524301	f
6.48525843039310	-0.09714514924483	2.37262343488628	f
1.71670461271106	0.24141896800531	-0.21027178461090	o
3.98729170666352	4.43820341247084	2.46190711353243	f
3.80091482958908	4.37886526365383	-2.70498711519183	f
6.16327595476637	-0.14227069899882	-2.77727219278510	f
-0.84287281979393	-5.44618831607860	-0.12016891050432	te
-0.13715644792381	-8.86037856961195	-1.19211948892991	f
2.69777397778573	-5.27994102626291	0.81162453786368	f
-1.84780661455333	-2.12751477821172	0.98601054029779	o
-0.00188298997080	-4.46570897503745	-3.52785102130546	f
-4.27813935344150	-6.06522565355789	-1.14004343196302	f
-1.57782851814716	-6.91437921963808	3.15045357771253	f
-4.14391510540228	3.47050189566201	-0.03236886716552	te
-6.62829452690156	5.08173367943024	-2.16468651427989	f
-3.14684272692553	1.59068508376009	-3.01497457975550	f
-1.73435616220920	2.09223392436254	2.41057871730229	o
-1.88953038326710	6.19055168133645	-1.00391715085811	f
-5.44539861668566	5.56710551638898	2.66478573568292	f
-6.74642687441547	1.00268348143821	0.71506106905697	f
1.14459420054982	-0.72070530622788	4.71989450414512	c
-0.38445015015329	-1.09905063592271	6.10685436127317	h
2.31821511448272	0.86387548893894	5.43270736806361	h
2.35260563908619	-2.43116872543579	4.54976246524868	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	18.26	0.02721	YES	YES
8		a	23.97	0.14900	YES	YES
9		a	30.65	0.00944	YES	YES
10		a	33.21	0.08388	YES	YES
11		a	42.56	0.01021	YES	YES
12		a	46.03	0.01336	YES	YES
13		a	68.68	0.07767	YES	YES
14		a	85.22	0.40779	YES	YES
15		a	93.84	0.10431	YES	YES
16		a	104.06	0.29122	YES	YES
17		a	109.89	0.07318	YES	YES
18		a	114.26	0.26790	YES	YES
19		a	155.04	1.20306	YES	YES
20		a	161.26	0.41244	YES	YES
21		a	167.39	0.07343	YES	YES
22		a	168.15	0.62130	YES	YES
23		a	176.12	0.17435	YES	YES
24		a	178.31	0.02297	YES	YES
25		a	187.81	5.19347	YES	YES

26	a	195.61	2.02623	YES	YES
27	a	197.86	2.00211	YES	YES
28	a	199.58	2.29883	YES	YES
29	a	206.25	0.37356	YES	YES
30	a	211.19	5.38660	YES	YES
31	a	241.34	3.85420	YES	YES
32	a	247.49	1.93514	YES	YES
33	a	249.12	1.37757	YES	YES
34	a	250.83	19.11669	YES	YES
35	a	258.74	1.27096	YES	YES
36	a	270.75	94.45021	YES	YES
37	a	273.08	86.56839	YES	YES
38	a	274.66	15.36444	YES	YES
39	a	278.79	24.92799	YES	YES
40	a	280.55	29.78974	YES	YES
41	a	281.89	15.21682	YES	YES
42	a	282.44	9.24328	YES	YES
43	a	284.48	30.33982	YES	YES
44	a	294.00	32.88248	YES	YES
45	a	329.16	10.97948	YES	YES
46	a	346.52	86.53524	YES	YES
47	a	398.94	34.21385	YES	YES
48	a	473.84	13.05295	YES	YES
49	a	500.78	8.22058	YES	YES
50	a	537.94	59.58866	YES	YES
51	a	557.30	38.47736	YES	YES
52	a	572.16	1.88665	YES	YES
53	a	575.73	0.15201	YES	YES
54	a	578.38	4.09279	YES	YES
55	a	579.54	2.15344	YES	YES
56	a	592.08	5.98269	YES	YES
57	a	598.56	54.47104	YES	YES
58	a	612.93	18.50893	YES	YES
59	a	617.45	132.00625	YES	YES
60	a	624.89	65.25382	YES	YES
61	a	629.04	66.87268	YES	YES
62	a	633.93	58.29311	YES	YES
63	a	635.68	70.35781	YES	YES
64	a	637.89	68.69009	YES	YES
65	a	639.56	129.67579	YES	YES
66	a	642.61	116.27891	YES	YES
67	a	754.01	139.75083	YES	YES
68	a	760.21	49.89921	YES	YES
69	a	783.11	88.13880	YES	YES
70	a	927.12	198.87189	YES	YES
71	a	968.16	91.82920	YES	YES
72	a	993.34	409.03187	YES	YES
73	a	1252.83	58.86203	YES	YES
74	a	1393.55	4.47883	YES	YES
75	a	1421.91	7.58007	YES	YES
76	a	2957.73	8.68809	YES	YES
77	a	3052.75	13.01186	YES	YES
78	a	3064.67	8.30699	YES	YES

As(OTeF₅)₅



Total energy = -5146.2368507750 H = -140036.3094412 eV

HOMO-LUMO Separation

HOMO: 164. 164 a -0.35657821 H = -9.70299 eV

LUMO: 165. 165 a -0.26820089 H = -7.29812 eV

Gap : +0.08837732 H = +2.40487 eV

Number of MOs= 517, Electrons= 328.00, Symmetry: c1

\$coord

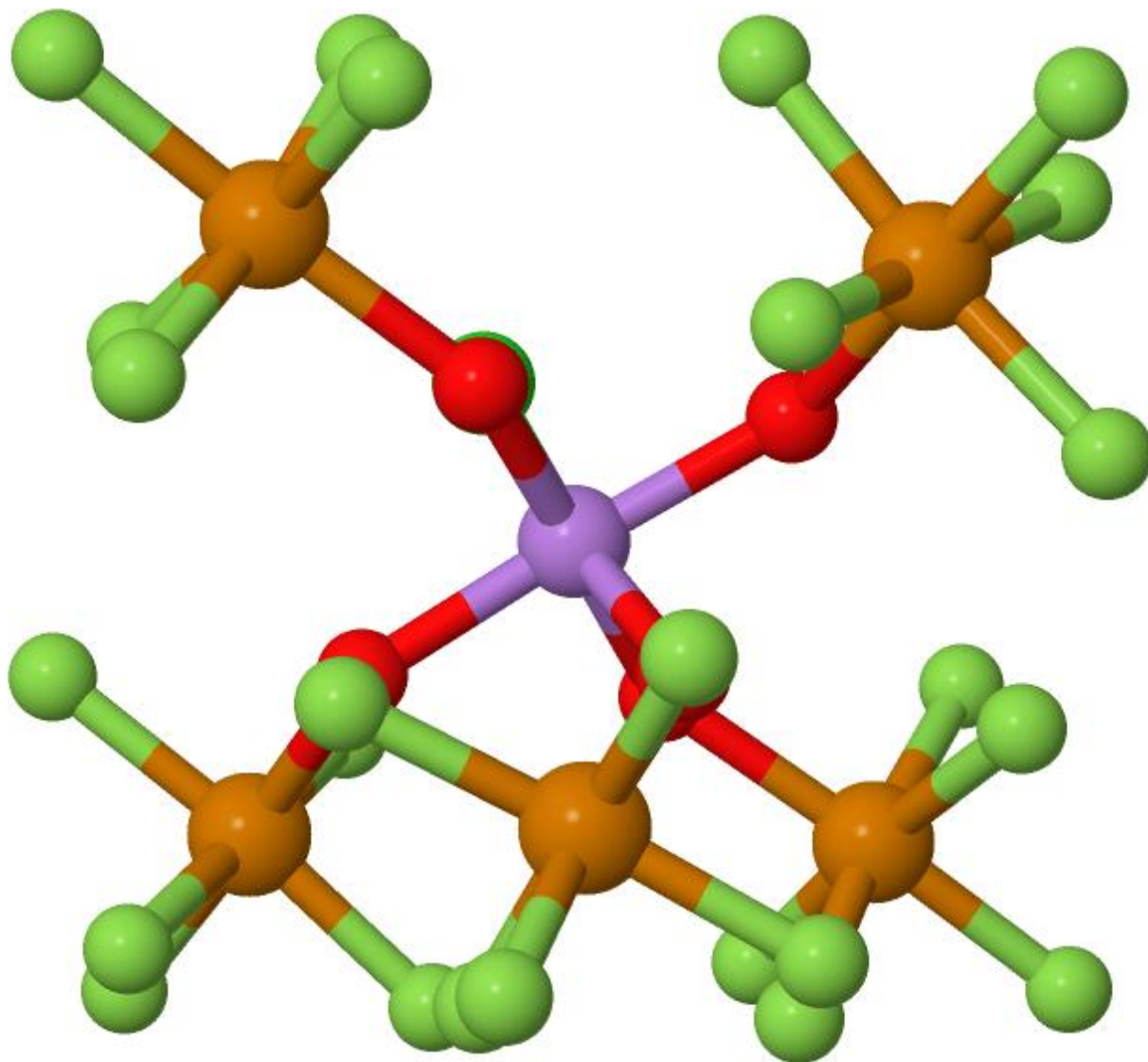
0.36295141344132	-0.12525906106568	0.05367024031579	as
2.00907484778771	-6.49721016355113	-0.51350231732782	te
-6.07939006544385	-1.83698316089429	0.14696529913818	te
-0.21619020704518	-3.43850320068858	0.01440328068149	o
-3.04297958123398	0.38523714400049	0.05048626949978	o
4.32113961900268	-5.61623654470203	2.13651016324308	f
-0.08906100631932	-8.15064931536800	1.92372601823362	f
-0.31793297087850	-7.47082986138482	-3.10618630685694	f
4.04521121625604	-4.88452232545448	-3.04721866959924	f
3.86347288726962	-9.54798470339863	-1.01981359382456	f
-4.85426202240496	-4.04940022236385	-2.45319488037145	f
-7.59078302138251	0.27484302838119	-2.37272354713434	f
-4.70024198126468	-3.95022821296566	2.75293532368184	f
-7.48458677583538	0.35683040962622	2.65748790363731	f
-9.10211950214024	-3.81025339904947	0.26996822019045	f
0.84879412961778	1.73352332181933	2.82040365851795	o
-1.40361970549411	3.53675364376318	5.29046259365553	te
0.94178653267697	1.49856302395392	-2.82882912113289	o
-1.26789843374360	3.32203024134207	-5.32231955977807	te
0.89052534870552	2.41621079663349	7.85072999822063	f
0.64388114567461	6.48170474512210	4.82919887944402	f
-3.69004234259289	4.80481326151793	2.77973059962790	f
-3.35877079687408	0.51402277305084	5.75542742872981	f
-3.36905849042367	5.20268966061547	7.81352222497851	f
-3.33403153665937	4.85568854962775	-2.76810988461332	f
-3.46474415148485	0.44411482010871	-5.58470972722876	f
1.00164327328924	6.12838249015446	-5.09061284559993	f
0.82899169768917	1.89683313662997	-7.89994898300254	f
-3.21198682787620	5.02662651972508	-7.83601256100729	f
3.74107519674296	-0.82621604311498	0.19163353952196	o
6.66246311161293	1.52147185385601	0.38454064805570	te
6.33981127723309	1.80334614268721	3.98533622999462	f
8.69725817112107	-1.43828406767668	0.78882187455591	f
7.10545406692022	1.33742983622797	-3.20795986845610	f
4.65165681593171	4.52230994145715	-0.03267432652605	f
9.62250866812484	3.57913494137770	0.58785579853521	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	5.93	0.00541	YES	YES
8		a	15.82	0.06575	YES	YES
9		a	19.80	0.02200	YES	YES
10		a	25.28	0.00233	YES	YES
11		a	26.57	0.01145	YES	YES
12		a	32.23	0.08140	YES	YES
13		a	35.98	0.20904	YES	YES
14		a	39.06	0.15978	YES	YES
15		a	41.60	0.01098	YES	YES
16		a	49.80	0.36708	YES	YES
17		a	51.46	0.15118	YES	YES

18	a	60.59	0.02098	YES	YES
19	a	64.64	0.03985	YES	YES
20	a	83.10	0.03462	YES	YES
21	a	85.69	0.21688	YES	YES
22	a	88.99	0.02244	YES	YES
23	a	92.80	0.26676	YES	YES
24	a	96.24	0.25962	YES	YES
25	a	99.22	0.45672	YES	YES
26	a	101.64	0.32921	YES	YES
27	a	103.96	0.81536	YES	YES
28	a	111.29	0.15199	YES	YES
29	a	112.75	0.58471	YES	YES
30	a	118.75	0.17800	YES	YES
31	a	151.57	0.55434	YES	YES
32	a	156.81	0.76663	YES	YES
33	a	157.77	0.11905	YES	YES
34	a	162.35	0.12341	YES	YES
35	a	167.05	0.17344	YES	YES
36	a	168.62	0.09827	YES	YES
37	a	171.16	1.90169	YES	YES
38	a	176.25	1.67557	YES	YES
39	a	177.07	1.44438	YES	YES
40	a	192.09	11.58034	YES	YES
41	a	195.09	6.27169	YES	YES
42	a	198.46	1.10047	YES	YES
43	a	202.30	1.58347	YES	YES
44	a	203.66	2.64849	YES	YES
45	a	206.55	0.49923	YES	YES
46	a	224.75	1.50459	YES	YES
47	a	234.20	42.93521	YES	YES
48	a	236.26	88.93763	YES	YES
49	a	240.27	32.22175	YES	YES
50	a	245.39	23.14642	YES	YES
51	a	251.17	3.93579	YES	YES
52	a	252.21	4.99527	YES	YES
53	a	254.24	7.73085	YES	YES
54	a	255.56	0.67694	YES	YES
55	a	256.43	15.67044	YES	YES
56	a	258.43	10.34734	YES	YES
57	a	261.70	9.00068	YES	YES
58	a	263.94	12.71941	YES	YES
59	a	265.38	5.22907	YES	YES
60	a	265.60	9.26585	YES	YES
61	a	268.81	11.09819	YES	YES
62	a	269.66	9.82075	YES	YES
63	a	270.76	11.46639	YES	YES
64	a	272.06	13.25319	YES	YES
65	a	272.76	7.00379	YES	YES
66	a	273.35	28.84212	YES	YES
67	a	276.66	99.64931	YES	YES
68	a	277.60	137.88549	YES	YES
69	a	287.18	55.67988	YES	YES
70	a	291.45	81.58227	YES	YES
71	a	293.60	170.20703	YES	YES
72	a	299.00	82.79089	YES	YES
73	a	339.28	20.09760	YES	YES
74	a	392.02	6.26368	YES	YES
75	a	460.59	8.97161	YES	YES
76	a	473.77	122.26537	YES	YES
77	a	489.63	61.19616	YES	YES
78	a	508.94	31.17585	YES	YES
79	a	583.19	0.96777	YES	YES

80	a	586.08	10.17742	YES	YES
81	a	587.03	16.69287	YES	YES
82	a	588.73	6.38059	YES	YES
83	a	590.64	15.76809	YES	YES
84	a	596.48	0.16493	YES	YES
85	a	596.66	0.72215	YES	YES
86	a	599.19	0.35363	YES	YES
87	a	600.16	0.10037	YES	YES
88	a	601.44	0.36159	YES	YES
89	a	633.51	15.24326	YES	YES
90	a	635.39	107.21285	YES	YES
91	a	640.91	100.94359	YES	YES
92	a	641.50	29.42875	YES	YES
93	a	641.60	132.51961	YES	YES
94	a	642.79	12.45072	YES	YES
95	a	646.62	15.74369	YES	YES
96	a	649.13	5.76159	YES	YES
97	a	650.75	4.53094	YES	YES
98	a	653.06	25.77198	YES	YES
99	a	653.62	13.03354	YES	YES
100	a	656.39	106.44642	YES	YES
101	a	657.78	94.84778	YES	YES
102	a	659.82	40.35902	YES	YES
103	a	660.25	112.15060	YES	YES
104	a	660.91	51.53243	YES	YES
105	a	706.60	547.11361	YES	YES
106	a	730.13	429.36940	YES	YES
107	a	735.41	454.66604	YES	YES
108	a	770.59	4.23433	YES	YES



Total energy = -5606.5495255980 H = -152562.0617609 eV

HOMO-LUMO Separation

HOMO: 173. 173 a -0.20499245 H = -5.57813 eV

LUMO: 174. 174 a -0.14269131 H = -3.88283 eV

Gap : +0.06230113 H = +1.69530 eV

Number of MOs= 535, Electrons= 346.00, Symmetry: c1

303

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$coord
-1.24261221832412      0.02923398496493      -0.17839852370225      as
-1.13396892083776      4.70431525678605      4.50297793224398      te
-0.80161493074430      4.27633245756146      -5.28079051272775      te
-0.13911912591796      3.01442147757007      1.36641647239797      o
 0.01565550267192      1.31601812298645      -3.22592873805776      o
 0.04475263970516      2.05739692928278      6.70051532979014      f
 2.14155346316829      6.26685033326196      4.49642325302104      f
-2.43067968569241      7.54385715753770      2.64194592905134      f
-4.52553306446626      3.41650516125549      4.75759024699043      f
-1.81376750455223      6.61233963571896      7.52276094872637      f
-2.38545791627142      6.25284426600456      -2.67078981755757      f
-4.04888425824741      3.02191258370860      -6.34362110920015      f
 2.37892517235186      5.85170038338401      -4.51660185477326      f
 0.76138366711654      2.56454091014102      -8.07273075373042      f
-1.40356397782939      7.07116155284914      -7.52864905643605      f
 1.92874954047828      -1.46835630706624      0.25090301909667      o
 5.32694563363886      -0.09730618635189      0.74594521813484      te
-2.12699314094008      -3.03877175522870      -1.69526796664769      o
-0.79755992163893      -4.80614843401340      -4.65969102885418      te
 4.56437645396217      1.33816038077719      3.99968727064442      f
 6.20005511633090      -3.25928295442517      2.29855797682662      f
 6.46422596779273      -1.44342138982252      -2.43039894179519      f
 4.80436261234572      3.12434555411022      -0.84959364147958      f
 8.76228947089073      0.94217644868768      1.32784788940783      f
 2.26799797864153      -2.93597405541781      -5.21364877826841      f
-2.59088061864193      -2.59282277390590      -6.93171824722871      f
 1.11287057109936      -7.22413653288839      -2.72903349683488      f
-3.73829734703273      -6.91914931312793      -4.35572271530440      f
 0.06142302413001      -6.76288033452504      -7.60159977428722      f
-2.35531222206568      -1.25560744174821      2.91486443146914      o
-1.52027561080350      -4.28934294333620      4.85207303671477      te
-5.18398637560890      1.34345892491121      -0.74158536796402      cl
 1.79651845361892      -3.14802021041895      5.83571926765229      f
-2.98424276025492      -2.63333858752821      7.73516276131011      f
-4.77725053850174      -5.70751981482732      4.06347506306420      f
-0.05395985492393      -6.26881694228880      2.18200587946279      f
-0.98976919435194      -7.15967556293765      7.01935165059012      f

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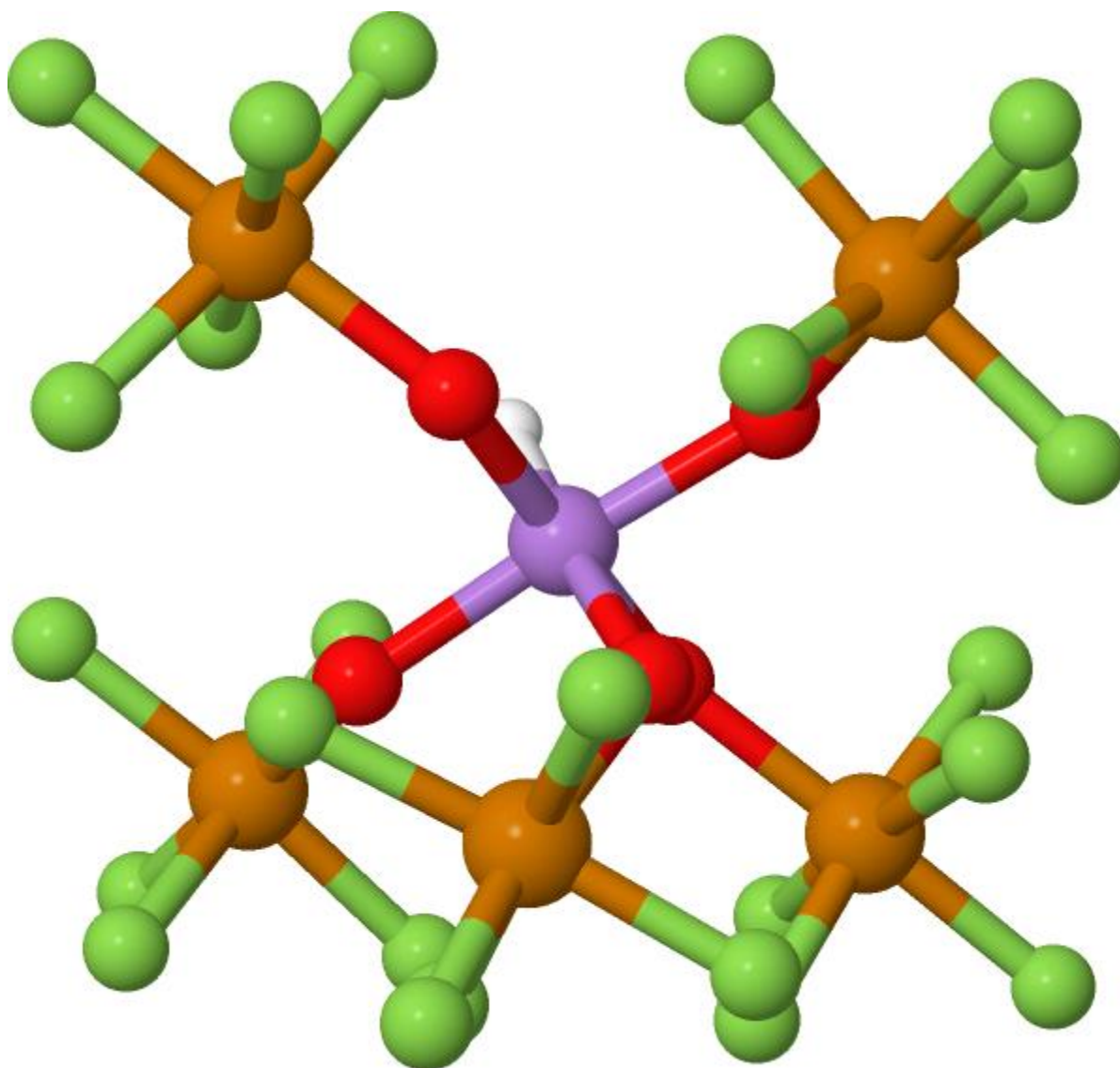
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$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#           #           cm** (-1)      km/mol      IR      RAMAN
 1           1           0.00           0.00000      -      -
 2           2           0.00           0.00000      -      -
 3           3           0.00           0.00000      -      -
 4           4           0.00           0.00000      -      -
 5           5           0.00           0.00000      -      -
 6           6           0.00           0.00000      -      -
 7           a          17.00           0.06786      YES      YES
 8           a          23.27           0.00406      YES      YES
 9           a          27.93           0.01572      YES      YES
10          a          30.19           0.03138      YES      YES
11          a          34.78           0.01428      YES      YES
12          a          38.07           0.12752      YES      YES
13          a          44.80           0.03243      YES      YES
14          a          45.78           0.16938      YES      YES
15          a          47.35           0.00934      YES      YES
16          a          52.40           0.02874      YES      YES

```

17	a	58.18	0.00424	YES	YES
18	a	64.16	0.03639	YES	YES
19	a	68.71	0.05349	YES	YES
20	a	75.94	0.07264	YES	YES
21	a	88.60	0.21612	YES	YES
22	a	90.77	0.19776	YES	YES
23	a	96.23	0.28864	YES	YES
24	a	99.81	0.07948	YES	YES
25	a	102.79	0.29843	YES	YES
26	a	106.92	0.28580	YES	YES
27	a	107.82	0.12090	YES	YES
28	a	109.93	0.10594	YES	YES
29	a	110.07	0.05654	YES	YES
30	a	116.38	0.27211	YES	YES
31	a	128.82	0.24891	YES	YES
32	a	139.45	1.33328	YES	YES
33	a	163.13	2.27894	YES	YES
34	a	165.87	0.21674	YES	YES
35	a	168.86	0.55259	YES	YES
36	a	171.03	1.72966	YES	YES
37	a	174.05	0.22848	YES	YES
38	a	176.22	0.22476	YES	YES
39	a	182.18	0.86168	YES	YES
40	a	183.69	2.33305	YES	YES
41	a	185.83	0.90504	YES	YES
42	a	190.52	11.61175	YES	YES
43	a	195.36	4.23874	YES	YES
44	a	197.12	6.27501	YES	YES
45	a	198.40	0.95795	YES	YES
46	a	201.82	2.18132	YES	YES
47	a	204.08	2.69799	YES	YES
48	a	211.28	1.97106	YES	YES
49	a	232.68	48.24247	YES	YES
50	a	236.53	89.08608	YES	YES
51	a	244.05	12.63255	YES	YES
52	a	247.92	20.61582	YES	YES
53	a	248.82	23.85841	YES	YES
54	a	249.26	23.29615	YES	YES
55	a	250.89	13.43498	YES	YES
56	a	254.83	1.45615	YES	YES
57	a	257.63	45.18277	YES	YES
58	a	264.15	96.17436	YES	YES
59	a	269.92	25.57829	YES	YES
60	a	273.30	19.37314	YES	YES
61	a	274.04	14.22310	YES	YES
62	a	275.51	9.84249	YES	YES
63	a	276.81	1.69200	YES	YES
64	a	277.27	2.44528	YES	YES
65	a	279.13	34.41564	YES	YES
66	a	279.33	63.39869	YES	YES
67	a	280.26	46.25937	YES	YES
68	a	281.99	1.29894	YES	YES
69	a	282.74	25.29022	YES	YES
70	a	284.07	76.38469	YES	YES
71	a	290.16	71.81475	YES	YES
72	a	294.01	89.61265	YES	YES
73	a	304.02	26.85885	YES	YES
74	a	306.73	41.01094	YES	YES
75	a	335.37	6.33293	YES	YES
76	a	363.54	24.41448	YES	YES
77	a	404.67	4.55004	YES	YES
78	a	451.79	11.77364	YES	YES

79	a	459.31	5.27720	YES	YES
80	a	467.59	113.05383	YES	YES
81	a	472.67	132.73920	YES	YES
82	a	576.70	1.46706	YES	YES
83	a	579.12	10.91504	YES	YES
84	a	581.10	10.98570	YES	YES
85	a	582.40	4.79858	YES	YES
86	a	584.82	2.32264	YES	YES
87	a	589.56	0.07335	YES	YES
88	a	589.75	0.64944	YES	YES
89	a	591.07	0.52201	YES	YES
90	a	591.70	0.06748	YES	YES
91	a	593.48	0.58738	YES	YES
92	a	613.02	27.63935	YES	YES
93	a	616.21	38.41724	YES	YES
94	a	617.20	77.82832	YES	YES
95	a	618.80	108.15457	YES	YES
96	a	619.44	39.53894	YES	YES
97	a	635.87	0.72089	YES	YES
98	a	637.51	11.16006	YES	YES
99	a	639.41	5.58542	YES	YES
100	a	640.64	26.94284	YES	YES
101	a	642.25	12.26399	YES	YES
102	a	643.56	3.43755	YES	YES
103	a	645.74	50.05555	YES	YES
104	a	648.30	56.90941	YES	YES
105	a	651.05	58.41014	YES	YES
106	a	652.06	46.00400	YES	YES
107	a	652.84	9.85308	YES	YES
108	a	654.68	375.30196	YES	YES
109	a	671.33	603.20616	YES	YES
110	a	676.62	568.95931	YES	YES
111	a	731.07	55.99257	YES	YES



Total energy = -5147.0223661700 H = -140057.6844148 eV

HOMO-LUMO Separation

HOMO: 165. 165 a -0.22007728 H = -5.98861 eV

LUMO: 166. 166 a -0.13734241 H = -3.73728 eV

Gap : +0.08273486 H = +2.25133 eV

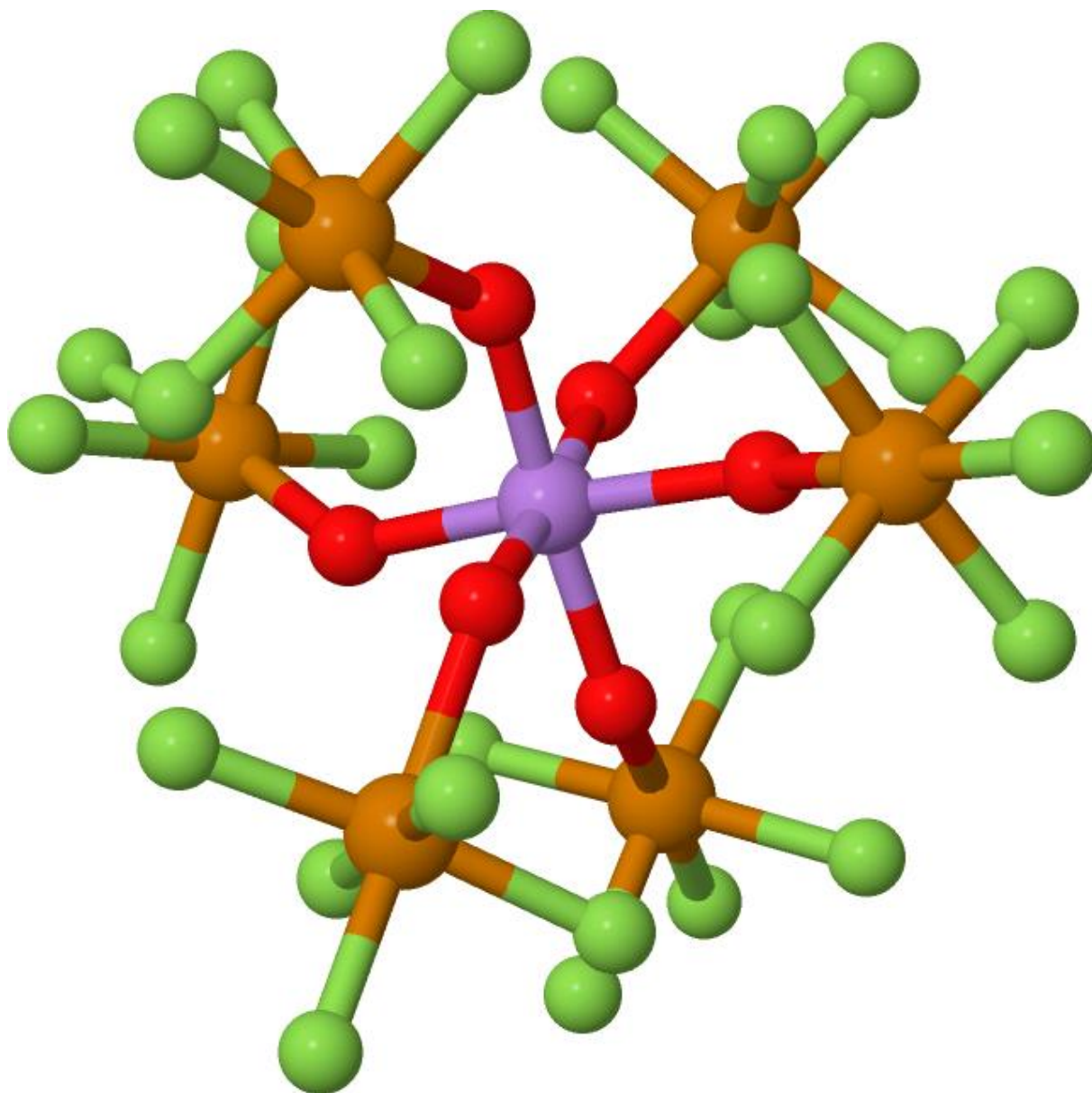
Number of MOs= 519, Electrons= 330.00, Symmetry: c1
307

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-1.20012680596952	0.06423229104817	-0.26041785264463	as
-1.30953447037022	4.48344689432148	4.57607330627593	te
-0.96018745756419	4.78773135851453	-4.67093178353713	te
0.13111985991860	2.78297089021776	1.67720945702430	o
0.21291290740127	1.65491107612145	-3.17054793627564	o
-0.89749117160454	1.67209790739166	6.84811730465750	f
1.97326837117751	5.72528595229647	5.50010200624103	f
-1.82879281760670	7.55121505865905	2.69276450121999	f
-4.73195961103413	3.44986029308624	3.81482283345786	f
-2.67047411060071	6.27432105008918	7.43404434745249	f
-3.33866179065442	5.52863678731073	-1.98082847212911	f
-3.72973672988938	3.22311992585527	-6.45061680733421	f
1.59798895981186	6.78878395261248	-3.04355510032568	f
1.23701654092181	4.22115927527828	-7.49956580738424	f
-2.02100560855329	7.88352491685753	-6.25438973604906	f
1.91517213561936	-1.53826508470786	0.06468334022699	o
5.29271724741597	-0.26265919444455	0.93982987073737	te
-2.19403771028097	-2.77206958537044	-2.16701615093963	o
-0.85009892093580	-4.36165756829873	-5.19519918153534	te
4.38246171434495	0.81721338314307	4.29347367464533	f
6.00030554723105	-3.59989564804023	2.18141318696647	f
6.60681648763103	-1.27462415376704	-2.29214817905347	f
4.96466584976859	3.12136877122248	-0.35239985167498	f
8.70405663172328	0.60650868761172	1.84691835227759	f
2.44453524934818	-2.82824520760117	-5.24083778384523	f
-2.12685770473656	-1.72611412609958	-7.36422497766160	f
0.51291434606522	-7.20714657009960	-3.39297911063618	f
-4.03803885250694	-6.09468915418964	-5.44322479064651	f
0.11972070909462	-6.08329053501076	-8.25058990802158	f
-2.51971873947277	-1.55567783932747	2.61293559386068	o
-1.81177103646090	-4.66798216100910	4.41114653971985	te
-3.83290285545437	1.18688208646875	-0.54960947312337	h
1.27890362555181	-3.45595604273005	5.90457887019429	f
-3.73079623342415	-3.35386901173400	7.20162582244238	f
-4.85368662089628	-6.19597593407459	3.11468303577135	f
0.09130127754756	-6.33682320407295	1.80323135503158	f
-1.36866711805145	-7.67819547402528	6.40417577011526	f

\$vibrational spectrum			wave number	IR intensity	selection rules	
#	mode	symmetry	cm** (-1)	km/mol	IR	RAMAN
#						
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		14.05	0.01500	YES	YES
8	a		22.09	0.02612	YES	YES
9	a		26.78	0.02001	YES	YES
10	a		28.09	0.00368	YES	YES
11	a		31.32	0.06272	YES	YES
12	a		37.03	0.01444	YES	YES
13	a		39.18	0.04819	YES	YES
14	a		42.56	0.01939	YES	YES

15	a	46.37	0.27442	YES	YES
16	a	47.31	0.07551	YES	YES
17	a	51.38	0.01333	YES	YES
18	a	56.12	0.03502	YES	YES
19	a	64.79	0.12989	YES	YES
20	a	73.80	0.14569	YES	YES
21	a	85.53	0.03826	YES	YES
22	a	88.77	0.11852	YES	YES
23	a	94.87	0.27518	YES	YES
24	a	98.43	0.02753	YES	YES
25	a	104.21	0.18812	YES	YES
26	a	105.68	0.04939	YES	YES
27	a	106.86	0.01099	YES	YES
28	a	109.68	0.15679	YES	YES
29	a	112.31	0.29222	YES	YES
30	a	115.28	0.28006	YES	YES
31	a	165.22	0.71225	YES	YES
32	a	166.15	1.60520	YES	YES
33	a	169.23	1.24169	YES	YES
34	a	171.27	1.88587	YES	YES
35	a	171.67	0.36096	YES	YES
36	a	175.77	3.56463	YES	YES
37	a	176.48	2.19700	YES	YES
38	a	179.80	5.25376	YES	YES
39	a	182.76	3.69512	YES	YES
40	a	186.24	3.72187	YES	YES
41	a	190.20	1.35206	YES	YES
42	a	192.94	8.11341	YES	YES
43	a	196.45	1.59371	YES	YES
44	a	198.04	0.42244	YES	YES
45	a	201.14	0.40003	YES	YES
46	a	217.26	8.98363	YES	YES
47	a	227.54	95.44990	YES	YES
48	a	230.85	64.80645	YES	YES
49	a	242.45	6.76737	YES	YES
50	a	247.20	5.96611	YES	YES
51	a	248.61	9.33547	YES	YES
52	a	249.75	5.37372	YES	YES
53	a	251.17	8.36144	YES	YES
54	a	252.65	0.41992	YES	YES
55	a	256.82	18.95294	YES	YES
56	a	266.09	94.73285	YES	YES
57	a	272.85	17.42442	YES	YES
58	a	274.31	12.90698	YES	YES
59	a	275.82	11.67344	YES	YES
60	a	276.64	30.13967	YES	YES
61	a	277.47	5.64135	YES	YES
62	a	277.90	21.11316	YES	YES
63	a	279.35	7.45950	YES	YES
64	a	280.65	56.34058	YES	YES
65	a	282.23	12.60653	YES	YES
66	a	282.79	16.92694	YES	YES
67	a	284.49	30.79531	YES	YES
68	a	285.17	158.45658	YES	YES
69	a	289.40	108.34010	YES	YES
70	a	293.63	52.20118	YES	YES
71	a	304.04	6.53142	YES	YES
72	a	305.57	52.79424	YES	YES
73	a	338.42	12.10506	YES	YES
74	a	398.74	3.90822	YES	YES
75	a	439.92	10.51301	YES	YES
76	a	455.85	27.08974	YES	YES

77	a	469.46	154.30873	YES	YES
78	a	482.28	152.15288	YES	YES
79	a	574.36	5.60073	YES	YES
80	a	577.04	22.59995	YES	YES
81	a	578.56	9.58074	YES	YES
82	a	581.12	16.40548	YES	YES
83	a	582.18	1.76940	YES	YES
84	a	585.20	4.38445	YES	YES
85	a	586.80	0.11602	YES	YES
86	a	589.03	0.09747	YES	YES
87	a	589.42	0.35207	YES	YES
88	a	591.91	0.99902	YES	YES
89	a	612.33	3.53439	YES	YES
90	a	613.78	9.94207	YES	YES
91	a	615.97	52.85956	YES	YES
92	a	616.92	59.61574	YES	YES
93	a	618.29	26.46006	YES	YES
94	a	629.87	199.48029	YES	YES
95	a	636.11	15.75800	YES	YES
96	a	637.40	12.88259	YES	YES
97	a	639.28	8.04066	YES	YES
98	a	639.81	54.29320	YES	YES
99	a	642.67	14.05715	YES	YES
100	a	643.47	29.58630	YES	YES
101	a	646.02	61.43106	YES	YES
102	a	647.62	67.29350	YES	YES
103	a	648.71	18.07923	YES	YES
104	a	651.07	148.47673	YES	YES
105	a	652.27	251.58882	YES	YES
106	a	656.86	570.43460	YES	YES
107	a	658.21	718.70367	YES	YES
108	a	738.33	33.45345	YES	YES
109	a	873.30	0.21185	YES	YES
110	a	908.93	7.53144	YES	YES
111	a	2208.50	18.02507	YES	YES



Total energy = -5728.5055676090 H = -155880.6564024 eV

HOMO-LUMO Separation

HOMO: 194. 194 a -0.22524295 H = -6.12918 eV

LUMO: 195. 195 a -0.15236701 H = -4.14612 eV

Gap : +0.07287594 H = +1.98306 eV

Number of MOs= 614, Electrons= 388.00, Symmetry: c1

\$coord

0.01692272863298	-0.00643132878467	0.06671393297257	as
2.71828975838887	-1.83917862307912	-1.12783946076123	o
-2.75655646226718	1.86635162186530	1.00543117436579	o
-2.02224126407225	-1.79538578848248	-2.16814739019204	o
0.84679074256876	2.55995824757841	-2.18814043899296	o
2.23029007555197	1.39708504248630	2.42776007297649	o
6.37056266703081	-1.14739923389413	-1.23730702446375	te
-1.06380107612073	5.22789164573264	-3.89083968956364	te
-6.03860795067503	0.90127136831615	2.47186562396465	te
-1.38770233621744	-3.57091141619914	-5.35039769409767	te
6.20895344416023	2.47251320242964	-0.98630126940010	f
9.97614109746361	-0.79279960556168	-1.47568443808139	f
6.85107901936522	-4.71738441343669	-1.62600037713062	f
6.82326636640124	-1.47179230200051	2.35314492570065	f
6.25743317352557	-0.83759486340620	-4.85192551603950	f
-1.08351314015603	-5.31968923472400	-8.52311941838804	f
1.19420597907700	-1.29108749277924	-6.50976135722864	f
-3.97913478103402	-5.94174165259207	-4.44405940519821	f
-3.91938087061909	-1.52999134329474	-6.96652352262149	f
1.14899057412155	-5.86687020463314	-4.11800229083241	f
-6.38961766246817	4.34949143001280	3.52916661690548	f
-9.32217925257628	0.28848303036090	3.89709948851534	f
-7.70736812276269	1.76373166689630	-0.63489145677223	f
-4.66892126162399	0.02820504278552	5.72200326211443	f
-6.05266148910262	-2.58229375508593	1.44163630196411	f
1.81351295191426	7.40659346568713	-3.53116731291356	f
-2.67752041839856	7.87096769725959	-5.79346301952975	f
-2.58269083071477	6.73694103194044	-0.94970539279579	f
0.28832320922947	4.08347361322879	-7.06079786586352	f
-4.04366438442302	3.21265326708986	-4.40317883852205	f
2.33306513219476	4.37094171052373	4.58083633428953	te
5.93040926932939	4.49396861536209	4.12050108448178	f
2.71701111387696	7.25880316673070	6.75178169759498	f
1.86213459055018	6.71055913050611	1.83443709442132	f
2.83237907459153	2.26530126627787	7.49681747090772	f
-1.21815234881744	4.50631962104108	5.35824509378601	f
-0.84881924417863	-2.26685439535688	2.63884435720569	o
-0.20163677673684	-5.78652564715409	3.47217886633350	te
3.15552579788272	-5.97416501659157	2.08662326398352	f
1.22381532652816	-4.80042192597970	6.66429180502930	f
-3.46887396347214	-5.91379244219516	5.04521454666710	f
0.23638451890339	-9.24341937558243	4.50152864295509	f
-1.60244297485190	-7.07577482329786	0.37113152225347	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules
#			cm** (-1)	km/mol	IR RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	17.38	0.00310	YES	YES
8	a	22.87	0.00851	YES	YES
9	a	25.75	0.03765	YES	YES
10	a	27.97	0.02319	YES	YES
11	a	30.55	0.05952	YES	YES
12	a	34.61	0.00395	YES	YES
13	a	38.02	0.01271	YES	YES
14	a	39.15	0.02057	YES	YES
15	a	40.04	0.02770	YES	YES
16	a	44.35	0.04562	YES	YES
17	a	45.83	0.00618	YES	YES
18	a	50.70	0.23850	YES	YES
19	a	53.89	0.11638	YES	YES
20	a	60.60	0.03002	YES	YES
21	a	65.23	0.08195	YES	YES
22	a	69.01	0.16344	YES	YES
23	a	87.04	0.06714	YES	YES
24	a	88.72	0.22538	YES	YES
25	a	89.78	0.10738	YES	YES
26	a	97.65	0.23700	YES	YES
27	a	98.86	0.03889	YES	YES
28	a	100.79	0.12757	YES	YES
29	a	104.25	0.08820	YES	YES
30	a	108.20	0.33582	YES	YES
31	a	109.28	0.16365	YES	YES
32	a	110.98	0.27008	YES	YES
33	a	112.32	0.60738	YES	YES
34	a	114.09	0.99018	YES	YES
35	a	115.52	0.21978	YES	YES
36	a	118.25	0.24474	YES	YES
37	a	145.35	0.64875	YES	YES
38	a	164.35	0.21955	YES	YES
39	a	166.21	0.04809	YES	YES
40	a	167.46	0.65638	YES	YES
41	a	169.43	0.08170	YES	YES
42	a	174.38	0.18998	YES	YES
43	a	176.21	0.35996	YES	YES
44	a	180.07	4.11137	YES	YES
45	a	182.09	1.00868	YES	YES
46	a	190.13	1.34088	YES	YES
47	a	193.18	6.38737	YES	YES
48	a	197.50	3.27195	YES	YES
49	a	199.03	3.29003	YES	YES
50	a	199.67	2.71860	YES	YES
51	a	200.57	3.40541	YES	YES
52	a	202.25	3.53240	YES	YES
53	a	203.68	1.32590	YES	YES
54	a	205.30	1.14434	YES	YES
55	a	220.21	1.96751	YES	YES
56	a	233.34	40.13399	YES	YES
57	a	237.40	52.51709	YES	YES
58	a	239.64	119.74498	YES	YES
59	a	247.23	40.16115	YES	YES
60	a	249.41	13.42293	YES	YES
61	a	250.13	17.50989	YES	YES
62	a	251.64	0.59217	YES	YES
63	a	253.21	11.98088	YES	YES
64	a	254.57	3.68689	YES	YES
65	a	259.21	18.50440	YES	YES
66	a	261.30	75.02545	YES	YES

67	a	265.80	19.04652	YES	YES
68	a	269.86	18.25254	YES	YES
69	a	270.77	31.04685	YES	YES
70	a	273.35	8.47690	YES	YES
71	a	275.23	21.34364	YES	YES
72	a	276.31	23.57024	YES	YES
73	a	276.73	2.16179	YES	YES
74	a	277.94	56.12844	YES	YES
75	a	279.07	27.38317	YES	YES
76	a	279.47	4.23758	YES	YES
77	a	280.58	10.84404	YES	YES
78	a	282.53	78.75802	YES	YES
79	a	282.81	35.53461	YES	YES
80	a	284.68	52.23039	YES	YES
81	a	285.73	16.71960	YES	YES
82	a	294.45	49.26650	YES	YES
83	a	298.52	10.67847	YES	YES
84	a	301.45	154.14780	YES	YES
85	a	308.40	93.17703	YES	YES
86	a	318.52	29.64216	YES	YES
87	a	341.82	20.29668	YES	YES
88	a	389.43	3.68070	YES	YES
89	a	431.12	13.71154	YES	YES
90	a	449.34	33.07634	YES	YES
91	a	465.13	143.42754	YES	YES
92	a	477.97	15.34413	YES	YES
93	a	487.39	89.67316	YES	YES
94	a	576.84	3.77063	YES	YES
95	a	579.90	6.68993	YES	YES
96	a	581.54	1.05970	YES	YES
97	a	583.86	8.65505	YES	YES
98	a	584.08	7.58264	YES	YES
99	a	584.87	0.47193	YES	YES
100	a	590.19	0.05798	YES	YES
101	a	590.37	0.16299	YES	YES
102	a	590.98	0.42934	YES	YES
103	a	591.34	0.07256	YES	YES
104	a	592.70	0.16388	YES	YES
105	a	594.61	1.15694	YES	YES
106	a	617.01	2.66385	YES	YES
107	a	618.30	40.22891	YES	YES
108	a	619.48	78.24805	YES	YES
109	a	619.95	121.11000	YES	YES
110	a	621.60	107.10855	YES	YES
111	a	622.19	45.89922	YES	YES
112	a	637.59	6.77699	YES	YES
113	a	640.22	17.33303	YES	YES
114	a	640.39	1.82422	YES	YES
115	a	641.40	6.63168	YES	YES
116	a	642.69	43.56147	YES	YES
117	a	643.18	0.53431	YES	YES
118	a	647.65	14.29692	YES	YES
119	a	650.06	26.66389	YES	YES
120	a	650.69	86.56007	YES	YES
121	a	651.90	108.68373	YES	YES
122	a	652.34	112.87655	YES	YES
123	a	654.27	4.71006	YES	YES
124	a	654.98	77.06794	YES	YES
125	a	655.77	58.73025	YES	YES
126	a	692.74	611.05435	YES	YES
127	a	695.02	591.61680	YES	YES
128	a	702.38	546.54855	YES	YES

129

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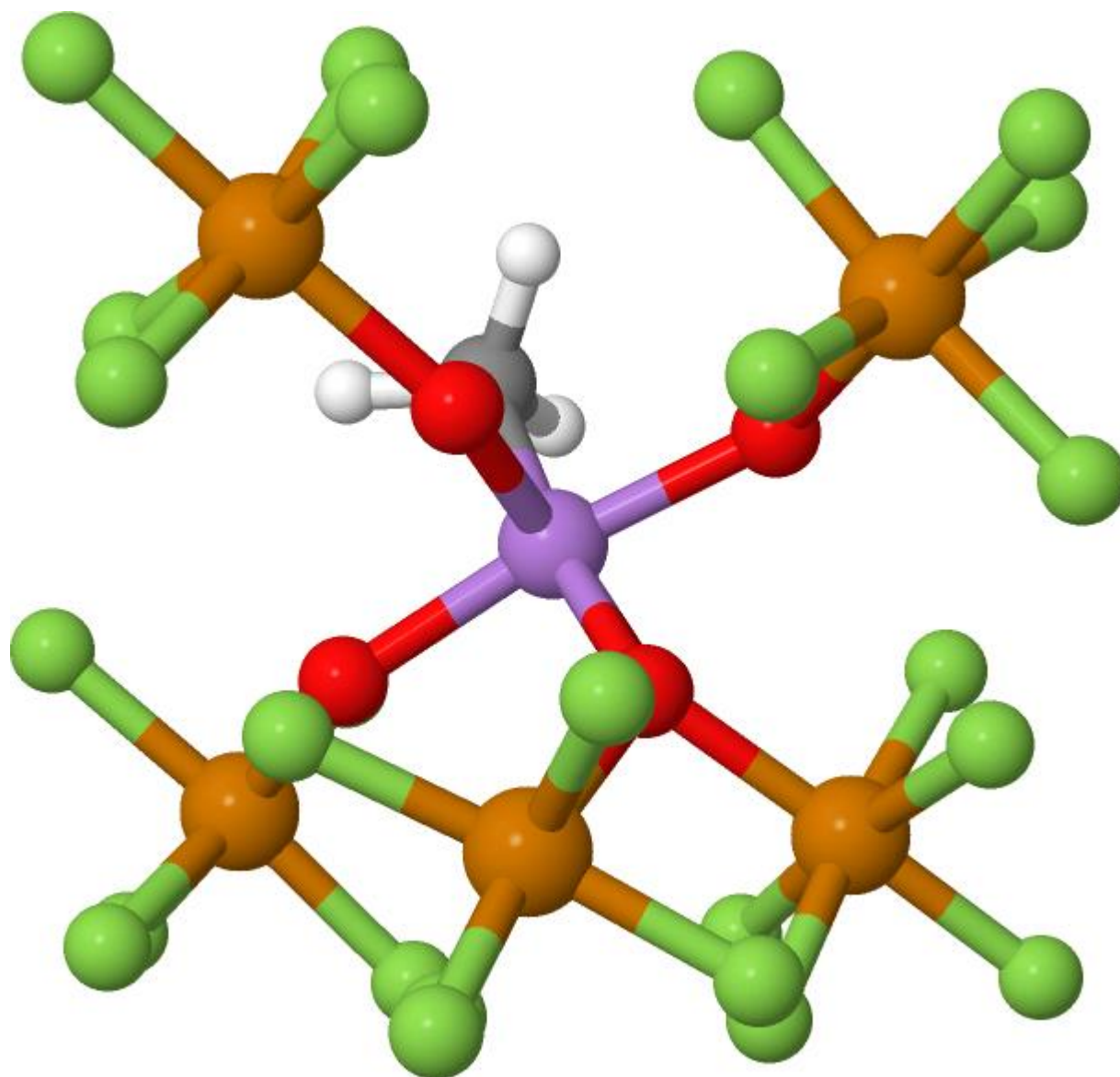
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4.64044

YES

YES

As(OTeF₅)₅Me⁻



Total energy = -5186.3157746290 H = -141126.9130697 eV

HOMO-LUMO Separation

HOMO: 169. 169 a -0.21653075 H = -5.89210 eV
315

LUMO: 170. 170 a -0.13649269 H = -3.71416 eV

Gap : +0.08003806 H = +2.17795 eV

Number of MOs= 537, Electrons= 338.00, Symmetry: c1

\$coord			
-1.36614341346048	0.01783557750818	-0.13503342283353	as
-1.41018656291138	4.66840319046367	4.55903905617883	te
-1.02835383143980	4.10594629658189	-5.44719820574723	te
-0.25727544789397	3.04515486979595	1.49309337188459	o
-0.03613555746226	1.36950117424140	-3.23666747221843	o
-0.20847201871095	2.10067800492863	6.83597199779273	f
1.74404151114136	6.44990945442673	4.77261678250879	f
-2.79910801441256	7.44368237444280	2.64799440541683	f
-4.74890045687403	3.17200372014013	4.58277488457375	f
-2.45145569222452	6.48502707881037	7.53527602811168	f
-2.63791700553634	6.13704171079525	-2.86096393384659	f
-4.31280693175598	2.70538609948954	-6.27111219017897	f
2.08744573329748	5.90043772687828	-4.94352312924180	f
0.44127836200844	2.34390976188426	-8.25918379266344	f
-1.90125222254035	6.75241458419446	-7.78983055601072	f
1.91974047669638	-1.26838848281906	0.22084306909801	o
5.21058144398366	0.37573388238719	0.67649638000151	te
-2.01211953262316	-3.18268636877097	-1.62814393539054	o
-0.75439519487403	-4.85587463528045	-4.63016338777945	te
4.46261581022280	1.59465707578439	4.02481578778683	f
6.32845435299902	-2.79563557539130	2.04809576345826	f
6.35209658046588	-0.69345043274053	-2.60563494701313	f
4.45686786128477	3.64303031471823	-0.72833040701624	f
8.59254485376629	1.58936472891045	1.23963749963226	f
2.29034781373887	-2.94996241919869	-5.17469266432096	f
-2.62346352200672	-2.58259361404780	-6.79797669058875	f
1.19466685144698	-7.32992636400886	-2.81651242109012	f
-3.67239350754627	-7.01625687315895	-4.38282012767104	f
0.06999553551380	-6.68477841824972	-7.66615951853720	f
-2.26358184106076	-1.41082798637596	3.01441367025458	o
-1.31028706958229	-4.37452370432613	4.92920214987180	te
1.95343186885511	-3.10531602151790	5.92325376049173	f
-2.84074959870674	-2.83739880821359	7.84734273802742	f
-4.50969653556276	-5.92898120960913	4.13412775186866	f
0.24598288413586	-6.28075117867742	2.25575085119351	f
-0.66402503049472	-7.24249808471272	7.07332002524611	f
-4.91701514456723	1.00283537554612	-0.69215860694380	c
-5.03183919847174	3.07875682220558	-0.48702731041984	h
-6.05529191818816	0.00519841373009	0.74513599865402	h
-5.36977164329198	0.38173058039778	-2.63403070689028	h

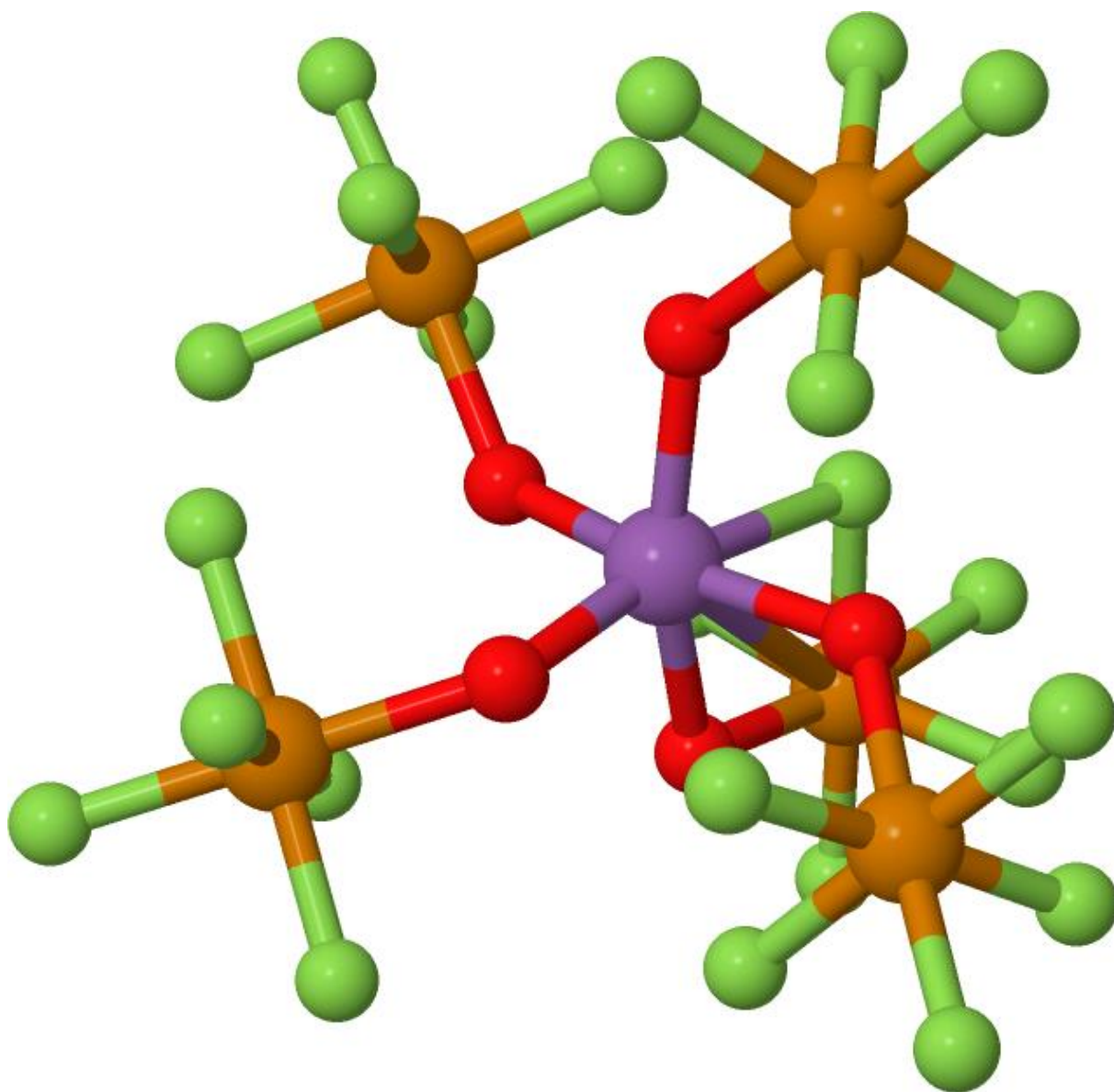
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1		0.00	0.00000	-	-
	2		0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	17.78	0.01975	YES	YES
8	a	20.88	0.03886	YES	YES
9	a	24.43	0.01702	YES	YES
10	a	30.73	0.01789	YES	YES
11	a	33.62	0.08801	YES	YES
12	a	37.82	0.08299	YES	YES
13	a	39.30	0.11885	YES	YES
14	a	41.60	0.04205	YES	YES
15	a	42.80	0.14963	YES	YES
16	a	49.09	0.06406	YES	YES
17	a	53.71	0.00136	YES	YES
18	a	62.94	0.15896	YES	YES
19	a	69.19	0.23582	YES	YES
20	a	73.96	0.27548	YES	YES
21	a	86.33	0.18042	YES	YES
22	a	87.91	0.03613	YES	YES
23	a	93.91	0.25331	YES	YES
24	a	96.65	0.16346	YES	YES
25	a	99.97	0.08232	YES	YES
26	a	104.48	0.07106	YES	YES
27	a	107.55	0.22335	YES	YES
28	a	109.37	0.13804	YES	YES
29	a	111.41	0.11924	YES	YES
30	a	114.17	0.24977	YES	YES
31	a	132.20	0.16216	YES	YES
32	a	158.99	2.52130	YES	YES
33	a	165.04	2.07683	YES	YES
34	a	168.10	0.81800	YES	YES
35	a	169.15	0.77845	YES	YES
36	a	172.59	1.09587	YES	YES
37	a	175.78	0.66173	YES	YES
38	a	178.82	0.92062	YES	YES
39	a	180.61	2.33044	YES	YES
40	a	182.84	11.98806	YES	YES
41	a	186.17	8.80758	YES	YES
42	a	189.51	2.30297	YES	YES
43	a	192.46	5.72395	YES	YES
44	a	196.40	0.18725	YES	YES
45	a	198.72	1.29715	YES	YES
46	a	202.82	1.24094	YES	YES
47	a	211.87	5.38185	YES	YES
48	a	218.39	9.65919	YES	YES
49	a	223.56	63.19483	YES	YES
50	a	229.45	85.63873	YES	YES
51	a	231.67	21.24508	YES	YES
52	a	246.52	3.04681	YES	YES
53	a	247.60	6.48564	YES	YES
54	a	248.73	9.08344	YES	YES
55	a	250.09	6.49669	YES	YES
56	a	252.77	5.88240	YES	YES
57	a	257.65	26.58958	YES	YES
58	a	263.44	72.36949	YES	YES
59	a	268.34	74.81450	YES	YES
60	a	272.78	13.96803	YES	YES
61	a	275.15	60.53551	YES	YES
62	a	275.93	9.52805	YES	YES
63	a	276.67	4.90011	YES	YES
64	a	278.74	1.75926	YES	YES
65	a	279.20	14.35382	YES	YES
66	a	279.93	35.36116	YES	YES

67	a	280.74	18.94148	YES	YES
68	a	283.06	30.28759	YES	YES
69	a	284.09	35.33428	YES	YES
70	a	285.36	55.46676	YES	YES
71	a	288.20	64.79481	YES	YES
72	a	292.69	83.31775	YES	YES
73	a	299.41	52.02739	YES	YES
74	a	307.42	21.92879	YES	YES
75	a	314.33	29.45785	YES	YES
76	a	337.25	19.57994	YES	YES
77	a	394.98	4.17675	YES	YES
78	a	435.01	21.81330	YES	YES
79	a	442.44	24.45399	YES	YES
80	a	456.40	109.15861	YES	YES
81	a	462.58	124.60996	YES	YES
82	a	557.32	0.53957	YES	YES
83	a	571.81	6.90042	YES	YES
84	a	575.55	13.02172	YES	YES
85	a	577.67	11.16644	YES	YES
86	a	578.45	5.26783	YES	YES
87	a	580.52	5.57448	YES	YES
88	a	582.26	2.89914	YES	YES
89	a	585.04	1.40338	YES	YES
90	a	587.54	0.71470	YES	YES
91	a	589.01	0.34295	YES	YES
92	a	590.20	1.21942	YES	YES
93	a	610.36	9.20585	YES	YES
94	a	611.39	2.25047	YES	YES
95	a	613.36	78.34328	YES	YES
96	a	615.33	77.80983	YES	YES
97	a	617.95	38.55135	YES	YES
98	a	631.35	134.68712	YES	YES
99	a	633.03	3.53665	YES	YES
100	a	635.63	15.35045	YES	YES
101	a	637.35	25.71337	YES	YES
102	a	638.69	27.03449	YES	YES
103	a	640.87	43.96018	YES	YES
104	a	642.23	47.99270	YES	YES
105	a	646.12	74.20770	YES	YES
106	a	647.52	106.43314	YES	YES
107	a	649.34	105.30683	YES	YES
108	a	649.80	63.99767	YES	YES
109	a	651.60	148.76567	YES	YES
110	a	668.03	648.46175	YES	YES
111	a	672.33	548.81450	YES	YES
112	a	733.91	84.00138	YES	YES
113	a	885.81	29.71281	YES	YES
114	a	889.14	37.82785	YES	YES
115	a	1231.11	5.10844	YES	YES
116	a	1387.98	8.58269	YES	YES
117	a	1397.10	8.25064	YES	YES
118	a	3007.85	2.01258	YES	YES
119	a	3141.11	4.35774	YES	YES
120	a	3146.63	5.42802	YES	YES

Sb(OTeF₅)₅



Total energy = -2915.8261622990 H = -79343.7120328 eV

HOMO-LUMO Separation

HOMO: 150. 150 a -0.35905532 H = -9.77040 eV

LUMO: 151. 151 a -0.28018143 H = -7.62413 eV

Gap : +0.07887388 H = +2.14627 eV

Number of MOs= 498, Electrons= 300.00, Symmetry: c1

\$coord

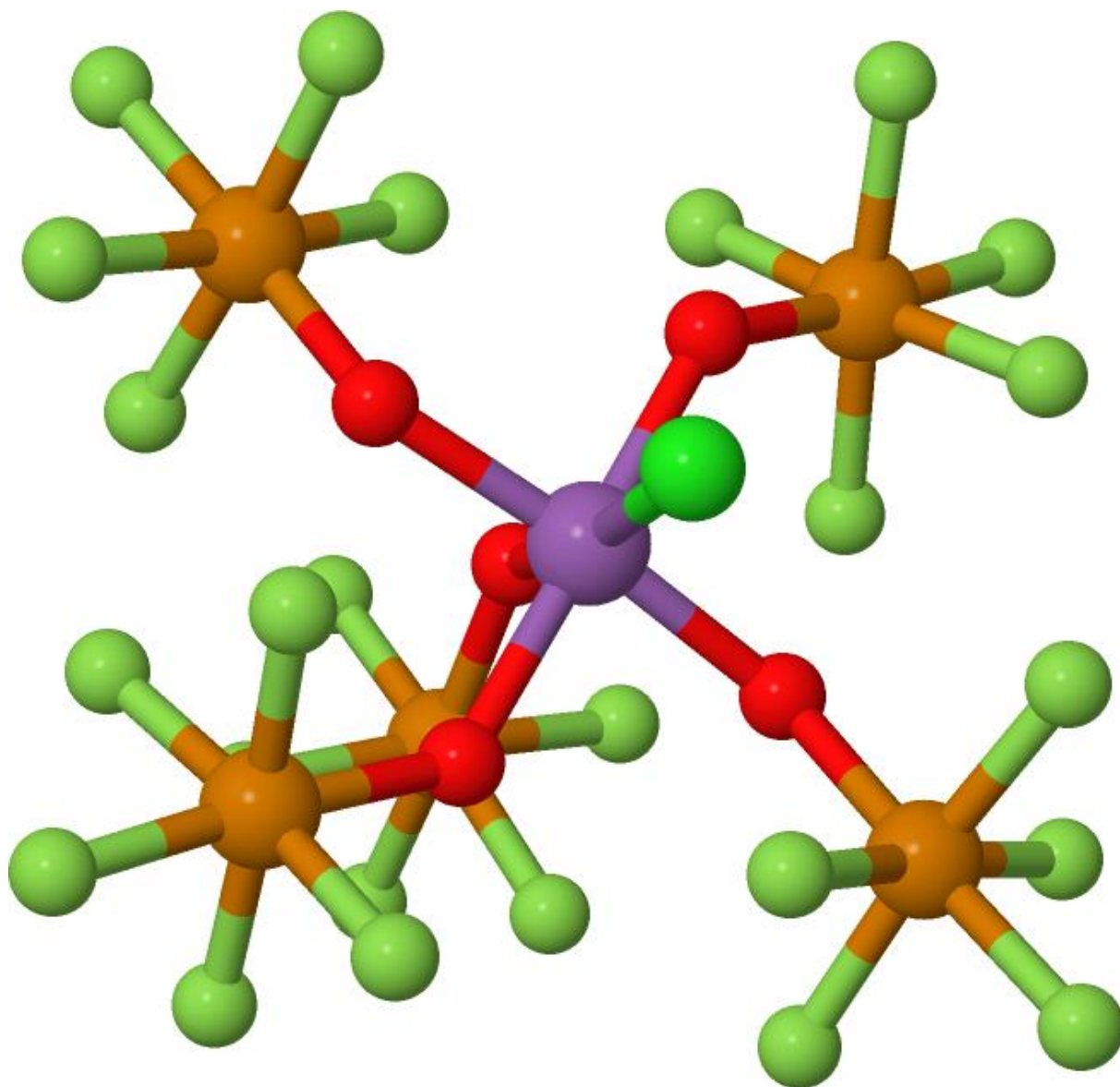
0.23855108176688	0.03159411324935	0.20193079803269	sb
-6.44979224185197	-1.60682491843970	0.34780436698231	te
-1.58880233199608	6.67793598813462	-0.32326594051145	te
-3.46102035920036	0.59900724208067	-0.12023191709535	o
0.75221692055215	3.77805963314522	-0.02409989053675	o
-5.17415434351823	-3.09993375215676	3.40289905628357	f
-7.94573703389120	1.03074228168356	2.31826205001760	f
-7.83570201617127	-0.11974067597002	-2.64528530956367	f
-5.03245898612414	-4.27543947916742	-1.66866787580026	f
-9.44849503792325	-3.58121525911384	0.73085093746323	f
-3.63092410147066	5.11577887038141	-2.88448686421543	f
0.57549876719948	8.05527997253436	-2.87434951541698	f
-3.76958969209830	5.45688059731517	2.31295455333260	f
0.40506585882370	8.36457450629177	2.18589420821822	f
-3.67965964653360	9.61268209241505	-0.58931313015200	f
3.74669260225136	-0.00204371364058	1.98871208398212	o
3.34498926553201	0.70866816995634	5.57600293757222	te
1.41869226520997	-0.91257867109148	-3.22765320960419	o
3.51410876505034	0.98675418304796	-5.67746368507688	te
2.90684550328509	-2.78139639149264	6.43399881676054	f
6.84568957907377	0.52407425393281	6.38536716644242	f
3.55636892628108	4.29571589128956	5.13947353353249	f
-0.37626361658031	0.80574826626300	4.48618841136357	f
2.24232410503129	1.42619822392222	8.93600590685933	f
5.28367505079362	2.76199486487166	-3.04575117551169	f
1.04077525344584	3.63686123529741	-5.86280611196514	f
6.01104781047113	-1.62448510899957	-5.56398002042727	f
1.79537657916228	-0.80174466868072	-8.30522025966223	f
5.49446899033206	2.74139625738229	-8.13448024293550	f
-0.39617294637398	-3.58296656947319	1.16744931243004	o
1.33180495012039	-6.70126328907902	0.05595248520140	te
2.43544407321672	-7.30302645569535	3.45399292564928	f
-1.74002956672049	-8.46988744138514	0.76744301141278	f
0.31059218730772	-6.27086874196457	-3.39645002660893	f
4.44891135556554	-4.94926593103829	-0.62033876369764	f
2.90166534257701	-9.80763716287272	-0.91296102853586	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	7.23	0.01007	YES	YES
8		a	13.50	0.06326	YES	YES
9		a	16.53	0.01836	YES	YES
10		a	19.26	0.00700	YES	YES
11		a	27.90	0.09111	YES	YES

12	a	29.42	0.33209	YES	YES
13	a	32.79	0.06185	YES	YES
14	a	37.36	0.19162	YES	YES
15	a	40.82	0.08363	YES	YES
16	a	45.12	0.08433	YES	YES
17	a	48.14	0.03083	YES	YES
18	a	50.18	0.31730	YES	YES
19	a	62.67	0.90889	YES	YES
20	a	69.32	0.28901	YES	YES
21	a	74.25	0.20638	YES	YES
22	a	80.70	0.15609	YES	YES
23	a	83.69	2.23311	YES	YES
24	a	86.73	0.40510	YES	YES
25	a	90.76	1.29870	YES	YES
26	a	91.90	1.16508	YES	YES
27	a	94.85	2.43492	YES	YES
28	a	105.56	0.51122	YES	YES
29	a	107.99	1.05067	YES	YES
30	a	112.21	0.07003	YES	YES
31	a	149.97	1.00342	YES	YES
32	a	154.27	3.96819	YES	YES
33	a	155.19	0.76598	YES	YES
34	a	156.20	2.47404	YES	YES
35	a	158.89	5.60848	YES	YES
36	a	163.41	10.40063	YES	YES
37	a	164.41	1.54843	YES	YES
38	a	168.76	3.51790	YES	YES
39	a	172.75	6.29536	YES	YES
40	a	176.64	13.13721	YES	YES
41	a	178.76	1.73899	YES	YES
42	a	183.49	14.67881	YES	YES
43	a	184.90	3.88591	YES	YES
44	a	193.53	4.33580	YES	YES
45	a	200.12	0.48781	YES	YES
46	a	208.63	13.59093	YES	YES
47	a	213.07	13.98997	YES	YES
48	a	216.09	25.74652	YES	YES
49	a	237.47	8.78232	YES	YES
50	a	245.60	19.65723	YES	YES
51	a	246.56	13.36093	YES	YES
52	a	249.85	3.54475	YES	YES
53	a	252.08	1.88909	YES	YES
54	a	253.29	8.64755	YES	YES
55	a	255.46	11.92839	YES	YES
56	a	257.55	28.87185	YES	YES
57	a	262.94	5.59693	YES	YES
58	a	264.08	20.61244	YES	YES
59	a	265.54	14.13505	YES	YES
60	a	267.33	12.21334	YES	YES
61	a	268.35	21.43369	YES	YES
62	a	270.76	2.35740	YES	YES
63	a	271.95	52.82558	YES	YES
64	a	273.56	13.64265	YES	YES
65	a	274.26	53.04587	YES	YES
66	a	276.32	80.83627	YES	YES
67	a	277.89	63.49832	YES	YES
68	a	279.80	173.92793	YES	YES
69	a	281.28	62.71317	YES	YES
70	a	282.91	63.24089	YES	YES
71	a	293.59	16.17873	YES	YES
72	a	304.64	37.78624	YES	YES
73	a	310.53	10.47576	YES	YES

74	a	387.06	6.75752	YES	YES
75	a	426.79	22.28721	YES	YES
76	a	436.86	68.23514	YES	YES
77	a	446.04	14.90668	YES	YES
78	a	483.16	59.02248	YES	YES
79	a	504.32	44.51666	YES	YES
80	a	582.09	1.92528	YES	YES
81	a	584.56	24.95756	YES	YES
82	a	585.41	17.80773	YES	YES
83	a	586.87	4.64904	YES	YES
84	a	594.58	4.68083	YES	YES
85	a	595.69	0.30871	YES	YES
86	a	597.26	0.41189	YES	YES
87	a	597.54	0.06352	YES	YES
88	a	597.84	1.63277	YES	YES
89	a	604.35	45.91168	YES	YES
90	a	633.97	0.88032	YES	YES
91	a	634.93	102.02342	YES	YES
92	a	636.72	46.76117	YES	YES
93	a	637.43	69.25421	YES	YES
94	a	641.81	116.17132	YES	YES
95	a	648.09	12.02544	YES	YES
96	a	648.56	14.73968	YES	YES
97	a	650.62	16.74059	YES	YES
98	a	650.81	24.32296	YES	YES
99	a	651.62	13.37093	YES	YES
100	a	654.75	89.78615	YES	YES
101	a	655.65	43.61381	YES	YES
102	a	656.21	94.70689	YES	YES
103	a	659.25	32.50091	YES	YES
104	a	660.17	86.40279	YES	YES
105	a	669.48	248.43359	YES	YES
106	a	691.25	640.39273	YES	YES
107	a	693.34	553.53380	YES	YES
108	a	730.36	58.29199	YES	YES



Total energy = -3376.1632390760 H = -91870.1283638 eV

HOMO-LUMO Separation

HOMO: 159. 159 a -0.21690092 H = -5.90218 eV

LUMO: 160. 160 a -0.14703357 H = -4.00099 eV

Gap : +0.06986734 H = +1.90119 eV

Number of MOs= 516, Electrons= 318.00, Symmetry: c1

\$coord

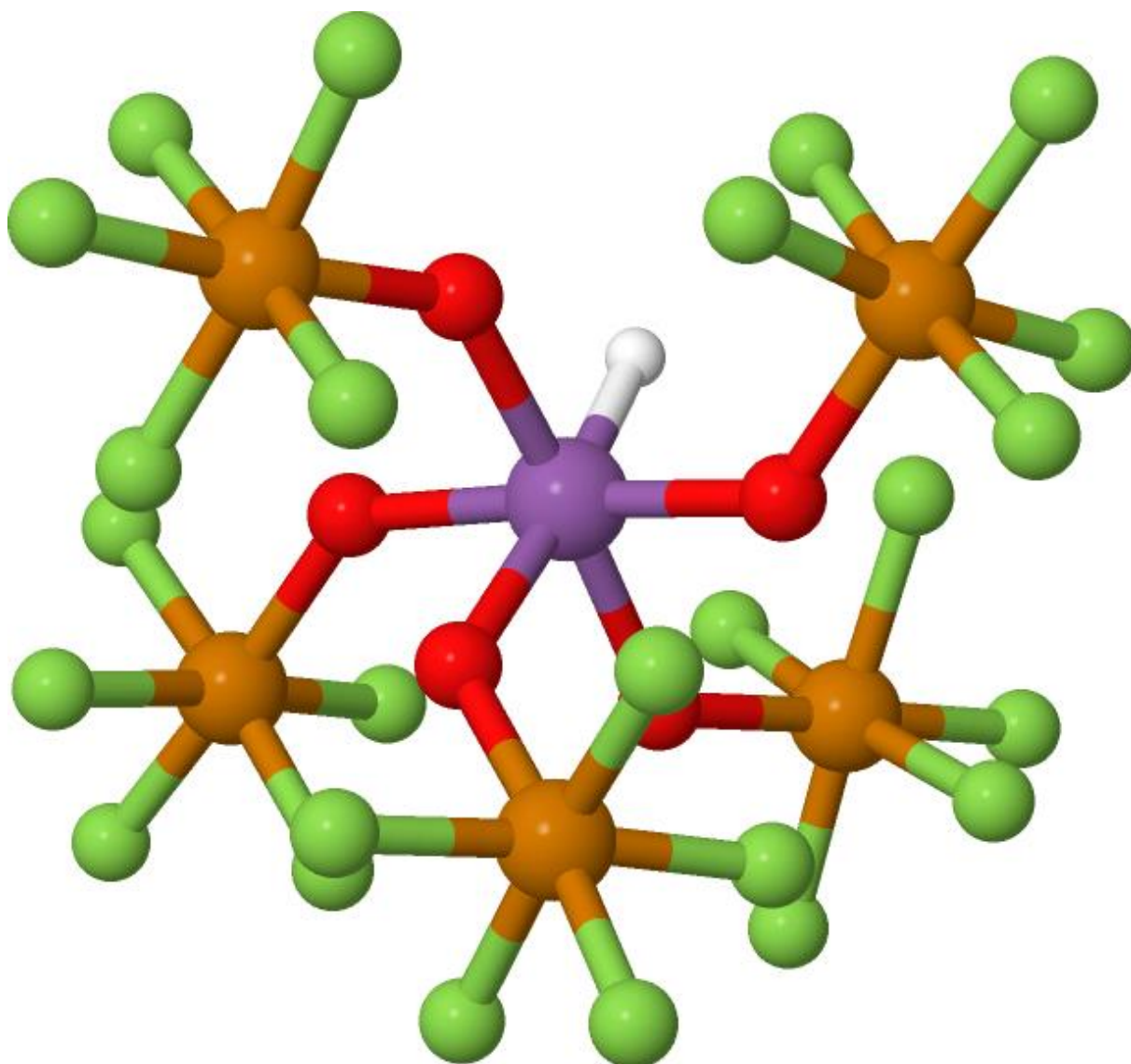
-1.28920482492804	0.02349090115673	-0.20970213378528	sb
-1.02361019241470	4.97122005450012	4.58118931497781	te
-0.85807271175710	4.49132979685344	-5.45379743138834	te
-0.09081610122394	3.33351361297485	1.43350629146752	o
0.03303544076463	1.49321873103790	-3.54673128213857	o
0.23144078074993	2.31255752677815	6.72026674716657	f
2.22698883388424	6.58386863881177	4.61619656798972	f
-2.35831893418800	7.83395500802332	2.78364761481714	f
-4.38364037178269	3.58173478005849	4.75953435374462	f
-1.77929763093650	6.78200255276873	7.64419875952496	f
-2.87270801606339	6.08130713071551	-2.87087068876206	f
-3.86788757460336	2.97820309504817	-6.83564108726937	f
2.04109874310206	6.33664657407918	-4.28387230701200	f
1.09193943373545	3.15873922045650	-8.20710406089128	f
-1.57795294687951	7.35752253453090	-7.57373345037029	f
2.22445466387840	-1.54534425332728	0.19299614012583	o
5.56967457152053	-0.10054289330393	0.60797690506152	te
-2.18651443933854	-3.38312917375253	-1.83250567491216	o
-0.77876221600333	-5.20483044936557	-4.68281503510387	te
4.79986827594338	1.38416146914248	3.83942819393777	f
6.58837983996212	-3.18360876770572	2.22914062014735	f
6.69221943917346	-1.47025082683620	-2.56300665381939	f
4.87852760781109	3.06800805806047	-1.03721610880585	f
8.97627522050953	1.07646686642441	1.09877346287562	f
2.20488030708825	-3.18451824360420	-5.15924384095224	f
-2.57149499859837	-3.11934809464769	-7.07322249811765	f
1.12533752246887	-7.51337747130029	-2.62065539068564	f
-3.65333304444010	-7.41505855070296	-4.45990559180832	f
0.30979054173891	-7.17872660060274	-7.53709399502153	f
-2.30099622725975	-1.32625784524056	3.27651837273871	o
-1.50315373807792	-4.35571726567432	5.15933254875668	te
-5.60865923647688	1.18087083597159	-0.76662875523032	cl
1.82094070072038	-3.23154636320061	6.12455189482422	f
-2.92090161348658	-2.75260822634390	8.09327089114955	f
-4.76174305989697	-5.77553122500529	4.38278362527982	f
-0.05863608750271	-6.25956942725689	2.42055312862918	f
-0.94286777429617	-7.26914614739658	7.26163078421505	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	13.21	0.03998	YES	YES
8		a	17.34	0.03952	YES	YES
9		a	22.25	0.01545	YES	YES
10		a	22.57	0.01531	YES	YES

11	a	32.93	0.02154	YES	YES
12	a	34.78	0.08690	YES	YES
13	a	35.74	0.13536	YES	YES
14	a	37.25	0.16760	YES	YES
15	a	38.49	0.06034	YES	YES
16	a	44.59	0.01895	YES	YES
17	a	52.96	0.04252	YES	YES
18	a	54.85	0.02868	YES	YES
19	a	61.56	0.15306	YES	YES
20	a	62.52	0.03618	YES	YES
21	a	73.05	0.23084	YES	YES
22	a	76.48	0.12544	YES	YES
23	a	79.30	0.39263	YES	YES
24	a	84.53	0.11462	YES	YES
25	a	89.84	1.32959	YES	YES
26	a	95.06	1.13322	YES	YES
27	a	97.00	1.03074	YES	YES
28	a	100.17	2.49412	YES	YES
29	a	104.48	0.66795	YES	YES
30	a	110.18	0.57899	YES	YES
31	a	111.33	1.60454	YES	YES
32	a	116.59	0.82588	YES	YES
33	a	147.57	7.90598	YES	YES
34	a	163.42	4.57296	YES	YES
35	a	164.03	0.29458	YES	YES
36	a	165.42	4.40940	YES	YES
37	a	166.93	6.13957	YES	YES
38	a	168.36	2.30907	YES	YES
39	a	170.12	15.57477	YES	YES
40	a	172.78	5.95233	YES	YES
41	a	176.36	9.64631	YES	YES
42	a	177.33	4.52642	YES	YES
43	a	179.59	2.45426	YES	YES
44	a	185.23	3.60286	YES	YES
45	a	186.79	10.50397	YES	YES
46	a	196.48	0.10964	YES	YES
47	a	198.72	3.04252	YES	YES
48	a	201.51	2.09559	YES	YES
49	a	216.46	37.49149	YES	YES
50	a	217.40	46.20266	YES	YES
51	a	246.51	22.24104	YES	YES
52	a	246.84	21.90790	YES	YES
53	a	248.82	0.78286	YES	YES
54	a	249.52	2.47826	YES	YES
55	a	251.80	0.06317	YES	YES
56	a	254.12	1.51553	YES	YES
57	a	255.48	16.27349	YES	YES
58	a	259.66	38.84685	YES	YES
59	a	268.08	68.40156	YES	YES
60	a	270.66	19.14106	YES	YES
61	a	272.58	8.18791	YES	YES
62	a	274.49	4.50389	YES	YES
63	a	274.98	1.98345	YES	YES
64	a	275.74	10.77837	YES	YES
65	a	276.18	10.83214	YES	YES
66	a	277.81	7.36775	YES	YES
67	a	278.71	58.22349	YES	YES
68	a	279.64	11.79198	YES	YES
69	a	280.13	24.06320	YES	YES
70	a	281.82	91.14630	YES	YES
71	a	284.40	92.84409	YES	YES
72	a	285.88	38.15541	YES	YES

73	a	287.74	132.02111	YES	YES
74	a	292.64	46.46822	YES	YES
75	a	301.64	3.02874	YES	YES
76	a	342.43	18.27059	YES	YES
77	a	382.20	1.53817	YES	YES
78	a	413.50	9.77516	YES	YES
79	a	417.22	3.84851	YES	YES
80	a	426.40	69.34406	YES	YES
81	a	429.48	84.37412	YES	YES
82	a	578.07	0.92150	YES	YES
83	a	579.34	11.07797	YES	YES
84	a	581.11	18.07403	YES	YES
85	a	581.68	10.83301	YES	YES
86	a	584.69	1.18666	YES	YES
87	a	589.73	0.49911	YES	YES
88	a	590.04	0.87890	YES	YES
89	a	590.78	0.55210	YES	YES
90	a	591.28	0.09936	YES	YES
91	a	592.72	0.04791	YES	YES
92	a	614.03	4.64710	YES	YES
93	a	614.85	60.68076	YES	YES
94	a	615.16	73.92965	YES	YES
95	a	616.32	52.85111	YES	YES
96	a	617.78	53.46514	YES	YES
97	a	639.71	1.76990	YES	YES
98	a	640.05	19.75556	YES	YES
99	a	642.72	35.43519	YES	YES
100	a	644.03	17.93844	YES	YES
101	a	647.30	39.06802	YES	YES
102	a	647.91	86.87010	YES	YES
103	a	651.20	158.87463	YES	YES
104	a	651.98	18.70242	YES	YES
105	a	652.48	72.70105	YES	YES
106	a	652.93	11.16039	YES	YES
107	a	663.59	31.85879	YES	YES
108	a	669.37	309.88348	YES	YES
109	a	683.97	633.89007	YES	YES
110	a	690.76	632.02520	YES	YES
111	a	734.58	76.29965	YES	YES



Total energy = -2916.6245915630 H = -79365.4384109 eV

HOMO-LUMO Separation

HOMO: 151. 151 a -0.22843304 H = -6.21598 eV

LUMO: 152. 152 a -0.13943223 H = -3.79415 eV

Gap : +0.08900082 H = +2.42184 eV

Number of MOs= 500, Electrons= 302.00, Symmetry: c1

\$coord

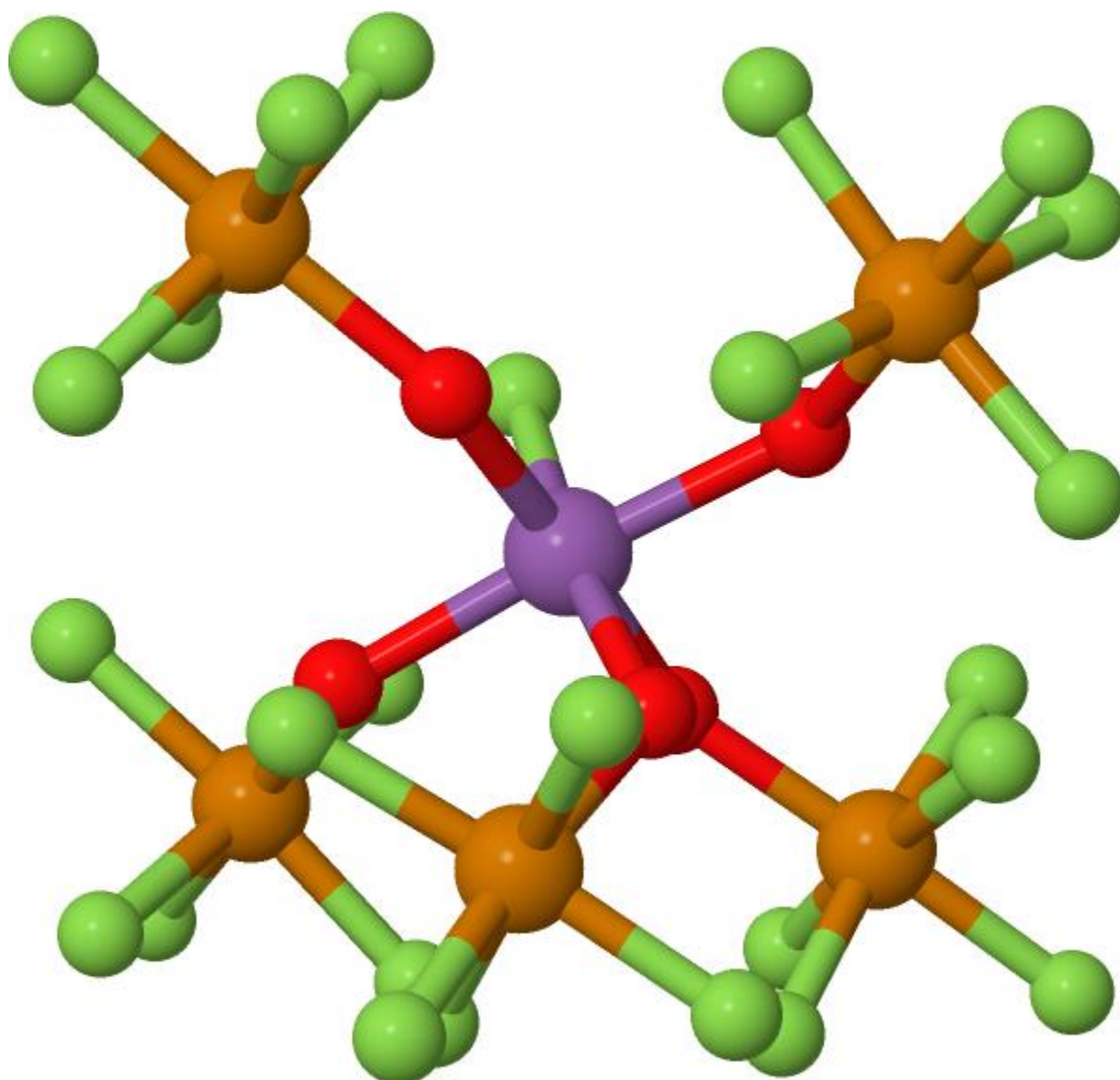
-1.28789782081077	0.13306122645959	-0.15750760285573	sb
-1.41224958918045	4.30326149001580	5.21568153369921	te
-0.82392990692581	5.36697088468865	-4.40723712166337	te
0.15608159987884	2.90433795164196	2.24320945334862	o
0.26189528101153	2.11716993901382	-3.18114947073541	o
-0.85954295131414	1.35206338136468	7.26728754759267	f
1.76646084187150	5.67803475038986	6.29613559674817	f
-2.15999006412568	7.46508756331965	3.57992437291787	f
-4.74756437620474	3.09040394627674	4.31319150722571	f
-2.93227962049845	5.76152290289381	8.18377305914639	f
-3.11484237422477	5.93197534609328	-1.60035409528836	f
-3.65224400283952	3.97937366425227	-6.24307190785813	f
1.78794895526879	7.20063443374974	-2.67377777966580	f
1.30814577255310	4.98787012164202	-7.31481347726770	f
-1.85942128151229	8.59048080296710	-5.73449745446640	f
2.15790424736722	-1.59662289022419	0.03379983064248	o
5.55537044678543	-0.33329771227728	0.65487251245567	te
-2.35750600453991	-2.81472809451603	-2.49269042899660	o
-1.15241821311633	-4.18192718407698	-5.63956183226869	te
4.92853077758172	0.53193256517237	4.13131340744677	f
6.47647876599075	-3.70088590784358	1.64629996493328	f
6.58423566343245	-1.10142730865826	-2.74240005061811	f
4.96655155837639	3.11535536360722	-0.33955782335176	f
9.01194072166305	0.61776800615458	1.26879453456684	f
2.11503497628459	-2.58382355020557	-5.62129757480822	f
-2.50871081627380	-1.39669368403355	-7.56223918463874	f
0.29323734167734	-7.14420292484271	-4.10947090894003	f
-4.32518017692620	-5.93025437369916	-5.95825996230677	f
-0.23187227250003	-5.64261180835379	-8.84376718545781	f
-2.53931452084722	-2.02452058728116	2.84189619724242	o
-1.52649644258035	-5.23037076210372	4.24374370747811	te
-4.30944968396869	1.29798113417721	-0.35172008840111	h
1.71295115154594	-4.04332927662787	5.40891178154742	f
-3.03315958578691	-4.28835426001053	7.41142109685023	f
-4.69248040342070	-6.73014010616444	3.25364975920867	f
0.01070213037646	-6.54977846663020	1.22281243040320	f
-0.70863829414074	-8.41531507433532	5.80201929775426	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	12.63	0.00087	YES	YES
8		a	18.42	0.05697	YES	YES
9		a	19.66	0.01797	YES	YES
10		a	23.32	0.00512	YES	YES
11		a	28.92	0.05663	YES	YES
12		a	33.90	0.31848	YES	YES
13		a	36.96	0.03138	YES	YES
14		a	37.64	0.05676	YES	YES

15	a	40.32	0.25644	YES	YES
16	a	41.96	0.00336	YES	YES
17	a	47.56	0.04279	YES	YES
18	a	49.49	0.01655	YES	YES
19	a	57.97	0.12537	YES	YES
20	a	65.22	0.30980	YES	YES
21	a	71.72	0.06904	YES	YES
22	a	73.97	0.42635	YES	YES
23	a	81.80	0.49737	YES	YES
24	a	84.49	0.28638	YES	YES
25	a	90.28	0.57159	YES	YES
26	a	95.52	1.19405	YES	YES
27	a	96.07	2.81281	YES	YES
28	a	101.55	0.88546	YES	YES
29	a	109.03	0.02497	YES	YES
30	a	110.35	0.44669	YES	YES
31	a	153.07	12.71570	YES	YES
32	a	161.94	14.55952	YES	YES
33	a	163.74	2.97639	YES	YES
34	a	163.84	15.35647	YES	YES
35	a	167.46	3.87033	YES	YES
36	a	168.05	0.25299	YES	YES
37	a	168.77	4.21218	YES	YES
38	a	171.85	0.45242	YES	YES
39	a	173.90	0.96310	YES	YES
40	a	175.65	2.12859	YES	YES
41	a	177.95	4.69033	YES	YES
42	a	180.44	1.31969	YES	YES
43	a	186.08	7.63446	YES	YES
44	a	193.72	0.23738	YES	YES
45	a	194.96	0.17948	YES	YES
46	a	206.83	3.77332	YES	YES
47	a	211.32	41.09505	YES	YES
48	a	213.57	41.88451	YES	YES
49	a	246.56	10.43904	YES	YES
50	a	246.84	5.05919	YES	YES
51	a	248.82	0.17937	YES	YES
52	a	249.97	2.86940	YES	YES
53	a	250.82	0.60874	YES	YES
54	a	253.91	1.23308	YES	YES
55	a	255.37	17.51799	YES	YES
56	a	263.27	54.66265	YES	YES
57	a	269.49	33.82201	YES	YES
58	a	271.60	35.37121	YES	YES
59	a	271.86	27.32839	YES	YES
60	a	275.76	4.72286	YES	YES
61	a	276.54	11.23417	YES	YES
62	a	277.22	8.83206	YES	YES
63	a	278.73	2.57041	YES	YES
64	a	280.33	32.31346	YES	YES
65	a	280.69	29.51678	YES	YES
66	a	281.92	31.29042	YES	YES
67	a	282.08	13.35053	YES	YES
68	a	283.67	113.65665	YES	YES
69	a	284.62	155.62141	YES	YES
70	a	288.27	24.10516	YES	YES
71	a	290.06	110.21687	YES	YES
72	a	293.72	19.66483	YES	YES
73	a	302.91	2.56474	YES	YES
74	a	381.01	8.32885	YES	YES
75	a	403.95	3.42257	YES	YES
76	a	419.92	26.83158	YES	YES

77	a	435.06	77.03637	YES	YES
78	a	444.49	94.55203	YES	YES
79	a	573.37	32.22966	YES	YES
80	a	576.16	23.75892	YES	YES
81	a	576.85	32.95968	YES	YES
82	a	578.25	18.63782	YES	YES
83	a	581.85	1.87781	YES	YES
84	a	585.46	4.92262	YES	YES
85	a	587.02	1.38720	YES	YES
86	a	588.47	1.08566	YES	YES
87	a	589.58	0.50333	YES	YES
88	a	591.25	0.47236	YES	YES
89	a	612.18	11.36497	YES	YES
90	a	613.51	8.97397	YES	YES
91	a	613.91	27.17374	YES	YES
92	a	614.65	28.94743	YES	YES
93	a	616.56	38.34621	YES	YES
94	a	623.45	295.84140	YES	YES
95	a	631.26	191.55968	YES	YES
96	a	638.09	7.74370	YES	YES
97	a	639.42	9.33016	YES	YES
98	a	641.46	42.51368	YES	YES
99	a	642.39	21.24072	YES	YES
100	a	646.65	113.48146	YES	YES
101	a	647.30	134.17699	YES	YES
102	a	649.04	197.91332	YES	YES
103	a	651.19	59.22760	YES	YES
104	a	653.30	320.10651	YES	YES
105	a	654.37	409.71559	YES	YES
106	a	664.00	189.46883	YES	YES
107	a	668.03	124.43427	YES	YES
108	a	722.67	105.51364	YES	YES
109	a	731.90	131.17499	YES	YES
110	a	751.36	82.03881	YES	YES
111	a	1960.88	3.66823	YES	YES



Total energy = -3015.8175409390 H = -82064.6174335 eV

HOMO-LUMO Separation

HOMO: 155. 155 a -0.23691767 H = -6.44686 eV

LUMO: 156. 156 a -0.14743945 H = -4.01203 eV

Gap : +0.08947822 H = +2.43483 eV

Number of MOs= 512, Electrons= 310.00, Symmetry: c1

\$coord

-1.18964527594156	0.04365043504069	-0.18972004867456	sb
-1.22574773593907	5.01330014079327	4.50581576062518	te
-1.06998826253983	4.40740990664128	-5.43278348420121	te
-0.00890959119756	3.31811729598622	1.48693110204433	o
0.06499281788512	1.47356726603503	-3.54473495769805	o
-0.04527317643602	2.44144181551974	6.78958090185638	f
1.97680671455634	6.70640267982282	4.72649155863789	f
-2.49705263451433	7.80387255021270	2.55919404162073	f
-4.54742329040156	3.52899212264377	4.47685790425071	f
-2.25565540062297	6.85913114810876	7.46433831219884	f
-3.00236567100838	5.93536337784589	-2.75531276452785	f
-4.07237442211418	2.75760526211255	-6.65392493353072	f
1.81801338864855	6.36713221929964	-4.42845997757379	f
0.79888329562329	3.12972535493634	-8.26749352491515	f
-2.01333451421149	7.22270084553498	-7.53259402516857	f
2.29523246546232	-1.58751159664667	0.24012931718496	o
5.64579627163879	-0.15419517515103	0.64832906914214	te
-2.18979628577356	-3.34165190121874	-1.74227278762057	o
-0.96951398930750	-5.09488965963021	-4.71566061068696	te
4.89443344200758	1.29615842264588	3.89927307225656	f
6.65934369500442	-3.25588020179786	2.23699303960892	f
6.73841530351873	-1.50034671332703	-2.54332660689980	f
4.93678371328522	3.02783434430551	-0.96397560354244	f
9.05743040175238	1.00962468891895	1.12779548382402	f
2.08725802614759	-3.18802483761303	-5.19516715031484	f
-2.73981377221057	-2.85902795880703	-6.97888175059082	f
0.89911199617883	-7.52751523429399	-2.77113400700280	f
-3.91538598401080	-7.20291934005788	-4.47018461121203	f
-0.04873445372445	-7.01332239428150	-7.66413266472854	f
-2.31641969062069	-1.27720734924308	3.24660297086333	o
-1.62199283645309	-4.34133388235898	5.11519554795226	te
-4.60780653058357	1.21995099495913	-0.73149265388518	f
1.69062960262329	-3.25562890758561	6.15438420390062	f
-3.07722910149544	-2.73474860326723	8.02498082835234	f
-4.88087427795468	-5.71067235075333	4.26386974097467	f
-0.13321329681576	-6.24641452502452	2.40295943932880	f
-1.13458094045533	-7.27069024030533	7.21152986815130	f

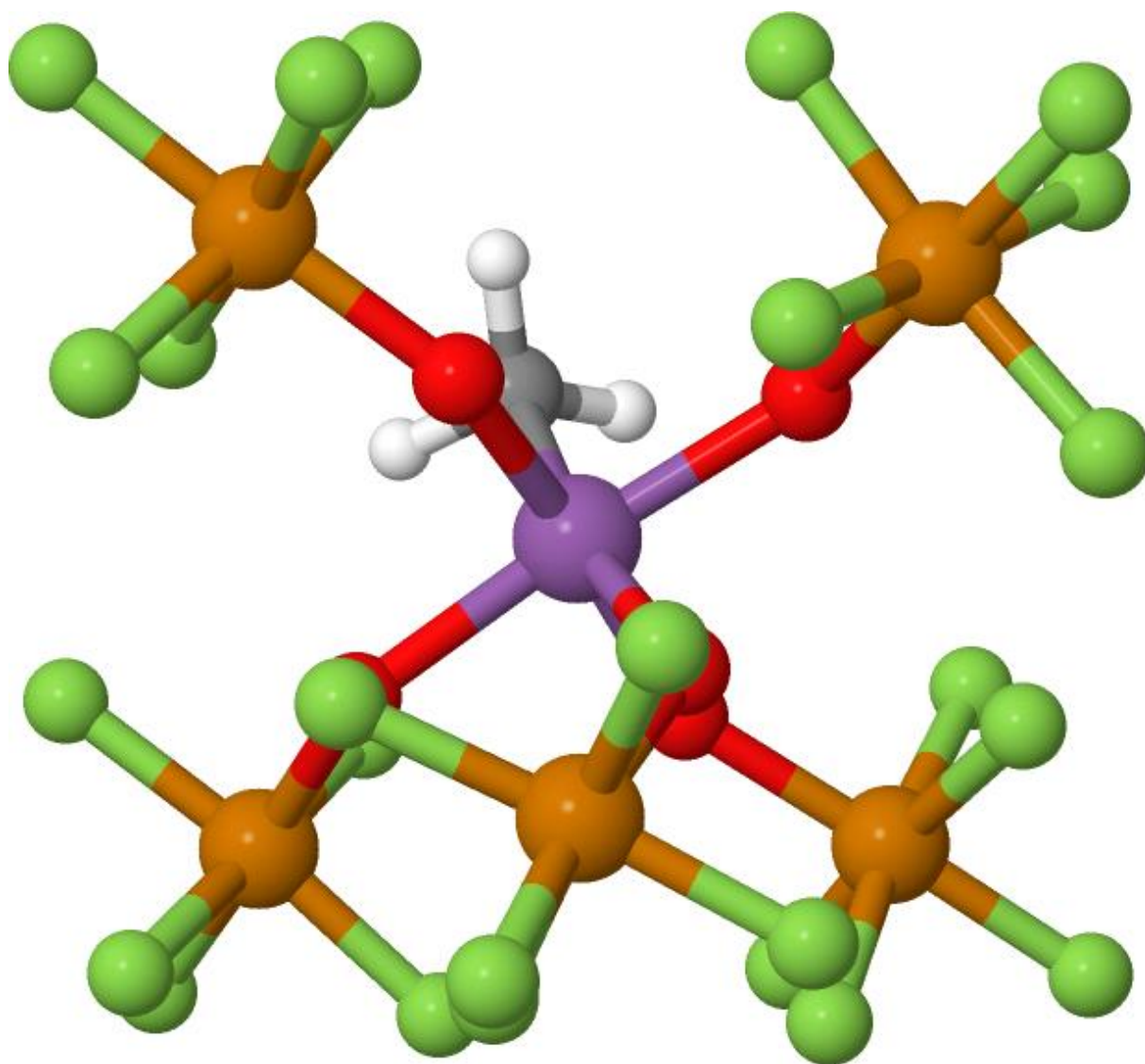
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\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
#						
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	10.20	0.00712	YES	YES
8		a	13.93	0.12582	YES	YES
9		a	18.66	0.04154	YES	YES
10		a	20.73	0.00398	YES	YES

11	a	23.41	0.03908	YES	YES
12	a	31.14	0.10301	YES	YES
13	a	31.85	0.00955	YES	YES
14	a	32.57	0.15045	YES	YES
15	a	35.98	0.08015	YES	YES
16	a	40.24	0.01537	YES	YES
17	a	48.88	0.11908	YES	YES
18	a	51.80	0.07143	YES	YES
19	a	57.14	0.06285	YES	YES
20	a	63.26	0.32049	YES	YES
21	a	73.77	0.07195	YES	YES
22	a	77.16	0.04287	YES	YES
23	a	79.16	0.13211	YES	YES
24	a	83.81	0.46314	YES	YES
25	a	87.85	2.18304	YES	YES
26	a	92.92	0.93850	YES	YES
27	a	96.66	2.04788	YES	YES
28	a	97.51	0.48439	YES	YES
29	a	107.38	0.05875	YES	YES
30	a	110.97	0.38698	YES	YES
31	a	140.84	1.28110	YES	YES
32	a	143.83	0.75176	YES	YES
33	a	154.68	5.14038	YES	YES
34	a	164.11	1.95361	YES	YES
35	a	164.47	0.96689	YES	YES
36	a	165.19	3.20375	YES	YES
37	a	168.07	2.54430	YES	YES
38	a	168.37	2.08630	YES	YES
39	a	171.04	7.46829	YES	YES
40	a	175.20	1.84233	YES	YES
41	a	178.63	5.40243	YES	YES
42	a	180.70	9.21511	YES	YES
43	a	185.05	6.55907	YES	YES
44	a	187.44	19.20228	YES	YES
45	a	195.32	8.11592	YES	YES
46	a	198.12	1.34106	YES	YES
47	a	200.60	1.26778	YES	YES
48	a	204.40	8.10818	YES	YES
49	a	220.42	55.45173	YES	YES
50	a	221.55	62.46905	YES	YES
51	a	248.25	14.23823	YES	YES
52	a	248.83	14.53998	YES	YES
53	a	249.02	35.23829	YES	YES
54	a	250.15	1.37279	YES	YES
55	a	250.96	2.33262	YES	YES
56	a	254.22	6.99321	YES	YES
57	a	257.84	22.28620	YES	YES
58	a	262.34	47.64431	YES	YES
59	a	267.97	23.33231	YES	YES
60	a	269.97	10.50994	YES	YES
61	a	272.42	19.37150	YES	YES
62	a	274.39	9.61092	YES	YES
63	a	275.17	22.93812	YES	YES
64	a	275.37	8.77357	YES	YES
65	a	276.20	2.66565	YES	YES
66	a	276.87	14.39167	YES	YES
67	a	277.96	43.60860	YES	YES
68	a	278.93	29.60191	YES	YES
69	a	280.18	59.78699	YES	YES
70	a	281.32	118.40819	YES	YES
71	a	285.13	109.03895	YES	YES
72	a	287.72	91.34872	YES	YES

73	a	295.42	22.52417	YES	YES
74	a	296.96	10.95355	YES	YES
75	a	306.27	9.03048	YES	YES
76	a	386.23	3.88633	YES	YES
77	a	420.45	5.04896	YES	YES
78	a	424.48	30.51970	YES	YES
79	a	433.65	45.35089	YES	YES
80	a	440.96	80.09628	YES	YES
81	a	579.29	0.19324	YES	YES
82	a	579.78	12.22262	YES	YES
83	a	582.24	14.05398	YES	YES
84	a	582.89	8.61932	YES	YES
85	a	584.74	0.11104	YES	YES
86	a	590.22	0.07400	YES	YES
87	a	590.43	0.92667	YES	YES
88	a	591.26	0.40360	YES	YES
89	a	592.03	0.12439	YES	YES
90	a	593.11	0.07613	YES	YES
91	a	609.76	22.20825	YES	YES
92	a	613.12	28.58364	YES	YES
93	a	614.36	48.28646	YES	YES
94	a	615.61	67.18823	YES	YES
95	a	618.53	60.02999	YES	YES
96	a	619.41	36.97527	YES	YES
97	a	640.63	2.14726	YES	YES
98	a	641.10	16.76956	YES	YES
99	a	643.68	25.34379	YES	YES
100	a	645.00	22.75507	YES	YES
101	a	648.39	48.01140	YES	YES
102	a	649.05	98.38222	YES	YES
103	a	652.15	94.61519	YES	YES
104	a	652.30	36.67677	YES	YES
105	a	653.02	156.70618	YES	YES
106	a	653.91	1.85159	YES	YES
107	a	667.95	54.34931	YES	YES
108	a	675.04	398.89586	YES	YES
109	a	694.31	612.52905	YES	YES
110	a	700.65	597.02317	YES	YES
111	a	744.95	40.27011	YES	YES



Total energy = -2955.9266259200 H = -80434.9017886 eV

HOMO-LUMO Separation

HOMO: 155. 155 a -0.22291256 H = -6.06576 eV

LUMO: 156. 156 a -0.13835420 H = -3.76481 eV

Gap : +0.08455836 H = +2.30095 eV

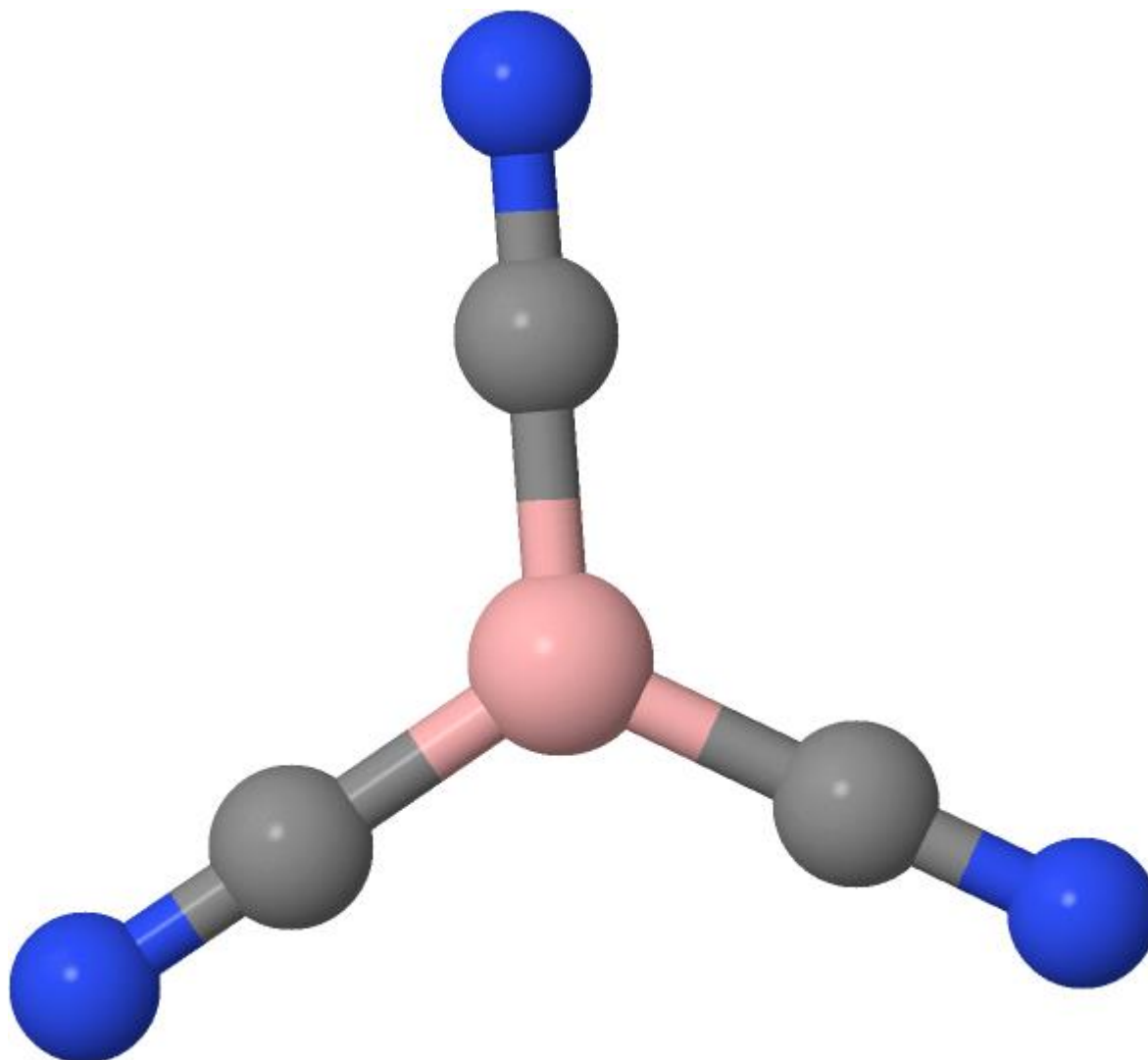
Number of MOs= 518, Electrons= 310.00, Symmetry: c1

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-1.38029802579089	0.09080218597636	-0.21946153379153	sb
-1.05268593505459	4.80679834040908	4.79417246307982	te
-1.12094721282659	4.66199895998317	-5.31090321738467	te
-0.00632009503832	3.27339751334499	1.67359181724726	o
0.08552214400495	1.75717318134683	-3.50615921220803	o
0.15746686316847	2.13172324290523	6.93983122579647	f
2.12555521199967	6.53693382519790	5.05395393846604	f
-2.42936578512611	7.69198427539168	3.04995761965280	f
-4.41081955194921	3.33017753042843	4.76530999132592	f
-2.05651848860879	6.47727219206169	7.86846877605218	f
-3.08022403749881	5.97795003574774	-2.50923567662159	f
-4.15133930599375	2.95748517811370	-6.48741609710810	f
1.68464836915420	6.76602136437571	-4.36783032207745	f
0.64452865858370	3.58812022220247	-8.29230426661909	f
-2.32847711464991	7.51115670561498	-7.22633909743662	f
2.15631469820329	-1.43861000916742	0.04951363275752	o
5.47977106814550	0.03768351384680	0.56708927828135	te
-2.18141823968760	-3.25002984077964	-2.12315646058132	o
-0.71159606324439	-5.02768790411601	-4.93167790363445	te
4.73161291236800	1.25760783749006	3.91409110037412	f
6.52381457728521	-3.14885503301932	1.95722663865800	f
6.62719285867133	-1.06753486306422	-2.69788570724148	f
4.77947993279495	3.32345083022844	-0.83084198877826	f
8.87769076205468	1.20035805819185	1.15112327226386	f
2.23811435668377	-2.94640376440523	-5.37685187900197	f
-2.52636122274019	-2.94672346289956	-7.32080255115555	f
1.22739215211217	-7.33834810813565	-2.90505253228294	f
-3.54048974782012	-7.31293747267582	-4.81292822497045	f
0.44392545012376	-6.92497129584288	-7.81706305973108	f
-2.28063576858321	-1.52892803573550	3.23310981204438	o
-1.57633568238328	-4.59557581613967	5.02302483593459	te
1.75320107791670	-3.59638836567994	6.10126217069405	f
-3.02547426434512	-3.13165634250291	8.02014303322578	f
-4.85780119634674	-5.93235757192746	4.15146264895240	f
-0.13732265315778	-6.40648754263096	2.21486643113549	f
-1.09658714242826	-7.61803366156474	6.99364560331548	f
-5.31386065968237	1.01890681614745	-0.64073676210172	c
-5.65459146970880	2.75302981072426	0.46881621607394	h
-6.29512266869883	-0.65010750132222	0.14835413272235	h
-5.62314829827715	1.25889176199655	-2.69417406444645	h

\$vibrational spectrum						
#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	2.44	0.03191	YES	YES
8		a	15.33	0.04178	YES	YES
9		a	19.60	0.01504	YES	YES
10		a	22.03	0.06067	YES	YES
11		a	25.69	0.02818	YES	YES
12		a	30.60	0.08882	YES	YES
13		a	32.78	0.01758	YES	YES
14		a	34.59	0.06953	YES	YES
15		a	35.70	0.08507	YES	YES
16		a	37.85	0.32104	YES	YES

17	a	47.02	0.00953	YES	YES
18	a	56.46	0.30274	YES	YES
19	a	58.66	0.08092	YES	YES
20	a	64.22	0.22303	YES	YES
21	a	67.45	0.16083	YES	YES
22	a	75.82	0.19876	YES	YES
23	a	82.46	0.08059	YES	YES
24	a	84.19	0.51625	YES	YES
25	a	88.58	0.50514	YES	YES
26	a	97.24	1.86170	YES	YES
27	a	99.38	1.10347	YES	YES
28	a	101.53	0.74068	YES	YES
29	a	108.38	0.01294	YES	YES
30	a	109.46	0.48740	YES	YES
31	a	140.98	0.48171	YES	YES
32	a	153.39	9.17895	YES	YES
33	a	154.06	7.41567	YES	YES
34	a	161.46	13.13363	YES	YES
35	a	163.63	8.43105	YES	YES
36	a	164.89	11.99742	YES	YES
37	a	165.94	4.65312	YES	YES
38	a	168.41	0.98309	YES	YES
39	a	169.64	4.46796	YES	YES
40	a	175.63	0.98370	YES	YES
41	a	176.94	2.01614	YES	YES
42	a	178.56	2.74369	YES	YES
43	a	179.26	5.11885	YES	YES
44	a	187.47	8.48231	YES	YES
45	a	189.67	1.63503	YES	YES
46	a	194.83	0.59484	YES	YES
47	a	196.44	2.26818	YES	YES
48	a	200.66	0.75066	YES	YES
49	a	202.97	3.56710	YES	YES
50	a	209.72	45.16615	YES	YES
51	a	210.10	51.51640	YES	YES
52	a	246.56	7.36261	YES	YES
53	a	247.28	5.72948	YES	YES
54	a	248.54	4.33693	YES	YES
55	a	249.27	1.81735	YES	YES
56	a	250.93	3.94508	YES	YES
57	a	254.79	10.75534	YES	YES
58	a	257.00	22.31505	YES	YES
59	a	264.28	52.88735	YES	YES
60	a	271.78	53.94098	YES	YES
61	a	275.43	10.29467	YES	YES
62	a	276.42	1.46046	YES	YES
63	a	276.76	5.75755	YES	YES
64	a	278.39	6.36897	YES	YES
65	a	279.05	30.13079	YES	YES
66	a	279.69	1.73318	YES	YES
67	a	280.29	17.05571	YES	YES
68	a	281.15	23.39080	YES	YES
69	a	282.25	35.09698	YES	YES
70	a	283.04	45.03060	YES	YES
71	a	284.83	91.90182	YES	YES
72	a	285.91	71.69497	YES	YES
73	a	289.75	106.34453	YES	YES
74	a	290.46	83.85271	YES	YES
75	a	296.55	18.12198	YES	YES
76	a	306.72	2.64620	YES	YES
77	a	374.34	5.43394	YES	YES
78	a	400.61	13.11738	YES	YES

79	a	413.34	18.65051	YES	YES
80	a	423.50	57.69951	YES	YES
81	a	428.30	90.29442	YES	YES
82	a	501.96	0.66338	YES	YES
83	a	570.22	7.68775	YES	YES
84	a	574.15	11.74358	YES	YES
85	a	576.69	16.55317	YES	YES
86	a	577.52	9.77154	YES	YES
87	a	579.93	6.30573	YES	YES
88	a	581.28	1.47861	YES	YES
89	a	584.91	2.77916	YES	YES
90	a	587.03	0.77917	YES	YES
91	a	588.24	0.34340	YES	YES
92	a	590.06	0.20966	YES	YES
93	a	611.56	10.95140	YES	YES
94	a	611.96	32.83541	YES	YES
95	a	612.75	69.85814	YES	YES
96	a	614.39	60.28179	YES	YES
97	a	616.09	38.91648	YES	YES
98	a	634.17	9.88951	YES	YES
99	a	637.37	5.50140	YES	YES
100	a	638.26	33.70433	YES	YES
101	a	639.50	33.30670	YES	YES
102	a	642.37	41.63541	YES	YES
103	a	643.44	92.76422	YES	YES
104	a	646.80	163.16978	YES	YES
105	a	648.77	43.18065	YES	YES
106	a	649.94	49.73155	YES	YES
107	a	650.14	23.02453	YES	YES
108	a	662.28	319.28227	YES	YES
109	a	671.00	189.34110	YES	YES
110	a	684.34	697.85761	YES	YES
111	a	694.03	479.66772	YES	YES
112	a	740.97	112.51297	YES	YES
113	a	831.79	21.99147	YES	YES
114	a	844.48	30.97001	YES	YES
115	a	1179.50	5.09177	YES	YES
116	a	1383.02	8.59517	YES	YES
117	a	1400.75	5.53738	YES	YES
118	a	3002.28	3.43313	YES	YES
119	a	3137.59	12.41644	YES	YES
120	a	3155.34	13.87943	YES	YES



Total energy = -303.1601383215 H = -8249.4117879 eV

HOMO-LUMO Separation

HOMO: 22. 22 a -0.34852414 H = -9.48383 eV

LUMO: 23. 23 a -0.21947944 H = -5.97234 eV

Gap : +0.12904470 H = +3.51149 eV

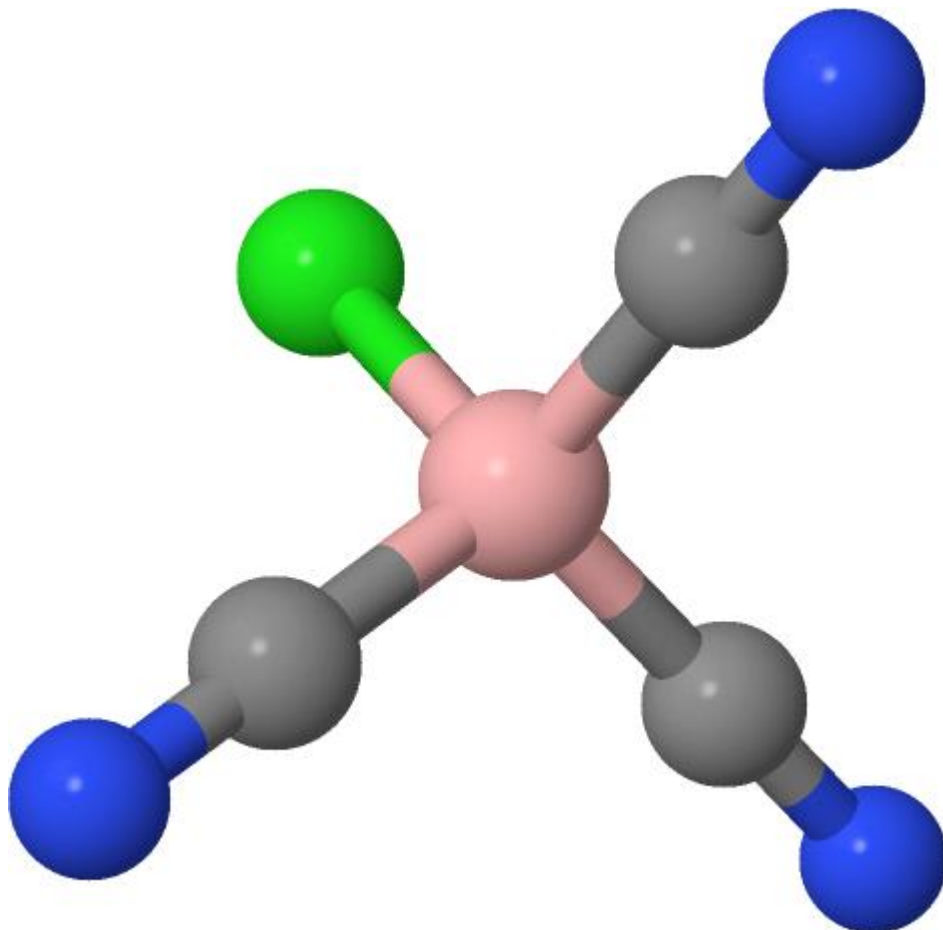
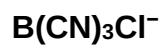
Number of MOs= 98, Electrons= 44.00, Symmetry: c1

\$coord

-0.48211422773238	2.26329562272605	4.25933763152281	b
-0.51242426599099	2.25635896322050	1.36093776418739	c
-0.53515416982813	2.25173333990239	-0.86079365219876	n
1.43237750215342	3.90761447558721	5.68523196283235	c
-2.36587369205775	0.62611259576093	5.73357644242162	c
2.89926901124414	5.16735809879555	6.77973365649179	n
-3.80924129090187	-0.62768645575890	6.86582287200414	n

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		113.08	4.99908	YES	YES
8	a		113.40	5.02552	YES	YES
9	a		144.02	26.09135	YES	YES
10	a		286.88	0.00005	YES	YES
11	a		287.13	0.00007	YES	YES
12	a		320.89	0.00005	YES	YES
13	a		501.14	1.11528	YES	YES
14	a		501.24	1.12069	YES	YES
15	a		536.35	0.00002	YES	YES
16	a		631.41	13.79087	YES	YES
17	a		1107.04	152.53103	YES	YES
18	a		1107.45	152.85346	YES	YES
19	a		2239.39	0.76257	YES	YES
20	a		2244.23	162.13964	YES	YES
21	a		2244.68	162.50528	YES	YES



Total energy = -763.4537695880 H = -20774.6459058 eV

HOMO-LUMO Separation

HOMO: 31. 31 a -0.11483702 H = -3.12488 eV

LUMO: 32. 32 a +0.08220926 H = +2.23703 eV

Gap : +0.19704628 H = +5.36191 eV

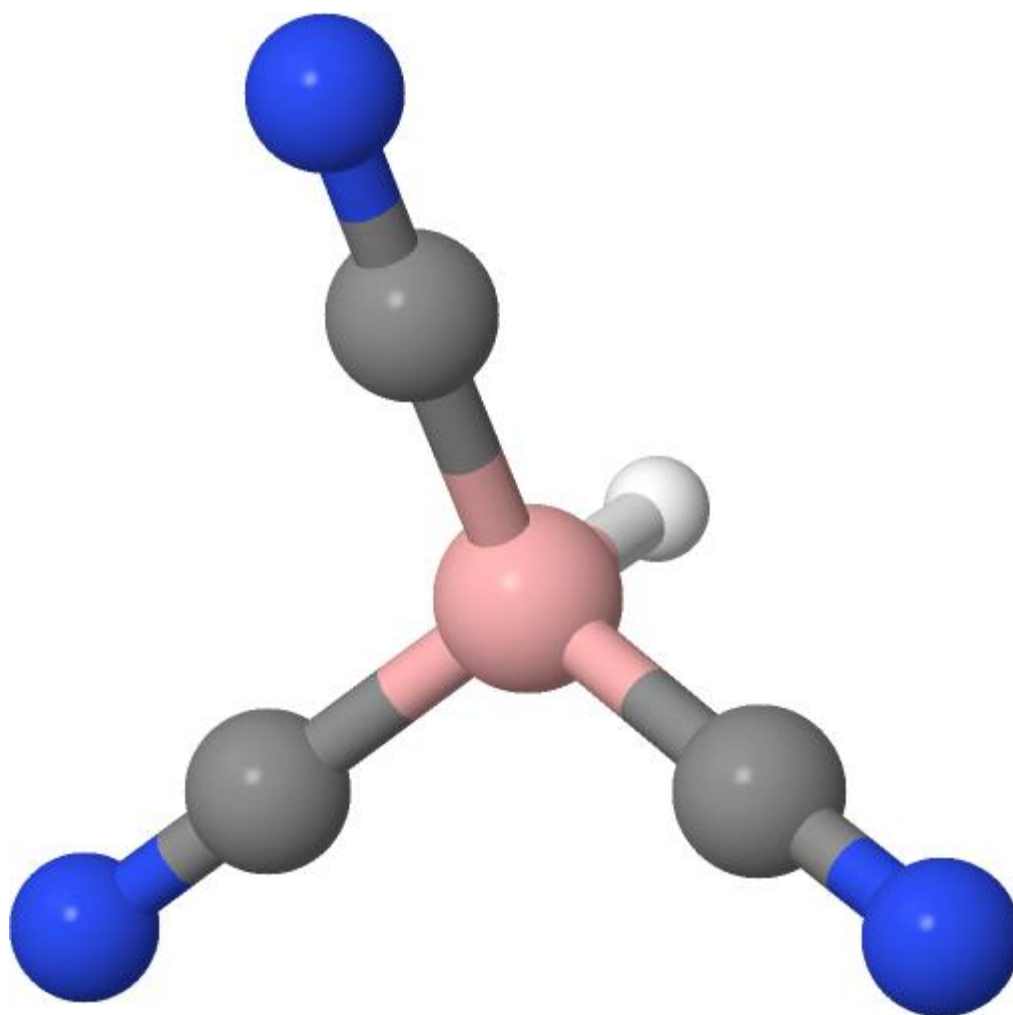
Number of MOs= 116, Electrons= 62.00, Symmetry: c1

\$coord

-0.33265092148535	1.96766741512416	4.18020825555980	b
-1.19669407629077	3.01648068968991	1.48065946090250	c
-1.82930672266234	3.77970516125614	-0.50497898013982	n
1.21304693496967	4.09548525009601	5.66891044646576	c
-2.75527729927704	1.14263544659924	5.78770219245752	c
2.35345234315028	5.65219152190685	6.76515434515536	n
-4.53234572731174	0.53172513873969	6.96842831202876	n
1.79080999027520	-0.90501497010241	3.69789902716715	cl

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		103.05	1.62145	YES	YES
8	a		103.26	1.59660	YES	YES
9	a		131.78	9.62549	YES	YES
10	a		167.70	4.07996	YES	YES
11	a		168.20	4.11928	YES	YES
12	a		334.66	0.00003	YES	YES
13	a		417.98	0.33521	YES	YES
14	a		418.23	0.32198	YES	YES
15	a		429.13	14.20039	YES	YES
16	a		489.55	4.58932	YES	YES
17	a		506.55	1.83123	YES	YES
18	a		506.69	1.83446	YES	YES
19	a		773.44	118.02427	YES	YES
20	a		939.01	76.75594	YES	YES
21	a		939.31	76.71093	YES	YES
22	a		2238.86	0.44557	YES	YES
23	a		2239.11	0.44691	YES	YES
24	a		2239.47	0.30612	YES	YES



Total energy = -303.8994536089 H = -8269.5295919 eV

HOMO-LUMO Separation

HOMO: 23. 23 a -0.10952702 H = -2.98038 eV

LUMO: 24. 24 a +0.12765469 H = +3.47366 eV

Gap : +0.23718171 H = +6.45405 eV

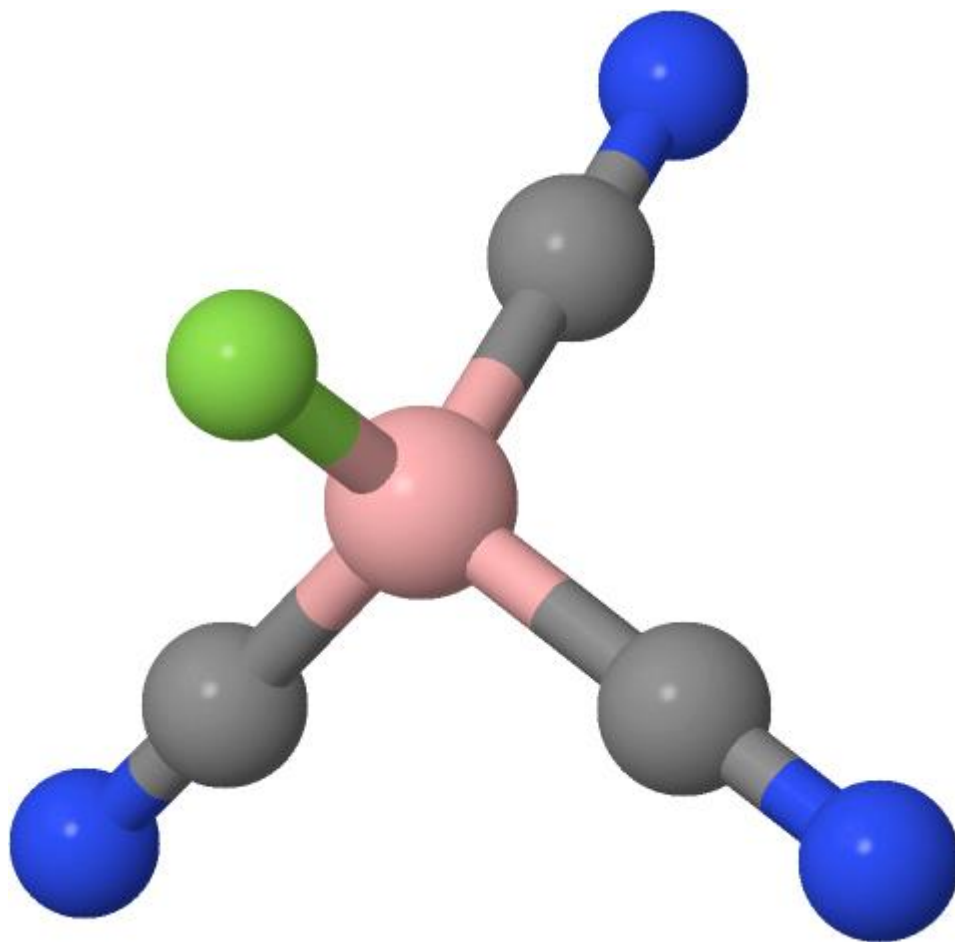
Number of MOs= 100, Electrons= 46.00, Symmetry: c1

\$coord

-0.32372635754649	1.97184497473399	4.18581237181172	b
-1.14079859907929	2.93870096465716	1.44439573376098	c
-1.68280082678350	3.59833199176224	-0.60574700503969	n
1.23282427364046	4.08884436073169	5.67358099100800	c
-2.70435064987640	1.03247779781814	5.78878552708133	c
2.43475828400660	5.60315160863671	6.76654184838673	n
-4.41532489530195	0.26808713523837	6.98047225234365	n
1.09974882937174	0.12317800186757	3.88610833046907	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		114.77	2.88651	YES	YES
8	a		115.46	2.81889	YES	YES
9	a		151.54	9.88639	YES	YES
10	a		339.73	3.98295	YES	YES
11	a		340.17	3.96327	YES	YES
12	a		343.89	0.07924	YES	YES
13	a		480.21	1.95594	YES	YES
14	a		507.54	0.56600	YES	YES
15	a		509.00	0.50273	YES	YES
16	a		709.76	0.06730	YES	YES
17	a		841.64	2.76198	YES	YES
18	a		842.91	2.70239	YES	YES
19	a		1033.55	63.75419	YES	YES
20	a		1034.15	65.01892	YES	YES
21	a		2231.56	11.00786	YES	YES
22	a		2231.75	11.05993	YES	YES
23	a		2234.88	1.92911	YES	YES
24	a		2359.88	122.36484	YES	YES



Total energy = -403.1235445733 H = -10969.5560208 eV

HOMO-LUMO Separation

HOMO: 27. 27 a -0.13533189 H = -3.68257 eV

LUMO: 28. 28 a +0.09082135 H = +2.47138 eV

Gap : +0.22615324 H = +6.15395 eV

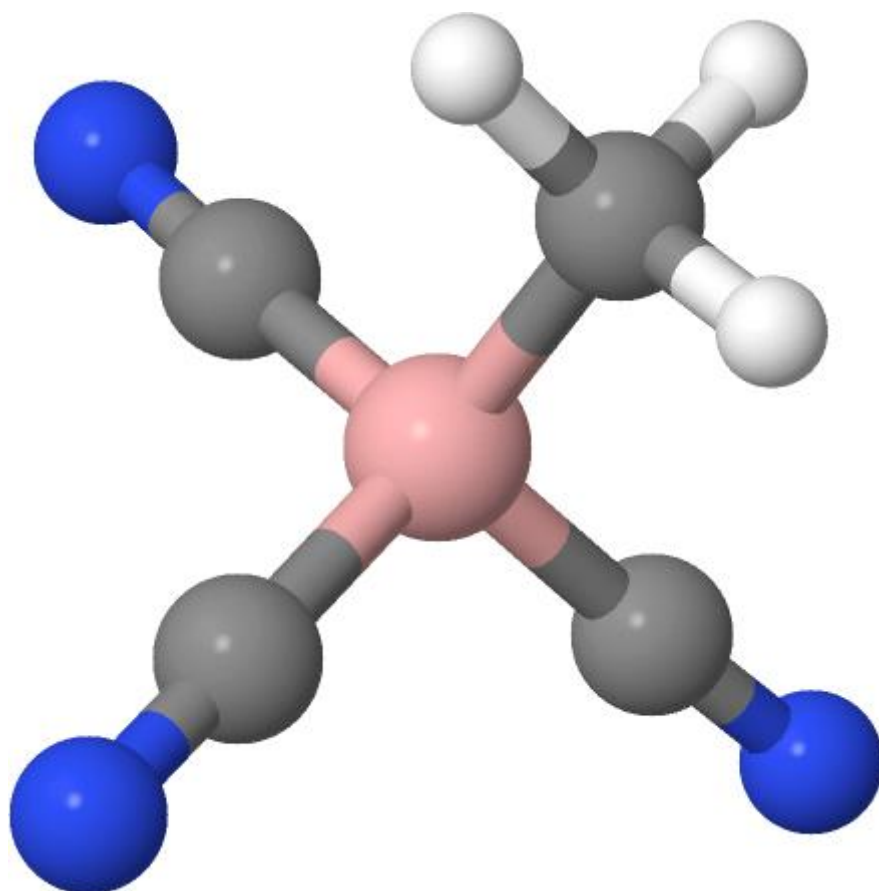
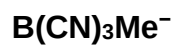
Number of MOs= 112, Electrons= 54.00, Symmetry: c1

\$coord

-0.24294114124192	1.86027510009992	4.16632914355490	b
-1.15844570661439	2.96743598804156	1.46317184476495	c
-1.79932072655482	3.74657564753118	-0.51358183383258	n
1.23546406747207	4.07817831628208	5.67099025803778	c
-2.72160330267651	1.08203515437000	5.78574630008382	c
2.33451692053944	5.66637715854274	6.76437766463917	n
-4.50444906495978	0.48668480635006	6.96564502477508	n
1.35710901246706	-0.26294533577158	3.81727164779866	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		104.75	2.01685	YES	YES
8	a		104.83	2.01190	YES	YES
9	a		132.00	10.56956	YES	YES
10	a		205.90	6.25381	YES	YES
11	a		208.57	6.15124	YES	YES
12	a		322.98	0.00010	YES	YES
13	a		448.04	0.05259	YES	YES
14	a		448.24	0.05943	YES	YES
15	a		467.27	4.35866	YES	YES
16	a		498.63	2.75992	YES	YES
17	a		498.88	2.69022	YES	YES
18	a		585.71	0.32995	YES	YES
19	a		913.85	132.25789	YES	YES
20	a		915.20	131.91244	YES	YES
21	a		1037.11	180.06662	YES	YES
22	a		2236.75	0.04148	YES	YES
23	a		2237.23	0.02363	YES	YES
24	a		2238.27	0.76887	YES	YES



Total energy = -343.1848002522 H = -9338.5388736 eV

HOMO-LUMO Separation

HOMO: 27. 27 a -0.11261695 H = -3.06446 eV

LUMO: 28. 28 a +0.12378190 H = +3.36828 eV

Gap : +0.23639886 H = +6.43274 eV

Number of MOs= 118, Electrons= 54.00, Symmetry: c1

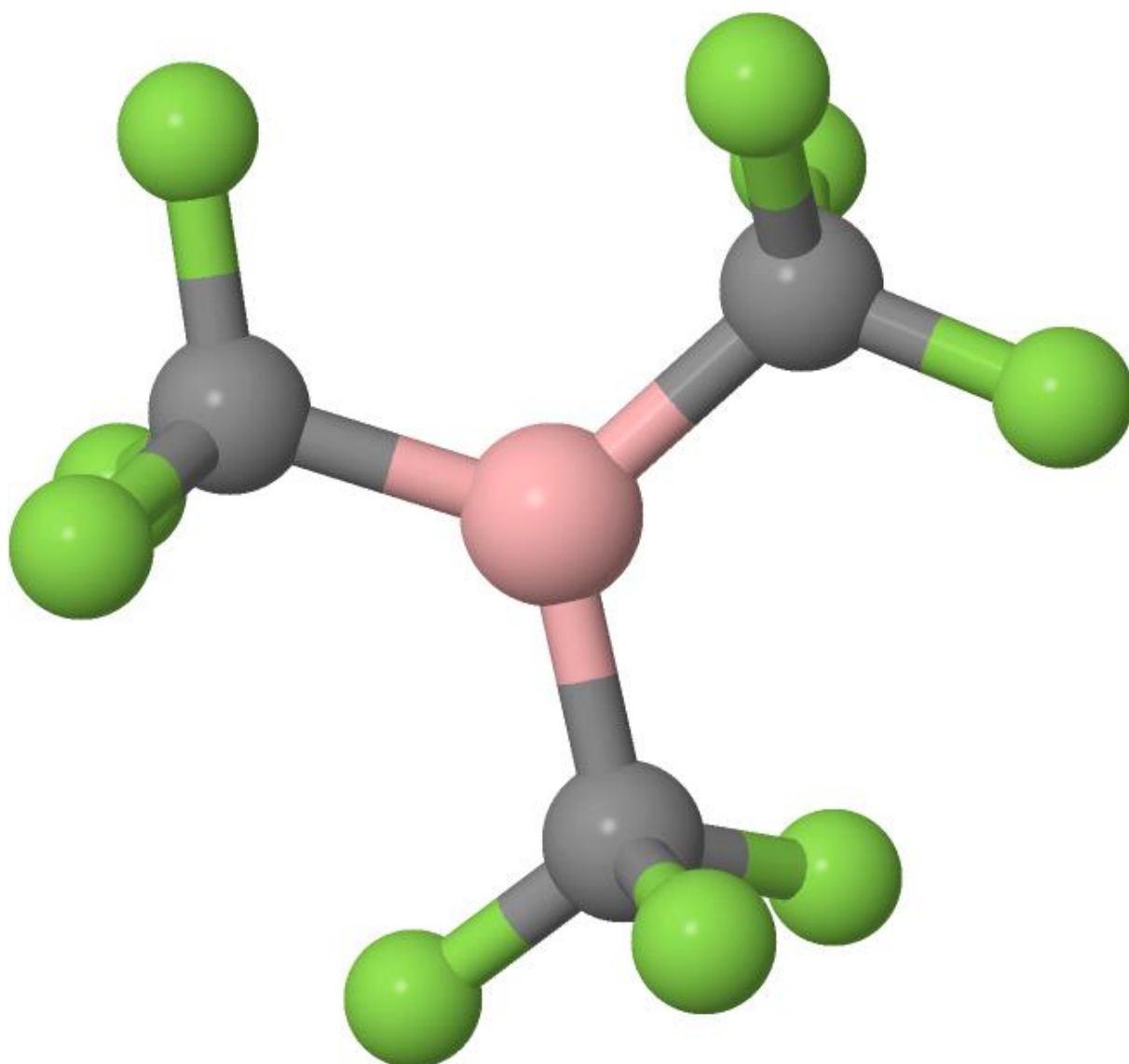
\$coord
-0.48044684994088 2.02824416043541 4.16820367439251 b

-1.40408866210606	3.14551040848302	1.49683228201120	c
-2.03092193668419	3.88910413435262	-0.50024327413270	n
1.14220319641620	4.14378382705132	5.62743729192530	c
-2.91494898242892	1.31313835288045	5.84119233551962	c
2.40102309275267	5.62927876793992	6.69657346469290	n
-4.66373286276902	0.69939912483208	7.06548827926875	n
1.26809186289826	-0.51513202966976	3.70222640896764	c
2.96381351991947	-0.05960416279663	2.54114714246843	h
0.17529090959986	-2.00614385054410	2.69562239806184	h
1.93140238249803	-1.31975895357174	5.53083073858481	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	106.84	2.79714	YES	YES
8		a	107.35	2.78220	YES	YES
9		a	137.72	11.15930	YES	YES
10		a	185.70	0.96177	YES	YES
11		a	186.97	0.98541	YES	YES
12		a	217.24	0.00127	YES	YES
13		a	344.37	0.00003	YES	YES
14		a	430.13	2.17649	YES	YES
15		a	430.39	2.14723	YES	YES
16		a	472.16	1.80215	YES	YES
17		a	508.00	0.73250	YES	YES
18		a	508.04	0.75826	YES	YES
19		a	557.00	0.01698	YES	YES
20		a	772.12	1.47503	YES	YES
21		a	773.83	1.51379	YES	YES
22		a	935.43	23.91269	YES	YES
23		a	1002.30	68.40278	YES	YES
24		a	1002.51	68.18185	YES	YES
25		a	1259.04	4.16204	YES	YES
26		a	1417.56	0.49405	YES	YES
27		a	1418.00	0.52476	YES	YES
28		a	2226.87	7.95407	YES	YES
29		a	2227.17	7.97449	YES	YES
30		a	2229.68	4.02297	YES	YES
31		a	2922.77	37.06420	YES	YES
32		a	3009.38	35.74329	YES	YES
33		a	3009.87	35.69289	YES	YES

B(CF₃)₃



Total energy = -1037.0098590190 H = -28218.4900777 eV

HOMO-LUMO Separation

HOMO: 52. 52 a -0.33036239 H = -8.98962 eV

LUMO: 53. 53 a -0.17530649 H = -4.77034 eV

Gap : +0.15505590 H = +4.21929 eV

Number of MOs= 182, Electrons= 104.00, Symmetry: c1

B(CF₃)₃Cl⁻

\$coord

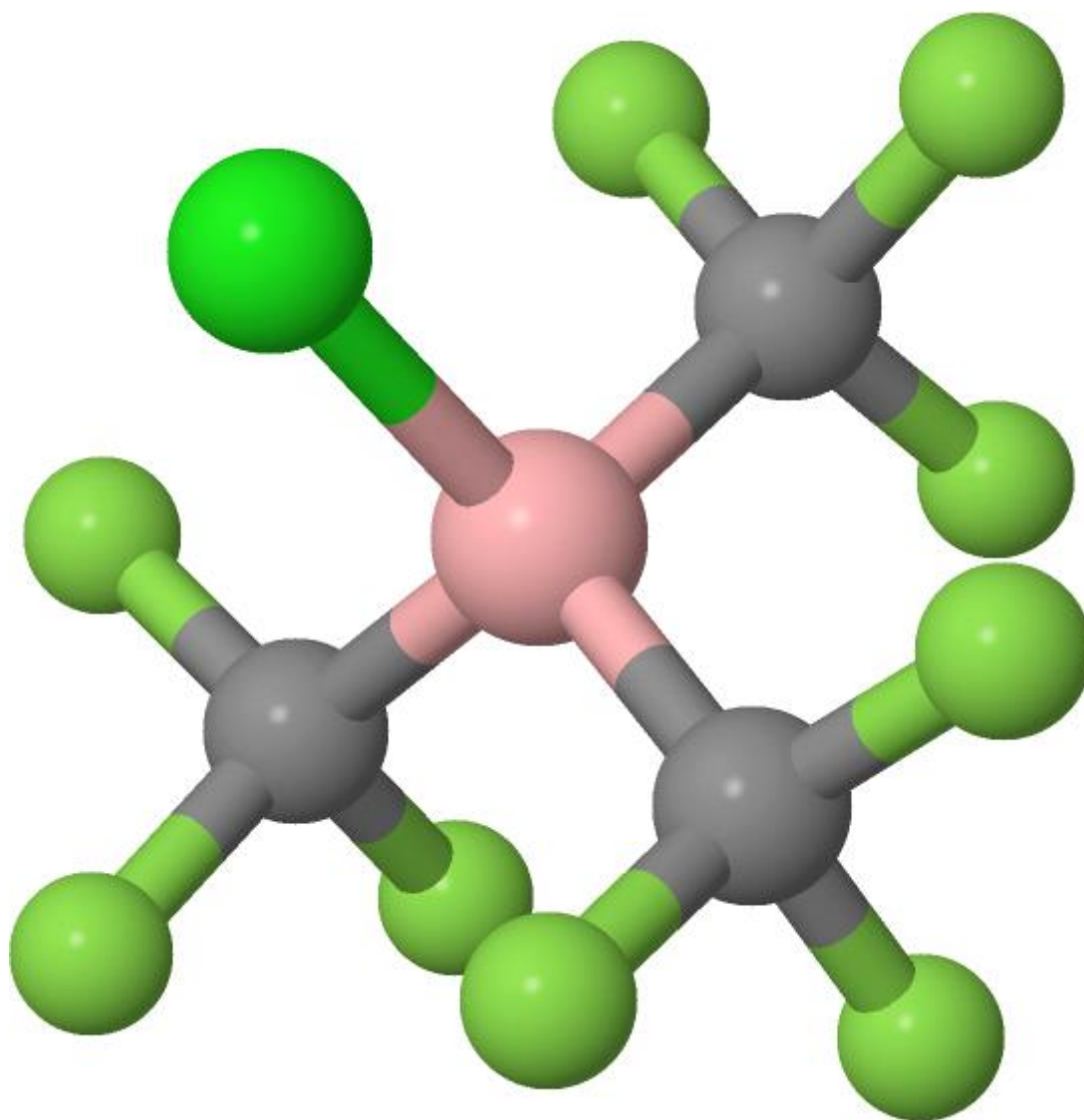
0.01035172514612	-0.00466066904979	-0.01616242011326	b
1.80406857659045	-2.44810996524684	0.02054651213016	c
1.20982984437085	2.78573408254051	-0.00960717657795	c
-3.00293957623767	-0.34802322409244	-0.02923040365239	c
-3.60074288090106	-1.03068760525411	2.39661398871021	f
-4.34656662440706	1.73677158686297	-0.59874743951709	f
-3.76858487185460	-2.21315481735277	-1.60160392399861	f
3.71226718103918	-2.23691457842259	1.70660092575837	f
2.81973960165037	-2.54845224203203	-2.36222069021563	f
0.63797061171703	-4.66723232449666	0.45937136771453	f
3.75455603112955	2.88052709670273	0.04613258529869	f
0.33870267167102	4.02477465185809	2.07431646823429	f
0.43983926212476	4.06359488936463	-2.09970212912684	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	19.11	0.22159	YES	YES
8		a	29.49	0.09821	YES	YES
9		a	44.49	0.75444	YES	YES
10		a	88.16	2.91301	YES	YES
11		a	109.50	1.01323	YES	YES
12		a	116.83	1.00452	YES	YES
13		a	163.07	0.60643	YES	YES
14		a	169.85	1.01012	YES	YES
15		a	232.44	0.02833	YES	YES
16		a	271.61	0.08525	YES	YES
17		a	281.28	1.45095	YES	YES
18		a	283.67	1.52289	YES	YES
19		a	476.37	3.84676	YES	YES
20		a	497.33	0.15361	YES	YES
21		a	502.30	8.59822	YES	YES
22		a	503.11	8.17627	YES	YES
23		a	509.57	0.00839	YES	YES
24		a	510.98	0.00685	YES	YES
25		a	657.05	40.46349	YES	YES
26		a	661.54	45.50438	YES	YES
27		a	672.97	10.82342	YES	YES
28		a	722.18	0.00531	YES	YES
29		a	930.99	148.22755	YES	YES
30		a	932.18	150.08760	YES	YES

31	a	1044.78	7.09667	YES	YES
32	a	1052.13	27.68662	YES	YES
33	a	1089.89	581.25563	YES	YES
34	a	1097.07	28.97892	YES	YES
35	a	1164.39	257.01262	YES	YES
36	a	1174.02	264.16062	YES	YES
37	a	1263.52	0.75142	YES	YES
38	a	1333.10	136.24269	YES	YES
39	a	1338.41	139.84942	YES	YES

B(CF₃)₃Cl⁻



Total energy = -1497.3058209050 H = -40743.7876150 eV

HOMO-LUMO Separation

HOMO: 61. 38 e -0.09029681 H = -2.45710 eV

LUMO: 62. 24 a +0.17035434 H = +4.63558 eV

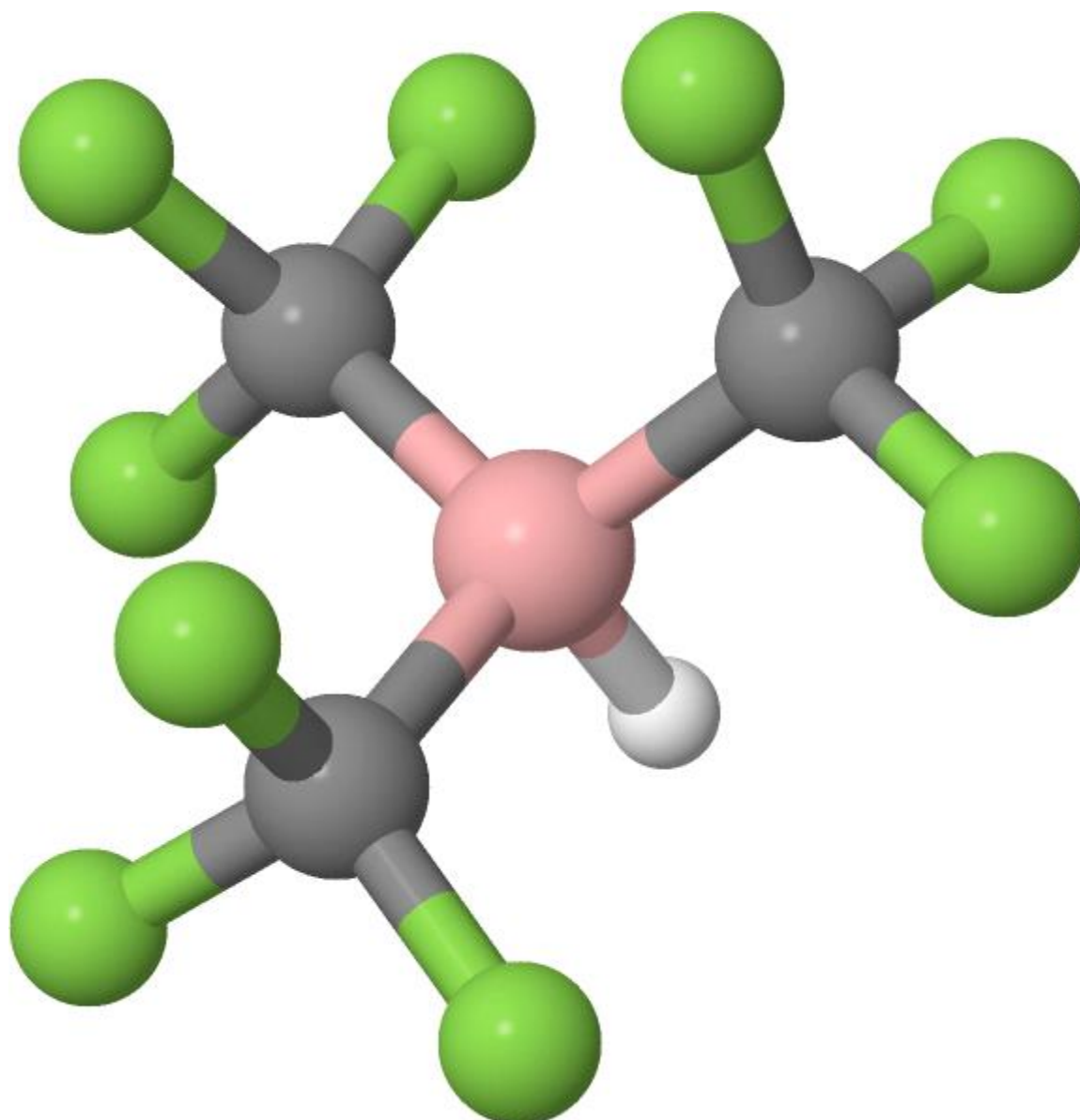
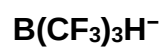
Gap : +0.26065115 H = +7.09268 eV

Number of MOs= 200, Electrons= 122.00, Symmetry: c3

```
$coord
  0.000000000000000  0.000000000000000  0.50923569490786  b
  0.000000000000000  0.000000000000000  4.08425566973058  c1
-2.39962428210978   -1.71718752374225   -0.45632200479821  c
-4.67328827944941   -0.99556456555209    0.55214297133339  f
-2.15996396837170   -4.23215889560168    0.13216136639977  f
-2.74833901040440   -1.64986839919581   -3.03295136788326  f
  2.68694015967737   -1.21954182597394   -0.45632200479821  c
-0.28731587756759    2.93672934971619   -0.45632200479821  c
  3.19882834460044   -3.54940408643521    0.55214297133339  f
  1.47445993484898    4.54496865198731    0.55214297133339  f
  4.74513910062920    0.24549577993190    0.13216136639977  f
-2.58517513225750    3.98666311566978    0.13216136639977  f
-0.05465844140253    3.20506560081990   -3.03295136788326  f
  2.80299745180694   -1.55519720162409   -3.03295136788326  f
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#          #          cm** (-1)      km/mol          IR          RAMAN
  1          0.00      0.00000      -          -
  2          0.00      0.00000      -          -
  3          0.00      0.00000      -          -
  4          0.00      0.00000      -          -
  5          0.00      0.00000      -          -
  6          0.00      0.00000      -          -
  7          a      12.62      0.00129      YES      YES
  8          e      54.10      0.00880      YES      YES
  9          e      54.10      0.00880      YES      YES
 10          e     107.64      0.00946      YES      YES
 11          e     107.64      0.00946      YES      YES
 12          a     144.66      0.02095      YES      YES
 13          e     167.94      0.25650      YES      YES
 14          e     167.94      0.25650      YES      YES
 15          a     246.55      0.01083      YES      YES
 16          e     265.72      0.22947      YES      YES
 17          e     265.72      0.22948      YES      YES
 18          a     274.22      0.07913      YES      YES
 19          e     298.83      0.08688      YES      YES
 20          e     298.83      0.08688      YES      YES
 21          a     344.07      0.27739      YES      YES
 22          e     504.39      2.61542      YES      YES
 23          e     504.39      2.61542      YES      YES
 24          a     505.00      0.08852      YES      YES
 25          a     513.22      3.21951      YES      YES
 26          e     522.43      0.30864      YES      YES
 27          e     522.43      0.30864      YES      YES
```

28	e	669.09	35.06491	YES	YES
29	e	669.09	35.06491	YES	YES
30	a	699.62	9.64075	YES	YES
31	a	846.66	158.59272	YES	YES
32	e	879.54	136.47689	YES	YES
33	e	879.54	136.47690	YES	YES
34	a	1017.73	0.75687	YES	YES
35	e	1035.50	37.55130	YES	YES
36	e	1035.50	37.55130	YES	YES
37	e	1104.10	193.64647	YES	YES
38	e	1104.10	193.64647	YES	YES
39	a	1104.65	523.92105	YES	YES
40	a	1251.60	30.24848	YES	YES
41	e	1252.86	237.20639	YES	YES
42	e	1252.86	237.20639	YES	YES



Total energy = -1037.7476066990 H = -28238.5652249 eV

HOMO-LUMO Separation

HOMO: 53. 19 a -0.10944840 H = -2.97824 eV

LUMO: 54. 20 a +0.22208431 H = +6.04322 eV

Gap : +0.33153271 H = +9.02147 eV

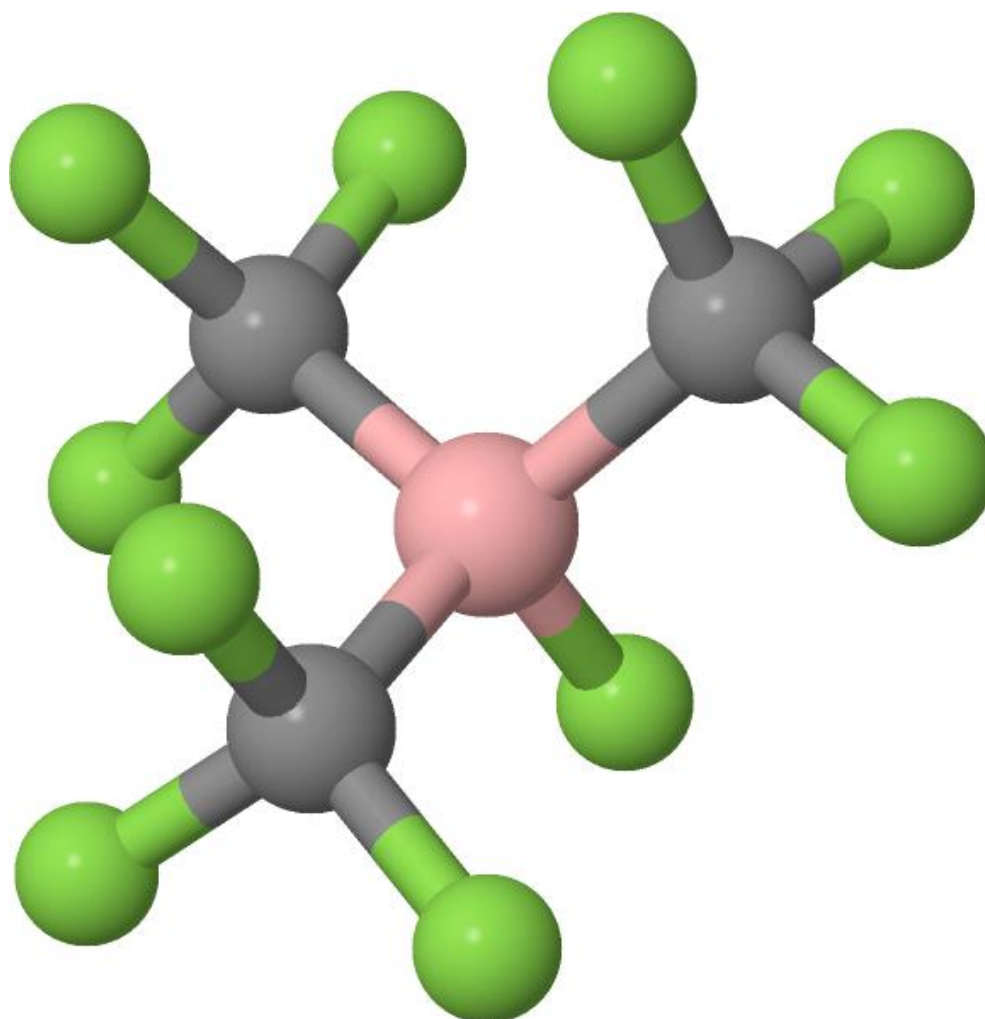
Number of MOs= 184, Electrons= 106.00, Symmetry: c3

```
$coord
  0.000000000000000  0.000000000000000  1.06282336402972  b
  0.000000000000000  0.000000000000000  3.40069114133002  h
 -2.84611579642362   0.75530729833883   0.16116600638524  c
 -3.77296922287898   2.87251050092773   1.36076977614040  f
 -4.60392052930796  -1.10318382676811   0.65505343161795  f
 -3.11756789145911   1.26703090442095  -2.37945637811365  f
  0.76894259018659  -2.84246223098445   0.16116600638524  c
  2.07717320623703   2.08715493264562   0.16116600638524  c
 -0.60118245500149  -4.70374244517389   1.36076977614040  f
  4.37415167788047   1.83123194424616   1.36076977614040  f
  3.25734548367929  -3.43552022200134   0.65505343161795  f
  1.34657504562867   4.53870404876945   0.65505343161795  f
  2.65606489633807   2.06637753981581  -2.37945637811365  f
  0.46150299512105  -3.33340844423675  -2.37945637811365  f
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#          #          cm** (-1)      km/mol          IR          RAMAN
  1          0.00          0.00000          -          -
  2          0.00          0.00000          -          -
  3          0.00          0.00000          -          -
  4          0.00          0.00000          -          -
  5          0.00          0.00000          -          -
  6          0.00          0.00000          -          -
  7          a          47.01          0.00027          YES          YES
  8          e          57.60          0.01828          YES          YES
  9          e          57.60          0.01828          YES          YES
 10          e          117.48          0.00248          YES          YES
 11          e          117.48          0.00248          YES          YES
 12          a          139.45          0.00217          YES          YES
 13          a          247.74          0.01677          YES          YES
 14          e          258.75          0.53268          YES          YES
 15          e          258.75          0.53268          YES          YES
 16          a          276.50          0.00230          YES          YES
 17          e          298.34          0.01967          YES          YES
 18          e          298.34          0.01967          YES          YES
```

19	a	483.06	1.00714	YES	YES
20	e	504.09	1.41300	YES	YES
21	e	504.09	1.41300	YES	YES
22	a	506.28	0.07485	YES	YES
23	e	514.07	0.06478	YES	YES
24	e	514.07	0.06478	YES	YES
25	e	650.61	26.99839	YES	YES
26	e	650.61	26.99839	YES	YES
27	a	685.78	8.86934	YES	YES
28	a	755.55	19.37651	YES	YES
29	e	797.23	10.71167	YES	YES
30	e	797.23	10.71169	YES	YES
31	e	971.95	224.92416	YES	YES
32	e	971.95	224.92413	YES	YES
33	a	996.52	0.05925	YES	YES
34	e	1070.56	0.42525	YES	YES
35	e	1070.56	0.42525	YES	YES
36	e	1084.95	206.90941	YES	YES
37	e	1084.95	206.90943	YES	YES
38	a	1095.52	602.48519	YES	YES
39	a	1238.98	63.04558	YES	YES
40	e	1263.49	232.16498	YES	YES
41	e	1263.49	232.16497	YES	YES
42	a	2417.35	144.00027	YES	YES

B(CF₃)₃F⁻



Total energy = -1136.9751643400 H = -30938.6859869 eV

HOMO-LUMO Separation

HOMO: 57. 36 e -0.09785882 H = -2.66288 eV

LUMO: 58. 22 a +0.18997395 H = +5.16946 eV

Gap : +0.28783277 H = +7.83233 eV

Number of MOs= 196, Electrons= 114.00, Symmetry: c3

\$coord

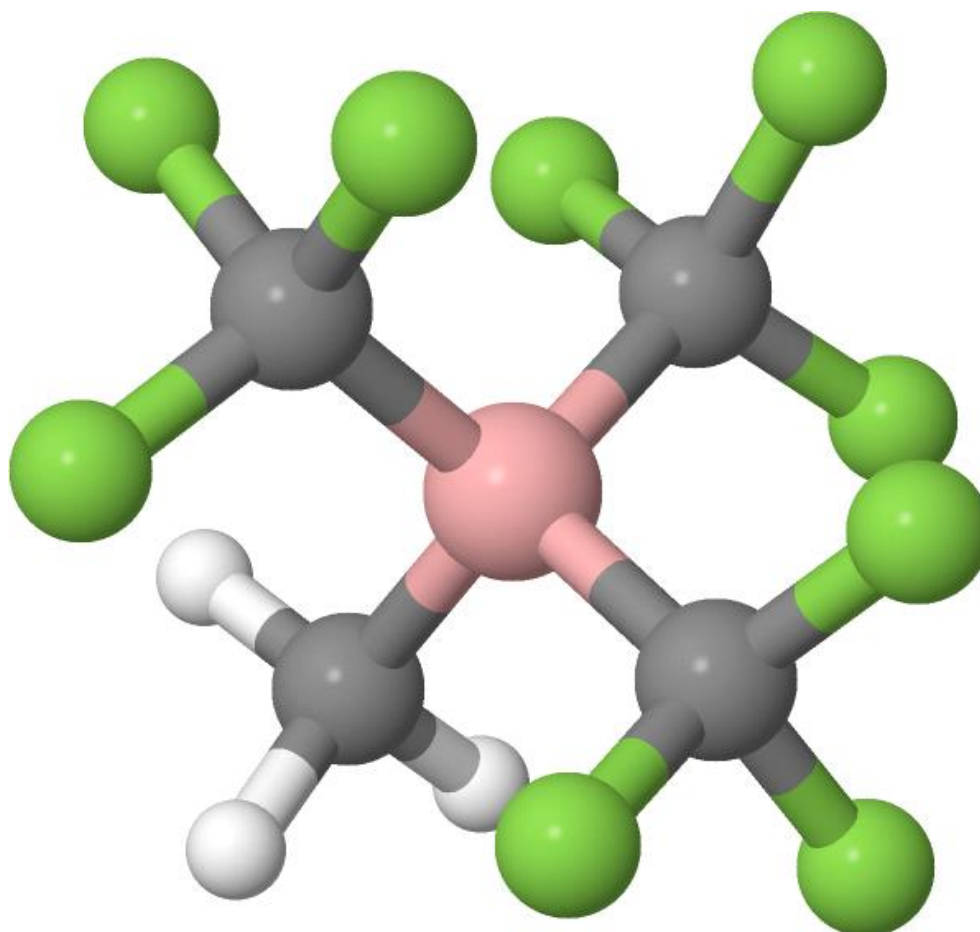
0.0000000000000000	0.0000000000000000	0.83437643333837	b
0.0000000000000000	0.0000000000000000	3.53264796575043	f
-2.41232998995185	-1.71545495827051	-0.14083916097205	c
-4.64194679123284	-1.05120715207663	1.00759935405342	f
-2.12940736284105	-4.24941642100460	0.36918895870015	f
-2.88765399861721	-1.58079534210457	-2.69162395147779	f
2.69179256788619	-1.23141157447412	-0.14083916097205	c
-0.27946257793431	2.94686653274466	-0.14083916097205	c
3.23134549395468	-3.49444026818499	1.00759935405342	f
1.41060129727818	4.54564742026162	1.00759935405342	f
4.74480625326927	0.28058733927632	0.36918895870015	f
-2.61539889042822	3.96882908172829	0.36918895870015	f
0.07481807486194	3.29117939119454	-2.69162395147779	f
2.81283592375530	-1.71038404908996	-2.69162395147779	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	34.55	0.01250	YES	YES
8		e	53.88	0.03410	YES	YES
9		e	53.88	0.03410	YES	YES
10		e	112.06	0.00407	YES	YES
11		e	112.06	0.00407	YES	YES
12		a	137.47	0.03831	YES	YES
13		e	205.94	1.09095	YES	YES
14		e	205.94	1.09095	YES	YES
15		a	236.39	0.00576	YES	YES
16		a	266.61	0.38812	YES	YES
17		e	279.99	0.17254	YES	YES
18		e	279.99	0.17254	YES	YES

19	e	304.37	0.20175	YES	YES
20	e	304.37	0.20175	YES	YES
21	a	439.51	1.31224	YES	YES
22	e	502.66	2.65051	YES	YES
23	e	502.66	2.65051	YES	YES
24	a	502.74	0.00950	YES	YES
25	e	522.18	0.08997	YES	YES
26	e	522.18	0.08997	YES	YES
27	a	559.91	0.23256	YES	YES
28	e	672.85	35.69802	YES	YES
29	e	672.85	35.69802	YES	YES
30	a	703.98	0.50289	YES	YES
31	e	890.19	202.57805	YES	YES
32	e	890.19	202.57805	YES	YES
33	a	1007.05	0.02275	YES	YES
34	e	1046.98	34.99177	YES	YES
35	e	1046.98	34.99177	YES	YES
36	a	1058.42	230.99852	YES	YES
37	e	1093.09	211.53029	YES	YES
38	e	1093.09	211.53029	YES	YES
39	a	1111.09	540.41812	YES	YES
40	e	1262.94	169.20820	YES	YES
41	e	1262.94	169.20820	YES	YES
42	a	1269.82	3.65696	YES	YES

B(CF₃)₃Me⁻



Total energy = -1077.0353608100 H = -29307.6400171 eV

HOMO-LUMO Separation

HOMO: 57. 36 e -0.10634758 H = -2.89387 eV

LUMO: 58. 22 a +0.20470965 H = +5.57044 eV

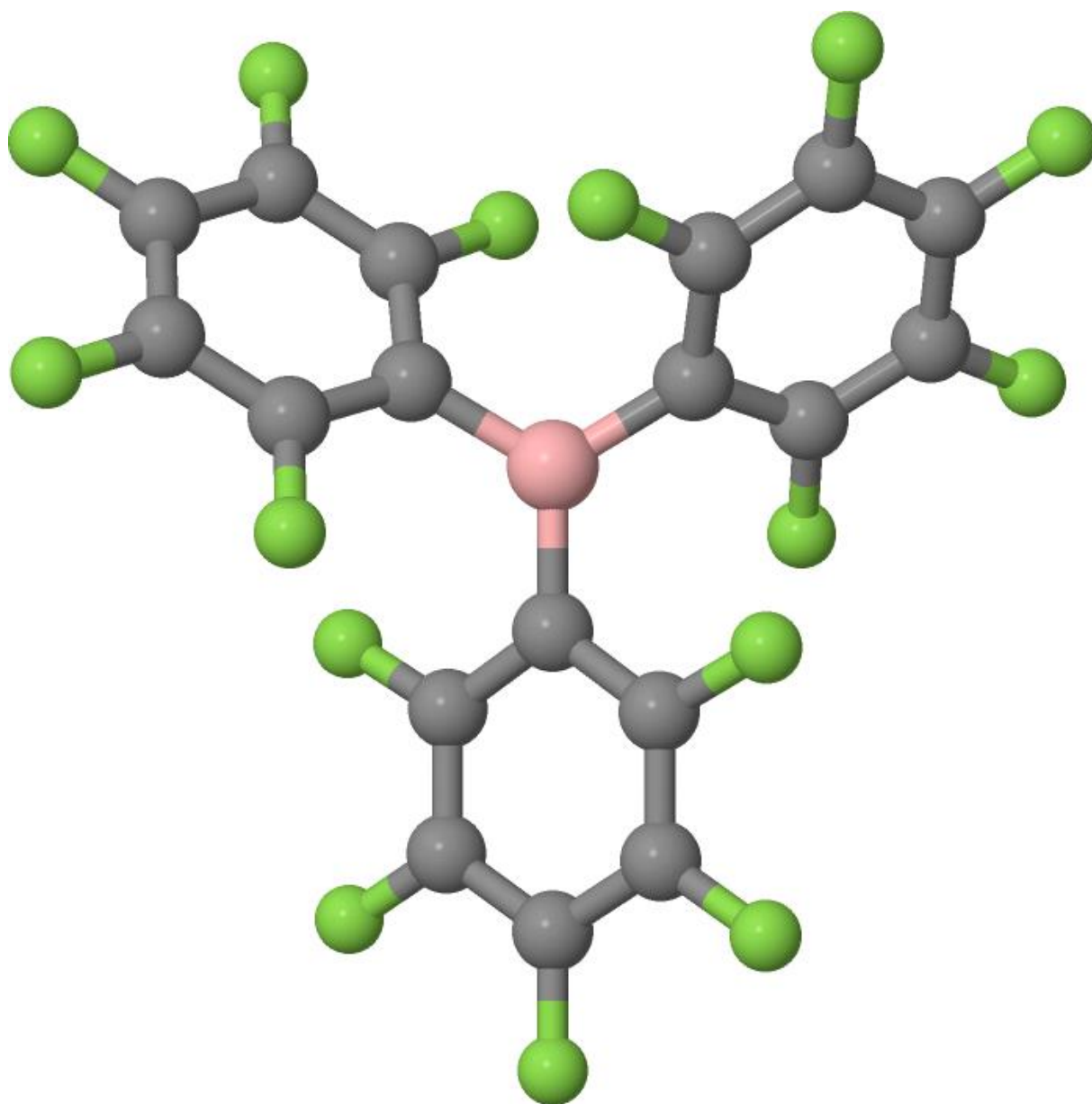
Gap : +0.31105723 H = +8.46430 eV

Number of MOs= 202, Electrons= 114.00, Symmetry: c3

```
$coord
0.000000000000000 0.000000000000000 0.93127368104726 b
2.45315675019152 1.60313287600232 -0.09292534701672 c
4.69146684053036 0.89174615151646 1.04100106198752 f
2.26929409746817 4.16201387722398 0.38071218744268 f
2.92787583293090 1.43560879199979 -2.64462198364106 f
-2.61493217135577 1.32292962712997 -0.09292534701672 c
0.16177542116426 -2.92606250313229 -0.09292534701672 c
-3.11800824120544 3.61705638915338 1.04100106198752 f
-1.57345859932492 -4.50880254066984 1.04100106198752 f
-4.73905679731342 -0.11574060154648 0.38071218744268 f
2.46976269984525 -4.04627327567751 0.38071218744268 f
-0.22066423269734 -3.25341924644458 -2.64462198364106 f
-2.70721160023356 1.81781045444478 -2.64462198364106 f
0.000000000000000 0.000000000000000 4.03432704566333 c
-1.75952699624664 -0.86365244973452 4.80286836355370 h
0.13181853661256 1.95562130226138 4.80286836355370 h
1.62770845963408 -1.09196885252685 4.80286836355370 h
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# # cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 a 38.59 0.00005 YES YES
8 e 57.00 0.00456 YES YES
9 e 57.00 0.00456 YES YES
10 e 115.32 0.00653 YES YES
11 e 115.32 0.00653 YES YES
12 a 143.60 0.04393 YES YES
13 a 185.16 0.01173 YES YES
14 e 209.23 0.00428 YES YES
15 e 209.23 0.00428 YES YES
```

16	a	248.51	0.03503	YES	YES
17	a	276.45	0.11473	YES	YES
18	e	277.78	0.56481	YES	YES
19	e	277.78	0.56481	YES	YES
20	e	302.59	0.01237	YES	YES
21	e	302.59	0.01237	YES	YES
22	a	440.99	4.64706	YES	YES
23	e	501.79	1.56229	YES	YES
24	e	501.79	1.56229	YES	YES
25	a	504.70	0.08752	YES	YES
26	e	520.98	0.00312	YES	YES
27	e	520.98	0.00312	YES	YES
28	a	549.12	2.33175	YES	YES
29	e	651.82	26.97244	YES	YES
30	e	651.82	26.97244	YES	YES
31	a	697.50	2.23139	YES	YES
32	e	760.82	3.29461	YES	YES
33	e	760.82	3.29461	YES	YES
34	e	957.28	226.00702	YES	YES
35	e	957.28	226.00702	YES	YES
36	a	981.36	75.36526	YES	YES
37	a	988.98	76.54476	YES	YES
38	e	1036.17	15.82072	YES	YES
39	e	1036.17	15.82072	YES	YES
40	e	1074.00	169.88390	YES	YES
41	e	1074.00	169.88390	YES	YES
42	a	1102.89	452.32496	YES	YES
43	a	1237.66	80.27651	YES	YES
44	e	1241.61	209.89522	YES	YES
45	e	1241.61	209.89523	YES	YES
46	a	1274.66	23.90912	YES	YES
47	e	1424.76	3.40755	YES	YES
48	e	1424.76	3.40755	YES	YES
49	a	2922.27	36.31021	YES	YES
50	e	3002.51	36.52452	YES	YES
51	e	3002.51	36.52452	YES	YES



Total energy = -2206.7527127110 H = -60048.8307667 eV

HOMO-LUMO Separation

HOMO: 124. 64 a -0.23771310 H = -6.46851 eV

LUMO: 125. 61 b -0.14460309 H = -3.93485 eV

Gap : +0.09311001 H = +2.53365 eV

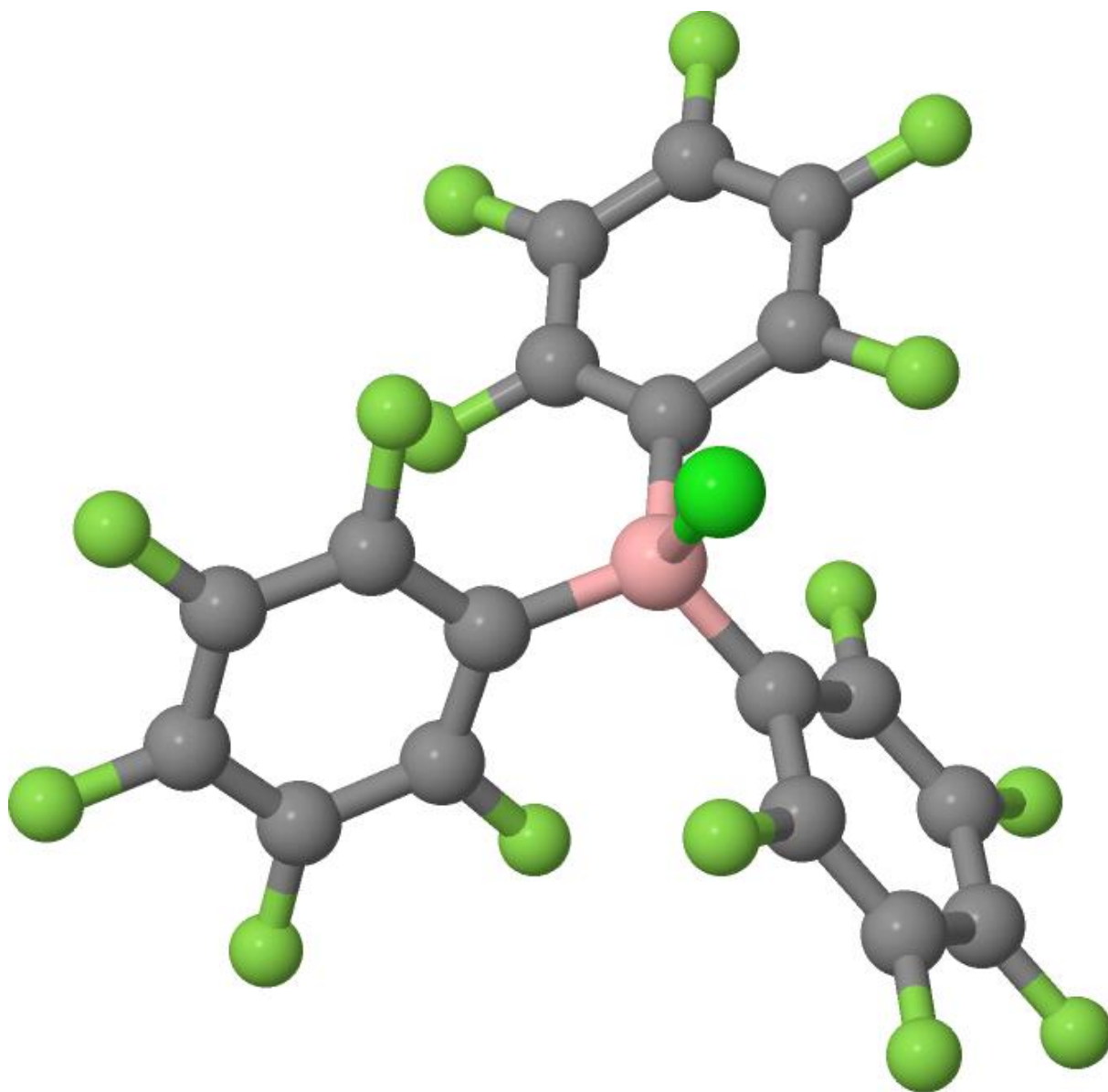
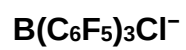
Number of MOs= 476, Electrons= 248.00, Symmetry: c2

```
$coord
0.0000000000000000 0.0000000000000000 -0.12238167035843 b
-0.06745327759709 -2.55175796948904 1.41179764389145 c
0.0000000000000000 0.0000000000000000 -3.08939276894972 c
0.06745327759709 2.55175796948904 1.41179764389145 c
1.38588277963181 -4.68358448091631 0.72854459413879 c
1.41870639080857 -6.91789682961215 2.15579872379210 c
-0.07858639915437 -7.07612478151046 4.34782645773904 c
-1.58714670364119 -5.01508316335341 5.08303225144601 c
-1.54088726380140 -2.80225632187844 3.62442325583791 c
-1.22329202922978 -1.90415525460493 -4.51750067650768 c
-1.25648927665460 -1.92921137708453 -7.16792219443953 c
0.0000000000000000 0.0000000000000000 -8.49678633229211 c
1.25648927665460 1.92921137708453 -7.16792219443953 c
1.22329202922978 1.90415525460493 -4.51750067650768 c
1.54088726380140 2.80225632187844 3.62442325583791 c
1.58714670364119 5.01508316335341 5.08303225144601 c
0.07858639915437 7.07612478151046 4.34782645773904 c
-1.41870639080857 6.91789682961215 2.15579872379210 c
-1.38588277963181 4.68358448091631 0.72854459413879 c
-0.07363453571465 -9.18302953732526 5.72302625097996 f
-3.02691884359086 -5.17708582291571 7.14988731377900 f
-3.02844272335426 -0.89294143245405 4.39237198964593 f
2.87094023658954 -4.60821371895568 -1.32850926332898 f
2.85241654302439 -8.87976892713136 1.47246849205302 f
2.48215903855411 3.77216450343252 -3.35575142456151 f
2.45921094173310 3.75137048691863 -8.43251133606173 f
0.0000000000000000 0.0000000000000000 -11.01162621617708 f
-2.45921094173310 -3.75137048691863 -8.43251133606173 f
-2.87094023658954 4.60821371895568 -1.32850926332898 f
3.02844272335426 0.89294143245405 4.39237198964593 f
3.02691884359086 5.17708582291571 7.14988731377900 f
0.07363453571465 9.18302953732526 5.72302625097996 f
-2.85241654302439 8.87976892713136 1.47246849205302 f
-2.48215903855411 -3.77216450343252 -3.35575142456151 f
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 a 19.70 0.43690 YES YES
8 b 23.31 0.49770 YES YES
9 a 32.98 0.00353 YES YES
10 b 34.58 0.01977 YES YES
11 b 36.98 0.00352 YES YES
12 a 38.83 0.00000 YES YES
```

13	b	100.04	0.14059	YES	YES
14	b	105.10	0.11058	YES	YES
15	a	107.98	0.03984	YES	YES
16	a	126.22	0.34894	YES	YES
17	b	126.96	0.45704	YES	YES
18	a	127.78	0.03517	YES	YES
19	a	138.93	0.02334	YES	YES
20	b	144.17	0.01695	YES	YES
21	b	148.34	0.03799	YES	YES
22	b	154.14	0.20651	YES	YES
23	a	154.85	0.00040	YES	YES
24	a	156.79	0.14630	YES	YES
25	b	221.32	3.47473	YES	YES
26	b	227.90	3.78120	YES	YES
27	a	232.11	3.69725	YES	YES
28	b	263.73	0.09730	YES	YES
29	a	264.02	0.15149	YES	YES
30	b	264.33	0.24992	YES	YES
31	b	269.57	0.12490	YES	YES
32	a	270.08	0.06561	YES	YES
33	a	273.18	0.12087	YES	YES
34	a	306.90	0.09328	YES	YES
35	b	307.29	1.06307	YES	YES
36	b	310.44	0.55913	YES	YES
37	b	339.90	2.65196	YES	YES
38	a	340.94	2.58436	YES	YES
39	b	347.08	0.10646	YES	YES
40	a	350.09	0.09702	YES	YES
41	b	377.00	6.25249	YES	YES
42	a	383.08	6.33828	YES	YES
43	a	391.62	1.20895	YES	YES
44	b	394.45	1.43983	YES	YES
45	a	394.72	0.24803	YES	YES
46	b	429.70	0.48050	YES	YES
47	a	430.79	0.23741	YES	YES
48	b	430.99	0.30773	YES	YES
49	a	458.60	5.15205	YES	YES
50	b	459.92	4.06223	YES	YES
51	a	484.82	0.00000	YES	YES
52	b	491.50	0.14940	YES	YES
53	b	509.56	0.01444	YES	YES
54	a	515.48	0.04014	YES	YES
55	b	536.36	1.99470	YES	YES
56	a	563.46	3.42701	YES	YES
57	b	563.82	2.67794	YES	YES
58	a	566.49	0.00297	YES	YES
59	b	617.93	27.73311	YES	YES
60	a	618.46	30.11916	YES	YES
61	a	633.84	1.96605	YES	YES
62	b	634.11	1.82692	YES	YES
63	a	636.26	0.00044	YES	YES
64	b	661.83	21.34984	YES	YES
65	a	668.43	24.27726	YES	YES
66	b	677.05	7.50509	YES	YES
67	a	768.81	23.23446	YES	YES
68	b	771.34	22.02897	YES	YES
69	b	774.15	3.87779	YES	YES
70	a	851.87	0.13594	YES	YES
71	b	984.04	130.42768	YES	YES
72	a	984.70	55.97345	YES	YES
73	b	985.18	109.92002	YES	YES
74	b	1021.28	128.56946	YES	YES

75	a	1022.67	100.06197	YES	YES
76	a	1117.56	0.69555	YES	YES
77	b	1154.56	7.20497	YES	YES
78	a	1156.45	19.62927	YES	YES
79	b	1159.04	24.90220	YES	YES
80	b	1175.37	193.78609	YES	YES
81	a	1184.46	234.61231	YES	YES
82	a	1305.29	0.00910	YES	YES
83	b	1316.56	148.99566	YES	YES
84	a	1319.95	198.64252	YES	YES
85	b	1345.79	0.10805	YES	YES
86	a	1349.11	9.17604	YES	YES
87	b	1349.96	6.43821	YES	YES
88	a	1377.78	322.14421	YES	YES
89	b	1380.75	240.52069	YES	YES
90	a	1397.07	1.90062	YES	YES
91	b	1471.58	459.26919	YES	YES
92	a	1480.70	530.61987	YES	YES
93	b	1482.66	683.00725	YES	YES
94	b	1521.21	232.80228	YES	YES
95	a	1521.64	293.99549	YES	YES
96	a	1523.88	3.16201	YES	YES
97	b	1609.11	21.26472	YES	YES
98	b	1611.45	11.31816	YES	YES
99	a	1611.71	5.65984	YES	YES
100	a	1630.89	204.26326	YES	YES
101	b	1631.75	177.13970	YES	YES
102	a	1633.16	18.56742	YES	YES



Total energy = -2667.0012065600 H = -72572.8366322 eV

HOMO-LUMO Separation

HOMO: 133. 133 a -0.10342383 H = -2.81431 eV

LUMO: 134. 134 a +0.04834064 H = +1.31542 eV

Gap : +0.15176447 H = +4.12972 eV

364

Number of MOs= 494, Electrons= 266.00, Symmetry: c1

\$coord

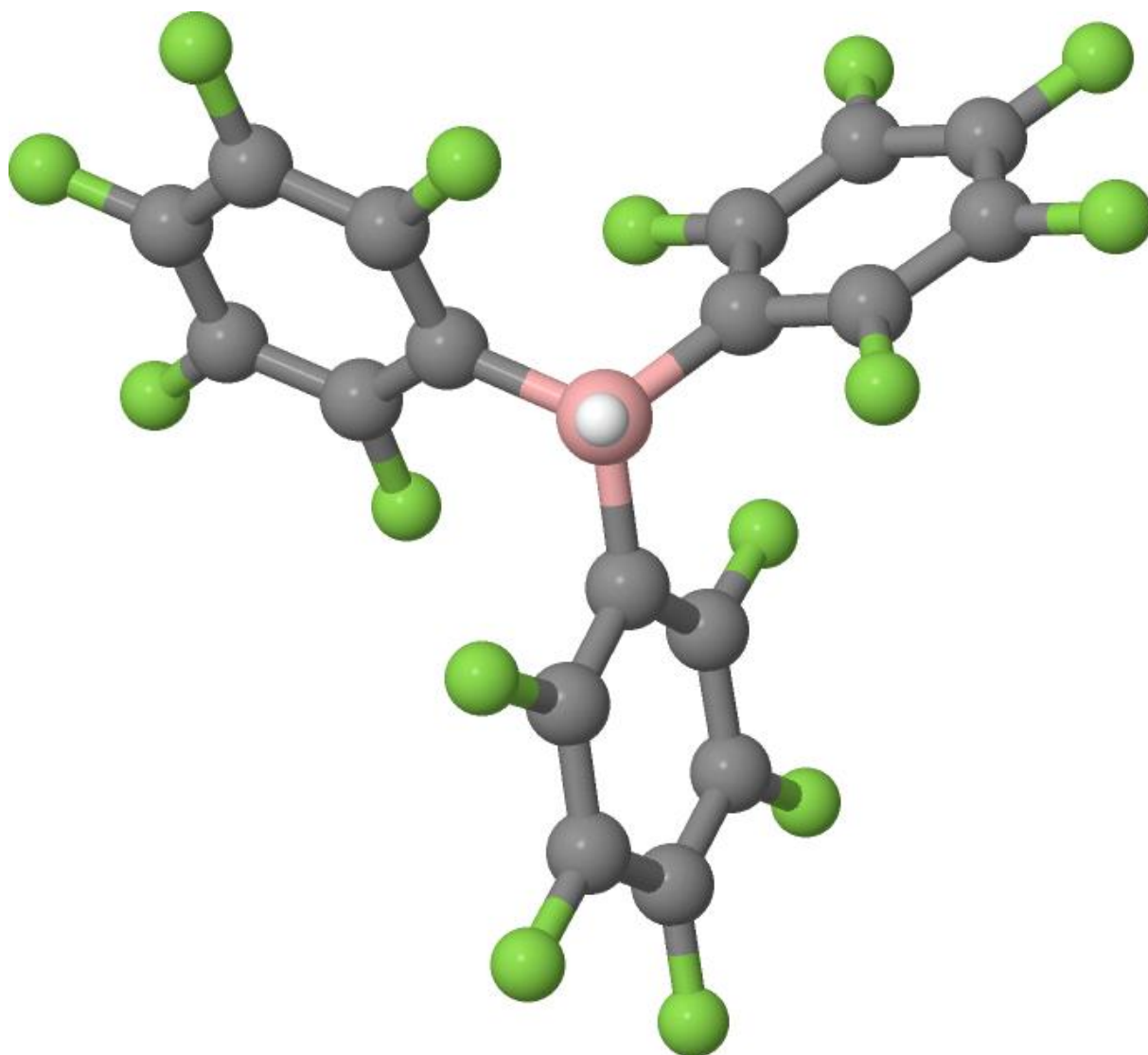
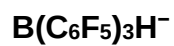
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-1.56480422798770	2.49942436330832	0.42348432399267	c
3.08291156233429	0.13119179380118	0.38993425442314	c
-1.34623240052495	-2.65621313473855	0.47940097872612	c
-1.19239621486138	4.88805114241329	1.54799652792893	c
-2.65066505099424	7.03303652460616	0.97384196151448	c
-4.55087257028953	6.86938545127839	-0.86753823490297	c
-4.95394749231919	4.55883360628313	-2.09217239180769	c
-3.44907579581625	2.46164103627153	-1.45186736538922	c
4.86611653952927	-1.61356178175611	1.33407612439484	c
7.46324017277047	-1.51137470149243	0.79900394651384	c
8.38926490555217	0.37676642289300	-0.81644814891637	c
6.69470410325560	2.12466205666429	-1.85126986608362	c
4.10504128882332	1.95327653465118	-1.25353735282522	c
-3.74164742079752	-3.23850440314101	1.49371958350090	c
-5.07080651619457	-5.47243344773235	0.96041883732580	c
-4.02852885726126	-7.23791492074832	-0.72075423434691	c
-1.67156319962545	-6.73434198316192	-1.81437550418392	c
-0.40785999122531	-4.46899525310876	-1.22037224321902	c
-5.95341360398080	8.90669133741668	-1.45860572302994	f
-6.74693949539634	4.37016555215133	-3.89052087397041	f
-3.92715213694408	0.35324555510325	-2.81813918747043	f
0.67684874775403	5.25902786377865	3.23037911709471	f
-2.21058640813612	9.26009973730880	2.12748263963306	f
2.62633981442850	3.68759546727901	-2.41194813667967	f
7.55065329549738	3.92917665435074	-3.43150760030677	f
10.86914098362738	0.49471104190445	-1.36924618109774	f
9.07119438605786	-3.23113000570045	1.76761234419871	f
1.80149425460878	-4.11406655084858	-2.45634782910074	f
-4.94090151546318	-1.58708980527578	3.01492215514787	f
-7.35885852940195	-5.90805591451349	1.98861648313407	f
-5.28228403387026	-9.37932179381483	-1.28164566947776	f
-0.66396372834510	-8.39749604036408	-3.45862230012738	f
4.12400537862672	-3.55543893803254	2.79968510160465	f
0.17566842318274	-0.03255779175665	4.95409029857671	c1

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	15.43	0.01321	YES	YES
8		a	20.81	0.01323	YES	YES
9		a	31.04	0.03485	YES	YES
10		a	33.02	0.06047	YES	YES
11		a	34.20	0.05327	YES	YES
12		a	47.49	0.03916	YES	YES
13		a	98.46	0.52706	YES	YES

14	a	102.70	0.38818	YES	YES
15	a	107.15	0.03207	YES	YES
16	a	123.71	0.01433	YES	YES
17	a	124.43	0.00709	YES	YES
18	a	134.30	0.01904	YES	YES
19	a	141.57	0.02771	YES	YES
20	a	147.90	0.35490	YES	YES
21	a	151.48	0.16284	YES	YES
22	a	155.84	0.87379	YES	YES
23	a	156.51	0.53222	YES	YES
24	a	159.40	0.09881	YES	YES
25	a	173.58	0.62791	YES	YES
26	a	175.23	0.50383	YES	YES
27	a	219.85	0.30976	YES	YES
28	a	231.78	1.32100	YES	YES
29	a	234.52	1.42026	YES	YES
30	a	258.05	2.92409	YES	YES
31	a	262.37	0.14513	YES	YES
32	a	263.32	0.60573	YES	YES
33	a	264.98	0.93100	YES	YES
34	a	274.14	0.05132	YES	YES
35	a	274.33	0.06684	YES	YES
36	a	274.90	0.01819	YES	YES
37	a	309.21	0.46851	YES	YES
38	a	309.87	0.54962	YES	YES
39	a	311.26	0.61615	YES	YES
40	a	342.43	3.48338	YES	YES
41	a	343.95	3.07427	YES	YES
42	a	346.53	0.05782	YES	YES
43	a	383.14	0.47417	YES	YES
44	a	383.75	0.08445	YES	YES
45	a	385.43	1.10157	YES	YES
46	a	385.56	0.34039	YES	YES
47	a	389.11	2.01189	YES	YES
48	a	391.63	3.62515	YES	YES
49	a	434.67	0.06313	YES	YES
50	a	434.72	0.21998	YES	YES
51	a	435.23	0.11593	YES	YES
52	a	460.33	2.50192	YES	YES
53	a	460.72	2.22706	YES	YES
54	a	477.04	0.16818	YES	YES
55	a	505.14	0.01518	YES	YES
56	a	508.31	0.02207	YES	YES
57	a	518.31	0.03994	YES	YES
58	a	561.22	4.13957	YES	YES
59	a	562.10	3.75022	YES	YES
60	a	563.56	1.74580	YES	YES
61	a	588.11	22.79737	YES	YES
62	a	606.20	34.06453	YES	YES
63	a	609.09	38.77205	YES	YES
64	a	629.24	0.83289	YES	YES
65	a	630.89	0.87222	YES	YES
66	a	633.38	0.61327	YES	YES
67	a	679.89	44.15659	YES	YES
68	a	685.98	49.76482	YES	YES
69	a	689.65	36.14028	YES	YES
70	a	757.68	23.81108	YES	YES
71	a	758.71	23.09797	YES	YES
72	a	771.78	23.60350	YES	YES
73	a	825.04	3.44907	YES	YES
74	a	926.11	0.28287	YES	YES
75	a	932.85	0.64312	YES	YES

76	a	973.02	175.99168	YES	YES
77	a	981.99	162.02930	YES	YES
78	a	983.31	188.23689	YES	YES
79	a	1086.04	22.35858	YES	YES
80	a	1097.85	251.57711	YES	YES
81	a	1098.94	287.24586	YES	YES
82	a	1129.17	2.95671	YES	YES
83	a	1131.58	2.30852	YES	YES
84	a	1132.23	0.81785	YES	YES
85	a	1265.75	35.24040	YES	YES
86	a	1267.68	40.47984	YES	YES
87	a	1268.46	30.36978	YES	YES
88	a	1342.82	6.98698	YES	YES
89	a	1344.83	7.88267	YES	YES
90	a	1345.88	8.55594	YES	YES
91	a	1374.93	14.74770	YES	YES
92	a	1375.69	15.23039	YES	YES
93	a	1379.90	8.56586	YES	YES
94	a	1457.20	415.00800	YES	YES
95	a	1462.51	420.28931	YES	YES
96	a	1464.43	454.33570	YES	YES
97	a	1509.88	238.39590	YES	YES
98	a	1510.20	218.58641	YES	YES
99	a	1513.36	15.42497	YES	YES
100	a	1615.68	7.01492	YES	YES
101	a	1617.09	3.51685	YES	YES
102	a	1617.90	4.85916	YES	YES
103	a	1624.47	54.58718	YES	YES
104	a	1625.07	55.58599	YES	YES
105	a	1626.76	9.44961	YES	YES



Total energy = -2207.4515475350 H = -60067.8470406 eV

HOMO-LUMO Separation

HOMO: 125. 125 a -0.09930279 H = -2.70217 eV

LUMO: 126. 126 a +0.05485666 H = +1.49273 eV

Gap : +0.15415945 H = +4.19489 eV

Number of MOs= 478, Electrons= 250.00, Symmetry: c1

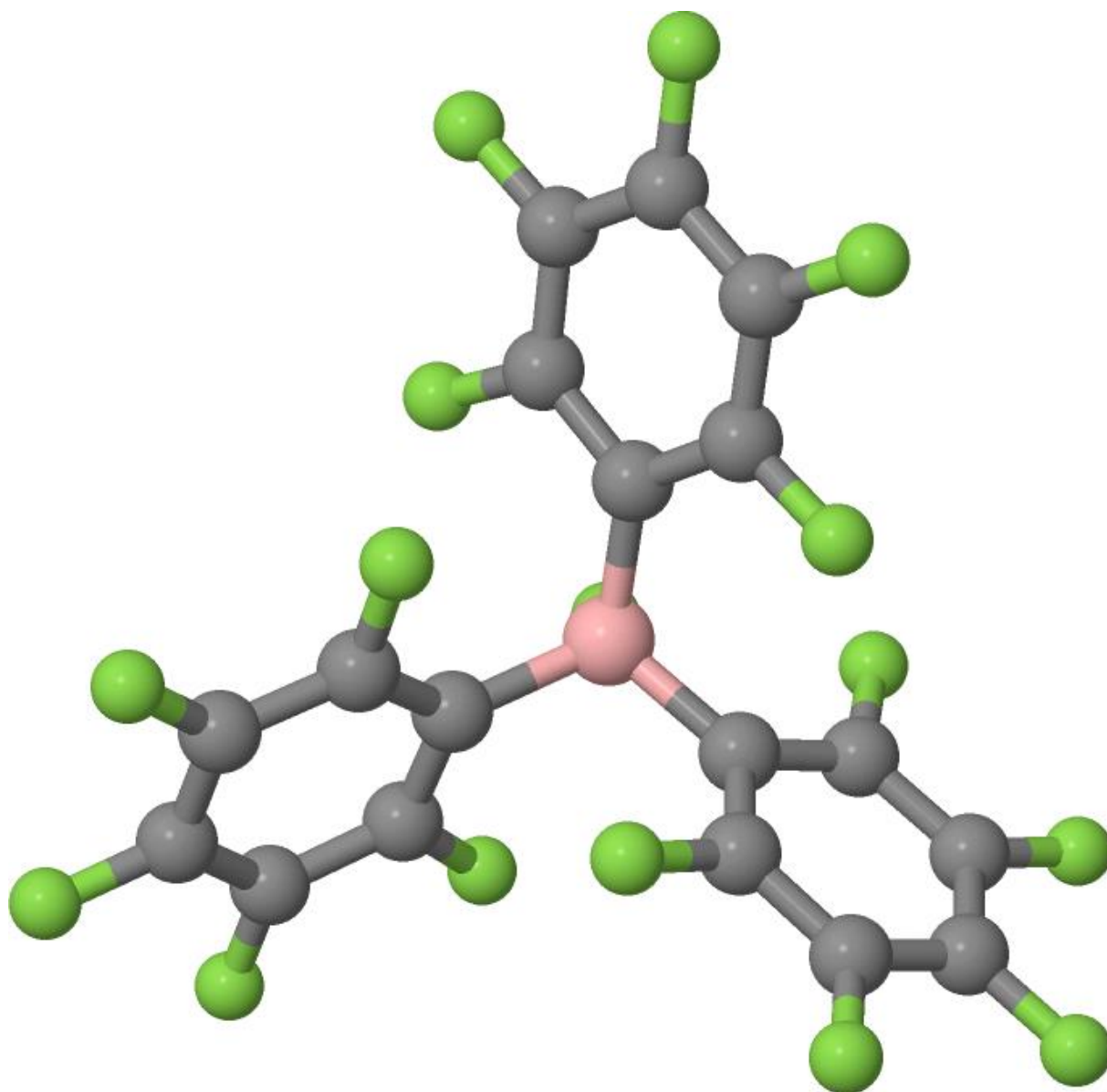
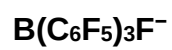
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1.07053282674827	-2.85551273346727	0.64457456145678	c	
-2.91705326734453	0.45290992414788	0.68053266503709	c	
4.03222651482134	2.89024482592888	2.16734609719616	c	
5.66062815641668	4.93497220226588	1.68224820157044	c	
5.19387313021211	6.49711408948150	-0.40859347525064	c	
3.11776957473058	5.97874630999079	-1.97203786255006	c	
1.55392755707693	3.90137568925989	-1.41754707807904	c	
0.24226528001051	-4.99894422329832	1.98768038923378	c	
1.10080226820691	-7.46790650288794	1.50964448214014	c	
2.86819297164398	-7.87149792834105	-0.42663222799704	c	
3.74083688800843	-5.80186129230199	-1.83413912250488	c	
2.81608580092729	-3.36749487687641	-1.29035909971861	c	
-4.48834877224268	1.93686548770350	2.22980891531186	c	
-7.03850773615450	2.44977558040941	1.67905047908184	c	
-8.11713192109665	1.44534968465479	-0.52505977421485	c	
-6.62998222462536	-0.04992589163670	-2.13284511989518	c	
-4.08664185651424	-0.50136829538456	-1.50466959515750	c	
6.72435699556578	8.46771970902122	-0.91344298600464	f	
2.66103753850618	7.45989371494648	-3.99482026678821	f	
-0.36008447801222	3.50294386610008	-3.06141262504704	f	
4.61199772765564	1.46851082004920	4.20544175929818	f	
7.65662771578643	5.41829263307768	3.19170678589195	f	
3.71366785736523	-1.49024948029367	-2.77234329975937	f	
5.43463926033392	-6.17567071100398	-3.70038652538959	f	
3.71979828438770	-10.21979325592762	-0.92226449450889	f	
0.25765701394937	-9.44775399869227	2.87629195058060	f	
-2.76293720377432	-1.90813003062533	-3.17455695682696	f	
-3.58140604899255	2.97865973812932	4.37515917917332	f	
-8.45853592485164	3.89287523354206	3.22770762190751	f	
-10.55348046786130	1.91993335929617	-1.09310421478111	f	
-7.64799565473893	-1.00230818799157	-4.26595384242448	f	
-1.46327904540513	-4.75075721014652	3.87054231605473	f	
0.06588335414562	-0.07403956603833	3.82571851952798	h	

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
#						
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	6.06	0.00848	YES	YES
8		a	13.49	0.00930	YES	YES
9		a	20.24	0.00867	YES	YES
10		a	28.05	0.01960	YES	YES
11		a	29.33	0.01791	YES	YES
12		a	39.35	0.10692	YES	YES
13		a	92.95	0.17263	YES	YES
14		a	100.80	0.20604	YES	YES
15		a	105.31	0.14494	YES	YES
16		a	123.07	0.00358	YES	YES

17	a	123.81	0.00192	YES	YES
18	a	125.22	0.00358	YES	YES
19	a	136.99	0.01859	YES	YES
20	a	139.56	0.03521	YES	YES
21	a	141.45	0.05790	YES	YES
22	a	156.95	0.01256	YES	YES
23	a	160.35	0.05645	YES	YES
24	a	161.51	0.03611	YES	YES
25	a	217.11	1.14420	YES	YES
26	a	223.27	1.35421	YES	YES
27	a	226.67	1.65021	YES	YES
28	a	257.52	0.04190	YES	YES
29	a	261.02	0.04025	YES	YES
30	a	262.58	0.03638	YES	YES
31	a	267.14	0.07239	YES	YES
32	a	270.45	0.06253	YES	YES
33	a	270.92	0.05272	YES	YES
34	a	304.52	0.38030	YES	YES
35	a	305.41	0.24968	YES	YES
36	a	305.59	1.02760	YES	YES
37	a	336.29	1.83056	YES	YES
38	a	336.40	1.27798	YES	YES
39	a	339.88	0.52545	YES	YES
40	a	349.07	0.00695	YES	YES
41	a	366.49	0.38707	YES	YES
42	a	373.16	0.36497	YES	YES
43	a	386.76	0.08491	YES	YES
44	a	388.09	0.03645	YES	YES
45	a	388.68	0.05143	YES	YES
46	a	432.67	0.00545	YES	YES
47	a	432.93	0.12645	YES	YES
48	a	432.94	0.07920	YES	YES
49	a	454.07	1.91345	YES	YES
50	a	454.37	2.03269	YES	YES
51	a	470.86	0.00595	YES	YES
52	a	494.07	0.04286	YES	YES
53	a	496.74	0.01711	YES	YES
54	a	505.22	0.02233	YES	YES
55	a	531.30	0.12163	YES	YES
56	a	558.82	5.93505	YES	YES
57	a	559.31	5.80828	YES	YES
58	a	563.95	0.05724	YES	YES
59	a	585.77	11.00509	YES	YES
60	a	587.42	11.26863	YES	YES
61	a	627.09	0.09023	YES	YES
62	a	629.44	0.04602	YES	YES
63	a	630.81	0.06763	YES	YES
64	a	659.46	3.72966	YES	YES
65	a	667.29	33.07194	YES	YES
66	a	675.07	34.10870	YES	YES
67	a	743.81	13.94446	YES	YES
68	a	748.35	14.05518	YES	YES
69	a	770.41	0.65738	YES	YES
70	a	827.15	1.41920	YES	YES
71	a	895.36	63.36607	YES	YES
72	a	898.15	73.74381	YES	YES
73	a	965.64	101.83934	YES	YES
74	a	969.31	104.94746	YES	YES
75	a	976.94	341.10198	YES	YES
76	a	1043.15	15.91148	YES	YES
77	a	1045.73	24.21822	YES	YES
78	a	1080.36	11.65925	YES	YES

79	a	1098.55	221.08200	YES	YES
80	a	1099.57	243.44265	YES	YES
81	a	1127.39	2.35399	YES	YES
82	a	1128.12	1.50684	YES	YES
83	a	1130.05	6.76409	YES	YES
84	a	1263.19	23.22418	YES	YES
85	a	1264.09	36.95870	YES	YES
86	a	1264.65	17.20768	YES	YES
87	a	1347.29	6.94718	YES	YES
88	a	1348.68	8.98874	YES	YES
89	a	1350.53	5.08563	YES	YES
90	a	1372.47	10.25811	YES	YES
91	a	1374.13	8.71327	YES	YES
92	a	1379.38	0.41507	YES	YES
93	a	1460.21	264.69082	YES	YES
94	a	1462.21	298.44040	YES	YES
95	a	1464.95	553.73868	YES	YES
96	a	1502.27	286.72574	YES	YES
97	a	1502.86	259.02618	YES	YES
98	a	1506.63	17.90895	YES	YES
99	a	1612.86	7.08497	YES	YES
100	a	1613.68	3.29907	YES	YES
101	a	1614.95	3.56302	YES	YES
102	a	1618.35	33.53367	YES	YES
103	a	1618.93	31.96868	YES	YES
104	a	1621.26	4.56527	YES	YES
105	a	2414.32	69.08808	YES	YES



Total energy = -2306.6769553810 H = -62767.9093037 eV

HOMO-LUMO Separation

HOMO: 129. 129 a -0.11020706 H = -2.99889 eV

LUMO: 130. 130 a +0.05365196 H = +1.45994 eV

Gap : +0.16385902 H = +4.45883 eV

372

Number of MOs= 490, Electrons= 258.00, Symmetry: c1

\$coord

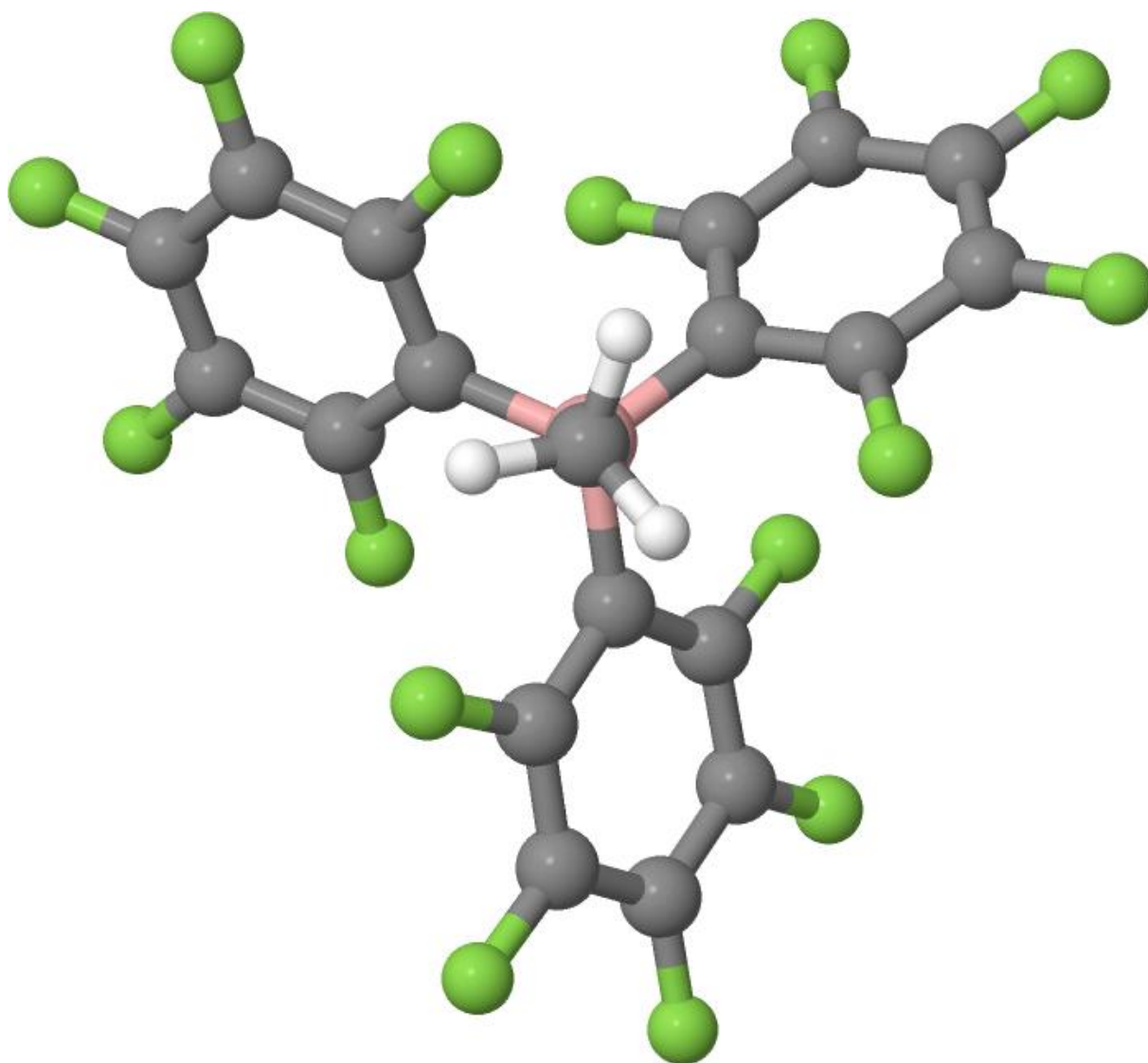
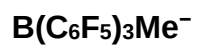
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-1.56521576770740	2.55957845613088	0.60368347765692	c
3.09192247376898	0.16921627072011	0.50267672551891	c
-1.34648596469009	-2.59283498460824	0.66849368042144	c
-1.60617396541859	4.79598979567895	2.04071391979752	c
-3.07079545248755	6.92117249115388	1.39605576870145	c
-4.54979016778503	6.86995450594557	-0.80190141331096	c
-4.53905223024735	4.69807100091849	-2.32035508991230	c
-3.04789700631357	2.62094801000094	-1.59665637809253	c
4.82678811291177	-1.58308390749388	1.49991489512978	c
7.41445216217909	-1.59978821430013	0.90625246717959	c
8.36216255468444	0.20086559633631	-0.79492774120982	c
6.70885503912721	1.97399651860895	-1.85889853277101	c
4.13054444973424	1.91944324571191	-1.19650747169458	c
-3.58244209884133	-3.27683659543168	1.93130812022268	c
-4.90475512887339	-5.53559691483388	1.46588631849311	c
-4.00076290201736	-7.20765704129898	-0.38230024681681	c
-1.79644391848614	-6.59411418927706	-1.71896836048898	c
-0.54366670343359	-4.31039146763411	-1.18471002130364	c
-5.95578754572984	8.88812301021737	-1.45315185984891	f
-5.93741496858467	4.64269752175058	-4.44865025901929	f
-3.08139082339434	0.62832334119311	-3.20002126932459	f
-0.18158177318815	5.04240866153539	4.13656361955635	f
-3.05234173249737	9.01521731884497	2.84622035973427	f
2.68178375491688	3.69205165279178	-2.33594310520618	f
7.60530470328156	3.70236274721791	-3.50136895362384	f
10.83294007433525	0.21858864031446	-1.40128473679454	f
8.99289332502840	-3.32652834699714	1.91371692497085	f
1.52465832978318	-3.83611683699842	-2.61050738626839	f
-4.60177699416894	-1.73374737211379	3.68576160308001	f
-7.03320370858692	-6.10346716410816	2.74567092014970	f
-5.23831619769746	-9.37782601215207	-0.86928730051438	f
-0.92155958608869	-8.18720853572974	-3.50416604603849	f
4.03473199317685	-3.41382425826081	3.08713968895821	f
0.23359194770133	0.05556403095657	4.22224880465722	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	11.09	0.00536	YES	YES
8		a	18.07	0.01022	YES	YES
9		a	25.40	0.00854	YES	YES
10		a	30.09	0.02314	YES	YES
11		a	33.08	0.02219	YES	YES
12		a	40.51	0.07996	YES	YES
13		a	96.74	0.35475	YES	YES

14	a	101.67	0.13197	YES	YES
15	a	104.38	0.21051	YES	YES
16	a	122.59	0.00171	YES	YES
17	a	123.20	0.01618	YES	YES
18	a	126.39	0.00578	YES	YES
19	a	135.48	0.06304	YES	YES
20	a	141.60	0.18264	YES	YES
21	a	147.44	0.18210	YES	YES
22	a	156.49	0.01669	YES	YES
23	a	159.35	0.11541	YES	YES
24	a	162.20	0.05384	YES	YES
25	a	207.83	2.70907	YES	YES
26	a	215.99	2.17369	YES	YES
27	a	224.48	2.09160	YES	YES
28	a	245.57	0.54572	YES	YES
29	a	247.91	0.64507	YES	YES
30	a	262.32	0.08135	YES	YES
31	a	264.31	0.04959	YES	YES
32	a	265.53	0.07466	YES	YES
33	a	272.15	0.07314	YES	YES
34	a	273.62	0.05408	YES	YES
35	a	273.96	0.08353	YES	YES
36	a	306.13	0.46191	YES	YES
37	a	307.97	0.24261	YES	YES
38	a	309.07	0.26602	YES	YES
39	a	312.14	0.96414	YES	YES
40	a	342.10	3.51225	YES	YES
41	a	343.44	2.49775	YES	YES
42	a	345.93	0.01651	YES	YES
43	a	380.85	1.32647	YES	YES
44	a	384.87	0.18248	YES	YES
45	a	389.14	0.30028	YES	YES
46	a	389.92	0.06919	YES	YES
47	a	390.76	1.23831	YES	YES
48	a	428.36	0.32994	YES	YES
49	a	433.36	0.09917	YES	YES
50	a	433.43	0.22417	YES	YES
51	a	434.50	0.14282	YES	YES
52	a	465.36	1.96942	YES	YES
53	a	466.11	1.76289	YES	YES
54	a	482.18	0.01960	YES	YES
55	a	493.06	0.08746	YES	YES
56	a	498.36	0.02486	YES	YES
57	a	511.84	0.00780	YES	YES
58	a	560.37	3.79233	YES	YES
59	a	561.51	2.85883	YES	YES
60	a	563.25	0.86738	YES	YES
61	a	598.89	34.21228	YES	YES
62	a	607.33	36.83111	YES	YES
63	a	628.20	0.19521	YES	YES
64	a	630.60	0.07190	YES	YES
65	a	633.33	0.03529	YES	YES
66	a	639.06	1.52739	YES	YES
67	a	689.90	67.24325	YES	YES
68	a	702.48	78.79681	YES	YES
69	a	745.99	2.98604	YES	YES
70	a	756.06	33.55485	YES	YES
71	a	758.77	34.73170	YES	YES
72	a	807.84	5.43779	YES	YES
73	a	915.26	10.25826	YES	YES
74	a	924.29	9.91886	YES	YES
75	a	969.03	316.24472	YES	YES

76	a	976.20	94.95977	YES	YES
77	a	979.83	146.23426	YES	YES
78	a	1011.43	0.51141	YES	YES
79	a	1084.44	59.65617	YES	YES
80	a	1089.22	300.05540	YES	YES
81	a	1091.74	334.17746	YES	YES
82	a	1128.07	0.89009	YES	YES
83	a	1129.93	0.52061	YES	YES
84	a	1131.70	1.47676	YES	YES
85	a	1260.03	46.51247	YES	YES
86	a	1263.18	43.12815	YES	YES
87	a	1267.34	31.68506	YES	YES
88	a	1348.44	7.93870	YES	YES
89	a	1351.49	5.59084	YES	YES
90	a	1351.68	6.26071	YES	YES
91	a	1370.27	25.30896	YES	YES
92	a	1371.96	19.52210	YES	YES
93	a	1380.30	0.49326	YES	YES
94	a	1460.33	386.36341	YES	YES
95	a	1464.00	387.01531	YES	YES
96	a	1465.71	594.67241	YES	YES
97	a	1506.86	191.26047	YES	YES
98	a	1508.18	228.27147	YES	YES
99	a	1511.15	13.71842	YES	YES
100	a	1617.98	15.03598	YES	YES
101	a	1618.36	5.19774	YES	YES
102	a	1619.52	4.08839	YES	YES
103	a	1622.77	62.78683	YES	YES
104	a	1623.42	41.44392	YES	YES
105	a	1625.47	8.95293	YES	YES



Total energy = -2246.7274023300 H = -61136.5980358 eV

HOMO-LUMO Separation

HOMO: 129. 129 a -0.10191487 H = -2.77325 eV

LUMO: 130. 130 a +0.05711504 H = +1.55418 eV

Gap : +0.15902991 H = +4.32743 eV

Number of MOs= 496, Electrons= 258.00, Symmetry: c1

\$coord

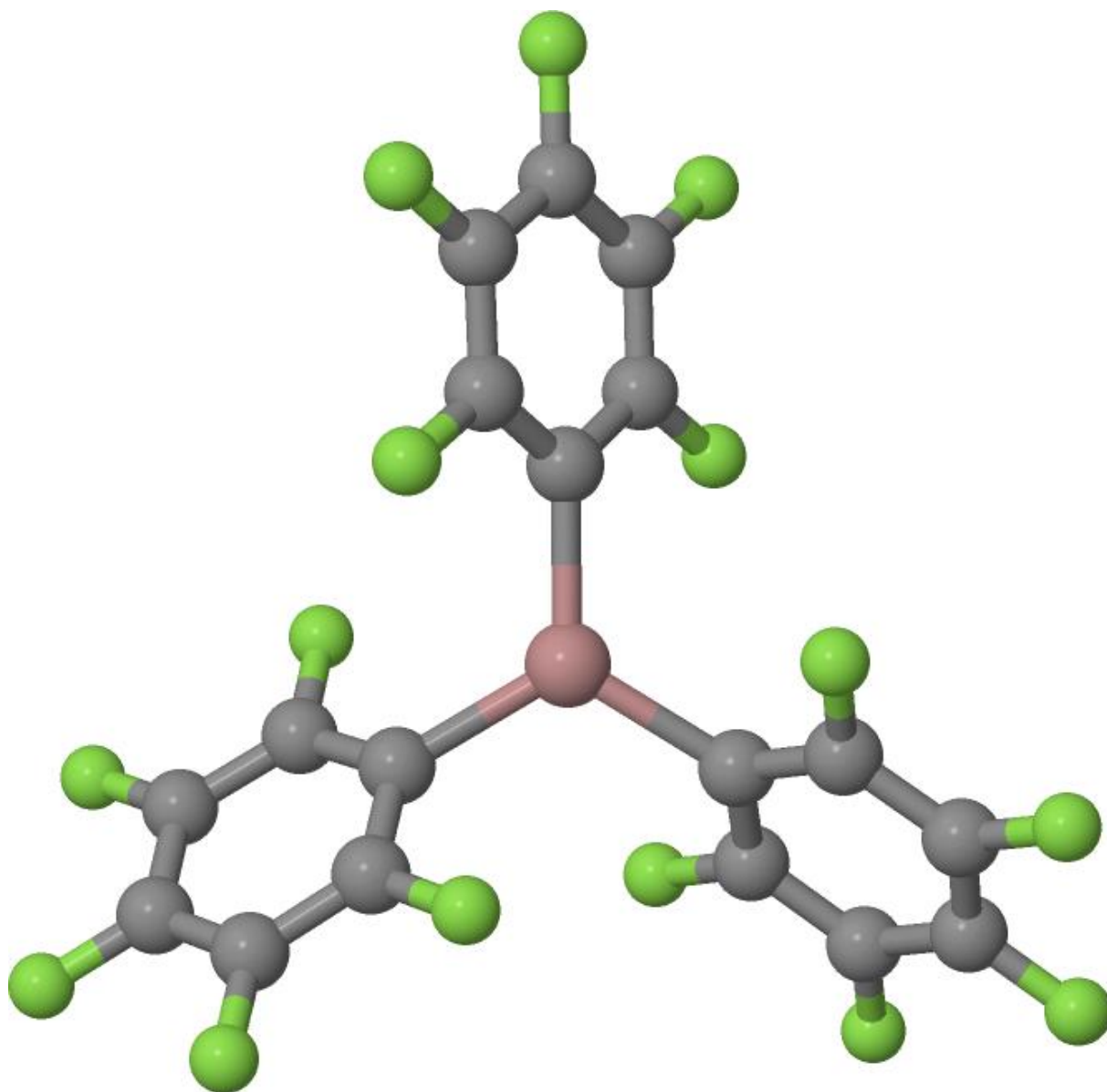
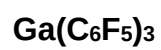
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-2.29929231363914	1.92537723730596	0.63470766004384	c
2.85884750605265	1.09528408914723	0.68219118229491	c
-2.39399058615714	-4.35215200869858	1.81993256726322	c
-2.90064769334522	-6.88563606348619	1.20799975884874	c
-1.43461128284989	-8.09210111518198	-0.64104464603515	c
0.49568729524309	-6.72754730456709	-1.83554609762310	c
0.91984265545941	-4.18919518676458	-1.15829767064286	c
-2.69656057465996	4.32709862620285	1.71430114928811	c
-4.72945103806288	5.92595334669023	1.11166857389208	c
-6.50218058044136	5.14474301159091	-0.69834499718143	c
-6.17550778717396	2.79772545500162	-1.87672163535483	c
-4.09400437948649	1.27590217765851	-1.21709103854521	c
5.08084895565121	0.02640644534260	1.68929191432420	c
7.53818740142339	0.84042270337217	1.10106469194934	c
7.86668704994434	2.83045829628690	-0.61988637652871	c
5.72662287080550	3.94643225533819	-1.70763689551090	c
3.30355860743608	3.05665105234126	-1.05482652542422	c
-1.88307876593746	-10.51951665689323	-1.26354815768502	f
1.89677954604004	-7.85176095796574	-3.64342031337689	f
2.76243086003750	-3.01675409800215	-2.48863620621816	f
-3.97347736126181	-3.31535243297318	3.54407570269508	f
-4.78841524600456	-8.15757147013009	2.35350191009054	f
-3.91869926509006	-0.90817827818185	-2.53698801706767	f
-7.84328677242161	2.02941564254103	-3.64354417459803	f
-8.47667838613305	6.63297116711460	-1.30335348061396	f
-4.99107041966735	8.20126095499404	2.22948046787943	f
1.37606450423301	4.22157848612640	-2.26575364288592	f
4.94477003961333	-1.96546760428045	3.28916420249117	f
9.57795461853522	-0.27536629195775	2.14500091818496	f
10.20210195482027	3.64455308215176	-1.22508187966771	f
6.01312156690244	5.83943326977974	-3.38914263919775	f
-1.03519415875873	5.26927824958779	3.41395826248102	f
0.05670745195180	0.12609447700253	4.80798463514731	c
1.20104783014908	1.72578078657260	5.55006695754289	h
0.87139180039019	-1.63910661572281	5.60701172481104	h
-1.87752241929864	0.32892349872194	5.60489040359470	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	10.65	0.00535	YES	YES
8		a	17.67	0.00257	YES	YES
9		a	27.04	0.04675	YES	YES
10		a	31.49	0.02865	YES	YES
11		a	32.57	0.02750	YES	YES
12		a	45.91	0.01331	YES	YES
13		a	101.66	0.06158	YES	YES

14	a	103.15	0.13827	YES	YES
15	a	105.08	0.13637	YES	YES
16	a	123.03	0.02174	YES	YES
17	a	124.47	0.01587	YES	YES
18	a	128.00	0.00012	YES	YES
19	a	131.75	0.03982	YES	YES
20	a	148.40	0.02178	YES	YES
21	a	149.13	0.02137	YES	YES
22	a	159.18	0.00081	YES	YES
23	a	161.43	0.11084	YES	YES
24	a	162.33	0.08531	YES	YES
25	a	213.86	0.48279	YES	YES
26	a	218.76	1.10569	YES	YES
27	a	220.30	1.10940	YES	YES
28	a	231.60	1.33034	YES	YES
29	a	249.48	0.34824	YES	YES
30	a	249.71	0.43182	YES	YES
31	a	261.21	0.06623	YES	YES
32	a	261.54	0.06832	YES	YES
33	a	262.69	0.05850	YES	YES
34	a	274.75	0.04596	YES	YES
35	a	275.62	0.02686	YES	YES
36	a	276.56	0.01788	YES	YES
37	a	311.50	0.22337	YES	YES
38	a	312.00	0.37929	YES	YES
39	a	312.89	0.41725	YES	YES
40	a	313.85	0.48161	YES	YES
41	a	344.07	2.69702	YES	YES
42	a	344.60	2.64653	YES	YES
43	a	349.55	0.06683	YES	YES
44	a	383.68	0.55853	YES	YES
45	a	384.98	0.32900	YES	YES
46	a	386.45	0.44582	YES	YES
47	a	387.29	0.33143	YES	YES
48	a	388.59	0.43640	YES	YES
49	a	431.40	0.00770	YES	YES
50	a	434.84	0.02026	YES	YES
51	a	435.14	0.06711	YES	YES
52	a	435.32	0.07799	YES	YES
53	a	459.33	1.33996	YES	YES
54	a	459.94	1.22586	YES	YES
55	a	479.27	0.01534	YES	YES
56	a	508.45	0.03455	YES	YES
57	a	514.33	0.06483	YES	YES
58	a	516.50	0.09024	YES	YES
59	a	560.15	5.04735	YES	YES
60	a	560.56	4.74460	YES	YES
61	a	563.58	0.08817	YES	YES
62	a	590.24	19.97024	YES	YES
63	a	590.92	20.01930	YES	YES
64	a	629.98	0.31996	YES	YES
65	a	631.30	0.27148	YES	YES
66	a	631.35	0.25074	YES	YES
67	a	652.82	0.65398	YES	YES
68	a	677.83	19.41885	YES	YES
69	a	681.36	20.89328	YES	YES
70	a	733.09	2.77405	YES	YES
71	a	751.56	8.83281	YES	YES
72	a	752.29	7.72688	YES	YES
73	a	794.97	11.79823	YES	YES
74	a	813.59	73.14034	YES	YES
75	a	819.21	67.16034	YES	YES

76	a	905.16	34.19875	YES	YES
77	a	954.67	53.18773	YES	YES
78	a	956.70	48.83920	YES	YES
79	a	973.85	191.02835	YES	YES
80	a	984.52	102.67703	YES	YES
81	a	985.08	124.38543	YES	YES
82	a	1078.00	21.35941	YES	YES
83	a	1085.62	255.99317	YES	YES
84	a	1086.30	275.38289	YES	YES
85	a	1123.15	4.11005	YES	YES
86	a	1124.68	0.04522	YES	YES
87	a	1125.27	0.47410	YES	YES
88	a	1258.36	7.17062	YES	YES
89	a	1260.26	35.77371	YES	YES
90	a	1260.93	32.90649	YES	YES
91	a	1273.14	4.16402	YES	YES
92	a	1343.28	13.30957	YES	YES
93	a	1344.29	16.13565	YES	YES
94	a	1345.17	14.60518	YES	YES
95	a	1364.34	6.28392	YES	YES
96	a	1364.98	6.04858	YES	YES
97	a	1369.45	2.41413	YES	YES
98	a	1423.28	12.34674	YES	YES
99	a	1428.66	13.99134	YES	YES
100	a	1452.23	433.43022	YES	YES
101	a	1456.65	360.55464	YES	YES
102	a	1457.96	368.67828	YES	YES
103	a	1505.36	257.01109	YES	YES
104	a	1506.11	247.68854	YES	YES
105	a	1509.71	23.59879	YES	YES
106	a	1612.37	8.07120	YES	YES
107	a	1613.76	7.88738	YES	YES
108	a	1613.99	4.19781	YES	YES
109	a	1621.45	39.61093	YES	YES
110	a	1622.01	34.53215	YES	YES
111	a	1623.98	9.07813	YES	YES
112	a	2936.45	32.95591	YES	YES
113	a	3018.79	32.63292	YES	YES
114	a	3019.81	31.87703	YES	YES



Total energy = -4106.8071600520 H = -111751.9723550 eV

HOMO-LUMO Separation

HOMO: 137. 137 a -0.24005910 H = -6.53234 eV

LUMO: 138. 138 a -0.12036461 H = -3.27529 eV

Gap : +0.11969448 H = +3.25705 eV
380

Number of MOs= 494, Electrons= 274.00, Symmetry: c1

\$coord

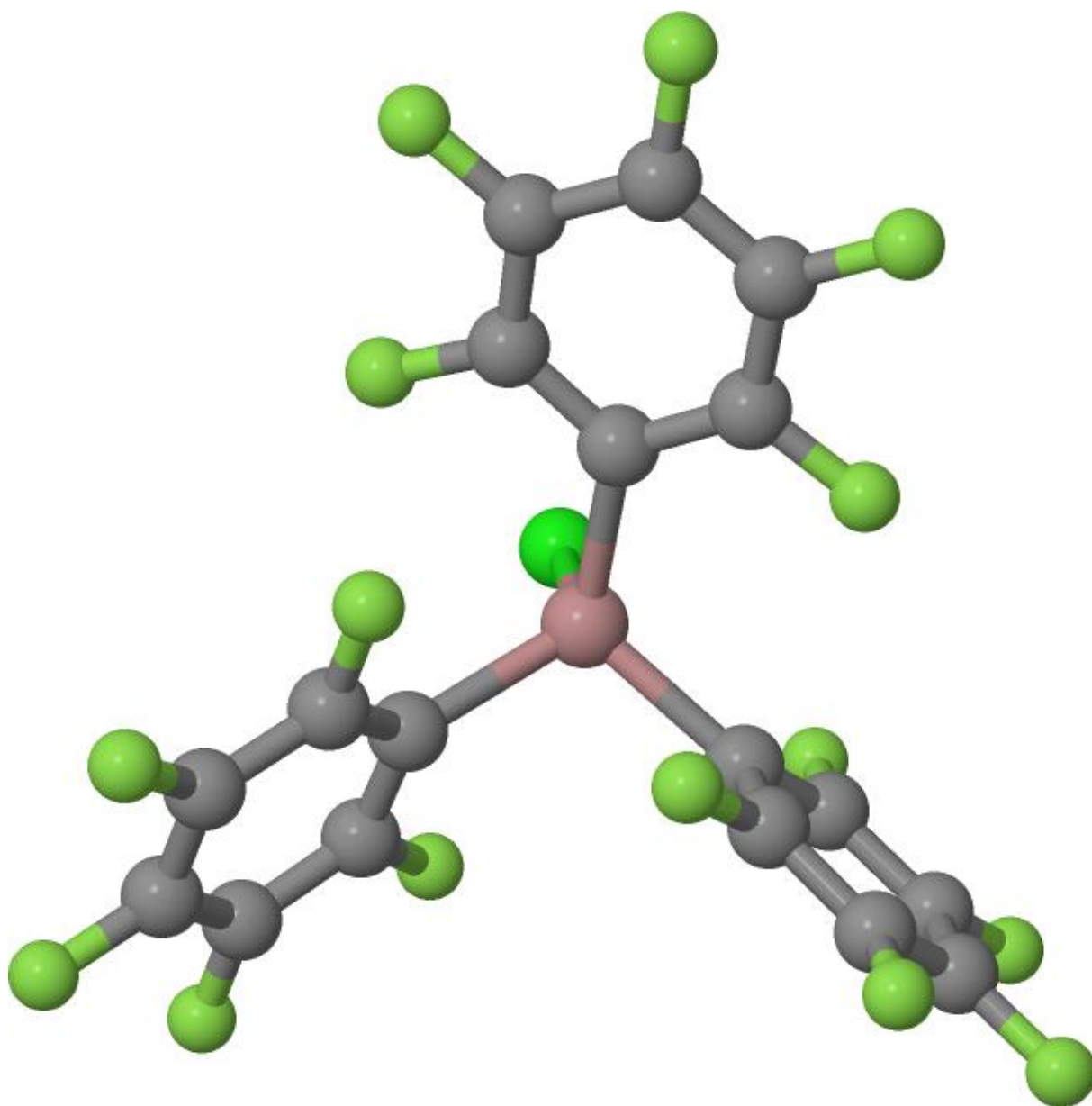
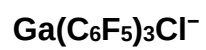
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-2.66190210443179	-2.60930764518208	0.03259855040850	c
-4.59763093156102	-2.81825488870879	-1.76067256695379	c
-6.29042740517233	-4.86435596124228	-1.77988458828705	c
-6.04225524377697	-6.75239861372222	0.07911846069129	c
-4.13188287998848	-6.58857245688517	1.92434974179177	c
-2.48040853586605	-4.51379216847704	1.86115431942820	c
-4.84203435908041	-1.04060969990547	-3.56999191458679	f
-8.10571183597612	-5.05427482509653	-3.52452049024874	f
-7.62481569037713	-8.71263200208168	0.09008857449750	f
-3.91832805151339	-8.38449190471821	3.68541983038442	f
-0.66337919246864	-4.36479758121898	3.64691703264972	f
3.47428639570042	-0.87525337377602	-0.04461636449207	c
-1.05801574152937	3.71458294810726	-0.05456975226836	c
4.40552440670920	-2.63314430067493	-1.79032633399075	c
0.03107554048639	5.40595664122270	-1.77710397103089	c
6.94409081839369	-3.40827393180374	-1.80585064656590	c
-0.57128940532226	7.99087925078064	-1.79921648519169	c
8.60398605587056	-2.38161199455896	0.00228908841902	c
-2.32511125744577	8.90953336593966	-0.02167083065344	c
7.73190012899671	-0.61100121049247	1.78660439921893	c
-3.45251277551351	7.26451057971922	1.73970565972811	c
5.17814033647903	0.11009524515137	1.72429256113990	c
-2.79870192712267	4.69247218472707	1.68452476859541	c
2.83558402287053	-3.61601129593593	-3.54342432410077	f
1.70072476403418	4.54548916290595	-3.49949700187175	f
7.80286623026491	-5.07900223929356	-3.49260237348637	f
0.47185233002193	9.57358902740807	-3.46655666331284	f
11.02082597282023	-3.09225818004224	0.02537426418050	f
-2.92222025819846	11.35629751725727	-0.00598445587733	f
9.32825027705060	0.33707699001627	3.49737271932247	f
-5.10353608119919	8.16728754279172	3.42203096708608	f
4.35555717356777	1.78337644072592	3.46389018477496	f
-3.86929998290770	3.14189464748072	3.40046747387652	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	8.97	0.09930	YES	YES
8		a	12.41	0.07937	YES	YES
9		a	14.87	0.01884	YES	YES
10		a	20.33	0.10284	YES	YES
11		a	20.83	0.11845	YES	YES
12		a	25.99	0.10397	YES	YES
13		a	69.09	0.00399	YES	YES
14		a	75.04	0.00525	YES	YES

15	a	75.97	0.00473	YES	YES
16	a	100.21	0.81635	YES	YES
17	a	101.25	0.93468	YES	YES
18	a	123.74	0.03277	YES	YES
19	a	124.01	0.02355	YES	YES
20	a	124.39	0.01822	YES	YES
21	a	126.51	0.00178	YES	YES
22	a	143.06	0.63630	YES	YES
23	a	150.22	0.02715	YES	YES
24	a	151.53	0.05902	YES	YES
25	a	172.87	3.84045	YES	YES
26	a	210.57	2.25149	YES	YES
27	a	212.45	0.23652	YES	YES
28	a	213.00	0.74227	YES	YES
29	a	241.61	27.98827	YES	YES
30	a	244.45	29.15821	YES	YES
31	a	262.38	0.08597	YES	YES
32	a	262.65	0.03383	YES	YES
33	a	262.98	0.10160	YES	YES
34	a	264.89	0.00145	YES	YES
35	a	272.11	11.80390	YES	YES
36	a	273.67	16.86966	YES	YES
37	a	301.09	0.16538	YES	YES
38	a	301.25	0.56288	YES	YES
39	a	302.02	0.45565	YES	YES
40	a	339.63	0.03559	YES	YES
41	a	345.98	0.40399	YES	YES
42	a	348.57	1.97741	YES	YES
43	a	353.30	2.54996	YES	YES
44	a	359.50	14.60840	YES	YES
45	a	360.61	16.05677	YES	YES
46	a	400.58	0.33021	YES	YES
47	a	401.68	0.26164	YES	YES
48	a	402.40	0.21991	YES	YES
49	a	429.77	0.01740	YES	YES
50	a	429.89	0.01570	YES	YES
51	a	430.05	0.22671	YES	YES
52	a	478.15	0.00964	YES	YES
53	a	483.80	4.27769	YES	YES
54	a	484.55	6.01606	YES	YES
55	a	485.50	1.97301	YES	YES
56	a	487.63	2.52013	YES	YES
57	a	492.56	1.82232	YES	YES
58	a	562.71	0.33796	YES	YES
59	a	562.92	0.40742	YES	YES
60	a	563.02	0.63049	YES	YES
61	a	607.93	1.93343	YES	YES
62	a	611.85	7.57823	YES	YES
63	a	612.67	7.66384	YES	YES
64	a	630.57	0.47591	YES	YES
65	a	631.03	0.55221	YES	YES
66	a	631.33	0.03707	YES	YES
67	a	739.94	4.11268	YES	YES
68	a	740.06	4.30653	YES	YES
69	a	741.42	0.08173	YES	YES
70	a	788.43	0.08846	YES	YES
71	a	801.28	4.23582	YES	YES
72	a	803.00	5.03042	YES	YES
73	a	972.76	69.98642	YES	YES
74	a	973.64	104.56831	YES	YES
75	a	974.98	253.58450	YES	YES
76	a	1086.38	118.49550	YES	YES

77	a	1086.87	244.86249	YES	YES
78	a	1088.17	285.73514	YES	YES
79	a	1150.45	0.22775	YES	YES
80	a	1151.13	3.09014	YES	YES
81	a	1152.23	5.90147	YES	YES
82	a	1283.54	37.89133	YES	YES
83	a	1284.33	38.15518	YES	YES
84	a	1284.86	16.01848	YES	YES
85	a	1357.37	1.39033	YES	YES
86	a	1357.71	2.72337	YES	YES
87	a	1358.34	1.31159	YES	YES
88	a	1372.65	126.09261	YES	YES
89	a	1373.01	115.08283	YES	YES
90	a	1385.44	0.01585	YES	YES
91	a	1479.70	289.70219	YES	YES
92	a	1480.33	355.63644	YES	YES
93	a	1483.93	752.84192	YES	YES
94	a	1513.95	313.61459	YES	YES
95	a	1514.75	331.26733	YES	YES
96	a	1517.11	10.33768	YES	YES
97	a	1617.62	1.50452	YES	YES
98	a	1618.13	4.33407	YES	YES
99	a	1619.09	8.21639	YES	YES
100	a	1623.74	85.22732	YES	YES
101	a	1624.34	68.73936	YES	YES
102	a	1625.14	28.74787	YES	YES



Total energy = -4567.0829316030 H = -124276.7204850 eV

HOMO-LUMO Separation

HOMO: 146. 146 a -0.11746231 H = -3.19631 eV

LUMO: 147. 147 a +0.04107064 H = +1.11759 eV

Gap : +0.15853295 H = +4.31390 eV

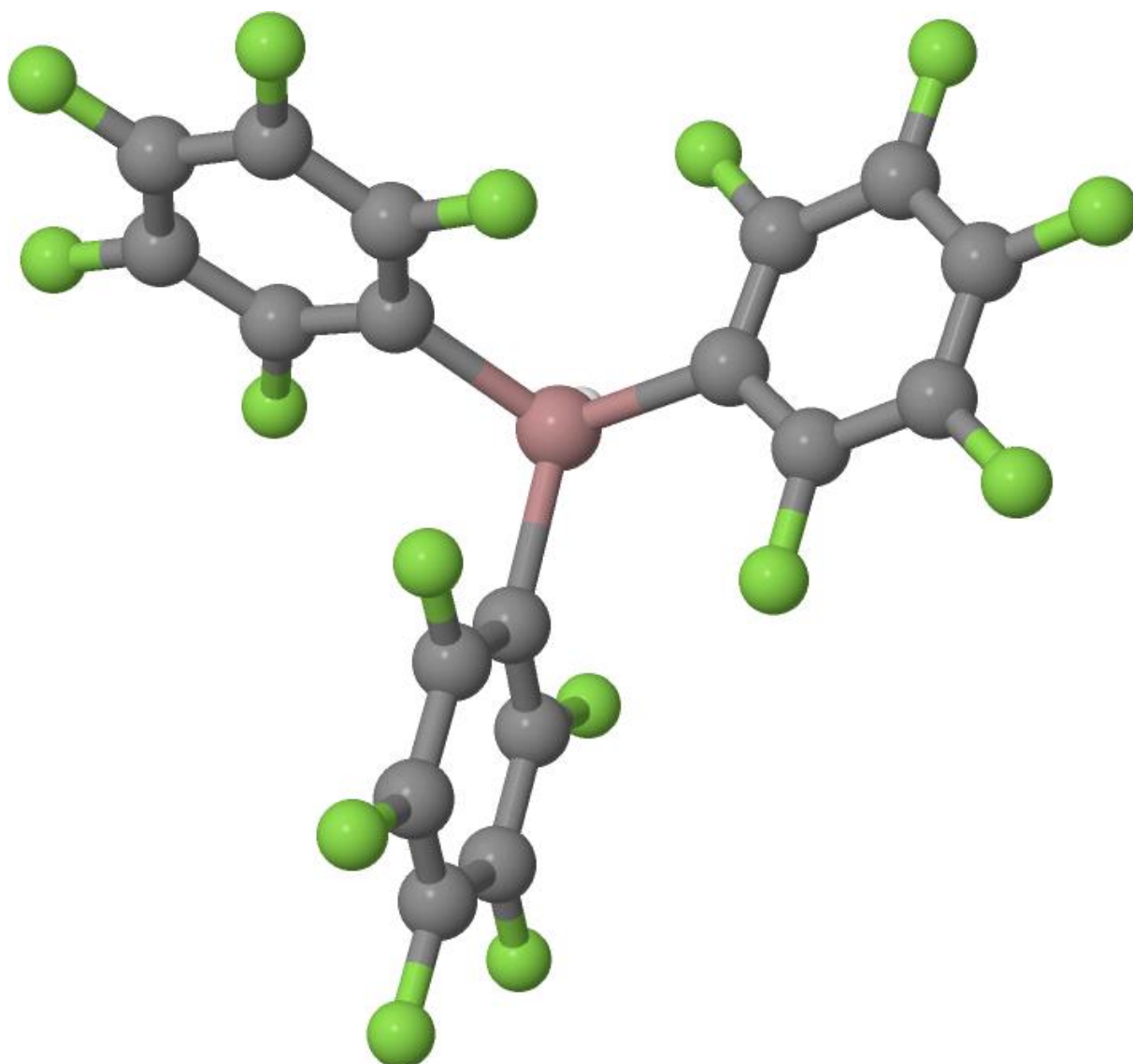
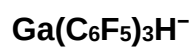
Number of MOs= 512, Electrons= 292.00, Symmetry: c1

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  0.04656643134245      -0.10834113965779      1.72926448737168      ga
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  -7.64517983985964      6.54129743433447      1.37005672309835      f
  -3.18001047657500      4.71335962436116      3.09889475844081      f
  -3.16147337732012      -5.14094852158178      2.00537683501564      f
  -2.14495216269638      -9.98734971774052      0.69684307035618      f
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  7.35928490046531      7.24530241763962      2.14542676733923      f
  4.21064302149374      3.90503844107717      4.36449839909808      f
  -0.11365294380824      -0.27195867790781      5.95138350823650      cl
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```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
  1      0.00      0.00000      -      -
  2      0.00      0.00000      -      -
  3      0.00      0.00000      -      -
  4      0.00      0.00000      -      -
  5      0.00      0.00000      -      -
  6      0.00      0.00000      -      -
  7      a      13.47      0.01649      YES      YES
  8      a      16.15      0.01245      YES      YES
  9      a      19.47      0.00352      YES      YES
  10     a      23.63      0.00544      YES      YES
  11     a      26.49      0.02792      YES      YES
```

12	a	34.40	0.06620	YES	YES
13	a	63.29	1.22859	YES	YES
14	a	76.15	0.66030	YES	YES
15	a	85.26	0.50061	YES	YES
16	a	100.54	0.13950	YES	YES
17	a	103.16	0.45938	YES	YES
18	a	109.92	1.73404	YES	YES
19	a	113.76	1.23525	YES	YES
20	a	116.67	0.35144	YES	YES
21	a	122.34	0.05733	YES	YES
22	a	123.11	0.02611	YES	YES
23	a	128.76	0.03916	YES	YES
24	a	151.88	0.12952	YES	YES
25	a	155.32	0.02360	YES	YES
26	a	157.16	0.00179	YES	YES
27	a	170.15	1.75528	YES	YES
28	a	211.49	4.26290	YES	YES
29	a	218.07	1.63541	YES	YES
30	a	219.00	0.49902	YES	YES
31	a	231.78	30.23201	YES	YES
32	a	238.71	40.81284	YES	YES
33	a	260.69	0.28662	YES	YES
34	a	261.67	0.05032	YES	YES
35	a	265.48	0.04025	YES	YES
36	a	267.72	0.63280	YES	YES
37	a	269.09	4.93050	YES	YES
38	a	271.03	3.91793	YES	YES
39	a	303.21	0.39106	YES	YES
40	a	303.32	0.47818	YES	YES
41	a	305.66	0.47143	YES	YES
42	a	340.84	2.78024	YES	YES
43	a	344.93	0.77035	YES	YES
44	a	345.15	2.93115	YES	YES
45	a	349.52	6.95898	YES	YES
46	a	355.59	5.11568	YES	YES
47	a	360.32	27.98279	YES	YES
48	a	364.88	28.71303	YES	YES
49	a	394.23	0.00847	YES	YES
50	a	396.59	0.06387	YES	YES
51	a	396.92	0.19007	YES	YES
52	a	432.10	0.05130	YES	YES
53	a	432.56	0.13675	YES	YES
54	a	433.24	0.02554	YES	YES
55	a	472.63	0.69061	YES	YES
56	a	474.03	4.93533	YES	YES
57	a	474.91	8.01273	YES	YES
58	a	476.22	1.58075	YES	YES
59	a	480.94	1.39616	YES	YES
60	a	491.66	1.07830	YES	YES
61	a	562.20	0.03035	YES	YES
62	a	563.03	0.00239	YES	YES
63	a	564.21	0.03304	YES	YES
64	a	601.72	8.53207	YES	YES
65	a	603.27	7.63241	YES	YES
66	a	612.66	11.19440	YES	YES
67	a	629.70	0.06889	YES	YES
68	a	632.22	0.19731	YES	YES
69	a	633.92	0.08884	YES	YES
70	a	729.44	0.69445	YES	YES
71	a	732.94	0.36622	YES	YES
72	a	734.65	0.68865	YES	YES
73	a	765.40	3.55940	YES	YES

74	a	766.30	10.34489	YES	YES
75	a	770.17	14.28699	YES	YES
76	a	961.66	110.34356	YES	YES
77	a	965.80	158.36238	YES	YES
78	a	967.04	205.61770	YES	YES
79	a	1068.31	280.67729	YES	YES
80	a	1068.71	312.44264	YES	YES
81	a	1071.30	108.72103	YES	YES
82	a	1126.23	1.10296	YES	YES
83	a	1130.05	0.26281	YES	YES
84	a	1131.69	5.53377	YES	YES
85	a	1254.75	40.10977	YES	YES
86	a	1256.59	31.21658	YES	YES
87	a	1259.36	24.05228	YES	YES
88	a	1354.18	13.68732	YES	YES
89	a	1355.66	5.27277	YES	YES
90	a	1356.57	6.28348	YES	YES
91	a	1358.84	33.68156	YES	YES
92	a	1363.28	27.91067	YES	YES
93	a	1371.04	6.21987	YES	YES
94	a	1453.79	237.72054	YES	YES
95	a	1462.29	385.48121	YES	YES
96	a	1464.28	734.25941	YES	YES
97	a	1502.81	191.76039	YES	YES
98	a	1503.40	235.75625	YES	YES
99	a	1505.39	50.20239	YES	YES
100	a	1613.49	26.00901	YES	YES
101	a	1615.83	22.01207	YES	YES
102	a	1616.45	45.86189	YES	YES
103	a	1617.38	11.81475	YES	YES
104	a	1618.78	19.86242	YES	YES
105	a	1619.60	18.47923	YES	YES



Total energy = -4107.5021793650 H = -111770.8848036 eV

HOMO-LUMO Separation

HOMO: 138. 138 a -0.11382206 H = -3.09726 eV

LUMO: 139. 139 a +0.04897712 H = +1.33274 eV

Gap : +0.16279918 H = +4.42999 eV

Number of MOs= 496, Electrons= 276.00, Symmetry: c1

\$coord

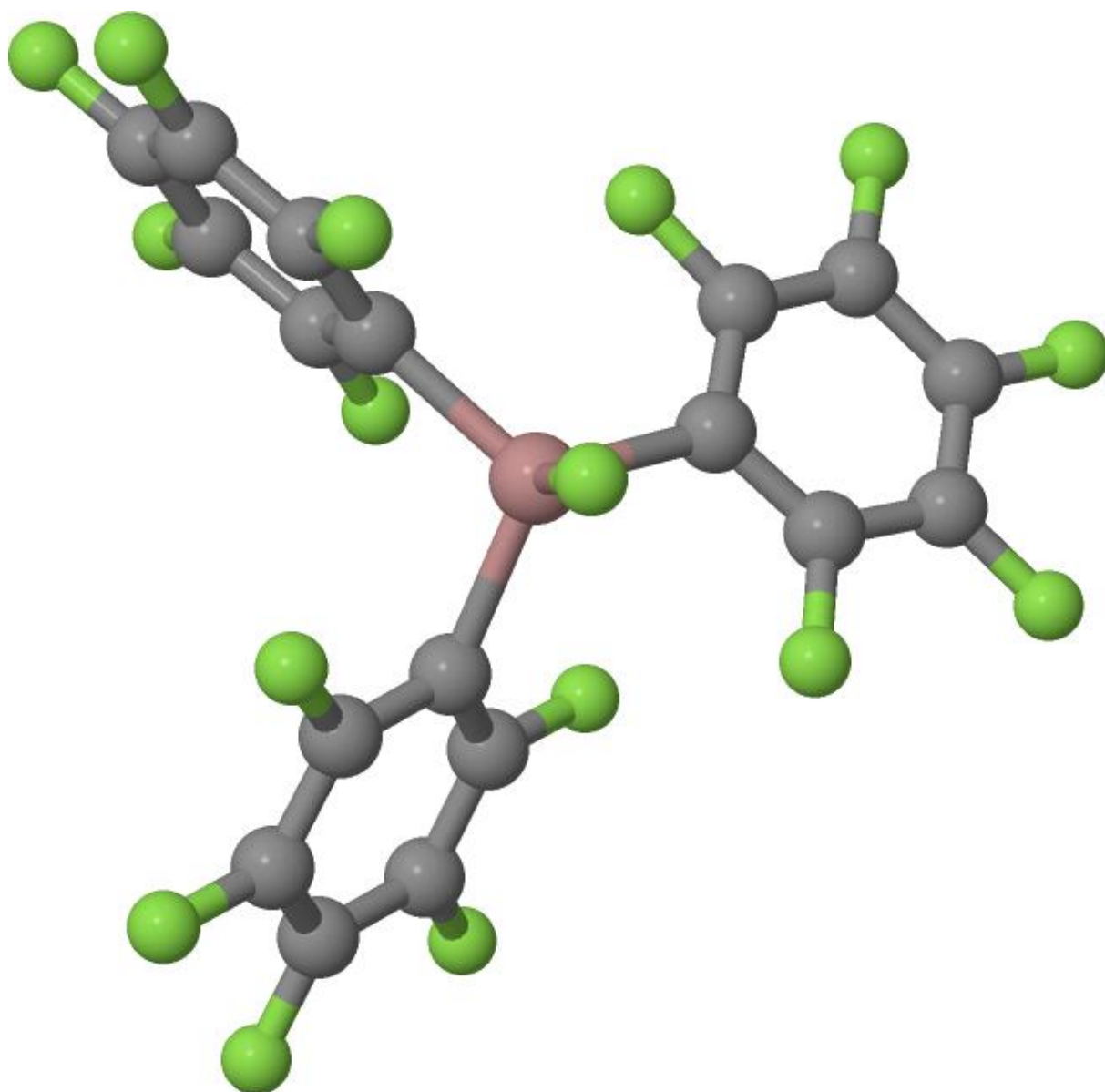
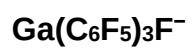
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1.96716386229754	3.04925909664991	0.70579081071852	c
3.51751177263792	4.59346105294521	2.19087563532191	c
4.76113508138084	6.74658205272050	1.24452166577078	c
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-9.20686309503190	4.11820129496209	1.81629640491261	f
-4.36842119321157	3.65045741935611	3.46600616895531	f
-1.32392940306902	-5.65403520110465	3.17228563945313	f
0.76902770266987	-10.15464090367554	1.85915332058251	f
4.98438130753044	-10.27016207667033	-1.16182343762181	f
7.10524334451142	-5.83597675642410	-2.83079577852609	f
5.05909008279042	-1.34848972896248	-1.52903165276961	f
0.29712404632578	2.36619726754422	-3.42880145508916	f
2.64660390605918	6.50924813869124	-5.32966717483948	f
5.61899978575040	9.44730522344507	-2.25676893732469	f
6.23966177730260	8.19139499187123	2.73396296327233	f
3.91393660026824	4.06073487816359	4.66001592500313	f
0.01019967574745	-0.02471939254797	5.12666553175289	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	5.79	0.00119	YES	YES
8		a	14.44	0.00219	YES	YES
9		a	18.86	0.00498	YES	YES
10		a	21.06	0.00202	YES	YES
11		a	24.81	0.00052	YES	YES
12		a	28.25	0.01416	YES	YES
13		a	75.91	0.12035	YES	YES

14	a	80.75	0.12047	YES	YES
15	a	90.79	0.13059	YES	YES
16	a	101.38	0.05874	YES	YES
17	a	107.94	0.05756	YES	YES
18	a	112.90	0.25760	YES	YES
19	a	119.89	0.00397	YES	YES
20	a	121.93	0.01295	YES	YES
21	a	122.92	0.00520	YES	YES
22	a	151.64	0.05694	YES	YES
23	a	153.35	0.07157	YES	YES
24	a	155.98	0.01629	YES	YES
25	a	190.31	4.12503	YES	YES
26	a	209.46	1.78597	YES	YES
27	a	213.87	8.42992	YES	YES
28	a	216.10	0.15097	YES	YES
29	a	223.58	17.34450	YES	YES
30	a	228.20	23.90320	YES	YES
31	a	260.93	0.07818	YES	YES
32	a	261.61	0.12344	YES	YES
33	a	262.20	0.15031	YES	YES
34	a	267.32	1.07936	YES	YES
35	a	268.19	1.52256	YES	YES
36	a	269.26	1.83659	YES	YES
37	a	301.87	0.48270	YES	YES
38	a	302.92	0.51392	YES	YES
39	a	304.36	0.27575	YES	YES
40	a	340.97	0.54227	YES	YES
41	a	342.79	0.80825	YES	YES
42	a	345.30	2.65827	YES	YES
43	a	346.14	1.39793	YES	YES
44	a	351.47	2.81286	YES	YES
45	a	358.60	6.81732	YES	YES
46	a	395.62	0.00884	YES	YES
47	a	396.68	0.05187	YES	YES
48	a	398.34	0.03876	YES	YES
49	a	431.88	0.00067	YES	YES
50	a	432.11	0.00054	YES	YES
51	a	432.43	0.00390	YES	YES
52	a	471.23	1.18341	YES	YES
53	a	472.00	7.09122	YES	YES
54	a	472.81	8.88127	YES	YES
55	a	473.53	0.62743	YES	YES
56	a	481.73	0.99922	YES	YES
57	a	488.50	0.76760	YES	YES
58	a	560.46	0.06426	YES	YES
59	a	561.22	0.63589	YES	YES
60	a	561.91	0.05782	YES	YES
61	a	571.49	56.47380	YES	YES
62	a	584.60	44.43744	YES	YES
63	a	604.92	14.92648	YES	YES
64	a	628.65	58.82118	YES	YES
65	a	629.01	9.90186	YES	YES
66	a	631.48	20.50425	YES	YES
67	a	633.82	0.43101	YES	YES
68	a	640.24	98.98329	YES	YES
69	a	730.91	1.16016	YES	YES
70	a	734.30	3.63921	YES	YES
71	a	735.12	4.24876	YES	YES
72	a	758.54	10.80973	YES	YES
73	a	760.85	15.60090	YES	YES
74	a	762.70	24.81283	YES	YES
75	a	959.17	120.59909	YES	YES

76	a	961.89	248.48372	YES	YES
77	a	962.75	121.19826	YES	YES
78	a	1061.97	299.72714	YES	YES
79	a	1062.85	287.59583	YES	YES
80	a	1065.10	86.62167	YES	YES
81	a	1120.67	1.05070	YES	YES
82	a	1123.82	0.93832	YES	YES
83	a	1124.86	4.65217	YES	YES
84	a	1246.83	29.34938	YES	YES
85	a	1249.80	34.95180	YES	YES
86	a	1251.29	14.03117	YES	YES
87	a	1351.64	37.08657	YES	YES
88	a	1352.38	46.15804	YES	YES
89	a	1356.90	0.88996	YES	YES
90	a	1357.00	1.60608	YES	YES
91	a	1361.29	10.90344	YES	YES
92	a	1362.99	4.26932	YES	YES
93	a	1450.18	281.87549	YES	YES
94	a	1456.26	507.95058	YES	YES
95	a	1457.92	548.12316	YES	YES
96	a	1499.17	202.35994	YES	YES
97	a	1499.77	251.92305	YES	YES
98	a	1502.04	34.25709	YES	YES
99	a	1612.50	44.65141	YES	YES
100	a	1613.28	37.59857	YES	YES
101	a	1614.20	14.87416	YES	YES
102	a	1615.61	6.70023	YES	YES
103	a	1616.58	7.79624	YES	YES
104	a	1617.16	9.32339	YES	YES
105	a	1863.93	208.05812	YES	YES



Total energy = -4206.7321069480 H = -114471.0700550 eV

HOMO-LUMO Separation

HOMO: 142. 142 a -0.11810516 H = -3.21381 eV

LUMO: 143. 143 a +0.04267243 H = +1.16118 eV

Gap : +0.16077758 H = +4.37498 eV

Number of MOs= 508, Electrons= 284.00, Symmetry: c1

\$scoord

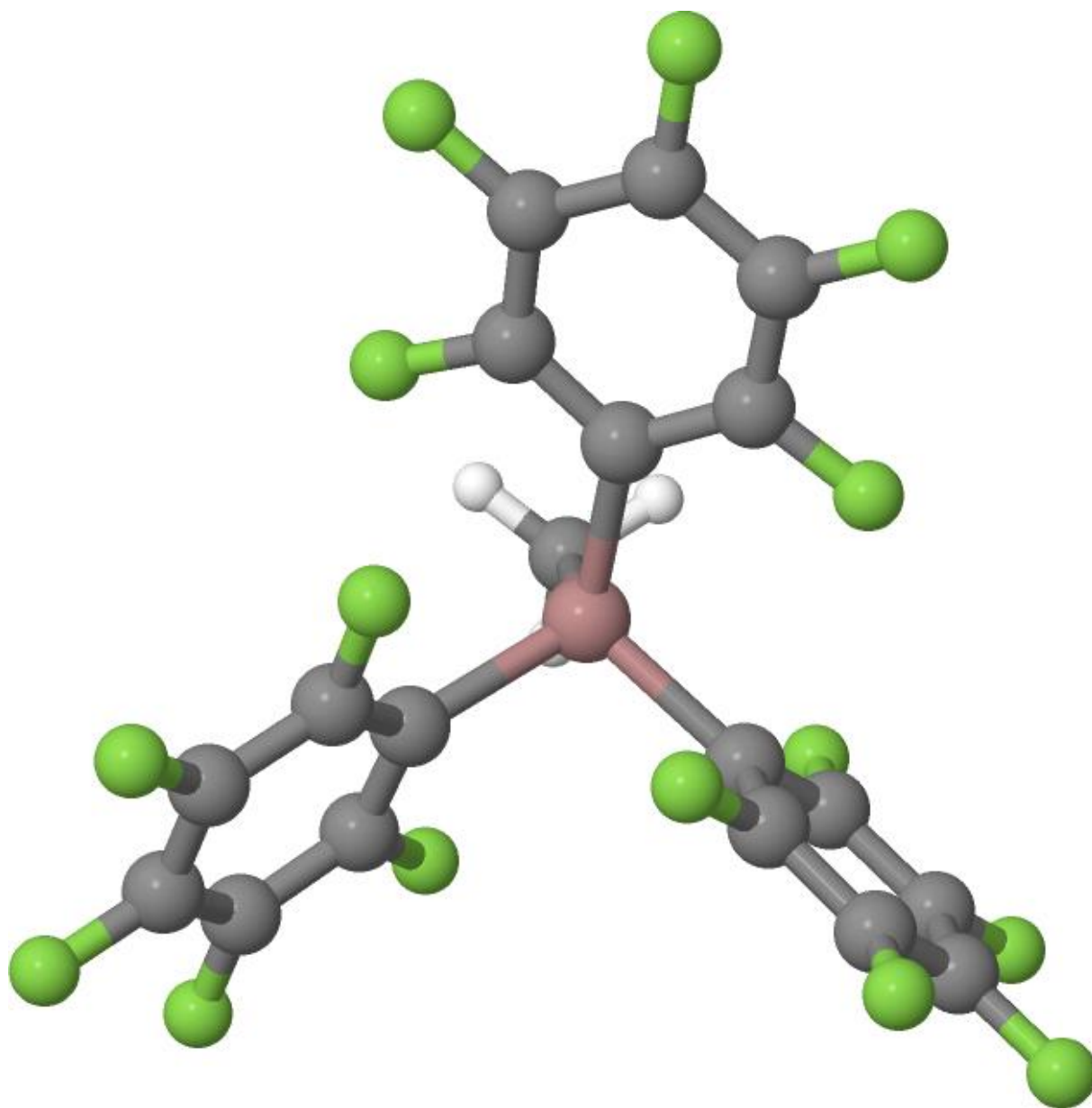
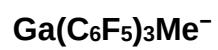
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2.61387234968923	2.44292362351052	0.70818678658011	c
4.17940835126740	3.98193593657511	2.18197397655896	c
5.86146910851055	5.75217183965732	1.12267190583176	c
5.99172880865880	6.00389781777098	-1.51528392361936	c
3.77347561837036	-6.98427794822392	-0.66567416849599	c
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-4.75166609133373	-0.14200627134608	-1.15406990100470	c
0.06116679122540	-0.11361438388502	2.05541338653133	ga
-3.87561245224839	-2.27916377281162	-2.24718297379797	f
-8.34532892887450	-0.43148530514852	-3.91432229121758	f
-10.27156039303334	3.93918676660041	-1.90744359561694	f
-7.67575863521572	6.47000570808486	1.80169800800409	f
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6.02602149574934	-7.63403946190295	-1.66052995410480	f
5.08329968456633	-2.76202889259621	-0.39549849851303	f
1.35920685249279	1.33306398034275	-3.47062359020319	f
4.58446860366466	4.73651121407397	-5.59530943206403	f
7.59302790444859	7.68316762587808	-2.55509633884108	f
7.34737465658801	7.20901678157535	2.58983050982915	f
4.15605475978773	3.83158036588880	4.72441984843303	f
0.01209507780021	-0.12128457245743	5.46926240356653	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	11.67	0.00258	YES	YES
8		a	15.79	0.01716	YES	YES
9		a	18.87	0.00165	YES	YES
10		a	22.65	0.00526	YES	YES
11		a	25.76	0.03337	YES	YES
12		a	33.60	0.05541	YES	YES
13		a	71.11	0.80196	YES	YES
14		a	76.53	0.91711	YES	YES
15		a	85.46	0.61790	YES	YES

16	a	100.32	0.06437	YES	YES
17	a	107.19	0.00690	YES	YES
18	a	115.89	0.23355	YES	YES
19	a	121.54	0.04105	YES	YES
20	a	122.71	0.08955	YES	YES
21	a	126.72	0.44850	YES	YES
22	a	133.84	4.72974	YES	YES
23	a	138.52	5.26747	YES	YES
24	a	153.11	0.25726	YES	YES
25	a	156.60	0.28092	YES	YES
26	a	157.71	0.48428	YES	YES
27	a	178.69	1.72113	YES	YES
28	a	210.98	4.95609	YES	YES
29	a	217.92	1.47397	YES	YES
30	a	218.89	0.88593	YES	YES
31	a	235.77	39.73556	YES	YES
32	a	241.27	51.64064	YES	YES
33	a	261.55	0.38002	YES	YES
34	a	261.94	0.32595	YES	YES
35	a	265.27	0.04074	YES	YES
36	a	267.10	0.83057	YES	YES
37	a	268.75	7.70968	YES	YES
38	a	270.62	6.39973	YES	YES
39	a	302.43	0.64654	YES	YES
40	a	302.74	0.25119	YES	YES
41	a	305.34	0.77285	YES	YES
42	a	341.21	0.35826	YES	YES
43	a	344.45	0.37053	YES	YES
44	a	344.50	1.93146	YES	YES
45	a	350.54	11.59419	YES	YES
46	a	356.58	1.83831	YES	YES
47	a	363.02	12.87094	YES	YES
48	a	395.62	0.01425	YES	YES
49	a	397.83	0.17967	YES	YES
50	a	398.36	0.06678	YES	YES
51	a	431.72	0.00570	YES	YES
52	a	432.24	0.03603	YES	YES
53	a	432.99	0.01601	YES	YES
54	a	472.15	1.33044	YES	YES
55	a	474.12	5.79767	YES	YES
56	a	474.60	7.68293	YES	YES
57	a	477.06	0.91197	YES	YES
58	a	479.49	1.49282	YES	YES
59	a	492.22	1.28577	YES	YES
60	a	562.00	0.03685	YES	YES
61	a	562.41	0.02902	YES	YES
62	a	563.80	0.03181	YES	YES
63	a	598.75	6.94755	YES	YES
64	a	600.87	5.45014	YES	YES
65	a	611.58	11.65568	YES	YES
66	a	618.36	57.25407	YES	YES
67	a	629.86	0.02744	YES	YES
68	a	633.06	0.18595	YES	YES
69	a	634.98	0.08329	YES	YES
70	a	729.30	1.02967	YES	YES
71	a	733.02	0.32627	YES	YES
72	a	734.14	0.92411	YES	YES
73	a	765.72	2.46003	YES	YES
74	a	766.58	9.60962	YES	YES
75	a	770.10	11.37477	YES	YES
76	a	960.67	109.36089	YES	YES
77	a	964.73	147.12064	YES	YES

78	a	966.00	239.05215	YES	YES
79	a	1067.42	285.41143	YES	YES
80	a	1067.74	323.01016	YES	YES
81	a	1070.28	100.37082	YES	YES
82	a	1125.16	0.63414	YES	YES
83	a	1128.68	0.54368	YES	YES
84	a	1130.47	3.89705	YES	YES
85	a	1253.87	43.86335	YES	YES
86	a	1255.26	31.26554	YES	YES
87	a	1258.01	24.41719	YES	YES
88	a	1355.09	25.23170	YES	YES
89	a	1356.71	30.34438	YES	YES
90	a	1357.44	1.54138	YES	YES
91	a	1359.04	13.05543	YES	YES
92	a	1362.69	24.08672	YES	YES
93	a	1371.43	1.42088	YES	YES
94	a	1454.10	246.42624	YES	YES
95	a	1462.02	361.64882	YES	YES
96	a	1464.56	784.68782	YES	YES
97	a	1502.01	184.84829	YES	YES
98	a	1502.38	232.81362	YES	YES
99	a	1504.39	41.07388	YES	YES
100	a	1613.83	31.36133	YES	YES
101	a	1615.53	43.16904	YES	YES
102	a	1616.34	30.64574	YES	YES
103	a	1617.11	15.11750	YES	YES
104	a	1618.64	13.09302	YES	YES
105	a	1620.07	13.22402	YES	YES



Total energy = -4146.7882634320 H = -112839.9141516 eV

HOMO-LUMO Separation

HOMO: 142. 142 a -0.10771306 H = -2.93102 eV

LUMO: 143. 143 a +0.04961621 H = +1.35013 eV

Gap : +0.15732926 H = +4.28115 eV

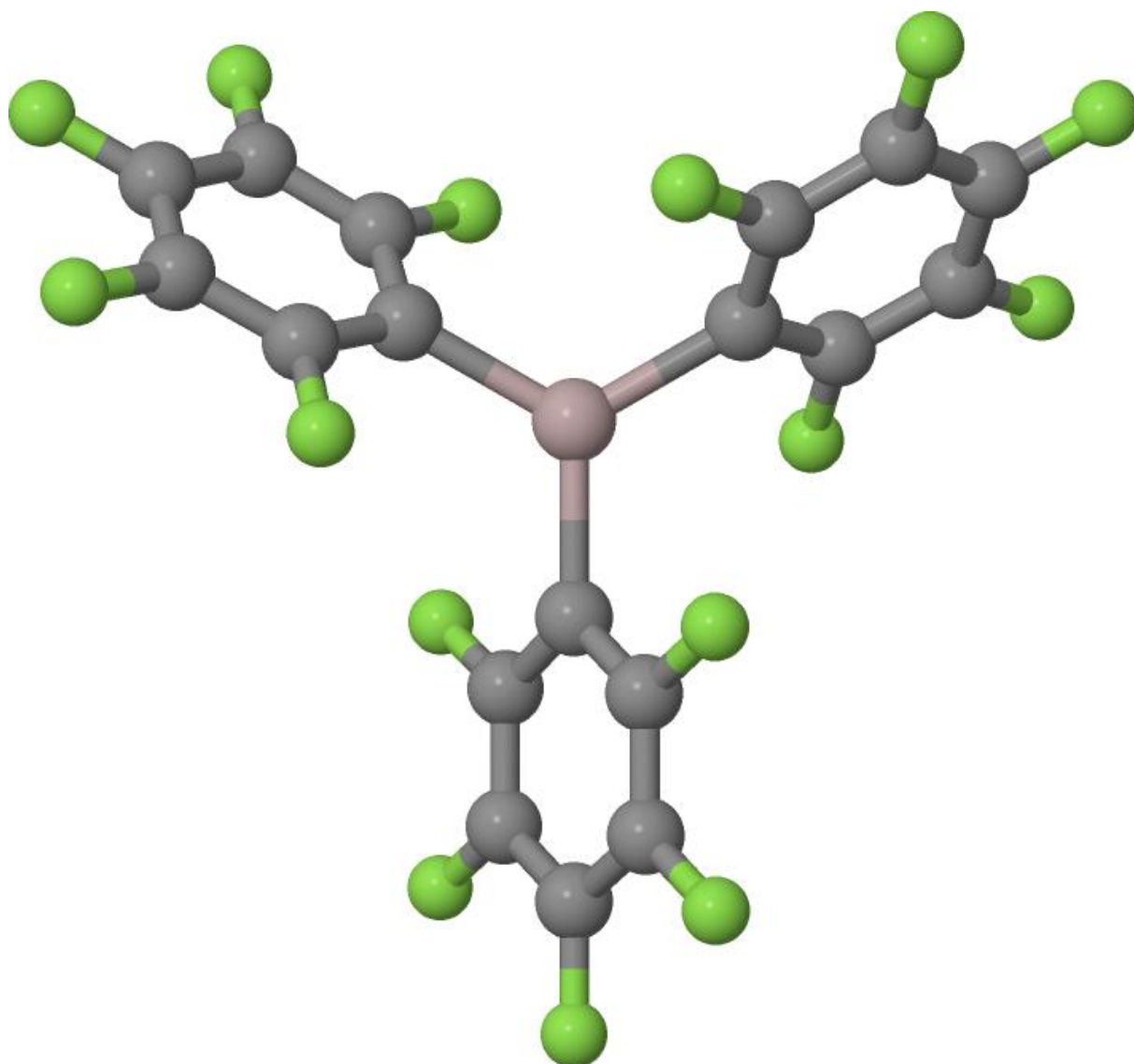
Number of MOs= 514, Electrons= 284.00, Symmetry: c1

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  4.15437404338545      4.00294455841961      1.97031860980120      c
  5.81341902971954      5.77045965753969      0.87494839757821      c
  5.89890841591749      5.99094274851793      -1.76739890450214      c
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 -3.09415306616200      -5.16857193617345      2.35224973678751      f
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$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#           #           cm** (-1)      km/mol      IR      RAMAN
  1           0.00      0.00000      -      -
  2           0.00      0.00000      -      -
  3           0.00      0.00000      -      -
  4           0.00      0.00000      -      -
  5           0.00      0.00000      -      -
  6           0.00      0.00000      -      -
  7           a      13.38      0.00203      YES      YES
  8           a      16.99      0.00202      YES      YES
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9	a	19.77	0.00058	YES	YES
10	a	23.01	0.00469	YES	YES
11	a	27.19	0.01005	YES	YES
12	a	33.20	0.00428	YES	YES
13	a	72.04	0.13745	YES	YES
14	a	81.98	0.00604	YES	YES
15	a	88.85	0.08646	YES	YES
16	a	100.28	0.06900	YES	YES
17	a	106.45	0.02246	YES	YES
18	a	113.63	0.25200	YES	YES
19	a	119.35	0.32576	YES	YES
20	a	121.29	0.02326	YES	YES
21	a	123.97	0.22332	YES	YES
22	a	127.12	0.07883	YES	YES
23	a	134.04	0.70020	YES	YES
24	a	137.86	0.51307	YES	YES
25	a	154.14	0.12652	YES	YES
26	a	156.64	0.03245	YES	YES
27	a	158.50	0.03346	YES	YES
28	a	183.45	5.76141	YES	YES
29	a	210.94	9.62557	YES	YES
30	a	216.80	7.77738	YES	YES
31	a	219.83	0.87930	YES	YES
32	a	222.11	17.96350	YES	YES
33	a	228.11	27.35878	YES	YES
34	a	260.85	0.13999	YES	YES
35	a	261.39	0.00762	YES	YES
36	a	265.59	0.06018	YES	YES
37	a	267.34	0.63206	YES	YES
38	a	268.07	2.64964	YES	YES
39	a	270.59	1.69318	YES	YES
40	a	303.38	0.10123	YES	YES
41	a	303.62	0.27546	YES	YES
42	a	306.01	0.17051	YES	YES
43	a	341.62	0.54531	YES	YES
44	a	344.03	0.65654	YES	YES
45	a	344.87	0.98610	YES	YES
46	a	347.63	4.25340	YES	YES
47	a	354.75	2.64345	YES	YES
48	a	362.54	6.89087	YES	YES
49	a	396.47	0.01911	YES	YES
50	a	398.33	0.08953	YES	YES
51	a	398.80	0.04289	YES	YES
52	a	431.97	0.01280	YES	YES
53	a	432.48	0.02651	YES	YES
54	a	433.23	0.00572	YES	YES
55	a	470.39	0.85875	YES	YES
56	a	471.59	5.10758	YES	YES
57	a	472.14	5.81353	YES	YES
58	a	485.76	0.77041	YES	YES
59	a	490.60	0.56513	YES	YES
60	a	496.47	0.75267	YES	YES
61	a	524.94	26.47225	YES	YES
62	a	561.06	0.01726	YES	YES
63	a	561.95	0.05764	YES	YES
64	a	563.08	0.01503	YES	YES
65	a	597.64	2.68253	YES	YES
66	a	600.40	8.21063	YES	YES
67	a	611.31	9.70363	YES	YES
68	a	630.35	0.01457	YES	YES
69	a	632.10	0.05178	YES	YES
70	a	633.45	0.22041	YES	YES

71	a	704.91	40.62784	YES	YES
72	a	711.81	71.53603	YES	YES
73	a	730.30	4.41425	YES	YES
74	a	734.52	7.03030	YES	YES
75	a	736.13	15.99867	YES	YES
76	a	756.62	9.78600	YES	YES
77	a	757.70	13.56364	YES	YES
78	a	760.38	13.93380	YES	YES
79	a	956.73	117.21263	YES	YES
80	a	961.02	141.36557	YES	YES
81	a	962.19	233.68375	YES	YES
82	a	1061.13	314.56981	YES	YES
83	a	1062.00	272.66643	YES	YES
84	a	1064.90	117.43292	YES	YES
85	a	1118.18	0.26680	YES	YES
86	a	1121.72	1.40736	YES	YES
87	a	1123.87	4.80547	YES	YES
88	a	1172.60	8.18978	YES	YES
89	a	1248.84	34.93563	YES	YES
90	a	1250.68	29.19778	YES	YES
91	a	1253.91	21.71315	YES	YES
92	a	1347.57	37.00596	YES	YES
93	a	1349.23	44.45218	YES	YES
94	a	1356.23	2.67059	YES	YES
95	a	1358.77	1.29388	YES	YES
96	a	1360.54	2.39486	YES	YES
97	a	1362.33	5.12201	YES	YES
98	a	1403.23	10.39119	YES	YES
99	a	1408.88	6.17585	YES	YES
100	a	1446.95	259.38906	YES	YES
101	a	1455.03	274.16125	YES	YES
102	a	1457.42	767.98159	YES	YES
103	a	1499.26	209.81804	YES	YES
104	a	1500.18	219.94734	YES	YES
105	a	1502.44	61.06415	YES	YES
106	a	1612.99	19.89571	YES	YES
107	a	1613.26	38.02859	YES	YES
108	a	1613.99	32.98798	YES	YES
109	a	1615.76	9.43503	YES	YES
110	a	1616.40	11.03151	YES	YES
111	a	1616.75	16.02998	YES	YES
112	a	2936.92	24.56960	YES	YES
113	a	3025.53	20.94895	YES	YES
114	a	3046.20	16.38532	YES	YES



Total energy = -2424.3162602240 H = -65969.0394835 eV

HOMO-LUMO Separation

HOMO: 86. 42 e -0.24028010 H = -6.53836 eV

LUMO: 87. 21 a2 -0.11290226 H = -3.07223 eV

Gap : +0.12737785 H = +3.46613 eV

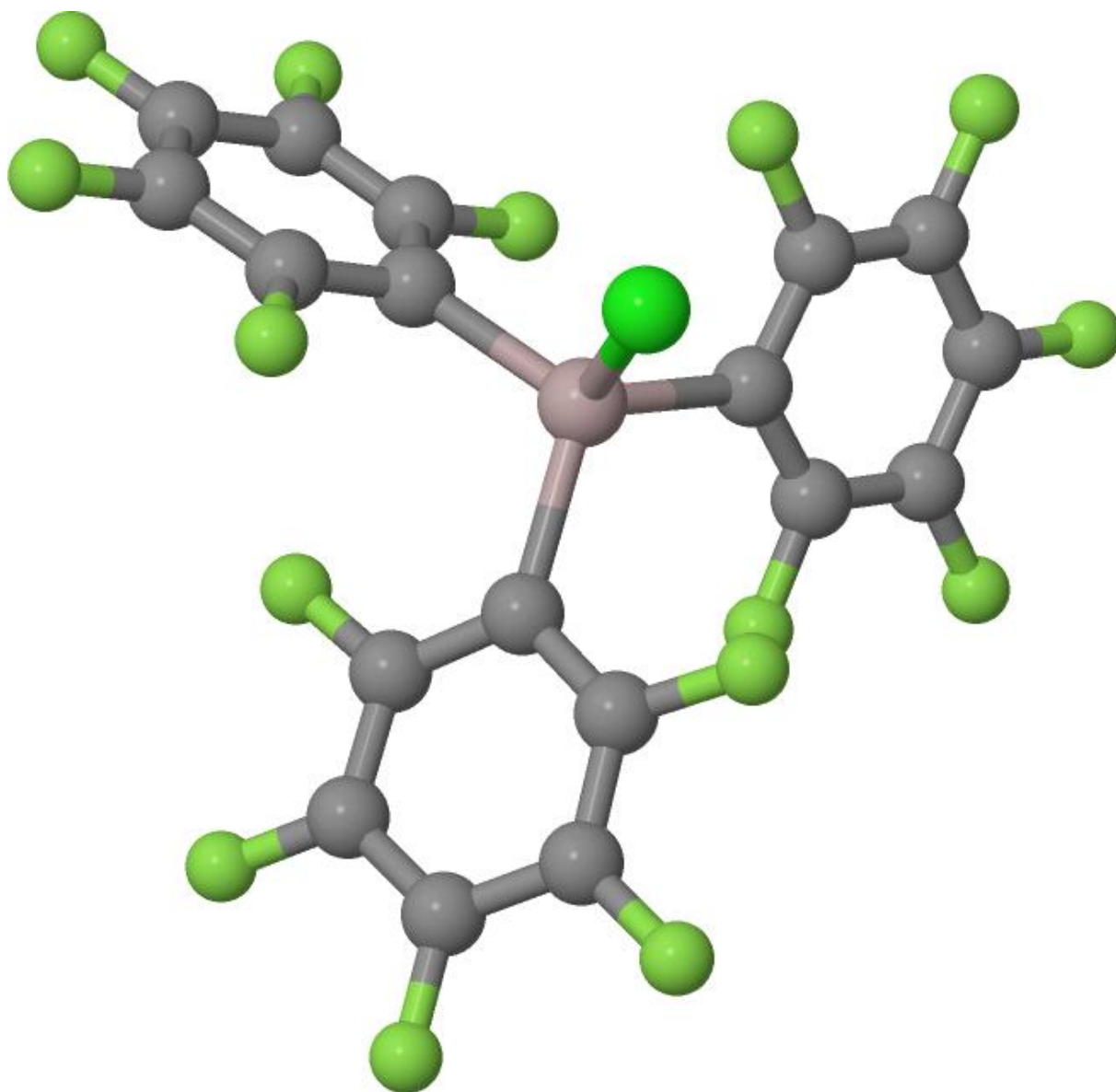
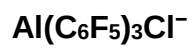
Number of MOs= 321, Electrons= 256.00, Symmetry: d3

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-9.02979166898323    -2.59850229520573    3.66135059129254    f
-3.85295330615184    -2.58629442782586    3.66533519891477    f
 1.85752380203565    -3.21732560139426    0.0000000000000000  c
 1.85752380203565    3.21732560139426    0.0000000000000000  c
 1.41358962001542    -5.07287951058056    -1.83798572117158    c
 3.68644771649262    3.76064427674962    -1.83798572117158    c
 2.71416554202941    -7.38551137691395    -1.88200570628317    c
 5.03895770133177    6.04329199793080    -1.88200570628317    c
 4.53658594160079    -7.85759734375526    0.0000000000000000  c
 4.53658594160079    7.85759734375526    0.0000000000000000  c
 5.03895770133177    -6.04329199793080    1.88200570628317    c
 2.71416554202941    7.38551137691395    1.88200570628317    c
 3.68644771649262    -3.76064427674962    1.83798572117158    c
 1.41358962001542    5.07287951058056    1.83798572117158    c
-0.31332002308742    -4.62990265663566    -3.66533519891477    f
 4.16627332923926    2.04360822880980    -3.66533519891477    f
 2.26452683505128    -9.11928012382342    -3.66135059129254    f
 6.76526483393195    6.52077782861769    -3.66135059129254    f
 5.79660756281364    -10.04001881033123   0.0000000000000000  f
 5.79660756281364    10.04001881033123    0.0000000000000000  f
 6.76526483393195    -6.52077782861769    3.66135059129254    f
 2.26452683505128    9.11928012382342    3.66135059129254    f
 4.16627332923926    -2.04360822880980    3.66533519891477    f
-0.31332002308742    4.62990265663566    3.66533519891477    f
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#           #           cm** (-1)         km/mol           IR      RAMAN
  1           0.00          0.00000          -      -
  2           0.00          0.00000          -      -
  3           0.00          0.00000          -      -
  4           0.00          0.00000          -      -
  5           0.00          0.00000          -      -
  6           0.00          0.00000          -      -
  7           e          11.53          0.05993        YES      YES
  8           e          11.53          0.05993        YES      YES
  9           e          15.07          0.08260        YES      YES
 10           e          15.07          0.08260        YES      YES
 11           e          16.30          0.00000        YES      YES
 12           a2         21.18          0.12865        YES      NO
 13           a2         60.49          0.01072        YES      NO
 14           e          63.55          0.01832        YES      YES
 15           e          63.55          0.01832        YES      YES
```

16	e	97.60	0.87372	YES	YES
17	e	97.60	0.87372	YES	YES
18	e	122.70	0.00000	YES	YES
19	e	122.74	0.00938	YES	YES
20	e	122.74	0.00938	YES	YES
21	a1	125.24	0.00000	NO	YES
22	a2	144.75	0.28705	YES	NO
23	e	150.62	0.08736	YES	YES
24	e	150.62	0.08736	YES	YES
25	a2	202.99	4.14280	YES	NO
26	e	209.82	0.58158	YES	YES
27	e	209.82	0.58158	YES	YES
28	a2	230.19	9.13545	YES	NO
29	e	257.06	2.60840	YES	YES
30	e	257.06	2.60840	YES	YES
31	e	259.55	0.01663	YES	YES
32	e	259.55	0.01663	YES	YES
33	e	259.57	0.01202	YES	YES
34	a1	261.89	0.00000	NO	YES
35	e	297.93	2.37942	YES	YES
36	e	297.93	2.37942	YES	YES
37	a2	301.63	0.17043	YES	NO
38	e	312.06	19.80534	YES	YES
39	e	312.06	19.80534	YES	YES
40	a1	337.73	0.00000	NO	YES
41	a2	352.86	5.55930	YES	NO
42	e	352.98	1.03120	YES	YES
43	e	352.98	1.03120	YES	YES
44	e	403.07	3.97521	YES	YES
45	e	403.07	3.97521	YES	YES
46	a1	403.35	0.00000	NO	YES
47	e	404.34	64.18119	YES	YES
48	e	404.34	64.18119	YES	YES
49	e	430.50	0.49750	YES	YES
50	e	430.50	0.49750	YES	YES
51	a2	430.88	0.15761	YES	NO
52	a1	478.61	0.00000	NO	YES
53	a2	493.49	0.82310	YES	NO
54	e	493.82	0.00636	YES	YES
55	e	493.82	0.00636	YES	YES
56	e	506.29	47.40866	YES	YES
57	e	506.29	47.40866	YES	YES
58	a1	562.90	0.00000	NO	YES
59	e	563.63	2.16465	YES	YES
60	e	563.63	2.16465	YES	YES
61	a2	606.50	2.59561	YES	NO
62	e	613.40	19.39042	YES	YES
63	e	613.40	19.39042	YES	YES
64	e	631.54	0.33210	YES	YES
65	e	631.54	0.33210	YES	YES
66	a1	632.13	0.00000	NO	YES
67	e	736.37	6.44964	YES	YES
68	e	736.37	6.44964	YES	YES
69	a2	738.73	0.42913	YES	NO
70	a1	791.01	0.00000	NO	YES
71	e	827.15	1.20527	YES	YES
72	e	827.15	1.20527	YES	YES
73	e	968.89	64.60181	YES	YES
74	e	968.89	64.60181	YES	YES
75	a2	970.58	294.52599	YES	NO
76	a1	1085.70	0.00000	NO	YES
77	e	1088.03	371.98781	YES	YES

78	e	1088.03	371.98781	YES	YES
79	e	1148.69	0.01998	YES	YES
80	e	1148.69	0.01998	YES	YES
81	a2	1150.29	10.03530	YES	NO
82	e	1285.53	65.08213	YES	YES
83	e	1285.53	65.08213	YES	YES
84	a1	1285.70	0.00000	NO	YES
85	e	1355.74	3.47886	YES	YES
86	e	1355.74	3.47886	YES	YES
87	a2	1356.16	0.42713	YES	NO
88	e	1367.49	104.60041	YES	YES
89	e	1367.49	104.60041	YES	YES
90	a1	1380.07	0.00000	NO	YES
91	e	1473.39	305.27448	YES	YES
92	e	1473.39	305.27449	YES	YES
93	a2	1479.67	835.71410	YES	NO
94	e	1512.02	308.83789	YES	YES
95	e	1512.02	308.83788	YES	YES
96	a1	1514.43	0.00000	NO	YES
97	e	1613.80	1.03516	YES	YES
98	e	1613.80	1.03516	YES	YES
99	a2	1614.80	16.21595	YES	NO
100	e	1624.21	104.38069	YES	YES
101	e	1624.21	104.38069	YES	YES
102	a1	1624.90	0.00000	NO	YES



Total energy = -2884.6075510910 H = -78494.2099158 eV

HOMO-LUMO Separation

HOMO: 137. 137 a -0.11785533 H = -3.20701 eV

LUMO: 138. 138 a +0.03940698 H = +1.07232 eV

Gap : +0.15726231 H = +4.27933 eV

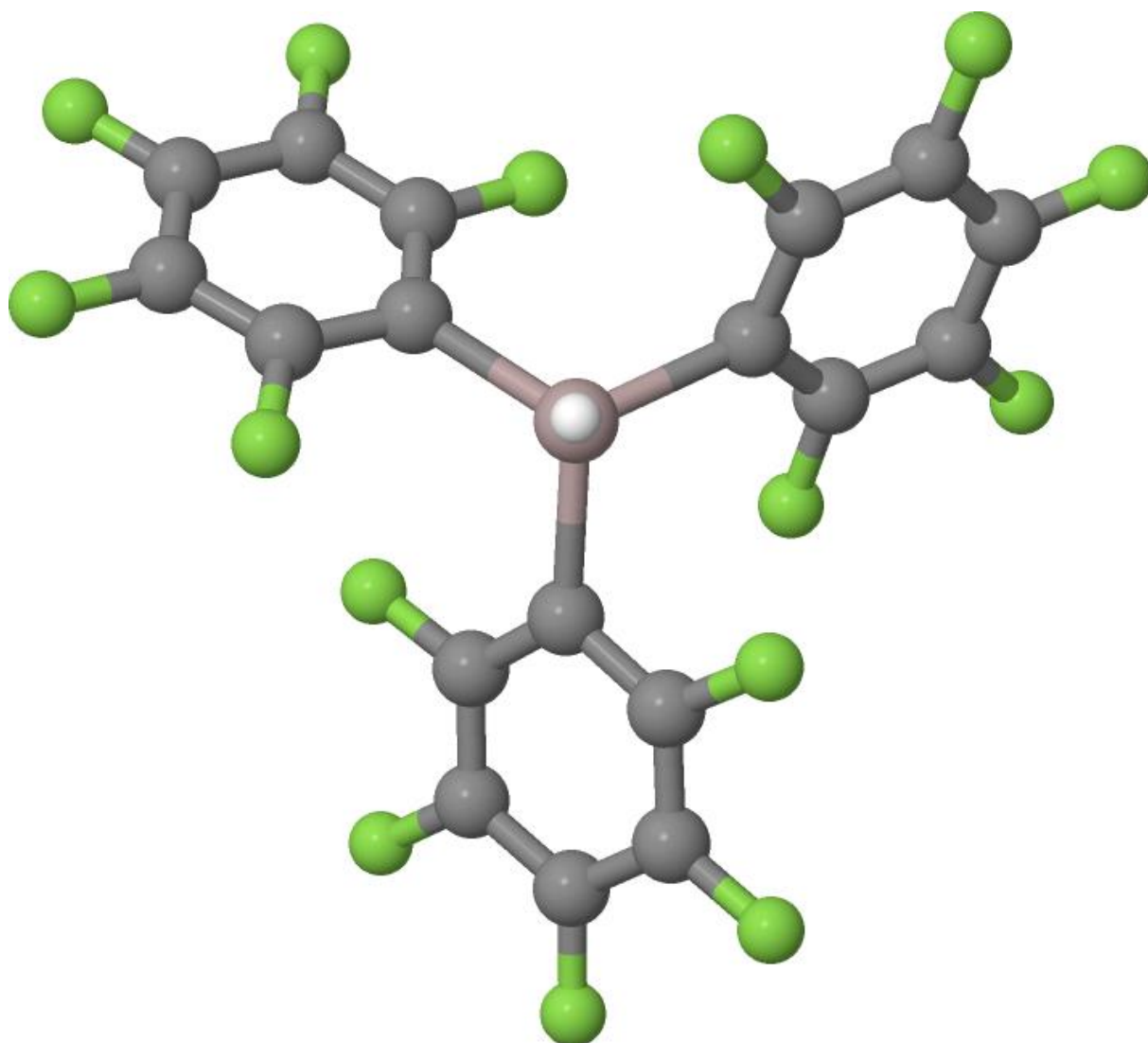
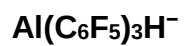
Number of MOs= 498, Electrons= 274.00, Symmetry: c1

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  5.47208268603407   -1.40912677156717    1.27052488871535     c
  7.68543173111320   -2.71967661366002    0.60995208443264     c
  7.49645906700981   -4.80745036841990   -1.01893002606239     c
  5.12480993642859   -5.53721552311244   -1.95632997345578     c
  2.97111710028733   -4.15529014311248   -1.22773266769417     c
  5.76935462892993    0.60379413552263    2.81561431249420     f
  9.96775141607492   -2.01699370366789    1.49157314047455     f
  9.58443349960839   -6.09412132820212   -1.68584288540949     f
  4.95495794307042   -7.52704195898771   -3.53668383513918     f
  0.75073408217480   -4.94887733319807   -2.22322477082638     f
  0.25105933735072    3.60967722145262    0.39550476833864     c
 -3.28539050145867   -1.63191173404101    0.37259492788419     c
 -1.55277616731815    5.36532190498315    1.22147184721234     c
 -4.02520334421555   -4.00505759436984    1.29201500820653     c
 -1.49584713299052    7.94508274028795    0.59553845382739     c
 -6.31848815176055   -5.18273313422721    0.65108083334997     c
  0.46138143236548    8.84198813282983   -0.95830709708049     c
 -7.97166672454816   -3.94466736115719   -1.01669447298679     c
  2.30094770523452    7.15611447705519   -1.85857075804711     c
 -7.30536772795978   -1.57932131338022   -2.01520694774186     c
  2.14791616438286    4.59158470578426   -1.16713493761214     c
 -4.98335058859796   -0.49072243421814   -1.30675610986116     c
 -3.49727481368093    4.60037963595952    2.69189121609983     f
 -2.49072413776074   -5.30161004461247    2.86905114430218     f
 -3.26466926372825    9.56265821962025    1.45073249883546     f
 -6.95725845641075   -7.46230060274746    1.58508942483225     f
  0.56081605708871   11.30195806436712   -1.59326299901037     f
 -10.17621524864799   -5.03034839395286   -1.66844719908990     f
  4.16679032238303    8.01392989707490   -3.36386425531818     f
 -8.88457874331922   -0.40529715409915   -3.63206396973754     f
  3.96138403524769    3.07158645487151   -2.14158746556231     f
 -4.44473322571733    1.76862447060626   -2.38274376639716     f
 -0.01661197895327   -0.03041928242219    5.72292892941075     c1
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#           #           cm** (-1)        km/mol           IR      RAMAN
  1           0.00        0.00000          -        -
  2           0.00        0.00000          -        -
  3           0.00        0.00000          -        -
  4           0.00        0.00000          -        -
  5           0.00        0.00000          -        -
  6           0.00        0.00000          -        -
  7           a          7.61          0.00316      YES      YES
  8           a          10.19         0.00440      YES      YES
  9           a          23.85         0.01617      YES      YES
 10           a          24.03         0.04005      YES      YES
 11           a          25.70         0.03421      YES      YES
 12           a          33.52         0.02361      YES      YES
 13           a          68.46         1.13367      YES      YES
 14           a          70.25         1.20267      YES      YES
 15           a          81.98         0.03870      YES      YES
```

16	a	98.71	0.21982	YES	YES
17	a	99.27	0.14186	YES	YES
18	a	108.94	0.15175	YES	YES
19	a	112.80	1.66834	YES	YES
20	a	113.52	1.56854	YES	YES
21	a	121.53	0.01976	YES	YES
22	a	121.67	0.02624	YES	YES
23	a	124.85	0.00851	YES	YES
24	a	151.24	0.01522	YES	YES
25	a	154.90	0.01985	YES	YES
26	a	155.86	0.01727	YES	YES
27	a	186.28	0.72761	YES	YES
28	a	212.98	0.55381	YES	YES
29	a	215.77	0.41001	YES	YES
30	a	221.07	0.43820	YES	YES
31	a	257.90	0.12709	YES	YES
32	a	261.71	0.22044	YES	YES
33	a	261.84	0.18256	YES	YES
34	a	262.66	0.34719	YES	YES
35	a	264.33	0.46759	YES	YES
36	a	266.48	0.18268	YES	YES
37	a	300.51	3.51952	YES	YES
38	a	301.63	4.45851	YES	YES
39	a	302.87	1.62932	YES	YES
40	a	318.34	26.47984	YES	YES
41	a	318.86	28.08520	YES	YES
42	a	338.74	0.57530	YES	YES
43	a	350.22	1.75138	YES	YES
44	a	352.06	1.44332	YES	YES
45	a	360.04	0.23880	YES	YES
46	a	385.66	58.01808	YES	YES
47	a	386.73	57.63032	YES	YES
48	a	393.87	0.48802	YES	YES
49	a	396.04	0.71226	YES	YES
50	a	396.22	0.21481	YES	YES
51	a	431.76	0.82400	YES	YES
52	a	433.01	0.42916	YES	YES
53	a	433.46	0.42184	YES	YES
54	a	461.63	21.69388	YES	YES
55	a	470.57	1.68744	YES	YES
56	a	472.34	1.18977	YES	YES
57	a	477.96	0.39944	YES	YES
58	a	485.25	31.14616	YES	YES
59	a	485.69	32.41144	YES	YES
60	a	491.31	68.10706	YES	YES
61	a	561.76	0.07571	YES	YES
62	a	562.08	0.30299	YES	YES
63	a	562.47	0.24787	YES	YES
64	a	599.39	10.58811	YES	YES
65	a	599.82	9.19341	YES	YES
66	a	603.40	22.02236	YES	YES
67	a	629.76	0.23785	YES	YES
68	a	631.13	0.36370	YES	YES
69	a	632.55	0.35031	YES	YES
70	a	727.33	1.16965	YES	YES
71	a	731.25	3.12507	YES	YES
72	a	732.50	3.30580	YES	YES
73	a	766.78	0.03388	YES	YES
74	a	778.96	2.01055	YES	YES
75	a	779.67	1.78234	YES	YES
76	a	958.34	156.92907	YES	YES
77	a	962.19	163.45983	YES	YES

78	a	963.27	162.14675	YES	YES
79	a	1067.62	345.09173	YES	YES
80	a	1068.65	364.68770	YES	YES
81	a	1069.98	75.95340	YES	YES
82	a	1122.76	1.21642	YES	YES
83	a	1126.03	0.82144	YES	YES
84	a	1127.01	0.74820	YES	YES
85	a	1252.49	54.79029	YES	YES
86	a	1253.60	49.29436	YES	YES
87	a	1255.31	19.43584	YES	YES
88	a	1348.37	19.79767	YES	YES
89	a	1349.26	17.47565	YES	YES
90	a	1352.04	3.22411	YES	YES
91	a	1357.99	16.65302	YES	YES
92	a	1359.04	14.87382	YES	YES
93	a	1364.13	6.92351	YES	YES
94	a	1446.89	433.18538	YES	YES
95	a	1454.43	522.54489	YES	YES
96	a	1455.86	536.55200	YES	YES
97	a	1501.78	199.34452	YES	YES
98	a	1502.98	210.32003	YES	YES
99	a	1504.80	31.06796	YES	YES
100	a	1612.13	2.02469	YES	YES
101	a	1613.33	13.56773	YES	YES
102	a	1613.90	11.70874	YES	YES
103	a	1614.95	54.49520	YES	YES
104	a	1616.47	54.92974	YES	YES
105	a	1617.49	41.45773	YES	YES



Total energy = -2425.0125199080 H = -65987.9856842 eV

HOMO-LUMO Separation

HOMO: 129. 129 a -0.11193708 H = -3.04596 eV

LUMO: 130. 130 a +0.04855310 H = +1.32120 eV

Gap : +0.16049018 H = +4.36716 eV

Number of MOs= 482, Electrons= 258.00, Symmetry: c1

\$coord

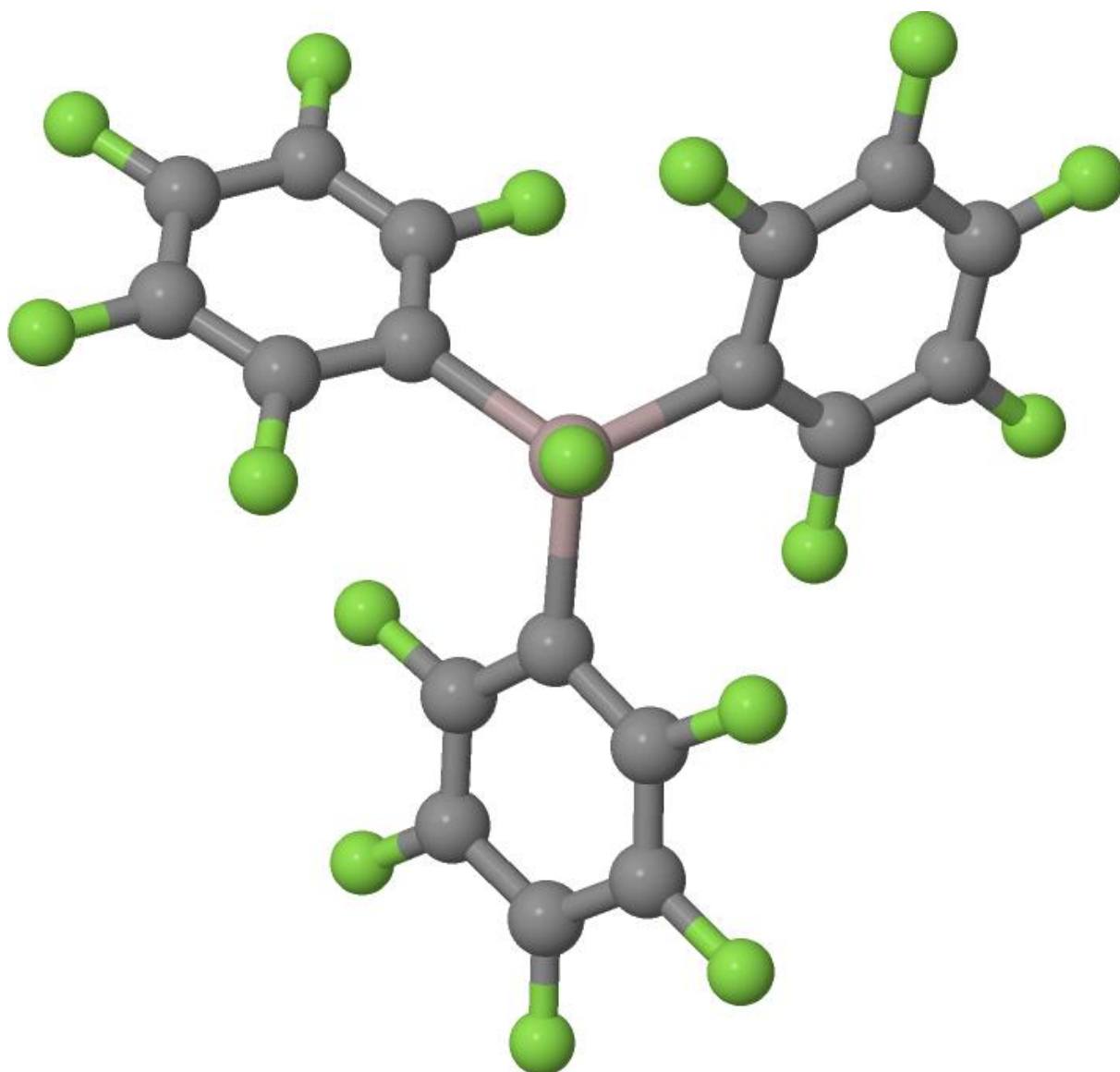
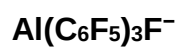
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5.75036802263584	-0.06546525136494	1.79911828802961	c
8.23762147526097	-0.71167481871295	1.12968179070589	c
8.61409308618008	-2.59580662128588	-0.70310965123414	c
6.52057060219477	-3.78183185402271	-1.82175794681844	c
4.07366950055383	-3.05676516228703	-1.07094604372225	c
5.48969932942894	1.77156631153889	3.56317624081096	f
10.25068737706487	0.42587615481701	2.19799892280854	f
10.97295781179893	-3.25614428698093	-1.38806132945904	f
6.89145651353250	-5.57948299723271	-3.58766838464811	f
2.14315185039959	-4.26241315256436	-2.24083394974009	f
-0.66277507838084	3.49375482754543	0.85853607923206	c
-2.65350645362685	-2.46104891389858	0.71035405666445	c
-2.91357602706890	4.60989490246352	1.69010132873393	c
-2.97869803316943	-4.85167655168248	1.80193125027927	c
-3.68389521762132	7.06468593025155	1.03348580322755	c
-4.95758704582032	-6.50879256070083	1.17055531525905	c
-2.12027755615624	8.50319615298568	-0.55887224892279	c
-6.70791684073174	-5.76127294424818	-0.68042137640941	c
0.15253673436588	7.46881941279066	-1.45504771635583	c
-6.44500078051076	-3.40009925325041	-1.86072625685288	c
0.82252170831457	4.99705347965435	-0.73166275533669	c
-4.42456776212199	-1.82406657037616	-1.15021814372916	c
-4.50221159777005	3.28761847220578	3.20630180553083	f
-1.33870193883811	-5.67871140258282	3.58769279797150	f
-5.87173486133032	8.05268067567361	1.88320881924096	f
-5.20879945582537	-8.78376386928791	2.28907816147452	f
-2.80106639967743	10.86127791073603	-1.22741663316912	f
-8.62658716907642	-7.30320312876406	-1.32157074924834	f
1.64013847814649	8.85729302818474	-2.98820754299099	f
-8.11407040035430	-2.69736717526302	-3.65288894667873	f
3.02400159148773	4.11207172585395	-1.69136941746446	f
-4.26775051795628	0.40859750116314	-2.39495037016620	f
0.11105627202312	-0.18541588844480	5.11250029624290	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		3.89	0.00640	YES	YES
8	a		13.74	0.00373	YES	YES
9	a		20.15	0.01628	YES	YES
10	a		21.85	0.01679	YES	YES
11	a		25.00	0.01089	YES	YES
12	a		31.36	0.04289	YES	YES
13	a		78.12	0.22649	YES	YES
14	a		79.36	0.16631	YES	YES
15	a		84.39	0.28191	YES	YES
16	a		101.66	0.06526	YES	YES
17	a		102.55	0.09575	YES	YES

18	a	108.42	0.13505	YES	YES
19	a	120.88	0.00695	YES	YES
20	a	122.17	0.00162	YES	YES
21	a	123.46	0.00016	YES	YES
22	a	152.42	0.03255	YES	YES
23	a	154.32	0.08576	YES	YES
24	a	155.37	0.07316	YES	YES
25	a	209.14	1.69356	YES	YES
26	a	212.35	0.84507	YES	YES
27	a	216.50	1.33914	YES	YES
28	a	259.17	0.61073	YES	YES
29	a	261.13	0.25200	YES	YES
30	a	262.19	0.06510	YES	YES
31	a	263.45	0.37245	YES	YES
32	a	265.74	0.50271	YES	YES
33	a	265.88	0.27595	YES	YES
34	a	270.67	1.48532	YES	YES
35	a	301.94	6.28037	YES	YES
36	a	303.25	3.48041	YES	YES
37	a	303.62	1.99141	YES	YES
38	a	306.08	12.99856	YES	YES
39	a	308.46	15.58350	YES	YES
40	a	340.09	0.28691	YES	YES
41	a	344.71	0.41831	YES	YES
42	a	346.21	0.78801	YES	YES
43	a	371.20	18.00446	YES	YES
44	a	372.14	17.91454	YES	YES
45	a	373.28	7.63966	YES	YES
46	a	395.59	0.07516	YES	YES
47	a	398.64	0.07948	YES	YES
48	a	401.51	0.04794	YES	YES
49	a	432.46	0.00275	YES	YES
50	a	432.65	0.00014	YES	YES
51	a	433.02	0.00512	YES	YES
52	a	471.65	0.49850	YES	YES
53	a	473.48	1.06311	YES	YES
54	a	478.37	1.35668	YES	YES
55	a	479.55	0.70277	YES	YES
56	a	481.01	10.53526	YES	YES
57	a	482.28	11.17271	YES	YES
58	a	561.29	0.67988	YES	YES
59	a	561.81	2.35238	YES	YES
60	a	561.90	0.65508	YES	YES
61	a	576.37	71.42195	YES	YES
62	a	580.26	67.12006	YES	YES
63	a	601.23	9.29307	YES	YES
64	a	630.37	5.77994	YES	YES
65	a	631.71	2.13871	YES	YES
66	a	633.53	5.13847	YES	YES
67	a	645.59	203.72519	YES	YES
68	a	646.21	182.17369	YES	YES
69	a	728.87	0.71690	YES	YES
70	a	734.39	15.66651	YES	YES
71	a	735.84	19.07832	YES	YES
72	a	762.66	0.63017	YES	YES
73	a	772.47	0.77056	YES	YES
74	a	774.63	0.68986	YES	YES
75	a	957.55	198.77719	YES	YES
76	a	960.32	133.51292	YES	YES
77	a	961.64	164.36375	YES	YES
78	a	1064.03	329.56813	YES	YES
79	a	1064.82	309.68106	YES	YES

80	a	1066.67	104.90653	YES	YES
81	a	1120.70	2.84656	YES	YES
82	a	1122.94	0.67192	YES	YES
83	a	1125.24	0.59591	YES	YES
84	a	1250.38	41.23873	YES	YES
85	a	1252.49	52.29238	YES	YES
86	a	1253.55	11.26603	YES	YES
87	a	1348.53	35.10416	YES	YES
88	a	1349.27	30.13270	YES	YES
89	a	1354.31	0.68589	YES	YES
90	a	1356.51	2.74780	YES	YES
91	a	1360.07	6.01193	YES	YES
92	a	1360.87	7.15074	YES	YES
93	a	1448.14	517.33491	YES	YES
94	a	1451.74	414.92112	YES	YES
95	a	1454.96	516.63248	YES	YES
96	a	1500.49	206.14712	YES	YES
97	a	1501.11	229.91502	YES	YES
98	a	1503.20	22.43870	YES	YES
99	a	1612.07	5.01873	YES	YES
100	a	1612.64	19.35068	YES	YES
101	a	1613.03	15.59744	YES	YES
102	a	1615.04	43.08258	YES	YES
103	a	1616.41	42.36950	YES	YES
104	a	1616.80	21.97884	YES	YES
105	a	1811.23	224.90495	YES	YES



Total energy = -2524.2728076890 H = -68688.9970791 eV

HOMO-LUMO Separation

HOMO: 133. 133 a -0.11657093 H = -3.17206 eV

LUMO: 134. 134 a +0.04107939 H = +1.11783 eV

Gap : +0.15765032 H = +4.28989 eV

Number of MOs= 494, Electrons= 266.00, Symmetry: c1

\$coord

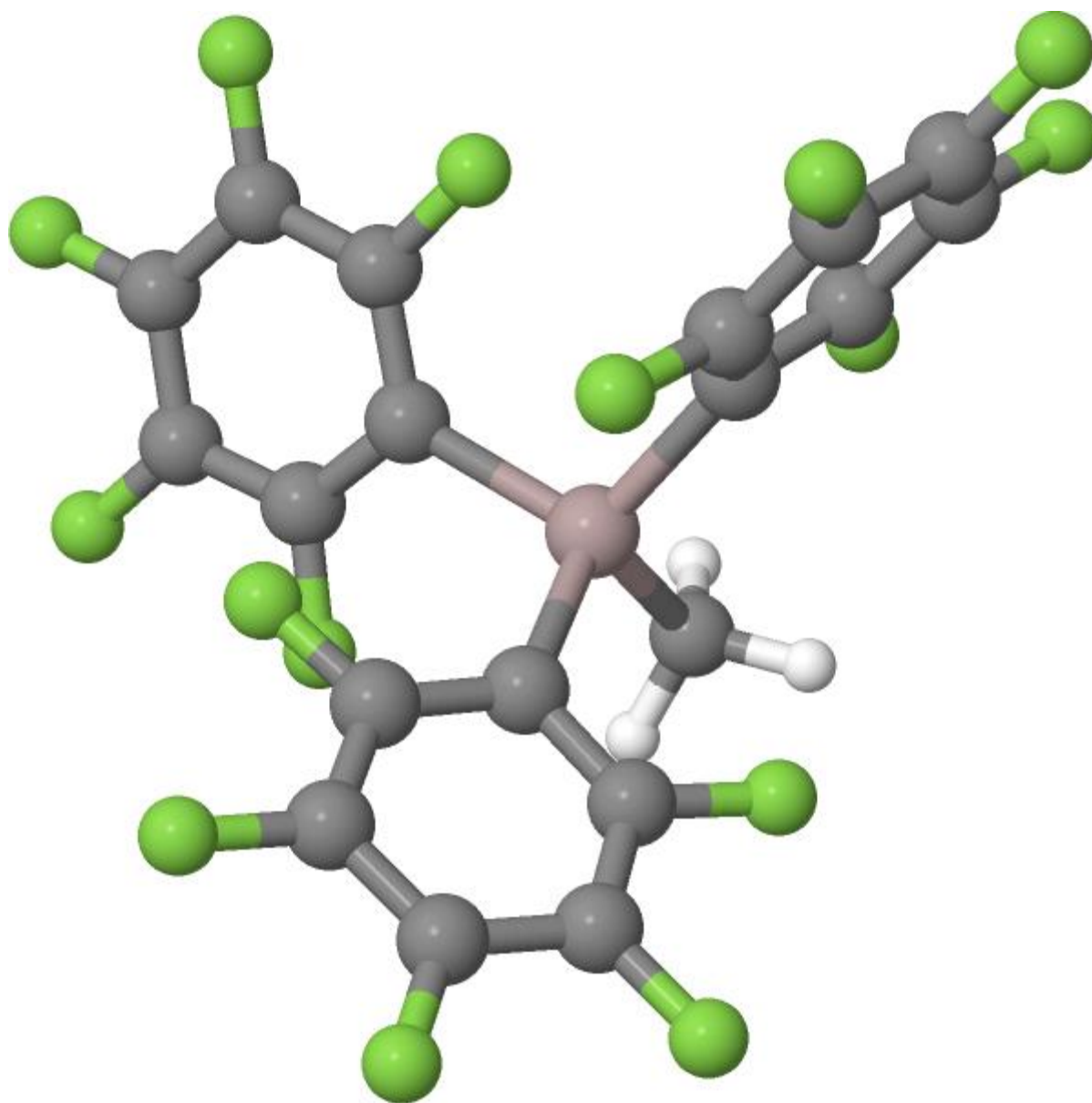
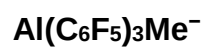
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5.37457373555841	-1.36381019735168	1.49854514993451	c
7.61305964412821	-2.64449309102313	0.86581247033751	c
7.45692429409923	-4.77521358946180	-0.71028703496481	c
5.09813739056775	-5.56719049756760	-1.62943129860273	c
2.92106503608604	-4.20425736712740	-0.93522358778174	c
5.62235524766760	0.68339755171908	3.01443469210211	f
9.88353899965234	-1.87952340135504	1.72661343786442	f
9.56206499921030	-6.05201671613515	-1.34512635983329	f
4.96801852658624	-7.60539504708748	-3.15153663349181	f
0.71437082594932	-5.05636849962892	-1.91223157050253	f
0.27269181722506	3.63064142656449	0.62592132003520	c
-3.34538140080357	-1.58610184787276	0.57497149656332	c
-1.41791219689935	5.42782808101941	1.58560048286785	c
-4.00459873397753	-3.98650807126876	1.47915475033700	c
-1.31739844328394	8.01368996404768	0.98746801797914	c
-6.24300811572824	-5.25083515636616	0.81405549886241	c
0.56921583672656	8.86659367388122	-0.67363810184857	c
-7.93161211054222	-4.05927142098799	-0.85254420496369	c
2.29832510575923	7.13868818670028	-1.70394203975266	c
-7.35500494024282	-1.65827766723423	-1.82264267889626	c
2.10494969960807	4.57101351253718	-1.03400024065433	c
-5.08440080356297	-0.48282475696584	-1.08522676983026	c
-3.28647501880353	4.70081908135046	3.17471082423085	f
-2.43195594191061	-5.22308762385097	3.07389280696130	f
-2.98061553791541	9.67911931371636	1.95760019952060	f
-6.80053293629915	-7.56122480876431	1.72849104506771	f
0.70973951750630	11.33097868375833	-1.28395279986208	f
-10.09010856192059	-5.22319417402082	-1.52580234625708	f
4.09275640504122	7.96726985234560	-3.31059808898013	f
-8.97682360897430	-0.53345905797021	-3.43286421368536	f
3.81335165373123	3.00376398132467	-2.12095469450453	f
-4.63971419064728	1.82121183338367	-2.10868959804993	f
-0.08886208041200	-0.02297697620832	5.06318385657482	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	11.82	0.00409	YES	YES
8		a	13.65	0.00466	YES	YES
9		a	22.27	0.03078	YES	YES
10		a	24.18	0.03110	YES	YES
11		a	26.52	0.03501	YES	YES
12		a	33.45	0.04147	YES	YES
13		a	72.88	0.95448	YES	YES

14	a	76.53	0.98490	YES	YES
15	a	79.21	0.07853	YES	YES
16	a	100.29	0.04828	YES	YES
17	a	101.36	0.05469	YES	YES
18	a	108.94	0.09325	YES	YES
19	a	120.74	0.00167	YES	YES
20	a	122.27	0.02962	YES	YES
21	a	124.44	0.00732	YES	YES
22	a	141.06	5.12738	YES	YES
23	a	141.09	5.11932	YES	YES
24	a	152.01	0.02306	YES	YES
25	a	157.34	1.22192	YES	YES
26	a	158.00	1.04367	YES	YES
27	a	200.31	1.54175	YES	YES
28	a	215.25	0.47374	YES	YES
29	a	217.73	0.30254	YES	YES
30	a	234.84	0.00872	YES	YES
31	a	258.39	0.12907	YES	YES
32	a	261.58	0.14416	YES	YES
33	a	262.01	0.41140	YES	YES
34	a	262.44	0.36290	YES	YES
35	a	264.62	0.63692	YES	YES
36	a	266.24	0.23876	YES	YES
37	a	299.96	3.95783	YES	YES
38	a	301.03	5.17075	YES	YES
39	a	302.02	0.96873	YES	YES
40	a	319.99	29.86409	YES	YES
41	a	320.85	31.15138	YES	YES
42	a	339.27	0.21273	YES	YES
43	a	349.23	1.25318	YES	YES
44	a	351.70	1.41275	YES	YES
45	a	367.64	3.05612	YES	YES
46	a	390.54	76.80854	YES	YES
47	a	391.40	75.83715	YES	YES
48	a	396.48	4.78874	YES	YES
49	a	399.33	2.44368	YES	YES
50	a	399.55	3.22655	YES	YES
51	a	431.88	0.06441	YES	YES
52	a	432.85	0.83735	YES	YES
53	a	433.19	0.85608	YES	YES
54	a	463.57	2.15838	YES	YES
55	a	467.08	1.58782	YES	YES
56	a	468.80	2.38526	YES	YES
57	a	473.21	0.29090	YES	YES
58	a	485.56	39.16759	YES	YES
59	a	485.81	41.01265	YES	YES
60	a	560.79	0.13498	YES	YES
61	a	561.44	0.26195	YES	YES
62	a	561.66	0.32535	YES	YES
63	a	594.18	3.63768	YES	YES
64	a	595.38	11.95811	YES	YES
65	a	595.77	13.18521	YES	YES
66	a	630.88	0.34943	YES	YES
67	a	631.72	0.33345	YES	YES
68	a	632.31	0.17812	YES	YES
69	a	724.68	5.10530	YES	YES
70	a	731.24	4.15323	YES	YES
71	a	732.21	3.90993	YES	YES
72	a	746.76	41.17978	YES	YES
73	a	778.51	0.67281	YES	YES
74	a	778.53	0.58377	YES	YES
75	a	784.98	33.08600	YES	YES

76	a	957.31	173.81901	YES	YES
77	a	961.01	170.99489	YES	YES
78	a	961.99	158.04350	YES	YES
79	a	1066.07	364.57496	YES	YES
80	a	1066.99	371.56932	YES	YES
81	a	1068.49	64.03901	YES	YES
82	a	1121.38	1.20751	YES	YES
83	a	1124.74	0.39086	YES	YES
84	a	1125.66	0.31137	YES	YES
85	a	1249.78	51.39947	YES	YES
86	a	1252.08	59.75841	YES	YES
87	a	1253.17	13.54183	YES	YES
88	a	1347.85	27.83637	YES	YES
89	a	1349.50	27.38520	YES	YES
90	a	1353.55	2.54837	YES	YES
91	a	1358.91	11.43870	YES	YES
92	a	1359.79	9.57474	YES	YES
93	a	1364.25	1.20990	YES	YES
94	a	1446.86	442.28756	YES	YES
95	a	1454.51	547.52919	YES	YES
96	a	1455.84	539.89204	YES	YES
97	a	1501.01	186.91697	YES	YES
98	a	1502.79	199.93564	YES	YES
99	a	1504.50	34.05651	YES	YES
100	a	1612.78	4.47521	YES	YES
101	a	1614.22	29.17905	YES	YES
102	a	1614.92	38.56862	YES	YES
103	a	1615.45	33.86441	YES	YES
104	a	1616.63	37.42316	YES	YES
105	a	1617.35	37.38229	YES	YES



Total energy = -2464.3031257990 H = -67057.1380774 eV

HOMO-LUMO Separation

HOMO: 133. 133 a -0.10696312 H = -2.91062 eV

LUMO: 134. 134 a +0.04852025 H = +1.32030 eV

Gap : +0.15548337 H = +4.23092 eV

Number of MOs= 500, Electrons= 266.00, Symmetry: c1

\$coord

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-0.75940679136775	-3.58136145793724	0.64262526808933	c
-0.07597802960935	0.07151735635053	5.81038974728688	c
3.88546952402784	2.91849524216945	-1.14604623336495	c
6.32411492040174	3.66902235822826	-1.89617817184479	c
8.43067686245677	2.52452428541613	-0.75824032268933	c
8.07153846230104	0.66015714020623	1.09618826738386	c
5.58824369548628	-0.00466558498320	1.76720737688002	c
-4.85544285652700	1.81618244912589	-0.80924750464950	c
-6.72932485942946	3.57045882991551	-1.51310230644895	c
-6.52563858811270	6.07930991192309	-0.67525065887008	c
-4.46834269888161	6.79623306582570	0.84257063376648	c
-2.66282177960969	4.95801295998011	1.48665600686316	c
-2.24823938639564	-5.30006678874941	1.99662152232890	c
-2.75320259925705	-7.78080946908908	1.18664458269951	c
-1.73158087330773	-8.60516086068853	-1.11927451153108	c
-0.24557730104693	-6.94860939117718	-2.56496313561086	c
0.19407348092975	-4.48909517880106	-1.65385729159103	c
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0.71274463938722	-7.74454885576051	-4.78714910894037	f
1.61281709265229	-2.97695517820832	-3.15646460397432	f
-5.17298564966209	-0.56565919542096	-1.69446881340457	f
-8.70914574688682	2.89361123050631	-2.96686541447533	f
-8.29393863803581	7.78997352200717	-1.32269457548203	f
-4.27554337096978	9.20724896358907	1.64371070940025	f
-0.71023812556339	5.75087010293217	2.95037758846894	f
1.94671682295452	4.07995614578266	-2.34701726638646	f
6.67781926647770	5.45033846266680	-3.68233753987790	f
10.78297210093740	3.20793064005141	-1.44534425081132	f
5.35217017243567	-1.83371816838025	3.55153784459618	f
10.09445993417057	-0.44637200791786	2.18041032110414	f
0.88275751035650	-1.60608646115697	6.64528897197655	h
-2.03882669814635	0.11281043161853	6.57349345103187	h
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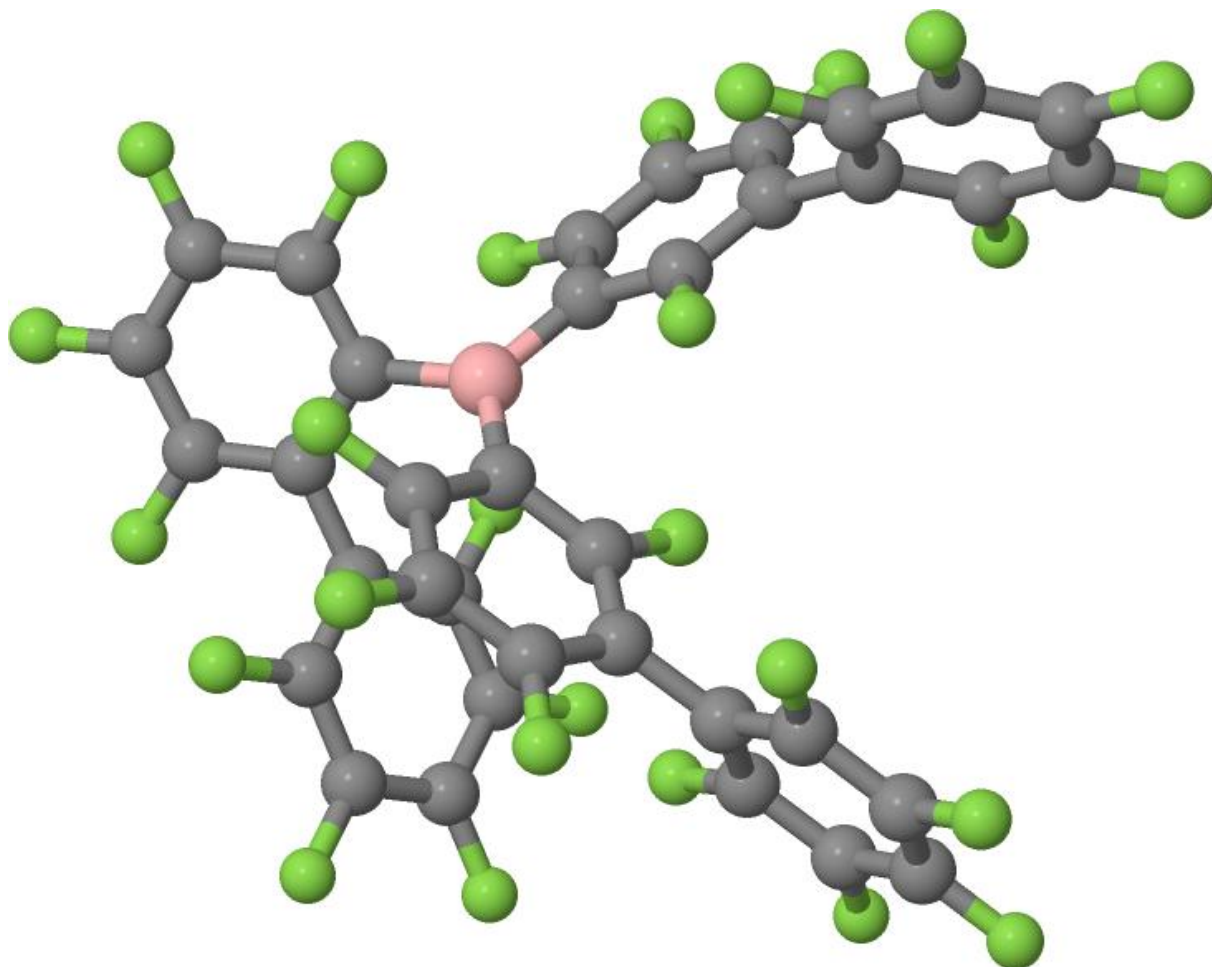
\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
#						
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	2.29	0.00673	YES	YES
8		a	12.50	0.00326	YES	YES

9	a	20.34	0.00832	YES	YES
10	a	20.81	0.01131	YES	YES
11	a	24.56	0.00422	YES	YES
12	a	28.82	0.01991	YES	YES
13	a	72.44	0.25267	YES	YES
14	a	77.36	0.02287	YES	YES
15	a	85.74	0.14591	YES	YES
16	a	97.40	0.10689	YES	YES
17	a	101.72	0.07105	YES	YES
18	a	107.11	0.15823	YES	YES
19	a	119.62	0.06623	YES	YES
20	a	121.36	0.00377	YES	YES
21	a	123.16	0.00835	YES	YES
22	a	129.11	0.77810	YES	YES
23	a	137.31	0.53607	YES	YES
24	a	143.95	0.83530	YES	YES
25	a	153.80	0.03701	YES	YES
26	a	156.76	0.04857	YES	YES
27	a	159.41	0.05788	YES	YES
28	a	207.94	2.53066	YES	YES
29	a	214.71	0.89569	YES	YES
30	a	219.06	0.87284	YES	YES
31	a	238.51	1.89405	YES	YES
32	a	259.68	0.14146	YES	YES
33	a	260.23	0.03502	YES	YES
34	a	261.03	0.08836	YES	YES
35	a	264.72	0.62283	YES	YES
36	a	266.05	0.39228	YES	YES
37	a	268.33	0.33205	YES	YES
38	a	300.76	6.67743	YES	YES
39	a	302.80	3.58523	YES	YES
40	a	304.01	3.93073	YES	YES
41	a	310.57	24.32900	YES	YES
42	a	313.38	25.05852	YES	YES
43	a	340.05	0.33127	YES	YES
44	a	348.07	0.45281	YES	YES
45	a	350.41	0.88077	YES	YES
46	a	362.38	3.78895	YES	YES
47	a	373.59	32.67505	YES	YES
48	a	379.32	33.31465	YES	YES
49	a	398.48	0.10155	YES	YES
50	a	399.92	0.08192	YES	YES
51	a	401.38	0.07404	YES	YES
52	a	432.30	0.05686	YES	YES
53	a	432.61	0.04652	YES	YES
54	a	432.96	0.07210	YES	YES
55	a	471.21	0.06243	YES	YES
56	a	479.20	14.18659	YES	YES
57	a	479.50	15.08632	YES	YES
58	a	487.28	0.90829	YES	YES
59	a	490.43	1.16574	YES	YES
60	a	494.50	1.47275	YES	YES
61	a	561.32	0.15907	YES	YES
62	a	561.75	0.03444	YES	YES
63	a	561.97	0.00716	YES	YES
64	a	585.54	16.17027	YES	YES
65	a	598.41	4.75321	YES	YES
66	a	606.88	7.52329	YES	YES
67	a	612.27	41.05520	YES	YES
68	a	632.29	0.02532	YES	YES
69	a	634.13	0.02113	YES	YES
70	a	634.48	0.01153	YES	YES

71	a	668.82	129.57859	YES	YES
72	a	671.98	94.80541	YES	YES
73	a	729.05	2.01535	YES	YES
74	a	732.18	10.37496	YES	YES
75	a	733.45	9.98399	YES	YES
76	a	761.72	0.05493	YES	YES
77	a	770.77	0.11687	YES	YES
78	a	771.01	0.06024	YES	YES
79	a	956.58	177.88828	YES	YES
80	a	958.53	152.12780	YES	YES
81	a	959.59	161.68111	YES	YES
82	a	1061.89	341.23295	YES	YES
83	a	1063.23	341.52086	YES	YES
84	a	1064.62	81.53011	YES	YES
85	a	1119.07	0.75208	YES	YES
86	a	1120.54	1.10140	YES	YES
87	a	1121.96	1.98665	YES	YES
88	a	1173.24	20.45543	YES	YES
89	a	1250.50	52.71028	YES	YES
90	a	1250.83	43.66993	YES	YES
91	a	1252.18	10.40694	YES	YES
92	a	1344.03	37.07811	YES	YES
93	a	1346.90	39.49766	YES	YES
94	a	1353.80	4.91700	YES	YES
95	a	1355.14	1.40553	YES	YES
96	a	1357.87	3.29097	YES	YES
97	a	1358.64	1.47824	YES	YES
98	a	1400.08	7.25889	YES	YES
99	a	1406.76	2.65496	YES	YES
100	a	1446.18	429.49473	YES	YES
101	a	1448.37	435.03640	YES	YES
102	a	1451.60	548.22658	YES	YES
103	a	1499.60	223.02953	YES	YES
104	a	1500.54	192.97869	YES	YES
105	a	1502.54	42.25027	YES	YES
106	a	1610.89	18.28752	YES	YES
107	a	1612.56	3.38215	YES	YES
108	a	1613.23	13.29101	YES	YES
109	a	1613.95	55.12081	YES	YES
110	a	1614.69	27.85775	YES	YES
111	a	1615.86	36.23002	YES	YES
112	a	2920.84	19.86364	YES	YES
113	a	3007.45	25.84397	YES	YES
114	a	3015.26	23.91738	YES	YES

B(C₁₂F₉)₃



Total energy = -4089.3961591880 H = -111278.1946461 eV

HOMO-LUMO Separation

HOMO: 232. 232 a -0.23824757 H = -6.48305 eV

LUMO: 233. 233 a -0.14522976 H = -3.95191 eV

Gap : +0.09301781 H = +2.53114 eV

Number of MOs= 896, Electrons= 464.00, Symmetry: c1

\$coord

6.00263941189047	2.61139408467599	-4.53304620290750	c
7.33314643062647	4.53263114349575	-3.27175234558662	c
8.42831660106832	4.05327979065630	-0.89819450734508	c
8.21272375587540	1.63861450260678	0.17784495774687	c
6.91082743327064	-0.33536500070418	-1.04880938970526	c
5.81925647725643	0.21236316592608	-3.41613112172818	c
4.52199445187570	-4.19436371079034	0.61755092408328	c
6.83357881192378	-2.93446785818137	0.03101180988152	c
9.14416315871018	-4.21723071258864	0.30955176504332	c
9.23877702138267	-6.72093546174032	1.19566887897858	c
6.97877763467264	-7.98907237693412	1.76361569614936	c
4.67254600013728	-6.71129149562529	1.45636881180614	c
-0.24068584586588	-5.82087671065659	-2.74047731017860	c
-0.47812123291952	-4.01225401013020	-0.77630333729217	c
-5.17198165225037	-4.48077810017947	-1.22079313375400	c
-4.76661480143754	-6.24983881457049	-3.17241553594712	c
-2.32308968627851	-6.92123575866025	-3.95481074914036	c
-7.76627859245083	-3.80099418488959	-0.40131806116669	c
-8.55896951890464	-4.16105983676913	2.11829966221766	c
-11.01005244865106	-3.52405929900602	2.91474252239136	c
-12.73593277332155	-2.52271586498637	1.15843435004210	c
-12.00102680503079	-2.15594328251566	-1.36946772428966	c
-9.53296191613865	-2.78292251699502	-2.11827486923413	c
1.41341242115582	4.53797230069153	4.52960724391324	c
2.62000939868915	2.47606914550810	5.67805713237844	c
2.77304806009833	0.18335314076572	4.35078787159456	c
1.71424684731725	-0.15829557695208	1.92541292242222	c
0.50237797469882	1.98263474249042	0.89751541702370	c
0.31874671481873	4.34704732350543	2.10352409588205	c
-2.98723307281780	7.78007524978394	2.12910536170245	c
-0.95391965337789	6.54777558916073	0.92208592942029	c
-0.16572026527253	7.50272051486983	-1.43623564774987	c
-1.34110148502390	9.59564592009582	-2.56646882206905	c
-3.35525438320831	10.79443786852040	-1.31319102180218	c
9.24858107956221	1.23944999229281	2.45254203451618	f
9.65168940742761	5.89740623585991	0.31524676564663	f
7.53921177799211	6.81775105409639	-4.30835378493550	f
4.95137732379216	3.06170077058456	-6.78104613840485	f
4.55841922882182	-1.59270635008466	-4.67530342391905	f
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7.04076073818252	-10.36638662013820	2.60038607550450	f
2.56020923517540	-7.98689798896630	2.07498198684923	f
-6.96530294255230	-5.15181006033225	3.81175088495998	f
-11.71489880146123	-3.88770977230611	5.31030336673411	f
-15.07037556177792	-1.92011875662739	1.88731023279121	f
-13.63987642114281	-1.19526438838442	-3.03005236645619	f
-8.86636781136614	-2.37334216084514	-4.52332933751193	f
-6.72853116139339	-7.35283985473876	-4.30294621708843	f
-1.99808169619942	-8.61133902517211	-5.79994336422111	f
2.03518779715452	-6.54321341885430	-3.56390943850568	f
1.77703388070533	6.42245283217326	-2.64956942107211	f
-0.54489030494489	10.46308326123450	-4.79670171540416	f
-4.48265000840658	12.78636662723459	-2.36371149779013	f
-3.83791651552558	6.92986994018077	4.35262085383342	f
1.32735728863982	6.72469954452671	5.78411639381387	f
3.61969268848346	2.70572915391083	7.98390887786681	f
3.90906718485720	-1.74766982992585	5.53255367793752	f
-0.53531036194431	1.76990843463201	-1.41789830924281	f
-4.17704226790004	9.89310208906159	1.04842451895206	c
-6.09316457660749	11.03009953846851	2.23181508031383	c

-3.00360003230239	-3.41851369457968	-0.10171958352526	c
-3.41310630917498	-1.74902240229212	1.76687493343975	f
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\$vibrational spectrum

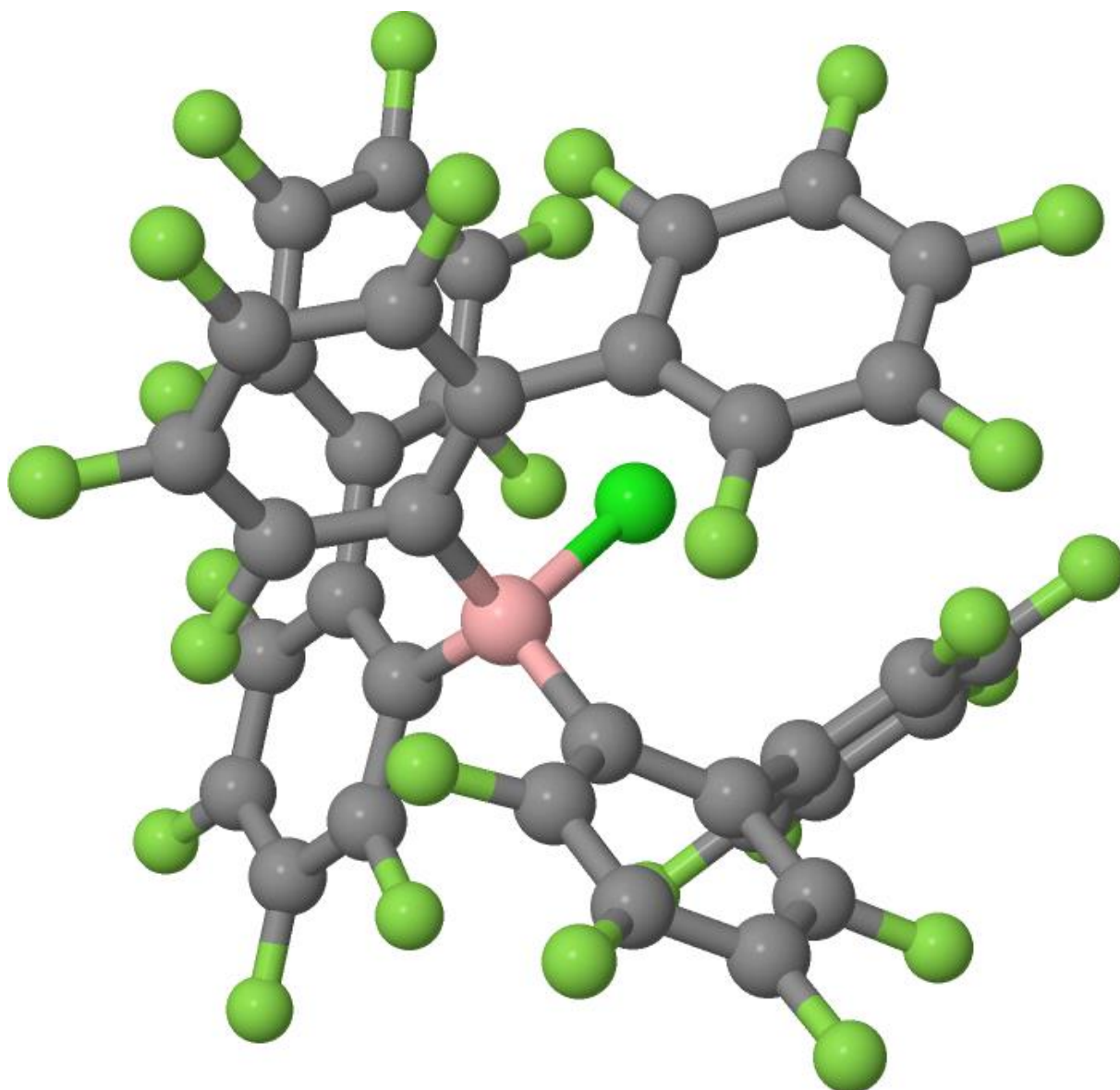
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2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	10.61	0.02259	YES	YES
8		a	13.21	0.03292	YES	YES
9		a	15.03	0.01425	YES	YES
10		a	19.47	0.02002	YES	YES
11		a	21.08	0.05597	YES	YES
12		a	25.32	0.01232	YES	YES
13		a	29.74	0.03805	YES	YES
14		a	33.06	0.00695	YES	YES
15		a	35.23	0.06696	YES	YES
16		a	36.93	0.00212	YES	YES
17		a	43.86	0.15188	YES	YES
18		a	46.83	0.27358	YES	YES
19		a	50.70	0.04350	YES	YES
20		a	54.37	0.09474	YES	YES
21		a	56.76	0.06146	YES	YES
22		a	91.60	0.10321	YES	YES
23		a	94.58	0.11228	YES	YES
24		a	97.77	0.02008	YES	YES
25		a	102.94	0.13360	YES	YES
26		a	108.05	0.13987	YES	YES
27		a	124.63	0.44818	YES	YES
28		a	125.78	0.35944	YES	YES
29		a	128.48	0.08071	YES	YES
30		a	131.02	0.03094	YES	YES
31		a	132.25	0.04708	YES	YES
32		a	134.77	0.04483	YES	YES
33		a	136.73	0.24242	YES	YES
34		a	138.27	0.08539	YES	YES
35		a	146.14	0.03932	YES	YES
36		a	151.03	0.10755	YES	YES
37		a	154.89	0.09930	YES	YES
38		a	158.49	0.08355	YES	YES
39		a	161.08	0.01083	YES	YES
40		a	168.36	0.18180	YES	YES
41		a	172.77	0.08765	YES	YES
42		a	175.79	0.26577	YES	YES
43		a	187.83	0.48828	YES	YES
44		a	202.43	0.45422	YES	YES
45		a	205.22	0.37490	YES	YES
46		a	233.78	1.63117	YES	YES
47		a	236.55	0.08536	YES	YES
48		a	242.84	0.51868	YES	YES
49		a	244.33	2.91247	YES	YES
50		a	248.38	3.78968	YES	YES

51	a	255.76	4.92061	YES	YES
52	a	262.49	0.14639	YES	YES
53	a	263.81	0.23921	YES	YES
54	a	265.17	0.17790	YES	YES
55	a	265.52	0.20374	YES	YES
56	a	267.33	0.18255	YES	YES
57	a	269.08	0.01709	YES	YES
58	a	270.12	0.22778	YES	YES
59	a	276.06	0.26781	YES	YES
60	a	279.84	0.44598	YES	YES
61	a	284.71	0.02707	YES	YES
62	a	301.82	0.64166	YES	YES
63	a	302.97	0.53596	YES	YES
64	a	303.87	0.59621	YES	YES
65	a	317.52	1.87122	YES	YES
66	a	323.27	1.28735	YES	YES
67	a	333.93	3.91330	YES	YES
68	a	341.16	2.38326	YES	YES
69	a	343.98	4.49617	YES	YES
70	a	348.69	0.15268	YES	YES
71	a	353.07	1.05679	YES	YES
72	a	366.06	1.03743	YES	YES
73	a	369.97	1.02408	YES	YES
74	a	375.28	0.41686	YES	YES
75	a	377.92	1.31519	YES	YES
76	a	381.15	1.54533	YES	YES
77	a	381.42	0.70218	YES	YES
78	a	383.84	0.13394	YES	YES
79	a	386.06	0.17419	YES	YES
80	a	389.95	8.37080	YES	YES
81	a	401.92	2.56736	YES	YES
82	a	408.50	0.88346	YES	YES
83	a	410.74	0.31606	YES	YES
84	a	414.71	0.45770	YES	YES
85	a	433.71	0.39177	YES	YES
86	a	434.98	0.23709	YES	YES
87	a	436.38	0.23881	YES	YES
88	a	446.57	1.28417	YES	YES
89	a	448.50	1.30338	YES	YES
90	a	453.90	1.68364	YES	YES
91	a	469.03	8.46759	YES	YES
92	a	473.37	5.20574	YES	YES
93	a	479.00	2.87176	YES	YES
94	a	501.72	0.18730	YES	YES
95	a	505.07	2.29510	YES	YES
96	a	508.57	0.01979	YES	YES
97	a	516.12	0.13780	YES	YES
98	a	539.99	6.52944	YES	YES
99	a	556.71	29.45951	YES	YES
100	a	565.39	4.77161	YES	YES
101	a	565.94	0.29114	YES	YES
102	a	566.43	0.09892	YES	YES
103	a	568.22	2.53815	YES	YES
104	a	571.08	1.84112	YES	YES
105	a	580.36	11.65480	YES	YES
106	a	584.80	51.92890	YES	YES
107	a	605.44	2.78567	YES	YES
108	a	609.81	5.82285	YES	YES
109	a	617.17	0.82058	YES	YES
110	a	619.10	2.85779	YES	YES
111	a	623.22	0.44400	YES	YES
112	a	625.17	2.65495	YES	YES

113	a	626.17	1.69548	YES	YES
114	a	628.38	0.33249	YES	YES
115	a	643.62	0.57778	YES	YES
116	a	655.31	3.66979	YES	YES
117	a	658.90	7.24829	YES	YES
118	a	676.84	1.06262	YES	YES
119	a	684.65	17.71863	YES	YES
120	a	697.01	14.48973	YES	YES
121	a	707.43	9.89497	YES	YES
122	a	721.16	43.39766	YES	YES
123	a	730.09	18.85927	YES	YES
124	a	763.85	4.38935	YES	YES
125	a	765.94	9.28130	YES	YES
126	a	775.70	10.75694	YES	YES
127	a	787.92	3.43566	YES	YES
128	a	794.44	14.17069	YES	YES
129	a	796.46	3.11245	YES	YES
130	a	860.73	68.43236	YES	YES
131	a	951.47	26.11737	YES	YES
132	a	954.17	38.69625	YES	YES
133	a	961.48	20.11781	YES	YES
134	a	990.01	80.23582	YES	YES
135	a	996.40	253.02930	YES	YES
136	a	1001.86	64.35859	YES	YES
137	a	1009.18	79.41846	YES	YES
138	a	1016.75	26.04558	YES	YES
139	a	1069.63	221.54692	YES	YES
140	a	1074.57	116.60363	YES	YES
141	a	1081.29	247.91675	YES	YES
142	a	1116.19	25.29195	YES	YES
143	a	1155.05	46.44633	YES	YES
144	a	1158.85	102.56005	YES	YES
145	a	1160.88	7.86999	YES	YES
146	a	1163.92	29.00442	YES	YES
147	a	1165.15	2.15697	YES	YES
148	a	1168.23	37.98783	YES	YES
149	a	1169.16	16.99981	YES	YES
150	a	1180.13	202.84863	YES	YES
151	a	1278.68	3.60821	YES	YES
152	a	1286.35	14.07763	YES	YES
153	a	1288.15	156.38424	YES	YES
154	a	1317.41	134.46234	YES	YES
155	a	1337.44	39.43584	YES	YES
156	a	1338.10	12.58152	YES	YES
157	a	1342.29	98.89130	YES	YES
158	a	1343.82	10.68453	YES	YES
159	a	1345.53	2.75708	YES	YES
160	a	1347.30	0.53174	YES	YES
161	a	1349.33	2.98080	YES	YES
162	a	1349.86	11.48229	YES	YES
163	a	1357.38	68.91985	YES	YES
164	a	1366.02	53.11363	YES	YES
165	a	1370.11	93.49859	YES	YES
166	a	1423.53	75.00068	YES	YES
167	a	1426.26	24.32831	YES	YES
168	a	1435.44	109.78098	YES	YES
169	a	1461.03	513.80762	YES	YES
170	a	1467.90	363.74013	YES	YES
171	a	1470.93	303.56878	YES	YES
172	a	1489.20	207.36214	YES	YES
173	a	1491.60	156.31243	YES	YES
174	a	1500.31	399.20701	YES	YES

175	a	1507.80	340.35224	YES	YES
176	a	1508.33	250.69777	YES	YES
177	a	1512.72	243.98882	YES	YES
178	a	1523.55	158.19316	YES	YES
179	a	1525.09	203.89382	YES	YES
180	a	1527.01	179.27305	YES	YES
181	a	1594.85	73.33430	YES	YES
182	a	1606.64	63.16790	YES	YES
183	a	1607.63	24.06189	YES	YES
184	a	1610.95	268.41360	YES	YES
185	a	1615.79	183.49774	YES	YES
186	a	1617.93	53.89739	YES	YES
187	a	1621.57	57.00767	YES	YES
188	a	1622.27	57.39457	YES	YES
189	a	1623.20	6.40646	YES	YES
190	a	1638.96	20.71605	YES	YES
191	a	1640.59	33.39574	YES	YES
192	a	1641.45	12.95870	YES	YES

B(C₁₂F₉)₃Cl⁻



Total energy = -4549.6263199190 H = -123801.7016418 eV

HOMO-LUMO Separation

HOMO: 241. 241 a -0.12373643 H = -3.36704 eV

LUMO: 242. 242 a +0.01550694 H = +0.42197 eV

Gap : +0.13924338 H = +3.78901 eV

Number of MOs= 914, Electrons= 482.00, Symmetry: c1

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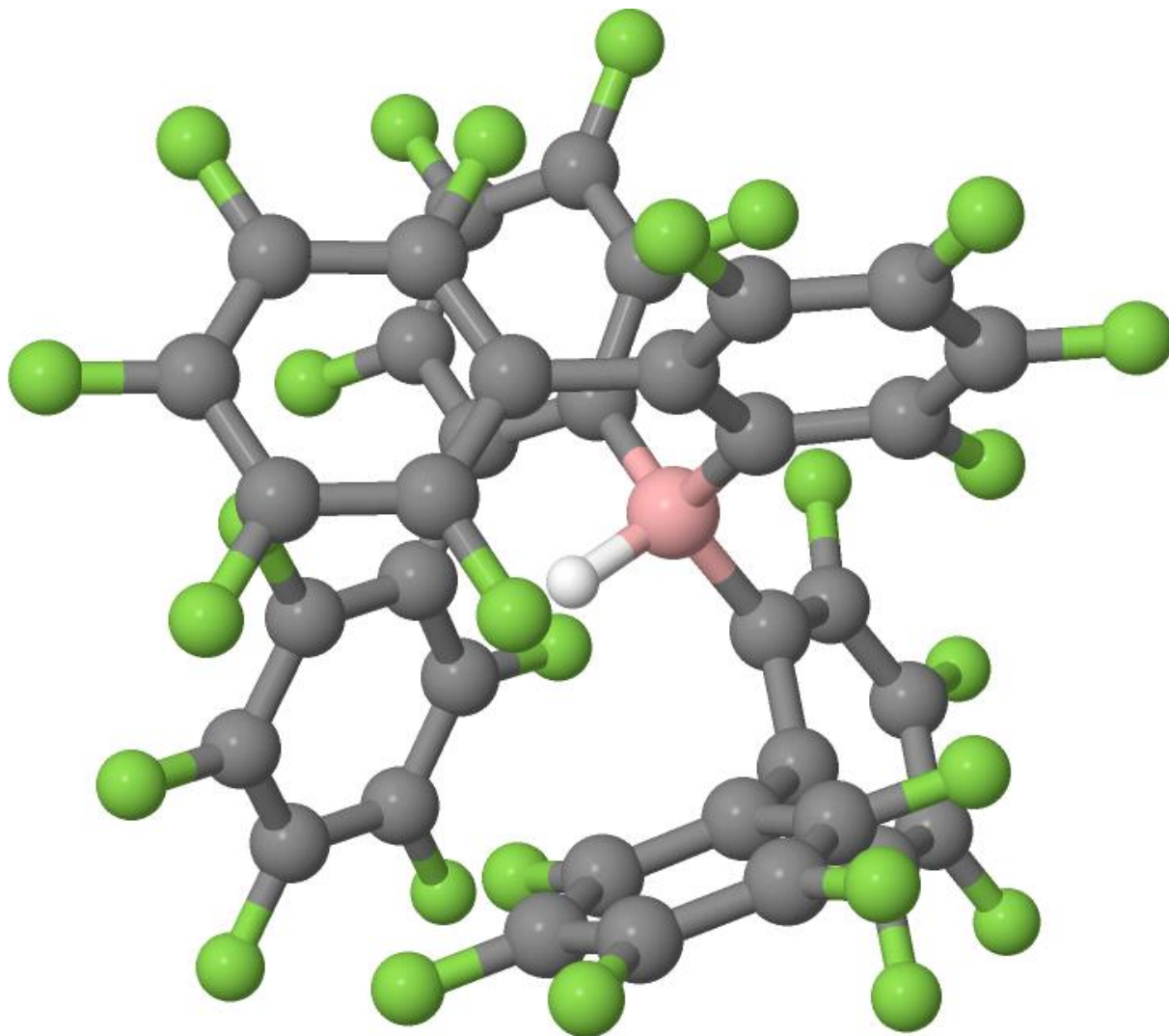
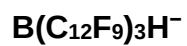
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		3.30	0.01507	YES	YES
8	a		7.94	0.00597	YES	YES
9	a		13.98	0.00420	YES	YES
10	a		21.59	0.01276	YES	YES
11	a		23.93	0.02396	YES	YES
12	a		26.68	0.01599	YES	YES
13	a		31.05	0.00409	YES	YES
14	a		34.03	0.00244	YES	YES
15	a		35.67	0.01738	YES	YES
16	a		36.72	0.00657	YES	YES
17	a		39.10	0.00372	YES	YES
18	a		46.73	0.00055	YES	YES
19	a		50.04	0.00071	YES	YES
20	a		52.92	0.00061	YES	YES
21	a		56.60	0.00019	YES	YES
22	a		94.89	0.25037	YES	YES
23	a		97.24	0.10493	YES	YES
24	a		99.74	0.09179	YES	YES
25	a		105.77	0.08299	YES	YES
26	a		107.66	0.04774	YES	YES
27	a		109.98	0.10965	YES	YES

28	a	122.98	0.05769	YES	YES
29	a	124.03	0.13733	YES	YES
30	a	126.91	0.12684	YES	YES
31	a	132.05	0.00449	YES	YES
32	a	134.16	0.00950	YES	YES
33	a	136.16	0.00553	YES	YES
34	a	139.35	0.02321	YES	YES
35	a	139.73	0.04714	YES	YES
36	a	153.53	0.02674	YES	YES
37	a	155.45	0.05917	YES	YES
38	a	157.04	0.27591	YES	YES
39	a	157.79	0.37890	YES	YES
40	a	167.98	0.43194	YES	YES
41	a	170.36	0.15531	YES	YES
42	a	174.03	0.09572	YES	YES
43	a	179.17	2.54060	YES	YES
44	a	186.31	3.46443	YES	YES
45	a	193.95	0.30371	YES	YES
46	a	216.95	0.70837	YES	YES
47	a	219.00	0.97451	YES	YES
48	a	242.06	0.43257	YES	YES
49	a	247.34	2.30322	YES	YES
50	a	248.62	1.76025	YES	YES
51	a	251.57	0.99112	YES	YES
52	a	253.23	3.43129	YES	YES
53	a	254.56	3.12596	YES	YES
54	a	261.54	0.23197	YES	YES
55	a	262.28	0.21567	YES	YES
56	a	262.81	0.25704	YES	YES
57	a	264.60	0.06868	YES	YES
58	a	265.91	0.05964	YES	YES
59	a	267.18	0.12700	YES	YES
60	a	267.45	0.10320	YES	YES
61	a	268.23	0.17014	YES	YES
62	a	270.16	0.23818	YES	YES
63	a	272.60	2.66726	YES	YES
64	a	291.45	0.15360	YES	YES
65	a	293.88	0.11529	YES	YES
66	a	297.46	0.13902	YES	YES
67	a	299.32	0.20673	YES	YES
68	a	299.78	0.25120	YES	YES
69	a	299.84	0.22526	YES	YES
70	a	335.96	4.07757	YES	YES
71	a	336.91	1.70618	YES	YES
72	a	337.15	1.02832	YES	YES
73	a	353.93	1.66854	YES	YES
74	a	354.75	1.37446	YES	YES
75	a	355.24	0.32994	YES	YES
76	a	378.10	0.10459	YES	YES
77	a	384.50	0.11251	YES	YES
78	a	386.48	0.12980	YES	YES
79	a	389.62	0.47388	YES	YES
80	a	395.80	0.94435	YES	YES
81	a	398.98	0.35309	YES	YES
82	a	406.43	0.83099	YES	YES
83	a	407.65	0.50629	YES	YES
84	a	407.87	0.47347	YES	YES
85	a	413.76	1.04520	YES	YES
86	a	415.20	1.33524	YES	YES
87	a	416.50	2.09947	YES	YES
88	a	434.80	0.01341	YES	YES
89	a	435.12	0.05951	YES	YES

90	a	435.83	0.12253	YES	YES
91	a	454.50	1.05076	YES	YES
92	a	454.76	0.87953	YES	YES
93	a	458.06	1.40046	YES	YES
94	a	469.96	1.11093	YES	YES
95	a	470.56	0.80364	YES	YES
96	a	476.02	0.46581	YES	YES
97	a	506.58	1.23508	YES	YES
98	a	507.31	1.67423	YES	YES
99	a	511.18	0.07580	YES	YES
100	a	513.80	0.14918	YES	YES
101	a	518.45	0.07290	YES	YES
102	a	520.46	0.24837	YES	YES
103	a	552.29	1.00895	YES	YES
104	a	554.51	1.16091	YES	YES
105	a	559.49	1.36280	YES	YES
106	a	566.25	0.47866	YES	YES
107	a	566.54	0.61826	YES	YES
108	a	567.11	0.65103	YES	YES
109	a	601.31	20.02747	YES	YES
110	a	601.82	18.42599	YES	YES
111	a	603.91	20.48440	YES	YES
112	a	619.54	9.93073	YES	YES
113	a	621.30	5.93122	YES	YES
114	a	622.62	6.98801	YES	YES
115	a	627.11	0.84874	YES	YES
116	a	629.65	3.62743	YES	YES
117	a	631.09	4.83143	YES	YES
118	a	640.86	0.58028	YES	YES
119	a	643.80	1.01983	YES	YES
120	a	649.54	2.93115	YES	YES
121	a	679.71	76.14601	YES	YES
122	a	698.35	57.60517	YES	YES
123	a	701.89	54.83436	YES	YES
124	a	713.13	25.52395	YES	YES
125	a	714.61	44.82449	YES	YES
126	a	718.19	24.74275	YES	YES
127	a	758.26	15.76224	YES	YES
128	a	761.78	16.86621	YES	YES
129	a	780.38	1.38866	YES	YES
130	a	781.78	3.61791	YES	YES
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132	a	787.63	8.77063	YES	YES
133	a	835.71	20.67307	YES	YES
134	a	905.30	4.88024	YES	YES
135	a	912.85	8.14967	YES	YES
136	a	948.19	4.73570	YES	YES
137	a	949.87	2.59996	YES	YES
138	a	951.80	3.86610	YES	YES
139	a	991.16	145.88494	YES	YES
140	a	992.64	146.34543	YES	YES
141	a	993.66	163.20148	YES	YES
142	a	1046.14	199.20448	YES	YES
143	a	1047.64	219.89278	YES	YES
144	a	1048.14	209.24353	YES	YES
145	a	1102.11	227.22960	YES	YES
146	a	1104.02	131.19331	YES	YES
147	a	1106.48	165.56671	YES	YES
148	a	1137.43	2.96391	YES	YES
149	a	1138.19	3.42727	YES	YES
150	a	1139.16	2.91459	YES	YES
151	a	1153.26	3.25348	YES	YES

152	a	1154.62	2.45469	YES	YES
153	a	1156.15	5.31895	YES	YES
154	a	1257.64	7.18973	YES	YES
155	a	1260.24	10.17747	YES	YES
156	a	1261.47	1.90094	YES	YES
157	a	1280.37	31.69077	YES	YES
158	a	1283.04	28.12840	YES	YES
159	a	1284.14	41.08289	YES	YES
160	a	1326.08	11.80736	YES	YES
161	a	1328.19	13.77732	YES	YES
162	a	1328.71	7.66543	YES	YES
163	a	1343.78	15.32707	YES	YES
164	a	1345.81	1.36480	YES	YES
165	a	1346.37	4.69019	YES	YES
166	a	1347.71	8.03008	YES	YES
167	a	1349.17	13.02191	YES	YES
168	a	1349.76	24.71295	YES	YES
169	a	1424.71	148.70931	YES	YES
170	a	1427.30	157.11235	YES	YES
171	a	1428.49	166.27464	YES	YES
172	a	1450.79	138.72005	YES	YES
173	a	1452.83	134.42846	YES	YES
174	a	1454.14	134.25637	YES	YES
175	a	1495.88	42.56262	YES	YES
176	a	1496.58	492.70003	YES	YES
177	a	1496.88	424.98981	YES	YES
178	a	1499.80	161.93930	YES	YES
179	a	1503.70	292.51237	YES	YES
180	a	1504.81	266.66157	YES	YES
181	a	1517.56	86.70922	YES	YES
182	a	1518.78	104.24637	YES	YES
183	a	1521.07	258.77316	YES	YES
184	a	1601.89	34.97588	YES	YES
185	a	1605.30	37.26180	YES	YES
186	a	1606.52	39.92658	YES	YES
187	a	1621.03	32.12933	YES	YES
188	a	1621.58	24.82206	YES	YES
189	a	1623.29	9.08044	YES	YES
190	a	1624.36	7.54457	YES	YES
191	a	1625.54	10.33553	YES	YES
192	a	1626.09	12.38926	YES	YES
193	a	1639.97	16.10357	YES	YES
194	a	1640.46	17.26172	YES	YES
195	a	1642.05	13.98139	YES	YES



Total energy = -4090.0824359930 H = -111296.8691988 eV

HOMO-LUMO Separation

HOMO: 233. 233 a -0.11503173 H = -3.13017 eV

LUMO: 234. 234 a +0.01926483 H = +0.52422 eV

Gap : +0.13429656 H = +3.65440 eV

Number of MOs= 898, Electrons= 466.00, Symmetry: c1

\$coord

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6.39077025603464	-0.01137769757334	5.69103087435317	c
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6.94792962294170	-2.76393334241505	2.11317407373079	c
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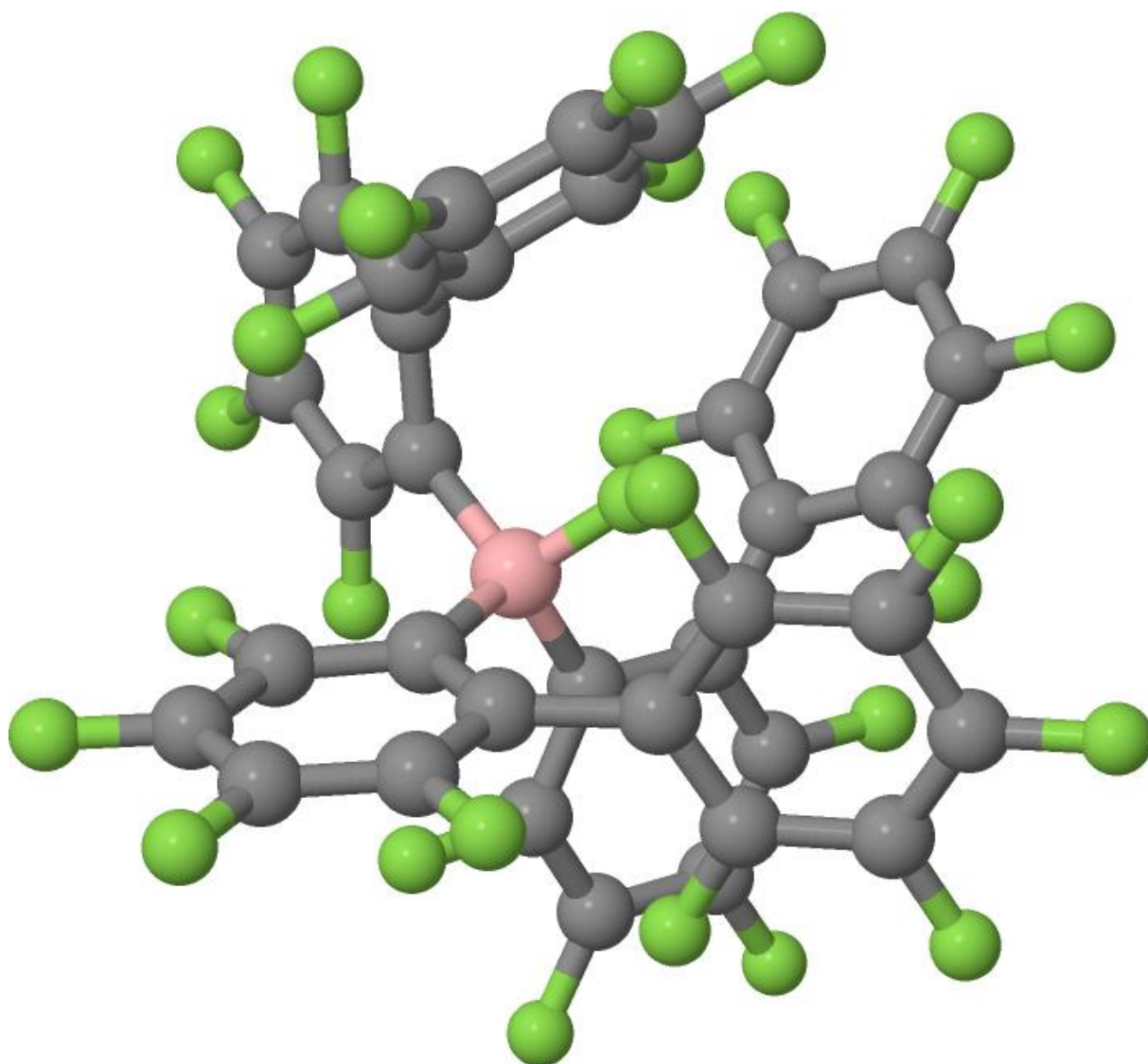
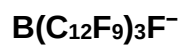
\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	12.62	0.02005	YES	YES
8		a	14.50	0.01858	YES	YES
9		a	15.98	0.01409	YES	YES
10		a	19.57	0.02737	YES	YES
11		a	21.85	0.02036	YES	YES
12		a	25.74	0.00228	YES	YES
13		a	28.05	0.00845	YES	YES
14		a	29.89	0.00227	YES	YES
15		a	40.13	0.02543	YES	YES
16		a	41.14	0.05038	YES	YES
17		a	42.22	0.03006	YES	YES
18		a	45.85	0.01195	YES	YES
19		a	47.35	0.03515	YES	YES
20		a	49.29	0.04885	YES	YES
21		a	50.91	0.00842	YES	YES
22		a	88.55	0.03438	YES	YES
23		a	92.79	0.25175	YES	YES
24		a	93.83	0.31025	YES	YES
25		a	101.94	0.07967	YES	YES
26		a	102.64	0.05260	YES	YES
27		a	104.26	0.00762	YES	YES
28		a	120.18	0.06713	YES	YES
29		a	120.79	0.04386	YES	YES
30		a	122.33	0.06184	YES	YES
31		a	131.43	0.00398	YES	YES
32		a	132.04	0.01157	YES	YES
33		a	132.64	0.01716	YES	YES
34		a	139.60	0.08411	YES	YES
35		a	140.45	0.08517	YES	YES
36		a	153.79	0.02749	YES	YES
37		a	156.18	0.01614	YES	YES
38		a	158.15	0.05760	YES	YES
39		a	158.80	0.06443	YES	YES
40		a	169.79	0.01862	YES	YES
41		a	170.47	0.01488	YES	YES
42		a	180.22	0.12011	YES	YES
43		a	190.35	0.00259	YES	YES
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45		a	210.50	1.38845	YES	YES
46		a	239.51	0.73019	YES	YES

47	a	241.61	0.59617	YES	YES
48	a	242.74	0.08683	YES	YES
49	a	247.54	1.99065	YES	YES
50	a	250.63	5.12096	YES	YES
51	a	251.43	3.50813	YES	YES
52	a	260.24	0.10513	YES	YES
53	a	261.08	0.01322	YES	YES
54	a	262.56	0.00702	YES	YES
55	a	262.97	0.06738	YES	YES
56	a	263.23	0.07707	YES	YES
57	a	264.50	0.06593	YES	YES
58	a	266.95	0.02027	YES	YES
59	a	268.23	0.01979	YES	YES
60	a	269.09	0.01473	YES	YES
61	a	284.57	0.04856	YES	YES
62	a	286.83	0.05193	YES	YES
63	a	287.27	0.03007	YES	YES
64	a	298.98	0.24513	YES	YES
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66	a	300.70	0.21703	YES	YES
67	a	333.17	1.09372	YES	YES
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73	a	358.00	0.03507	YES	YES
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75	a	379.15	0.62391	YES	YES
76	a	383.21	0.14053	YES	YES
77	a	386.11	0.31589	YES	YES
78	a	387.09	0.32216	YES	YES
79	a	402.75	0.08897	YES	YES
80	a	404.52	0.52212	YES	YES
81	a	405.88	0.12595	YES	YES
82	a	407.20	0.44615	YES	YES
83	a	408.09	0.24404	YES	YES
84	a	409.51	0.41978	YES	YES
85	a	434.87	0.12813	YES	YES
86	a	435.02	0.10038	YES	YES
87	a	435.54	0.12297	YES	YES
88	a	450.33	0.79870	YES	YES
89	a	450.77	0.83232	YES	YES
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91	a	467.95	0.79916	YES	YES
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106	a	568.61	0.03932	YES	YES
107	a	593.21	11.75311	YES	YES
108	a	593.99	11.66500	YES	YES

109	a	621.69	0.95625	YES	YES
110	a	622.38	0.42125	YES	YES
111	a	624.19	0.42133	YES	YES
112	a	627.87	0.03743	YES	YES
113	a	628.49	0.03067	YES	YES
114	a	629.60	0.06636	YES	YES
115	a	635.99	0.77759	YES	YES
116	a	636.41	0.69932	YES	YES
117	a	640.25	0.90240	YES	YES
118	a	676.61	29.53423	YES	YES
119	a	679.82	31.50216	YES	YES
120	a	682.27	32.93138	YES	YES
121	a	712.14	21.15965	YES	YES
122	a	712.85	22.69867	YES	YES
123	a	715.50	97.53490	YES	YES
124	a	759.62	10.29631	YES	YES
125	a	761.15	10.44723	YES	YES
126	a	773.79	0.05658	YES	YES
127	a	782.12	1.03394	YES	YES
128	a	782.45	2.08527	YES	YES
129	a	789.73	0.10976	YES	YES
130	a	833.88	0.32811	YES	YES
131	a	895.57	86.60210	YES	YES
132	a	900.31	80.62216	YES	YES
133	a	942.51	3.99309	YES	YES
134	a	943.49	4.00067	YES	YES
135	a	948.08	0.26041	YES	YES
136	a	990.58	174.33256	YES	YES
137	a	992.17	155.60128	YES	YES
138	a	993.73	127.62323	YES	YES
139	a	1029.11	17.62247	YES	YES
140	a	1042.76	93.67475	YES	YES
141	a	1044.62	275.21518	YES	YES
142	a	1048.71	160.28945	YES	YES
143	a	1051.94	98.65817	YES	YES
144	a	1099.25	182.34954	YES	YES
145	a	1105.93	141.49140	YES	YES
146	a	1107.12	145.26293	YES	YES
147	a	1138.86	5.60181	YES	YES
148	a	1140.47	6.40751	YES	YES
149	a	1141.54	6.62711	YES	YES
150	a	1152.77	1.62548	YES	YES
151	a	1154.95	1.04569	YES	YES
152	a	1156.31	2.21132	YES	YES
153	a	1258.02	7.46163	YES	YES
154	a	1258.99	8.37635	YES	YES
155	a	1260.40	0.94998	YES	YES
156	a	1285.77	28.48565	YES	YES
157	a	1286.90	26.89577	YES	YES
158	a	1288.80	26.65680	YES	YES
159	a	1331.56	6.92188	YES	YES
160	a	1333.02	12.45262	YES	YES
161	a	1334.84	15.11689	YES	YES
162	a	1346.46	0.17655	YES	YES
163	a	1348.69	0.98015	YES	YES
164	a	1349.56	1.43924	YES	YES
165	a	1350.03	30.91629	YES	YES
166	a	1351.67	9.30394	YES	YES
167	a	1352.84	11.98062	YES	YES
168	a	1428.43	103.26593	YES	YES
169	a	1430.48	116.47882	YES	YES
170	a	1432.15	109.72311	YES	YES

171	a	1456.64	171.91791	YES	YES
172	a	1457.60	167.77734	YES	YES
173	a	1459.04	189.76197	YES	YES
174	a	1491.41	220.70579	YES	YES
175	a	1493.22	194.09283	YES	YES
176	a	1496.28	182.91895	YES	YES
177	a	1496.65	424.82867	YES	YES
178	a	1498.89	368.47764	YES	YES
179	a	1499.83	304.66331	YES	YES
180	a	1518.28	100.68896	YES	YES
181	a	1520.29	104.12495	YES	YES
182	a	1523.13	265.67917	YES	YES
183	a	1595.09	26.84378	YES	YES
184	a	1597.80	25.54903	YES	YES
185	a	1598.15	23.43298	YES	YES
186	a	1618.10	21.76436	YES	YES
187	a	1619.98	21.05566	YES	YES
188	a	1620.75	16.65025	YES	YES
189	a	1623.26	4.24074	YES	YES
190	a	1625.05	4.68030	YES	YES
191	a	1626.05	6.98593	YES	YES
192	a	1640.45	19.49461	YES	YES
193	a	1642.19	16.95170	YES	YES
194	a	1643.20	14.15683	YES	YES
195	a	2353.01	100.89996	YES	YES



Total energy = -4189.3122086860 H = -113997.0502354 eV

HOMO-LUMO Separation

HOMO: 237. 237 a -0.12579436 H = -3.42304 eV

LUMO: 238. 238 a +0.02180808 H = +0.59343 eV

Gap : +0.14760243 H = +4.01647 eV

Number of MOs= 910, Electrons= 474.00, Symmetry: c1

437

\$coord

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4.25924917449602	-5.00938700046819	-5.54934034244173	c
6.49986406019985	-5.02989881850265	-4.14085981868533	c
6.67810787805913	-3.44111467967628	-2.03064220151061	c
4.67665094152929	-1.83777636836746	-1.32120761804810	c
5.20668287330097	-0.19543970639489	0.92034073087456	c
6.11291968377066	2.28399517272319	0.63895175976866	c
6.75166297450643	3.79035059827084	2.73061170188362	c
6.50024141379988	2.80025124902568	5.17699674397462	c
5.61492304342699	0.32069660507244	5.51620234735714	c
5.01239539941073	-1.14397942190448	3.39225756513689	c
0.16942580611219	2.94356636744656	-2.84103599224348	c
1.48010861176824	3.62140136885952	-5.04770917258818	c
1.81974488534732	6.13119498493788	-5.85192398725052	c
0.77981668795159	8.10985760993889	-4.43644571339948	c
-0.57621739366919	7.51033276322885	-2.24302433413708	c
-0.89694277681847	4.99017755395984	-1.45124589937387	c
-2.46838133563240	4.66695383883189	0.87871132332862	c
-1.43057994555301	4.99133895267364	3.30160523052926	c
-2.91084556426744	4.83568153096582	5.49467443857946	c
-5.51910665783298	4.38810948496455	5.28067892606620	c
-6.61431686959695	4.07674961637222	2.88690824594219	c
-5.08396300549201	4.23851657515406	0.72243240795069	c
-2.84416527338600	-1.32623040696005	-2.48535262229760	c
-4.31391234000056	-0.60824925537594	-4.57454378284734	c
-6.74036655124083	-1.56931064966421	-5.07412008970715	c
-7.79334032625223	-3.36590916460511	-3.44179718477401	c
-6.36928735934423	-4.16334912779186	-1.35806226108032	c
-3.93548070859177	-3.19944792199700	-0.88720860670554	c
-2.60637669346421	-4.36504651153150	1.32133685338713	c
-3.09438934171055	-3.58529590115586	3.81269212404278	c
-1.96254888694688	-4.76806051070013	5.89839275425534	c
-0.33286112013423	-6.82755276987586	5.50540697611296	c
0.16639705602725	-7.66870461529311	3.04170918001777	c
-0.99224636638614	-6.44775505586839	0.98875367032150	c
0.06031718574924	0.11642428823012	0.93416532839643	f
0.20764730477901	-3.48060461048466	-6.31751918623989	f
4.04655946293941	-6.50845643913644	-7.58788313746282	f
8.43274056291508	-6.53782763707485	-4.80565498606903	f
8.85385564609459	-3.46804416308839	-0.69559119828626	f
6.42629970861760	3.27404090025215	-1.67480975329055	f
7.62609689064383	6.14738699275232	2.40732104998130	f
7.10801478633122	4.21360030101516	7.18832129219933	f
5.38131489259331	-0.62964665583164	7.85495104162874	f
4.22226915183455	-3.52566123965631	3.77379447331858	f
2.50748325838787	1.85518523434688	-6.57592251899482	f
3.12335757544978	6.65417850824911	-7.96720369390383	f
1.07373652865674	10.52259050119098	-5.17559428342852	f
-1.60395041297373	9.43174803083534	-0.91178491961278	f
1.04679589930594	5.46627683057179	3.56596086046598	f
-1.86928017107166	5.13682791771373	7.78638100110398	f
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-9.10765045719764	3.66904437797638	2.68007519043401	f
-6.20548594158791	4.00953745830245	-1.54165725901949	f

-3.44820815915958	1.08649460301369	-6.27332915541501	f
-8.05953103548642	-0.79105179342741	-7.09946752113843	f
-10.11230562796628	-4.30830368428002	-3.87442767751761	f
-7.38905939808986	-5.92499368544206	0.18334943255991	f
-4.67945246817356	-1.65358792291973	4.24784625899883	f
-2.44183534136351	-3.97401360182635	8.25889349528227	f
0.75820702245405	-7.97535774083974	7.48146970787595	f
1.71834810842349	-9.63785648334813	2.66756369336641	f
-0.53593527527993	-7.34787405322203	-1.33923461373457	f

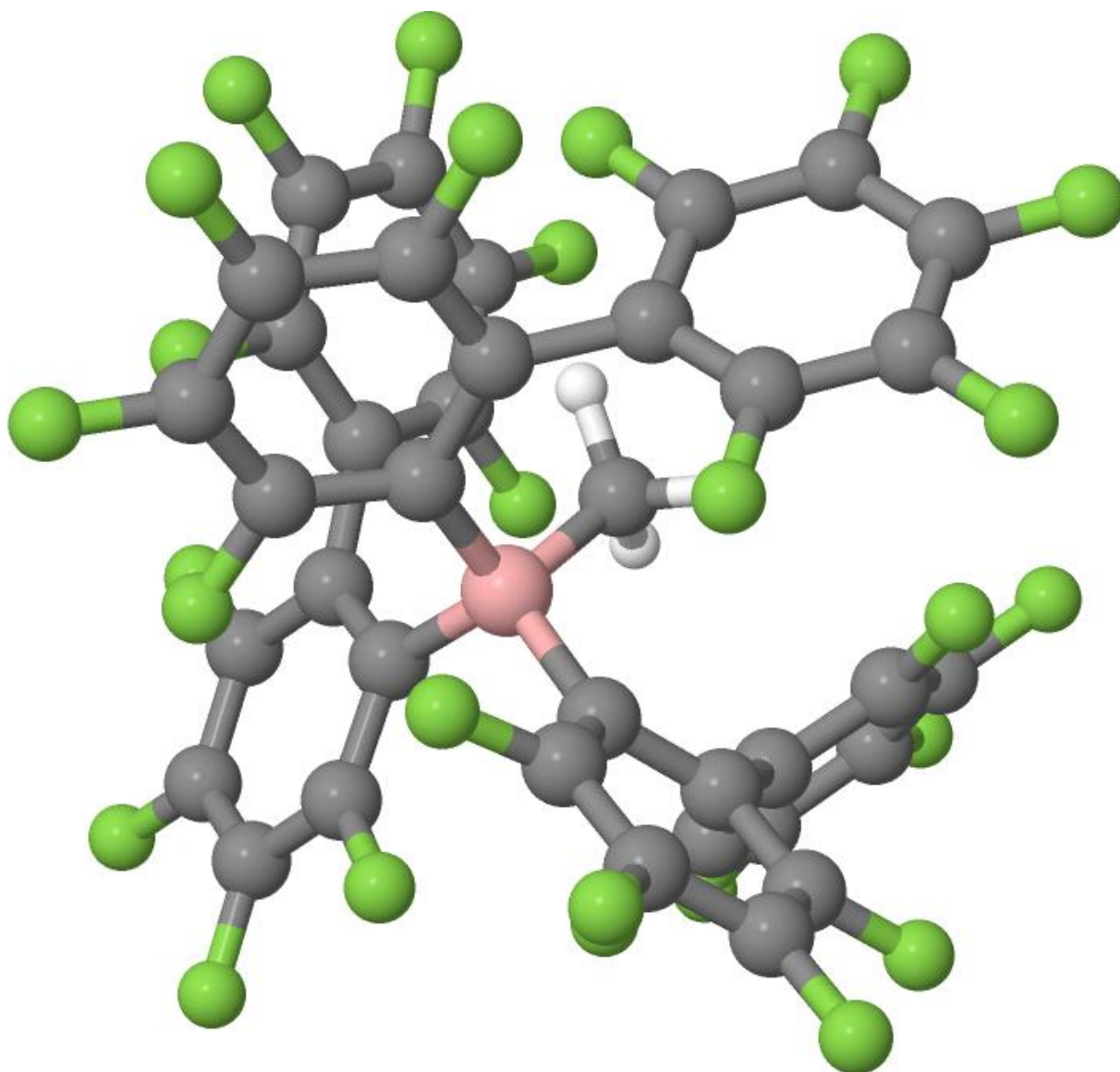
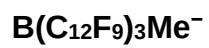
\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	7.41	0.00425	YES	YES
8		a	11.80	0.00709	YES	YES
9		a	13.06	0.00175	YES	YES
10		a	19.64	0.02334	YES	YES
11		a	21.96	0.02066	YES	YES
12		a	22.99	0.01199	YES	YES
13		a	29.49	0.00964	YES	YES
14		a	32.91	0.00605	YES	YES
15		a	35.05	0.02326	YES	YES
16		a	37.88	0.06439	YES	YES
17		a	40.74	0.00299	YES	YES
18		a	43.84	0.06584	YES	YES
19		a	47.10	0.00163	YES	YES
20		a	48.62	0.00222	YES	YES
21		a	52.84	0.00372	YES	YES
22		a	89.85	0.03287	YES	YES
23		a	94.28	0.26435	YES	YES
24		a	95.60	0.29188	YES	YES
25		a	102.54	0.24602	YES	YES
26		a	102.69	0.18437	YES	YES
27		a	103.08	0.05235	YES	YES
28		a	119.52	0.09147	YES	YES
29		a	122.48	0.10206	YES	YES
30		a	123.67	0.12402	YES	YES
31		a	129.74	0.00797	YES	YES
32		a	131.82	0.01050	YES	YES
33		a	132.74	0.00480	YES	YES
34		a	138.73	0.12148	YES	YES
35		a	139.20	0.13056	YES	YES
36		a	154.26	0.02260	YES	YES
37		a	154.88	0.08196	YES	YES
38		a	157.53	0.12573	YES	YES
39		a	158.44	0.10276	YES	YES
40		a	167.85	0.01658	YES	YES
41		a	168.86	0.01453	YES	YES
42		a	177.89	0.12780	YES	YES
43		a	188.92	0.06695	YES	YES
44		a	201.69	3.93790	YES	YES
45		a	203.29	3.95733	YES	YES
46		a	232.11	0.11459	YES	YES
47		a	234.66	0.12729	YES	YES
48		a	240.55	1.08472	YES	YES

49	a	247.06	2.11504	YES	YES
50	a	248.56	3.93488	YES	YES
51	a	249.45	5.02362	YES	YES
52	a	260.59	1.02675	YES	YES
53	a	261.02	1.09486	YES	YES
54	a	262.12	0.27632	YES	YES
55	a	262.81	0.75329	YES	YES
56	a	263.45	0.87925	YES	YES
57	a	264.53	0.44039	YES	YES
58	a	265.65	0.20561	YES	YES
59	a	266.19	0.29728	YES	YES
60	a	266.69	0.51301	YES	YES
61	a	267.63	0.34004	YES	YES
62	a	268.49	0.52988	YES	YES
63	a	287.15	0.15304	YES	YES
64	a	287.85	0.07508	YES	YES
65	a	289.23	0.02085	YES	YES
66	a	299.05	0.21033	YES	YES
67	a	299.69	0.21628	YES	YES
68	a	300.14	0.20340	YES	YES
69	a	325.99	0.00993	YES	YES
70	a	335.07	3.86735	YES	YES
71	a	335.51	1.59061	YES	YES
72	a	336.11	2.40969	YES	YES
73	a	353.97	1.51891	YES	YES
74	a	354.42	1.24200	YES	YES
75	a	356.12	0.35293	YES	YES
76	a	379.03	0.06773	YES	YES
77	a	382.37	0.16000	YES	YES
78	a	383.02	0.08839	YES	YES
79	a	395.04	1.01137	YES	YES
80	a	395.67	1.17363	YES	YES
81	a	401.87	0.16364	YES	YES
82	a	405.26	0.24434	YES	YES
83	a	407.90	0.40789	YES	YES
84	a	408.49	0.59412	YES	YES
85	a	410.03	0.44551	YES	YES
86	a	411.02	0.78765	YES	YES
87	a	432.18	0.16866	YES	YES
88	a	435.59	0.06762	YES	YES
89	a	435.88	0.05149	YES	YES
90	a	442.18	0.01017	YES	YES
91	a	455.86	0.59596	YES	YES
92	a	455.99	0.56799	YES	YES
93	a	460.65	1.64351	YES	YES
94	a	471.84	1.23519	YES	YES
95	a	472.15	1.25010	YES	YES
96	a	480.00	0.84388	YES	YES
97	a	506.43	1.18215	YES	YES
98	a	507.16	1.25241	YES	YES
99	a	512.16	0.28462	YES	YES
100	a	521.29	0.04218	YES	YES
101	a	522.75	0.02655	YES	YES
102	a	523.64	0.07826	YES	YES
103	a	559.68	0.90717	YES	YES
104	a	561.19	1.16373	YES	YES
105	a	563.43	0.72417	YES	YES
106	a	566.70	0.16599	YES	YES
107	a	566.87	0.31036	YES	YES
108	a	567.11	0.44011	YES	YES
109	a	606.69	19.29461	YES	YES
110	a	607.80	19.44637	YES	YES

111	a	623.12	0.00943	YES	YES
112	a	625.36	0.55859	YES	YES
113	a	626.72	0.80703	YES	YES
114	a	628.16	1.42364	YES	YES
115	a	632.41	8.39433	YES	YES
116	a	633.70	8.14744	YES	YES
117	a	639.07	0.64422	YES	YES
118	a	640.60	3.53021	YES	YES
119	a	642.25	2.70631	YES	YES
120	a	653.26	2.30182	YES	YES
121	a	705.31	71.02680	YES	YES
122	a	705.52	63.71453	YES	YES
123	a	710.68	138.59880	YES	YES
124	a	718.81	20.71033	YES	YES
125	a	720.64	24.82867	YES	YES
126	a	757.29	1.22370	YES	YES
127	a	762.83	22.49757	YES	YES
128	a	763.97	22.37640	YES	YES
129	a	780.18	0.52623	YES	YES
130	a	782.42	4.68734	YES	YES
131	a	783.06	5.17424	YES	YES
132	a	813.06	0.23992	YES	YES
133	a	920.15	5.75003	YES	YES
134	a	921.98	5.51514	YES	YES
135	a	938.11	38.56683	YES	YES
136	a	951.72	1.24694	YES	YES
137	a	952.31	1.22726	YES	YES
138	a	967.01	70.46682	YES	YES
139	a	990.62	162.89013	YES	YES
140	a	991.78	172.42349	YES	YES
141	a	992.32	164.21136	YES	YES
142	a	1045.81	203.25832	YES	YES
143	a	1046.12	187.50203	YES	YES
144	a	1050.62	187.64215	YES	YES
145	a	1101.80	199.65628	YES	YES
146	a	1105.53	177.54466	YES	YES
147	a	1106.22	181.52000	YES	YES
148	a	1139.97	2.99981	YES	YES
149	a	1140.02	4.39518	YES	YES
150	a	1140.87	3.36916	YES	YES
151	a	1151.90	1.04540	YES	YES
152	a	1153.14	1.17500	YES	YES
153	a	1155.10	2.52004	YES	YES
154	a	1258.87	13.20305	YES	YES
155	a	1260.39	12.52225	YES	YES
156	a	1262.63	2.96070	YES	YES
157	a	1285.91	37.84947	YES	YES
158	a	1286.47	37.69759	YES	YES
159	a	1288.02	35.43780	YES	YES
160	a	1333.68	12.68334	YES	YES
161	a	1335.28	16.61986	YES	YES
162	a	1335.97	3.12288	YES	YES
163	a	1347.13	0.20099	YES	YES
164	a	1348.41	0.96695	YES	YES
165	a	1349.43	0.36221	YES	YES
166	a	1351.65	15.72983	YES	YES
167	a	1352.62	17.74877	YES	YES
168	a	1355.06	31.04821	YES	YES
169	a	1430.50	130.54743	YES	YES
170	a	1431.28	108.77876	YES	YES
171	a	1434.35	149.90387	YES	YES
172	a	1456.51	174.30211	YES	YES

173	a	1456.88	169.39401	YES	YES
174	a	1457.91	179.35512	YES	YES
175	a	1496.48	405.58074	YES	YES
176	a	1497.02	446.07461	YES	YES
177	a	1497.72	18.67847	YES	YES
178	a	1500.10	85.40529	YES	YES
179	a	1500.79	278.39993	YES	YES
180	a	1501.85	422.67302	YES	YES
181	a	1518.60	104.00764	YES	YES
182	a	1519.90	84.20003	YES	YES
183	a	1522.62	243.02704	YES	YES
184	a	1599.72	29.79722	YES	YES
185	a	1600.40	31.48860	YES	YES
186	a	1601.19	29.51400	YES	YES
187	a	1622.05	26.24931	YES	YES
188	a	1623.05	22.92467	YES	YES
189	a	1623.86	12.17683	YES	YES
190	a	1624.72	11.99617	YES	YES
191	a	1625.95	3.09027	YES	YES
192	a	1626.17	2.77610	YES	YES
193	a	1641.51	19.51258	YES	YES
194	a	1642.43	14.77281	YES	YES
195	a	1644.01	13.77366	YES	YES



Total energy = -4129.3450777730 H = -112365.2606493 eV

HOMO-LUMO Separation

HOMO: 237. 237 a -0.11897338 H = -3.23743 eV

LUMO: 238. 238 a +0.01542600 H = +0.41976 eV

Gap : +0.13439939 H = +3.65720 eV

Number of MOs= 916, Electrons= 474.00, Symmetry: c1

\$coord

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-3.07843866872444	-2.12570426709536	4.80744738938891	c
-5.37081045441982	-3.05509396326687	5.77238198015813	c
-7.63603859533465	-2.51162226195417	4.52627567970990	c
-7.51600993823230	-1.03283943105571	2.33931359744477	c
-5.20109213728828	-0.12747289284690	1.37888531549841	c
-5.51391252730861	1.48375619082728	-0.92898256947033	c
-5.60645239715684	4.13480680928765	-0.77459848681824	c
-6.04971987791418	5.65707159494517	-2.90737381603866	c
-6.49212749705241	4.51153538573510	-5.25851282859784	c
-6.45106981048571	1.86448893460188	-5.46741920649546	c
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1.86492403767224	8.34470883844729	3.57193285011916	c
3.12574682486669	7.14687200838411	1.58125714960317	c
2.60263619506894	4.62563313044320	0.90265940679299	c
4.19051991983944	3.69873269172074	-1.25220865848921	c
3.59539053448952	4.33367812790971	-3.76547988948921	c
5.10328170401158	3.57391693569988	-5.80931825805761	c
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8.01161894916394	1.59291100620079	-2.85874081979730	c
6.46813117606061	2.39108142179860	-0.84839633869445	c
2.24186122100717	-1.84777066389792	2.45473859726878	c
3.79668861231615	-1.27042470651652	4.53973718536782	c
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6.22107989607667	-5.14994258496130	4.26673762510269	c
4.69484680059122	-5.83639799671291	2.22155803761405	c
2.74735212062751	-4.25310732488201	1.32874766816351	c
1.28250353410080	-5.37835346439644	-0.81666295707928	c
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0.96555690332643	-6.48205126649965	-5.32162927602174	c
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10.16072999988854	0.32820730321308	-2.41134387416850	f
7.25313214180765	1.88431715806448	1.50603924032464	f
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7.15477834399721	-2.12573330251272	7.43480014545937	f
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-1.96081882703543	-6.90461409246407	1.90985925723309	f
-0.12296917884604	0.00459947015354	-1.72159932644596	c
-0.79549250687512	1.80063690833100	-2.57653978361923	h
-1.41302046651487	-1.50656582649226	-2.39769620408639	h
1.75590965014833	-0.39440983308948	-2.56677709897265	h

\$vibrational spectrum

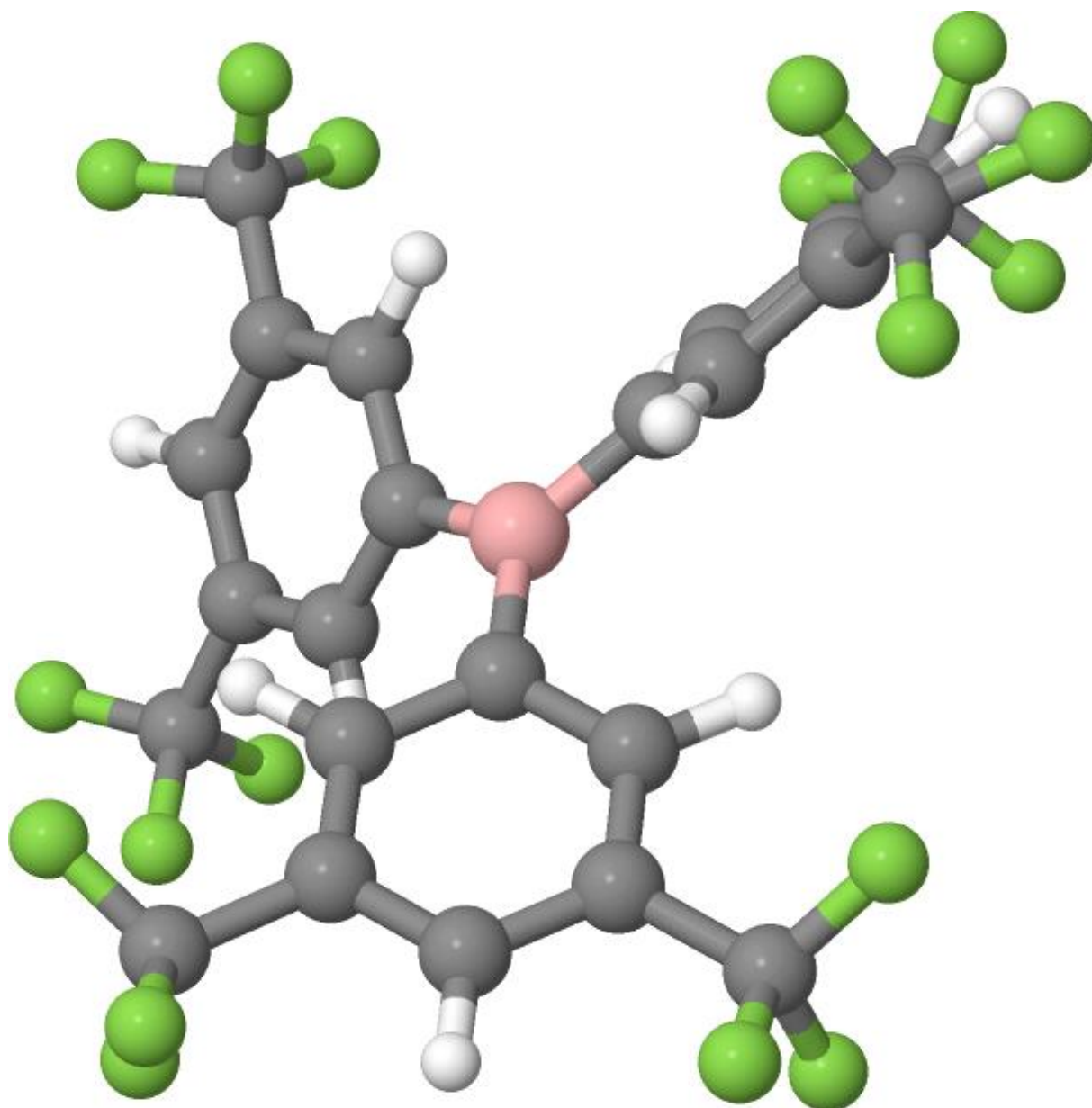
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3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		8.31	0.01373	YES	YES
8	a		10.02	0.01286	YES	YES
9	a		16.42	0.01176	YES	YES
10	a		20.90	0.01084	YES	YES
11	a		23.06	0.01457	YES	YES
12	a		25.33	0.00825	YES	YES
13	a		33.25	0.00698	YES	YES
14	a		33.98	0.00504	YES	YES
15	a		36.30	0.02030	YES	YES
16	a		37.18	0.01507	YES	YES
17	a		37.40	0.00914	YES	YES
18	a		46.77	0.00018	YES	YES
19	a		51.52	0.00045	YES	YES
20	a		52.42	0.00071	YES	YES
21	a		56.26	0.00986	YES	YES
22	a		95.26	0.01310	YES	YES
23	a		97.11	0.07224	YES	YES
24	a		97.81	0.08670	YES	YES
25	a		106.57	0.09390	YES	YES
26	a		107.14	0.05544	YES	YES
27	a		108.13	0.10419	YES	YES
28	a		121.30	0.04155	YES	YES
29	a		122.27	0.11527	YES	YES
30	a		123.32	0.11980	YES	YES
31	a		134.03	0.00986	YES	YES
32	a		134.57	0.00751	YES	YES
33	a		135.22	0.00681	YES	YES
34	a		140.45	0.17498	YES	YES
35	a		141.22	0.15833	YES	YES
36	a		152.98	0.00442	YES	YES
37	a		156.79	0.01907	YES	YES
38	a		158.03	0.05460	YES	YES
39	a		158.93	0.04646	YES	YES
40	a		173.66	0.09230	YES	YES
41	a		173.78	0.08004	YES	YES
42	a		176.37	0.06349	YES	YES

43	a	197.35	0.01784	YES	YES
44	a	215.03	1.24349	YES	YES
45	a	215.89	1.37443	YES	YES
46	a	236.78	0.35875	YES	YES
47	a	237.78	0.59231	YES	YES
48	a	244.69	1.66700	YES	YES
49	a	247.02	0.05118	YES	YES
50	a	248.90	3.98621	YES	YES
51	a	251.65	4.08787	YES	YES
52	a	261.48	0.03266	YES	YES
53	a	261.73	0.01609	YES	YES
54	a	262.21	0.03959	YES	YES
55	a	266.26	0.06709	YES	YES
56	a	266.49	0.08742	YES	YES
57	a	267.84	0.00785	YES	YES
58	a	268.04	0.06033	YES	YES
59	a	268.06	0.04869	YES	YES
60	a	268.74	0.05514	YES	YES
61	a	290.70	0.48406	YES	YES
62	a	291.76	0.40568	YES	YES
63	a	293.52	0.10744	YES	YES
64	a	294.77	0.13520	YES	YES
65	a	296.57	0.19847	YES	YES
66	a	300.29	0.30407	YES	YES
67	a	300.53	0.23237	YES	YES
68	a	300.75	0.25969	YES	YES
69	a	328.29	0.02185	YES	YES
70	a	336.61	4.81342	YES	YES
71	a	338.25	1.23145	YES	YES
72	a	338.91	1.21361	YES	YES
73	a	354.69	1.18533	YES	YES
74	a	355.43	1.06617	YES	YES
75	a	356.80	0.00214	YES	YES
76	a	382.35	0.04307	YES	YES
77	a	382.50	0.01647	YES	YES
78	a	383.43	0.03634	YES	YES
79	a	398.14	0.64008	YES	YES
80	a	399.71	0.57642	YES	YES
81	a	402.77	0.21859	YES	YES
82	a	406.20	0.25503	YES	YES
83	a	406.51	0.15864	YES	YES
84	a	407.72	0.37934	YES	YES
85	a	415.62	1.29329	YES	YES
86	a	416.13	1.23138	YES	YES
87	a	426.40	0.16292	YES	YES
88	a	433.71	0.12417	YES	YES
89	a	435.36	0.08060	YES	YES
90	a	435.66	0.08669	YES	YES
91	a	452.35	0.41703	YES	YES
92	a	454.47	0.85891	YES	YES
93	a	454.96	0.83686	YES	YES
94	a	461.82	0.92643	YES	YES
95	a	469.81	0.79346	YES	YES
96	a	470.18	0.62045	YES	YES
97	a	477.88	0.98736	YES	YES
98	a	507.05	0.95594	YES	YES
99	a	507.67	1.12178	YES	YES
100	a	513.06	0.35274	YES	YES
101	a	542.36	0.22631	YES	YES
102	a	544.85	0.15634	YES	YES
103	a	545.35	0.22764	YES	YES
104	a	554.86	1.90209	YES	YES

105	a	555.14	1.62346	YES	YES
106	a	559.93	0.14963	YES	YES
107	a	566.58	0.30078	YES	YES
108	a	566.75	0.44629	YES	YES
109	a	566.82	0.47286	YES	YES
110	a	588.88	13.87265	YES	YES
111	a	591.00	15.27915	YES	YES
112	a	627.26	0.10949	YES	YES
113	a	629.08	2.35411	YES	YES
114	a	630.52	2.22531	YES	YES
115	a	631.34	0.12060	YES	YES
116	a	631.94	0.31749	YES	YES
117	a	632.04	0.11030	YES	YES
118	a	640.50	0.25711	YES	YES
119	a	641.33	0.09314	YES	YES
120	a	643.12	0.19252	YES	YES
121	a	663.90	3.88315	YES	YES
122	a	695.05	29.33548	YES	YES
123	a	695.75	36.84606	YES	YES
124	a	706.38	129.01324	YES	YES
125	a	711.18	22.61059	YES	YES
126	a	712.28	23.46494	YES	YES
127	a	750.49	1.54686	YES	YES
128	a	761.24	4.98337	YES	YES
129	a	762.43	4.47721	YES	YES
130	a	780.59	0.24374	YES	YES
131	a	782.00	4.88413	YES	YES
132	a	782.53	3.48580	YES	YES
133	a	797.27	0.13147	YES	YES
134	a	806.18	60.71806	YES	YES
135	a	813.08	54.77458	YES	YES
136	a	921.37	12.17102	YES	YES
137	a	934.51	9.44267	YES	YES
138	a	937.91	8.83854	YES	YES
139	a	957.48	16.85987	YES	YES
140	a	961.05	1.77822	YES	YES
141	a	963.78	3.36354	YES	YES
142	a	990.82	148.06618	YES	YES
143	a	992.10	150.95294	YES	YES
144	a	992.25	156.92115	YES	YES
145	a	1042.33	212.96518	YES	YES
146	a	1043.11	239.43212	YES	YES
147	a	1047.60	191.86635	YES	YES
148	a	1098.44	223.46775	YES	YES
149	a	1099.40	132.89442	YES	YES
150	a	1100.57	147.26439	YES	YES
151	a	1136.10	3.85599	YES	YES
152	a	1136.35	6.01354	YES	YES
153	a	1136.99	3.77312	YES	YES
154	a	1152.55	3.49305	YES	YES
155	a	1153.26	3.50134	YES	YES
156	a	1154.57	3.82527	YES	YES
157	a	1253.28	7.72907	YES	YES
158	a	1255.94	9.76295	YES	YES
159	a	1257.58	1.34590	YES	YES
160	a	1276.59	13.17356	YES	YES
161	a	1277.74	19.55338	YES	YES
162	a	1278.51	18.31544	YES	YES
163	a	1281.51	25.37940	YES	YES
164	a	1325.55	16.84318	YES	YES
165	a	1326.50	18.56438	YES	YES
166	a	1327.36	10.89149	YES	YES

167	a	1340.51	7.15687	YES	YES
168	a	1341.40	7.12303	YES	YES
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170	a	1344.26	1.66812	YES	YES
171	a	1344.72	1.51871	YES	YES
172	a	1344.87	2.58243	YES	YES
173	a	1421.64	157.34880	YES	YES
174	a	1422.58	137.85426	YES	YES
175	a	1423.30	133.14892	YES	YES
176	a	1441.24	90.68951	YES	YES
177	a	1445.49	138.63748	YES	YES
178	a	1449.16	91.53293	YES	YES
179	a	1451.37	69.66892	YES	YES
180	a	1452.82	16.58594	YES	YES
181	a	1492.95	310.99563	YES	YES
182	a	1493.84	146.51615	YES	YES
183	a	1493.94	433.31239	YES	YES
184	a	1497.35	144.93895	YES	YES
185	a	1498.31	76.46230	YES	YES
186	a	1499.96	552.79904	YES	YES
187	a	1517.15	105.82869	YES	YES
188	a	1517.57	115.14839	YES	YES
189	a	1519.87	294.44358	YES	YES
190	a	1599.20	32.05525	YES	YES
191	a	1600.47	29.80910	YES	YES
192	a	1601.30	37.39869	YES	YES
193	a	1621.54	22.77230	YES	YES
194	a	1621.83	13.86915	YES	YES
195	a	1622.07	9.60702	YES	YES
196	a	1622.57	11.33583	YES	YES
197	a	1623.03	30.52878	YES	YES
198	a	1623.91	6.16949	YES	YES
199	a	1638.42	18.31593	YES	YES
200	a	1639.01	16.32416	YES	YES
201	a	1639.72	13.82930	YES	YES
202	a	2949.57	14.10782	YES	YES
203	a	3026.75	29.89144	YES	YES
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B(C₆H₃-3,5-(CF₃)₂)₃



Total energy = -2740.1651999490 H = -74563.7313219 eV

HOMO-LUMO Separation

HOMO: 160. 160 a -0.27536303 H = -7.49301 eV

LUMO: 161. 161 a -0.14850672 H = -4.04108 eV

Gap : +0.12685631 H = +3.45194 eV

Number of MOs= 620, Electrons= 320.00, Symmetry: c1

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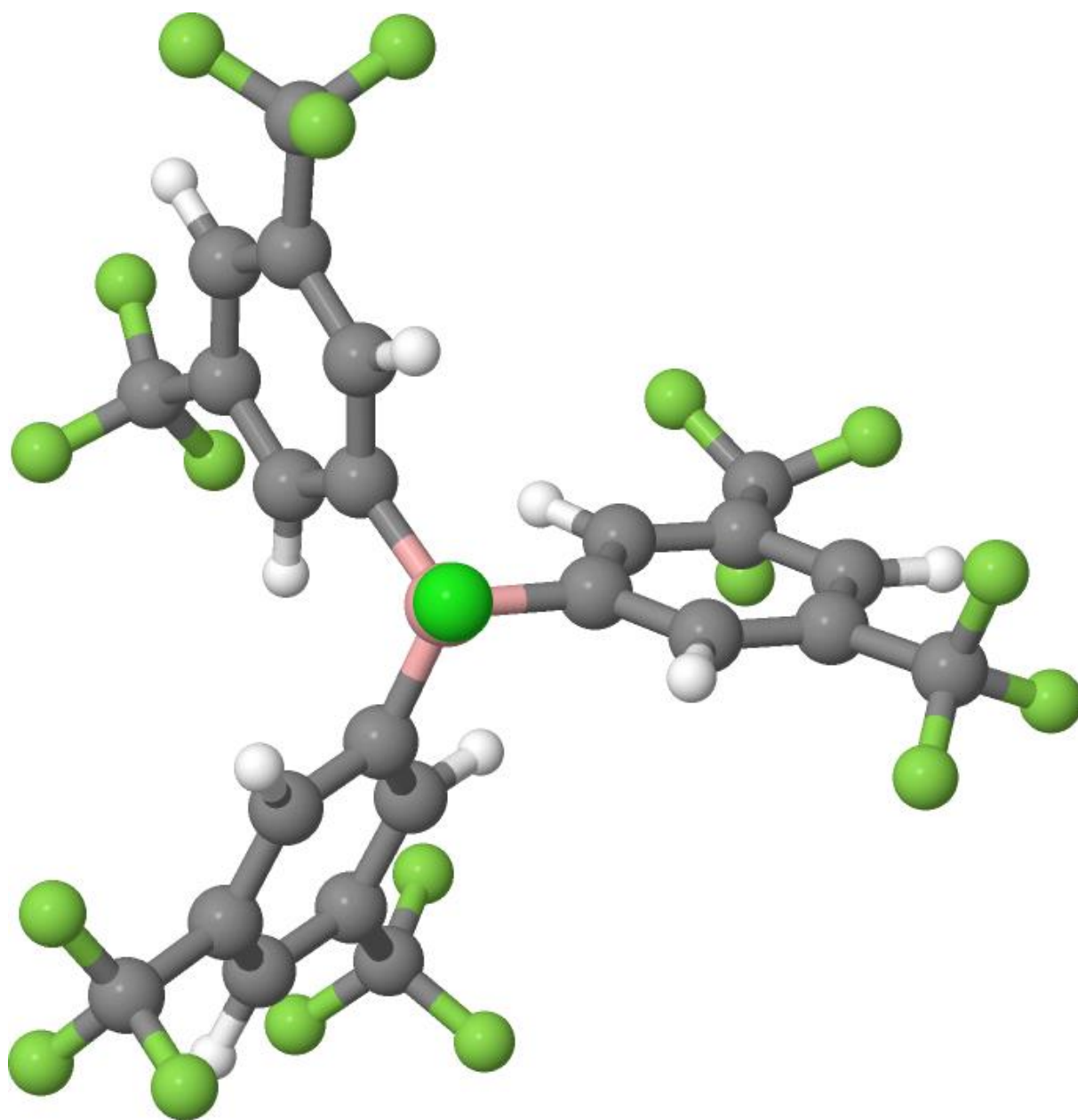
\$vibrational spectrum

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3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
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9		a	14.50	0.00824	YES	YES
10		a	20.18	0.00022	YES	YES
11		a	24.13	0.06909	YES	YES
12		a	25.52	0.09277	YES	YES
13		a	25.63	0.10704	YES	YES
14		a	26.53	0.07113	YES	YES
15		a	27.80	0.10063	YES	YES
16		a	28.79	0.02963	YES	YES
17		a	29.51	0.23532	YES	YES
18		a	36.91	0.03228	YES	YES
19		a	83.21	0.18869	YES	YES
20		a	84.03	0.08728	YES	YES
21		a	85.95	0.00153	YES	YES
22		a	87.42	0.52864	YES	YES
23		a	96.74	1.29522	YES	YES
24		a	98.93	1.57026	YES	YES
25		a	126.65	0.30938	YES	YES
26		a	129.22	0.33570	YES	YES
27		a	138.59	0.69161	YES	YES
28		a	143.94	0.51892	YES	YES
29		a	144.64	0.63917	YES	YES
30		a	159.24	0.06950	YES	YES
31		a	183.21	0.00840	YES	YES
32		a	202.75	0.13753	YES	YES
33		a	206.18	0.15792	YES	YES
34		a	247.29	0.10128	YES	YES
35		a	252.48	0.12279	YES	YES
36		a	254.62	0.21347	YES	YES
37		a	274.67	1.45111	YES	YES
38		a	276.10	1.87312	YES	YES
39		a	278.89	0.06262	YES	YES
40		a	303.25	1.79125	YES	YES
41		a	303.87	1.25343	YES	YES
42		a	318.73	0.79971	YES	YES
43		a	324.13	0.93674	YES	YES
44		a	333.81	0.20981	YES	YES
45		a	334.82	0.46117	YES	YES
46		a	354.15	1.96905	YES	YES
47		a	362.98	8.12136	YES	YES
48		a	363.45	7.70975	YES	YES
49		a	396.01	0.13814	YES	YES
50		a	397.69	0.20944	YES	YES
51		a	402.10	0.03537	YES	YES
52		a	425.83	2.53399	YES	YES
53		a	438.47	1.67596	YES	YES
54		a	438.64	2.42539	YES	YES
55		a	462.21	0.12169	YES	YES
56		a	489.09	0.31200	YES	YES
57		a	489.35	1.41239	YES	YES

58	a	491.22	0.35969	YES	YES
59	a	492.43	1.30214	YES	YES
60	a	493.44	0.79567	YES	YES
61	a	545.64	1.95921	YES	YES
62	a	554.71	0.77119	YES	YES
63	a	555.42	0.57632	YES	YES
64	a	556.72	0.05110	YES	YES
65	a	575.99	16.61125	YES	YES
66	a	577.12	14.02061	YES	YES
67	a	585.77	1.14222	YES	YES
68	a	586.41	1.47112	YES	YES
69	a	589.63	0.41069	YES	YES
70	a	647.06	47.44758	YES	YES
71	a	648.44	42.78875	YES	YES
72	a	654.47	7.70002	YES	YES
73	a	655.22	3.70372	YES	YES
74	a	656.57	1.60586	YES	YES
75	a	667.43	35.03577	YES	YES
76	a	668.71	30.49431	YES	YES
77	a	669.19	24.72273	YES	YES
78	a	686.83	5.37933	YES	YES
79	a	696.73	0.03352	YES	YES
80	a	707.54	10.88612	YES	YES
81	a	708.58	5.42678	YES	YES
82	a	721.30	31.83868	YES	YES
83	a	728.76	0.41692	YES	YES
84	a	729.23	0.40210	YES	YES
85	a	815.79	0.01636	YES	YES
86	a	837.26	15.08430	YES	YES
87	a	837.49	15.15783	YES	YES
88	a	837.88	13.78572	YES	YES
89	a	897.71	17.39960	YES	YES
90	a	901.00	18.27793	YES	YES
91	a	901.65	37.58978	YES	YES
92	a	921.64	1.50948	YES	YES
93	a	924.44	0.20611	YES	YES
94	a	925.17	0.18828	YES	YES
95	a	932.92	7.78864	YES	YES
96	a	934.96	7.78756	YES	YES
97	a	941.79	2.05365	YES	YES
98	a	974.45	20.19818	YES	YES
99	a	975.90	20.14103	YES	YES
100	a	984.07	0.07389	YES	YES
101	a	988.99	15.04380	YES	YES
102	a	989.57	20.15850	YES	YES
103	a	1091.49	9.39727	YES	YES
104	a	1092.99	0.75641	YES	YES
105	a	1093.40	0.17731	YES	YES
106	a	1094.63	0.53745	YES	YES
107	a	1096.41	20.07715	YES	YES
108	a	1097.34	16.57130	YES	YES
109	a	1141.65	77.33825	YES	YES
110	a	1145.55	35.86275	YES	YES
111	a	1146.29	65.51857	YES	YES
112	a	1149.55	38.60940	YES	YES
113	a	1150.26	674.92089	YES	YES
114	a	1151.15	197.65894	YES	YES
115	a	1151.70	164.83349	YES	YES
116	a	1173.22	168.40156	YES	YES
117	a	1174.94	137.86051	YES	YES
118	a	1175.64	113.62109	YES	YES
119	a	1181.56	423.30064	YES	YES

120	a	1181.98	462.00403	YES	YES
121	a	1186.95	3.68213	YES	YES
122	a	1208.36	539.46356	YES	YES
123	a	1212.64	576.41509	YES	YES
124	a	1248.45	500.18020	YES	YES
125	a	1250.49	635.07484	YES	YES
126	a	1251.48	583.04795	YES	YES
127	a	1261.61	56.61307	YES	YES
128	a	1265.34	135.31338	YES	YES
129	a	1269.73	124.55487	YES	YES
130	a	1344.85	0.70102	YES	YES
131	a	1352.99	51.53275	YES	YES
132	a	1356.17	39.78455	YES	YES
133	a	1358.39	12.35461	YES	YES
134	a	1367.43	8.30272	YES	YES
135	a	1370.30	9.72919	YES	YES
136	a	1416.65	0.12128	YES	YES
137	a	1422.40	1.83085	YES	YES
138	a	1424.26	1.61025	YES	YES
139	a	1447.55	0.33636	YES	YES
140	a	1450.45	1.42137	YES	YES
141	a	1451.62	1.72509	YES	YES
142	a	1605.18	19.14066	YES	YES
143	a	1606.28	18.97372	YES	YES
144	a	1606.99	54.16040	YES	YES
145	a	1607.11	53.22596	YES	YES
146	a	1607.81	37.16000	YES	YES
147	a	1608.74	60.80326	YES	YES
148	a	3111.84	1.05760	YES	YES
149	a	3117.67	0.71546	YES	YES
150	a	3118.68	0.82334	YES	YES
151	a	3119.38	0.84783	YES	YES
152	a	3121.48	0.59045	YES	YES
153	a	3121.94	0.52030	YES	YES
154	a	3136.16	1.15427	YES	YES
155	a	3137.10	1.32720	YES	YES
156	a	3140.03	1.44463	YES	YES

B(C₆H₃-3,5-(CF₃)₂)₃Cl⁻



Total energy = -3200.4307213990 H = -87088.2005323 eV

HOMO-LUMO Separation

HOMO: 169. 169 a -0.12629663 H = -3.43671 eV

LUMO: 170. 170 a +0.01393169 H = +0.37910 eV

Gap : +0.14022832 H = +3.81581 eV

Number of MOs= 638, Electrons= 338.00, Symmetry: c1

\$coord

-1.88348659952856	6.20779956622850	-1.35584049522051	c
-1.03531097217867	3.91748937011974	-0.28418829756175	c
1.21536225494494	2.72849548304113	-1.08304468781323	c
2.59355793161167	3.96397857020048	-3.01561803597875	c
1.76425007152319	6.24242313831126	-4.09946607126189	c
-0.48869424872616	7.38811245468875	-3.27354402589346	c
-2.23975521543533	-4.17895666033848	-4.47927094681957	c
-0.78675445948503	-6.36464736649947	-4.86375355730331	c
1.60148238560433	-6.52494535978548	-3.71360557117042	c
2.50545851400873	-4.53592722476933	-2.19726588262452	c
1.08394442083627	-2.31125300928896	-1.78451246543154	c
-1.30590718839925	-2.18936247074375	-2.97406710996728	c
1.20378257304914	-0.41086798033169	2.97708724977780	c
2.70587044411338	0.42436928942099	5.02520802626259	c
1.90164416153539	0.19473165646118	7.54840787379024	c
-0.45907808982568	-0.87920731567971	8.11717383038621	c
-1.98337371555463	-1.73158023574248	6.12207058459096	c
-1.15512728744533	-1.50016933723669	3.59986147830627	c
2.11959767581126	-0.02046505526324	0.03709974511849	b
3.21608836394177	7.42077456736406	-6.25184063167806	c
-4.26578014140855	7.41764339927826	-0.36428330819889	c
-6.11839258081571	5.69227937853327	0.05132164996531	f
-5.22078465405243	9.17178806700320	-1.98398255287381	f
-3.87937593520299	8.62506738526728	1.87599169721388	f
2.35629967776228	6.61368651108618	-8.54151501922194	f
5.71556667911343	6.86741074360784	-6.17432010900607	f
3.00970357306491	9.98776415908281	-6.27186685711435	f
-4.46752591596434	-2.99707660037726	6.71615982812721	c
-6.21150370579581	-2.65206871043169	4.87111950405150	f
-5.49768242878627	-2.11995406587762	8.90487563186721	f
-4.20576833047065	-5.54209476143610	7.01162399370860	f
3.61221090106087	1.01266141727592	9.67754920717090	c
2.28699940705841	1.69685986546723	11.77598295266885	f
5.08857427010663	3.00577063246755	9.03809355722845	f
5.20308881953981	-0.87415320137617	10.41539402257135	f
3.25313504110931	-8.79744956469862	-4.20332518396617	c
4.90177537087347	-8.39597142960387	-6.13999046290862	f
1.87997433751665	-10.87854461757812	-4.84285978214029	f
4.66902022746255	-9.43025783640393	-2.16340514186327	f
-4.85069683179876	-4.01187394956621	-5.61088297778685	c
-5.07372478971967	-5.41693166798115	-7.75453872650152	f
-5.50027433259922	-1.60735936441675	-6.21494007757453	f
-6.65675056185515	-4.87419739772316	-3.98953732674416	f
-2.17509450140367	3.04323756901411	1.22656629488245	h
4.38352003668606	3.11239095401498	-3.65139799597033	h
-1.14317960448839	9.17202100302886	-4.11146920980347	h
-1.49871932040229	-7.91476067105940	-6.04919951928488	h
4.39228059560309	-4.67464029835350	-1.32729856725378	h
-2.47399498025698	-0.47718237734759	-2.75914977894756	h
4.56968952378425	1.25340076758736	4.60665857727658	h
-1.10568792634448	-1.03575820812535	10.08513646098721	h
-2.39722712146378	-2.19857876194153	2.07993093674049	h

5.79530195821073

-0.09594268628607

-0.02070406935207

c1

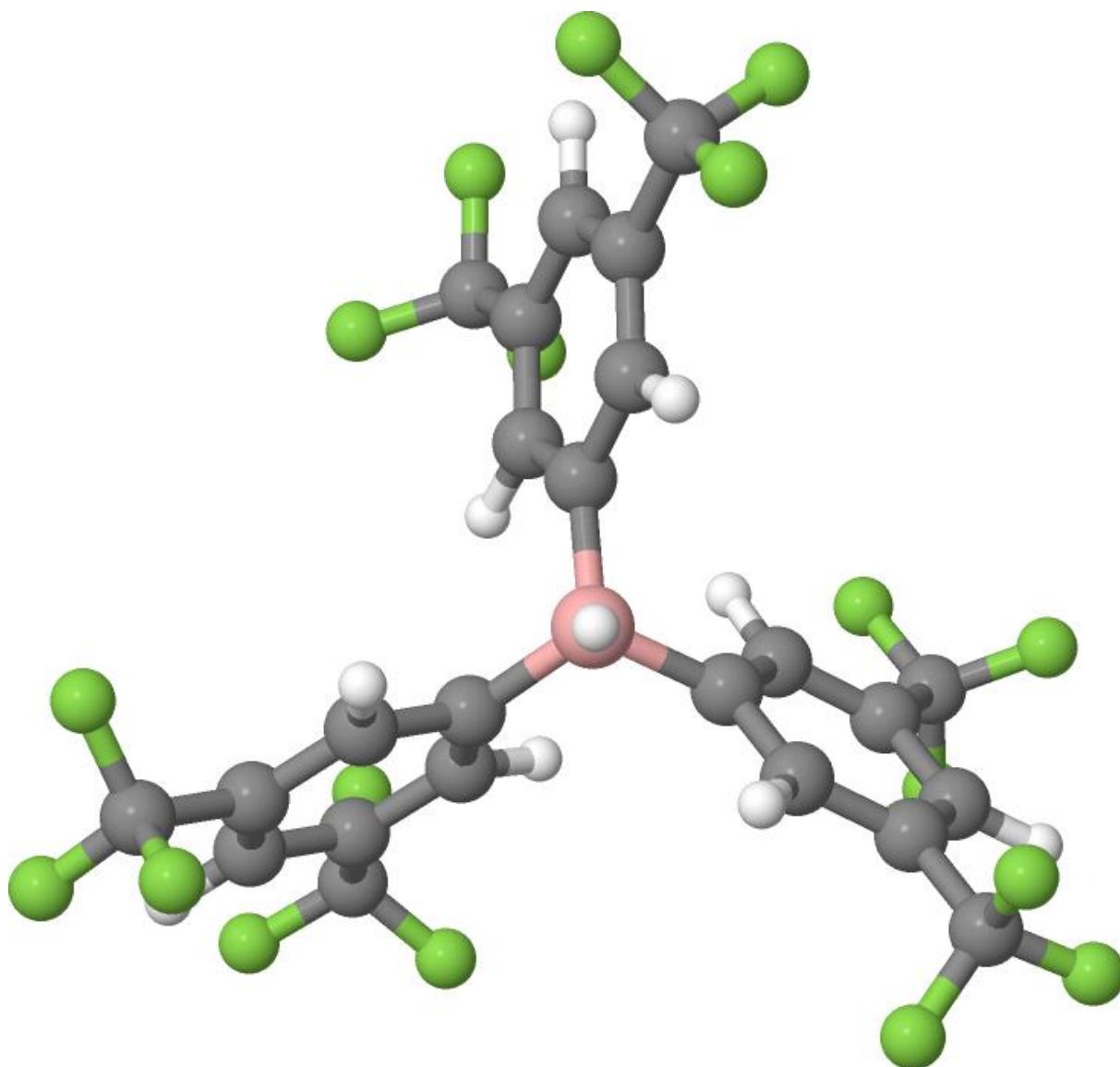
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	1.95	0.00815	YES	YES
8		a	6.62	0.01071	YES	YES
9		a	8.81	0.00017	YES	YES
10		a	20.45	0.01430	YES	YES
11		a	21.39	0.01285	YES	YES
12		a	29.59	0.01609	YES	YES
13		a	29.78	0.02544	YES	YES
14		a	30.31	0.00421	YES	YES
15		a	31.93	0.00940	YES	YES
16		a	34.63	0.02893	YES	YES
17		a	37.19	0.01622	YES	YES
18		a	42.59	0.02606	YES	YES
19		a	82.88	0.05182	YES	YES
20		a	84.41	0.55583	YES	YES
21		a	85.85	0.62106	YES	YES
22		a	88.99	0.14064	YES	YES
23		a	95.20	0.28445	YES	YES
24		a	97.44	0.22072	YES	YES
25		a	110.89	0.06423	YES	YES
26		a	112.04	0.04837	YES	YES
27		a	140.07	0.01843	YES	YES
28		a	141.29	0.01424	YES	YES
29		a	143.62	0.07938	YES	YES
30		a	144.45	0.15382	YES	YES
31		a	164.12	2.49020	YES	YES
32		a	168.11	2.79151	YES	YES
33		a	190.58	0.44501	YES	YES
34		a	221.29	0.08495	YES	YES
35		a	223.85	0.07060	YES	YES
36		a	237.15	1.16080	YES	YES
37		a	259.49	0.22092	YES	YES
38		a	260.01	0.37376	YES	YES
39		a	275.06	0.71266	YES	YES
40		a	276.32	2.37130	YES	YES
41		a	278.50	2.48047	YES	YES
42		a	282.62	0.82681	YES	YES
43		a	300.25	0.44637	YES	YES
44		a	300.91	0.07402	YES	YES
45		a	303.30	0.27353	YES	YES
46		a	339.29	1.60408	YES	YES
47		a	341.16	1.64914	YES	YES
48		a	343.02	0.32399	YES	YES
49		a	372.27	3.65137	YES	YES
50		a	373.23	3.82611	YES	YES
51		a	379.93	15.83580	YES	YES
52		a	392.87	3.71692	YES	YES
53		a	393.97	4.43986	YES	YES
54		a	401.23	1.17640	YES	YES
55		a	437.69	1.44089	YES	YES
56		a	440.90	1.38306	YES	YES

57	a	441.01	1.32237	YES	YES
58	a	488.87	0.19265	YES	YES
59	a	489.16	0.54323	YES	YES
60	a	489.69	0.24633	YES	YES
61	a	497.70	0.56891	YES	YES
62	a	502.84	0.03266	YES	YES
63	a	504.25	0.20396	YES	YES
64	a	553.09	2.13154	YES	YES
65	a	553.42	2.07071	YES	YES
66	a	555.10	0.32662	YES	YES
67	a	570.78	6.91661	YES	YES
68	a	571.84	7.16865	YES	YES
69	a	575.97	4.20031	YES	YES
70	a	588.58	2.00947	YES	YES
71	a	591.41	2.62575	YES	YES
72	a	592.82	3.79065	YES	YES
73	a	650.20	5.71675	YES	YES
74	a	651.06	1.15383	YES	YES
75	a	651.32	3.66217	YES	YES
76	a	656.25	45.56319	YES	YES
77	a	657.41	31.70857	YES	YES
78	a	666.21	83.65462	YES	YES
79	a	667.32	20.86888	YES	YES
80	a	667.67	13.88078	YES	YES
81	a	679.07	2.17238	YES	YES
82	a	705.33	15.81969	YES	YES
83	a	705.68	18.12981	YES	YES
84	a	706.18	5.15464	YES	YES
85	a	724.68	4.44682	YES	YES
86	a	725.35	5.52824	YES	YES
87	a	732.89	31.89460	YES	YES
88	a	819.97	38.78527	YES	YES
89	a	832.89	8.05291	YES	YES
90	a	833.10	10.10167	YES	YES
91	a	845.90	10.34713	YES	YES
92	a	876.90	23.67681	YES	YES
93	a	877.17	22.12441	YES	YES
94	a	877.89	11.55565	YES	YES
95	a	889.20	1.69987	YES	YES
96	a	891.52	3.10038	YES	YES
97	a	909.40	1.47150	YES	YES
98	a	928.46	11.47397	YES	YES
99	a	932.90	10.36110	YES	YES
100	a	942.01	7.99110	YES	YES
101	a	943.15	0.81607	YES	YES
102	a	943.76	9.33488	YES	YES
103	a	984.17	2.78481	YES	YES
104	a	984.43	4.77741	YES	YES
105	a	984.74	4.56866	YES	YES
106	a	1082.78	2.52635	YES	YES
107	a	1083.37	4.38987	YES	YES
108	a	1086.95	21.41213	YES	YES
109	a	1092.12	13.35396	YES	YES
110	a	1093.70	16.90818	YES	YES
111	a	1095.04	47.54454	YES	YES
112	a	1123.26	93.26504	YES	YES
113	a	1124.07	33.18615	YES	YES
114	a	1125.16	98.77260	YES	YES
115	a	1126.51	219.24356	YES	YES
116	a	1128.25	80.12286	YES	YES
117	a	1129.31	521.04734	YES	YES
118	a	1130.07	397.65893	YES	YES

119	a	1131.40	280.34919	YES	YES
120	a	1133.67	607.15588	YES	YES
121	a	1155.72	70.94200	YES	YES
122	a	1157.49	62.14166	YES	YES
123	a	1159.82	118.34297	YES	YES
124	a	1167.99	88.23290	YES	YES
125	a	1169.20	113.04651	YES	YES
126	a	1172.29	40.68267	YES	YES
127	a	1249.20	224.38880	YES	YES
128	a	1249.70	252.96984	YES	YES
129	a	1251.69	904.39795	YES	YES
130	a	1256.79	200.27622	YES	YES
131	a	1262.29	124.35444	YES	YES
132	a	1266.06	248.38132	YES	YES
133	a	1335.36	371.13972	YES	YES
134	a	1337.00	368.66177	YES	YES
135	a	1344.44	53.75714	YES	YES
136	a	1360.39	0.84801	YES	YES
137	a	1361.76	4.10400	YES	YES
138	a	1363.68	10.28836	YES	YES
139	a	1419.30	2.83201	YES	YES
140	a	1420.37	3.78696	YES	YES
141	a	1422.96	8.17086	YES	YES
142	a	1448.33	0.56769	YES	YES
143	a	1450.17	0.71534	YES	YES
144	a	1451.42	1.01705	YES	YES
145	a	1591.62	0.61639	YES	YES
146	a	1593.23	0.88111	YES	YES
147	a	1596.73	3.22631	YES	YES
148	a	1606.00	14.55454	YES	YES
149	a	1607.24	13.02519	YES	YES
150	a	1608.13	31.39295	YES	YES
151	a	3092.06	1.53990	YES	YES
152	a	3095.56	1.55550	YES	YES
153	a	3098.06	1.97363	YES	YES
154	a	3111.18	4.02846	YES	YES
155	a	3112.43	3.15000	YES	YES
156	a	3116.36	2.61864	YES	YES
157	a	3137.82	0.42424	YES	YES
158	a	3138.94	0.39435	YES	YES
159	a	3140.68	0.43672	YES	YES

B(C₆H₃-3,5-(CF₃)₂)₃H⁻



Total energy = -2740.8644218920 H = -74582.7581299 eV

HOMO-LUMO Separation

HOMO: 161. 161 a -0.12139259 H = -3.30326 eV

LUMO: 162. 162 a +0.01897146 H = +0.51624 eV

Gap : +0.14036405 H = +3.81950 eV

Number of MOs= 622, Electrons= 322.00, Symmetry: c1

\$coord

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1.35044341211697	-1.87122750726142	2.09353924346237	c
-3.06041714662886	-0.48387043677802	-0.04397468872702	c
3.42461846016456	-2.21216506900966	0.44899818365908	c
5.11125752036676	-4.26735385839993	0.69333994288236	c
4.78731193545936	-6.04587115698883	2.62734613256752	c
2.74738606638739	-5.74032446990161	4.31051507535043	c
1.07280404678148	-3.70009570872902	4.03332078109538	c
-5.56917639526742	0.26886064915595	0.47647449762139	c
-2.71210685912240	-1.98124557672017	-2.23717923599290	c
-4.73219940989309	-2.66192050419341	-3.82445958039777	c
-7.21211738714732	-1.89110551509880	-3.25304018864770	c
-7.61710168817805	-0.42418920254155	-1.08236658389073	c
1.36609080679589	4.85985974043543	2.62551010795701	c
0.99442791986988	3.63213009877406	-1.72348927656970	c
2.19588457371594	5.88967783707031	-2.47483921081492	c
2.96607122557645	7.66882754328777	-0.66425364978062	c
2.52906045392731	7.14042800989131	1.90057709030492	c
-5.93055679485348	1.42071830570333	2.17650172774542	h
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-1.65740500068897	0.79226732337694	3.95529396145312	h
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-0.51202107836537	-3.49826072394483	5.36777393874270	h
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4.33748123186253	11.14694420626821	2.93934923170362	f
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2.12758195084461	-10.03434977711085	5.49216555023194	f
8.77017546613266	-2.46445593265886	-1.19579571122279	f
8.75480401076804	-6.55859544189338	-0.67124191078943	f
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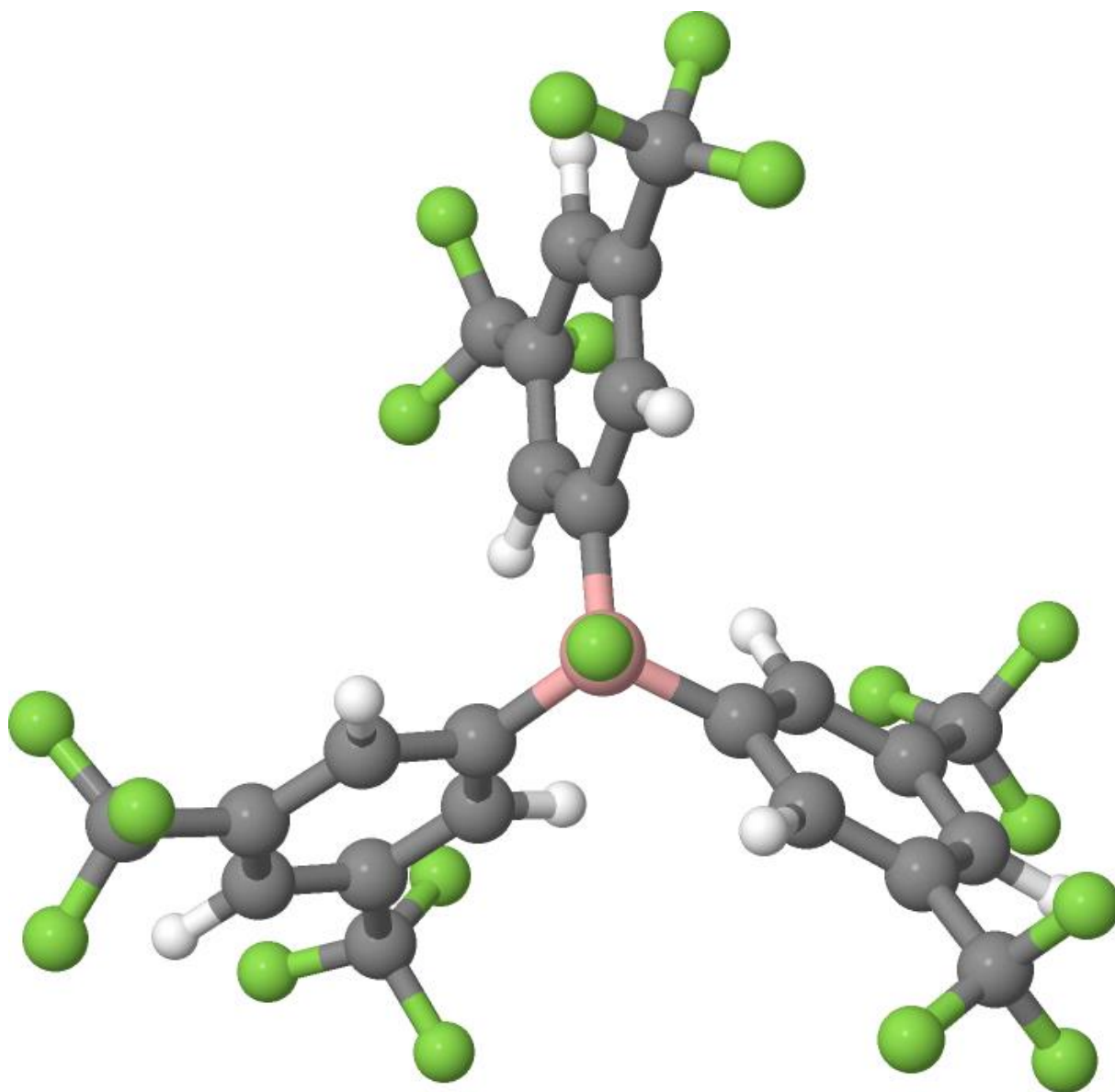
\$vibrational spectrum

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5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
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8		a	8.40	0.01012	YES	YES
9		a	10.18	0.00352	YES	YES
10		a	19.74	0.00758	YES	YES
11		a	20.35	0.00713	YES	YES
12		a	24.88	0.00954	YES	YES
13		a	26.32	0.02894	YES	YES
14		a	27.20	0.02537	YES	YES
15		a	28.48	0.01211	YES	YES
16		a	31.26	0.02064	YES	YES
17		a	35.54	0.00756	YES	YES
18		a	36.68	0.02759	YES	YES
19		a	81.74	0.02500	YES	YES
20		a	84.51	0.21449	YES	YES
21		a	86.15	0.19702	YES	YES
22		a	87.22	0.12759	YES	YES
23		a	97.08	0.39366	YES	YES
24		a	98.00	0.36975	YES	YES
25		a	116.93	0.04816	YES	YES
26		a	119.26	0.06213	YES	YES
27		a	138.67	0.03440	YES	YES
28		a	142.87	0.03834	YES	YES
29		a	143.68	0.01375	YES	YES
30		a	150.05	0.01958	YES	YES
31		a	184.74	0.19109	YES	YES
32		a	210.22	0.31033	YES	YES
33		a	212.43	0.29332	YES	YES
34		a	237.50	0.64903	YES	YES
35		a	253.49	0.80641	YES	YES
36		a	257.27	0.07690	YES	YES
37		a	269.21	1.83268	YES	YES
38		a	279.83	2.11221	YES	YES
39		a	280.62	0.25778	YES	YES
40		a	293.24	0.04177	YES	YES
41		a	298.98	0.05073	YES	YES
42		a	299.88	0.06707	YES	YES
43		a	333.95	1.43096	YES	YES
44		a	339.01	0.20497	YES	YES
45		a	341.35	2.67592	YES	YES
46		a	346.33	0.39299	YES	YES
47		a	361.87	2.13741	YES	YES
48		a	363.49	1.81662	YES	YES
49		a	382.29	3.00597	YES	YES
50		a	387.58	2.34192	YES	YES
51		a	400.77	0.11580	YES	YES
52		a	431.25	9.32271	YES	YES
53		a	439.74	0.73385	YES	YES
54		a	440.34	3.42607	YES	YES
55		a	486.66	0.13166	YES	YES
56		a	487.56	0.07639	YES	YES
57		a	488.61	0.00919	YES	YES
58		a	489.59	0.23343	YES	YES
59		a	494.82	0.66560	YES	YES

60	a	498.07	0.57247	YES	YES
61	a	546.97	2.38275	YES	YES
62	a	547.86	2.59728	YES	YES
63	a	554.09	0.05031	YES	YES
64	a	560.09	1.86714	YES	YES
65	a	561.17	1.70621	YES	YES
66	a	562.16	0.11693	YES	YES
67	a	586.05	0.84029	YES	YES
68	a	586.27	0.99741	YES	YES
69	a	587.00	0.34162	YES	YES
70	a	643.46	18.97077	YES	YES
71	a	644.99	20.51240	YES	YES
72	a	648.45	0.78924	YES	YES
73	a	649.27	2.17478	YES	YES
74	a	649.69	2.58307	YES	YES
75	a	664.19	72.08113	YES	YES
76	a	666.60	9.65036	YES	YES
77	a	667.23	9.51922	YES	YES
78	a	673.25	14.19697	YES	YES
79	a	702.61	5.87685	YES	YES
80	a	703.40	21.92971	YES	YES
81	a	703.51	23.34947	YES	YES
82	a	714.30	0.42794	YES	YES
83	a	715.39	0.11063	YES	YES
84	a	716.29	0.03837	YES	YES
85	a	813.90	4.97743	YES	YES
86	a	831.91	5.35833	YES	YES
87	a	832.27	5.27653	YES	YES
88	a	840.65	61.08556	YES	YES
89	a	861.97	10.70180	YES	YES
90	a	863.60	1.60289	YES	YES
91	a	865.54	28.33912	YES	YES
92	a	868.26	51.07157	YES	YES
93	a	878.75	44.72247	YES	YES
94	a	895.47	4.01730	YES	YES
95	a	901.19	28.71480	YES	YES
96	a	907.03	36.35354	YES	YES
97	a	923.09	0.53996	YES	YES
98	a	931.24	2.82911	YES	YES
99	a	932.20	5.15255	YES	YES
100	a	981.83	4.00852	YES	YES
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102	a	983.52	1.70763	YES	YES
103	a	1035.42	4.37332	YES	YES
104	a	1043.44	1.79749	YES	YES
105	a	1083.88	3.50166	YES	YES
106	a	1086.30	6.10051	YES	YES
107	a	1087.69	5.05344	YES	YES
108	a	1090.95	7.45397	YES	YES
109	a	1092.08	25.80604	YES	YES
110	a	1093.07	28.87972	YES	YES
111	a	1116.75	134.54839	YES	YES
112	a	1118.52	170.57871	YES	YES
113	a	1125.83	88.55087	YES	YES
114	a	1127.47	176.39293	YES	YES
115	a	1128.38	27.93424	YES	YES
116	a	1130.48	289.75537	YES	YES
117	a	1131.73	824.13614	YES	YES
118	a	1133.14	43.12158	YES	YES
119	a	1137.19	450.28430	YES	YES
120	a	1150.93	127.94898	YES	YES
121	a	1152.71	106.41749	YES	YES

122	a	1154.94	142.69826	YES	YES
123	a	1164.08	63.51483	YES	YES
124	a	1167.80	97.48344	YES	YES
125	a	1169.70	53.79832	YES	YES
126	a	1247.23	357.63285	YES	YES
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129	a	1260.94	127.72593	YES	YES
130	a	1263.89	53.80458	YES	YES
131	a	1265.85	318.16143	YES	YES
132	a	1332.94	389.76246	YES	YES
133	a	1333.97	436.40232	YES	YES
134	a	1342.85	38.01095	YES	YES
135	a	1360.40	6.20142	YES	YES
136	a	1361.10	4.47222	YES	YES
137	a	1364.37	28.62374	YES	YES
138	a	1417.07	6.28019	YES	YES
139	a	1422.00	6.84228	YES	YES
140	a	1423.42	12.30710	YES	YES
141	a	1448.02	0.72892	YES	YES
142	a	1449.12	0.91074	YES	YES
143	a	1454.54	0.21204	YES	YES
144	a	1587.17	1.31156	YES	YES
145	a	1588.18	1.81483	YES	YES
146	a	1592.38	1.61458	YES	YES
147	a	1605.04	15.96075	YES	YES
148	a	1606.19	20.06614	YES	YES
149	a	1608.51	22.04661	YES	YES
150	a	2300.93	152.47652	YES	YES
151	a	3079.49	2.98655	YES	YES
152	a	3081.23	4.10961	YES	YES
153	a	3093.38	5.72303	YES	YES
154	a	3094.10	6.87053	YES	YES
155	a	3096.93	1.70984	YES	YES
156	a	3114.12	3.31158	YES	YES
157	a	3132.62	0.78313	YES	YES
158	a	3133.46	0.82137	YES	YES
159	a	3150.14	0.03916	YES	YES

B(C₆H₃-3,5-(CF₃)₂)₃F⁻



Total energy = -2840.1006536720 H = -77283.1149273 eV

HOMO-LUMO Separation

HOMO: 165. 165 a -0.12906823 H = -3.51213 eV

LUMO: 166. 166 a +0.01843522 H = +0.50165 eV

Gap : +0.14750345 H = +4.01378 eV

Number of MOs= 634, Electrons= 330.00, Symmetry: c1

\$coord

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1.10305341448710	2.70319435917006	-1.12645542218192	c
2.66259304980737	4.02134935941884	-2.85267887492171	c
1.93004668989240	6.34555673532889	-3.91588104608047	c
-0.40224379611812	7.44691513435258	-3.26762192934366	c
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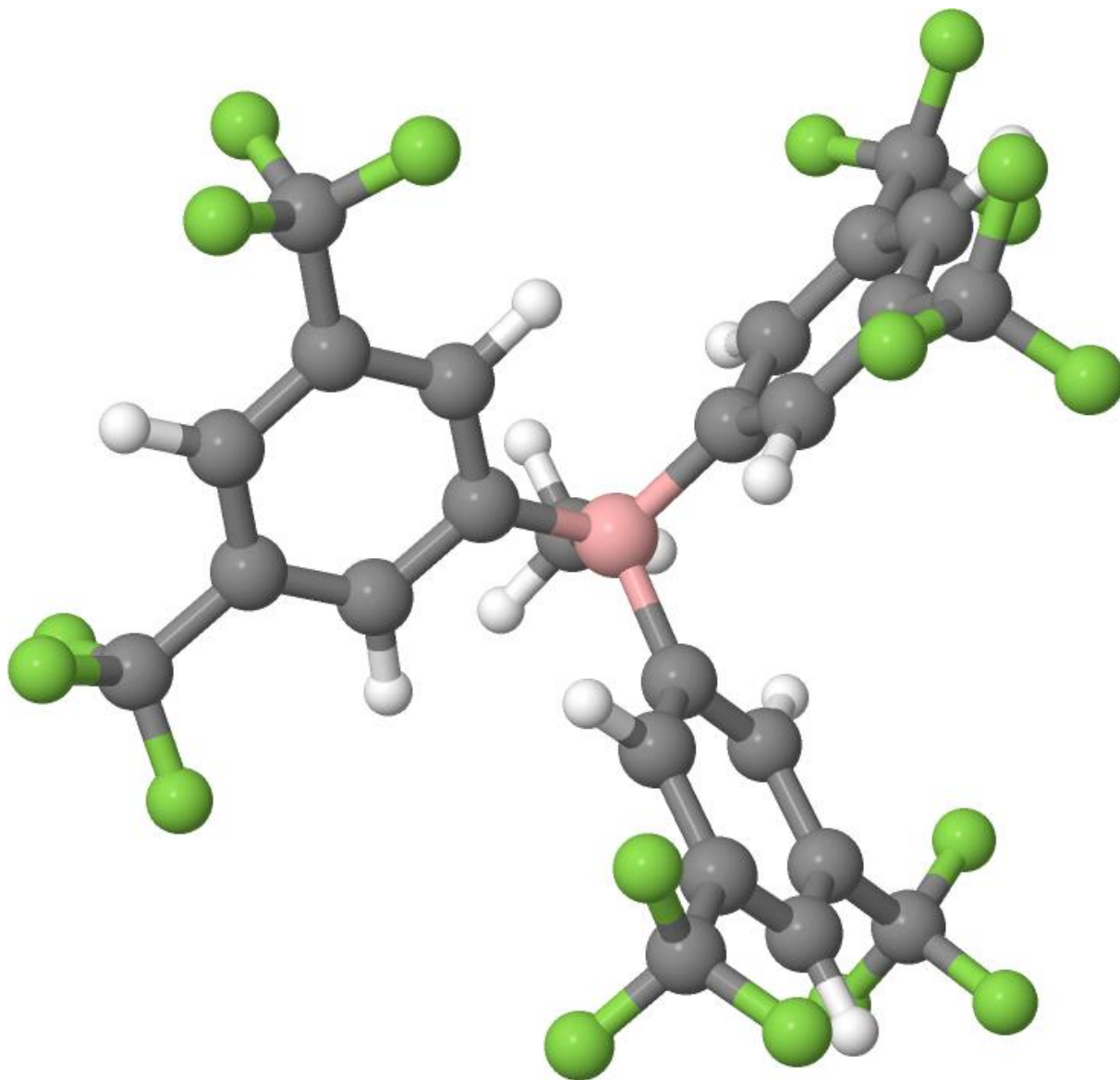
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1		0.00	0.00000	-	-
	2		0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	3.65	0.00304	YES	YES
	8	a	8.82	0.00427	YES	YES
	9	a	11.04	0.00542	YES	YES
	10	a	18.35	0.00527	YES	YES
	11	a	20.50	0.01614	YES	YES
	12	a	21.32	0.01019	YES	YES
	13	a	21.78	0.00882	YES	YES
	14	a	23.33	0.00520	YES	YES
	15	a	28.80	0.01691	YES	YES
	16	a	30.70	0.01840	YES	YES
	17	a	32.61	0.00745	YES	YES
	18	a	37.65	0.02197	YES	YES
	19	a	80.79	0.06396	YES	YES
	20	a	82.59	0.43305	YES	YES
	21	a	83.81	0.44883	YES	YES
	22	a	87.66	0.17962	YES	YES
	23	a	95.45	0.37494	YES	YES
	24	a	96.61	0.26718	YES	YES
	25	a	115.08	0.03059	YES	YES
	26	a	115.53	0.05010	YES	YES
	27	a	140.72	0.04205	YES	YES
	28	a	142.41	0.02289	YES	YES
	29	a	144.52	0.03568	YES	YES
	30	a	147.88	0.03978	YES	YES
	31	a	186.83	0.19856	YES	YES
	32	a	206.28	1.41372	YES	YES
	33	a	207.17	1.22680	YES	YES
	34	a	232.54	0.99034	YES	YES
	35	a	235.82	1.15809	YES	YES
	36	a	238.46	0.84527	YES	YES
	37	a	261.42	0.27477	YES	YES
	38	a	262.91	0.44480	YES	YES
	39	a	276.90	3.71891	YES	YES
	40	a	277.19	1.24563	YES	YES
	41	a	280.40	2.99303	YES	YES
	42	a	298.97	0.42782	YES	YES
	43	a	300.04	0.02036	YES	YES
	44	a	301.05	0.08298	YES	YES
	45	a	318.32	1.44723	YES	YES
	46	a	338.67	1.59278	YES	YES
	47	a	342.27	0.86397	YES	YES
	48	a	343.67	0.25910	YES	YES
	49	a	372.65	3.22875	YES	YES
	50	a	375.37	3.15182	YES	YES
	51	a	397.50	3.82825	YES	YES
	52	a	398.12	5.05049	YES	YES
	53	a	398.58	0.99283	YES	YES
	54	a	422.77	11.65778	YES	YES
	55	a	438.53	1.22543	YES	YES
	56	a	438.99	1.32726	YES	YES
	57	a	469.07	0.67218	YES	YES
	58	a	487.49	0.24511	YES	YES
	59	a	488.09	0.40037	YES	YES
	60	a	488.66	0.24644	YES	YES

61	a	503.20	0.05164	YES	YES
62	a	503.69	0.22083	YES	YES
63	a	513.97	0.49539	YES	YES
64	a	553.06	1.44497	YES	YES
65	a	553.48	1.46876	YES	YES
66	a	554.58	0.13376	YES	YES
67	a	573.34	6.30758	YES	YES
68	a	574.06	8.40996	YES	YES
69	a	585.20	1.04678	YES	YES
70	a	590.81	4.01064	YES	YES
71	a	592.58	5.18060	YES	YES
72	a	602.82	0.55836	YES	YES
73	a	650.45	4.31572	YES	YES
74	a	650.97	1.19943	YES	YES
75	a	651.03	2.46922	YES	YES
76	a	663.05	64.71845	YES	YES
77	a	663.62	53.29237	YES	YES
78	a	666.62	30.09389	YES	YES
79	a	667.21	22.21713	YES	YES
80	a	667.77	37.55782	YES	YES
81	a	689.68	2.08235	YES	YES
82	a	705.86	15.03554	YES	YES
83	a	706.50	14.31626	YES	YES
84	a	706.79	8.48041	YES	YES
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87	a	789.92	4.75316	YES	YES
88	a	830.81	49.08746	YES	YES
89	a	831.46	25.07918	YES	YES
90	a	831.76	13.16047	YES	YES
91	a	874.82	28.03029	YES	YES
92	a	875.40	27.20738	YES	YES
93	a	875.84	14.12014	YES	YES
94	a	887.70	0.50624	YES	YES
95	a	888.44	1.17925	YES	YES
96	a	900.92	5.02969	YES	YES
97	a	930.63	1.62772	YES	YES
98	a	933.79	2.01870	YES	YES
99	a	938.96	2.63031	YES	YES
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101	a	945.35	6.52577	YES	YES
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104	a	984.39	4.67536	YES	YES
105	a	994.06	11.94574	YES	YES
106	a	1081.60	4.81111	YES	YES
107	a	1082.05	1.78118	YES	YES
108	a	1087.32	8.11584	YES	YES
109	a	1090.19	22.43236	YES	YES
110	a	1091.78	43.59388	YES	YES
111	a	1093.24	17.14565	YES	YES
112	a	1122.09	92.55108	YES	YES
113	a	1122.17	55.39806	YES	YES
114	a	1124.42	26.85620	YES	YES
115	a	1125.30	177.44322	YES	YES
116	a	1126.55	395.47746	YES	YES
117	a	1127.58	334.90842	YES	YES
118	a	1128.15	580.62871	YES	YES
119	a	1129.26	269.47739	YES	YES
120	a	1130.44	424.50039	YES	YES
121	a	1153.02	68.37844	YES	YES
122	a	1155.45	73.44875	YES	YES

123	a	1157.43	141.08095	YES	YES
124	a	1163.54	119.41737	YES	YES
125	a	1165.23	135.21699	YES	YES
126	a	1169.69	28.65856	YES	YES
127	a	1248.92	179.38080	YES	YES
128	a	1249.06	191.31691	YES	YES
129	a	1251.32	949.70297	YES	YES
130	a	1254.66	261.68384	YES	YES
131	a	1260.45	82.16814	YES	YES
132	a	1264.83	296.84836	YES	YES
133	a	1335.32	349.64095	YES	YES
134	a	1336.66	348.08016	YES	YES
135	a	1344.34	36.50051	YES	YES
136	a	1364.25	4.89695	YES	YES
137	a	1365.99	10.53734	YES	YES
138	a	1369.39	4.71588	YES	YES
139	a	1419.31	2.11888	YES	YES
140	a	1420.39	2.65104	YES	YES
141	a	1424.00	12.86315	YES	YES
142	a	1446.64	0.16091	YES	YES
143	a	1448.50	0.48244	YES	YES
144	a	1449.78	0.55630	YES	YES
145	a	1589.38	0.09852	YES	YES
146	a	1591.11	0.22910	YES	YES
147	a	1595.44	0.73894	YES	YES
148	a	1606.31	14.81725	YES	YES
149	a	1606.95	15.51626	YES	YES
150	a	1608.69	37.12136	YES	YES
151	a	3086.30	2.52417	YES	YES
152	a	3091.08	2.15955	YES	YES
153	a	3093.01	3.05480	YES	YES
154	a	3113.98	2.67300	YES	YES
155	a	3115.38	2.34077	YES	YES
156	a	3116.85	2.09840	YES	YES
157	a	3135.30	0.48409	YES	YES
158	a	3136.63	0.47643	YES	YES
159	a	3139.51	0.36575	YES	YES

B(C₆H₃-3,5-(CF₃)₂)₃Me⁻



Total energy = -2780.1474082730 H = -75651.7031855 eV

HOMO-LUMO Separation

HOMO: 165. 165 a -0.12109279 H = -3.29510 eV

LUMO: 166. 166 a +0.01701921 H = +0.46312 eV

Gap : +0.13811200 H = +3.75822 eV

Number of MOs= 640, Electrons= 330.00, Symmetry: c1

\$coord

-0.07629003698812	-0.03105227725786	2.33086839454135	b
0.78305332441158	-2.81169121731556	1.18431821236454	c
-2.88536983444407	0.60872716354362	1.12487936556545	c
1.98539588804909	2.18171423357871	1.56593275073112	c
-4.99922223421429	1.19128242417459	2.64926757198290	c
-7.38928925600367	1.76528216723685	1.62087111650282	c
-7.74979635594939	1.78488840512873	-1.00745212890925	c
-5.68441786098565	1.20477095325382	-2.57723939437173	c
-3.31390760559084	0.62517670068563	-1.51809252550358	c
-0.20144698244440	-5.07958740986494	2.21171716624656	c
0.39096774072183	-7.47404672759637	1.21723776824924	c
2.01889561799930	-7.69829394746973	-0.86884446468937	c
3.03144238521653	-5.48794936146465	-1.92777573770150	c
2.41146590794878	-3.10179453581837	-0.91858367511177	c
4.58243773868352	1.85084308680674	2.13460236413982	c
6.40053123603037	3.73499338459638	1.66748983820972	c
5.68684450619993	6.04585877751835	0.56864464543374	c
3.12770477912344	6.43608921618522	-0.01199731160289	c
1.32454855718958	4.54061847089582	0.49394352561025	c
2.32754193812750	8.94469493252189	-1.10612076375167	c
0.16573483657460	8.78734932073793	-2.47059472899007	f
4.12572470617397	9.94108209955880	-2.65815703854282	f
1.91154126778122	10.70840928346515	0.72730581408653	f
9.11361657042432	3.34079744655630	2.44646659949662	c
9.81529424823318	0.87706199806314	2.36268861711557	f
10.75694155211223	4.64688326545252	0.95696865188553	f
9.54536685110076	4.13900642467940	4.86080859358906	f
4.86501376678258	-5.71077747860664	-4.09788473352864	c
7.28182451738651	-6.08033220401852	-3.28163954896709	f
4.31444955493700	-7.70495907806366	-5.63053124330566	f
4.90356096997389	-3.61715200598938	-5.57335319242946	f
-0.63611344622546	-9.84039170753535	2.42750125844946	c
-0.97374347523378	-11.73534832868639	0.71942896419519	f
-2.89385160818075	-9.46081693343698	3.58180372042030	f
0.95722168678458	-10.77398303830907	4.22762608516014	f
-6.05867438522893	1.12403177119404	-5.40407422141119	c
-3.90036682795619	1.61829767644076	-6.69420384029112	f
-7.81858854463909	2.82575692542518	-6.20142161946230	f
-6.88041182167652	-1.18266786724692	-6.20382651001090	f
-9.59534294424585	2.28280137216482	3.34978725584021	c
-11.28370153404318	3.92744137886560	2.31612636450600	f
-8.86459400096789	3.27471657223183	5.59997672672215	f
-10.92282955653320	0.14197965576509	3.89672408744280	f
-0.16532610351134	-0.12882049762385	5.45862699257167	c
-4.77895678405331	1.22386854664688	4.71814716600983	h
-9.59935532130966	2.26663259266048	-1.82426749551336	h
-1.73416928767854	0.18189210350537	-2.80412849297113	h
-1.50526364548529	-4.97512385264114	3.83248707113372	h
2.46965654066733	-9.56264186806045	-1.66832006558997	h
3.23219093462914	-1.40698327532589	-1.80900645484247	h
5.21226118780363	0.04784660075107	2.97001777227872	h
7.10600030176906	7.50631615354670	0.15507111537059	h
-0.66614725709299	4.91005025109403	0.00621276312255	h
-0.66734671417552	1.74402462694300	6.29031518325850	h

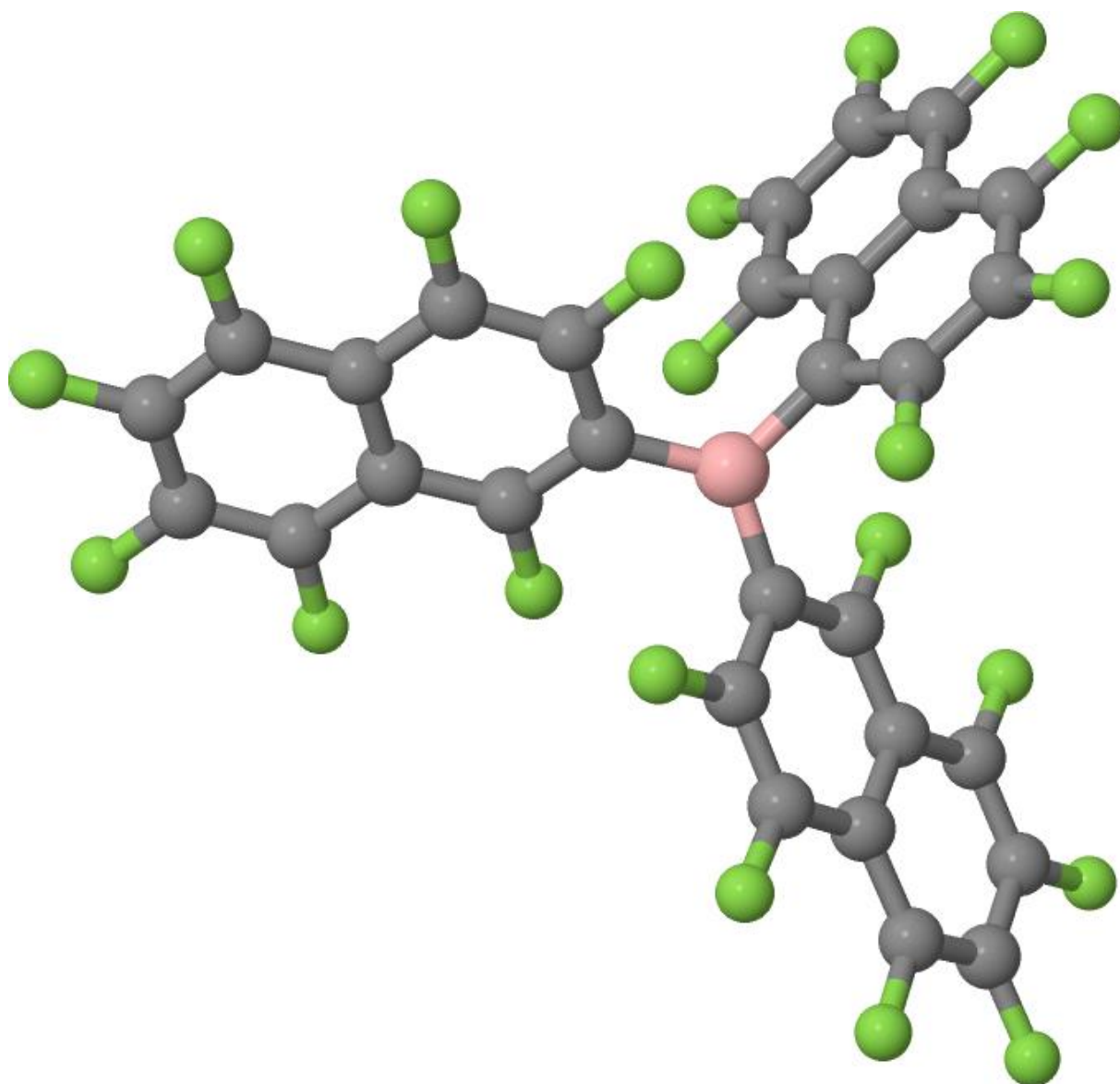
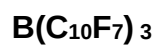
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-1.56287612974219	-1.52020563359894	6.21260449165133	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	6.68	0.00148	YES	YES
8		a	10.71	0.00504	YES	YES
9		a	11.37	0.00041	YES	YES
10		a	15.03	0.01218	YES	YES
11		a	20.79	0.00426	YES	YES
12		a	24.03	0.00607	YES	YES
13		a	27.04	0.00780	YES	YES
14		a	28.44	0.01591	YES	YES
15		a	31.77	0.00817	YES	YES
16		a	32.20	0.03792	YES	YES
17		a	33.99	0.00810	YES	YES
18		a	35.84	0.02019	YES	YES
19		a	84.09	0.03812	YES	YES
20		a	85.86	0.12177	YES	YES
21		a	87.01	0.19938	YES	YES
22		a	88.65	0.15863	YES	YES
23		a	96.09	0.38629	YES	YES
24		a	98.71	0.21246	YES	YES
25		a	114.71	0.07259	YES	YES
26		a	124.72	0.05001	YES	YES
27		a	137.50	0.18985	YES	YES
28		a	142.75	0.08772	YES	YES
29		a	144.92	0.05294	YES	YES
30		a	148.56	0.04190	YES	YES
31		a	173.37	0.51533	YES	YES
32		a	182.41	0.24852	YES	YES
33		a	212.70	0.36816	YES	YES
34		a	231.64	0.12523	YES	YES
35		a	237.73	0.13247	YES	YES
36		a	248.18	0.68461	YES	YES
37		a	253.07	0.49193	YES	YES
38		a	259.25	0.31256	YES	YES
39		a	274.72	0.33456	YES	YES
40		a	279.38	2.26678	YES	YES
41		a	280.96	1.72192	YES	YES
42		a	283.02	0.80631	YES	YES
43		a	297.92	0.32346	YES	YES
44		a	303.14	0.28537	YES	YES
45		a	304.09	0.63438	YES	YES
46		a	320.41	0.97765	YES	YES
47		a	338.80	0.40509	YES	YES
48		a	343.39	1.57770	YES	YES
49		a	346.15	1.15885	YES	YES
50		a	363.58	3.96720	YES	YES
51		a	379.24	4.87419	YES	YES
52		a	389.60	3.01707	YES	YES
53		a	395.52	1.02329	YES	YES
54		a	397.37	0.27659	YES	YES
55		a	421.09	5.32370	YES	YES

56	a	437.61	2.27742	YES	YES
57	a	442.26	1.19984	YES	YES
58	a	453.31	0.16416	YES	YES
59	a	486.97	0.47480	YES	YES
60	a	487.52	0.36074	YES	YES
61	a	488.47	0.26509	YES	YES
62	a	494.64	0.41731	YES	YES
63	a	508.01	0.18610	YES	YES
64	a	515.95	1.27853	YES	YES
65	a	549.83	2.01408	YES	YES
66	a	552.36	0.96309	YES	YES
67	a	554.67	0.17354	YES	YES
68	a	562.45	1.99864	YES	YES
69	a	568.53	2.73214	YES	YES
70	a	586.89	0.44017	YES	YES
71	a	587.90	0.24021	YES	YES
72	a	591.78	1.73455	YES	YES
73	a	613.68	2.50624	YES	YES
74	a	636.03	17.78820	YES	YES
75	a	647.79	4.63405	YES	YES
76	a	649.04	1.44126	YES	YES
77	a	649.43	4.35381	YES	YES
78	a	650.79	19.20707	YES	YES
79	a	666.67	28.72185	YES	YES
80	a	667.25	22.48399	YES	YES
81	a	667.49	47.47118	YES	YES
82	a	686.64	2.49075	YES	YES
83	a	703.23	19.33084	YES	YES
84	a	703.61	22.72656	YES	YES
85	a	704.85	11.76768	YES	YES
86	a	709.17	2.74569	YES	YES
87	a	714.49	2.08426	YES	YES
88	a	778.84	5.01172	YES	YES
89	a	796.82	43.54560	YES	YES
90	a	801.68	27.88782	YES	YES
91	a	830.50	41.14828	YES	YES
92	a	831.43	24.57152	YES	YES
93	a	833.12	13.75270	YES	YES
94	a	868.53	31.81596	YES	YES
95	a	869.22	18.66909	YES	YES
96	a	871.21	21.83358	YES	YES
97	a	887.04	10.47839	YES	YES
98	a	890.44	3.59145	YES	YES
99	a	902.24	4.05278	YES	YES
100	a	928.03	1.28484	YES	YES
101	a	930.40	0.84042	YES	YES
102	a	932.46	1.74016	YES	YES
103	a	950.86	6.43727	YES	YES
104	a	964.79	7.89792	YES	YES
105	a	972.13	2.96132	YES	YES
106	a	983.85	1.81907	YES	YES
107	a	984.42	4.33947	YES	YES
108	a	985.64	2.28685	YES	YES
109	a	1083.04	1.57362	YES	YES
110	a	1084.61	5.78498	YES	YES
111	a	1086.80	20.17089	YES	YES
112	a	1090.92	3.70190	YES	YES
113	a	1092.69	65.26861	YES	YES
114	a	1093.09	52.07204	YES	YES
115	a	1117.51	49.71687	YES	YES
116	a	1119.60	41.68515	YES	YES
117	a	1120.36	13.43056	YES	YES

118	a	1121.02	219.32079	YES	YES
119	a	1122.36	460.51812	YES	YES
120	a	1123.64	135.60104	YES	YES
121	a	1123.77	405.04325	YES	YES
122	a	1126.56	344.97727	YES	YES
123	a	1132.03	529.74685	YES	YES
124	a	1154.05	33.43063	YES	YES
125	a	1155.74	62.98194	YES	YES
126	a	1157.48	88.07818	YES	YES
127	a	1167.52	194.03189	YES	YES
128	a	1168.51	85.56675	YES	YES
129	a	1171.32	71.55164	YES	YES
130	a	1248.63	315.15752	YES	YES
131	a	1250.24	511.78523	YES	YES
132	a	1251.69	698.07309	YES	YES
133	a	1258.09	160.17297	YES	YES
134	a	1261.74	57.92841	YES	YES
135	a	1263.71	87.62316	YES	YES
136	a	1272.66	130.86501	YES	YES
137	a	1330.50	383.37445	YES	YES
138	a	1332.00	389.22054	YES	YES
139	a	1341.22	63.54527	YES	YES
140	a	1352.06	5.55132	YES	YES
141	a	1358.64	2.65440	YES	YES
142	a	1360.12	6.30762	YES	YES
143	a	1416.96	0.88986	YES	YES
144	a	1417.80	10.06746	YES	YES
145	a	1421.33	10.59348	YES	YES
146	a	1424.55	4.24164	YES	YES
147	a	1427.64	2.00657	YES	YES
148	a	1447.40	0.22276	YES	YES
149	a	1449.31	0.22258	YES	YES
150	a	1449.75	0.62006	YES	YES
151	a	1586.93	0.95170	YES	YES
152	a	1587.66	1.01763	YES	YES
153	a	1590.75	0.28683	YES	YES
154	a	1602.86	19.43096	YES	YES
155	a	1604.81	14.80611	YES	YES
156	a	1605.66	23.68285	YES	YES
157	a	2895.76	37.64400	YES	YES
158	a	2967.90	54.48132	YES	YES
159	a	2978.61	41.94211	YES	YES
160	a	3093.23	3.48198	YES	YES
161	a	3094.46	6.02095	YES	YES
162	a	3102.16	2.10892	YES	YES
163	a	3105.40	3.31324	YES	YES
164	a	3105.60	2.96399	YES	YES
165	a	3117.31	2.99495	YES	YES
166	a	3130.88	0.82461	YES	YES
167	a	3133.03	0.71773	YES	YES
168	a	3133.43	0.77666	YES	YES



Total energy = -3262.3479715010 H = -88773.0555917 eV

HOMO-LUMO Separation

HOMO: 187. 187 a -0.21737460 H = -5.91507 eV

LUMO: 188. 188 a -0.14355289 H = -3.90628 eV

Gap : +0.07382171 H = +2.00879 eV

Number of MOs= 728, Electrons= 374.00, Symmetry: c1

\$coord

-7.33993959393358	-2.31575814101557	0.31746728325670	c
-4.79134586405751	-2.36031893431214	0.93794198233931	c
-2.90986089263619	-1.01986258053307	-0.45353894624130	c
-3.79778107923068	0.39793939617161	-2.50487047424631	c
-6.38954458058140	0.57042282126266	-3.22581679566458	c
-8.22612789306732	-0.84879173965668	-1.76208203864930	c
-10.82278254158684	-0.71974527873834	-2.46146817581733	c
-7.25941302955205	2.06433392025667	-5.30160690175106	c
-9.80898863244553	2.14447646554606	-5.93313877345091	c
-11.59641076632311	0.74483368305099	-4.50577896185300	c
-14.02742492746336	0.85385382716102	-5.14884404494791	f
-12.58949740859283	-1.99088307308728	-1.17944126161204	f
-8.95320037395049	-3.67832490800953	1.71116748306009	f
-10.60817298899570	3.53893693253449	-7.87469823514712	f
-5.66147402566422	3.42601537890367	-6.70225668698093	f
-2.12520670470290	1.74455523820449	-3.85537102025116	f
8.53430348611012	-0.71800461427023	-6.72959868388185	c
10.65681583988063	0.71844386173971	-6.13261915252182	c
10.71590392630123	2.19782784650252	-3.89698791860234	c
8.64920125706854	2.22181537130640	-2.27437330726795	c
6.45264643044134	0.74804701338428	-2.80734830687419	c
6.38484708458336	-0.74294512520572	-5.10789559216904	c
4.16813401856779	-2.18639946468475	-5.63224563773868	c
4.31602136165963	0.62545959883163	-1.16761526582162	c
2.15008657298413	-0.79944029814532	-1.65687237187357	c
2.13804177393539	-2.17225507152977	-3.97158421950848	c
0.11884957942151	-3.59353532397686	-4.55732643682675	f
4.02372493356038	-3.59469063259777	-7.72969221442706	f
8.57825613486768	-2.07530447894782	-8.85970606240625	f
4.38797115861416	2.00674533346429	0.96417968176296	f
8.79366194242346	3.65170681347730	-0.19811720285621	f
12.77281627378244	3.56037874300184	-3.38018657126233	f
0.75517875409466	-1.49603394125012	3.19016520130441	c
1.82333109430892	-3.81621638537954	3.77399765461571	c
2.55935197796280	-4.51411210975881	6.25552536888681	c
2.22767392755571	-2.81818442664334	8.23365467640068	c
1.18020341030200	-0.37190627111037	7.79322908586446	c
0.45386553044096	0.26422579120034	5.23027855762309	c
-0.49042291886061	2.73762513038990	4.77552112320862	c
0.85972773115942	1.46368161005896	9.74226441312604	c
-0.10858108025273	3.84888122842134	9.20587333930544	c
-0.78171867544084	4.50483892864317	6.69230149428360	c
-1.67096798603558	6.81669905130299	6.21936679447644	f
-1.08799123031747	3.41248354741391	2.39024015754317	f
-0.40240574339804	5.56196428624097	11.03322362135321	f
1.49305352832200	0.94498368144118	12.13412310341416	f
2.92983142292963	-3.53240179863577	10.55155530018633	f
3.54937799638339	-6.79694742605084	6.67359374593722	f
-4.10977343921753	-3.79179390658183	2.91668953419605	f
12.66629190011440	0.72380098630369	-7.64985934607083	f
2.13931771588613	-5.56989043581481	1.95465735073036	f
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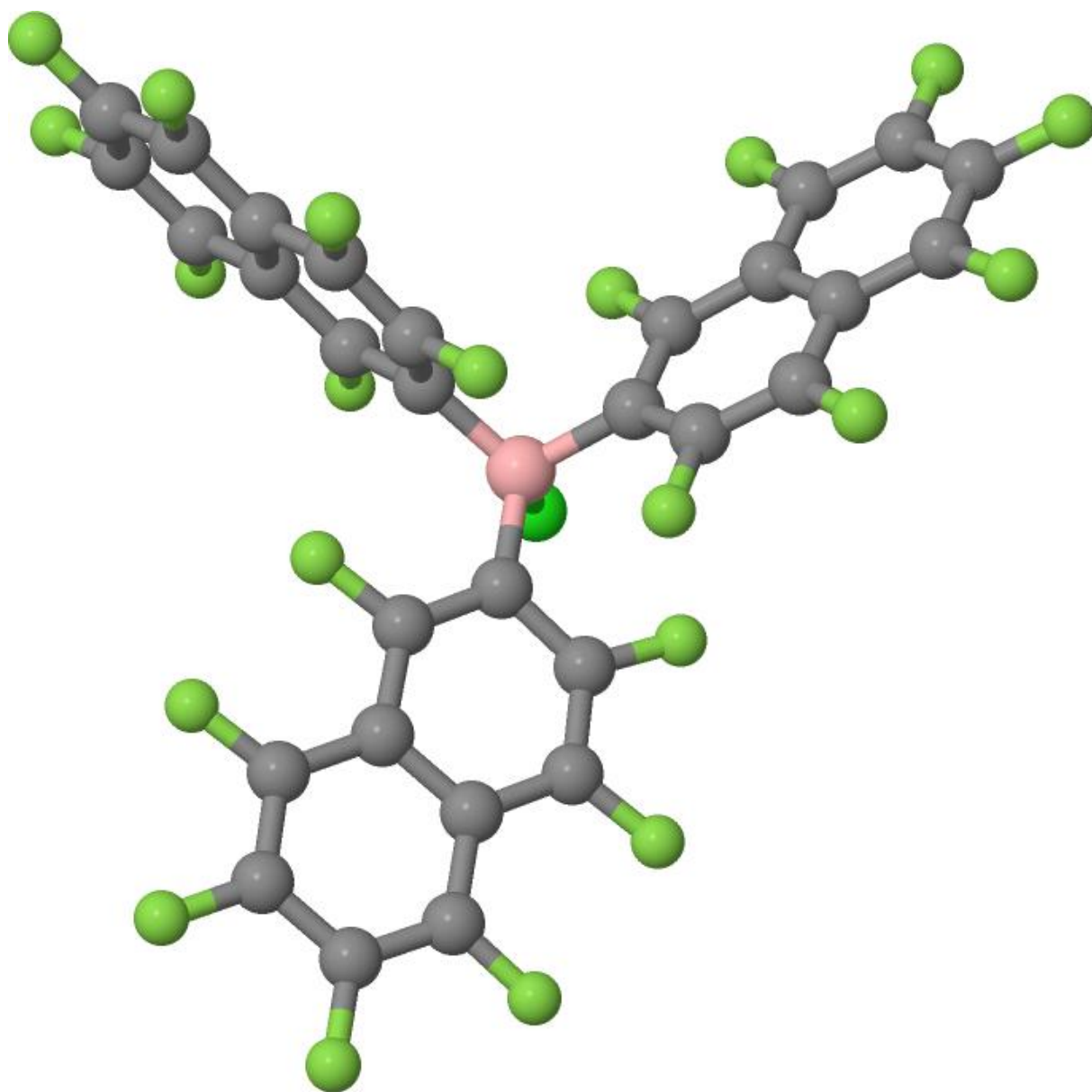
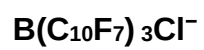
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules

#		cm** (-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.96	0.18536	YES	YES
8	a	15.06	0.13268	YES	YES
9	a	15.87	0.00093	YES	YES
10	a	19.20	0.09545	YES	YES
11	a	22.86	0.08363	YES	YES
12	a	28.55	0.03823	YES	YES
13	a	56.39	0.13082	YES	YES
14	a	60.08	0.01931	YES	YES
15	a	64.44	0.07627	YES	YES
16	a	72.20	0.57901	YES	YES
17	a	74.82	0.35719	YES	YES
18	a	78.62	0.25517	YES	YES
19	a	91.62	0.28002	YES	YES
20	a	100.24	0.02733	YES	YES
21	a	104.99	0.18389	YES	YES
22	a	111.62	0.09243	YES	YES
23	a	112.63	0.22154	YES	YES
24	a	120.22	0.05859	YES	YES
25	a	124.94	0.01522	YES	YES
26	a	128.49	0.11314	YES	YES
27	a	140.98	0.19917	YES	YES
28	a	146.33	0.01696	YES	YES
29	a	148.19	0.02684	YES	YES
30	a	151.52	0.13109	YES	YES
31	a	183.26	1.86849	YES	YES
32	a	184.44	2.14511	YES	YES
33	a	186.87	2.85083	YES	YES
34	a	195.41	1.02732	YES	YES
35	a	206.68	0.13058	YES	YES
36	a	210.56	0.18434	YES	YES
37	a	265.07	0.31686	YES	YES
38	a	267.42	0.13060	YES	YES
39	a	268.13	0.74061	YES	YES
40	a	269.31	0.02020	YES	YES
41	a	273.05	0.29901	YES	YES
42	a	274.54	0.14015	YES	YES
43	a	278.51	1.82441	YES	YES
44	a	283.68	0.28845	YES	YES
45	a	284.11	0.63859	YES	YES
46	a	288.51	1.04864	YES	YES
47	a	293.30	1.16725	YES	YES
48	a	300.58	0.13391	YES	YES
49	a	302.19	0.10567	YES	YES
50	a	310.44	0.99367	YES	YES
51	a	313.12	1.39562	YES	YES
52	a	313.55	0.92530	YES	YES
53	a	330.32	1.06258	YES	YES
54	a	331.15	0.06538	YES	YES
55	a	336.78	7.82552	YES	YES
56	a	340.54	2.54439	YES	YES
57	a	350.74	0.61053	YES	YES
58	a	355.09	0.51660	YES	YES
59	a	368.57	2.42705	YES	YES
60	a	371.29	1.21653	YES	YES
61	a	375.92	1.09122	YES	YES

62	a	377.80	2.94425	YES	YES
63	a	387.04	2.59066	YES	YES
64	a	400.54	1.18940	YES	YES
65	a	403.16	4.53050	YES	YES
66	a	420.70	2.17462	YES	YES
67	a	425.74	1.44276	YES	YES
68	a	429.01	3.16869	YES	YES
69	a	434.03	0.16123	YES	YES
70	a	441.88	0.14794	YES	YES
71	a	442.51	0.18314	YES	YES
72	a	463.20	2.12930	YES	YES
73	a	492.52	0.83800	YES	YES
74	a	498.40	1.00354	YES	YES
75	a	502.86	0.08197	YES	YES
76	a	503.95	0.21819	YES	YES
77	a	506.06	0.11252	YES	YES
78	a	506.81	0.84860	YES	YES
79	a	508.51	0.90255	YES	YES
80	a	509.23	2.05167	YES	YES
81	a	512.13	1.97495	YES	YES
82	a	535.83	1.38887	YES	YES
83	a	556.44	34.92003	YES	YES
84	a	572.27	18.83526	YES	YES
85	a	582.00	38.47953	YES	YES
86	a	589.28	1.18906	YES	YES
87	a	593.55	23.25342	YES	YES
88	a	623.13	9.65501	YES	YES
89	a	624.92	2.80411	YES	YES
90	a	633.15	1.89174	YES	YES
91	a	636.59	2.47032	YES	YES
92	a	655.75	3.20597	YES	YES
93	a	659.53	1.51505	YES	YES
94	a	669.86	2.60278	YES	YES
95	a	688.18	3.44683	YES	YES
96	a	693.36	3.71523	YES	YES
97	a	701.03	16.11416	YES	YES
98	a	726.60	20.16856	YES	YES
99	a	739.99	26.57402	YES	YES
100	a	751.92	21.64387	YES	YES
101	a	785.90	20.15909	YES	YES
102	a	792.00	39.96458	YES	YES
103	a	798.22	28.79942	YES	YES
104	a	811.87	15.08806	YES	YES
105	a	828.12	26.63355	YES	YES
106	a	901.48	92.99809	YES	YES
107	a	945.91	107.87384	YES	YES
108	a	952.69	163.51727	YES	YES
109	a	995.13	28.61754	YES	YES
110	a	1045.69	24.92214	YES	YES
111	a	1049.01	9.48966	YES	YES
112	a	1053.74	11.42406	YES	YES
113	a	1063.76	57.28247	YES	YES
114	a	1073.15	232.75302	YES	YES
115	a	1121.03	169.38895	YES	YES
116	a	1136.21	51.32127	YES	YES
117	a	1140.08	22.57192	YES	YES
118	a	1182.35	62.41471	YES	YES
119	a	1201.28	49.57915	YES	YES
120	a	1208.45	150.09561	YES	YES
121	a	1214.46	265.21489	YES	YES
122	a	1249.83	7.29675	YES	YES
123	a	1250.85	4.11298	YES	YES

124	a	1275.70	5.52045	YES	YES
125	a	1280.32	83.80565	YES	YES
126	a	1286.81	183.49829	YES	YES
127	a	1334.99	3.38972	YES	YES
128	a	1335.75	4.18276	YES	YES
129	a	1339.58	28.29028	YES	YES
130	a	1379.78	9.75671	YES	YES
131	a	1382.18	19.75756	YES	YES
132	a	1384.64	16.42560	YES	YES
133	a	1403.91	28.50351	YES	YES
134	a	1407.59	109.68328	YES	YES
135	a	1409.88	86.42008	YES	YES
136	a	1421.77	419.64238	YES	YES
137	a	1425.00	646.26562	YES	YES
138	a	1445.93	561.47293	YES	YES
139	a	1457.60	21.03614	YES	YES
140	a	1463.67	12.73054	YES	YES
141	a	1481.98	207.08496	YES	YES
142	a	1491.05	842.20827	YES	YES
143	a	1493.60	198.40934	YES	YES
144	a	1506.06	50.17343	YES	YES
145	a	1528.77	183.86734	YES	YES
146	a	1530.54	167.92592	YES	YES
147	a	1532.91	152.24180	YES	YES
148	a	1584.74	219.61783	YES	YES
149	a	1591.09	164.48322	YES	YES
150	a	1600.87	20.78684	YES	YES
151	a	1628.15	145.32149	YES	YES
152	a	1634.50	110.88308	YES	YES
153	a	1635.96	156.84962	YES	YES
154	a	1644.30	136.93463	YES	YES
155	a	1645.85	108.69822	YES	YES
156	a	1652.57	75.99163	YES	YES



Total energy = -3722.6076654260 H = -101297.3662270 eV

HOMO-LUMO Separation

HOMO: 196. 196 a -0.10895310 H = -2.96477 eV

LUMO: 197. 197 a -0.00235065 H = -0.06396 eV

Gap : +0.10660244 H = +2.90080 eV

Number of MOs= 746, Electrons= 392.00, Symmetry: c1

\$coord

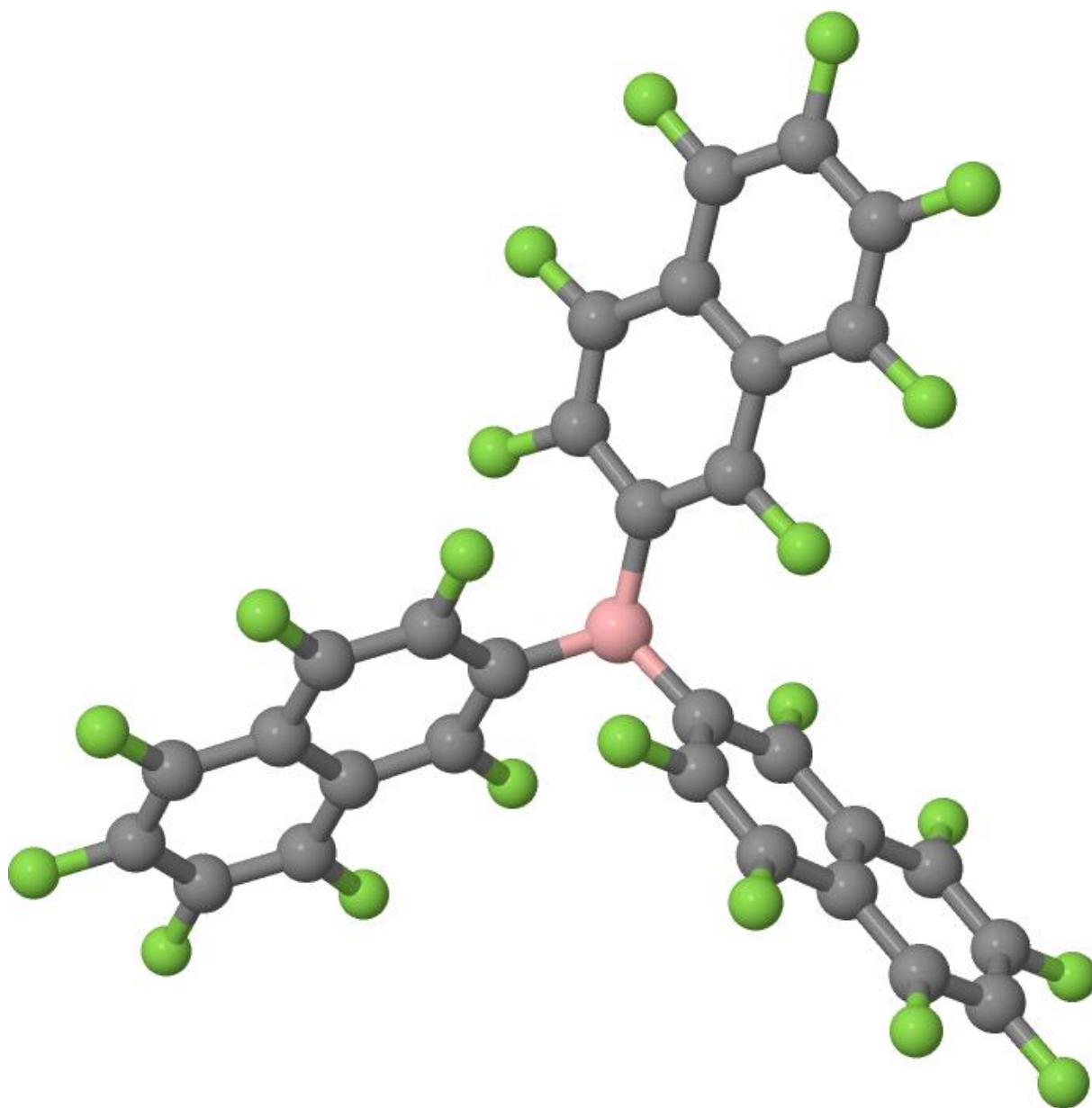
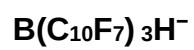
0.84984380135873	-1.43628091026715	11.84609580672873	c
0.62873507324250	1.22502560085723	11.63015309521162	c
0.40255820368330	2.35492123250951	9.26853739307172	c
0.38129726911748	0.88180343844439	7.00344539998204	c
0.59618054823691	-1.84187657381881	7.24145986550692	c
0.83366262551953	-2.93628931796849	9.69348123447837	c
0.14081584020730	1.95468858136027	4.52376502970647	c
0.11749076225654	0.55626426335286	2.28960368483779	c
0.30828986444076	-2.09700996977671	2.65086987023072	c
0.54077602005180	-3.28573455155712	4.97994067716105	c
-0.05790513858839	1.60073893573997	-0.65368162071715	b
2.45350664025251	0.46901890287679	-2.15217081606752	c
-2.79442767022682	1.00413327289231	-2.02648782136641	c
4.87164782942716	1.34637715032530	-1.56364101292419	c
7.14234775848562	0.61230676355181	-2.83672811887128	c
6.95215017710083	-1.26023463797210	-4.83230257157131	c
4.52114071061397	-2.26584524220800	-5.35619356954523	c
2.40046946021056	-1.43344791673509	-4.04073275211202	c
9.58307691053595	1.62085591746097	-2.26506164942213	c
11.71740803254850	0.86041891863962	-3.59490703676944	c
11.51580005120163	-0.95764174519968	-5.55565644040699	c
9.18278761803869	-1.99591038082532	-6.15755561923933	c
-4.99662175263993	0.26834781873684	-0.78846816814967	c
-7.43168476079522	0.03330560674251	-1.94859384533519	c
-7.64778667580564	0.59111707504631	-4.62463187491083	c
-5.41686868958972	1.35664151322442	-5.91111766120704	c
-3.12783092174204	1.54297859678067	-4.64043287399199	c
-9.66104754299744	-0.71535072144451	-0.62190817510831	c
-11.97730312703697	-0.90884981343892	-1.84755936293348	c
-12.17343170012022	-0.37780939663169	-4.46564095177252	c
-10.05057301775978	0.35917623193850	-5.82324951330415	c
1.04659503064480	-5.45010568328119	9.99178826037810	f
1.07867481953325	-2.47302402929619	14.15046659054134	f
0.64299101259424	2.63378340750303	13.74121882773212	f
0.20839152500265	4.88109403963983	9.22070735617471	f
0.68944457729063	-5.82703587803518	5.05989618271521	f
0.20167284585212	-3.63110831446301	0.61619397387330	f
-0.10810354429244	4.47720345484172	4.44547404876689	f
-4.91332777263096	-0.24684569418250	1.71416405647431	f
-9.61996702402918	-1.25857618524206	1.85401575759138	f
-14.05964603839561	-1.60380648513667	-0.57301928650811	f
-14.43164090225618	-0.59809107645071	-5.60211136839678	f
-10.33342920691651	0.84406226472943	-8.30102036666507	f
-5.48932307225080	1.91017386132536	-8.39584097603562	f
-1.13792619871901	2.29320250948928	-6.02952383950245	f
5.13496403169204	3.02019524595506	0.33381974899054	f
0.21068131592500	-2.57479516345170	-4.65422780026310	f
4.22674727823024	-4.06538477418402	-7.13318466820635	f
9.08662031959634	-3.70519817576585	-8.03450037252937	f
13.60607386601514	-1.64028036162940	-6.82166023450147	f
13.99871473303790	1.83664303087609	-3.05734899909149	f
9.90757348656200	3.35625280166494	-0.44810299120974	f
0.09332657935490	5.21935459036119	-0.93896634481076	c1

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	10.64	0.07004	YES	YES
8		a	13.50	0.00361	YES	YES
9		a	18.72	0.03777	YES	YES
10		a	19.83	0.01406	YES	YES
11		a	26.06	0.02163	YES	YES
12		a	27.90	0.04267	YES	YES
13		a	56.51	0.24505	YES	YES
14		a	62.48	0.07697	YES	YES
15		a	67.60	0.08165	YES	YES
16		a	69.78	0.12306	YES	YES
17		a	77.15	0.14988	YES	YES
18		a	79.88	0.20035	YES	YES
19		a	100.24	0.09535	YES	YES
20		a	102.49	0.33363	YES	YES
21		a	104.24	0.19238	YES	YES
22		a	108.07	0.18037	YES	YES
23		a	112.74	0.05141	YES	YES
24		a	115.03	0.05888	YES	YES
25		a	122.39	0.05194	YES	YES
26		a	129.06	0.21208	YES	YES
27		a	134.51	2.11966	YES	YES
28		a	148.88	0.17679	YES	YES
29		a	150.73	0.07989	YES	YES
30		a	152.82	0.05525	YES	YES
31		a	159.05	0.60352	YES	YES
32		a	167.75	1.02161	YES	YES
33		a	181.20	1.86937	YES	YES
34		a	183.65	1.25171	YES	YES
35		a	185.36	1.44043	YES	YES
36		a	205.50	0.12175	YES	YES
37		a	212.11	0.45787	YES	YES
38		a	214.69	0.17597	YES	YES
39		a	239.74	1.21237	YES	YES
40		a	267.12	0.03899	YES	YES
41		a	267.35	0.02148	YES	YES
42		a	268.23	0.00641	YES	YES
43		a	278.85	0.39856	YES	YES
44		a	282.60	0.24679	YES	YES
45		a	283.20	0.73510	YES	YES
46		a	284.36	0.78826	YES	YES
47		a	288.33	1.27162	YES	YES
48		a	296.37	0.13835	YES	YES
49		a	303.52	0.76371	YES	YES
50		a	306.18	0.53047	YES	YES
51		a	307.31	0.15547	YES	YES
52		a	313.56	0.61787	YES	YES
53		a	314.87	1.14656	YES	YES
54		a	318.74	1.28171	YES	YES
55		a	332.68	0.42114	YES	YES
56		a	335.01	0.35841	YES	YES
57		a	337.67	1.35488	YES	YES

58	a	340.61	6.05966	YES	YES
59	a	342.66	2.04907	YES	YES
60	a	350.25	0.38887	YES	YES
61	a	363.96	0.12284	YES	YES
62	a	364.91	0.06809	YES	YES
63	a	365.36	0.26508	YES	YES
64	a	382.35	0.88539	YES	YES
65	a	395.85	10.98985	YES	YES
66	a	401.70	3.33686	YES	YES
67	a	414.37	1.68989	YES	YES
68	a	417.05	2.36040	YES	YES
69	a	423.96	0.59784	YES	YES
70	a	426.52	1.60385	YES	YES
71	a	428.35	0.70252	YES	YES
72	a	430.67	0.16341	YES	YES
73	a	441.58	0.23386	YES	YES
74	a	442.04	0.09969	YES	YES
75	a	443.72	0.36638	YES	YES
76	a	495.14	0.09413	YES	YES
77	a	500.56	0.36649	YES	YES
78	a	500.98	0.06589	YES	YES
79	a	501.98	0.33677	YES	YES
80	a	502.21	0.23217	YES	YES
81	a	502.90	0.26248	YES	YES
82	a	506.91	4.03172	YES	YES
83	a	508.36	2.13906	YES	YES
84	a	509.92	0.35967	YES	YES
85	a	549.28	56.81065	YES	YES
86	a	567.88	36.31604	YES	YES
87	a	572.72	4.02946	YES	YES
88	a	582.91	19.59936	YES	YES
89	a	586.73	27.35574	YES	YES
90	a	611.29	8.48609	YES	YES
91	a	622.67	6.76703	YES	YES
92	a	629.12	9.46133	YES	YES
93	a	634.48	11.83849	YES	YES
94	a	654.34	7.74189	YES	YES
95	a	657.84	3.12598	YES	YES
96	a	660.16	9.01110	YES	YES
97	a	669.58	4.34387	YES	YES
98	a	679.13	9.37441	YES	YES
99	a	689.49	3.03551	YES	YES
100	a	701.78	55.02174	YES	YES
101	a	714.78	7.80080	YES	YES
102	a	728.23	80.67348	YES	YES
103	a	758.75	23.25523	YES	YES
104	a	777.42	12.84127	YES	YES
105	a	791.32	4.17334	YES	YES
106	a	808.07	25.38374	YES	YES
107	a	812.88	21.98629	YES	YES
108	a	815.78	8.80820	YES	YES
109	a	907.38	132.31436	YES	YES
110	a	923.89	65.95337	YES	YES
111	a	938.69	112.21437	YES	YES
112	a	952.59	186.44221	YES	YES
113	a	975.93	81.54902	YES	YES
114	a	992.85	218.17676	YES	YES
115	a	1039.60	3.74533	YES	YES
116	a	1043.91	6.26287	YES	YES
117	a	1045.20	21.71955	YES	YES
118	a	1112.42	45.55333	YES	YES
119	a	1114.36	52.63079	YES	YES

120	a	1118.50	41.52264	YES	YES
121	a	1153.41	48.11435	YES	YES
122	a	1156.98	55.64242	YES	YES
123	a	1160.19	131.33254	YES	YES
124	a	1235.44	5.25072	YES	YES
125	a	1239.63	0.11969	YES	YES
126	a	1241.53	1.84268	YES	YES
127	a	1251.03	45.03302	YES	YES
128	a	1252.88	35.48073	YES	YES
129	a	1254.89	43.54400	YES	YES
130	a	1327.33	33.63554	YES	YES
131	a	1330.51	79.23327	YES	YES
132	a	1334.81	23.82979	YES	YES
133	a	1379.00	17.43783	YES	YES
134	a	1379.61	3.29169	YES	YES
135	a	1381.93	28.30474	YES	YES
136	a	1392.98	147.37021	YES	YES
137	a	1396.26	88.51014	YES	YES
138	a	1400.46	220.97638	YES	YES
139	a	1404.71	106.23768	YES	YES
140	a	1406.30	613.11692	YES	YES
141	a	1409.29	536.44958	YES	YES
142	a	1446.88	15.12542	YES	YES
143	a	1450.51	14.27218	YES	YES
144	a	1452.67	0.58112	YES	YES
145	a	1488.07	460.76117	YES	YES
146	a	1489.47	275.29261	YES	YES
147	a	1492.00	177.63917	YES	YES
148	a	1525.53	119.46843	YES	YES
149	a	1527.94	31.23465	YES	YES
150	a	1529.17	62.05046	YES	YES
151	a	1585.57	129.71356	YES	YES
152	a	1590.64	89.59199	YES	YES
153	a	1593.01	93.96094	YES	YES
154	a	1620.47	37.46924	YES	YES
155	a	1624.35	43.08075	YES	YES
156	a	1626.20	60.31629	YES	YES
157	a	1646.60	77.62979	YES	YES
158	a	1647.54	79.20873	YES	YES
159	a	1647.99	93.45719	YES	YES



Total energy = -3263.0600035810 H = -88792.4309814 eV

HOMO-LUMO Separation

HOMO: 188. 188 a -0.10414180 H = -2.83384 eV

LUMO: 189. 189 a +0.00080193 H = +0.02182 eV

Gap : +0.10494373 H = +2.85567 eV

Number of MOs= 730, Electrons= 376.00, Symmetry: c1

\$coord

-0.87668182939269	-0.71342850149867	12.11043140013359	c
-1.42886344059685	1.85432980336375	11.57533539722798	c
-1.38267660774887	2.73363469352189	9.10025996084978	c
-0.78936827966725	1.09287678534770	7.03791686363398	c
-0.23977511012398	-1.53943308094378	7.59593384377728	c
-0.29643360767263	-2.37076311451336	10.16088346437762	c
-0.69870574581113	1.88858812780664	4.45295326986986	c
-0.11804305337251	0.32009986449166	2.42093792657747	c
0.35415458474820	-2.23387507389002	3.07198095045638	c
0.32007297240159	-3.16351415820607	5.53050052431647	c
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7.43485673366776	0.83772452151976	-2.18357300900984	c
7.49903737104575	-1.08755912201428	-4.14265324768086	c
5.17315954162383	-2.24467856109983	-4.82586868842237	c
2.92186422757505	-1.53242534832025	-3.66478601703574	c
9.76248898394270	2.01466811366579	-1.47522201869663	c
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-9.08643217887405	0.95870735577893	-7.04539802213905	c
0.22060106852106	-4.78330777991763	10.76692951072988	f
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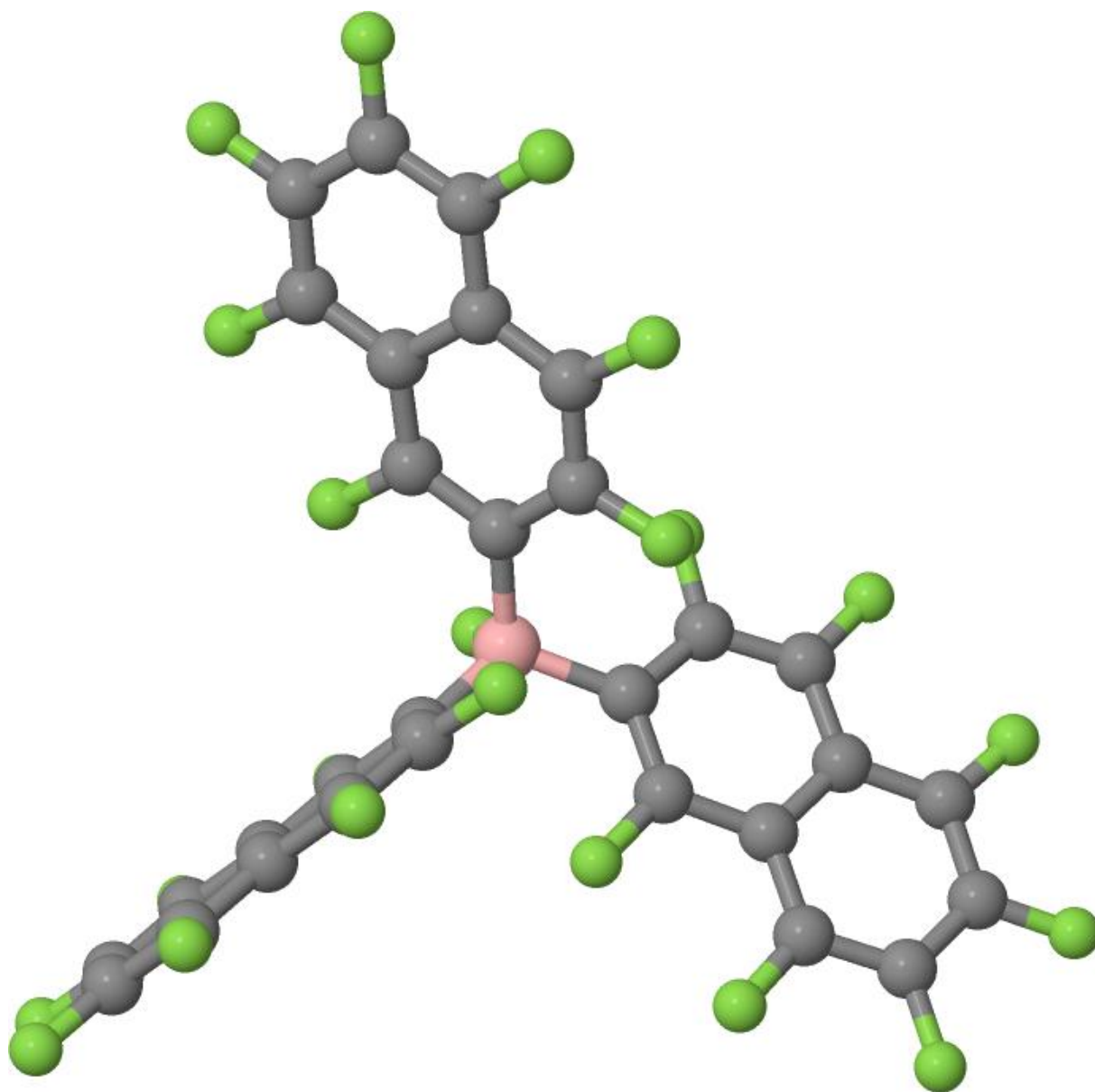
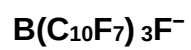
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\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
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2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	6.89	0.02046	YES	YES
8		a	10.17	0.00209	YES	YES
9		a	15.18	0.02080	YES	YES
10		a	17.38	0.00674	YES	YES
11		a	21.08	0.03819	YES	YES
12		a	24.16	0.01391	YES	YES
13		a	58.73	0.08704	YES	YES
14		a	60.43	0.03505	YES	YES
15		a	64.16	0.04067	YES	YES
16		a	67.61	0.03231	YES	YES
17		a	71.89	0.06953	YES	YES
18		a	72.50	0.13371	YES	YES
19		a	101.76	0.10584	YES	YES
20		a	103.37	0.04505	YES	YES
21		a	104.09	0.13590	YES	YES
22		a	106.97	0.03244	YES	YES
23		a	110.52	0.01680	YES	YES
24		a	113.29	0.01218	YES	YES
25		a	119.21	0.06399	YES	YES
26		a	125.86	0.15730	YES	YES
27		a	130.23	0.24781	YES	YES
28		a	151.27	0.01552	YES	YES
29		a	152.25	0.04331	YES	YES
30		a	153.88	0.02190	YES	YES
31		a	177.84	1.49760	YES	YES
32		a	181.98	1.69305	YES	YES
33		a	182.09	1.14753	YES	YES
34		a	199.71	0.04846	YES	YES
35		a	207.95	0.09951	YES	YES
36		a	209.82	0.38431	YES	YES
37		a	262.94	0.09952	YES	YES
38		a	266.29	0.00995	YES	YES
39		a	267.06	0.00388	YES	YES
40		a	268.20	0.01957	YES	YES
41		a	271.08	0.49693	YES	YES
42		a	276.53	0.43246	YES	YES
43		a	281.90	0.25364	YES	YES
44		a	282.45	0.62228	YES	YES
45		a	283.27	0.16957	YES	YES
46		a	296.95	0.27777	YES	YES
47		a	300.64	0.32858	YES	YES
48		a	304.58	0.12088	YES	YES
49		a	309.34	0.14295	YES	YES
50		a	309.95	1.58124	YES	YES
51		a	312.64	1.20628	YES	YES
52		a	327.24	0.44195	YES	YES
53		a	328.98	0.13107	YES	YES
54		a	332.92	0.25095	YES	YES
55		a	336.04	4.33620	YES	YES
56		a	338.85	2.51248	YES	YES

57	a	344.77	0.04918	YES	YES
58	a	353.91	0.19254	YES	YES
59	a	361.29	0.17424	YES	YES
60	a	364.35	0.01550	YES	YES
61	a	369.30	0.20763	YES	YES
62	a	375.78	0.72225	YES	YES
63	a	384.37	2.05375	YES	YES
64	a	411.15	1.80910	YES	YES
65	a	411.96	1.86801	YES	YES
66	a	419.58	1.46562	YES	YES
67	a	423.33	0.23763	YES	YES
68	a	426.66	0.71838	YES	YES
69	a	427.79	0.59071	YES	YES
70	a	441.78	0.23747	YES	YES
71	a	442.47	0.08700	YES	YES
72	a	443.01	0.09322	YES	YES
73	a	497.71	0.11478	YES	YES
74	a	498.62	0.14671	YES	YES
75	a	500.00	0.04290	YES	YES
76	a	500.53	0.02680	YES	YES
77	a	501.10	0.08945	YES	YES
78	a	501.58	0.61130	YES	YES
79	a	504.23	2.03024	YES	YES
80	a	507.57	1.63738	YES	YES
81	a	508.89	0.49460	YES	YES
82	a	526.58	0.37186	YES	YES
83	a	537.99	23.00575	YES	YES
84	a	553.62	23.48966	YES	YES
85	a	579.96	13.07992	YES	YES
86	a	582.64	6.65152	YES	YES
87	a	583.02	6.76831	YES	YES
88	a	621.24	7.49042	YES	YES
89	a	624.19	1.06392	YES	YES
90	a	627.51	7.18867	YES	YES
91	a	650.72	8.90452	YES	YES
92	a	653.80	2.66045	YES	YES
93	a	657.01	5.18444	YES	YES
94	a	667.65	4.67909	YES	YES
95	a	670.25	7.16685	YES	YES
96	a	680.36	15.05633	YES	YES
97	a	685.60	9.71997	YES	YES
98	a	704.69	6.33819	YES	YES
99	a	728.44	68.26429	YES	YES
100	a	746.41	13.69175	YES	YES
101	a	766.94	49.97318	YES	YES
102	a	783.76	39.28086	YES	YES
103	a	796.25	81.79878	YES	YES
104	a	800.70	3.82686	YES	YES
105	a	806.50	4.05858	YES	YES
106	a	901.08	104.34078	YES	YES
107	a	923.02	94.68133	YES	YES
108	a	937.64	167.45529	YES	YES
109	a	946.12	108.27955	YES	YES
110	a	953.77	3.38132	YES	YES
111	a	963.04	65.65170	YES	YES
112	a	1022.18	52.89506	YES	YES
113	a	1029.88	103.45275	YES	YES
114	a	1041.51	8.27528	YES	YES
115	a	1050.78	95.83609	YES	YES
116	a	1059.29	57.43818	YES	YES
117	a	1109.69	13.36094	YES	YES
118	a	1111.40	82.47444	YES	YES

119	a	1115.95	33.63469	YES	YES
120	a	1153.16	51.16782	YES	YES
121	a	1156.10	60.54121	YES	YES
122	a	1159.38	98.52722	YES	YES
123	a	1230.37	1.29900	YES	YES
124	a	1232.85	1.63896	YES	YES
125	a	1234.77	2.98290	YES	YES
126	a	1247.30	29.79572	YES	YES
127	a	1250.35	13.78307	YES	YES
128	a	1251.54	60.98831	YES	YES
129	a	1331.95	66.63944	YES	YES
130	a	1335.57	48.56994	YES	YES
131	a	1336.61	48.88642	YES	YES
132	a	1377.84	2.03330	YES	YES
133	a	1378.54	3.38819	YES	YES
134	a	1380.60	3.12889	YES	YES
135	a	1391.22	174.68242	YES	YES
136	a	1396.33	29.49155	YES	YES
137	a	1399.23	137.09964	YES	YES
138	a	1400.97	304.45829	YES	YES
139	a	1401.88	617.49889	YES	YES
140	a	1403.99	488.99359	YES	YES
141	a	1448.28	25.36839	YES	YES
142	a	1450.68	5.47314	YES	YES
143	a	1451.90	8.02416	YES	YES
144	a	1487.06	380.90283	YES	YES
145	a	1488.48	339.14830	YES	YES
146	a	1490.21	118.71112	YES	YES
147	a	1523.55	105.27131	YES	YES
148	a	1526.45	64.11700	YES	YES
149	a	1527.12	48.43394	YES	YES
150	a	1584.69	115.23987	YES	YES
151	a	1590.67	61.81759	YES	YES
152	a	1591.79	100.92689	YES	YES
153	a	1615.56	30.10437	YES	YES
154	a	1619.53	56.01876	YES	YES
155	a	1621.94	50.74026	YES	YES
156	a	1645.75	75.53958	YES	YES
157	a	1646.98	83.39535	YES	YES
158	a	1647.29	82.36375	YES	YES
159	a	2391.53	63.23961	YES	YES



Total energy = -3362.2842089550 H = -91492.4605236 eV

HOMO-LUMO Separation

HOMO: 192. 192 a -0.10710869 H = -2.91458 eV

LUMO: 193. 193 a -0.00050458 H = -0.01373 eV

Gap : +0.10660411 H = +2.90085 eV

Number of MOs= 742, Electrons= 384.00, Symmetry: c1

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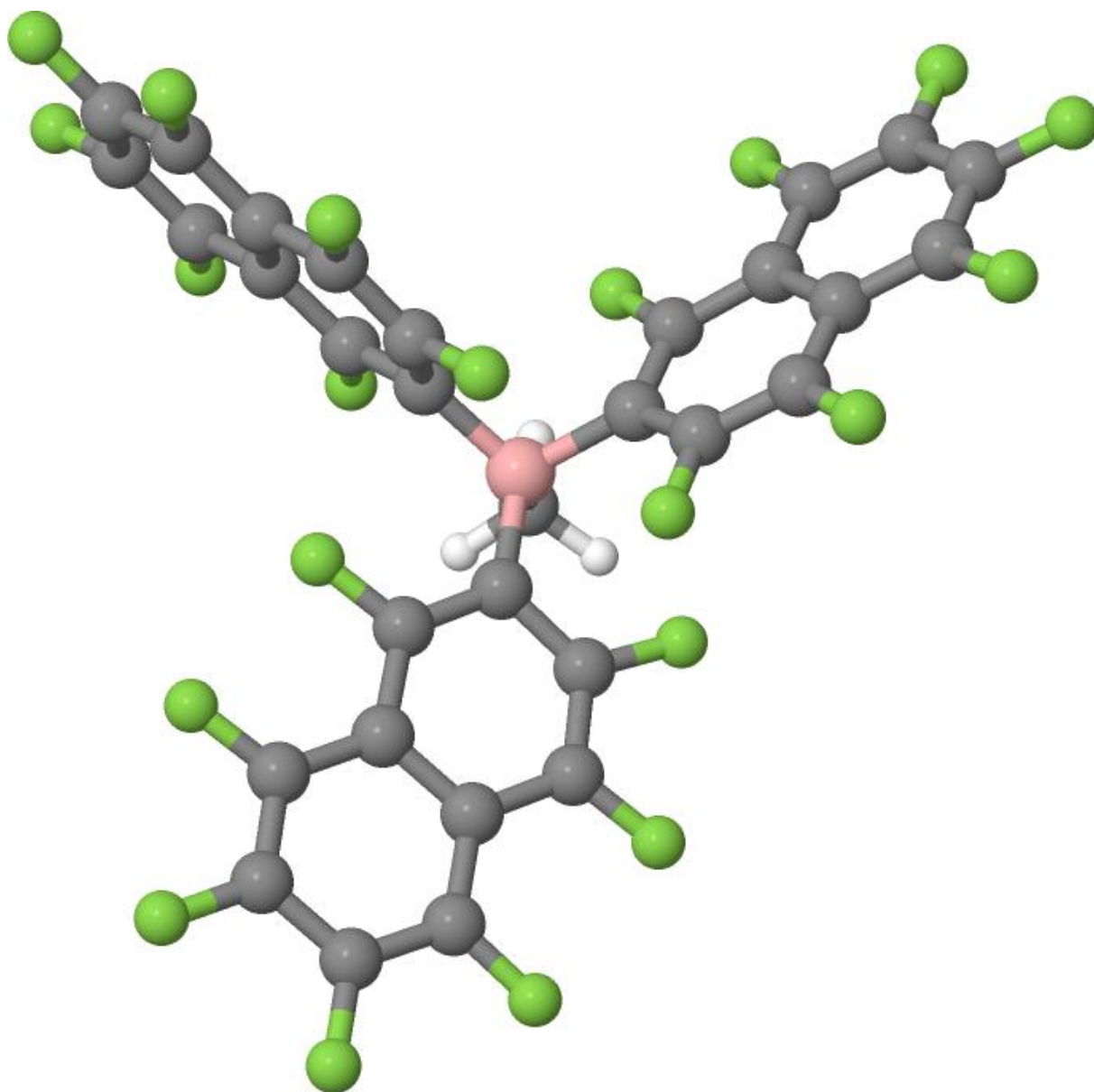
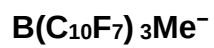
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\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	9.90	0.02072	YES	YES
8		a	12.53	0.01981	YES	YES
9		a	17.13	0.02439	YES	YES
10		a	19.19	0.01207	YES	YES
11		a	24.08	0.02055	YES	YES
12		a	24.87	0.02950	YES	YES
13		a	58.14	0.09787	YES	YES
14		a	62.32	0.07701	YES	YES
15		a	66.71	0.05140	YES	YES
16		a	69.62	0.09835	YES	YES
17		a	72.97	0.10011	YES	YES
18		a	75.93	0.14873	YES	YES
19		a	98.62	0.19398	YES	YES
20		a	102.26	0.18507	YES	YES
21		a	104.68	0.01171	YES	YES
22		a	107.51	0.03395	YES	YES
23		a	110.50	0.10547	YES	YES
24		a	113.89	0.03243	YES	YES
25		a	118.97	0.07042	YES	YES
26		a	125.67	0.10049	YES	YES
27		a	132.71	0.29463	YES	YES
28		a	151.36	0.03283	YES	YES
29		a	152.51	0.06100	YES	YES
30		a	153.93	0.02753	YES	YES
31		a	178.90	1.60396	YES	YES
32		a	181.43	1.94497	YES	YES
33		a	183.75	1.73070	YES	YES
34		a	199.49	0.75055	YES	YES
35		a	204.33	0.76282	YES	YES
36		a	210.77	0.01411	YES	YES
37		a	214.07	1.71528	YES	YES
38		a	232.31	1.69499	YES	YES
39		a	262.70	0.02446	YES	YES
40		a	265.93	0.07234	YES	YES
41		a	267.61	0.02156	YES	YES
42		a	268.40	0.02150	YES	YES
43		a	279.97	0.66372	YES	YES
44		a	282.17	0.34622	YES	YES
45		a	283.55	0.65048	YES	YES
46		a	284.46	1.05530	YES	YES
47		a	291.77	0.23537	YES	YES
48		a	303.25	0.47474	YES	YES
49		a	304.62	0.50445	YES	YES
50		a	305.20	0.10286	YES	YES
51		a	309.83	1.32384	YES	YES
52		a	311.24	0.61860	YES	YES
53		a	315.35	0.76585	YES	YES
54		a	325.44	1.38280	YES	YES
55		a	332.42	0.27465	YES	YES
56		a	333.40	1.36244	YES	YES
57		a	334.89	0.63044	YES	YES

58	a	342.45	3.70870	YES	YES
59	a	346.38	2.04848	YES	YES
60	a	353.13	0.53346	YES	YES
61	a	364.20	0.03351	YES	YES
62	a	365.36	0.11905	YES	YES
63	a	366.73	0.00520	YES	YES
64	a	381.43	3.27179	YES	YES
65	a	398.50	6.55941	YES	YES
66	a	413.43	1.52052	YES	YES
67	a	417.04	1.99233	YES	YES
68	a	419.32	1.28450	YES	YES
69	a	426.10	0.45549	YES	YES
70	a	428.59	0.53422	YES	YES
71	a	431.00	0.15275	YES	YES
72	a	441.74	0.27808	YES	YES
73	a	442.06	0.12186	YES	YES
74	a	443.08	0.31529	YES	YES
75	a	451.36	0.29355	YES	YES
76	a	491.94	0.09094	YES	YES
77	a	501.42	0.13307	YES	YES
78	a	501.69	0.04444	YES	YES
79	a	502.18	0.32737	YES	YES
80	a	502.47	0.22332	YES	YES
81	a	503.12	0.19935	YES	YES
82	a	507.49	2.40570	YES	YES
83	a	509.26	1.58989	YES	YES
84	a	510.17	0.67789	YES	YES
85	a	552.88	53.49652	YES	YES
86	a	570.09	32.27272	YES	YES
87	a	576.74	0.77442	YES	YES
88	a	586.78	27.25916	YES	YES
89	a	591.76	42.74778	YES	YES
90	a	621.29	6.45005	YES	YES
91	a	622.80	2.69404	YES	YES
92	a	628.22	8.05696	YES	YES
93	a	649.88	6.76938	YES	YES
94	a	654.02	14.01783	YES	YES
95	a	659.03	11.85233	YES	YES
96	a	665.84	3.52102	YES	YES
97	a	674.13	10.25907	YES	YES
98	a	674.63	9.48817	YES	YES
99	a	685.35	8.07654	YES	YES
100	a	716.12	15.80237	YES	YES
101	a	727.79	79.89044	YES	YES
102	a	731.57	28.58955	YES	YES
103	a	779.01	2.99012	YES	YES
104	a	790.92	5.10525	YES	YES
105	a	793.63	8.47305	YES	YES
106	a	817.06	9.50809	YES	YES
107	a	820.29	16.21357	YES	YES
108	a	894.33	122.48541	YES	YES
109	a	917.16	132.95829	YES	YES
110	a	932.68	147.44495	YES	YES
111	a	951.29	190.91870	YES	YES
112	a	968.56	120.20744	YES	YES
113	a	981.51	259.22278	YES	YES
114	a	1027.70	55.22577	YES	YES
115	a	1039.29	3.42518	YES	YES
116	a	1042.29	6.94484	YES	YES
117	a	1044.80	20.62805	YES	YES
118	a	1111.31	53.82170	YES	YES
119	a	1113.73	32.71141	YES	YES

120	a	1117.08	33.63281	YES	YES
121	a	1152.81	28.25702	YES	YES
122	a	1153.90	88.62797	YES	YES
123	a	1157.41	153.21500	YES	YES
124	a	1233.93	8.09537	YES	YES
125	a	1237.76	1.74825	YES	YES
126	a	1240.48	0.86126	YES	YES
127	a	1249.17	55.42117	YES	YES
128	a	1251.92	39.61950	YES	YES
129	a	1254.11	45.53597	YES	YES
130	a	1328.33	46.21032	YES	YES
131	a	1332.88	46.59137	YES	YES
132	a	1336.42	38.77665	YES	YES
133	a	1377.00	9.80052	YES	YES
134	a	1378.14	14.72399	YES	YES
135	a	1382.28	14.26351	YES	YES
136	a	1393.10	127.32266	YES	YES
137	a	1395.86	100.19894	YES	YES
138	a	1398.85	283.97856	YES	YES
139	a	1403.56	50.79006	YES	YES
140	a	1404.78	510.22102	YES	YES
141	a	1409.62	670.51995	YES	YES
142	a	1449.47	18.86581	YES	YES
143	a	1452.77	0.66152	YES	YES
144	a	1453.73	14.96498	YES	YES
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146	a	1489.61	350.83090	YES	YES
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148	a	1526.12	123.77101	YES	YES
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151	a	1587.42	140.88267	YES	YES
152	a	1591.61	157.57182	YES	YES
153	a	1594.86	78.88680	YES	YES
154	a	1619.94	33.66815	YES	YES
155	a	1622.94	62.35568	YES	YES
156	a	1625.02	41.01838	YES	YES
157	a	1646.46	80.81739	YES	YES
158	a	1647.75	60.11489	YES	YES
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Total energy = -3302.3365579200 H = -89861.2010122 eV

HOMO-LUMO Separation

HOMO: 192. 192 a -0.10579079 H = -2.87872 eV

LUMO: 193. 193 a +0.00050382 H = +0.01371 eV

Gap : +0.10629461 H = +2.89243 eV

Number of MOs= 748, Electrons= 384.00, Symmetry: c1

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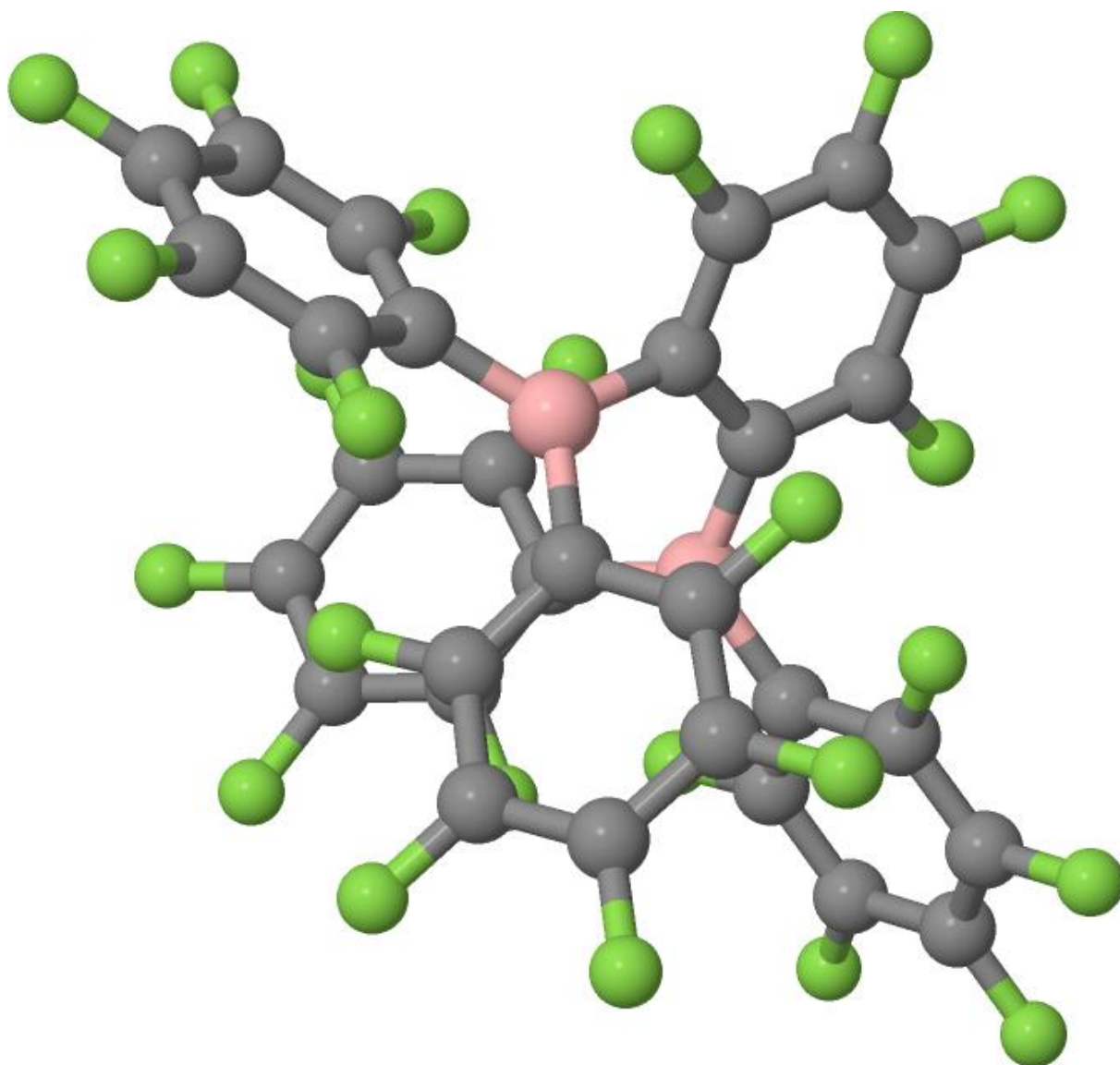
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3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	11.42	0.02737	YES	YES
8		a	14.57	0.00227	YES	YES
9		a	18.82	0.02186	YES	YES
10		a	19.67	0.01165	YES	YES
11		a	25.16	0.02181	YES	YES
12		a	28.00	0.00641	YES	YES
13		a	57.41	0.03545	YES	YES
14		a	64.07	0.03732	YES	YES
15		a	67.62	0.03180	YES	YES
16		a	70.65	0.05587	YES	YES
17		a	76.93	0.13563	YES	YES
18		a	80.29	0.03092	YES	YES
19		a	101.14	0.09673	YES	YES
20		a	103.29	0.03867	YES	YES
21		a	105.12	0.11877	YES	YES
22		a	108.23	0.04755	YES	YES
23		a	111.91	0.04031	YES	YES
24		a	115.18	0.00178	YES	YES
25		a	121.71	0.14928	YES	YES
26		a	128.66	0.14987	YES	YES
27		a	145.88	0.15532	YES	YES
28		a	151.79	0.01165	YES	YES
29		a	152.66	0.02075	YES	YES
30		a	154.93	0.24521	YES	YES
31		a	179.18	0.97843	YES	YES
32		a	181.51	1.72638	YES	YES
33		a	183.15	1.63469	YES	YES
34		a	198.80	0.23634	YES	YES
35		a	202.95	0.12633	YES	YES
36		a	212.36	0.32100	YES	YES
37		a	214.70	0.12526	YES	YES
38		a	240.98	0.30679	YES	YES
39		a	261.70	0.29976	YES	YES
40		a	267.08	0.01600	YES	YES
41		a	267.42	0.02171	YES	YES
42		a	268.26	0.01151	YES	YES
43		a	277.30	0.29716	YES	YES
44		a	279.50	0.57020	YES	YES
45		a	283.43	0.38886	YES	YES
46		a	283.95	0.40728	YES	YES
47		a	285.84	0.75778	YES	YES
48		a	292.96	0.02326	YES	YES
49		a	305.63	0.58585	YES	YES
50		a	306.96	0.13445	YES	YES
51		a	308.83	0.13233	YES	YES
52		a	313.67	1.23942	YES	YES
53		a	313.82	0.63951	YES	YES
54		a	319.65	0.83633	YES	YES
55		a	324.50	0.81030	YES	YES

56	a	335.16	0.53729	YES	YES
57	a	338.11	3.59875	YES	YES
58	a	338.73	1.79461	YES	YES
59	a	343.55	1.06920	YES	YES
60	a	344.93	0.64160	YES	YES
61	a	356.53	0.21418	YES	YES
62	a	363.85	0.01105	YES	YES
63	a	364.93	0.05757	YES	YES
64	a	366.25	0.06765	YES	YES
65	a	382.58	1.93290	YES	YES
66	a	397.26	3.80065	YES	YES
67	a	413.49	0.57444	YES	YES
68	a	415.56	2.40661	YES	YES
69	a	418.11	0.75445	YES	YES
70	a	425.17	0.56633	YES	YES
71	a	427.27	0.02788	YES	YES
72	a	430.41	0.58200	YES	YES
73	a	441.70	0.18172	YES	YES
74	a	442.15	0.08645	YES	YES
75	a	443.03	0.08039	YES	YES
76	a	448.27	0.10214	YES	YES
77	a	495.24	0.02560	YES	YES
78	a	499.27	0.22715	YES	YES
79	a	500.31	0.08200	YES	YES
80	a	500.37	0.15931	YES	YES
81	a	501.65	0.12384	YES	YES
82	a	502.06	0.23940	YES	YES
83	a	506.62	3.08188	YES	YES
84	a	508.72	1.69355	YES	YES
85	a	510.02	0.22609	YES	YES
86	a	539.27	27.19220	YES	YES
87	a	556.63	28.59682	YES	YES
88	a	577.09	1.05520	YES	YES
89	a	580.72	10.05018	YES	YES
90	a	584.22	6.19533	YES	YES
91	a	621.41	3.45871	YES	YES
92	a	623.00	1.89768	YES	YES
93	a	629.56	7.93031	YES	YES
94	a	653.99	1.54540	YES	YES
95	a	655.78	3.44597	YES	YES
96	a	660.35	6.51148	YES	YES
97	a	662.56	4.49429	YES	YES
98	a	676.24	7.15460	YES	YES
99	a	679.70	5.98045	YES	YES
100	a	689.70	21.57298	YES	YES
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102	a	723.36	26.11722	YES	YES
103	a	726.38	69.43744	YES	YES
104	a	747.48	39.39331	YES	YES
105	a	755.02	80.84187	YES	YES
106	a	787.60	10.58805	YES	YES
107	a	790.63	15.57885	YES	YES
108	a	798.35	0.65328	YES	YES
109	a	866.19	65.25222	YES	YES
110	a	875.37	50.34534	YES	YES
111	a	882.90	15.76173	YES	YES
112	a	925.64	47.25782	YES	YES
113	a	936.30	102.97772	YES	YES
114	a	948.50	240.71055	YES	YES
115	a	954.06	46.39879	YES	YES
116	a	987.70	90.98208	YES	YES
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118	a	1035.92	3.31480	YES	YES
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123	a	1113.22	39.84281	YES	YES
124	a	1148.90	71.01911	YES	YES
125	a	1150.14	33.99835	YES	YES
126	a	1155.13	111.36283	YES	YES
127	a	1231.59	5.59744	YES	YES
128	a	1234.00	6.62944	YES	YES
129	a	1236.13	4.60841	YES	YES
130	a	1247.10	35.39808	YES	YES
131	a	1248.75	25.37946	YES	YES
132	a	1249.91	55.29480	YES	YES
133	a	1266.81	12.27991	YES	YES
134	a	1326.19	119.56686	YES	YES
135	a	1328.29	38.28552	YES	YES
136	a	1331.99	39.83553	YES	YES
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138	a	1375.92	3.32097	YES	YES
139	a	1378.84	10.01152	YES	YES
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142	a	1396.83	197.94560	YES	YES
143	a	1397.25	58.39323	YES	YES
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146	a	1422.05	27.64429	YES	YES
147	a	1430.39	3.72148	YES	YES
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161	a	1620.24	38.86213	YES	YES
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163	a	1647.04	43.16560	YES	YES
164	a	1647.16	111.22061	YES	YES
165	a	1647.77	87.06683	YES	YES
166	a	2937.15	32.54824	YES	YES
167	a	3008.34	32.39754	YES	YES
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F₄C₆(1,2-(B(C₆F₅)₂)₃



Total energy = -3586.4464055570 H = -97592.2277202 eV

HOMO-LUMO Separation

HOMO: 203. 102 a -0.23890667 H = -6.50098 eV

LUMO: 204. 103 a -0.15096874 H = -4.10807 eV

Gap : +0.08793793 H = +2.39291 eV

Number of MOs= 784, Electrons= 406.00, Symmetry: c2

\$coord

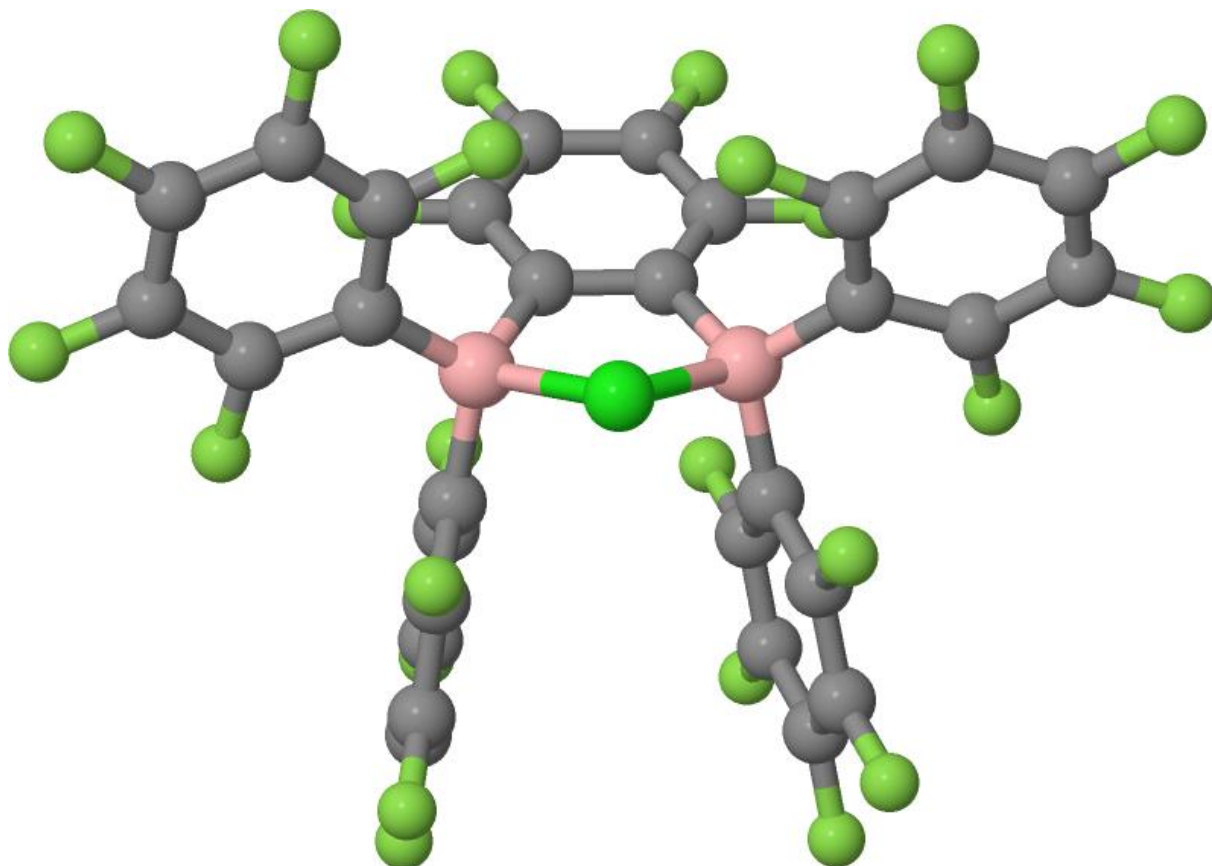
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10.56389729776061	3.26075653972911	-1.43822958216954	f
13.14364016256616	-0.45952197040489	1.05927455065946	f
10.68778714120631	-4.74686430525339	2.59882960739704	f
5.73662679938236	-5.32688836616576	1.69067785465065	f
-5.60220867974645	-2.71888550134706	-2.41283323142093	f
-10.56389729776061	-3.26075653972911	-1.43822958216954	f
-13.14364016256616	0.45952197040489	1.05927455065946	f
-10.68778714120631	4.74686430525339	2.59882960739704	f
-5.73662679938236	5.32688836616576	1.69067785465065	f
-2.53706195735110	1.37108228845145	4.60565769887503	f
0.41756758594082	4.17645022961252	7.69972695975563	f
3.71125131360849	7.62840670467124	5.69615530586129	f
4.03804897584512	8.26110222654316	0.58260452994461	f
1.07044167232866	5.51244491885485	-2.53264944662827	f
-2.27418849504914	-6.23538176147946	4.17107006257720	c
-3.71125131360849	-7.62840670467124	5.69615530586129	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	12.98	0.03757	YES	YES
8		a	15.43	0.02245	YES	YES
9		a	21.52	0.12830	YES	YES
10		a	26.03	0.35172	YES	YES
11		a	29.11	0.13548	YES	YES
12		a	31.70	0.04176	YES	YES
13		a	33.03	0.01987	YES	YES
14		a	37.01	0.12972	YES	YES
15		a	38.10	0.05942	YES	YES
16		a	40.21	0.02288	YES	YES
17		a	50.30	0.00455	YES	YES
18		a	55.28	0.02849	YES	YES
19		a	78.69	0.03870	YES	YES
20		a	84.57	0.26869	YES	YES
21		a	99.51	0.32633	YES	YES
22		a	107.76	0.01144	YES	YES
23		a	108.53	0.14235	YES	YES
24		a	112.63	0.33578	YES	YES
25		a	118.95	0.16278	YES	YES
26		a	121.80	0.00745	YES	YES
27		a	128.06	0.31195	YES	YES
28		a	129.24	0.01848	YES	YES
29		a	135.55	0.03364	YES	YES
30		a	139.50	0.13043	YES	YES
31		a	143.64	0.01102	YES	YES
32		a	144.02	0.04449	YES	YES
33		a	147.35	0.01518	YES	YES
34		a	149.83	0.05029	YES	YES
35		a	152.51	0.10444	YES	YES
36		a	160.07	0.10193	YES	YES
37		a	160.44	0.03908	YES	YES
38		a	173.89	0.06842	YES	YES
39		a	182.80	1.18031	YES	YES
40		a	219.84	0.85665	YES	YES
41		a	222.51	4.64661	YES	YES
42		a	228.86	4.65134	YES	YES
43		a	231.19	0.75830	YES	YES
44		a	240.98	7.06228	YES	YES
45		a	262.67	0.18240	YES	YES
46		a	262.73	0.18525	YES	YES
47		a	263.19	0.18084	YES	YES
48		a	263.51	0.12315	YES	YES
49		a	265.06	0.15540	YES	YES
50		a	269.54	0.00512	YES	YES
51		a	270.04	0.03311	YES	YES
52		a	271.27	0.26659	YES	YES
53		a	271.46	0.00207	YES	YES
54		a	284.83	0.12131	YES	YES
55		a	306.12	0.41419	YES	YES
56		a	306.79	0.61532	YES	YES
57		a	308.61	0.43252	YES	YES

58	a	308.76	0.82490	YES	YES
59	a	335.14	2.02689	YES	YES
60	a	336.99	6.04642	YES	YES
61	a	340.60	0.00299	YES	YES
62	a	342.56	0.55070	YES	YES
63	a	346.54	0.86960	YES	YES
64	a	348.47	0.06395	YES	YES
65	a	354.05	0.23226	YES	YES
66	a	371.83	0.69425	YES	YES
67	a	378.95	13.89321	YES	YES
68	a	380.02	3.28974	YES	YES
69	a	390.97	0.96328	YES	YES
70	a	391.29	1.50151	YES	YES
71	a	394.27	0.88081	YES	YES
72	a	395.35	1.63823	YES	YES
73	a	409.95	3.72242	YES	YES
74	a	429.80	0.29896	YES	YES
75	a	430.43	0.67211	YES	YES
76	a	431.30	0.38947	YES	YES
77	a	431.36	0.36804	YES	YES
78	a	452.29	0.67865	YES	YES
79	a	458.54	0.00363	YES	YES
80	a	461.29	7.93502	YES	YES
81	a	466.34	2.58772	YES	YES
82	a	480.12	0.72307	YES	YES
83	a	495.37	0.52668	YES	YES
84	a	505.56	0.05031	YES	YES
85	a	507.00	0.48364	YES	YES
86	a	516.17	0.06406	YES	YES
87	a	516.59	0.08560	YES	YES
88	a	532.92	12.30206	YES	YES
89	a	533.98	0.84557	YES	YES
90	a	563.21	1.52815	YES	YES
91	a	564.02	2.73643	YES	YES
92	a	565.36	1.13201	YES	YES
93	a	565.43	1.25103	YES	YES
94	a	572.30	4.78890	YES	YES
95	a	614.74	26.05043	YES	YES
96	a	617.14	36.07149	YES	YES
97	a	621.86	6.78195	YES	YES
98	a	624.69	33.66563	YES	YES
99	a	631.17	2.74496	YES	YES
100	a	633.95	0.00091	YES	YES
101	a	634.89	1.84321	YES	YES
102	a	635.48	0.80235	YES	YES
103	a	649.10	12.18160	YES	YES
104	a	660.92	18.35628	YES	YES
105	a	665.94	23.31617	YES	YES
106	a	669.03	27.27405	YES	YES
107	a	691.57	3.13891	YES	YES
108	a	700.32	1.77588	YES	YES
109	a	758.45	62.69136	YES	YES
110	a	767.30	15.31264	YES	YES
111	a	770.46	20.83810	YES	YES
112	a	775.16	2.22053	YES	YES
113	a	775.61	2.74035	YES	YES
114	a	842.85	2.97443	YES	YES
115	a	856.59	0.12596	YES	YES
116	a	974.20	2.67870	YES	YES
117	a	982.69	0.08201	YES	YES
118	a	984.52	95.21096	YES	YES
119	a	985.73	172.34635	YES	YES

120	a	997.17	149.73430	YES	YES
121	a	1014.36	5.86401	YES	YES
122	a	1017.56	117.99084	YES	YES
123	a	1030.94	106.35771	YES	YES
124	a	1097.75	1.49158	YES	YES
125	a	1122.44	0.15913	YES	YES
126	a	1152.97	77.17227	YES	YES
127	a	1154.07	53.48685	YES	YES
128	a	1154.72	35.34760	YES	YES
129	a	1156.47	21.21631	YES	YES
130	a	1162.06	16.09094	YES	YES
131	a	1164.06	95.23587	YES	YES
132	a	1177.74	12.50668	YES	YES
133	a	1178.62	539.86761	YES	YES
134	a	1288.54	18.35231	YES	YES
135	a	1299.44	82.68366	YES	YES
136	a	1307.49	94.48110	YES	YES
137	a	1311.50	173.64272	YES	YES
138	a	1316.33	23.58195	YES	YES
139	a	1317.00	378.48040	YES	YES
140	a	1346.09	1.55430	YES	YES
141	a	1346.31	0.90607	YES	YES
142	a	1350.74	4.62358	YES	YES
143	a	1351.29	4.89058	YES	YES
144	a	1367.41	175.20391	YES	YES
145	a	1372.81	3.00211	YES	YES
146	a	1376.52	413.84741	YES	YES
147	a	1380.53	106.48097	YES	YES
148	a	1392.53	75.55987	YES	YES
149	a	1430.30	231.67724	YES	YES
150	a	1466.75	1.62209	YES	YES
151	a	1472.59	332.92218	YES	YES
152	a	1474.98	798.44159	YES	YES
153	a	1482.43	930.19033	YES	YES
154	a	1496.34	22.56662	YES	YES
155	a	1519.09	172.58280	YES	YES
156	a	1520.22	44.63038	YES	YES
157	a	1521.79	513.78502	YES	YES
158	a	1524.17	86.06002	YES	YES
159	a	1586.08	71.73190	YES	YES
160	a	1602.99	107.01049	YES	YES
161	a	1608.79	2.07374	YES	YES
162	a	1609.36	27.97329	YES	YES
163	a	1610.07	1.71247	YES	YES
164	a	1611.10	37.93888	YES	YES
165	a	1628.87	277.87366	YES	YES
166	a	1629.23	2.77722	YES	YES
167	a	1633.85	63.45160	YES	YES
168	a	1634.11	145.11706	YES	YES



Total energy = -3586.4464055570 H = -97592.2277202 eV

HOMO-LUMO Separation

HOMO: 203. 102 a -0.23890667 H = -6.50098 eV

LUMO: 204. 103 a -0.15096874 H = -4.10807 eV

Gap : +0.08793793 H = +2.39291 eV

Number of MOs= 784, Electrons= 406.00, Symmetry: c2

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3.14688341741517 -6.83090860818297 -1.44082283251747 c
3.10853157230810 -6.86304730859153 1.20958010693992 c
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1.52068776193723	-2.49796332472160	1.26309402235713	c
1.54889235658254	-2.47249357956337	-1.42715287657541	c
2.37195555908409	-4.63430000056298	-2.71219565642732	c
0.55802371659451	-0.00013049566915	-2.92709632053981	b
0.61339915784694	-0.01153033068803	2.79426427660630	b
6.54818956224712	2.19565013352863	-6.89228258036812	c
4.93234960797043	1.40588176195971	-4.93567432081301	c
2.32776744112128	0.94173835774014	-5.26682554450174	c
1.45773107865419	1.23191542207611	-7.76711802486380	c
3.00939412868058	2.00497987932262	-9.78239875950370	c
5.57593269644369	2.49041099407713	-9.34150916248930	c
-4.07673515757483	-2.00249702270213	-3.49024604396861	c
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-3.70711700319000	2.45472746423037	-3.85761453180242	c
-6.32459877574890	2.70343771566822	-4.19810210431196	c
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6.47509734170079	2.42247604685099	6.90394486398468	c
5.58118040414968	2.15092772046413	9.38334400428165	c
3.14606958390672	1.18582241659592	9.78011785161369	c
1.64785571050301	0.52861814673777	7.68815226471443	c
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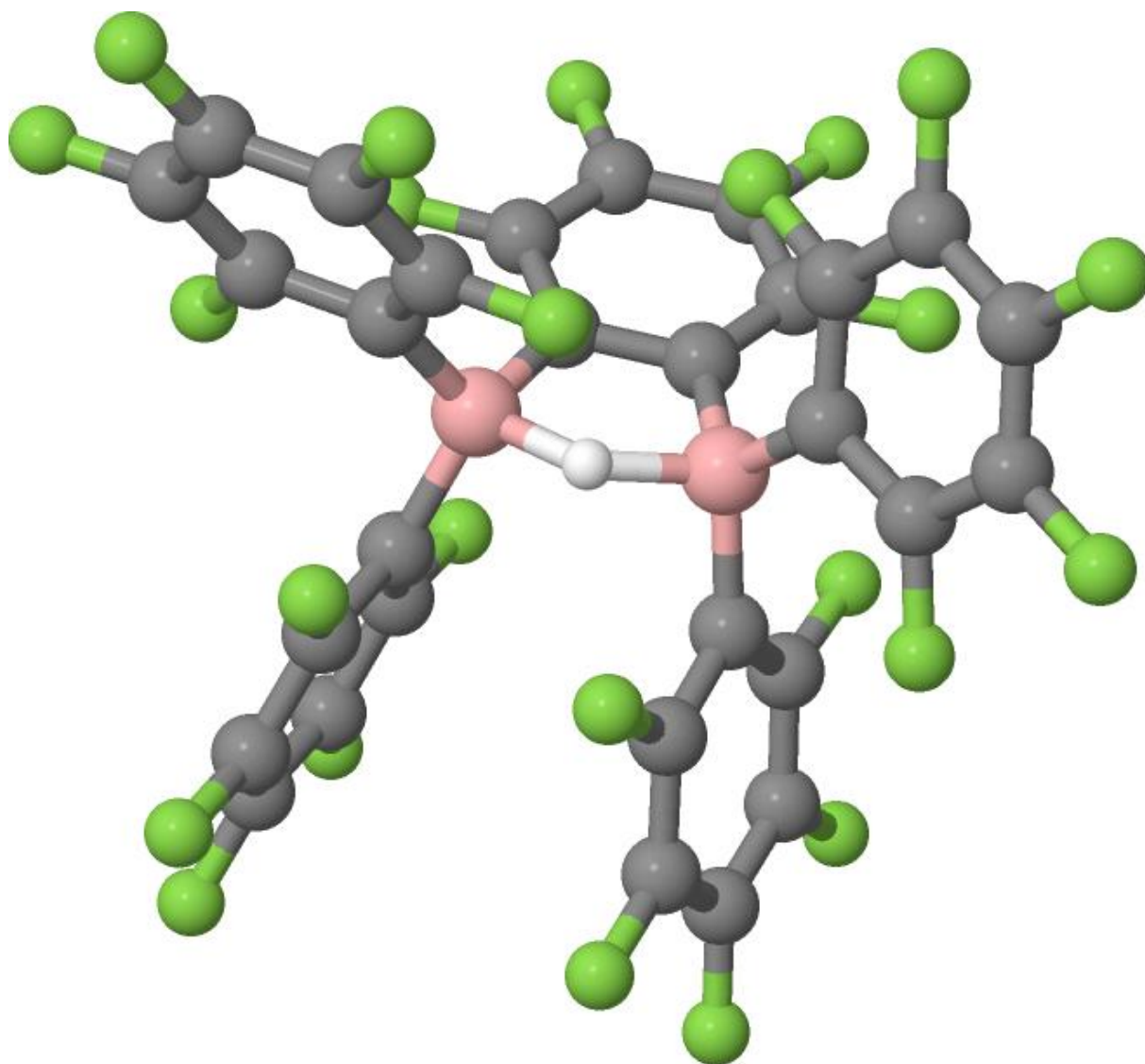
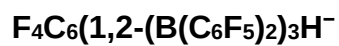
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1		0.00	0.00000	-	-
	2		0.00	0.00000	-	-

3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	12.44	0.00204	YES	YES
8	a	14.64	0.04695	YES	YES
9	a	17.29	0.01189	YES	YES
10	a	19.68	0.00567	YES	YES
11	a	27.37	0.00404	YES	YES
12	a	28.50	0.00156	YES	YES
13	a	31.23	0.00237	YES	YES
14	a	34.07	0.02149	YES	YES
15	a	41.33	0.04967	YES	YES
16	a	42.62	0.23122	YES	YES
17	a	46.60	0.04076	YES	YES
18	a	49.59	0.01314	YES	YES
19	a	87.01	0.00926	YES	YES
20	a	95.66	0.15040	YES	YES
21	a	99.36	0.22667	YES	YES
22	a	104.26	0.05562	YES	YES
23	a	114.38	0.13948	YES	YES
24	a	119.14	0.04982	YES	YES
25	a	120.38	0.32648	YES	YES
26	a	122.19	0.15161	YES	YES
27	a	125.85	0.09794	YES	YES
28	a	130.02	0.11642	YES	YES
29	a	132.93	0.21222	YES	YES
30	a	135.88	0.14269	YES	YES
31	a	146.27	0.34130	YES	YES
32	a	149.63	0.18612	YES	YES
33	a	151.96	0.14558	YES	YES
34	a	155.69	0.00310	YES	YES
35	a	159.13	0.29329	YES	YES
36	a	159.57	0.04329	YES	YES
37	a	163.17	0.00470	YES	YES
38	a	166.75	0.16508	YES	YES
39	a	191.67	0.67973	YES	YES
40	a	198.69	1.51163	YES	YES
41	a	217.77	1.73342	YES	YES
42	a	224.00	1.66069	YES	YES
43	a	229.46	1.45710	YES	YES
44	a	231.41	1.72405	YES	YES
45	a	243.23	1.41858	YES	YES
46	a	245.80	25.96559	YES	YES
47	a	261.83	0.20088	YES	YES
48	a	261.97	0.03086	YES	YES
49	a	262.52	0.06866	YES	YES
50	a	262.65	0.15840	YES	YES
51	a	263.41	0.02210	YES	YES
52	a	265.98	0.90577	YES	YES
53	a	271.57	0.04830	YES	YES
54	a	273.52	0.03790	YES	YES
55	a	274.07	0.18667	YES	YES
56	a	274.43	0.08584	YES	YES
57	a	281.08	0.66800	YES	YES
58	a	306.57	0.40456	YES	YES
59	a	308.58	0.72722	YES	YES
60	a	309.19	1.00293	YES	YES
61	a	310.60	0.53536	YES	YES
62	a	337.03	5.45771	YES	YES
63	a	340.81	3.93363	YES	YES
64	a	341.62	1.25237	YES	YES

65	a	345.31	0.09651	YES	YES
66	a	348.40	0.37487	YES	YES
67	a	360.92	24.87155	YES	YES
68	a	365.78	8.81029	YES	YES
69	a	380.70	3.46743	YES	YES
70	a	383.58	0.09784	YES	YES
71	a	383.80	0.34007	YES	YES
72	a	387.42	0.41896	YES	YES
73	a	388.31	1.91411	YES	YES
74	a	390.30	0.96690	YES	YES
75	a	393.37	0.56347	YES	YES
76	a	406.57	0.05244	YES	YES
77	a	433.03	0.15140	YES	YES
78	a	433.79	0.07892	YES	YES
79	a	433.89	0.33740	YES	YES
80	a	435.31	0.18603	YES	YES
81	a	457.19	0.32999	YES	YES
82	a	458.58	1.70575	YES	YES
83	a	465.80	6.89866	YES	YES
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86	a	476.00	29.00879	YES	YES
87	a	506.43	64.64504	YES	YES
88	a	512.21	4.69622	YES	YES
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90	a	516.23	2.10363	YES	YES
91	a	519.53	0.09387	YES	YES
92	a	556.93	1.81469	YES	YES
93	a	561.72	11.98501	YES	YES
94	a	563.77	3.53119	YES	YES
95	a	565.09	0.25069	YES	YES
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97	a	567.86	11.10601	YES	YES
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99	a	614.42	40.85502	YES	YES
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101	a	621.96	18.56902	YES	YES
102	a	629.87	0.54151	YES	YES
103	a	631.31	0.74827	YES	YES
104	a	632.62	0.61241	YES	YES
105	a	634.91	0.09073	YES	YES
106	a	659.83	14.51872	YES	YES
107	a	667.49	42.43509	YES	YES
108	a	682.08	39.04562	YES	YES
109	a	685.96	34.22022	YES	YES
110	a	703.94	66.94630	YES	YES
111	a	709.49	3.82225	YES	YES
112	a	748.31	72.36602	YES	YES
113	a	759.47	18.17801	YES	YES
114	a	763.00	30.16159	YES	YES
115	a	764.72	8.80958	YES	YES
116	a	766.48	16.74192	YES	YES
117	a	835.08	2.42124	YES	YES
118	a	836.36	0.83953	YES	YES
119	a	948.36	4.94700	YES	YES
120	a	953.90	3.33924	YES	YES
121	a	960.37	9.31914	YES	YES
122	a	965.42	21.76014	YES	YES
123	a	981.06	16.17295	YES	YES
124	a	983.89	276.78371	YES	YES
125	a	986.33	195.71597	YES	YES
126	a	999.02	141.65106	YES	YES

127	a	1068.84	1.95371	YES	YES
128	a	1098.99	6.67559	YES	YES
129	a	1106.16	229.02032	YES	YES
130	a	1113.02	198.04623	YES	YES
131	a	1117.19	396.77709	YES	YES
132	a	1121.18	107.55466	YES	YES
133	a	1136.75	2.48591	YES	YES
134	a	1139.86	2.94241	YES	YES
135	a	1141.90	14.38383	YES	YES
136	a	1144.46	0.57433	YES	YES
137	a	1254.61	16.45808	YES	YES
138	a	1277.98	38.07569	YES	YES
139	a	1279.35	36.60546	YES	YES
140	a	1281.40	31.18441	YES	YES
141	a	1283.81	93.58047	YES	YES
142	a	1316.52	79.40861	YES	YES
143	a	1342.73	1.89667	YES	YES
144	a	1343.12	3.67419	YES	YES
145	a	1344.81	3.11778	YES	YES
146	a	1346.11	5.66770	YES	YES
147	a	1359.23	62.78431	YES	YES
148	a	1381.38	8.33116	YES	YES
149	a	1383.68	41.62044	YES	YES
150	a	1386.08	18.35776	YES	YES
151	a	1389.84	19.44507	YES	YES
152	a	1438.25	250.76589	YES	YES
153	a	1461.12	150.65399	YES	YES
154	a	1467.14	306.27273	YES	YES
155	a	1468.74	602.43764	YES	YES
156	a	1474.86	671.79895	YES	YES
157	a	1491.98	120.20854	YES	YES
158	a	1512.67	12.74944	YES	YES
159	a	1514.76	267.24119	YES	YES
160	a	1515.49	287.98528	YES	YES
161	a	1518.13	104.17902	YES	YES
162	a	1593.57	24.44773	YES	YES
163	a	1615.53	2.27000	YES	YES
164	a	1616.54	4.47570	YES	YES
165	a	1617.28	3.25015	YES	YES
166	a	1618.39	10.87098	YES	YES
167	a	1621.22	31.75917	YES	YES
168	a	1626.27	56.60066	YES	YES
169	a	1627.00	70.52681	YES	YES
170	a	1628.43	16.81732	YES	YES
171	a	1630.02	52.93216	YES	YES



Total energy = -3587.1648975880 H = -97611.7788942 eV

HOMO-LUMO Separation

HOMO: 204. 204 a -0.11496864 H = -3.12846 eV

LUMO: 205. 205 a +0.00221597 H = +0.06030 eV

Gap : +0.11718461 H = +3.18876 eV

Number of MOs= 786, Electrons= 408.00, Symmetry: c1

\$scoord

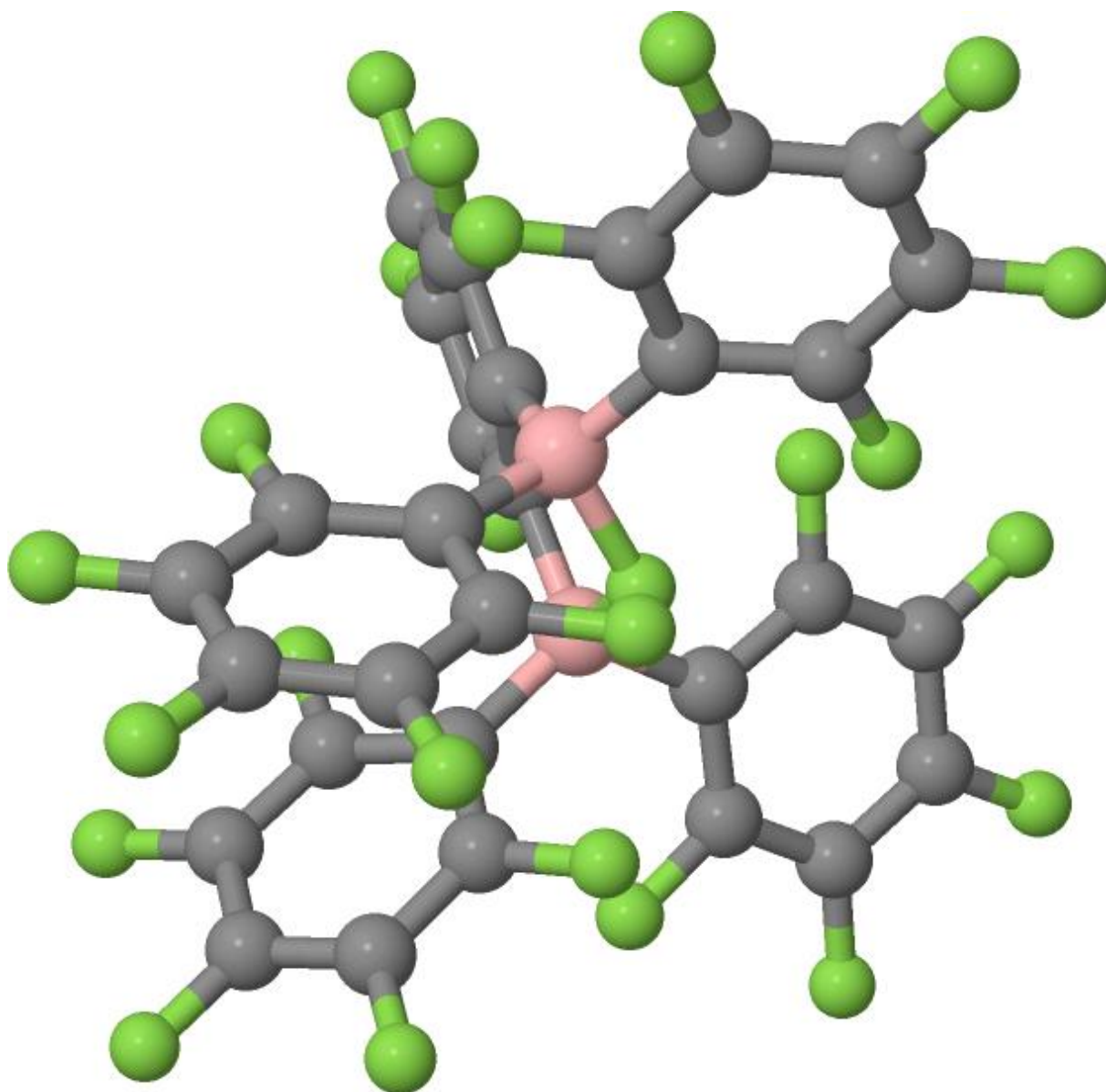
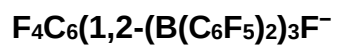
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1.25394377140711	-0.61725944384930	-3.37286570509424	c
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8.72404113562226	-3.32874533243517	0.96398664878668	c
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4.24466081475665	-1.99668016701045	0.64571656467483	c
3.66934652963762	-4.06829438157690	2.20070515565676	c
5.49833991326276	-5.77292189371705	3.10217678921876	c
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3.47134662264206	3.53919691159729	2.75616779988837	c
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3.73091197209479	8.01396917759043	1.82906765153975	c
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-3.84087467239688	-3.07388293603871	0.76393626615677	c
-3.53560583290396	2.14166628100228	0.18256685353130	c
-4.86326363690592	3.67677322052262	-1.53209117733539	c
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-5.15191417622366	7.16020037357004	1.43860932462579	c
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9.82027593467245	-7.00811691485476	3.32116233618855	f
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5.10028131065534	-0.55235427463756	-5.79484079068485	f
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\$vibrational spectrum

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2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	12.79	0.00988	YES	YES
8		a	16.24	0.01585	YES	YES
9		a	19.49	0.00277	YES	YES
10		a	22.16	0.01721	YES	YES
11		a	25.11	0.02330	YES	YES
12		a	28.11	0.00950	YES	YES
13		a	30.72	0.01941	YES	YES
14		a	34.99	0.00800	YES	YES
15		a	39.84	0.03392	YES	YES
16		a	40.40	0.01555	YES	YES
17		a	47.84	0.01844	YES	YES
18		a	57.49	0.13788	YES	YES
19		a	88.04	0.00833	YES	YES
20		a	92.37	0.07552	YES	YES
21		a	102.39	0.08014	YES	YES
22		a	107.37	0.03675	YES	YES
23		a	113.87	0.11382	YES	YES
24		a	117.90	0.22489	YES	YES
25		a	118.49	0.04473	YES	YES
26		a	122.65	0.01707	YES	YES
27		a	126.11	0.03968	YES	YES
28		a	128.23	0.02696	YES	YES
29		a	137.01	0.10898	YES	YES
30		a	138.57	0.03939	YES	YES
31		a	145.53	0.16671	YES	YES
32		a	147.69	0.00677	YES	YES
33		a	156.17	0.01361	YES	YES
34		a	157.03	0.12768	YES	YES
35		a	158.77	0.05563	YES	YES
36		a	163.65	0.04585	YES	YES
37		a	164.67	0.02405	YES	YES
38		a	173.59	0.03166	YES	YES
39		a	182.47	3.08171	YES	YES
40		a	220.56	1.73162	YES	YES
41		a	221.30	1.30525	YES	YES
42		a	226.23	0.08242	YES	YES
43		a	228.39	1.47879	YES	YES
44		a	240.48	3.09514	YES	YES
45		a	260.29	0.11010	YES	YES
46		a	260.94	0.11855	YES	YES
47		a	261.78	0.10016	YES	YES
48		a	262.17	0.09786	YES	YES
49		a	263.31	0.05444	YES	YES
50		a	268.19	0.02078	YES	YES
51		a	270.87	0.03019	YES	YES
52		a	271.54	0.00890	YES	YES
53		a	275.50	0.09995	YES	YES
54		a	277.32	1.08816	YES	YES
55		a	304.62	0.67704	YES	YES
56		a	305.42	0.31684	YES	YES
57		a	308.73	0.60117	YES	YES
58		a	311.66	0.42565	YES	YES
59		a	322.33	1.62812	YES	YES

60	a	334.81	4.44278	YES	YES
61	a	338.15	0.54554	YES	YES
62	a	343.99	1.25079	YES	YES
63	a	348.30	1.00345	YES	YES
64	a	352.48	1.34076	YES	YES
65	a	360.52	0.38403	YES	YES
66	a	372.50	0.75480	YES	YES
67	a	373.22	0.03220	YES	YES
68	a	386.15	0.26104	YES	YES
69	a	386.67	0.01072	YES	YES
70	a	388.07	0.46326	YES	YES
71	a	388.30	0.50630	YES	YES
72	a	390.06	2.09786	YES	YES
73	a	408.53	0.26819	YES	YES
74	a	432.49	1.46847	YES	YES
75	a	433.01	0.14202	YES	YES
76	a	433.79	0.48906	YES	YES
77	a	434.89	0.24240	YES	YES
78	a	452.47	1.22380	YES	YES
79	a	460.43	0.47926	YES	YES
80	a	461.88	5.01756	YES	YES
81	a	466.57	5.59862	YES	YES
82	a	476.23	0.04288	YES	YES
83	a	480.71	22.86552	YES	YES
84	a	501.78	31.53172	YES	YES
85	a	510.33	23.60781	YES	YES
86	a	515.58	12.53431	YES	YES
87	a	528.75	0.05352	YES	YES
88	a	533.36	0.08021	YES	YES
89	a	551.81	0.84530	YES	YES
90	a	561.52	1.54611	YES	YES
91	a	562.63	6.20385	YES	YES
92	a	563.69	0.60339	YES	YES
93	a	565.36	0.13338	YES	YES
94	a	566.37	4.54769	YES	YES
95	a	600.34	28.63224	YES	YES
96	a	607.36	29.80299	YES	YES
97	a	612.37	12.21342	YES	YES
98	a	623.72	11.54305	YES	YES
99	a	630.52	0.25392	YES	YES
100	a	630.56	0.20110	YES	YES
101	a	631.93	0.45129	YES	YES
102	a	634.68	0.49161	YES	YES
103	a	652.15	41.86779	YES	YES
104	a	657.21	31.16583	YES	YES
105	a	667.14	37.56391	YES	YES
106	a	688.75	6.42889	YES	YES
107	a	698.17	49.34980	YES	YES
108	a	721.42	13.55650	YES	YES
109	a	744.36	35.16588	YES	YES
110	a	758.05	20.35653	YES	YES
111	a	761.50	29.32392	YES	YES
112	a	762.38	11.04028	YES	YES
113	a	767.23	44.74816	YES	YES
114	a	831.75	4.46752	YES	YES
115	a	838.84	0.32066	YES	YES
116	a	936.83	51.04544	YES	YES
117	a	953.29	14.72060	YES	YES
118	a	960.91	58.33519	YES	YES
119	a	971.17	23.44186	YES	YES
120	a	976.36	73.08615	YES	YES
121	a	979.29	51.67954	YES	YES

122	a	985.43	192.07265	YES	YES
123	a	997.57	239.42782	YES	YES
124	a	1025.48	12.55171	YES	YES
125	a	1067.44	1.30968	YES	YES
126	a	1098.03	23.48130	YES	YES
127	a	1105.12	210.17554	YES	YES
128	a	1113.97	193.26071	YES	YES
129	a	1118.96	332.11962	YES	YES
130	a	1132.86	78.02440	YES	YES
131	a	1135.39	10.94362	YES	YES
132	a	1138.33	19.65576	YES	YES
133	a	1140.71	11.78788	YES	YES
134	a	1143.18	2.20611	YES	YES
135	a	1255.72	6.35006	YES	YES
136	a	1277.17	52.23061	YES	YES
137	a	1278.96	11.76099	YES	YES
138	a	1279.98	16.77174	YES	YES
139	a	1281.35	114.97745	YES	YES
140	a	1325.10	64.67539	YES	YES
141	a	1341.66	11.74899	YES	YES
142	a	1343.24	78.23687	YES	YES
143	a	1345.53	44.98013	YES	YES
144	a	1347.96	0.21525	YES	YES
145	a	1365.98	259.90925	YES	YES
146	a	1376.84	100.18034	YES	YES
147	a	1378.30	8.47957	YES	YES
148	a	1384.65	35.35853	YES	YES
149	a	1390.23	1.04058	YES	YES
150	a	1446.26	275.45904	YES	YES
151	a	1454.81	138.01726	YES	YES
152	a	1460.52	405.93091	YES	YES
153	a	1464.62	273.68357	YES	YES
154	a	1472.65	571.98577	YES	YES
155	a	1480.43	602.36884	YES	YES
156	a	1490.98	37.10293	YES	YES
157	a	1510.76	19.67735	YES	YES
158	a	1512.16	259.68092	YES	YES
159	a	1513.83	419.92495	YES	YES
160	a	1516.35	44.65691	YES	YES
161	a	1590.28	576.15510	YES	YES
162	a	1602.12	101.66898	YES	YES
163	a	1615.20	3.95335	YES	YES
164	a	1616.15	17.13742	YES	YES
165	a	1617.32	6.94080	YES	YES
166	a	1619.05	38.69182	YES	YES
167	a	1623.11	182.99852	YES	YES
168	a	1624.39	16.05120	YES	YES
169	a	1628.22	83.46383	YES	YES
170	a	1628.85	53.06693	YES	YES
171	a	1629.70	108.65837	YES	YES



Total energy = -3686.3980761920 H = -100312.0526105 eV

HOMO-LUMO Separation

HOMO: 208. 208 a -0.11886245 H = -3.23441 eV

LUMO: 209. 209 a +0.01412282 H = +0.38430 eV

Gap : +0.13298528 H = +3.61872 eV

Number of MOs= 798, Electrons= 416.00, Symmetry: c1

\$coord

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-1.55629635725092	-1.10980218502168	-2.97332927698308	c
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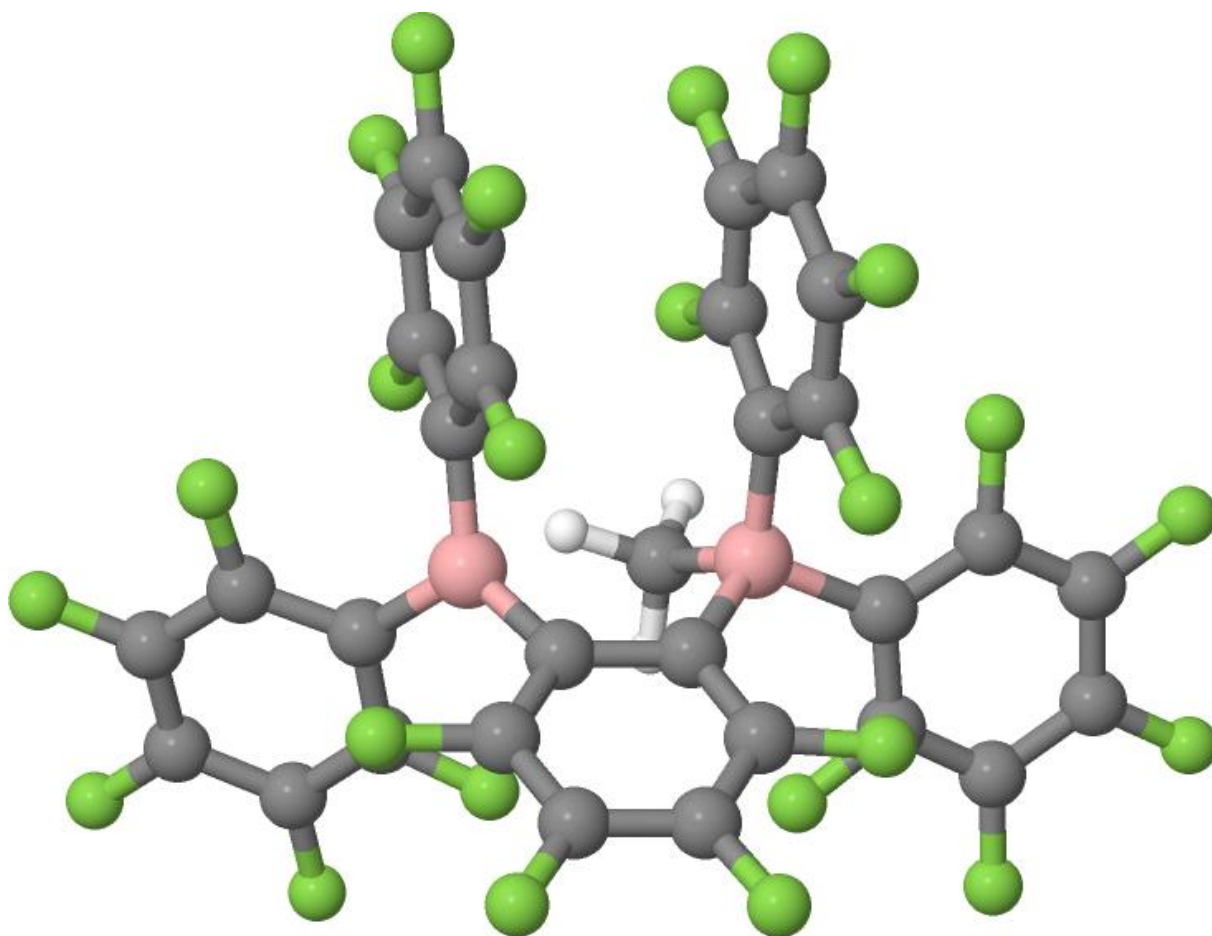
1.38610171233265 f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	6.73	0.00729	YES	YES
8		a	13.58	0.01689	YES	YES
9		a	19.82	0.00917	YES	YES
10		a	23.18	0.01078	YES	YES
11		a	24.29	0.03536	YES	YES
12		a	26.72	0.01801	YES	YES
13		a	27.56	0.00127	YES	YES
14		a	30.90	0.00820	YES	YES
15		a	36.37	0.02344	YES	YES
16		a	41.73	0.00798	YES	YES
17		a	50.40	0.03352	YES	YES
18		a	51.51	0.13080	YES	YES
19		a	87.42	0.03851	YES	YES
20		a	92.76	0.05611	YES	YES
21		a	101.60	0.01664	YES	YES
22		a	107.50	0.02874	YES	YES
23		a	112.58	0.08189	YES	YES
24		a	118.25	0.05971	YES	YES
25		a	121.13	0.03338	YES	YES
26		a	122.66	0.00918	YES	YES
27		a	126.45	0.04668	YES	YES
28		a	127.46	0.01359	YES	YES
29		a	134.59	0.06497	YES	YES
30		a	134.81	0.07811	YES	YES
31		a	144.15	0.18825	YES	YES
32		a	148.01	0.12518	YES	YES
33		a	155.38	0.03502	YES	YES
34		a	157.55	0.00863	YES	YES
35		a	159.89	0.04828	YES	YES
36		a	160.84	0.00231	YES	YES
37		a	162.98	0.00194	YES	YES
38		a	169.13	0.01542	YES	YES
39		a	190.56	1.08223	YES	YES
40		a	216.98	1.01486	YES	YES
41		a	219.47	1.37289	YES	YES
42		a	227.09	0.30256	YES	YES
43		a	228.98	1.70805	YES	YES
44		a	238.86	3.92564	YES	YES
45		a	261.30	0.10687	YES	YES
46		a	261.82	0.05457	YES	YES
47		a	261.97	0.14240	YES	YES
48		a	263.01	0.10677	YES	YES
49		a	264.04	0.06139	YES	YES
50		a	270.27	0.06752	YES	YES
51		a	270.79	0.08508	YES	YES
52		a	272.14	0.01117	YES	YES
53		a	273.57	0.01374	YES	YES
54		a	278.49	0.03541	YES	YES
55		a	281.61	0.80135	YES	YES

56	a	305.58	0.28919	YES	YES
57	a	307.08	0.07172	YES	YES
58	a	307.63	0.90353	YES	YES
59	a	310.45	0.56482	YES	YES
60	a	317.91	1.04432	YES	YES
61	a	331.09	2.50555	YES	YES
62	a	340.49	0.92334	YES	YES
63	a	342.17	5.54106	YES	YES
64	a	346.17	0.93419	YES	YES
65	a	347.98	0.31211	YES	YES
66	a	359.94	0.46495	YES	YES
67	a	377.58	0.63938	YES	YES
68	a	382.93	0.63820	YES	YES
69	a	384.97	1.19899	YES	YES
70	a	385.30	0.58269	YES	YES
71	a	389.06	1.07374	YES	YES
72	a	391.30	0.04217	YES	YES
73	a	395.40	2.78535	YES	YES
74	a	408.34	4.14242	YES	YES
75	a	413.72	31.37904	YES	YES
76	a	426.54	35.56542	YES	YES
77	a	432.73	0.68000	YES	YES
78	a	433.17	0.01822	YES	YES
79	a	434.20	0.27718	YES	YES
80	a	434.50	1.16149	YES	YES
81	a	460.96	1.02269	YES	YES
82	a	469.89	3.90497	YES	YES
83	a	471.07	24.11795	YES	YES
84	a	473.28	0.77139	YES	YES
85	a	480.60	12.13242	YES	YES
86	a	483.36	33.27864	YES	YES
87	a	503.41	30.79730	YES	YES
88	a	512.70	118.62305	YES	YES
89	a	518.82	4.91520	YES	YES
90	a	522.63	0.19378	YES	YES
91	a	529.68	0.23690	YES	YES
92	a	556.05	2.44114	YES	YES
93	a	563.37	2.38333	YES	YES
94	a	564.19	0.25640	YES	YES
95	a	564.48	0.89978	YES	YES
96	a	565.32	0.26737	YES	YES
97	a	604.45	15.94888	YES	YES
98	a	611.14	36.89055	YES	YES
99	a	618.32	12.60536	YES	YES
100	a	624.04	21.85352	YES	YES
101	a	629.69	1.09217	YES	YES
102	a	629.97	0.21206	YES	YES
103	a	631.74	14.98460	YES	YES
104	a	634.26	1.09495	YES	YES
105	a	639.30	1.61553	YES	YES
106	a	657.94	4.42971	YES	YES
107	a	674.67	69.13437	YES	YES
108	a	695.14	52.06581	YES	YES
109	a	698.20	59.94167	YES	YES
110	a	717.19	18.54497	YES	YES
111	a	722.96	79.94456	YES	YES
112	a	747.19	51.28049	YES	YES
113	a	760.89	45.10760	YES	YES
114	a	764.53	26.02845	YES	YES
115	a	768.17	4.15149	YES	YES
116	a	783.34	17.20384	YES	YES
117	a	836.07	2.13675	YES	YES

118	a	853.68	4.92031	YES	YES
119	a	951.31	11.95072	YES	YES
120	a	957.66	7.82998	YES	YES
121	a	967.17	15.30677	YES	YES
122	a	974.15	80.47370	YES	YES
123	a	981.90	52.17895	YES	YES
124	a	982.51	128.29429	YES	YES
125	a	986.97	202.10388	YES	YES
126	a	1005.11	153.49488	YES	YES
127	a	1073.05	5.27943	YES	YES
128	a	1101.00	21.50338	YES	YES
129	a	1108.03	304.90800	YES	YES
130	a	1112.04	155.53758	YES	YES
131	a	1120.21	436.77883	YES	YES
132	a	1131.11	105.87231	YES	YES
133	a	1137.79	8.09076	YES	YES
134	a	1140.13	18.56195	YES	YES
135	a	1142.19	14.71023	YES	YES
136	a	1144.91	1.65303	YES	YES
137	a	1259.22	25.03346	YES	YES
138	a	1278.80	58.08253	YES	YES
139	a	1279.87	30.79314	YES	YES
140	a	1282.15	15.07904	YES	YES
141	a	1283.71	121.68612	YES	YES
142	a	1311.72	95.96564	YES	YES
143	a	1342.09	1.65047	YES	YES
144	a	1346.41	3.21058	YES	YES
145	a	1348.14	1.16577	YES	YES
146	a	1348.84	2.73643	YES	YES
147	a	1376.94	74.24255	YES	YES
148	a	1381.28	8.27310	YES	YES
149	a	1385.24	24.69901	YES	YES
150	a	1386.77	20.75958	YES	YES
151	a	1393.24	13.01044	YES	YES
152	a	1453.89	83.91467	YES	YES
153	a	1463.92	582.09611	YES	YES
154	a	1467.64	126.11733	YES	YES
155	a	1471.59	385.41465	YES	YES
156	a	1477.20	853.99669	YES	YES
157	a	1488.80	113.84134	YES	YES
158	a	1512.44	51.82673	YES	YES
159	a	1513.76	176.48458	YES	YES
160	a	1515.61	298.75572	YES	YES
161	a	1518.01	93.87292	YES	YES
162	a	1595.08	15.97959	YES	YES
163	a	1616.25	4.26318	YES	YES
164	a	1617.42	2.98893	YES	YES
165	a	1618.84	0.82524	YES	YES
166	a	1620.05	6.65297	YES	YES
167	a	1625.92	79.04390	YES	YES
168	a	1626.77	90.56656	YES	YES
169	a	1627.32	15.49709	YES	YES
170	a	1629.40	10.79253	YES	YES
171	a	1630.95	40.67365	YES	YES



Total energy = -3626.4241882470 H = -98680.0791561 eV

HOMO-LUMO Separation

HOMO: 208. 208 a -0.11369727 H = -3.09386 eV

LUMO: 209. 209 a -0.03087883 H = -0.84026 eV

Gap : +0.08281844 H = +2.25361 eV

Number of MOs= 804, Electrons= 416.00, Symmetry: c1

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 -1.87248489392827   -4.02341389101284   -6.02476389821798    c
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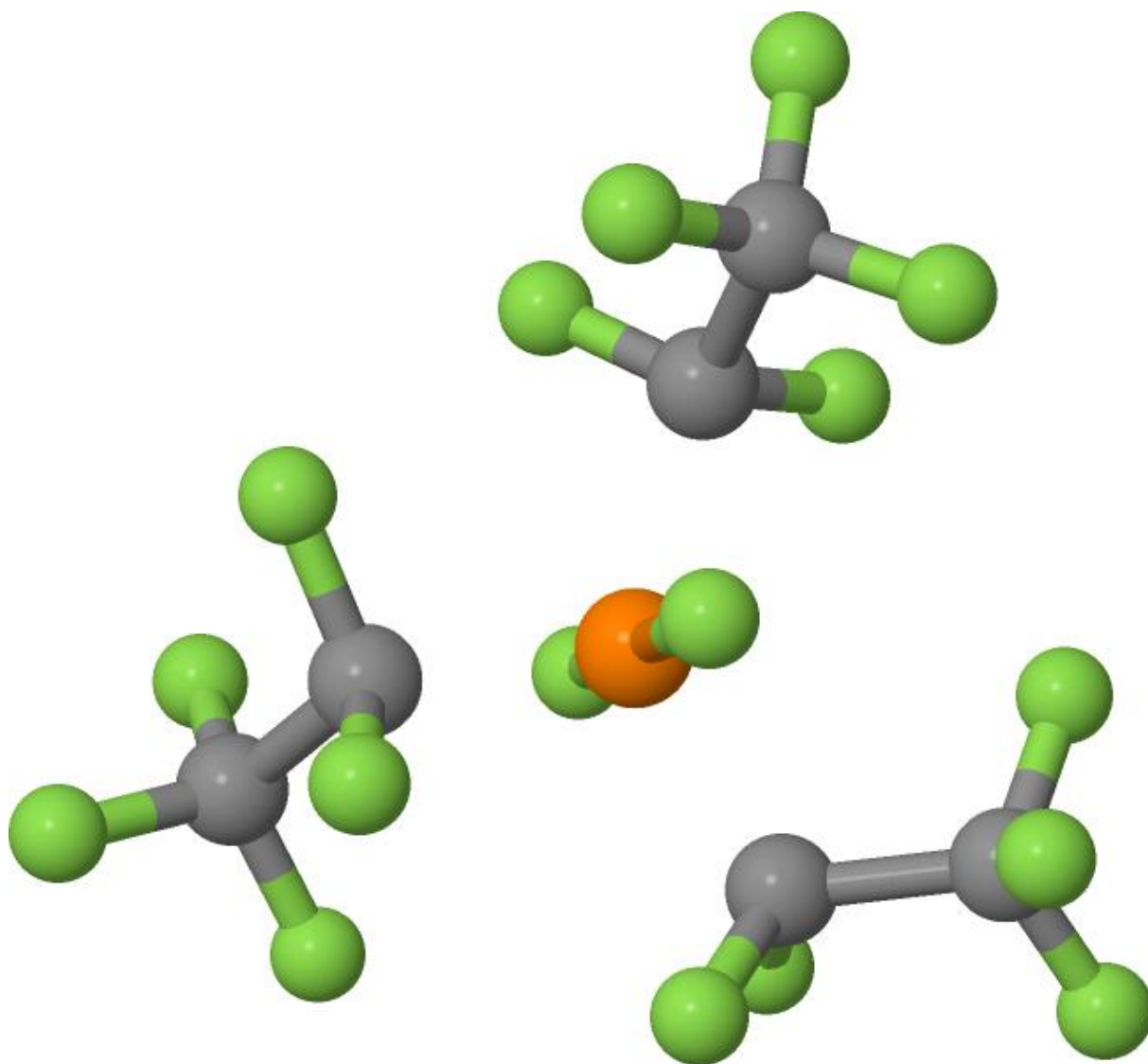
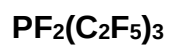
\$vibrational spectrum

mode symmetry wave number IR intensity selection rules

#		cm** (-1)	km/mol	IR	RAMAN
1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	16.59	0.02758	YES	YES
8	a	20.29	0.09671	YES	YES
9	a	23.11	0.00974	YES	YES
10	a	26.32	0.02413	YES	YES
11	a	28.83	0.02280	YES	YES
12	a	30.27	0.01116	YES	YES
13	a	35.49	0.13406	YES	YES
14	a	38.50	0.33235	YES	YES
15	a	41.87	0.22695	YES	YES
16	a	44.69	0.06447	YES	YES
17	a	50.90	0.02423	YES	YES
18	a	53.30	0.08178	YES	YES
19	a	84.40	6.56484	YES	YES
20	a	89.77	0.47364	YES	YES
21	a	100.08	2.05212	YES	YES
22	a	106.43	0.46224	YES	YES
23	a	112.42	0.21879	YES	YES
24	a	116.98	0.61285	YES	YES
25	a	119.04	2.71293	YES	YES
26	a	124.86	0.03090	YES	YES
27	a	127.29	0.08026	YES	YES
28	a	130.06	0.63471	YES	YES
29	a	133.34	0.03299	YES	YES
30	a	134.87	0.03129	YES	YES
31	a	144.25	0.18361	YES	YES
32	a	145.65	0.79181	YES	YES
33	a	153.58	0.04986	YES	YES
34	a	156.47	0.03571	YES	YES
35	a	160.08	2.99054	YES	YES
36	a	161.86	0.44560	YES	YES
37	a	165.43	0.91259	YES	YES
38	a	166.02	1.22527	YES	YES
39	a	188.11	17.49759	YES	YES
40	a	208.96	7.52253	YES	YES
41	a	221.00	2.66678	YES	YES
42	a	228.48	4.58435	YES	YES
43	a	229.11	3.10854	YES	YES
44	a	238.58	5.65733	YES	YES
45	a	247.37	15.00874	YES	YES
46	a	260.14	0.38009	YES	YES
47	a	262.08	0.17828	YES	YES
48	a	262.25	0.13205	YES	YES
49	a	263.02	0.23067	YES	YES
50	a	264.81	0.12968	YES	YES
51	a	267.55	1.48552	YES	YES
52	a	270.59	0.04868	YES	YES
53	a	273.48	0.07418	YES	YES
54	a	274.55	0.10213	YES	YES
55	a	284.89	0.21477	YES	YES
56	a	286.36	0.24031	YES	YES
57	a	307.38	3.17267	YES	YES
58	a	308.96	1.39194	YES	YES
59	a	309.85	0.78170	YES	YES
60	a	313.82	1.06828	YES	YES
61	a	318.00	11.31523	YES	YES

62	a	334.95	16.08943	YES	YES
63	a	336.05	1.39326	YES	YES
64	a	341.18	2.74330	YES	YES
65	a	347.73	2.63668	YES	YES
66	a	348.89	2.52125	YES	YES
67	a	353.01	2.19096	YES	YES
68	a	358.38	10.96772	YES	YES
69	a	370.45	1.47016	YES	YES
70	a	383.70	0.46462	YES	YES
71	a	387.47	0.07888	YES	YES
72	a	387.89	0.33581	YES	YES
73	a	391.43	4.53266	YES	YES
74	a	392.34	3.12305	YES	YES
75	a	396.24	0.68307	YES	YES
76	a	406.44	0.31640	YES	YES
77	a	423.14	3.68506	YES	YES
78	a	431.77	0.27131	YES	YES
79	a	432.92	0.08531	YES	YES
80	a	434.87	0.04196	YES	YES
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82	a	453.73	2.38928	YES	YES
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91	a	519.47	5.37735	YES	YES
92	a	537.99	0.12711	YES	YES
93	a	552.85	3.88369	YES	YES
94	a	561.91	2.06604	YES	YES
95	a	564.08	3.30560	YES	YES
96	a	564.22	2.27762	YES	YES
97	a	566.09	0.98972	YES	YES
98	a	580.63	22.33629	YES	YES
99	a	589.34	10.65898	YES	YES
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101	a	619.38	26.95443	YES	YES
102	a	629.01	0.11415	YES	YES
103	a	633.31	0.61705	YES	YES
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105	a	636.22	0.29138	YES	YES
106	a	648.50	7.42380	YES	YES
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110	a	680.14	28.03896	YES	YES
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112	a	729.32	23.86251	YES	YES
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114	a	752.39	3.02866	YES	YES
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116	a	765.16	20.22902	YES	YES
117	a	781.41	59.67752	YES	YES
118	a	793.53	11.73529	YES	YES
119	a	811.34	38.77719	YES	YES
120	a	839.28	1.16763	YES	YES
121	a	933.37	35.20706	YES	YES
122	a	944.69	42.76132	YES	YES
123	a	957.61	66.04837	YES	YES

124	a	972.27	56.74575	YES	YES
125	a	975.58	27.44610	YES	YES
126	a	981.88	90.42750	YES	YES
127	a	982.50	77.69051	YES	YES
128	a	994.25	88.16756	YES	YES
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135	a	1125.82	2.53057	YES	YES
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137	a	1145.59	16.42210	YES	YES
138	a	1147.82	178.61400	YES	YES
139	a	1151.44	89.49737	YES	YES
140	a	1241.92	9.80032	YES	YES
141	a	1257.75	25.52988	YES	YES
142	a	1264.66	27.26298	YES	YES
143	a	1269.24	5.72680	YES	YES
144	a	1288.83	21.20540	YES	YES
145	a	1297.29	153.55451	YES	YES
146	a	1302.53	147.93033	YES	YES
147	a	1340.60	57.13008	YES	YES
148	a	1341.58	11.17305	YES	YES
149	a	1341.99	17.53668	YES	YES
150	a	1344.02	9.10247	YES	YES
151	a	1347.61	0.08575	YES	YES
152	a	1352.75	6.81999	YES	YES
153	a	1362.62	2.23022	YES	YES
154	a	1367.46	12.51433	YES	YES
155	a	1379.77	97.39047	YES	YES
156	a	1386.41	54.15143	YES	YES
157	a	1405.81	13.02206	YES	YES
158	a	1415.63	273.80940	YES	YES
159	a	1452.00	224.05298	YES	YES
160	a	1454.53	295.13806	YES	YES
161	a	1467.17	486.09349	YES	YES
162	a	1476.90	663.41855	YES	YES
163	a	1485.23	77.22394	YES	YES
164	a	1507.50	228.87082	YES	YES
165	a	1509.73	98.22084	YES	YES
166	a	1517.26	221.67525	YES	YES
167	a	1519.95	171.89284	YES	YES
168	a	1590.12	44.76769	YES	YES
169	a	1612.40	4.42890	YES	YES
170	a	1612.87	7.04791	YES	YES
171	a	1613.53	13.52798	YES	YES
172	a	1614.80	15.20130	YES	YES
173	a	1616.62	39.50599	YES	YES
174	a	1622.17	32.74649	YES	YES
175	a	1624.08	17.72868	YES	YES
176	a	1626.24	108.68595	YES	YES
177	a	1632.42	74.86289	YES	YES
178	a	2703.42	643.20277	YES	YES
179	a	3003.48	25.98211	YES	YES
180	a	3065.76	6.95819	YES	YES



Total energy = -2265.8841913580 H = -61657.8810847 eV

HOMO-LUMO Separation

HOMO: 102. 102 a -0.31314572 H = -8.52113 eV

LUMO: 103. 103 a -0.08838644 H = -2.40512 eV

Gap : +0.22475928 H = +6.11601 eV

Number of MOs= 340, Electrons= 204.00, Symmetry: c1

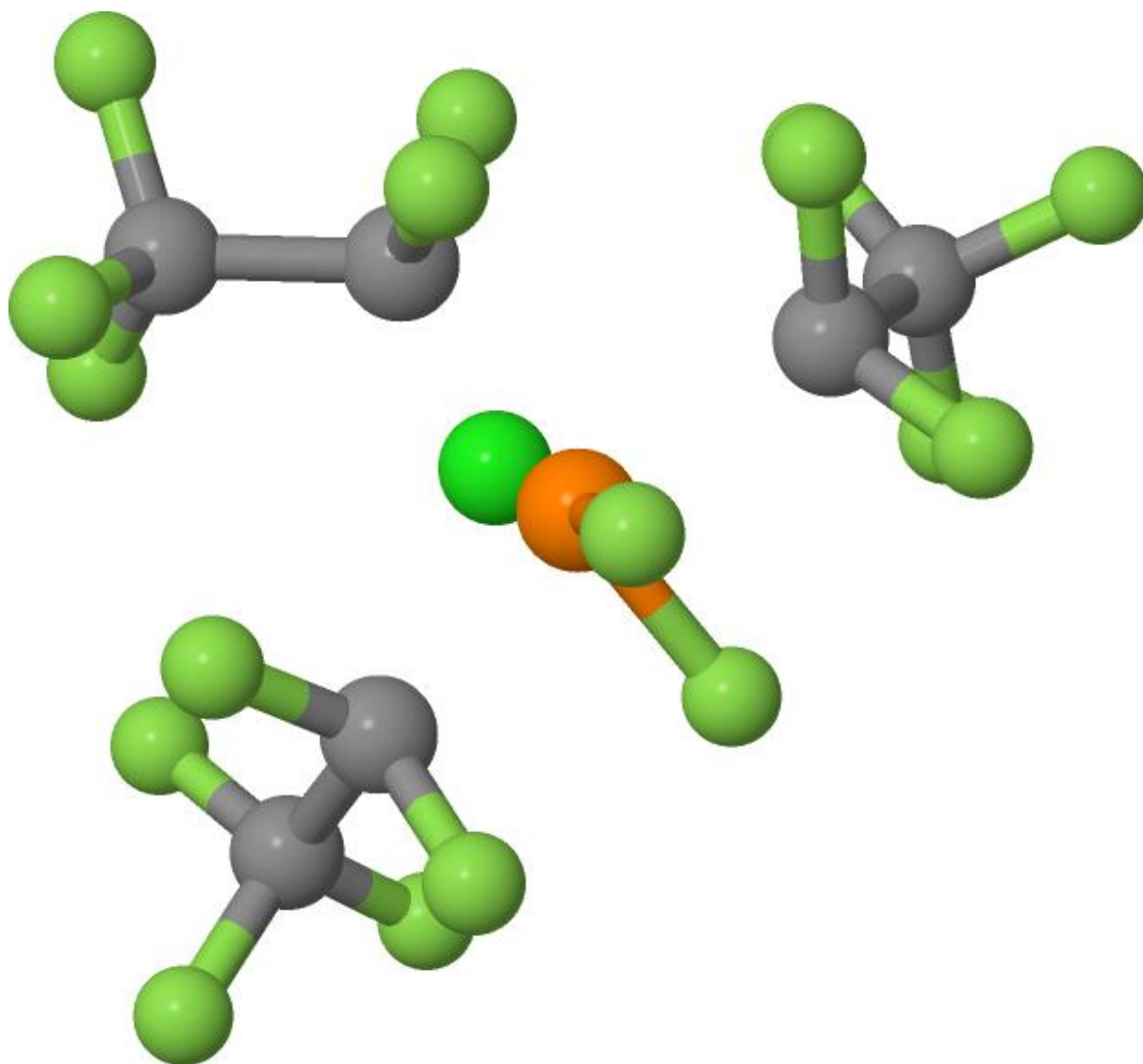
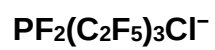
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-0.20008998270229	0.17269874310491	0.03943630312668	p
-3.13685615667977	1.31254963368664	0.12123676764158	f
2.67337446783471	-1.15200523220400	0.02847815697971	f
-1.45249663684118	-2.19271245473883	-2.47087692683356	c
0.46838776900139	-4.05111931333260	-3.72084347134166	c
-0.08048510179297	0.03739736392725	3.70932701581481	c
0.34472575451979	-2.69550782935406	4.76765651805210	c
1.19701805828962	3.23583604070924	-1.35334818540075	c
-0.36262002030590	5.70160055880005	-0.90068221979866	c
1.44075486014702	2.88176621650118	-3.88556513990228	f
3.51026732651999	3.59432535880333	-0.34673564493076	f
1.05183302341502	7.70311867238385	-1.56265799054681	f
-0.94180638285620	5.89954247236149	1.56996831954762	f
-2.47711639997625	5.71801854566002	-2.27904573044831	f
2.34950169607433	-2.77603340914889	-4.83979806198397	f
-0.76720930098030	-5.38985736892860	-5.49560190105459	f
1.41464026341814	-5.66067889760690	-2.01265931580794	f
-2.48343469958099	-0.78077010991224	-4.34061814182916	f
-3.30013177536610	-3.58318613792388	-1.37704587825772	f
1.87818014988931	1.52596824226266	4.42972358219224	f
-2.22491676488763	0.94854425898706	4.70904373140477	f
-1.01433565852632	-4.33490626080403	3.35251549084945	f
2.77464760191699	-3.35640930206981	4.69960468790690	f
-0.47402210606797	-2.82169898475516	7.16185263224626	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	19.76	0.01539	YES	YES
8		a	22.81	0.02668	YES	YES
9		a	26.18	0.00417	YES	YES
10		a	48.42	0.16277	YES	YES
11		a	57.53	0.01570	YES	YES
12		a	67.11	0.00627	YES	YES
13		a	82.19	0.06837	YES	YES
14		a	96.57	0.13197	YES	YES
15		a	101.75	0.44875	YES	YES
16		a	122.36	0.37602	YES	YES
17		a	136.56	1.68315	YES	YES
18		a	196.44	6.11308	YES	YES
19		a	201.32	0.75824	YES	YES
20		a	203.07	0.59749	YES	YES
21		a	210.53	0.47358	YES	YES
22		a	230.15	1.23076	YES	YES
23		a	231.33	0.26975	YES	YES
24		a	238.12	1.70254	YES	YES
25		a	241.81	1.35444	YES	YES
26		a	248.92	2.35237	YES	YES
27		a	268.89	6.93844	YES	YES
28		a	277.81	2.04146	YES	YES
29		a	290.13	7.14720	YES	YES

30	a	305.05	0.04116	YES	YES
31	a	323.88	1.22818	YES	YES
32	a	336.68	0.62728	YES	YES
33	a	355.66	0.15264	YES	YES
34	a	357.78	0.15159	YES	YES
35	a	365.34	1.15335	YES	YES
36	a	412.18	8.81012	YES	YES
37	a	417.96	5.95470	YES	YES
38	a	432.81	4.83055	YES	YES
39	a	503.01	48.80768	YES	YES
40	a	511.15	41.23627	YES	YES
41	a	522.51	1.51686	YES	YES
42	a	550.87	40.41266	YES	YES
43	a	562.06	21.15608	YES	YES
44	a	574.86	0.42783	YES	YES
45	a	581.52	18.57387	YES	YES
46	a	590.97	49.59006	YES	YES
47	a	603.81	6.08699	YES	YES
48	a	623.15	4.60710	YES	YES
49	a	630.09	31.35252	YES	YES
50	a	634.03	37.40120	YES	YES
51	a	732.86	2.94322	YES	YES
52	a	740.02	10.62865	YES	YES
53	a	740.25	15.04617	YES	YES
54	a	827.22	132.05543	YES	YES
55	a	944.33	84.40549	YES	YES
56	a	964.16	52.32460	YES	YES
57	a	973.83	171.38768	YES	YES
58	a	1107.52	29.45173	YES	YES
59	a	1117.50	199.15105	YES	YES
60	a	1126.36	58.56400	YES	YES
61	a	1139.31	165.98961	YES	YES
62	a	1156.29	124.46018	YES	YES
63	a	1181.84	96.98993	YES	YES
64	a	1194.40	205.11426	YES	YES
65	a	1201.43	74.84533	YES	YES
66	a	1202.95	168.40023	YES	YES
67	a	1231.13	322.61188	YES	YES
68	a	1232.06	285.62857	YES	YES
69	a	1239.02	381.17650	YES	YES
70	a	1284.57	266.52907	YES	YES
71	a	1289.53	196.03203	YES	YES
72	a	1300.97	7.03081	YES	YES



Total energy = -2726.1028977580 H = -74181.0763921 eV

HOMO-LUMO Separation

HOMO: 111. 111 a -0.11089425 H = -3.01759 eV

LUMO: 112. 112 a +0.07373214 H = +2.00635 eV

Gap : +0.18462639 H = +5.02394 eV

Number of MOs= 358, Electrons= 222.00, Symmetry: c1

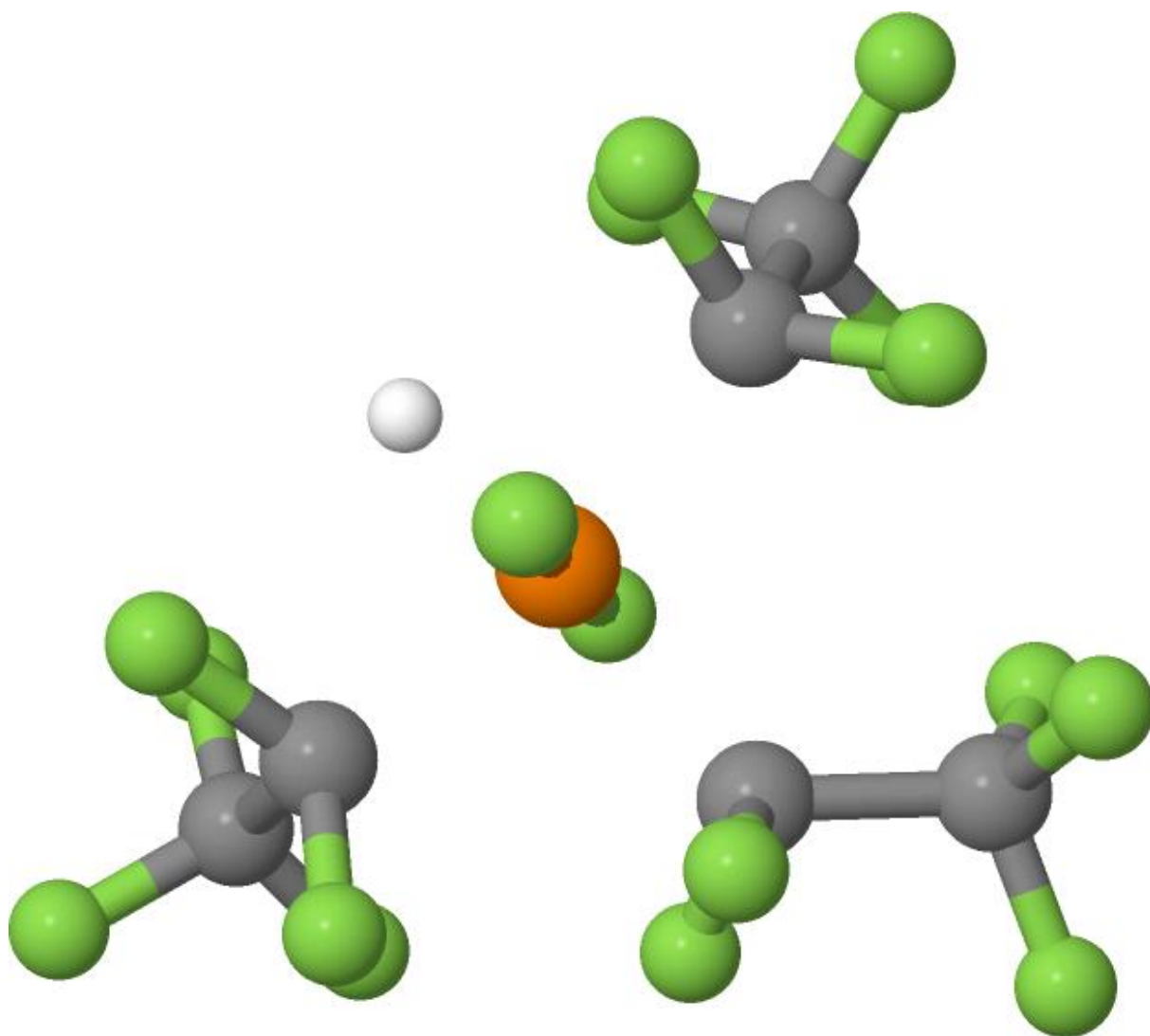
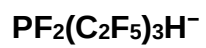
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-5.27688518554497	1.53433594347773	0.51861317041150	p
-2.12996836604343	1.37892385268269	0.17508384344493	f
-5.31324158455764	4.67761960374555	0.92559481250118	f
-5.29451308215221	2.38781295171828	-3.15910603045089	c
-4.52923722598366	1.42859787165367	4.26999047183813	c
-7.62655209451867	3.57108811636228	-4.52488769947859	c
-4.64401720867254	0.31053039919955	-4.57263122217613	f
-3.41892177785802	4.12804826436114	-3.52244090342245	f
-9.53361271049945	1.92660979717197	-4.83885365626131	f
-6.89905000587352	4.30639470540911	-6.88929691763421	f
-8.49430880484466	5.63783577472296	-3.33830502209578	f
-6.59635814930933	2.01927582784397	6.27983585925530	c
-2.71328385925756	3.22845860415890	4.66527941051518	f
-3.47605272279279	-0.81706570801405	5.01449838962543	f
-7.75468306250606	4.23637738796640	5.85107430415940	f
-5.47298793256388	2.19637366067276	8.59650846460167	f
-8.34240818131588	0.18467932534634	6.45709205825944	f
-5.41914709897093	-2.33145505301917	0.32016412327738	c
-6.55163945074165	-3.89809377570757	-1.94155693269553	c
-6.82383472829156	-3.07042524254769	2.36522801283269	f
-3.04609514158945	-3.30575603567503	0.62969600183457	f
-8.53777297240823	-2.78890632883181	-3.05787072864724	f
-7.35702853962563	-6.17746652594731	-1.06393275759780	f
-4.79160425561212	-4.39677008909460	-3.71312220454174	f
-9.47381659408392	1.48389656687084	0.88732917819850	c1

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		30.32	0.06907	YES	YES
8	a		56.07	0.07116	YES	YES
9	a		68.22	0.01486	YES	YES
10	a		70.41	0.01765	YES	YES
11	a		79.15	0.07586	YES	YES
12	a		82.46	0.00618	YES	YES
13	a		91.70	0.10003	YES	YES
14	a		120.79	0.06456	YES	YES
15	a		124.04	0.22281	YES	YES
16	a		140.46	0.28052	YES	YES
17	a		155.10	0.45407	YES	YES
18	a		165.50	0.33501	YES	YES
19	a		177.76	0.44736	YES	YES
20	a		196.19	0.64996	YES	YES
21	a		205.02	2.66162	YES	YES
22	a		214.05	0.30721	YES	YES
23	a		220.56	0.91486	YES	YES
24	a		224.90	0.37020	YES	YES
25	a		244.58	2.52154	YES	YES

26	a	258.12	1.24617	YES	YES
27	a	265.93	2.50467	YES	YES
28	a	282.33	1.27325	YES	YES
29	a	290.13	0.49266	YES	YES
30	a	298.27	5.97651	YES	YES
31	a	305.72	0.11593	YES	YES
32	a	327.85	0.64540	YES	YES
33	a	330.85	0.68242	YES	YES
34	a	339.51	2.67040	YES	YES
35	a	351.31	6.82084	YES	YES
36	a	366.27	0.96269	YES	YES
37	a	371.89	3.73038	YES	YES
38	a	375.88	13.47534	YES	YES
39	a	397.62	19.82955	YES	YES
40	a	431.27	3.42931	YES	YES
41	a	438.26	0.88794	YES	YES
42	a	466.02	9.09382	YES	YES
43	a	511.30	78.55984	YES	YES
44	a	518.66	1.28434	YES	YES
45	a	522.75	3.76578	YES	YES
46	a	540.03	135.98444	YES	YES
47	a	574.57	3.07777	YES	YES
48	a	577.08	6.91544	YES	YES
49	a	579.18	5.76920	YES	YES
50	a	611.69	1.24732	YES	YES
51	a	618.47	11.82472	YES	YES
52	a	622.45	41.35424	YES	YES
53	a	705.51	135.32124	YES	YES
54	a	720.00	36.48694	YES	YES
55	a	724.96	75.09105	YES	YES
56	a	727.98	44.85856	YES	YES
57	a	736.94	34.53680	YES	YES
58	a	906.27	63.41342	YES	YES
59	a	927.36	96.60766	YES	YES
60	a	936.11	97.83989	YES	YES
61	a	1069.49	23.70927	YES	YES
62	a	1089.78	93.03556	YES	YES
63	a	1097.52	118.18226	YES	YES
64	a	1101.96	32.18569	YES	YES
65	a	1107.01	135.76782	YES	YES
66	a	1115.60	91.25756	YES	YES
67	a	1146.26	287.10795	YES	YES
68	a	1153.86	300.39594	YES	YES
69	a	1161.23	228.96578	YES	YES
70	a	1205.66	318.72230	YES	YES
71	a	1217.75	267.24541	YES	YES
72	a	1224.61	193.54206	YES	YES
73	a	1248.05	293.48341	YES	YES
74	a	1278.16	166.93260	YES	YES
75	a	1289.10	56.99864	YES	YES



Total energy = -2266.5622624690 H = -61676.3323489 eV

HOMO-LUMO Separation

HOMO: 103. 103 a -0.08274957 H = -2.25173 eV

LUMO: 104. 104 a +0.12302798 H = +3.34776 eV

Gap : +0.20577755 H = +5.59950 eV

Number of MOs= 342, Electrons= 206.00, Symmetry: c1

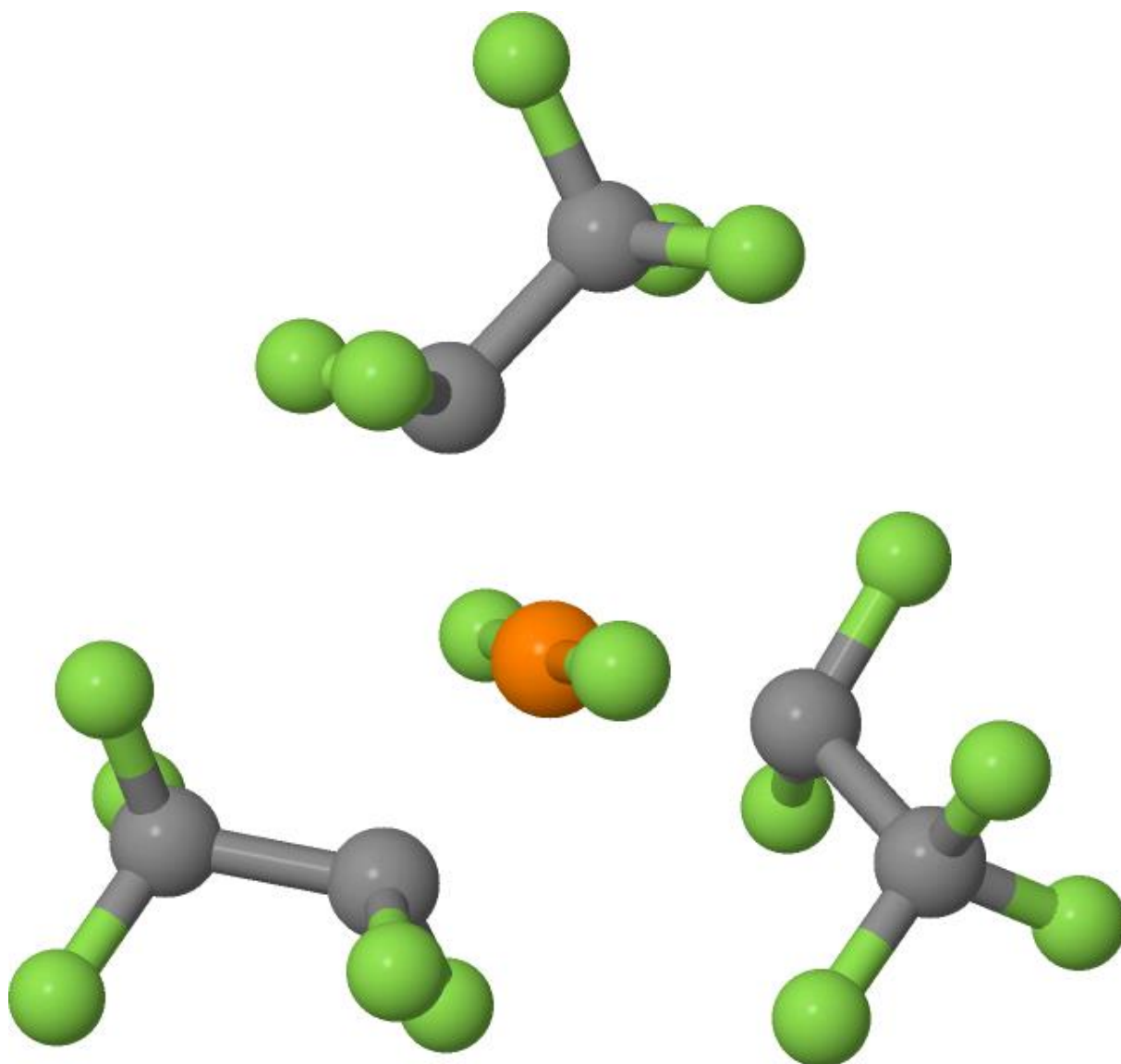
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-5.11813900937793	1.52115865424052	0.47359765675489	p
-1.96701607162769	1.24863569291834	0.09637621144512	f
-4.98438057479376	4.22928200224812	0.81811637763176	h
-5.29501373012624	2.34305465374039	-3.19999160957783	c
-4.53218202161665	1.39952849177220	4.24049061922955	c
-7.75543697627421	3.55347096496414	-4.24040668250129	c
-4.69973382386553	0.39244429954955	-4.80474591866990	f
-3.48751234511211	4.18099509177103	-3.57027255043701	f
-9.72837845690769	1.95793004889411	-4.27895487322828	f
-7.39881108386734	4.35107868642596	-6.66884533890217	f
-8.40573111599275	5.60874507427476	-2.87392245592750	f
-6.78270385110616	2.03284437593667	6.00360814006151	c
-2.81920226479098	3.32336298255490	4.66251574626832	f
-3.44825106111853	-0.75407162312208	5.18834638824056	f
-7.85095684844057	4.26280393564121	5.36441096602681	f
-5.96967863249595	2.26706552294580	8.44348552911523	f
-8.58705349981520	0.24675114602951	6.00199404878088	f
-5.36223003774896	-2.32053535477147	0.34495536707853	c
-6.49853629258077	-3.88292988824240	-1.88507378936570	c
-6.88387582362556	-2.94788456163227	2.36062223285442	f
-3.04965045122325	-3.40186284478465	0.76804919054621	f
-8.54667925094125	-2.77812955020276	-2.90853948733420	f
-7.24479127006805	-6.19783057074595	-1.03773998257680	f
-4.78836826882299	-4.31288285966643	-3.72006643399680	f
-8.31270797327769	1.52789552378778	0.75597467423714	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	27.72	0.03603	YES	YES
8		a	50.79	0.02306	YES	YES
9		a	55.26	0.00620	YES	YES
10		a	58.73	0.00265	YES	YES
11		a	70.22	0.02805	YES	YES
12		a	81.23	0.06328	YES	YES
13		a	93.25	0.07034	YES	YES
14		a	113.38	0.35387	YES	YES
15		a	121.87	0.58953	YES	YES
16		a	133.61	0.03991	YES	YES
17		a	147.03	0.42221	YES	YES
18		a	167.97	0.14693	YES	YES
19		a	196.96	0.92593	YES	YES
20		a	204.47	0.28306	YES	YES
21		a	210.71	1.05425	YES	YES
22		a	214.00	3.05501	YES	YES
23		a	223.39	0.31143	YES	YES
24		a	238.20	0.83192	YES	YES
25		a	247.33	0.35756	YES	YES

26	a	255.50	1.22369	YES	YES
27	a	269.23	1.00409	YES	YES
28	a	273.98	0.76631	YES	YES
29	a	297.15	0.14611	YES	YES
30	a	308.46	0.72509	YES	YES
31	a	321.51	0.83479	YES	YES
32	a	337.45	1.17361	YES	YES
33	a	356.40	0.86394	YES	YES
34	a	358.38	0.35474	YES	YES
35	a	364.78	0.03217	YES	YES
36	a	412.36	16.59829	YES	YES
37	a	421.80	0.90490	YES	YES
38	a	437.50	2.35930	YES	YES
39	a	499.66	130.07945	YES	YES
40	a	513.08	11.90749	YES	YES
41	a	516.86	6.79877	YES	YES
42	a	529.58	77.55530	YES	YES
43	a	533.89	58.68666	YES	YES
44	a	570.83	1.08261	YES	YES
45	a	571.76	2.86784	YES	YES
46	a	576.50	5.15604	YES	YES
47	a	590.71	39.34077	YES	YES
48	a	604.59	4.14658	YES	YES
49	a	611.37	20.14617	YES	YES
50	a	615.33	30.34879	YES	YES
51	a	717.68	13.04431	YES	YES
52	a	721.32	5.50568	YES	YES
53	a	724.30	7.74294	YES	YES
54	a	787.96	124.99779	YES	YES
55	a	909.23	72.40367	YES	YES
56	a	920.64	34.50089	YES	YES
57	a	922.54	110.37099	YES	YES
58	a	1042.90	26.16904	YES	YES
59	a	1071.57	105.98200	YES	YES
60	a	1076.43	54.20109	YES	YES
61	a	1083.07	109.22098	YES	YES
62	a	1098.75	16.29258	YES	YES
63	a	1112.15	59.01078	YES	YES
64	a	1120.81	136.32413	YES	YES
65	a	1139.39	400.52916	YES	YES
66	a	1149.63	233.32447	YES	YES
67	a	1153.20	134.65381	YES	YES
68	a	1194.20	160.84413	YES	YES
69	a	1199.53	329.04980	YES	YES
70	a	1218.59	295.51069	YES	YES
71	a	1237.21	248.61722	YES	YES
72	a	1256.59	275.08025	YES	YES
73	a	1285.46	94.87304	YES	YES
74	a	1293.36	96.86605	YES	YES
75	a	2220.54	147.34010	YES	YES



Total energy = -2265.8836870100 H = -61657.8673607 eV

HOMO-LUMO Separation

HOMO: 102. 102 a -0.31047383 H = -8.44843 eV

LUMO: 103. 103 a -0.08275215 H = -2.25180 eV

Gap : +0.22772167 H = +6.19663 eV

Number of MOs= 340, Electrons= 204.00, Symmetry: c1

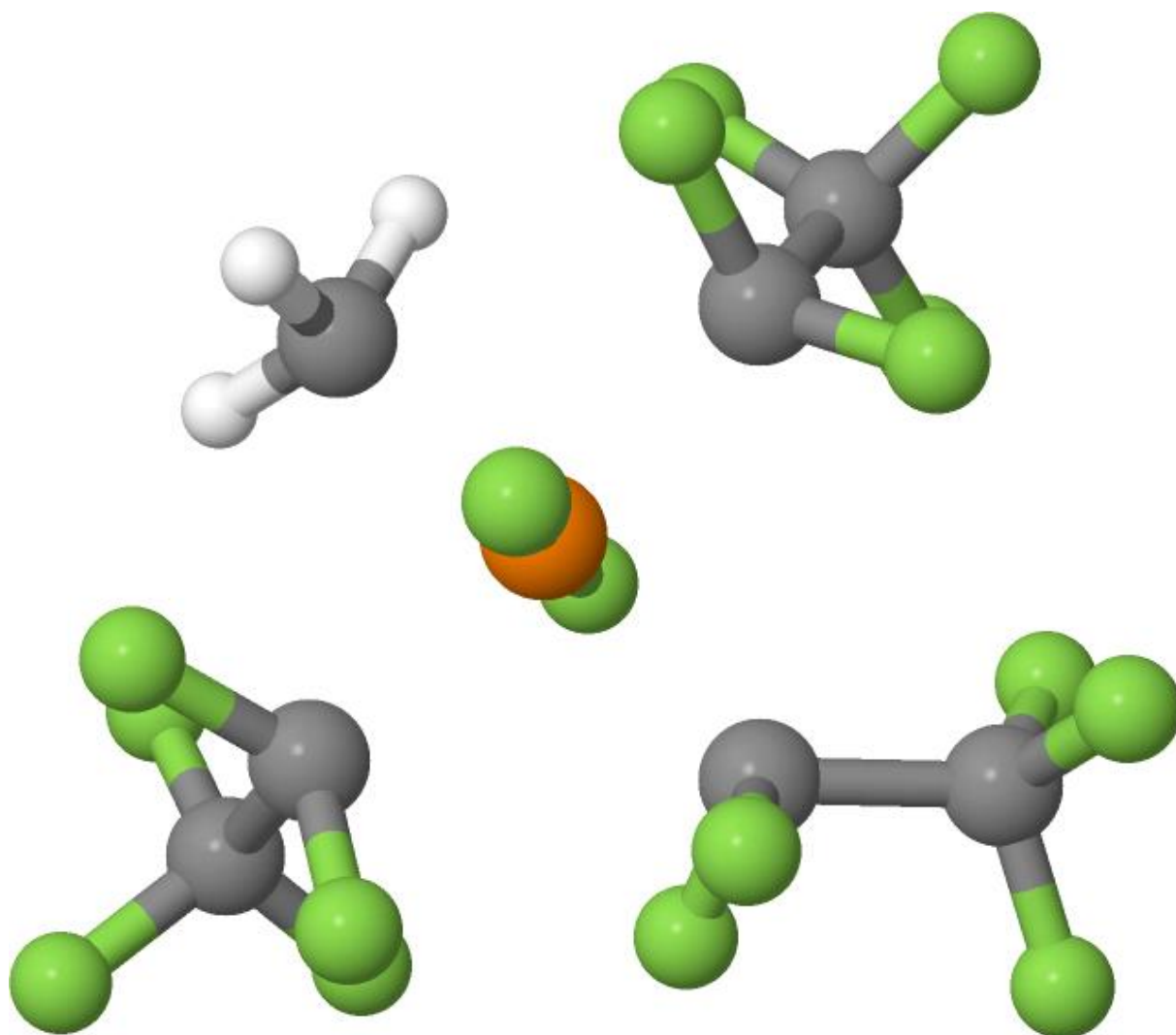
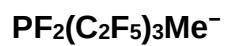
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-0.95533817497016	3.11422454868447	0.29908249895047	f
0.81114119534013	-2.90504961948289	-0.19038978623820	f
-0.09412836978623	0.10255575626710	-0.02589481544522	p
3.30005331911459	1.22068508527366	-0.88529380922159	c
4.84669931972434	-0.56960571432911	-2.66330257733581	c
4.62307698075702	1.49228031256701	1.30132431396555	f
3.14124301332393	3.48297365129123	-2.03633450479754	f
5.63425451727665	-2.63905509260373	-1.45269712852027	f
6.88275436377998	0.69416476793085	-3.50738155201468	f
3.42032676922618	-1.23650147837110	-4.66233579378302	f
-2.25819175866544	-0.19511613986826	-2.95857395648486	c
-5.12703539697715	0.24545203945159	-2.40799517735044	c
-2.01926567242818	-2.50241019247767	-3.99712081024784	f
-1.46792331835584	1.57263222264791	-4.64083035141807	f
-5.81354877252994	-1.21782061948597	-0.43226938974614	f
-6.48644861006708	-0.43422309945138	-4.43541439274446	f
-5.62128209528515	2.65764447099299	-1.86420464719806	f
-1.39794183663221	-0.56939881403906	3.37175586322717	c
0.60734263757503	-0.18269215762291	5.49743211888959	c
2.56017503937281	-1.76604080963505	5.15050717076118	f
-0.44818327038685	-0.65544446849998	7.75139895129402	f
-2.22010002378988	-2.97977624411865	3.48142450537359	f
-3.35343044972156	0.99724611628849	3.84617993678691	f
1.45076317943477	2.20982003909015	5.46958437060806	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	11.73	0.01444	YES	YES
8		a	25.73	0.01193	YES	YES
9		a	39.36	0.00611	YES	YES
10		a	50.82	0.13177	YES	YES
11		a	60.60	0.01277	YES	YES
12		a	61.70	0.02473	YES	YES
13		a	70.12	0.10845	YES	YES
14		a	79.17	0.13969	YES	YES
15		a	110.23	0.44150	YES	YES
16		a	117.19	0.54820	YES	YES
17		a	128.97	0.83485	YES	YES
18		a	176.16	4.99101	YES	YES
19		a	200.98	0.60572	YES	YES
20		a	206.88	0.31980	YES	YES
21		a	211.85	0.20393	YES	YES
22		a	218.09	1.14378	YES	YES
23		a	220.05	2.01662	YES	YES
24		a	241.64	0.75900	YES	YES
25		a	263.66	7.97239	YES	YES
26		a	266.45	0.17545	YES	YES
27		a	273.05	6.30543	YES	YES

28	a	284.25	0.25703	YES	YES
29	a	295.15	1.12886	YES	YES
30	a	304.36	1.12513	YES	YES
31	a	329.21	1.16377	YES	YES
32	a	340.60	0.91109	YES	YES
33	a	354.38	0.08391	YES	YES
34	a	358.48	0.99894	YES	YES
35	a	360.58	0.53317	YES	YES
36	a	418.58	7.06766	YES	YES
37	a	433.46	3.49835	YES	YES
38	a	447.56	2.86047	YES	YES
39	a	496.42	70.27575	YES	YES
40	a	507.45	56.37376	YES	YES
41	a	522.52	0.72478	YES	YES
42	a	547.49	45.05356	YES	YES
43	a	554.28	34.46098	YES	YES
44	a	577.45	6.64871	YES	YES
45	a	578.70	3.68463	YES	YES
46	a	583.45	16.44467	YES	YES
47	a	609.66	4.74882	YES	YES
48	a	614.83	0.99957	YES	YES
49	a	631.98	26.57098	YES	YES
50	a	634.85	29.64275	YES	YES
51	a	731.07	1.98165	YES	YES
52	a	737.63	13.60675	YES	YES
53	a	740.19	16.26964	YES	YES
54	a	836.30	109.30141	YES	YES
55	a	930.21	55.92868	YES	YES
56	a	947.19	73.10627	YES	YES
57	a	959.95	126.41954	YES	YES
58	a	1108.69	38.37158	YES	YES
59	a	1118.18	180.08718	YES	YES
60	a	1122.95	215.68032	YES	YES
61	a	1157.14	90.13912	YES	YES
62	a	1177.32	20.96499	YES	YES
63	a	1183.92	84.28074	YES	YES
64	a	1195.60	124.82256	YES	YES
65	a	1201.54	156.15639	YES	YES
66	a	1212.02	202.06457	YES	YES
67	a	1215.38	190.83810	YES	YES
68	a	1230.20	308.61353	YES	YES
69	a	1239.59	528.57755	YES	YES
70	a	1278.68	252.36052	YES	YES
71	a	1281.24	284.25456	YES	YES
72	a	1291.67	7.37800	YES	YES



Total energy = -2305.8376753020 H = -62745.0713177 eV

HOMO-LUMO Separation

HOMO: 107. 107 a -0.08131184 H = -2.21261 eV

LUMO: 108. 108 a +0.11315709 H = +3.07916 eV

Gap : +0.19446892 H = +5.29177 eV

Number of MOs= 360, Electrons= 214.00, Symmetry: c1

\$scoord

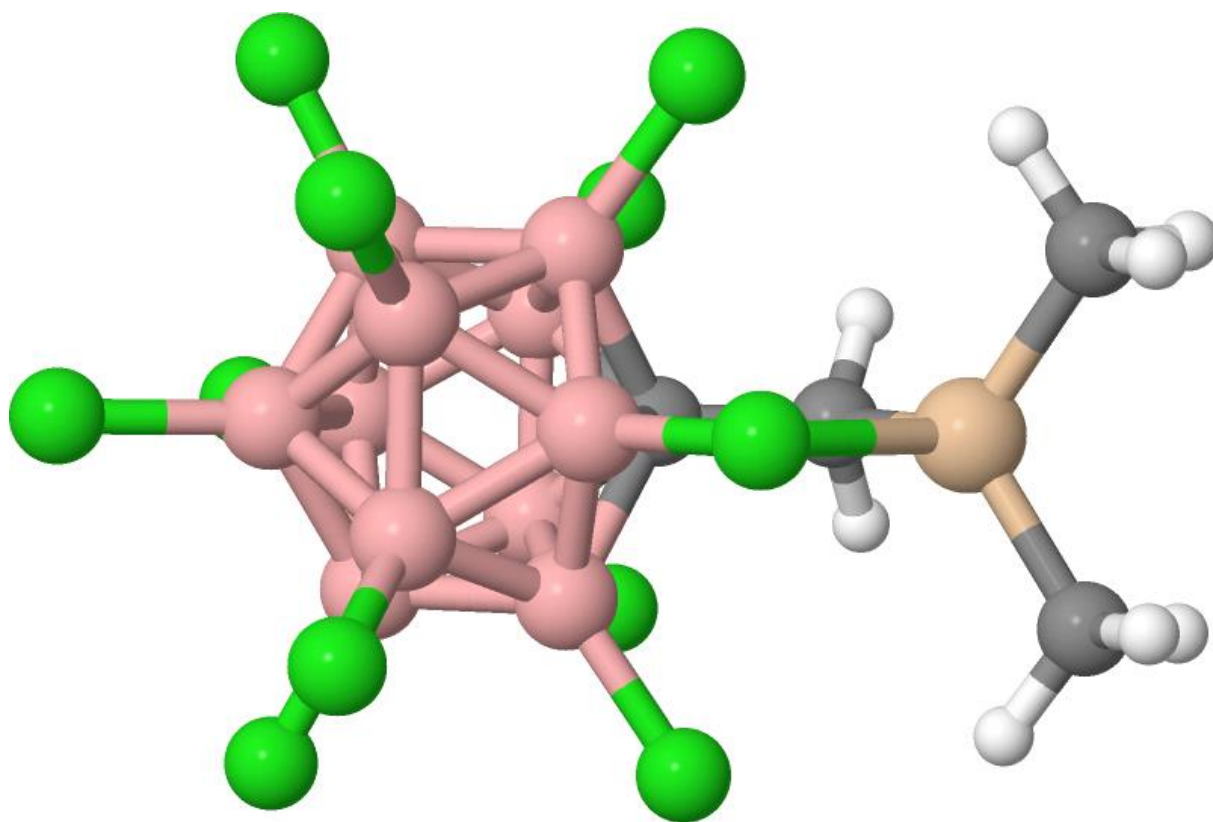
-5.10194327202871	1.77800142686379	0.49066045350846	p
-1.95383459472301	1.39415029846399	0.09269930533788	f
-4.89717716319831	5.32843405877613	0.96404723489797	c
-5.24563289093768	2.32713623927102	-3.28532221607625	c
-4.44544947392895	1.30602900107225	4.31354279147262	c
-7.68113883855829	3.29867470838036	-4.63703216320606	c
-4.57125138741153	0.17878484683442	-4.57010957422804	f
-3.43919249235510	4.11019796569790	-3.89123350257411	f
-9.70870575127098	1.82868953789249	-4.26089613125761	f
-7.27838941829740	3.39769758664909	-7.18034026268595	f
-8.30430200299319	5.67558146214418	-3.91113051980801	f
-6.62815975964760	1.67627479846330	6.25725005920241	c
-2.70312333542882	3.14648158177748	4.96679446712376	f
-3.32396521202272	-0.93425994831487	4.96395931689281	f
-7.69529125320208	3.99850458385173	6.06729429278178	f
-5.69838253429367	1.49519661963076	8.65716170453696	f
-8.48041719558167	-0.03893230669992	6.05440722929667	f
-5.46100967879114	-2.16621326353047	0.27034403391307	c
-6.70957653213309	-3.82062059383541	-1.85505597543489	c
-6.92763768198514	-2.75604720189900	2.34084274636419	f
-3.14806370784912	-3.27899551413886	0.61170727597388	f
-8.77057962981853	-2.73625278759637	-2.87396857118012	f
-7.48218392119525	-6.06669072116541	-0.85133473984561	f
-5.08911731588251	-4.42252667483650	-3.72459510597408	f
-8.29458944510165	1.85316472010708	0.81333349605841	f
-2.90078164688342	5.95165136110215	0.91665603731097	h
-5.75009028857185	5.85912603606649	2.79487936194322	h
-5.96426442521587	6.30419698412971	-0.54286619639991	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
#						
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	27.38	0.00388	YES	YES
8		a	30.07	0.09124	YES	YES
9		a	51.39	0.00282	YES	YES
10		a	60.27	0.02287	YES	YES
11		a	65.24	0.03359	YES	YES
12		a	94.59	0.11242	YES	YES
13		a	98.92	0.09455	YES	YES
14		a	124.14	1.20575	YES	YES
15		a	130.31	0.05038	YES	YES
16		a	142.19	0.17379	YES	YES
17		a	144.65	0.39057	YES	YES
18		a	170.12	0.10297	YES	YES
19		a	190.68	0.82862	YES	YES
20		a	200.07	1.36263	YES	YES
21		a	201.83	0.18269	YES	YES
22		a	211.37	1.71292	YES	YES
23		a	220.32	0.99067	YES	YES
24		a	226.24	0.48401	YES	YES
25		a	233.89	0.59266	YES	YES
26		a	243.88	0.23690	YES	YES
27		a	258.79	1.09031	YES	YES
28		a	262.81	0.37504	YES	YES

29	a	277.30	0.90403	YES	YES
30	a	288.36	0.18510	YES	YES
31	a	297.96	0.86889	YES	YES
32	a	317.83	0.74926	YES	YES
33	a	330.76	2.98591	YES	YES
34	a	337.06	5.51522	YES	YES
35	a	342.13	1.69078	YES	YES
36	a	362.98	0.55837	YES	YES
37	a	370.98	0.28372	YES	YES
38	a	382.02	2.72729	YES	YES
39	a	401.00	28.90040	YES	YES
40	a	433.22	5.38400	YES	YES
41	a	439.28	0.19316	YES	YES
42	a	464.57	22.35399	YES	YES
43	a	496.21	164.92495	YES	YES
44	a	515.58	2.19799	YES	YES
45	a	519.74	0.69491	YES	YES
46	a	526.42	34.69312	YES	YES
47	a	563.74	0.56419	YES	YES
48	a	570.69	0.01078	YES	YES
49	a	572.35	0.89007	YES	YES
50	a	577.16	2.86113	YES	YES
51	a	607.11	3.39490	YES	YES
52	a	610.02	8.83136	YES	YES
53	a	614.13	13.33475	YES	YES
54	a	660.99	166.39512	YES	YES
55	a	716.27	5.29560	YES	YES
56	a	719.44	10.13831	YES	YES
57	a	723.22	14.19166	YES	YES
58	a	763.83	93.07757	YES	YES
59	a	885.00	76.75466	YES	YES
60	a	890.10	45.93910	YES	YES
61	a	898.06	172.17076	YES	YES
62	a	913.88	3.27811	YES	YES
63	a	930.69	4.72891	YES	YES
64	a	1043.42	40.90769	YES	YES
65	a	1067.10	218.27646	YES	YES
66	a	1072.40	40.50494	YES	YES
67	a	1087.78	20.20786	YES	YES
68	a	1104.74	99.62450	YES	YES
69	a	1116.43	108.78928	YES	YES
70	a	1136.90	276.22523	YES	YES
71	a	1143.57	230.71397	YES	YES
72	a	1150.64	336.20195	YES	YES
73	a	1184.18	168.68973	YES	YES
74	a	1195.31	326.08130	YES	YES
75	a	1216.38	294.37799	YES	YES
76	a	1239.05	189.60737	YES	YES
77	a	1266.51	192.08403	YES	YES
78	a	1278.18	134.04409	YES	YES
79	a	1281.78	19.29763	YES	YES
80	a	1417.75	0.95847	YES	YES
81	a	1434.69	2.48703	YES	YES
82	a	3004.00	7.79665	YES	YES
83	a	3110.30	4.00307	YES	YES
84	a	3119.22	1.47916	YES	YES

SiMe₂CH₂CB₁₁Cl₁₁



Total energy = -5781.5570173570 H = -157324.2606221 eV

HOMO-LUMO Separation

HOMO: 144. 144 a -0.24060313 H = -6.54715 eV

LUMO: 145. 145 a -0.11125121 H = -3.02730 eV

Gap : +0.12935192 H = +3.51985 eV

Number of MOs= 442, Electrons= 288.00, Symmetry: c1

```
$coord
  1.83335612821959    0.73821314598232    0.28594142561850    b
  3.32941928786780   -2.47737709953755    0.51560303426022    c1
 -0.62952159041704   -6.71007757333771    2.90711753268591    c
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-2.42301848233539	-7.81298948184911	2.80859416050480	h
-0.67939119146221	-5.51896143623394	4.63025288627981	h
0.95360882487987	-8.08458336261877	3.05140341856209	h
5.19330309676473	3.38632291099895	4.31404941942970	cl
3.28482590991392	9.06010013109773	0.48973955927125	cl
0.72350610350256	6.68949410350636	-5.64386303218777	cl
0.94903291976297	-0.38746727381243	-5.41340598104977	cl
6.21440263432683	3.37502599051146	-2.61096249770173	cl
2.59951890066935	3.41312733130144	2.13974976803919	b
1.65535470160273	6.11260280367735	0.25092284929415	b
0.41586767259020	4.98404695248732	-2.74307221516879	b
0.58868061553427	1.61997433529033	-2.70588096064459	b
3.10316049125994	3.40870546242564	-1.27722852435342	b
-1.33211621258567	0.63341336643610	-0.17996694452898	c
-2.59500787753374	-1.95188852062512	-0.36620849763746	c
-3.57004508747541	-2.09567774246494	-2.22541026564348	h
-4.07317401267404	-2.09010674643355	1.12546070787044	h
-0.36403362083129	-4.75993519773090	-0.02875294263378	si
0.22881261474889	-6.72284395039404	-2.90726582650223	c
1.80058034880728	-8.07973237522529	-2.58484407790850	h
0.65982833578169	-5.53894723939647	-4.58116953890351	h
-1.50729780374702	-7.84727712503721	-3.31349128668591	h
-4.97122126633312	2.65154209329714	-4.16166908213975	cl
-3.68949208957379	8.69195503023544	-0.53686762021204	cl
-0.93740267665166	6.70524963162461	5.62370890608098	cl
-0.65740529190065	-0.36971238521959	5.49177322379837	cl
-5.96610913630896	2.66418333627218	2.57099168385610	cl
-2.37544341719216	3.14587158748287	-2.06306149616215	b
-1.74095854629071	5.94713256256786	-0.24959401020568	b
-0.39722736607831	4.99075500433789	2.76283156316611	b
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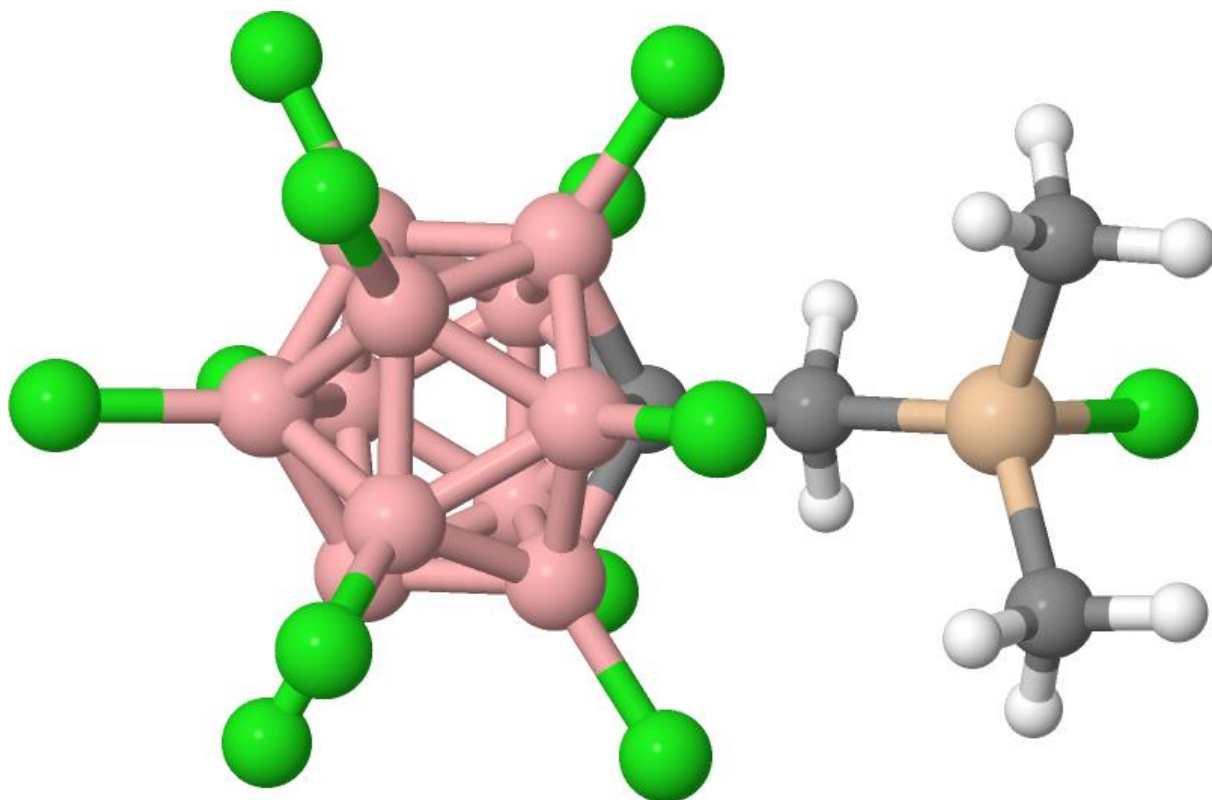
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		73.53	1.03020	YES	YES
8	a		79.90	0.10363	YES	YES
9	a		82.43	1.50546	YES	YES
10	a		101.94	0.05675	YES	YES
11	a		105.15	0.03556	YES	YES
12	a		105.85	0.02989	YES	YES
13	a		108.80	0.00892	YES	YES
14	a		109.03	0.02264	YES	YES
15	a		111.08	0.15396	YES	YES
16	a		111.54	0.04134	YES	YES
17	a		112.85	0.10144	YES	YES
18	a		113.17	0.16981	YES	YES
19	a		114.39	0.65831	YES	YES
20	a		116.07	0.03826	YES	YES
21	a		116.56	0.98266	YES	YES
22	a		119.57	0.11460	YES	YES
23	a		120.32	0.00705	YES	YES
24	a		120.60	0.20382	YES	YES
25	a		121.42	0.15970	YES	YES

26	a	129.84	0.18262	YES	YES
27	a	142.98	3.80256	YES	YES
28	a	147.86	2.63634	YES	YES
29	a	150.06	0.40610	YES	YES
30	a	175.17	1.80666	YES	YES
31	a	190.17	2.25505	YES	YES
32	a	196.90	0.77987	YES	YES
33	a	239.77	0.32509	YES	YES
34	a	255.05	3.40203	YES	YES
35	a	276.18	0.03478	YES	YES
36	a	280.41	0.52933	YES	YES
37	a	285.89	0.52707	YES	YES
38	a	287.63	0.10036	YES	YES
39	a	290.80	2.15100	YES	YES
40	a	307.07	0.84815	YES	YES
41	a	313.39	1.66601	YES	YES
42	a	315.50	0.02191	YES	YES
43	a	319.76	54.27898	YES	YES
44	a	405.25	0.00493	YES	YES
45	a	416.98	2.63625	YES	YES
46	a	427.13	0.26156	YES	YES
47	a	453.86	4.09062	YES	YES
48	a	515.04	1.41129	YES	YES
49	a	516.24	41.65472	YES	YES
50	a	527.90	30.39718	YES	YES
51	a	532.04	11.70403	YES	YES
52	a	555.68	14.42322	YES	YES
53	a	564.07	24.11549	YES	YES
54	a	590.42	0.53260	YES	YES
55	a	606.80	26.09420	YES	YES
56	a	625.55	14.13684	YES	YES
57	a	641.69	18.58878	YES	YES
58	a	662.75	0.10530	YES	YES
59	a	662.99	2.43315	YES	YES
60	a	674.58	0.98378	YES	YES
61	a	694.71	18.13073	YES	YES
62	a	696.16	0.50541	YES	YES
63	a	696.70	0.64300	YES	YES
64	a	703.25	0.85935	YES	YES
65	a	706.87	11.34686	YES	YES
66	a	722.59	0.66422	YES	YES
67	a	738.00	6.70595	YES	YES
68	a	739.90	2.05799	YES	YES
69	a	745.94	3.01815	YES	YES
70	a	749.80	5.48744	YES	YES
71	a	767.17	2.49168	YES	YES
72	a	793.07	5.25188	YES	YES
73	a	801.13	0.25767	YES	YES
74	a	811.48	74.62627	YES	YES
75	a	834.19	67.34821	YES	YES
76	a	865.84	169.24191	YES	YES
77	a	911.79	9.89160	YES	YES
78	a	942.31	0.08359	YES	YES
79	a	953.12	1.17192	YES	YES
80	a	966.34	5.82806	YES	YES
81	a	974.83	8.07681	YES	YES
82	a	989.03	10.07650	YES	YES
83	a	991.19	1.66539	YES	YES
84	a	1011.80	323.13873	YES	YES
85	a	1036.88	323.92665	YES	YES
86	a	1043.81	336.32946	YES	YES
87	a	1065.26	25.88262	YES	YES

88	a	1142.21	3.10827	YES	YES
89	a	1151.68	19.81502	YES	YES
90	a	1189.93	16.07352	YES	YES
91	a	1238.94	40.50925	YES	YES
92	a	1245.89	44.75723	YES	YES
93	a	1375.40	12.24260	YES	YES
94	a	1377.77	5.07105	YES	YES
95	a	1388.30	0.42201	YES	YES
96	a	1392.44	0.01538	YES	YES
97	a	1408.34	10.00778	YES	YES
98	a	2944.32	1.43692	YES	YES
99	a	2946.61	0.29905	YES	YES
100	a	2948.69	10.84895	YES	YES
101	a	3002.63	2.93236	YES	YES
102	a	3032.94	0.05063	YES	YES
103	a	3035.09	1.68703	YES	YES
104	a	3077.82	3.84969	YES	YES
105	a	3078.91	2.28902	YES	YES

ClSiMe₂CH₂CB₁₁Cl₁₁⁻



Total energy = -6241.8687147780 H = -169849.9863453 eV

HOMO-LUMO Separation

HOMO: 153. 153 a -0.13375598 H = -3.63969 eV

LUMO: 154. 154 a +0.02725881 H = +0.74175 eV

Gap : +0.16101479 H = +4.38144 eV

Number of MOs= 460, Electrons= 306.00, Symmetry: c1

\$coord

2.24929412108643	0.20042198687503	0.33498467954276	b
4.06884843832296	-2.65913056140546	0.60939427859320	c1
-0.48134917640453	-7.00597895633366	2.95080775439956	c
-0.36164568257832	-9.10439117171960	2.85807279646392	h
-1.88113601040145	-6.48843355938626	4.42689352886119	h
1.38323701370096	-6.23221817233811	3.51745433488594	h
5.46882581204146	3.05535421360737	4.37576653551705	c1
3.56925887843234	8.65333243037544	0.52916655950480	c1
1.05055806509550	6.24436611869325	-5.61646039142830	c1
1.28567878354875	-0.79520684580454	-5.40767841108538	c1
6.52340441092857	3.04890831036226	-2.57675273625283	c1
2.88869183811864	2.97488181298733	2.15961296669795	b
1.95491238548439	5.67042073491875	0.28390161800934	b
0.74087514022642	4.52487369670956	-2.69765505608791	b
0.91978857995693	1.13202238429360	-2.63877297391411	b
3.40192820102154	2.97228081150209	-1.22461091385815	b
-1.00099391727649	0.12738050327098	-0.15626177901684	c
-2.56750094758393	-2.29014501954583	-0.39171070180020	c
-3.58782372997250	-2.19064706199125	-2.22932584867731	h
-4.08939018787228	-2.18284707600372	1.05800735591296	h
-1.51942487668767	-5.76023324784458	-0.22499940014930	si
0.40500855406189	-7.01613378262061	-2.95210855585316	c
2.36116052184714	-6.26186721655983	-2.93139868974628	h
-0.48289698259008	-6.47930530914850	-4.77706774953400	h
0.47054969976315	-9.11587869935400	-2.83990467037935	h
-4.62934577233723	2.30840825371416	-4.16684850673692	c1
-3.39088997590816	8.25160553093479	-0.52596583257187	c1
-0.65736310667650	6.25715221300332	5.64821974203254	c1
-0.37399450383263	-0.78118498544325	5.53802062432966	c1
-5.65494061956243	2.31581483519202	2.58792458343717	c1
-2.02695354729561	2.69921571936238	-2.02908080054923	b
-1.41630858305540	5.49780618797635	-0.22723643186468	b
-0.08982951882405	4.52997878263156	2.77348303270994	b
0.09749843415396	1.13733481272442	2.77937782529671	b
-2.53523899512861	2.70250957303873	1.31938830679149	b
-5.14552482271202	-7.48044613950682	-0.76492565661375	c1

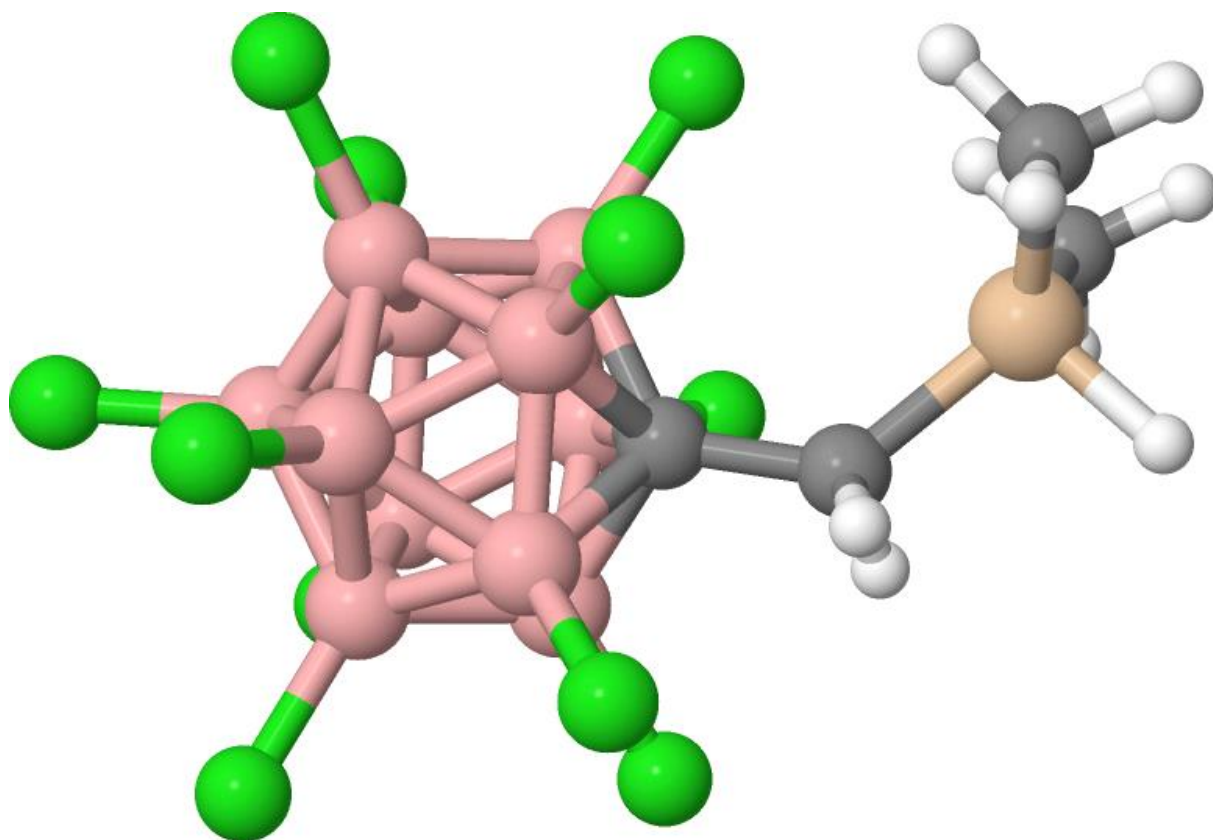
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	42.32	0.15585	YES	YES
8	a	60.27	0.48985	YES	YES
9	a	60.63	0.37300	YES	YES
10	a	105.81	0.00688	YES	YES
11	a	106.37	0.03639	YES	YES
12	a	107.15	0.00994	YES	YES
13	a	108.91	0.03178	YES	YES
14	a	109.07	0.06216	YES	YES
15	a	112.37	0.17678	YES	YES
16	a	112.65	0.03496	YES	YES
17	a	113.54	0.50450	YES	YES
18	a	114.52	0.02292	YES	YES
19	a	115.05	0.01849	YES	YES
20	a	117.04	0.01267	YES	YES
21	a	117.40	0.14678	YES	YES
22	a	118.60	0.08494	YES	YES
23	a	119.88	0.03904	YES	YES
24	a	120.75	0.66016	YES	YES
25	a	123.02	0.13366	YES	YES
26	a	123.62	0.05449	YES	YES
27	a	142.40	1.40253	YES	YES
28	a	144.92	1.00346	YES	YES
29	a	156.20	3.14176	YES	YES
30	a	166.07	0.71338	YES	YES
31	a	169.87	0.91961	YES	YES
32	a	173.82	0.22776	YES	YES
33	a	184.54	0.48993	YES	YES
34	a	203.49	0.12916	YES	YES
35	a	215.01	2.32392	YES	YES
36	a	216.52	1.75447	YES	YES
37	a	270.65	10.29874	YES	YES
38	a	274.45	0.03604	YES	YES
39	a	277.11	0.17197	YES	YES
40	a	284.79	0.03116	YES	YES
41	a	286.40	0.00231	YES	YES
42	a	291.85	0.06893	YES	YES
43	a	304.67	0.02966	YES	YES
44	a	312.87	0.00102	YES	YES
45	a	313.57	0.00527	YES	YES
46	a	403.95	12.75435	YES	YES
47	a	409.87	0.01888	YES	YES
48	a	426.62	0.60409	YES	YES
49	a	446.49	70.40918	YES	YES
50	a	468.00	23.07544	YES	YES
51	a	519.55	10.61945	YES	YES
52	a	523.77	28.63054	YES	YES
53	a	527.60	7.29622	YES	YES
54	a	529.49	27.96578	YES	YES
55	a	548.14	32.36558	YES	YES
56	a	561.88	18.10376	YES	YES
57	a	594.99	0.01999	YES	YES
58	a	613.92	0.80508	YES	YES
59	a	620.23	51.77980	YES	YES
60	a	644.10	17.17733	YES	YES
61	a	668.80	16.52628	YES	YES
62	a	678.13	0.04705	YES	YES
63	a	682.07	3.22848	YES	YES
64	a	687.87	1.53311	YES	YES
65	a	693.31	4.09740	YES	YES

66	a	710.30	13.10514	YES	YES
67	a	712.99	0.32769	YES	YES
68	a	716.18	1.18245	YES	YES
69	a	731.67	0.13202	YES	YES
70	a	736.35	1.17879	YES	YES
71	a	751.74	0.05780	YES	YES
72	a	757.06	0.16490	YES	YES
73	a	758.56	15.99893	YES	YES
74	a	779.36	1.63946	YES	YES
75	a	786.57	0.04679	YES	YES
76	a	790.54	0.09072	YES	YES
77	a	824.39	115.39165	YES	YES
78	a	825.72	162.70284	YES	YES
79	a	857.22	87.70402	YES	YES
80	a	929.11	0.29216	YES	YES
81	a	932.60	0.34326	YES	YES
82	a	947.93	0.14814	YES	YES
83	a	974.40	3.04557	YES	YES
84	a	977.31	3.11032	YES	YES
85	a	985.15	0.71676	YES	YES
86	a	987.66	0.30017	YES	YES
87	a	1017.81	314.98966	YES	YES
88	a	1041.35	336.51870	YES	YES
89	a	1043.69	346.05497	YES	YES
90	a	1065.25	4.60557	YES	YES
91	a	1128.85	2.91511	YES	YES
92	a	1194.52	6.80484	YES	YES
93	a	1210.43	16.24876	YES	YES
94	a	1235.03	37.67919	YES	YES
95	a	1242.41	29.78955	YES	YES
96	a	1376.00	2.92363	YES	YES
97	a	1389.22	0.30327	YES	YES
98	a	1398.85	1.59345	YES	YES
99	a	1401.06	6.84848	YES	YES
100	a	1407.00	14.09872	YES	YES
101	a	2943.94	15.71716	YES	YES
102	a	2951.42	3.03917	YES	YES
103	a	2952.70	15.50165	YES	YES
104	a	2993.33	1.29026	YES	YES
105	a	3044.31	0.82991	YES	YES
106	a	3045.20	16.53554	YES	YES
107	a	3068.68	0.76711	YES	YES
108	a	3069.05	1.60460	YES	YES

HSiMe₂CH₂CB₁₁Cl₁₁⁻



Total energy = -5782.2971551060 H = -157344.4008065 eV

HOMO-LUMO Separation

HOMO: 145. 145 a -0.13018282 H = -3.54246 eV

LUMO: 146. 146 a +0.03137161 H = +0.85367 eV

Gap : +0.16155443 H = +4.39612 eV

Number of MOs= 444, Electrons= 290.00, Symmetry: c1

```
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  2.25214156485880      0.20844538159741      0.32826491233587      b
  4.08405710827693     -2.63935771878737      0.60046094834048      c1
 -0.52655064710001     -7.01052755397886      2.94022317548790      c
 -0.45300704732167     -9.11443373354895      2.87314722195475      h
 -1.87159226055215     -6.45149519557870      4.45406570290070      h
```

1.36941010357973	-6.28433160740720	3.46458675569892	h
5.47877629949821	3.05974217556102	4.36872875865797	cl
3.58840892680060	8.66365619369398	0.53224082850750	cl
1.05402488446293	6.26859228143102	-5.61346361926112	cl
1.27196067311247	-0.77065803369839	-5.41651272304110	cl
6.52314590101889	3.06145984501223	-2.58802873845917	cl
2.89579028079065	2.98298371394423	2.15444936491332	b
1.96613404174403	5.68387592932667	0.28513617537045	b
0.74492118387400	4.54483842576327	-2.69559188521169	b
0.91539566264233	1.14886750050627	-2.64035413469836	b
3.40363550947484	2.98412191561279	-1.22927063044631	b
-1.00551738024946	0.14435420123305	-0.15902485935646	c
-2.58387690155493	-2.26558113607397	-0.39800827752912	c
-3.60002019519653	-2.14366090466988	-2.23804235506843	h
-4.10892582183218	-2.13377606779621	1.04786307806733	h
-1.62622352294731	-5.77479376896539	-0.24118479393636	si
0.36371273273228	-7.02876735357099	-2.94783611548083	c
2.33286796202377	-6.31163618393066	-2.88676979974217	h
-0.46575433246162	-6.47094042254431	-4.79582988064778	h
0.40394379711790	-9.13257742186360	-2.85592062322530	h
-4.63326833367426	2.35156718258456	-4.16192662669029	cl
-3.37460982432338	8.28092236150503	-0.51265744235832	cl
-0.63690366264514	6.26829340421070	5.65478788166191	cl
-0.37063408415846	-0.76583971241803	5.53623094841651	cl
-5.64908448861383	2.35116684003193	2.59642918662509	cl
-2.02456591518530	2.72605112550131	-2.02444685714658	b
-1.40490662059749	5.52101633833820	-0.22089765731013	b
-0.07717935452470	4.54364847650298	2.77541846857528	b
0.10212343479510	1.14840301596668	2.77419207218336	b
-2.52717643453666	2.72540155541649	1.32166991030536	b
-4.23558381799033	-6.91933769336726	-0.63289471870092	h

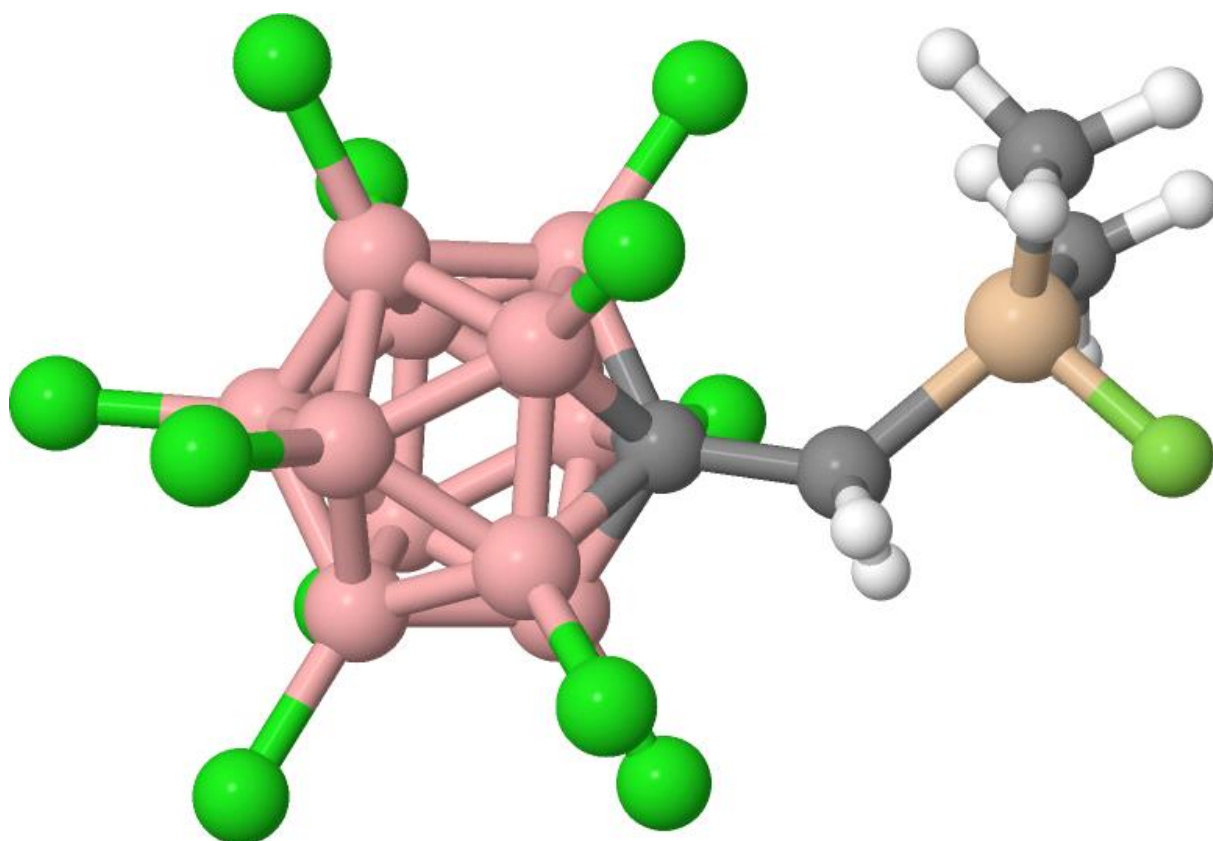
\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	53.05	0.03462	YES	YES
8		a	75.93	0.24085	YES	YES
9		a	78.55	0.01729	YES	YES
10		a	105.93	0.00562	YES	YES
11		a	106.57	0.01277	YES	YES
12		a	107.19	0.00166	YES	YES
13		a	109.00	0.01085	YES	YES
14		a	109.39	0.02141	YES	YES
15		a	112.62	0.00868	YES	YES
16		a	112.87	0.01502	YES	YES
17		a	114.58	0.01442	YES	YES
18		a	115.05	0.02555	YES	YES
19		a	115.25	0.02276	YES	YES
20		a	116.83	0.00406	YES	YES
21		a	119.38	0.09766	YES	YES
22		a	119.85	0.01757	YES	YES
23		a	121.70	0.04014	YES	YES
24		a	124.62	0.27160	YES	YES
25		a	125.61	0.00754	YES	YES

26	a	141.24	0.83250	YES	YES
27	a	144.78	0.58363	YES	YES
28	a	154.96	3.31602	YES	YES
29	a	156.02	0.05305	YES	YES
30	a	165.03	0.27764	YES	YES
31	a	171.21	0.02047	YES	YES
32	a	182.73	0.26913	YES	YES
33	a	199.04	0.00416	YES	YES
34	a	219.06	1.91536	YES	YES
35	a	270.88	6.41182	YES	YES
36	a	274.36	0.07958	YES	YES
37	a	276.78	0.06790	YES	YES
38	a	284.55	0.01505	YES	YES
39	a	286.23	0.00036	YES	YES
40	a	292.17	0.29174	YES	YES
41	a	306.26	0.50495	YES	YES
42	a	312.63	0.00412	YES	YES
43	a	313.41	0.01014	YES	YES
44	a	389.75	1.83551	YES	YES
45	a	410.05	0.00303	YES	YES
46	a	425.16	0.16035	YES	YES
47	a	452.15	2.98120	YES	YES
48	a	517.94	16.20068	YES	YES
49	a	519.64	38.57508	YES	YES
50	a	526.51	1.34913	YES	YES
51	a	529.21	22.34516	YES	YES
52	a	543.89	46.03217	YES	YES
53	a	558.38	19.50010	YES	YES
54	a	595.01	0.03861	YES	YES
55	a	605.48	23.02602	YES	YES
56	a	611.78	1.71611	YES	YES
57	a	622.91	0.17661	YES	YES
58	a	644.13	16.31821	YES	YES
59	a	664.74	21.46918	YES	YES
60	a	677.60	0.05706	YES	YES
61	a	680.43	1.25424	YES	YES
62	a	681.70	1.13707	YES	YES
63	a	685.04	17.14568	YES	YES
64	a	689.99	9.12962	YES	YES
65	a	713.25	0.10892	YES	YES
66	a	716.62	0.28061	YES	YES
67	a	727.09	3.64824	YES	YES
68	a	736.54	2.11606	YES	YES
69	a	751.18	5.51001	YES	YES
70	a	751.81	1.42465	YES	YES
71	a	765.74	9.15219	YES	YES
72	a	786.09	7.35125	YES	YES
73	a	787.06	18.18489	YES	YES
74	a	791.92	0.28277	YES	YES
75	a	811.97	31.55482	YES	YES
76	a	849.78	39.49907	YES	YES
77	a	898.48	261.09875	YES	YES
78	a	903.06	99.83352	YES	YES
79	a	927.80	0.79340	YES	YES
80	a	932.26	0.43013	YES	YES
81	a	947.81	1.13216	YES	YES
82	a	974.00	2.97742	YES	YES
83	a	977.02	2.76813	YES	YES
84	a	984.67	0.78522	YES	YES
85	a	987.20	0.39202	YES	YES
86	a	1017.66	318.77617	YES	YES
87	a	1040.52	339.23162	YES	YES

88	a	1043.43	344.20039	YES	YES
89	a	1064.68	4.02762	YES	YES
90	a	1125.99	2.13686	YES	YES
91	a	1200.70	6.92303	YES	YES
92	a	1206.94	6.16380	YES	YES
93	a	1232.00	35.00932	YES	YES
94	a	1240.17	28.48296	YES	YES
95	a	1382.56	4.58169	YES	YES
96	a	1391.92	0.48105	YES	YES
97	a	1402.51	9.01475	YES	YES
98	a	1405.01	0.71782	YES	YES
99	a	1412.99	11.35935	YES	YES
100	a	2094.37	216.81593	YES	YES
101	a	2936.36	18.28790	YES	YES
102	a	2941.66	6.65743	YES	YES
103	a	2942.98	26.66771	YES	YES
104	a	2984.99	0.40757	YES	YES
105	a	3031.22	4.08434	YES	YES
106	a	3031.81	22.22977	YES	YES
107	a	3063.62	2.02042	YES	YES
108	a	3064.68	2.06629	YES	YES

FSiMe₂CH₂CB₁₁Cl₁₁⁻



Total energy = -5881.5383326600 H = -160044.8921853 eV

HOMO-LUMO Separation

HOMO: 149. 149 a -0.13243170 H = -3.60365 eV

LUMO: 150. 150 a +0.02887397 H = +0.78570 eV

Gap : +0.16130567 H = +4.38935 eV

Number of MOs= 456, Electrons= 298.00, Symmetry: c1

\$coord

2.21856304807319	0.19122651040588	0.32749984001559	b
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-0.50785247255291	-9.10418285675342	2.86402231716469	h
-1.99925747723158	-6.46322332408111	4.41412481620230	h
1.27804492512461	-6.27254549305070	3.55771628388199	h
5.46296084477064	3.01353639967900	4.37131165581538	c1
3.59959979091588	8.63378995238839	0.54041308021509	c1
1.05470656153898	6.25867182800717	-5.60763069484274	c1
1.23775260227019	-0.78467062153450	-5.41508087800183	c1
6.50840228555557	3.01688374686167	-2.58386110479613	c1
2.87976394276381	2.95625048409906	2.15755643847016	b
1.96261698721356	5.66311978544592	0.29027819695086	b
0.73597205054756	4.53375582776979	-2.69239027079290	b
0.89104440627438	1.13946539421186	-2.64144880768679	b
3.38832145837626	2.95824660111892	-1.22687983646313	b
-1.03419395587028	0.14346966785304	-0.15965650466970	c
-2.59162007989188	-2.27159195716532	-0.39775832531925	c
-3.60139637309188	-2.18071437170400	-2.24340087424794	h
-4.12450112466259	-2.16501030914543	1.04257659778352	h
-1.58907329221491	-5.74294582327809	-0.22414669938999	si
0.29511277902857	-7.02994534563461	-2.95661948866307	c
2.27180485875167	-6.33499725234282	-2.96993781076608	h
-0.59571758375653	-6.47006438400188	-4.77517067317420	h
0.31069689236884	-9.13275657681304	-2.85380057083148	h
-4.65271593168058	2.35616529224401	-4.15926111393180	c1
-3.36486215335905	8.28667144683394	-0.50581718961051	c1
-0.63833763672960	6.25510106974680	5.66003853385028	c1
-0.40655782135943	-0.78081946827736	5.53280835183494	c1
-5.66936590066188	2.35415403516762	2.59424809011886	c1
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-0.08736905375309	4.53111959625435	2.77944152904939	b
0.07611709017932	1.13764187298440	2.77606791090853	b
-2.54746749183230	2.72436470399736	1.32349800827353	b
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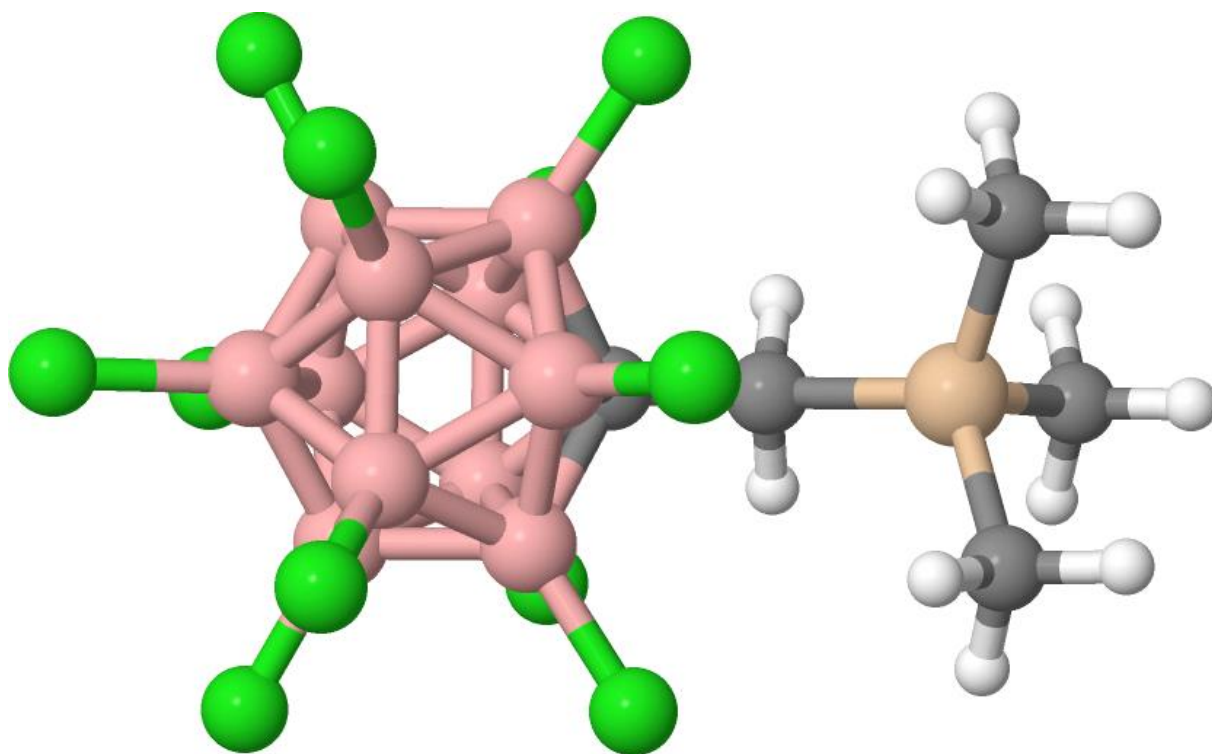
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules
#			cm** (-1)	km/mol	IR RAMAN

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2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	48.69	0.00513	YES	YES
8	a	67.79	0.33129	YES	YES
9	a	69.21	0.31788	YES	YES
10	a	105.85	0.00567	YES	YES
11	a	106.46	0.02066	YES	YES
12	a	107.22	0.00776	YES	YES
13	a	108.86	0.01263	YES	YES
14	a	109.30	0.03051	YES	YES
15	a	112.52	0.01368	YES	YES
16	a	112.72	0.01518	YES	YES
17	a	114.48	0.02354	YES	YES
18	a	114.98	0.01508	YES	YES
19	a	115.35	0.04900	YES	YES
20	a	116.95	0.00580	YES	YES
21	a	118.83	0.07359	YES	YES
22	a	119.91	0.01332	YES	YES
23	a	120.64	0.14154	YES	YES
24	a	123.19	0.15318	YES	YES
25	a	124.07	0.02463	YES	YES
26	a	140.90	0.91059	YES	YES
27	a	144.49	0.98114	YES	YES
28	a	145.01	1.42655	YES	YES
29	a	150.70	0.20157	YES	YES
30	a	152.24	0.95200	YES	YES
31	a	165.01	0.54118	YES	YES
32	a	173.87	0.55591	YES	YES
33	a	195.07	1.16712	YES	YES
34	a	200.49	0.00593	YES	YES
35	a	217.91	2.57304	YES	YES
36	a	268.53	7.36068	YES	YES
37	a	274.63	0.00658	YES	YES
38	a	276.87	0.08934	YES	YES
39	a	284.50	0.21748	YES	YES
40	a	286.30	0.01688	YES	YES
41	a	290.96	5.34850	YES	YES
42	a	293.53	11.28958	YES	YES
43	a	305.22	0.16331	YES	YES
44	a	312.78	0.00133	YES	YES
45	a	313.51	0.02394	YES	YES
46	a	408.20	13.12162	YES	YES
47	a	409.88	0.00636	YES	YES
48	a	426.10	0.63174	YES	YES
49	a	458.84	14.86908	YES	YES
50	a	519.53	11.89897	YES	YES
51	a	522.40	31.28742	YES	YES
52	a	527.75	3.83678	YES	YES
53	a	529.36	25.52875	YES	YES
54	a	548.24	41.97759	YES	YES
55	a	561.43	19.45017	YES	YES
56	a	594.77	0.02878	YES	YES
57	a	611.62	0.60214	YES	YES
58	a	619.62	23.85981	YES	YES
59	a	642.60	16.83420	YES	YES
60	a	669.46	15.64162	YES	YES
61	a	677.64	0.08785	YES	YES
62	a	682.10	3.14292	YES	YES

63	a	682.87	0.19447	YES	YES
64	a	692.24	4.39271	YES	YES
65	a	707.32	23.71098	YES	YES
66	a	713.18	0.17196	YES	YES
67	a	716.05	1.03086	YES	YES
68	a	731.39	0.80266	YES	YES
69	a	735.55	0.62827	YES	YES
70	a	749.89	4.38933	YES	YES
71	a	754.66	14.47868	YES	YES
72	a	757.24	0.66941	YES	YES
73	a	758.12	11.26484	YES	YES
74	a	782.02	2.84332	YES	YES
75	a	786.88	0.07273	YES	YES
76	a	790.71	0.07955	YES	YES
77	a	824.54	89.01256	YES	YES
78	a	847.72	260.27955	YES	YES
79	a	867.92	119.94476	YES	YES
80	a	928.34	0.27706	YES	YES
81	a	932.61	0.22883	YES	YES
82	a	948.19	0.26800	YES	YES
83	a	973.64	2.73885	YES	YES
84	a	976.80	2.92347	YES	YES
85	a	985.31	0.64268	YES	YES
86	a	987.29	0.29569	YES	YES
87	a	1017.51	317.12451	YES	YES
88	a	1040.57	336.48272	YES	YES
89	a	1043.70	352.31547	YES	YES
90	a	1065.47	3.55421	YES	YES
91	a	1137.54	3.30988	YES	YES
92	a	1188.26	10.73357	YES	YES
93	a	1211.52	18.06033	YES	YES
94	a	1238.80	45.95786	YES	YES
95	a	1243.49	34.67342	YES	YES
96	a	1379.96	3.43880	YES	YES
97	a	1390.03	0.31255	YES	YES
98	a	1400.11	0.50916	YES	YES
99	a	1401.88	11.34016	YES	YES
100	a	1407.76	11.57536	YES	YES
101	a	2935.75	14.77910	YES	YES
102	a	2946.60	3.47968	YES	YES
103	a	2948.03	21.84995	YES	YES
104	a	2984.92	0.49752	YES	YES
105	a	3035.26	2.87277	YES	YES
106	a	3036.24	20.01986	YES	YES
107	a	3071.31	0.69603	YES	YES
108	a	3071.79	3.17347	YES	YES

MeSiMe₂CH₂CB₁₁Cl₁₁⁻



Total energy = -5821.5878199090 H = -158413.5548027 eV

HOMO-LUMO Separation

HOMO: 149. 149 a -0.12916836 H = -3.51485 eV

LUMO: 150. 150 a +0.03267325 H = +0.88908 eV

Gap : +0.16184161 H = +4.40394 eV

Number of MOs= 462, Electrons= 298.00, Symmetry: c1

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 -0.07713217808779   -6.92516746919712    2.94820075179948    c
 -1.46277133110437   -6.45647714612820    4.45672170194616    h
  1.75738883889234   -6.05778745135091    3.47580827302463    h
  0.15786408352138   -9.01849116128193    2.90230205207604    h
  5.41363883449226    3.41061186677921    4.50176889755586    c1
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-2.29432912986128	-2.30799530362246	-0.42592481592854	c
-3.26509748760475	-2.21521670524353	-2.29212870226715	h
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-0.87460727740612	6.30570408050832	5.66543142395078	cl
-0.25743248752121	-0.70309882279236	5.55949523614974	cl
-5.62557671489314	2.15273991338491	2.51613821932495	cl
-1.93434125757156	2.70222916090391	-2.03466356785874	b
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-0.17440560924309	4.61085558744251	2.79894882460573	b
0.17389056279245	1.22750973830376	2.80181184637785	b
-2.50063755677653	2.67474100079648	1.29918133128017	b
-4.42752319658970	-7.44277787293231	-0.79828566160383	c
-4.19210326718595	-9.53483300262284	-0.76831729644185	h
-5.26235713721421	-6.92569558313120	-2.66054270758767	h
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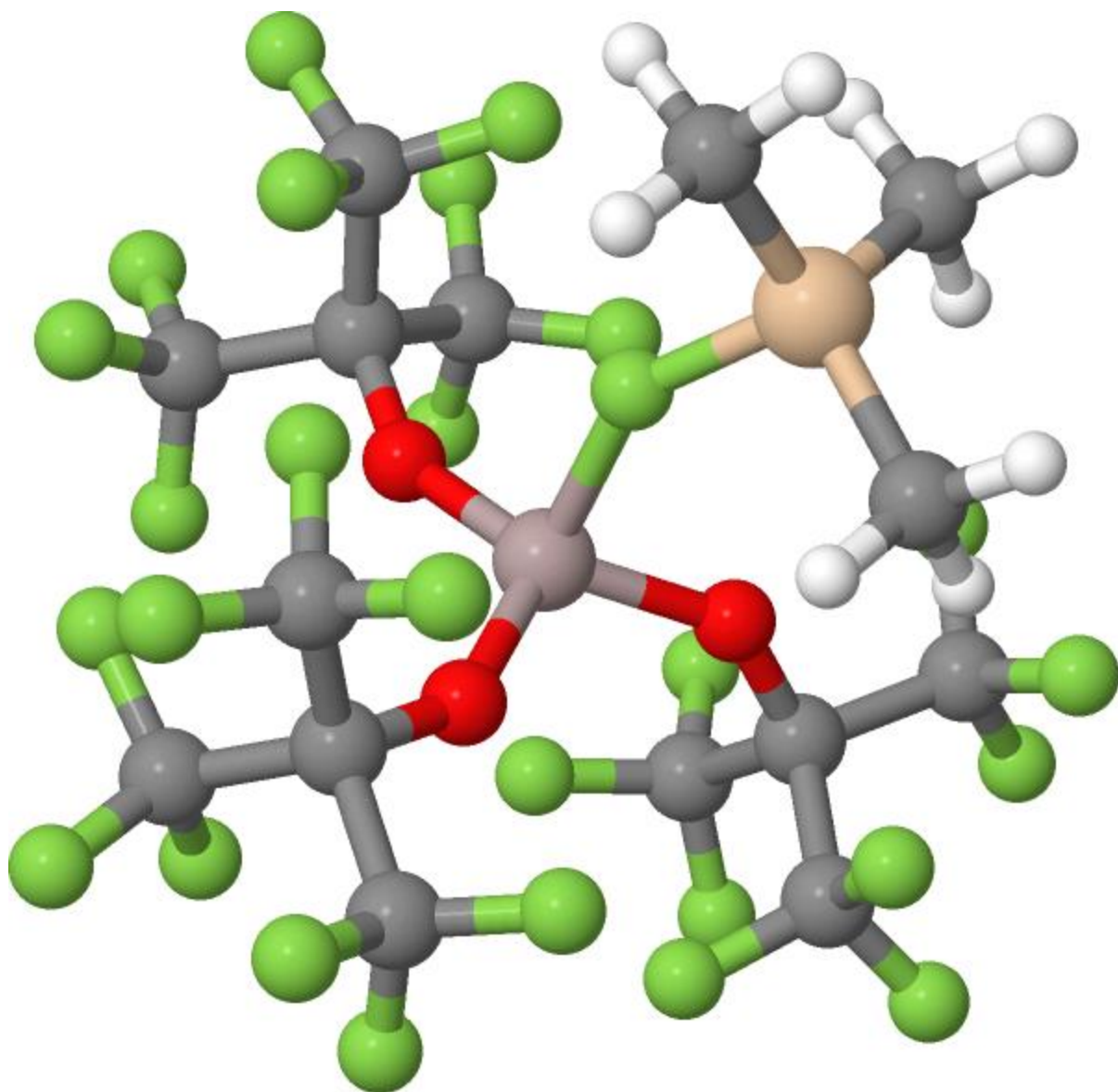
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#	mode	symmetry	wave number	IR intensity	selection rules	
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6			0.00	0.00000	-	-
7		a	42.55	0.03388	YES	YES
8		a	57.00	0.00116	YES	YES
9		a	67.82	0.19734	YES	YES
10		a	105.96	0.00759	YES	YES
11		a	106.74	0.01415	YES	YES
12		a	107.17	0.00183	YES	YES
13		a	108.99	0.01241	YES	YES
14		a	109.06	0.01454	YES	YES
15		a	112.46	0.04442	YES	YES
16		a	112.63	0.02043	YES	YES
17		a	113.96	0.06366	YES	YES
18		a	114.55	0.00657	YES	YES
19		a	115.24	0.01429	YES	YES
20		a	116.96	0.00099	YES	YES
21		a	117.55	0.04465	YES	YES
22		a	120.06	0.01179	YES	YES
23		a	120.53	0.06889	YES	YES
24		a	122.64	0.01477	YES	YES
25		a	123.42	0.18055	YES	YES

26	a	134.97	0.58450	YES	YES
27	a	142.97	0.66888	YES	YES
28	a	144.20	1.46948	YES	YES
29	a	147.64	1.12607	YES	YES
30	a	155.39	1.24252	YES	YES
31	a	162.69	0.22329	YES	YES
32	a	170.08	0.10614	YES	YES
33	a	180.61	0.09757	YES	YES
34	a	183.62	0.31122	YES	YES
35	a	190.55	0.01313	YES	YES
36	a	217.70	1.07932	YES	YES
37	a	218.21	1.65308	YES	YES
38	a	271.97	9.88086	YES	YES
39	a	274.03	0.03748	YES	YES
40	a	276.98	0.15333	YES	YES
41	a	285.32	0.02107	YES	YES
42	a	286.28	0.00444	YES	YES
43	a	291.60	0.22350	YES	YES
44	a	304.64	0.10723	YES	YES
45	a	311.71	0.00063	YES	YES
46	a	312.44	0.00730	YES	YES
47	a	400.62	5.70057	YES	YES
48	a	411.90	0.02211	YES	YES
49	a	427.86	0.28262	YES	YES
50	a	457.49	7.41666	YES	YES
51	a	517.68	34.15542	YES	YES
52	a	518.47	15.75557	YES	YES
53	a	529.71	0.52933	YES	YES
54	a	531.09	22.13693	YES	YES
55	a	545.28	49.09802	YES	YES
56	a	561.12	21.03278	YES	YES
57	a	596.98	0.03642	YES	YES
58	a	597.38	1.41018	YES	YES
59	a	614.89	17.52243	YES	YES
60	a	640.67	14.52132	YES	YES
61	a	648.15	24.52989	YES	YES
62	a	665.24	19.17820	YES	YES
63	a	669.89	3.00990	YES	YES
64	a	677.00	0.79957	YES	YES
65	a	679.44	6.17423	YES	YES
66	a	680.41	7.06743	YES	YES
67	a	683.33	2.00389	YES	YES
68	a	688.11	5.63932	YES	YES
69	a	715.54	0.02544	YES	YES
70	a	720.32	0.33033	YES	YES
71	a	729.94	2.14873	YES	YES
72	a	739.18	1.92974	YES	YES
73	a	753.92	1.93007	YES	YES
74	a	755.76	5.36350	YES	YES
75	a	766.98	15.12995	YES	YES
76	a	779.62	3.32145	YES	YES
77	a	788.34	0.06115	YES	YES
78	a	794.92	0.02911	YES	YES
79	a	798.26	6.26357	YES	YES
80	a	842.94	118.79200	YES	YES
81	a	848.73	79.88728	YES	YES
82	a	861.14	196.50412	YES	YES
83	a	927.57	0.31859	YES	YES
84	a	929.99	0.05869	YES	YES
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86	a	978.64	2.96049	YES	YES
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88	a	985.86	0.55000	YES	YES
89	a	989.81	0.99620	YES	YES
90	a	1020.63	313.83230	YES	YES
91	a	1042.95	336.03673	YES	YES
92	a	1045.07	342.98321	YES	YES
93	a	1064.71	5.41113	YES	YES
94	a	1124.09	3.76874	YES	YES
95	a	1200.85	11.02278	YES	YES
96	a	1214.78	10.23956	YES	YES
97	a	1231.20	27.17628	YES	YES
98	a	1234.36	35.52402	YES	YES
99	a	1244.10	25.13033	YES	YES
100	a	1381.29	2.10159	YES	YES
101	a	1389.57	0.02515	YES	YES
102	a	1400.76	2.17314	YES	YES
103	a	1401.01	3.00110	YES	YES
104	a	1403.27	3.06040	YES	YES
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106	a	1418.56	15.56026	YES	YES
107	a	2928.36	8.46544	YES	YES
108	a	2931.57	20.37780	YES	YES
109	a	2937.87	7.81481	YES	YES
110	a	2939.61	35.76184	YES	YES
111	a	2980.56	0.25046	YES	YES
112	a	3017.26	11.66326	YES	YES
113	a	3020.86	8.97859	YES	YES
114	a	3026.35	5.93285	YES	YES
115	a	3027.17	30.75731	YES	YES
116	a	3063.00	0.40340	YES	YES
117	a	3063.09	3.49823	YES	YES

TMS-F-Al(OC(CF₃)₃)₃



Total energy = -4127.8800966700 H = -112325.3964625 eV

HOMO-LUMO Separation

HOMO: 201. 201 a -0.27278682 H = -7.42291 eV

LUMO: 202. 202 a -0.04457452 H = -1.21294 eV

Gap : +0.22821230 H = +6.20998 eV

Number of MOs= 698, Electrons= 402.00, Symmetry: c1

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8.93623122684794	2.03014455248795	0.26761938160407	c
0.43368546365244	-0.07578011112304	0.01878671558926	al
0.64345198602344	-3.36337416970007	-0.27706049697769	o
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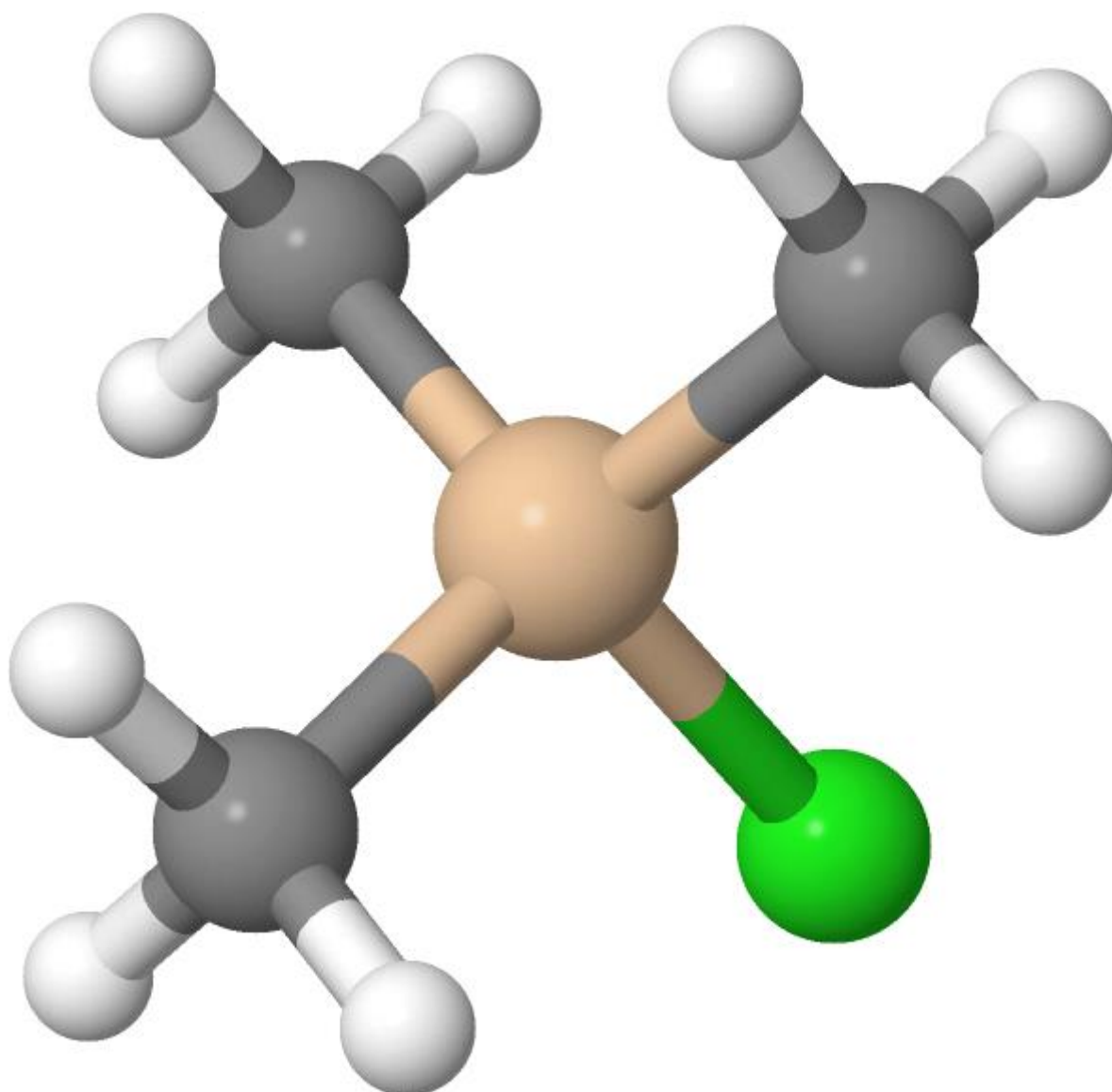
\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
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5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	12.62	0.24025	YES	YES
8		a	14.68	0.07260	YES	YES
9		a	15.45	0.03834	YES	YES
10		a	21.31	0.48230	YES	YES
11		a	25.97	0.26329	YES	YES
12		a	29.87	0.26490	YES	YES
13		a	32.90	0.31310	YES	YES
14		a	36.71	0.20968	YES	YES
15		a	37.08	0.34762	YES	YES
16		a	41.32	0.92825	YES	YES
17		a	45.85	0.21725	YES	YES
18		a	55.76	1.48577	YES	YES
19		a	64.00	0.60639	YES	YES
20		a	64.29	0.43303	YES	YES
21		a	69.58	0.23029	YES	YES
22		a	70.86	0.03676	YES	YES
23		a	73.07	0.52643	YES	YES
24		a	76.01	0.50868	YES	YES
25		a	78.56	0.34427	YES	YES
26		a	80.10	0.72458	YES	YES
27		a	82.40	0.04798	YES	YES
28		a	84.04	0.09243	YES	YES
29		a	88.17	1.05207	YES	YES
30		a	94.98	3.86500	YES	YES
31		a	104.78	0.41006	YES	YES
32		a	106.18	0.22928	YES	YES
33		a	118.64	6.10350	YES	YES
34		a	138.82	0.51453	YES	YES
35		a	153.03	0.29667	YES	YES
36		a	155.96	0.57589	YES	YES
37		a	157.39	1.23773	YES	YES
38		a	157.80	0.06079	YES	YES
39		a	160.19	0.44953	YES	YES
40		a	162.35	0.56168	YES	YES
41		a	164.99	0.36649	YES	YES
42		a	168.61	0.05378	YES	YES
43		a	181.62	6.15349	YES	YES
44		a	188.18	3.41282	YES	YES
45		a	198.34	3.52513	YES	YES
46		a	203.45	3.50205	YES	YES
47		a	213.24	0.53170	YES	YES
48		a	229.44	4.52327	YES	YES
49		a	252.04	5.81338	YES	YES
50		a	265.09	0.21748	YES	YES
51		a	268.74	3.75344	YES	YES
52		a	272.54	1.40889	YES	YES
53		a	277.20	6.41222	YES	YES
54		a	280.59	5.80182	YES	YES
55		a	282.60	8.37779	YES	YES
56		a	284.01	0.28109	YES	YES

57	a	284.63	0.14327	YES	YES
58	a	285.63	3.41513	YES	YES
59	a	290.21	0.96104	YES	YES
60	a	306.24	5.35255	YES	YES
61	a	306.54	7.90458	YES	YES
62	a	310.95	0.33161	YES	YES
63	a	315.76	0.23001	YES	YES
64	a	318.83	1.62206	YES	YES
65	a	319.18	1.36681	YES	YES
66	a	319.77	3.28184	YES	YES
67	a	324.47	0.05876	YES	YES
68	a	325.45	1.49909	YES	YES
69	a	345.03	0.08158	YES	YES
70	a	353.51	4.32153	YES	YES
71	a	355.82	2.13935	YES	YES
72	a	360.79	7.56826	YES	YES
73	a	366.84	19.05356	YES	YES
74	a	388.75	20.16933	YES	YES
75	a	428.37	72.74510	YES	YES
76	a	443.97	61.75438	YES	YES
77	a	456.92	42.40651	YES	YES
78	a	516.79	4.11153	YES	YES
79	a	519.08	0.87636	YES	YES
80	a	520.29	4.56292	YES	YES
81	a	520.88	4.42923	YES	YES
82	a	521.40	1.00320	YES	YES
83	a	521.98	9.28002	YES	YES
84	a	522.52	8.96008	YES	YES
85	a	524.64	0.32062	YES	YES
86	a	526.00	1.88204	YES	YES
87	a	529.11	0.69334	YES	YES
88	a	552.39	2.81086	YES	YES
89	a	554.64	3.21909	YES	YES
90	a	555.21	0.19231	YES	YES
91	a	555.66	0.66793	YES	YES
92	a	555.90	0.37173	YES	YES
93	a	556.59	1.26724	YES	YES
94	a	562.93	18.17516	YES	YES
95	a	568.33	24.26800	YES	YES
96	a	594.93	70.05654	YES	YES
97	a	632.14	175.38895	YES	YES
98	a	687.90	0.14139	YES	YES
99	a	690.62	0.87377	YES	YES
100	a	693.19	0.98596	YES	YES
101	a	706.96	15.64793	YES	YES
102	a	707.94	12.51327	YES	YES
103	a	708.78	39.41522	YES	YES
104	a	709.60	32.85471	YES	YES
105	a	711.02	42.47071	YES	YES
106	a	711.62	63.64120	YES	YES
107	a	728.44	1.64262	YES	YES
108	a	739.50	1.49034	YES	YES
109	a	741.00	0.76249	YES	YES
110	a	761.86	24.46990	YES	YES
111	a	766.00	19.77639	YES	YES
112	a	793.96	3.55007	YES	YES
113	a	856.13	109.12370	YES	YES
114	a	858.22	55.66747	YES	YES
115	a	870.15	56.86778	YES	YES
116	a	875.57	113.65405	YES	YES
117	a	878.86	81.14924	YES	YES
118	a	957.10	35.97126	YES	YES

119	a	957.93	26.14124	YES	YES
120	a	962.00	62.08419	YES	YES
121	a	963.26	221.10580	YES	YES
122	a	966.41	222.59513	YES	YES
123	a	967.99	275.84752	YES	YES
124	a	1103.64	5.33576	YES	YES
125	a	1104.43	4.77093	YES	YES
126	a	1108.88	6.03983	YES	YES
127	a	1152.11	2.03272	YES	YES
128	a	1157.65	10.69337	YES	YES
129	a	1159.90	28.90965	YES	YES
130	a	1162.97	13.27112	YES	YES
131	a	1168.08	4.82562	YES	YES
132	a	1172.79	7.91201	YES	YES
133	a	1178.77	8.47978	YES	YES
134	a	1189.18	13.74753	YES	YES
135	a	1193.33	20.88672	YES	YES
136	a	1198.58	7.24552	YES	YES
137	a	1201.71	69.06831	YES	YES
138	a	1203.45	109.24820	YES	YES
139	a	1207.99	90.67458	YES	YES
140	a	1211.08	60.23208	YES	YES
141	a	1222.44	38.28146	YES	YES
142	a	1236.26	310.65755	YES	YES
143	a	1240.17	1227.40633	YES	YES
144	a	1243.26	333.49926	YES	YES
145	a	1245.45	1075.07837	YES	YES
146	a	1249.03	268.63631	YES	YES
147	a	1254.27	147.22380	YES	YES
148	a	1256.04	839.99438	YES	YES
149	a	1259.01	100.45652	YES	YES
150	a	1260.36	14.41007	YES	YES
151	a	1263.63	805.63391	YES	YES
152	a	1266.17	608.18886	YES	YES
153	a	1270.52	32.68668	YES	YES
154	a	1318.08	63.42014	YES	YES
155	a	1334.30	194.52342	YES	YES
156	a	1343.57	85.94007	YES	YES
157	a	1384.49	0.37785	YES	YES
158	a	1395.86	1.45470	YES	YES
159	a	1398.46	0.22359	YES	YES
160	a	1400.00	4.53764	YES	YES
161	a	1402.16	3.37976	YES	YES
162	a	1417.40	31.22302	YES	YES
163	a	2951.11	0.11973	YES	YES
164	a	2952.75	0.41582	YES	YES
165	a	2955.33	4.09812	YES	YES
166	a	3042.61	0.11144	YES	YES
167	a	3043.36	0.11352	YES	YES
168	a	3044.44	0.84975	YES	YES
169	a	3054.87	0.14608	YES	YES
170	a	3061.50	0.45070	YES	YES
171	a	3069.37	2.03786	YES	YES

CITMS



Total energy = -869.2582785558 H = -23653.7347211 eV

HOMO-LUMO Separation

HOMO: 21. 8 e -0.25291432 H = -6.88215 eV

LUMO: 22. 13 a1 +0.01863263 H = +0.50702 eV

Gap : +0.27154694 H = +7.38917 eV

Number of MOs= 66, Electrons= 58.00, Symmetry: c3v

\$scoord

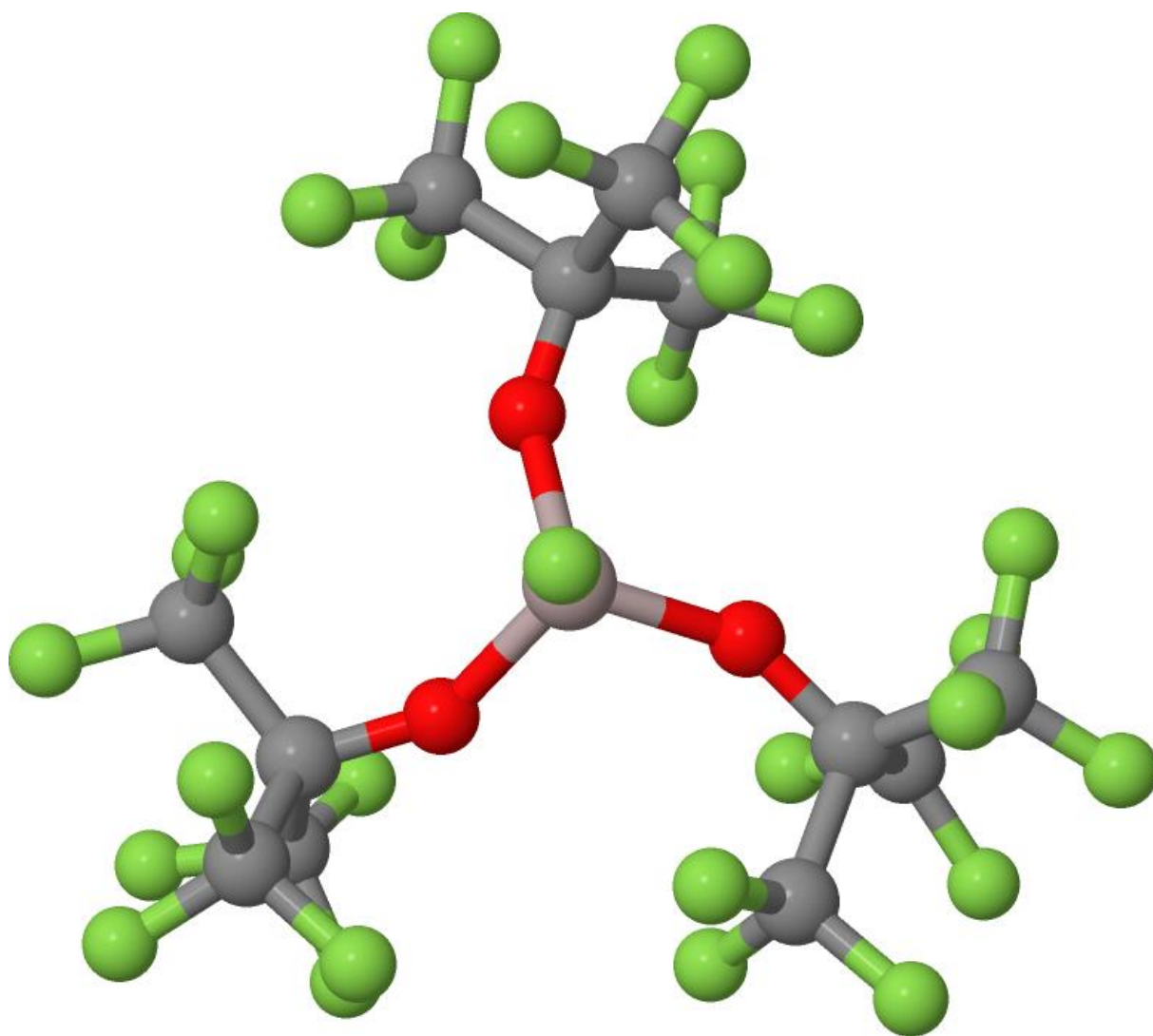
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\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a2		167.59	0.00000	NO	NO
8	e		169.75	0.56506	YES	YES
9	e		169.75	0.56506	YES	YES
10	e		181.86	0.03874	YES	YES
11	e		181.86	0.03874	YES	YES
12	a1		215.25	0.45808	YES	YES
13	e		225.98	4.85775	YES	YES
14	e		225.98	4.85775	YES	YES
15	a1		466.25	40.64007	YES	YES
16	a1		612.98	28.15153	YES	YES
17	e		677.71	6.20935	YES	YES
18	e		677.71	6.20935	YES	YES
19	a2		677.97	0.00000	NO	NO
20	e		756.41	22.38776	YES	YES
21	e		756.41	22.38776	YES	YES
22	e		852.84	96.11182	YES	YES
23	e		852.84	96.11182	YES	YES
24	a1		858.55	145.93862	YES	YES
25	e		1241.56	36.03086	YES	YES
26	e		1241.56	36.03086	YES	YES
27	a1		1250.43	7.07521	YES	YES
28	a2		1391.12	0.00000	NO	NO
29	e		1399.13	0.01460	YES	YES
30	e		1399.13	0.01460	YES	YES
31	e		1404.83	6.86986	YES	YES
32	e		1404.83	6.86986	YES	YES
33	a1		1416.12	11.72855	YES	YES
34	e		2941.81	3.32593	YES	YES
35	e		2941.81	3.32593	YES	YES
36	a1		2943.97	4.20141	YES	YES
37	e		3032.45	0.58492	YES	YES

38	e	3032.45	0.58492	YES	YES
39	a1	3034.48	15.25008	YES	YES
40	a2	3044.70	0.00000	NO	NO
41	e	3045.23	5.79433	YES	YES
42	e	3045.23	5.79433	YES	YES

FAI(OC(CF₃)₃)₃⁻



Total energy = -3718.8776135480 H = -101195.8662933 eV

HOMO-LUMO Separation

HOMO: 181. 181 a -0.14375246 H = -3.91171 eV

LUMO: 182. 182 a +0.11122499 H = +3.02659 eV

Gap : +0.25497745 H = +6.93829 eV

Number of MOs= 620, Electrons= 362.00, Symmetry: c1

\$coord

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0.14249518817913	-0.05409654866787	1.47404131492463	al
-1.86459567828278	2.44794876139331	0.48911515676764	o
3.12418125935236	0.51581452741118	0.04837066468845	o
-1.07309445457296	-2.82520701509676	0.02131566047243	o
-2.34073875764628	4.94849024599138	0.56099879429810	c
5.39627664445371	-0.45532240011258	-0.56162198284903	c
-3.03195393769768	-4.44682747609399	-0.12763471278766	c
-3.97291095421675	5.61850762263540	2.97129017606763	c
-3.88974163367911	5.65971663074597	-1.88923456202461	c
0.17084121496695	6.55648992790797	0.61658707748265	c
7.16251820349435	1.81084599565098	-1.36192481600398	c
6.63342740296138	-1.88369139241509	1.74483832673080	c
5.15499121314534	-2.35345401450855	-2.85811944589698	c
-2.37661425057502	-6.93235880789035	1.39317883371945	c
-3.46970676167315	-5.14384040866304	-2.99591292951873	c
-5.55074288369706	-3.27596843344866	0.96030925314957	c
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-0.24778156503186	9.00894640670963	1.23891704679849	f
1.32232025479234	6.52928641378149	-1.65676521543654	f
1.79110211012780	5.59569285457400	2.31943643305465	f
6.94674023946382	3.73360094755229	0.27673476807043	f
9.63808908860875	1.14633325961217	-1.45896408477229	f
6.51435861751769	2.68598986952345	-3.67102591885757	f
7.44130577417370	-0.23171562648259	3.51381029789693	f
8.64654008321948	-3.31344337100415	1.05583053273564	f
4.93535851937853	-3.41981509147561	2.84528109266494	f
4.30087860310935	-4.62475103250125	-2.08344411720924	f
3.52206359657519	-1.45226008611606	-4.57476782120569	f
7.40034549699601	-2.74570511254882	-4.04267419890899	f
-2.61910102480174	-6.54477033834395	3.90605293248824	f
-3.89267836135420	-8.90578868076719	0.77033482926628	f
0.01961547380686	-7.63154910785209	0.95374339900669	f
-1.65196067458402	-6.72604132850220	-3.83996267611924	f
-3.40595037349531	-3.06245750447239	-4.43747641836353	f
-5.72758247955043	-6.30086204452937	-3.38504664439456	f
-7.33557614161197	-5.05265037175027	1.43438738393507	f
-6.55794258020827	-1.59784545218498	-0.67059916480375	f
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\$vibrational spectrum

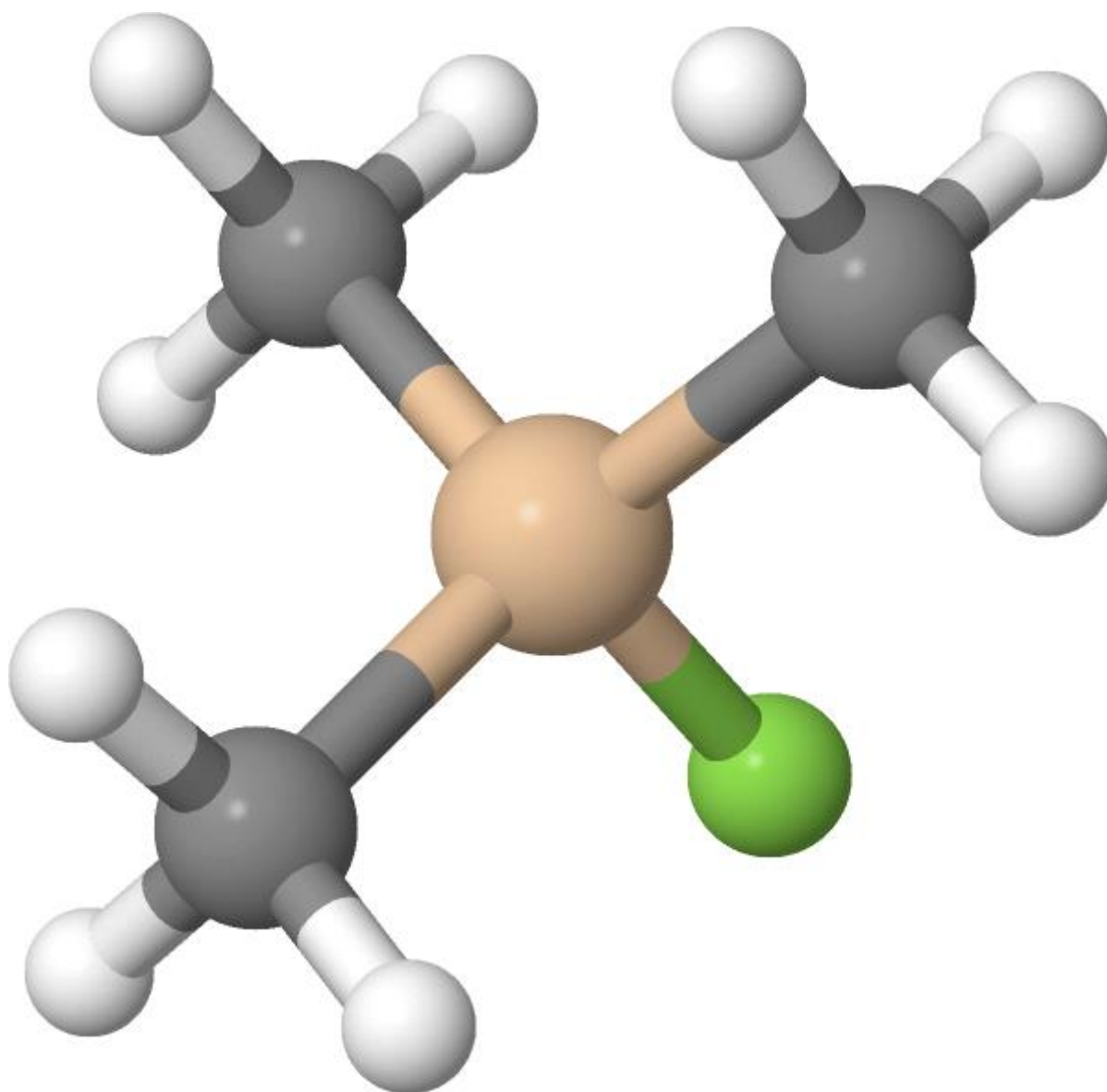
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2			0.00	0.00000	- -
3			0.00	0.00000	- -

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
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8	a	13.68	0.05381	YES	YES
9	a	14.66	0.01989	YES	YES
10	a	20.26	0.08596	YES	YES
11	a	20.65	0.25473	YES	YES
12	a	23.35	0.04668	YES	YES
13	a	38.16	0.03944	YES	YES
14	a	41.65	0.05069	YES	YES
15	a	50.19	0.01088	YES	YES
16	a	64.26	0.09805	YES	YES
17	a	66.62	0.10106	YES	YES
18	a	67.23	0.05905	YES	YES
19	a	69.28	0.12251	YES	YES
20	a	71.53	0.18751	YES	YES
21	a	76.33	0.02693	YES	YES
22	a	79.22	0.03553	YES	YES
23	a	80.32	0.02406	YES	YES
24	a	81.21	0.06444	YES	YES
25	a	86.16	0.30506	YES	YES
26	a	88.55	0.29950	YES	YES
27	a	95.96	0.20234	YES	YES
28	a	136.52	1.87105	YES	YES
29	a	139.13	0.83635	YES	YES
30	a	149.62	0.18893	YES	YES
31	a	157.96	0.19724	YES	YES
32	a	159.05	0.38562	YES	YES
33	a	159.61	0.06422	YES	YES
34	a	167.35	1.11665	YES	YES
35	a	169.57	1.29508	YES	YES
36	a	192.57	0.42704	YES	YES
37	a	195.26	7.67277	YES	YES
38	a	196.11	6.96653	YES	YES
39	a	227.77	0.30616	YES	YES
40	a	268.70	1.81978	YES	YES
41	a	269.90	0.97191	YES	YES
42	a	272.86	3.41237	YES	YES
43	a	277.80	4.03156	YES	YES
44	a	278.64	2.65491	YES	YES
45	a	283.08	0.14257	YES	YES
46	a	283.18	0.12308	YES	YES
47	a	283.23	0.04690	YES	YES
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51	a	307.62	0.12510	YES	YES
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53	a	316.04	0.47893	YES	YES
54	a	317.79	0.62096	YES	YES
55	a	319.97	3.34089	YES	YES
56	a	320.87	3.44461	YES	YES
57	a	325.97	0.38381	YES	YES
58	a	350.08	1.51337	YES	YES
59	a	350.94	1.73666	YES	YES
60	a	357.50	3.96417	YES	YES
61	a	358.51	27.53161	YES	YES
62	a	360.62	27.87293	YES	YES
63	a	403.17	8.00795	YES	YES
64	a	438.90	88.28145	YES	YES
65	a	440.55	81.69046	YES	YES

66	a	514.91	0.56556	YES	YES
67	a	518.01	4.26075	YES	YES
68	a	518.16	3.13927	YES	YES
69	a	518.64	5.04067	YES	YES
70	a	519.93	1.10655	YES	YES
71	a	520.03	12.30277	YES	YES
72	a	520.21	4.51585	YES	YES
73	a	523.41	2.28774	YES	YES
74	a	523.87	3.22276	YES	YES
75	a	527.51	0.18392	YES	YES
76	a	545.78	31.36959	YES	YES
77	a	546.53	35.23349	YES	YES
78	a	553.14	0.92782	YES	YES
79	a	553.52	2.36891	YES	YES
80	a	553.97	1.71295	YES	YES
81	a	554.55	0.54900	YES	YES
82	a	555.00	7.39276	YES	YES
83	a	555.87	10.23631	YES	YES
84	a	705.84	0.03737	YES	YES
85	a	706.72	16.44491	YES	YES
86	a	707.36	6.83986	YES	YES
87	a	707.67	59.48800	YES	YES
88	a	707.85	51.89921	YES	YES
89	a	708.85	74.15914	YES	YES
90	a	716.72	0.33398	YES	YES
91	a	734.26	6.24667	YES	YES
92	a	734.56	5.90964	YES	YES
93	a	759.56	7.71743	YES	YES
94	a	808.24	31.65465	YES	YES
95	a	809.62	34.11769	YES	YES
96	a	843.37	54.08006	YES	YES
97	a	954.26	26.08440	YES	YES
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99	a	955.93	50.42854	YES	YES
100	a	960.29	174.48568	YES	YES
101	a	960.76	342.02541	YES	YES
102	a	961.91	203.40871	YES	YES
103	a	1111.63	4.85880	YES	YES
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105	a	1115.47	1.90235	YES	YES
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107	a	1130.72	12.74535	YES	YES
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111	a	1136.36	9.08792	YES	YES
112	a	1194.00	14.21742	YES	YES
113	a	1197.67	51.67712	YES	YES
114	a	1199.73	15.27127	YES	YES
115	a	1202.17	54.46917	YES	YES
116	a	1205.41	27.09850	YES	YES
117	a	1208.52	61.45659	YES	YES
118	a	1214.45	939.71507	YES	YES
119	a	1214.92	993.78969	YES	YES
120	a	1230.74	568.24944	YES	YES
121	a	1231.58	450.28097	YES	YES
122	a	1236.25	13.30706	YES	YES
123	a	1237.89	98.61985	YES	YES
124	a	1243.32	14.50596	YES	YES
125	a	1246.65	10.53791	YES	YES
126	a	1248.81	64.02413	YES	YES
127	a	1253.51	553.59788	YES	YES

128	a	1255.14	810.43711	YES	YES
129	a	1261.68	1011.16601	YES	YES
130	a	1334.95	293.63674	YES	YES
131	a	1337.24	307.78202	YES	YES
132	a	1356.42	19.73884	YES	YES

FTMS



Total energy = -508.9275711884 H = -13848.6317106 eV

HOMO-LUMO Separation

HOMO: 18. 7 e -0.26548305 H = -7.22417 eV

LUMO: 19. 11 a1 +0.02663142 H = +0.72468 eV

Gap : +0.29211447 H = +7.94884 eV

Number of MOs= 63, Electrons= 50.00, Symmetry: c3v

\$coord

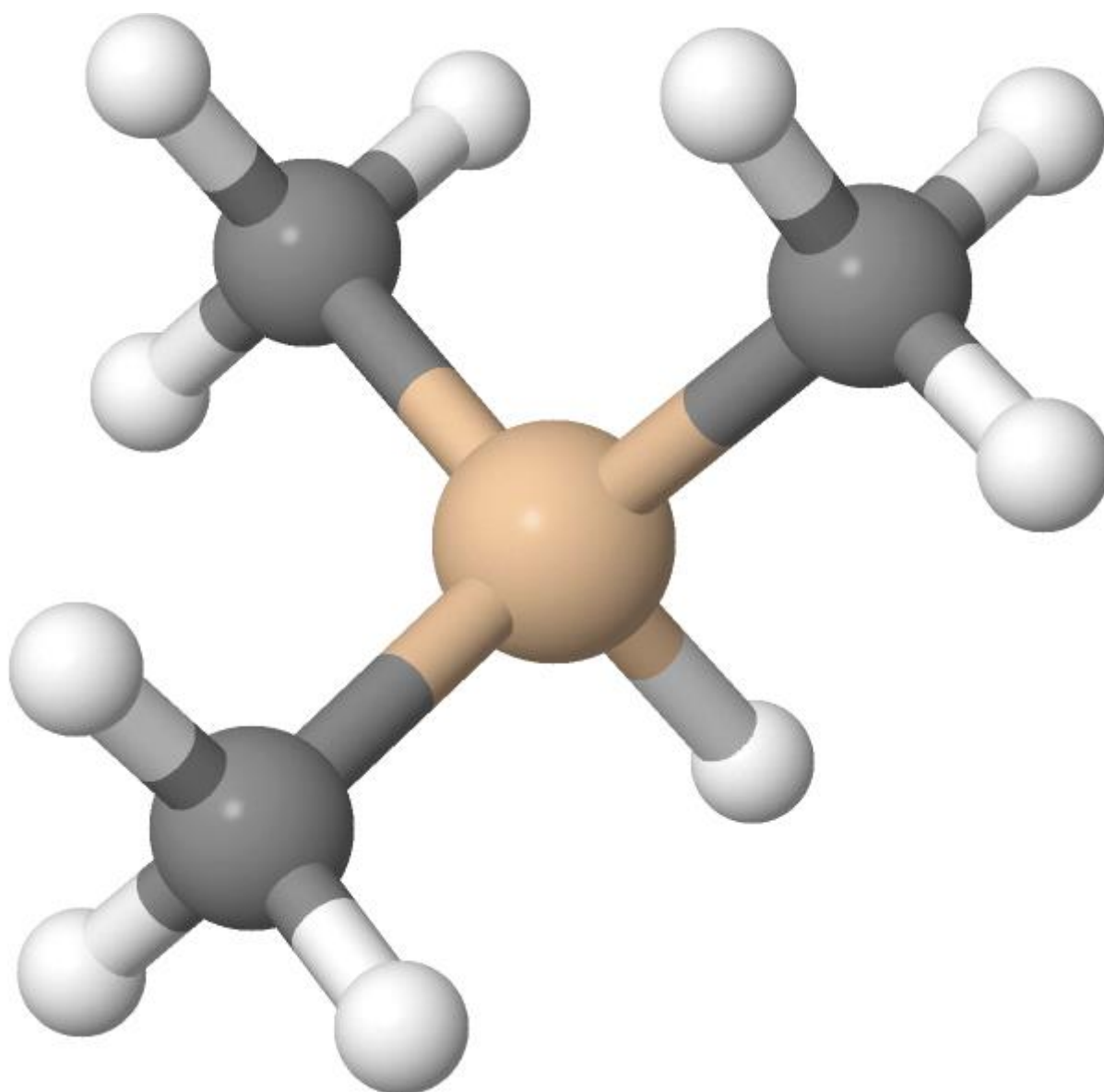
0.0000000000000000	0.0000000000000000	0.80170237140333	si
-1.70407079611717	-2.95153719856927	-0.23906941923149	c
-1.70407079611717	2.95153719856927	-0.23906941923149	c
3.40814159223432	0.0000000000000000	-0.23906941923149	c
0.0000000000000000	0.0000000000000000	3.93047173780635	f
-0.73842105846497	-4.67607142834268	0.47943585164706	h
-1.78138127455104	-3.08544287517417	-2.33745402199301	h
-3.68038611762287	-2.97752710949138	0.47943585164706	h
-0.73842105846497	4.67607142834268	0.47943585164706	h
-3.68038611762287	2.97752710949138	0.47943585164706	h
-1.78138127455104	3.08544287517417	-2.33745402199301	h
4.41880717608783	1.69854431885129	0.47943585164706	h
3.56276254910205	0.0000000000000000	-2.33745402199301	h
4.41880717608783	-1.69854431885129	0.47943585164706	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a2		149.85	0.00000	NO	NO
8	e		166.53	0.00055	YES	YES
9	e		166.53	0.00055	YES	YES
10	e		187.10	0.03229	YES	YES
11	e		187.10	0.03229	YES	YES
12	a1		227.98	0.11541	YES	YES
13	e		269.12	11.96812	YES	YES
14	e		269.12	11.96812	YES	YES
15	a1		585.17	0.01850	YES	YES
16	a2		667.52	0.00000	NO	NO
17	e		676.00	3.90793	YES	YES
18	e		676.00	3.90793	YES	YES
19	e		754.37	29.70240	YES	YES
20	e		754.37	29.70240	YES	YES
21	a1		770.96	4.25989	YES	YES
22	e		852.18	136.51484	YES	YES
23	e		852.18	136.51484	YES	YES
24	a1		909.00	166.80255	YES	YES
25	e		1246.64	46.39760	YES	YES

26	e	1246.64	46.39760	YES	YES
27	a1	1253.80	15.04985	YES	YES
28	a2	1391.91	0.00000	NO	NO
29	e	1399.66	0.03409	YES	YES
30	e	1399.66	0.03409	YES	YES
31	e	1405.49	4.81520	YES	YES
32	e	1405.49	4.81520	YES	YES
33	a1	1416.74	16.47970	YES	YES
34	e	2941.58	3.57362	YES	YES
35	e	2941.58	3.57362	YES	YES
36	a1	2943.79	1.09387	YES	YES
37	e	3032.50	0.46593	YES	YES
38	e	3032.50	0.46593	YES	YES
39	a1	3034.93	16.83549	YES	YES
40	a2	3037.19	0.00000	NO	NO
41	e	3037.88	8.86774	YES	YES
42	e	3037.88	8.86774	YES	YES

HTMS



Total energy = -409.6891298663 H = -11148.2147884 eV

HOMO-LUMO Separation

HOMO: 15. 6 e -0.26679090 H = -7.25975 eV

LUMO: 16. 9 a1 +0.03241712 H = +0.88212 eV

Gap : +0.29920802 H = +8.14187 eV

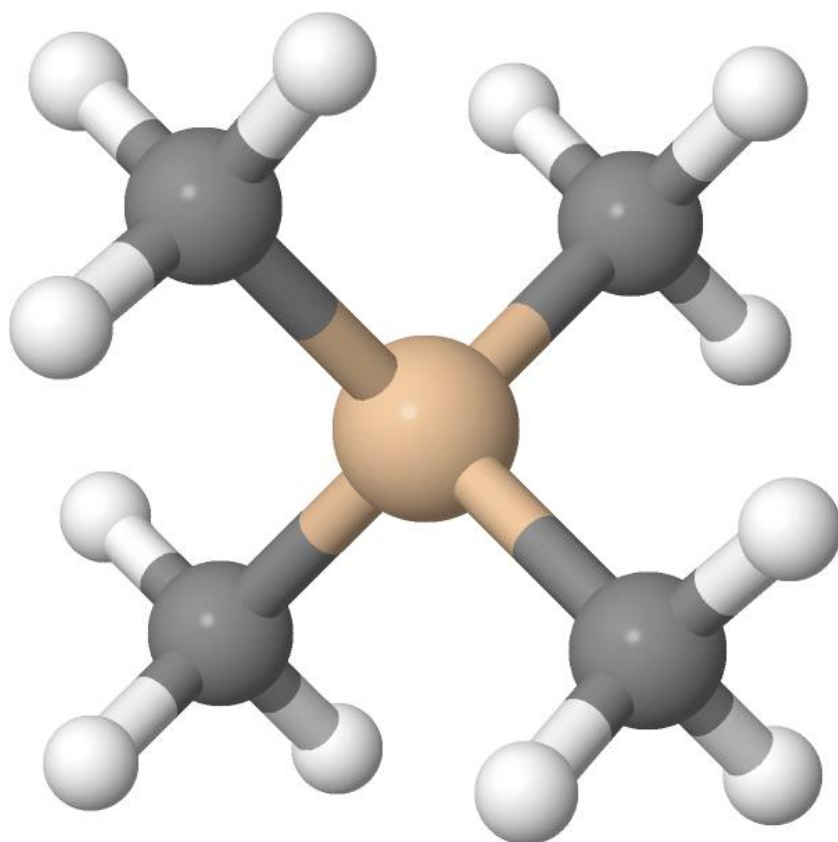
Number of MOs= 55, Electrons= 42.00, Symmetry: c3v

```
$coord
  0.0000000000000000  0.0000000000000000  0.91349788552103  si
-1.70389413050220    2.95123120474819    -0.21945234505776  c
-1.70389413050220   -2.95123120474819    -0.21945234505776  c
  3.40778826100438    0.0000000000000000   -0.21945234505776  c
  0.0000000000000000  0.0000000000000000   3.77587450047056  h
-0.74878831958580    4.69286519733812    0.47249253277433  h
-3.68974631763778    2.99490230548743    0.47249253277433  h
-1.75489133275006    3.03956095008537   -2.32117774767042  h
-0.74878831958580   -4.69286519733812    0.47249253277433  h
-1.75489133275006   -3.03956095008537   -2.32117774767042  h
-3.68974631763778   -2.99490230548743    0.47249253277433  h
  4.43853463722359   -1.69796289185070    0.47249253277433  h
  4.43853463722359    1.69796289185070    0.47249253277433  h
  3.50978266550014    0.0000000000000000   -2.32117774767042  h
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#          #          cm** (-1)      km/mol          IR          RAMAN
  1          0.00          0.00000          -          -
  2          0.00          0.00000          -          -
  3          0.00          0.00000          -          -
  4          0.00          0.00000          -          -
  5          0.00          0.00000          -          -
  6          0.00          0.00000          -          -
  7          a2          165.26          0.00000          NO          NO
  8          e          175.75          0.00201          YES          YES
  9          e          175.75          0.00201          YES          YES
 10          e          198.36          0.59466          YES          YES
 11          e          198.36          0.59466          YES          YES
 12          a1          232.64          0.93581          YES          YES
 13          a1          594.45          1.51266          YES          YES
 14          e          605.14          7.10460          YES          YES
 15          e          605.14          7.10460          YES          YES
 16          a2          670.21          0.00000          NO          NO
 17          e          685.16          12.17947          YES          YES
 18          e          685.16          12.17947          YES          YES
```

19	e	835.10	16.79420	YES	YES
20	e	835.10	16.79420	YES	YES
21	a1	857.85	69.13100	YES	YES
22	e	889.59	161.56294	YES	YES
23	e	889.59	161.56294	YES	YES
24	e	1238.71	30.57305	YES	YES
25	e	1238.71	30.57305	YES	YES
26	a1	1248.84	5.63688	YES	YES
27	a2	1397.02	0.00000	NO	NO
28	e	1401.66	0.31651	YES	YES
29	e	1401.66	0.31651	YES	YES
30	e	1410.54	5.00856	YES	YES
31	e	1410.54	5.00856	YES	YES
32	a1	1417.52	14.17313	YES	YES
33	a1	2137.51	161.56304	YES	YES
34	e	2938.50	8.45536	YES	YES
35	e	2938.50	8.45536	YES	YES
36	a1	2939.51	2.46195	YES	YES
37	e	3029.10	0.48297	YES	YES
38	e	3029.10	0.48297	YES	YES
39	a1	3030.55	22.13846	YES	YES
40	a2	3032.88	0.00000	NO	NO
41	e	3033.33	12.42138	YES	YES
42	e	3033.33	12.42138	YES	YES

SiMe₄



Total energy = -448.9813133214 H = -12217.4101093 eV

HOMO-LUMO Separation

HOMO: 12. 5 t2 -0.25792252 H = -7.01843 eV

LUMO: 13. 6 a1 +0.02724223 H = +0.74130 eV

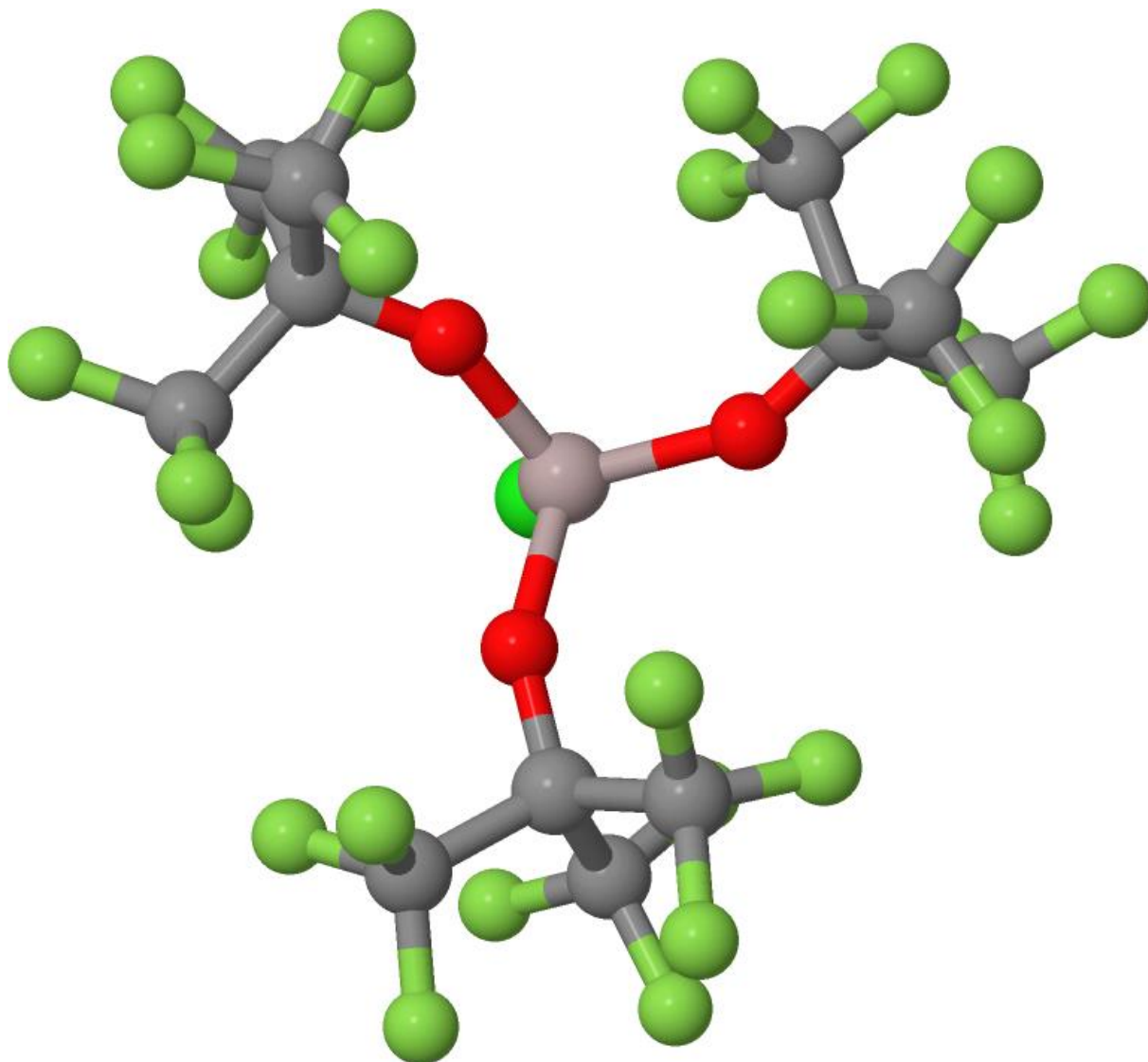
Gap : +0.28516475 H = +7.75973 eV

Number of MOs= 43, Electrons= 50.00, Symmetry: td

```
$coord
  0.000000000000000  0.000000000000000  0.000000000000000  si
  2.07667375478765 -2.07667375478765  2.07667375478765  c
 -2.07667375478765  2.07667375478765  2.07667375478765  c
  2.07667375478765  2.07667375478765 -2.07667375478765  c
 -2.07667375478765 -2.07667375478765 -2.07667375478765  c
  3.31775967033017 -3.31775967033017  0.91622601920978  h
  0.91622601920978 -3.31775967033017  3.31775967033017  h
  3.31775967033017 -0.91622601920978  3.31775967033017  h
 -3.31775967033017  3.31775967033017  0.91622601920978  h
 -0.91622601920978  3.31775967033017  3.31775967033017  h
 -3.31775967033017  0.91622601920978  3.31775967033017  h
  0.91622601920978  3.31775967033017 -3.31775967033017  h
  3.31775967033017  0.91622601920978 -3.31775967033017  h
  3.31775967033017  3.31775967033017 -0.91622601920978  h
 -3.31775967033017 -0.91622601920978 -3.31775967033017  h
 -3.31775967033017 -3.31775967033017 -0.91622601920978  h
 -0.91622601920978 -3.31775967033017 -3.31775967033017  h
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#          #          cm** (-1)      km/mol          IR          RAMAN
  1          0.00          0.00000          -          -
  2          0.00          0.00000          -          -
  3          0.00          0.00000          -          -
  4          0.00          0.00000          -          -
  5          0.00          0.00000          -          -
  6          0.00          0.00000          -          -
  7          a2          163.78          0.00000          NO          NO
  8          t1          179.09          0.00000          NO          NO
  9          t1          179.09          0.00000          NO          NO
 10          t1          179.09          0.00000          NO          NO
 11          e          180.46          0.00000          NO          YES
 12          e          180.46          0.00000          NO          YES
 13          t2          224.92          2.15460          YES          YES
 14          t2          224.92          2.15460          YES          YES
 15          t2          224.92          2.15460          YES          YES
```

16	a1	562.22	0.00000	NO	YES
17	t1	669.66	0.00000	NO	NO
18	t1	669.66	0.00000	NO	NO
19	t1	669.66	0.00000	NO	NO
20	t2	672.44	12.08215	YES	YES
21	t2	672.44	12.08215	YES	YES
22	t2	672.44	12.08215	YES	YES
23	e	812.31	0.00000	NO	YES
24	e	812.31	0.00000	NO	YES
25	t2	864.33	132.35779	YES	YES
26	t2	864.33	132.35779	YES	YES
27	t2	864.33	132.35779	YES	YES
28	t2	1237.34	31.53159	YES	YES
29	t2	1237.34	31.53159	YES	YES
30	t2	1237.34	31.53159	YES	YES
31	a1	1250.59	0.00000	NO	YES
32	t1	1399.17	0.00000	NO	NO
33	t1	1399.17	0.00000	NO	NO
34	t1	1399.17	0.00000	NO	NO
35	e	1404.15	0.00000	NO	YES
36	e	1404.15	0.00000	NO	YES
37	t2	1417.64	9.47506	YES	YES
38	t2	1417.64	9.47506	YES	YES
39	t2	1417.64	9.47506	YES	YES
40	t2	2934.96	10.65240	YES	YES
41	t2	2934.96	10.65240	YES	YES
42	t2	2934.96	10.65240	YES	YES
43	a1	2937.33	0.00000	NO	YES
44	e	3025.93	0.00000	NO	YES
45	e	3025.93	0.00000	NO	YES
46	t1	3026.72	0.00000	NO	NO
47	t1	3026.72	0.00000	NO	NO
48	t1	3026.72	0.00000	NO	NO
49	t2	3028.30	26.91845	YES	YES
50	t2	3028.30	26.91845	YES	YES
51	t2	3028.30	26.91845	YES	YES



Total energy = -4079.2112791130 H = -111001.0498005 eV

HOMO-LUMO Separation

HOMO: 185. 185 a -0.13511297 H = -3.67661 eV

LUMO: 186. 186 a +0.10784539 H = +2.93462 eV

Gap : +0.24295836 H = +6.61124 eV

Number of MOs= 624, Electrons= 370.00, Symmetry: c1

\$coord

0.60411238049247	-0.21494114592801	5.75630591001399	cl
0.22668980200892	-0.09319022570564	1.71089827677981	al
-1.81531032871220	2.35078415370744	0.66530648180540	o
3.17542193974833	0.41208118118945	0.20884499029095	o
-1.03117486142098	-2.93279228600977	0.46004501994507	o
-2.33721487321745	4.84308229700501	0.56040863190383	c
5.43758692952068	-0.45891784875892	-0.56813982153078	c
-3.05605632813735	-4.40801115769188	0.00047056528468	c
-4.03088424283241	5.63447346565454	2.88932683072636	c
-3.84485008943101	5.36289823311660	-1.96309997979985	c
0.14396457446037	6.49829020310995	0.55710391322435	c
7.07668577365075	1.88883408528616	-1.41027569235805	c
6.86381544030520	-1.90449167090316	1.61811850391696	c
5.11847116925414	-2.30220446353169	-2.89767579843285	c
-2.64617690834377	-7.04183067391757	1.34626072484094	c
-3.29736489749847	-4.83315240531560	-2.94538082466453	c
-5.60556140748740	-3.21030945331386	0.99879200437594	c
-2.63078662285268	5.81467926599760	5.01302163070642	f
-5.18706792672540	7.89876300491794	2.53710086510560	f
-5.83397616421995	3.90130016930154	3.29948295618968	f
-6.24624744062295	4.51693679886883	-1.78062907918023	f
-2.75231776992286	4.16508998644829	-3.90971375143280	f
-3.95647627652052	7.85993042991458	-2.54063106586365	f
-0.32620328688995	8.97083100577933	1.04188225259374	f
1.32248448772328	6.37017683339865	-1.69950559318698	f
1.76084876344782	5.65850485108439	2.32523614592416	f
6.88593613927456	3.76299921748823	0.28572144022717	f
9.56375859137177	1.31372176306031	-1.66284900114482	f
6.27021956624725	2.79235098278894	-3.65597016191571	f
7.73949727424382	-0.26776525071109	3.36727932419499	f
8.86845879319895	-3.25565808145934	0.76202424548056	f
5.28946377788023	-3.51729066373952	2.78626557580368	f
4.33275585280120	-4.60325340169774	-2.13719444011289	f
3.39450656839844	-1.38949211241453	-4.51755112702376	f
7.31201707024856	-2.62857728002033	-4.19143145271021	f
-3.05853822851312	-6.84121431303476	3.85816622742164	f
-4.21545828368499	-8.86139425233870	0.44885428701642	f
-0.26462250619551	-7.84863031008092	1.02457948299868	f
-1.50937693064560	-6.45083123576487	-3.78446816356648	f
-2.99330691124294	-2.64263741410972	-4.18157382950825	f
-5.57642955493498	-5.80628375737757	-3.61140308744708	f
-7.46054862825319	-4.95879925320064	1.27249301595488	f
-6.47549673375176	-1.42484618815913	-0.59688996366084	f
-5.23524958194544	-2.11921686238497	3.26039542053986	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
	1		0.00	0.00000	-	-
	2		0.00	0.00000	-	-
	3		0.00	0.00000	-	-
	4		0.00	0.00000	-	-
	5		0.00	0.00000	-	-
	6		0.00	0.00000	-	-
	7	a	12.14	0.02452	YES	YES

8	a	12.97	0.06737	YES	YES
9	a	15.42	0.02039	YES	YES
10	a	18.84	0.09030	YES	YES
11	a	22.66	0.17533	YES	YES
12	a	24.13	0.08486	YES	YES
13	a	34.01	0.06976	YES	YES
14	a	40.00	0.03619	YES	YES
15	a	49.29	0.03102	YES	YES
16	a	62.56	0.14897	YES	YES
17	a	64.35	0.03386	YES	YES
18	a	67.13	0.01638	YES	YES
19	a	68.09	0.18365	YES	YES
20	a	71.13	0.13613	YES	YES
21	a	73.26	0.01239	YES	YES
22	a	76.12	0.11236	YES	YES
23	a	78.53	0.03337	YES	YES
24	a	80.48	0.07602	YES	YES
25	a	84.73	0.27506	YES	YES
26	a	87.83	0.03518	YES	YES
27	a	96.07	0.42406	YES	YES
28	a	100.42	1.71117	YES	YES
29	a	102.67	2.19412	YES	YES
30	a	145.84	0.24903	YES	YES
31	a	157.99	0.13441	YES	YES
32	a	158.56	0.46610	YES	YES
33	a	158.77	0.73047	YES	YES
34	a	160.28	0.17843	YES	YES
35	a	162.11	1.03166	YES	YES
36	a	181.66	0.39192	YES	YES
37	a	189.87	4.91979	YES	YES
38	a	191.06	4.50989	YES	YES
39	a	223.01	0.30814	YES	YES
40	a	265.36	1.35123	YES	YES
41	a	267.95	1.27397	YES	YES
42	a	272.19	5.28124	YES	YES
43	a	274.76	3.00362	YES	YES
44	a	274.94	2.95546	YES	YES
45	a	282.22	1.66618	YES	YES
46	a	282.76	1.22978	YES	YES
47	a	283.68	0.19427	YES	YES
48	a	283.86	0.20517	YES	YES
49	a	301.59	10.75891	YES	YES
50	a	302.54	10.26450	YES	YES
51	a	307.48	0.48467	YES	YES
52	a	314.28	0.48783	YES	YES
53	a	315.32	0.62631	YES	YES
54	a	317.85	0.94078	YES	YES
55	a	318.46	1.60857	YES	YES
56	a	319.46	2.44338	YES	YES
57	a	323.48	0.08331	YES	YES
58	a	346.72	2.53403	YES	YES
59	a	348.70	8.13468	YES	YES
60	a	350.25	13.48835	YES	YES
61	a	350.82	6.25018	YES	YES
62	a	357.92	4.98735	YES	YES
63	a	376.31	0.98940	YES	YES
64	a	430.76	75.02432	YES	YES
65	a	434.82	72.31732	YES	YES
66	a	490.44	41.20377	YES	YES
67	a	517.46	3.35830	YES	YES
68	a	517.69	3.69445	YES	YES
69	a	518.02	4.30920	YES	YES

70	a	519.52	7.26801	YES	YES
71	a	520.04	1.84416	YES	YES
72	a	520.46	8.32914	YES	YES
73	a	523.06	2.14189	YES	YES
74	a	523.63	3.73252	YES	YES
75	a	524.37	2.98829	YES	YES
76	a	543.14	26.67855	YES	YES
77	a	544.11	28.29919	YES	YES
78	a	546.98	56.32710	YES	YES
79	a	552.89	0.85445	YES	YES
80	a	553.14	1.37221	YES	YES
81	a	553.50	1.10492	YES	YES
82	a	554.19	2.42985	YES	YES
83	a	554.48	3.58555	YES	YES
84	a	555.47	11.34836	YES	YES
85	a	706.08	4.95420	YES	YES
86	a	706.48	6.50106	YES	YES
87	a	706.95	17.19038	YES	YES
88	a	707.82	68.58714	YES	YES
89	a	708.45	50.03689	YES	YES
90	a	708.96	56.59546	YES	YES
91	a	728.78	6.31563	YES	YES
92	a	734.42	4.15253	YES	YES
93	a	734.57	4.74694	YES	YES
94	a	785.25	9.82000	YES	YES
95	a	810.21	24.17069	YES	YES
96	a	812.22	24.91894	YES	YES
97	a	953.46	18.18212	YES	YES
98	a	954.21	17.22147	YES	YES
99	a	955.28	57.69105	YES	YES
100	a	959.08	265.75324	YES	YES
101	a	960.04	221.00348	YES	YES
102	a	961.34	198.39565	YES	YES
103	a	1111.39	7.95299	YES	YES
104	a	1113.15	9.05770	YES	YES
105	a	1116.52	1.79052	YES	YES
106	a	1127.47	3.56977	YES	YES
107	a	1129.33	5.45031	YES	YES
108	a	1130.42	3.90568	YES	YES
109	a	1133.90	17.49664	YES	YES
110	a	1134.45	15.72367	YES	YES
111	a	1134.75	7.05374	YES	YES
112	a	1194.99	7.84682	YES	YES
113	a	1198.12	56.68358	YES	YES
114	a	1199.91	21.63861	YES	YES
115	a	1201.73	19.76530	YES	YES
116	a	1204.30	24.25450	YES	YES
117	a	1207.97	28.65211	YES	YES
118	a	1213.40	992.19163	YES	YES
119	a	1214.10	947.41308	YES	YES
120	a	1230.50	562.55252	YES	YES
121	a	1231.36	472.14020	YES	YES
122	a	1235.18	33.55649	YES	YES
123	a	1238.18	131.20731	YES	YES
124	a	1242.26	45.62421	YES	YES
125	a	1245.84	20.86766	YES	YES
126	a	1247.41	82.31426	YES	YES
127	a	1253.96	571.82446	YES	YES
128	a	1254.93	687.54267	YES	YES
129	a	1260.83	1060.46921	YES	YES
130	a	1336.04	300.46247	YES	YES
131	a	1339.22	319.63191	YES	YES

132

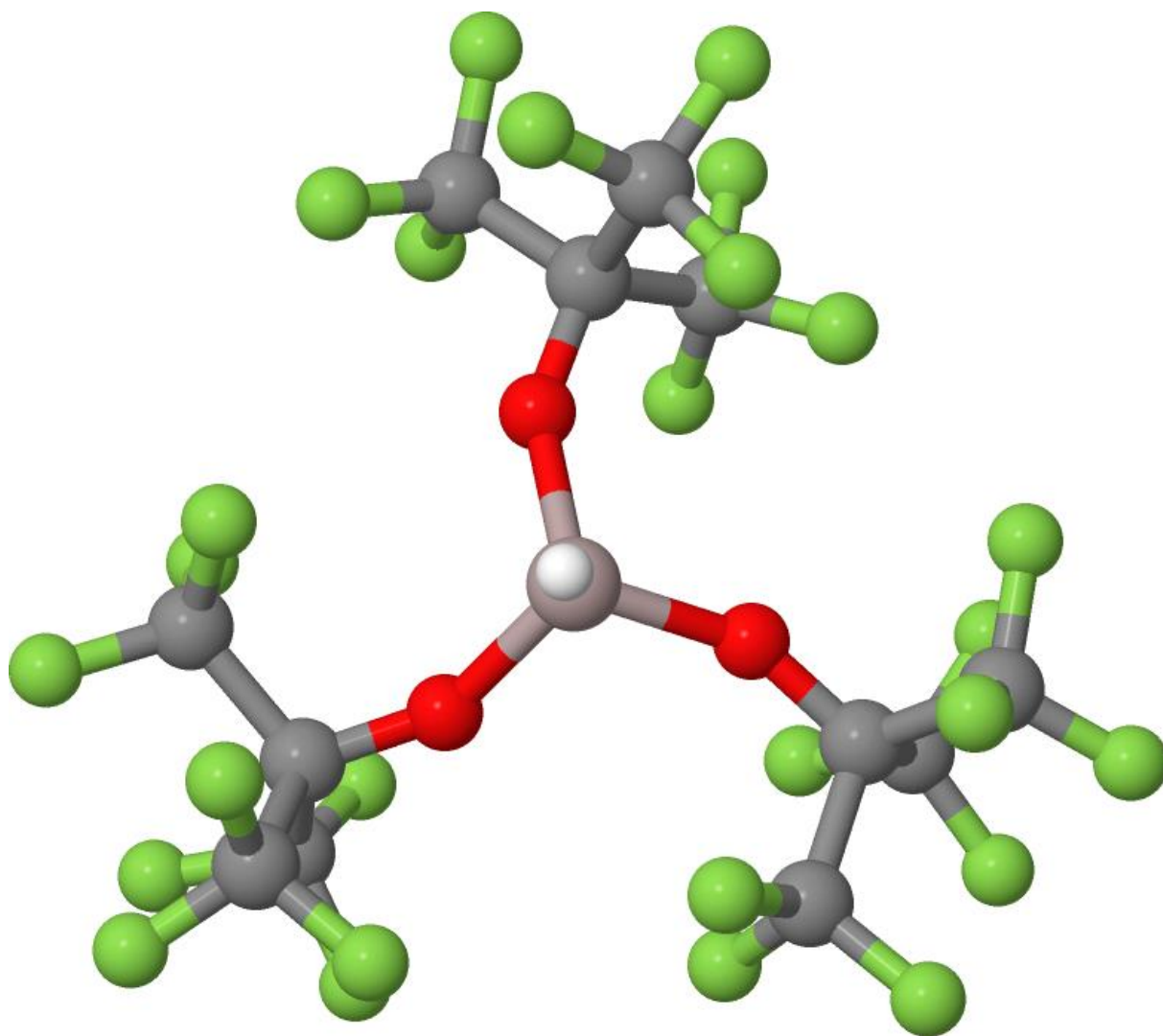
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1357.26

66.93543

YES

YES

HAl(OC(CF₃)₃)₃⁻

Total energy = -3619.6183801390 H = -98494.8835893 eV

HOMO-LUMO Separation

HOMO: 177. 177 a -0.12359009 H = -3.36306 eV

LUMO: 178. 178 a +0.11814901 H = +3.21500 eV

Gap : +0.24173910 H = +6.57806 eV

Number of MOs= 608, Electrons= 354.00, Symmetry: c1

\$coord

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-1.78409804408132	2.55890190131698	0.44626426741426	o
3.16247311031582	0.50261998728824	0.13310155495364	o
-1.08967247213987	-2.73654178560693	0.07194787365775	o
-2.35200523824774	5.03480092717226	0.57551185428094	c
5.38254880114635	-0.53350830840816	-0.54934545258973	c
-2.98234172251626	-4.42082416499759	-0.13934805234408	c
-3.98735112015923	5.61766095784275	3.00971707713021	c
-3.94824102146282	5.74250977470467	-1.84603957606184	c
0.10313700747861	6.73082760401189	0.64175941119722	c
7.18174247515567	1.66858922306004	-1.45588679706405	c
6.66762687325081	-1.95112402624992	1.74015774180302	c
5.02585820087134	-2.46836484187482	-2.80289396370553	c
-2.31438545244090	-6.88608082378726	1.41119051754898	c
-3.29144904786709	-5.14084226345940	-3.02061153105522	c
-5.57369423337133	-3.32788496124174	0.85659220849567	c
-2.52140936313176	5.64780599180111	5.10204189415212	f
-5.18637023197766	7.88239514022380	2.88308299226362	f
-5.75274751447349	3.82855465086205	3.34444861106058	f
-6.33099450161309	4.84197504248488	-1.65503188254712	f
-2.91162014277555	4.73372111362026	-3.92544537873947	f
-4.11920832747870	8.27838218468815	-2.20642681043630	f
-0.38831215325694	9.15376907300496	1.32767224602264	f
1.23155033645448	6.79895593454669	-1.64240452991904	f
1.77667611835577	5.78741632954314	2.30507752779387	f
7.06853839661506	3.63737427092999	0.13871211099125	f
9.63700431003187	0.93717281154985	-1.61090196875140	f
6.48624248244588	2.50682658797249	-3.76463145385205	f
7.59813374575521	-0.28309146190338	3.43613100172004	f
8.60356436710946	-3.46703929783237	1.01891011642642	f
4.96397144393126	-3.39687069917703	2.95596701904870	f
4.15168049929711	-4.70631957904154	-1.95807642681200	f
3.36204729894407	-1.56300057080566	-4.48544055880700	f
7.22468796684564	-2.93460001206362	-4.05128677310160	f
-2.64097782288253	-6.49260437480131	3.91677319444935	f
-3.76512643547671	-8.89787885627835	0.75792388620441	f
0.10938159271119	-7.53438915755856	1.05225686007672	f
-1.38039932859615	-6.64997661700593	-3.78887298442667	f
-3.25890761277289	-3.06254207749885	-4.46631145164425	f
-5.48543066648432	-6.39034476001217	-3.49297369942382	f
-7.33380292137757	-5.14975003426389	1.24760575957682	f
-6.55791719659863	-1.65813416476551	-0.79569500986969	f
-5.22158144397318	-2.11326833905456	3.06497703280545	f

\$vibrational spectrum

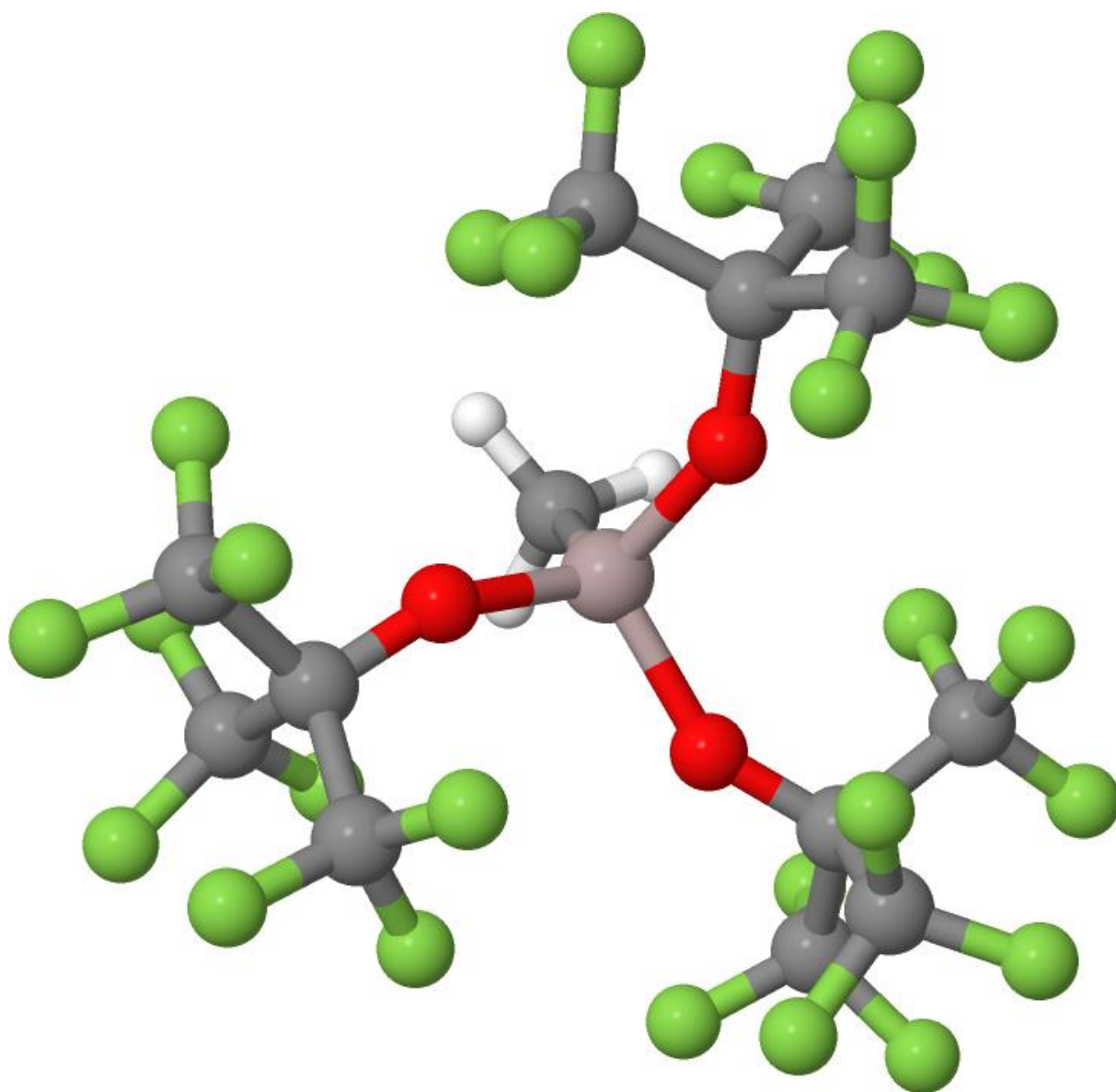
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3			0.00	0.00000	- -

4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	9.32	0.06733	YES	YES
8	a	11.09	0.01614	YES	YES
9	a	15.44	0.06647	YES	YES
10	a	17.78	0.02447	YES	YES
11	a	18.98	0.17016	YES	YES
12	a	23.44	0.13067	YES	YES
13	a	35.91	0.03509	YES	YES
14	a	39.23	0.01404	YES	YES
15	a	47.72	0.03251	YES	YES
16	a	65.52	0.03067	YES	YES
17	a	67.34	0.17696	YES	YES
18	a	67.49	0.02302	YES	YES
19	a	69.58	0.09612	YES	YES
20	a	71.83	0.18941	YES	YES
21	a	76.03	0.02169	YES	YES
22	a	79.09	0.06906	YES	YES
23	a	80.99	0.02548	YES	YES
24	a	81.29	0.04092	YES	YES
25	a	85.82	0.19724	YES	YES
26	a	87.88	0.39871	YES	YES
27	a	93.68	0.18738	YES	YES
28	a	151.80	0.11341	YES	YES
29	a	153.85	0.03803	YES	YES
30	a	155.47	0.09387	YES	YES
31	a	157.94	0.20613	YES	YES
32	a	159.27	0.52707	YES	YES
33	a	159.76	0.41747	YES	YES
34	a	185.67	2.33104	YES	YES
35	a	186.53	2.06114	YES	YES
36	a	200.21	0.35708	YES	YES
37	a	242.76	0.40631	YES	YES
38	a	255.95	0.08584	YES	YES
39	a	257.14	0.78497	YES	YES
40	a	267.79	2.37342	YES	YES
41	a	270.06	2.56658	YES	YES
42	a	272.14	1.80839	YES	YES
43	a	282.65	0.11866	YES	YES
44	a	283.16	0.10223	YES	YES
45	a	283.57	0.15435	YES	YES
46	a	296.24	4.66291	YES	YES
47	a	298.80	7.90047	YES	YES
48	a	299.59	9.04886	YES	YES
49	a	306.92	0.43508	YES	YES
50	a	307.77	0.25780	YES	YES
51	a	308.46	0.44903	YES	YES
52	a	315.43	0.39458	YES	YES
53	a	315.91	0.33165	YES	YES
54	a	318.29	1.35560	YES	YES
55	a	328.96	1.14281	YES	YES
56	a	333.66	0.66739	YES	YES
57	a	334.24	1.04735	YES	YES
58	a	347.94	2.39954	YES	YES
59	a	349.37	3.00565	YES	YES
60	a	355.58	4.01860	YES	YES
61	a	417.93	25.34889	YES	YES
62	a	424.15	45.29194	YES	YES
63	a	426.33	40.55181	YES	YES
64	a	516.71	3.47742	YES	YES
65	a	517.66	3.41338	YES	YES

66	a	518.13	4.21701	YES	YES
67	a	518.48	0.96744	YES	YES
68	a	519.74	3.41285	YES	YES
69	a	520.60	12.17359	YES	YES
70	a	520.90	2.47010	YES	YES
71	a	522.23	1.61688	YES	YES
72	a	522.96	2.40530	YES	YES
73	a	529.09	2.78251	YES	YES
74	a	535.56	4.41480	YES	YES
75	a	537.15	6.35897	YES	YES
76	a	553.10	1.18962	YES	YES
77	a	553.26	0.78464	YES	YES
78	a	553.41	0.18229	YES	YES
79	a	554.10	0.85963	YES	YES
80	a	554.14	0.54155	YES	YES
81	a	554.61	0.98725	YES	YES
82	a	652.73	252.10705	YES	YES
83	a	673.86	237.85270	YES	YES
84	a	705.88	1.11465	YES	YES
85	a	706.44	5.97055	YES	YES
86	a	707.23	13.83265	YES	YES
87	a	707.43	85.33042	YES	YES
88	a	707.93	64.38711	YES	YES
89	a	708.86	74.57971	YES	YES
90	a	724.20	4.41872	YES	YES
91	a	732.47	21.30823	YES	YES
92	a	732.75	23.03245	YES	YES
93	a	774.12	3.64185	YES	YES
94	a	793.21	42.36171	YES	YES
95	a	793.99	46.37055	YES	YES
96	a	951.81	25.41613	YES	YES
97	a	952.25	30.57357	YES	YES
98	a	954.23	59.39342	YES	YES
99	a	958.17	289.17877	YES	YES
100	a	958.86	189.79634	YES	YES
101	a	960.17	219.03985	YES	YES
102	a	1109.98	4.53988	YES	YES
103	a	1110.90	12.06132	YES	YES
104	a	1113.46	1.45540	YES	YES
105	a	1123.70	12.03009	YES	YES
106	a	1129.01	15.97110	YES	YES
107	a	1129.60	9.92281	YES	YES
108	a	1131.13	2.69560	YES	YES
109	a	1134.13	9.56440	YES	YES
110	a	1135.61	7.51467	YES	YES
111	a	1191.74	16.02478	YES	YES
112	a	1195.46	65.01428	YES	YES
113	a	1198.50	15.84457	YES	YES
114	a	1201.40	55.98963	YES	YES
115	a	1204.81	26.03959	YES	YES
116	a	1208.12	75.91068	YES	YES
117	a	1213.07	1066.04428	YES	YES
118	a	1213.69	909.57487	YES	YES
119	a	1228.75	484.78520	YES	YES
120	a	1230.42	410.31455	YES	YES
121	a	1233.78	49.48752	YES	YES
122	a	1235.68	124.78882	YES	YES
123	a	1242.41	11.86565	YES	YES
124	a	1244.77	19.34449	YES	YES
125	a	1247.39	175.07761	YES	YES
126	a	1251.04	461.64384	YES	YES
127	a	1253.43	781.68270	YES	YES

128	a	1261.74	947.12703	YES	YES
129	a	1332.10	319.76637	YES	YES
130	a	1333.38	272.23659	YES	YES
131	a	1351.35	34.59720	YES	YES
132	a	1891.95	208.41763	YES	YES

MeAl(OC(CF₃)₃)₃⁻



Total energy = -3658.9105172040 H = -99564.0776478 eV

HOMO-LUMO Separation

HOMO: 181. 181 a -0.11542630 H = -3.14091 eV

LUMO: 182. 182 a +0.11791573 H = +3.20865 eV

Gap : +0.23334203 H = +6.34956 eV

Number of MOs= 626, Electrons= 362.00, Symmetry: c1

\$coord

0.61867741914137	-0.02511046409293	5.40119189913152	c
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-1.77616345860286	2.36397677989724	0.42210241450778	o
3.19961944321064	0.39889169742324	0.04455286631521	o
-1.01873260056805	-2.91870069883791	0.41720565033733	o
-2.36568822200824	4.83707767081486	0.40988896461096	c
5.46192609026950	-0.48082338430805	-0.69507436984879	c
-3.03202501812983	-4.38735499519829	-0.06971166954573	c
-4.02879041497692	5.52446002303452	2.79515552738712	c
-3.94284852929214	5.40731533784574	-2.06042222761395	c
0.07177944532590	6.56021946690046	0.40991464925456	c
7.13053755550839	1.84795597765635	-1.53713425987942	c
6.85986090406227	-1.91358203815287	1.52046350543142	c
5.17266483713372	-2.34642533414140	-3.01308838581619	c
-2.60281727109682	-7.05079981200582	1.21234616877930	c
-3.30794433954636	-4.75752998227309	-3.02210571163269	c
-5.58465400181940	-3.23090144043624	0.97553733788671	c
-2.58534708781699	5.63072932950048	4.90361123857875	f
-5.21673198869654	7.78668010444217	2.56762575423435	f
-5.80506357536717	3.75653586420221	3.18221116762652	f
-6.31853262180185	4.49347566901483	-1.85352592771200	f
-2.86979991929033	4.31059002494540	-4.07492318843148	f
-4.13593040899163	7.92196635589309	-2.54562137930179	f
-0.44250308431649	9.00779125897031	0.97881750471271	f
1.21723435936519	6.52927077487281	-1.86573298548057	f
1.74339882574007	5.71106590507512	2.12852831350855	f
6.93542342452831	3.73917527790417	0.14263496792975	f
9.61968272142583	1.25760212788201	-1.75516686292087	f
6.35791630605038	2.74198565198447	-3.79813988086915	f
7.72819505783615	-0.26290114729035	3.26627174231001	f
8.86126480315169	-3.29819480794767	0.71871957176783	f
5.25616504046891	-3.49616138487318	2.70387703226751	f
4.37209799789916	-4.63962548785853	-2.24073075970777	f
3.47563965054453	-1.44601945694465	-4.66544443554788	f
7.38451198953442	-2.69497218519038	-4.27552532639607	f
-2.97409341921766	-6.89676876918379	3.73945762391894	f
-4.18299887248817	-8.85980402713310	0.31302198637356	f
-0.22588792365605	-7.85226252343949	0.84423844864103	f
-1.53061280852308	-6.36286152045492	-3.91077252388778	f
-3.01775525826368	-2.54756212631127	-4.22316821012502	f
-5.59556172326645	-5.72127379402085	-3.68403395241475	f
-7.42867951244058	-4.99361367405423	1.24478524830078	f
-6.48688469181936	-1.42153011956658	-0.57237269784813	f
-5.19950023318501	-2.17688984768975	3.25863112020440	f
-1.24703291952744	0.08588224005479	6.36796666905103	h
1.76107672129149	1.61722481292876	6.05612203135207	h
1.57744190978000	-1.76806316548148	6.09034993626299	h

\$vibrational spectrum

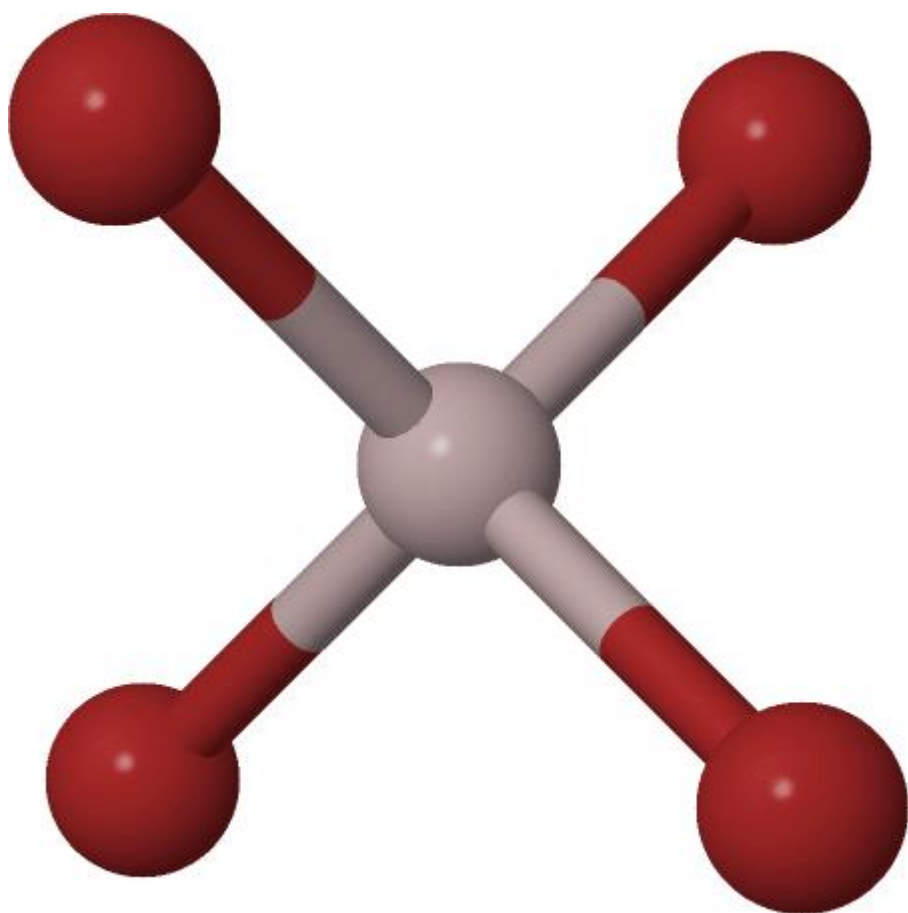
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5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	10.89	0.08172	YES	YES
8		a	12.28	0.01771	YES	YES
9		a	15.97	0.05234	YES	YES
10		a	19.01	0.04635	YES	YES
11		a	21.92	0.13589	YES	YES
12		a	24.66	0.07933	YES	YES
13		a	32.74	0.09570	YES	YES
14		a	41.67	0.03780	YES	YES
15		a	50.11	0.02283	YES	YES
16		a	62.99	0.16406	YES	YES
17		a	64.52	0.03389	YES	YES
18		a	66.30	0.04607	YES	YES
19		a	68.63	0.15979	YES	YES
20		a	71.66	0.10482	YES	YES
21		a	73.89	0.02184	YES	YES
22		a	77.70	0.00279	YES	YES
23		a	78.56	0.06097	YES	YES
24		a	80.63	0.10423	YES	YES
25		a	85.71	0.33888	YES	YES
26		a	88.34	0.28022	YES	YES
27		a	93.67	0.24775	YES	YES
28		a	101.11	0.16542	YES	YES
29		a	122.94	0.21149	YES	YES
30		a	133.98	0.12090	YES	YES
31		a	149.81	0.30954	YES	YES
32		a	157.15	0.15280	YES	YES
33		a	157.83	0.41112	YES	YES
34		a	159.28	0.75696	YES	YES
35		a	159.80	0.07045	YES	YES
36		a	164.50	0.60170	YES	YES
37		a	188.85	3.88922	YES	YES
38		a	189.77	3.15283	YES	YES
39		a	193.50	1.34427	YES	YES
40		a	233.94	0.00461	YES	YES
41		a	261.66	1.94700	YES	YES
42		a	264.34	1.04312	YES	YES
43		a	269.29	4.76431	YES	YES
44		a	271.82	2.63375	YES	YES
45		a	272.26	2.62129	YES	YES
46		a	282.51	0.11722	YES	YES
47		a	283.11	0.21961	YES	YES
48		a	283.67	0.09227	YES	YES
49		a	287.94	7.09888	YES	YES
50		a	298.85	12.61618	YES	YES
51		a	300.36	12.35731	YES	YES
52		a	306.82	0.25316	YES	YES
53		a	311.39	0.36514	YES	YES
54		a	312.11	0.72142	YES	YES
55		a	315.94	1.01157	YES	YES
56		a	317.30	1.54025	YES	YES
57		a	318.10	1.32818	YES	YES

58	a	325.64	1.08122	YES	YES
59	a	338.69	6.77715	YES	YES
60	a	339.61	7.24194	YES	YES
61	a	346.28	3.45172	YES	YES
62	a	349.90	3.19702	YES	YES
63	a	354.99	4.46828	YES	YES
64	a	391.50	15.63292	YES	YES
65	a	418.27	56.11029	YES	YES
66	a	426.88	54.88100	YES	YES
67	a	510.14	0.13869	YES	YES
68	a	516.62	4.27268	YES	YES
69	a	517.20	3.87818	YES	YES
70	a	517.25	3.18406	YES	YES
71	a	519.11	6.66958	YES	YES
72	a	519.59	0.70624	YES	YES
73	a	519.95	7.84513	YES	YES
74	a	521.50	3.08981	YES	YES
75	a	522.15	4.48375	YES	YES
76	a	525.73	0.01101	YES	YES
77	a	533.23	9.21282	YES	YES
78	a	534.91	10.75200	YES	YES
79	a	551.93	0.29458	YES	YES
80	a	552.63	0.65376	YES	YES
81	a	553.02	0.65683	YES	YES
82	a	553.41	0.62127	YES	YES
83	a	553.50	0.56869	YES	YES
84	a	553.69	1.04432	YES	YES
85	a	622.03	47.76256	YES	YES
86	a	677.13	79.62937	YES	YES
87	a	681.89	80.75232	YES	YES
88	a	705.52	7.46611	YES	YES
89	a	705.66	5.30812	YES	YES
90	a	706.68	22.66403	YES	YES
91	a	707.06	68.04194	YES	YES
92	a	707.87	52.30510	YES	YES
93	a	708.48	61.55947	YES	YES
94	a	727.05	9.30171	YES	YES
95	a	732.24	17.79181	YES	YES
96	a	732.51	22.74704	YES	YES
97	a	777.16	11.96981	YES	YES
98	a	790.74	41.90100	YES	YES
99	a	793.14	39.45892	YES	YES
100	a	950.46	5.04939	YES	YES
101	a	951.10	24.42025	YES	YES
102	a	953.19	66.54058	YES	YES
103	a	955.84	270.97837	YES	YES
104	a	957.69	211.06784	YES	YES
105	a	959.05	223.86575	YES	YES
106	a	1107.54	6.92332	YES	YES
107	a	1108.76	8.31710	YES	YES
108	a	1111.86	1.72076	YES	YES
109	a	1122.74	6.10281	YES	YES
110	a	1126.60	12.90391	YES	YES
111	a	1128.55	19.27743	YES	YES
112	a	1129.70	1.01412	YES	YES
113	a	1132.03	12.24228	YES	YES
114	a	1133.84	7.35276	YES	YES
115	a	1189.77	9.93435	YES	YES
116	a	1193.66	66.86844	YES	YES
117	a	1194.61	56.40223	YES	YES
118	a	1197.69	18.00314	YES	YES
119	a	1199.65	43.88731	YES	YES

120	a	1203.41	39.66473	YES	YES
121	a	1206.75	36.09775	YES	YES
122	a	1212.78	1057.70663	YES	YES
123	a	1213.91	1098.60669	YES	YES
124	a	1227.38	344.96944	YES	YES
125	a	1228.49	310.94068	YES	YES
126	a	1232.31	16.94767	YES	YES
127	a	1234.57	218.47877	YES	YES
128	a	1241.30	104.94015	YES	YES
129	a	1243.88	75.89120	YES	YES
130	a	1245.15	58.69669	YES	YES
131	a	1249.67	577.81671	YES	YES
132	a	1252.49	588.83049	YES	YES
133	a	1260.17	1003.28231	YES	YES
134	a	1331.53	284.30524	YES	YES
135	a	1337.20	321.52458	YES	YES
136	a	1354.80	72.66855	YES	YES
137	a	1405.75	1.60626	YES	YES
138	a	1409.58	1.73525	YES	YES
139	a	2930.43	12.07578	YES	YES
140	a	3018.31	22.40280	YES	YES
141	a	3021.09	22.69920	YES	YES

Stability of WCAs:

Anions (not mentioned earlier):



Total energy = -10539.2894607700 H = -286788.8212328 eV

HOMO-LUMO Separation

HOMO: 34. 5 t1 -0.09205524 H = -2.50495 eV

LUMO: 35. 11 a1 +0.11686828 H = +3.18015 eV

Gap : +0.20892351 H = +5.68510 eV

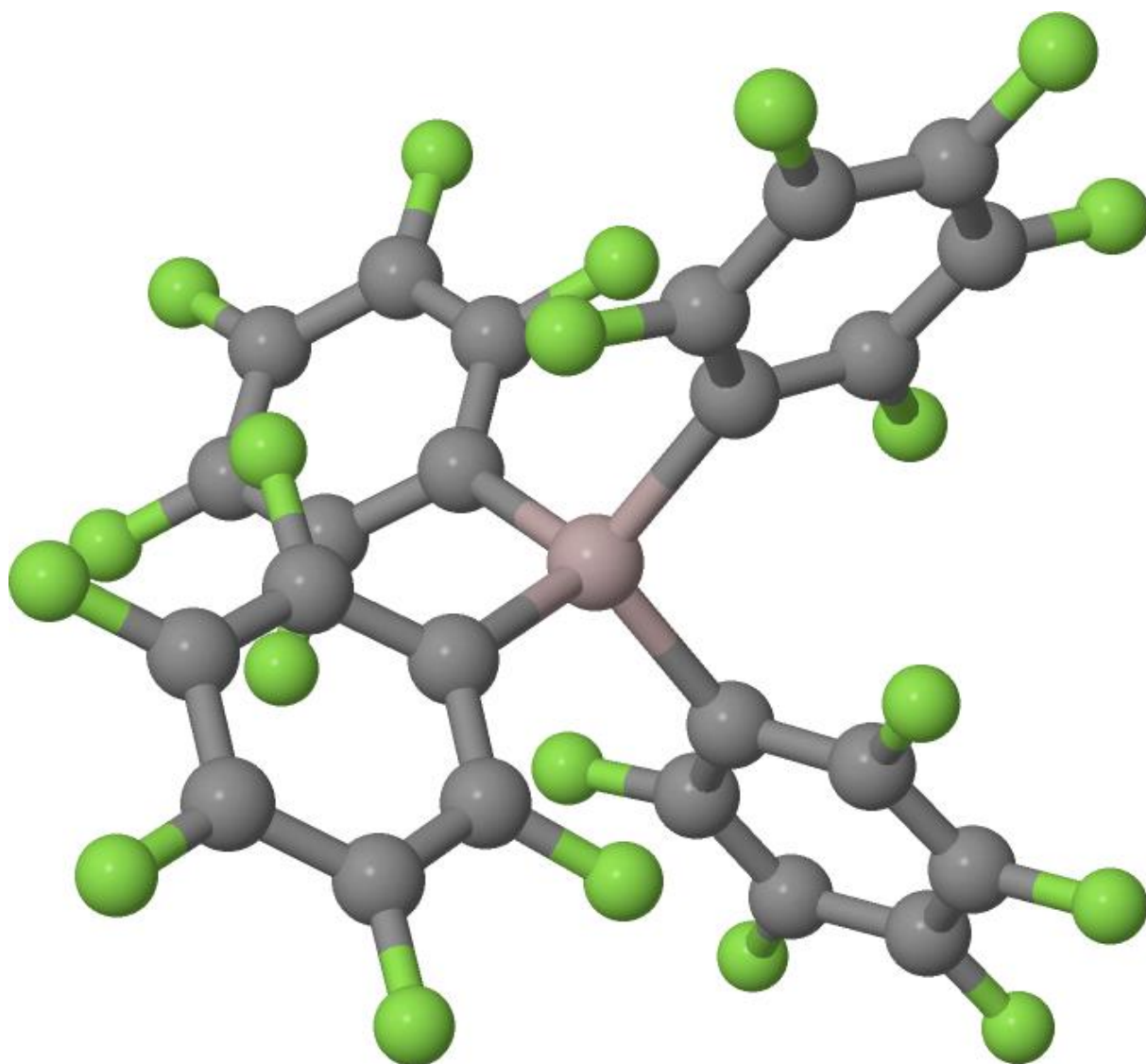
Number of MOs= 63, Electrons= 154.00, Symmetry: td

\$coord

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2.56376033078424	-2.56376033078424	2.56376033078424	br
-2.56376033078424	-2.56376033078424	-2.56376033078424	br
2.56376033078424	2.56376033078424	-2.56376033078424	br

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	60.14	0.00000	NO	YES
8		e	60.14	0.00000	NO	YES
9		t2	99.41	1.13891	YES	YES
10		t2	99.41	1.13891	YES	YES
11		t2	99.41	1.13891	YES	YES
12		a1	191.78	0.00000	NO	YES
13		t2	382.90	121.95570	YES	YES
14		t2	382.90	121.95570	YES	YES
15		t2	382.90	121.95570	YES	YES



Total energy = -3151.7455478390 H = -85763.4088005 eV

HOMO-LUMO Separation

HOMO: 169. 43 a -0.12142939 H = -3.30426 eV

LUMO: 170. 43 b +0.03479621 H = +0.94685 eV

Gap : +0.15622561 H = +4.25112 eV

Number of MOs= 634, Electrons= 338.00, Symmetry: s4

\$coord

-7.15345483466457	2.51761464954907	3.36747478561551	c
-5.29837285946126	1.53879577232121	1.73011622881528	c
-2.70584631090107	1.57435489450462	2.26516512559887	c
-2.05185289147101	2.70568495635583	4.57013806983447	c
-3.81536378109857	3.71145487752631	6.28038938183107	c
-6.39482554831174	3.60531981099269	5.66431484389411	c
3.60531981099269	6.39482554831174	-5.66431484389411	c
2.51761464954907	7.15345483466457	-3.36747478561551	c
1.53879577232121	5.29837285946126	-1.73011622881528	c
1.57435489450462	2.70584631090107	-2.26516512559887	c
2.70568495635583	2.05185289147101	-4.57013806983447	c
3.71145487752631	3.81536378109857	-6.28038938183107	c
-3.60531981099269	-6.39482554831174	-5.66431484389411	c
-3.71145487752631	-3.81536378109857	-6.28038938183107	c
-2.70568495635583	-2.05185289147101	-4.57013806983447	c
-1.57435489450462	-2.70584631090107	-2.26516512559887	c
-1.53879577232121	-5.29837285946126	-1.73011622881528	c
-2.51761464954907	-7.15345483466457	-3.36747478561551	c
6.39482554831174	-3.60531981099269	5.66431484389411	c
7.15345483466457	-2.51761464954907	3.36747478561551	c
5.29837285946126	-1.53879577232121	1.73011622881528	c
2.70584631090107	-1.57435489450462	2.26516512559887	c
2.05185289147101	-2.70568495635583	4.57013806983447	c
3.81536378109857	-3.71145487752631	6.28038938183107	c
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-2.87801641491169	0.40571669741032	-5.26414626237334	f
-4.76425112734051	-3.08828573306534	-8.47956596559275	f
-4.54974728333712	-8.12668959310103	-7.26501252212337	f
-2.43443131586773	-9.62625842482987	-2.77012725257387	f
-0.53317359047229	-6.16687520694613	0.45585973060652	f
2.87801641491169	-0.40571669741032	-5.26414626237334	f
4.76425112734051	3.08828573306534	-8.47956596559275	f
4.54974728333712	8.12668959310103	-7.26501252212337	f
2.43443131586773	9.62625842482987	-2.77012725257387	f
0.53317359047229	6.16687520694613	0.45585973060652	f
9.62625842482987	-2.43443131586773	2.77012725257387	f
6.16687520694613	-0.53317359047229	-0.45585973060652	f
8.12668959310103	-4.54974728333712	7.26501252212337	f
3.08828573306534	-4.76425112734051	8.47956596559275	f
-0.40571669741032	-2.87801641491169	5.26414626237334	f
-6.16687520694613	0.53317359047229	-0.45585973060652	f
-9.62625842482987	2.43443131586773	2.77012725257387	f
-8.12668959310103	4.54974728333712	7.26501252212337	f
-3.08828573306534	4.76425112734051	8.47956596559275	f
0.40571669741032	2.87801641491169	5.26414626237334	f

\$vibrational spectrum

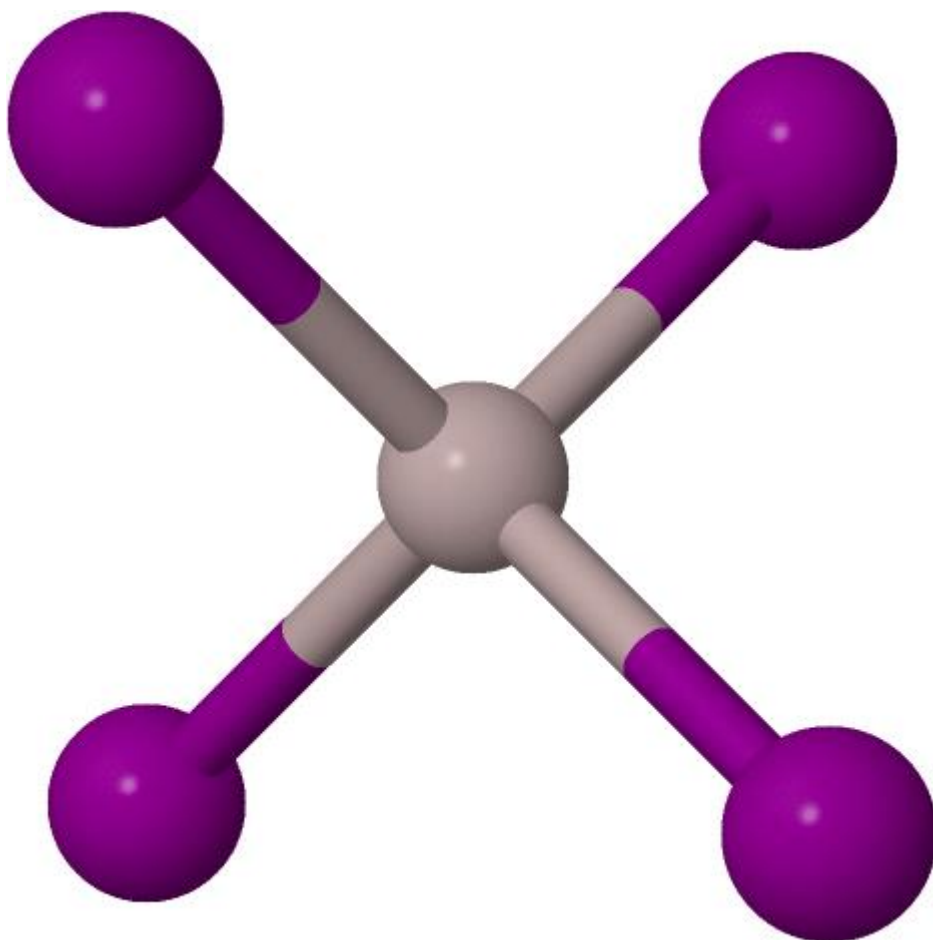
#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	11.97	0.00000	NO	YES
8	e	18.47	0.00999	YES	YES
9	e	18.47	0.00999	YES	YES
10	b	20.72	0.00437	YES	YES
11	a	29.46	0.00000	NO	YES
12	e	29.89	0.00719	YES	YES
13	e	29.89	0.00719	YES	YES
14	b	30.42	0.01529	YES	YES
15	b	39.61	0.03286	YES	YES
16	e	84.01	0.01422	YES	YES
17	e	84.01	0.01422	YES	YES
18	a	92.32	0.00000	NO	YES
19	a	97.53	0.00000	NO	YES
20	b	101.37	0.08712	YES	YES
21	e	104.97	0.25638	YES	YES
22	e	104.97	0.25638	YES	YES
23	b	114.67	0.21868	YES	YES
24	e	124.21	0.03900	YES	YES
25	e	124.21	0.03900	YES	YES
26	a	124.51	0.00000	NO	YES
27	b	129.29	0.06307	YES	YES
28	a	129.41	0.00000	NO	YES
29	e	154.71	0.00550	YES	YES
30	e	154.71	0.00550	YES	YES
31	a	155.99	0.00000	NO	YES
32	b	159.06	0.00354	YES	YES
33	a	215.05	0.00000	NO	YES
34	e	217.34	1.68378	YES	YES
35	e	217.34	1.68378	YES	YES
36	b	218.49	0.70973	YES	YES
37	e	261.51	0.23440	YES	YES
38	e	261.51	0.23440	YES	YES
39	a	261.64	0.00000	NO	YES
40	b	261.65	0.30288	YES	YES
41	b	265.05	0.21761	YES	YES
42	e	265.75	0.33150	YES	YES
43	e	265.75	0.33150	YES	YES
44	a	267.11	0.00000	NO	YES
45	e	304.13	2.74202	YES	YES
46	e	304.13	2.74202	YES	YES
47	a	304.26	0.00000	NO	YES
48	b	304.27	5.19692	YES	YES
49	e	315.89	22.24201	YES	YES
50	e	315.89	22.24201	YES	YES
51	b	320.71	20.54066	YES	YES
52	a	340.97	0.00000	NO	YES
53	e	347.60	1.65609	YES	YES
54	e	347.60	1.65609	YES	YES
55	a	354.40	0.00000	NO	YES
56	b	360.86	2.54953	YES	YES
57	b	391.38	53.60599	YES	YES
58	e	394.45	31.87671	YES	YES
59	e	394.45	31.87671	YES	YES
60	a	395.26	0.00000	NO	YES
61	b	395.84	0.60282	YES	YES
62	e	396.35	18.06519	YES	YES
63	e	396.35	18.06519	YES	YES
64	a	433.34	0.00000	NO	YES
65	e	433.40	0.42280	YES	YES
66	e	433.40	0.42280	YES	YES

67	b	434.75	0.51321	YES	YES
68	a	471.92	0.00000	NO	YES
69	e	482.83	14.01419	YES	YES
70	e	482.83	14.01419	YES	YES
71	b	484.96	20.89219	YES	YES
72	a	489.01	0.00000	NO	YES
73	e	489.68	12.95065	YES	YES
74	e	489.68	12.95065	YES	YES
75	b	490.05	9.16781	YES	YES
76	a	563.11	0.00000	NO	YES
77	b	563.21	0.26397	YES	YES
78	e	563.27	0.29458	YES	YES
79	e	563.27	0.29458	YES	YES
80	a	601.84	0.00000	NO	YES
81	e	607.58	23.59877	YES	YES
82	e	607.58	23.59877	YES	YES
83	b	614.25	13.73218	YES	YES
84	e	633.55	0.33153	YES	YES
85	e	633.55	0.33153	YES	YES
86	a	634.44	0.00000	NO	YES
87	b	634.49	0.38611	YES	YES
88	e	729.51	3.72425	YES	YES
89	e	729.51	3.72425	YES	YES
90	a	730.35	0.00000	NO	YES
91	b	735.27	4.26581	YES	YES
92	a	763.82	0.00000	NO	YES
93	e	776.96	2.54988	YES	YES
94	e	776.96	2.54988	YES	YES
95	b	777.86	3.37761	YES	YES
96	e	959.69	202.90687	YES	YES
97	e	959.69	202.90687	YES	YES
98	a	960.42	0.00000	NO	YES
99	b	965.68	213.84702	YES	YES
100	b	1069.00	402.15429	YES	YES
101	e	1069.23	321.87759	YES	YES
102	e	1069.23	321.87759	YES	YES
103	a	1071.48	0.00000	NO	YES
104	a	1123.38	0.00000	NO	YES
105	e	1124.20	1.06292	YES	YES
106	e	1124.20	1.06292	YES	YES
107	b	1129.24	1.98071	YES	YES
108	e	1256.66	50.56342	YES	YES
109	e	1256.66	50.56342	YES	YES
110	b	1257.00	54.18398	YES	YES
111	a	1258.72	0.00000	NO	YES
112	b	1344.73	53.76688	YES	YES
113	e	1350.68	6.99189	YES	YES
114	e	1350.68	6.99189	YES	YES
115	a	1353.36	0.00000	NO	YES
116	e	1357.03	24.78642	YES	YES
117	e	1357.03	24.78642	YES	YES
118	b	1358.35	9.32821	YES	YES
119	a	1365.54	0.00000	NO	YES
120	a	1446.54	0.00000	NO	YES
121	e	1449.43	616.21006	YES	YES
122	e	1449.43	616.21006	YES	YES
123	b	1460.80	716.14772	YES	YES
124	e	1505.26	174.28680	YES	YES
125	e	1505.26	174.28680	YES	YES
126	b	1505.29	263.23003	YES	YES
127	a	1508.07	0.00000	NO	YES
128	e	1613.22	3.98025	YES	YES

129	e	1613.22	3.98025	YES	YES
130	a	1613.41	0.00000	NO	YES
131	b	1615.02	25.68393	YES	YES
132	e	1618.37	76.12881	YES	YES
133	e	1618.37	76.12881	YES	YES
134	b	1618.42	55.01668	YES	YES
135	a	1619.33	0.00000	NO	YES

[AlI₄]⁻



Total energy = -288.5702666634 H = -7852.4009543 eV

HOMO-LUMO Separation

HOMO: 10. 1 t1 -0.09768834 H = -2.65824 eV

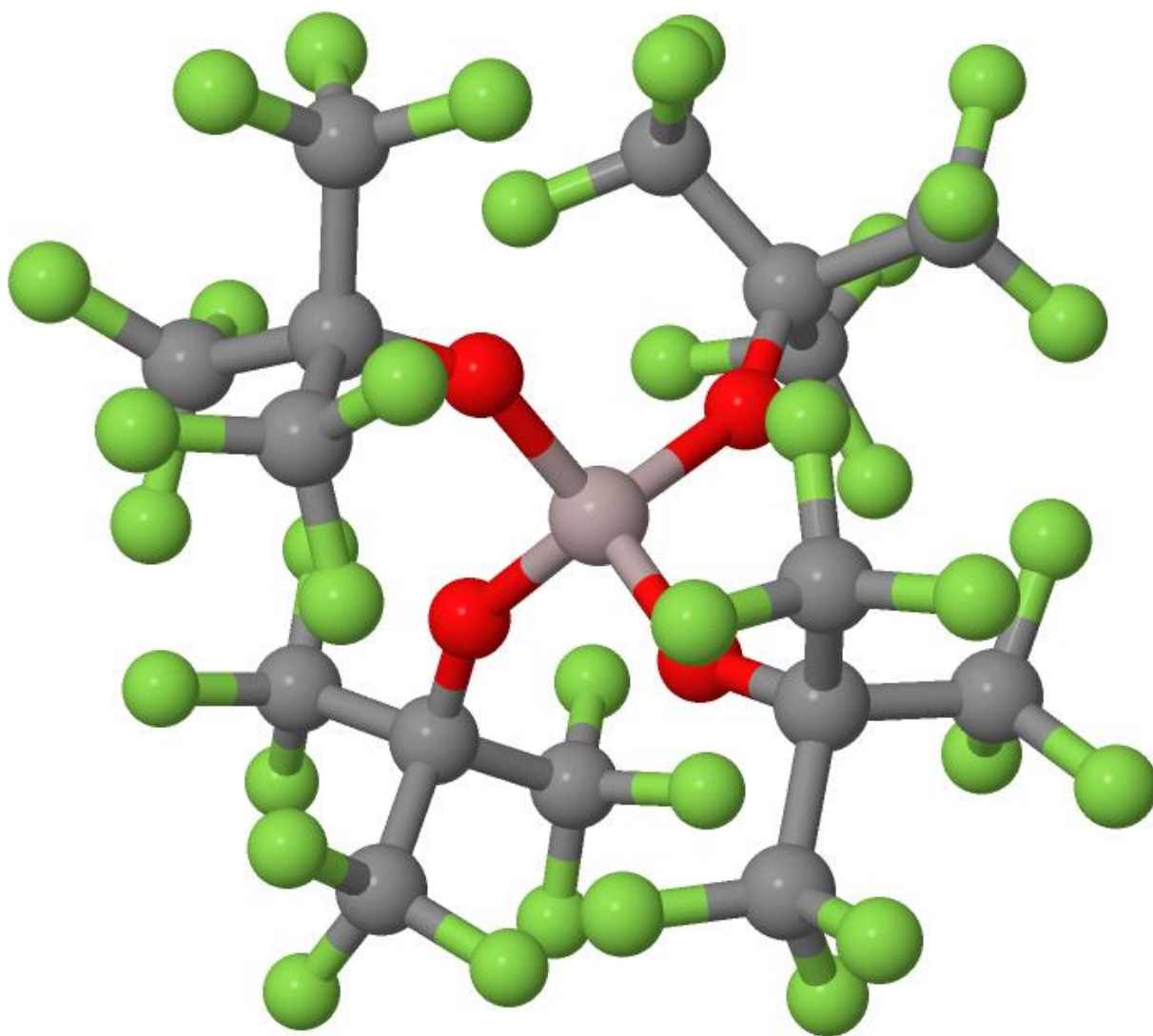
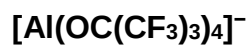
LUMO: 11. 5 a1 +0.04831976 H = +1.31485 eV

Gap : +0.14600810 H = +3.97308 eV

Number of MOs= 31, Electrons= 42.00, Symmetry: td

```
$coord
  0.0000000000000000    0.0000000000000000    0.0000000000000000    a1
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  2.83007097237831     -2.83007097237831      2.83007097237831      i
-2.83007097237831     -2.83007097237831     -2.83007097237831      i
  2.83007097237831      2.83007097237831     -2.83007097237831      i
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#          #          cm** (-1)      km/mol          IR          RAMAN
  1          0.00          0.00000          -            -
  2          0.00          0.00000          -            -
  3          0.00          0.00000          -            -
  4          0.00          0.00000          -            -
  5          0.00          0.00000          -            -
  6          0.00          0.00000          -            -
  7          e          45.02          0.00000          NO          YES
  8          e          45.02          0.00000          NO          YES
  9          t2         73.75          0.19891          YES          YES
 10          t2         73.75          0.19891          YES          YES
 11          t2         73.75          0.19891          YES          YES
 12          a1        135.00          0.00000          NO          YES
 13          t2        327.76         123.56282          YES          YES
 14          t2        327.76         123.56282          YES          YES
 15          t2        327.76         123.56282          YES          YES
```



Total energy = -4744.5497306140 H = -129105.8405396 eV

HOMO-LUMO Separation

HOMO: 233. 233 a -0.15053081 H = -4.09615 eV

LUMO: 234. 234 a +0.09704685 H = +2.64078 eV

Gap : +0.24757766 H = +6.73693 eV

Number of MOs= 802, Electrons= 466.00, Symmetry: c1

\$scoord

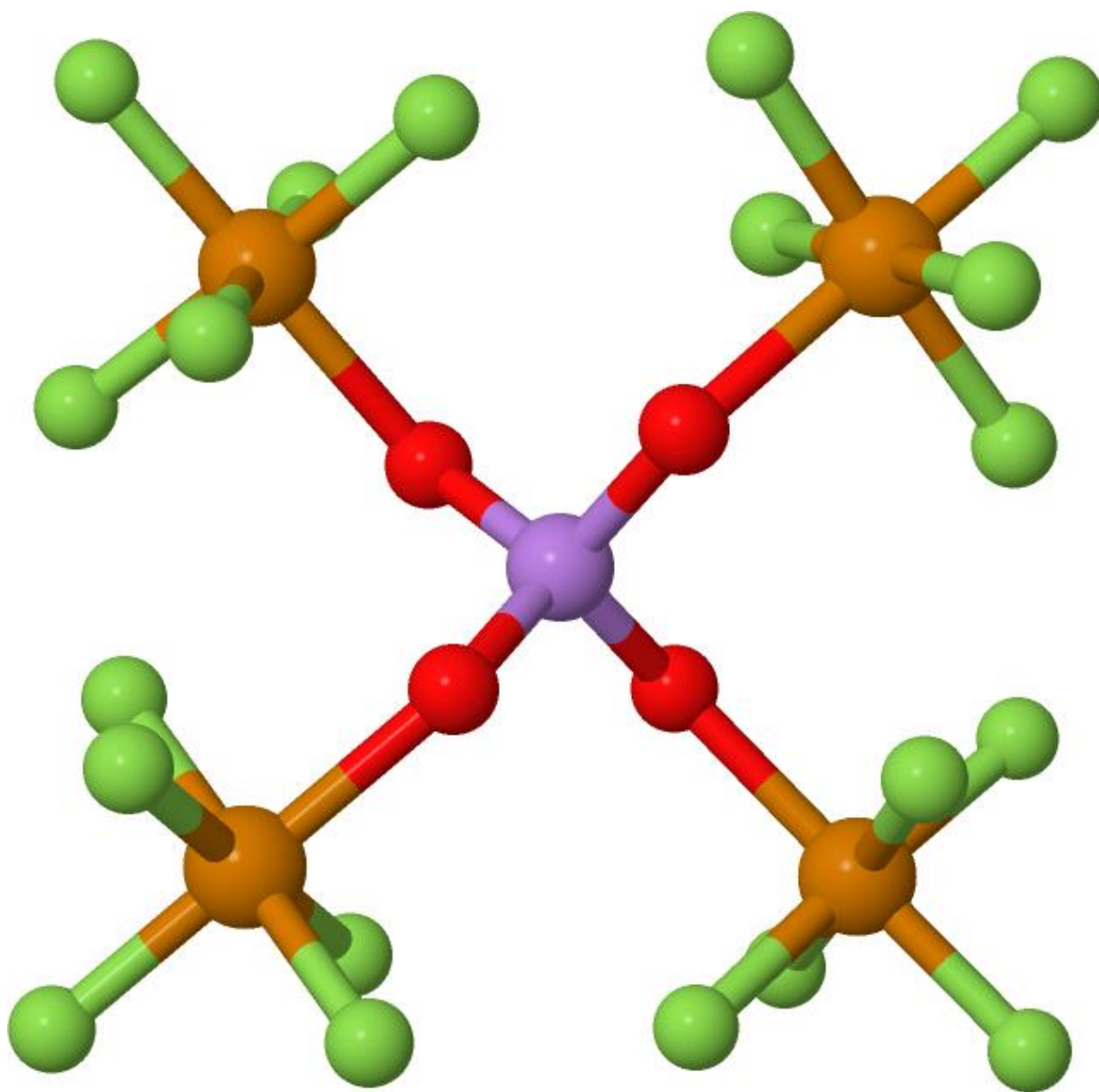
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3.18708334517494	-2.59754154780716	-3.73023180655749	c
-4.74734642549584	1.47954377005787	-0.90822175465813	c
-0.93720715030782	-5.10148431364029	4.22254286833166	c
6.20377454553358	3.30525764852588	3.37387728580533	c
6.91705257514809	4.66639963240628	1.33651754853153	f
7.31641021009726	4.36002739057563	5.42822502420671	f
7.13418164942086	0.96413603307004	3.10486439912302	f
2.16568482501656	6.00009618470727	3.20462940125027	c
-0.24418441768962	6.16502471354231	4.02712348672270	f
2.18870304219891	6.61194969748909	0.74615413080348	f
3.52814982423467	7.76853028384793	4.46501481781989	f
2.49017785059465	2.30663121864178	6.33588130565928	c
3.87782276784842	0.27766599436675	7.00946171773927	f
0.04433296388316	1.63698769449050	6.40187150673190	f
2.85350668006903	4.11286905020557	8.11477925066813	f
1.91667582402554	-3.59294567796858	-6.24316973859765	c
-0.11683590617250	-5.00457866501234	-5.70858186085961	f
1.14969834752980	-1.64279934998283	-7.70088413618717	f
3.51477565860140	-5.01909083414917	-7.65084087315618	f
5.05130283792302	-0.36404351421927	-4.41298108316070	c
3.76261106401545	1.77698719256990	-4.83074617138778	f
6.43583210985245	-0.87172511316489	-6.51186333007092	f
6.69158172402362	0.06915976741301	-2.50871010108992	f
4.76075289971964	-4.81225265339979	-2.49809164616465	c
6.98517354864693	-5.22725359299419	-3.69912382768641	f
3.44556187834539	-6.99704564111163	-2.55162472230491	f
5.27538693596587	-4.27857197780255	-0.07046403097912	f
-3.79925228043977	4.02213461987795	-2.14827710795493	c
-5.39717464324714	4.89157400349753	-3.95023194039877	f
-3.55853285505943	5.85422515362240	-0.38968031963203	f
-1.52375563412724	3.68328687487817	-3.21977293379178	f
-5.77210116198984	-0.31931913164587	-3.06430099541022	c
-4.20313139650040	-0.32119927186003	-5.07614859341568	f
-8.08704405310241	0.39656705216851	-3.90192899474375	f
-5.94898594313488	-2.70136906924494	-2.22095786583681	f
-6.98133195835292	2.10165817373525	0.97586066607435	c
-8.63825588400236	3.79526670010720	-0.00404100728775	f
-6.07884514016415	3.05930046932519	3.13840710163608	f
-8.30114269279238	-0.00545997141272	1.55206716977753	f
0.62651236924798	-5.81927790102791	6.65925092615752	c
0.23125711864678	-4.11806397213763	8.52012086206554	f
-0.00948395350336	-8.12641579654245	7.57951608057153	f
3.10891206091839	-5.84438201619324	6.15306184955386	f
-1.03648251321715	-7.47033754396462	2.40865930469001	c
-1.74966786357495	-6.76356070129625	0.07817474733435	f
-2.67562675327638	-9.26204936259831	3.22444024224562	f
1.25849471182182	-8.56782606491925	2.21796370454430	f
-3.73009109100376	-4.40962239739972	5.02797584170977	c
-5.29088479890329	-4.47876361705263	3.01544878335610	f
-3.82918442510681	-2.07702269419168	6.01170033864418	f
-4.66419001009916	-6.03577139212195	6.77814909297554	f
2.30892799364966	1.69710205301371	1.78842971331048	o
1.32864303126099	-1.80729565940796	-2.17704967917386	o
-2.89285812173366	0.34175282627726	0.41733822829050	o
0.23570775042874	-3.14033037288371	3.08869210370986	o

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	9.31	0.00298	YES	YES
8		a	12.11	0.01149	YES	YES
9		a	17.18	0.00596	YES	YES
10		a	20.81	0.00851	YES	YES
11		a	25.54	0.01063	YES	YES
12		a	25.95	0.05046	YES	YES
13		a	29.64	0.01874	YES	YES
14		a	32.32	0.06795	YES	YES
15		a	35.27	0.02103	YES	YES
16		a	38.32	0.14707	YES	YES
17		a	41.73	0.08382	YES	YES
18		a	49.07	0.01652	YES	YES
19		a	62.36	0.20016	YES	YES
20		a	64.43	0.02050	YES	YES
21		a	68.21	0.12375	YES	YES
22		a	69.69	0.05069	YES	YES
23		a	70.05	0.15513	YES	YES
24		a	71.82	0.07159	YES	YES
25		a	72.75	0.07952	YES	YES
26		a	73.11	0.26980	YES	YES
27		a	75.78	0.08728	YES	YES
28		a	80.49	0.00841	YES	YES
29		a	81.88	0.11657	YES	YES
30		a	84.17	0.03365	YES	YES
31		a	85.36	0.04037	YES	YES
32		a	87.15	0.03079	YES	YES
33		a	92.49	0.84785	YES	YES
34		a	93.32	0.86410	YES	YES
35		a	94.39	0.79441	YES	YES
36		a	109.16	0.00114	YES	YES
37		a	153.55	0.05571	YES	YES
38		a	154.20	0.03240	YES	YES
39		a	157.58	0.48105	YES	YES
40		a	158.90	0.34492	YES	YES
41		a	159.71	0.42880	YES	YES
42		a	160.71	0.28103	YES	YES
43		a	162.65	0.32817	YES	YES
44		a	164.29	0.55985	YES	YES
45		a	191.68	4.37621	YES	YES
46		a	193.17	3.96155	YES	YES
47		a	193.50	3.81455	YES	YES
48		a	217.91	0.00060	YES	YES
49		a	258.00	0.88358	YES	YES
50		a	258.66	0.74711	YES	YES
51		a	270.15	4.34102	YES	YES
52		a	271.06	0.36200	YES	YES
53		a	275.32	3.77336	YES	YES
54		a	276.09	4.10496	YES	YES
55		a	278.51	5.44216	YES	YES
56		a	280.00	0.18405	YES	YES
57		a	283.71	0.11065	YES	YES
58		a	283.88	0.11729	YES	YES
59		a	284.22	0.08777	YES	YES

60	a	284.35	0.09773	YES	YES
61	a	302.37	8.51590	YES	YES
62	a	303.09	7.95369	YES	YES
63	a	303.49	8.49238	YES	YES
64	a	308.08	0.15984	YES	YES
65	a	311.11	0.05580	YES	YES
66	a	311.61	0.07036	YES	YES
67	a	315.54	0.10853	YES	YES
68	a	317.66	0.23773	YES	YES
69	a	318.52	1.99239	YES	YES
70	a	318.96	2.55101	YES	YES
71	a	321.19	2.22807	YES	YES
72	a	322.73	0.03351	YES	YES
73	a	340.51	0.53309	YES	YES
74	a	340.93	0.30927	YES	YES
75	a	347.23	2.26815	YES	YES
76	a	352.86	7.41309	YES	YES
77	a	353.78	11.25007	YES	YES
78	a	355.10	2.30468	YES	YES
79	a	367.24	27.04879	YES	YES
80	a	371.28	1.17967	YES	YES
81	a	426.87	73.20723	YES	YES
82	a	434.98	74.85171	YES	YES
83	a	436.58	80.86729	YES	YES
84	a	513.40	0.33620	YES	YES
85	a	517.67	2.88968	YES	YES
86	a	518.24	1.28896	YES	YES
87	a	518.70	0.81196	YES	YES
88	a	519.27	7.22128	YES	YES
89	a	519.64	9.18410	YES	YES
90	a	520.04	8.30011	YES	YES
91	a	520.59	4.26505	YES	YES
92	a	521.14	2.85298	YES	YES
93	a	524.35	3.12542	YES	YES
94	a	524.46	1.97098	YES	YES
95	a	524.99	1.57843	YES	YES
96	a	527.15	0.36215	YES	YES
97	a	542.30	24.36524	YES	YES
98	a	545.51	25.51433	YES	YES
99	a	546.85	27.43797	YES	YES
100	a	552.96	0.52366	YES	YES
101	a	553.76	0.61603	YES	YES
102	a	554.09	0.93692	YES	YES
103	a	554.16	0.79959	YES	YES
104	a	554.75	0.49770	YES	YES
105	a	554.98	3.09759	YES	YES
106	a	555.09	3.46859	YES	YES
107	a	555.93	4.82226	YES	YES
108	a	706.68	7.34124	YES	YES
109	a	707.07	2.30329	YES	YES
110	a	707.90	1.91137	YES	YES
111	a	708.32	5.82397	YES	YES
112	a	709.14	87.68927	YES	YES
113	a	709.19	26.78592	YES	YES
114	a	709.59	58.66085	YES	YES
115	a	710.52	74.28500	YES	YES
116	a	724.07	0.29584	YES	YES
117	a	735.56	2.53877	YES	YES
118	a	735.90	3.70157	YES	YES
119	a	736.85	3.53581	YES	YES
120	a	777.45	0.03035	YES	YES
121	a	816.17	18.67393	YES	YES

122	a	821.09	20.61015	YES	YES
123	a	823.15	22.79364	YES	YES
124	a	950.74	16.56934	YES	YES
125	a	951.98	12.19250	YES	YES
126	a	955.79	11.28353	YES	YES
127	a	956.66	14.09231	YES	YES
128	a	959.06	305.61093	YES	YES
129	a	960.39	92.00180	YES	YES
130	a	962.64	285.20490	YES	YES
131	a	962.94	260.55427	YES	YES
132	a	1109.97	10.70120	YES	YES
133	a	1112.27	8.96378	YES	YES
134	a	1113.47	11.18426	YES	YES
135	a	1118.35	0.67197	YES	YES
136	a	1128.89	7.17884	YES	YES
137	a	1130.83	3.39337	YES	YES
138	a	1131.92	0.94332	YES	YES
139	a	1135.41	10.46656	YES	YES
140	a	1136.75	10.14333	YES	YES
141	a	1138.73	17.60451	YES	YES
142	a	1139.95	6.67783	YES	YES
143	a	1140.63	17.55410	YES	YES
144	a	1192.97	10.13368	YES	YES
145	a	1194.65	4.94389	YES	YES
146	a	1195.23	11.76794	YES	YES
147	a	1200.26	30.44208	YES	YES
148	a	1202.70	43.94960	YES	YES
149	a	1203.79	43.72737	YES	YES
150	a	1208.40	60.70347	YES	YES
151	a	1210.11	30.32748	YES	YES
152	a	1214.11	631.95945	YES	YES
153	a	1215.35	742.91014	YES	YES
154	a	1216.51	763.60564	YES	YES
155	a	1231.34	775.71794	YES	YES
156	a	1231.88	811.68331	YES	YES
157	a	1233.32	680.91215	YES	YES
158	a	1234.75	381.40273	YES	YES
159	a	1239.82	22.83372	YES	YES
160	a	1242.10	9.23978	YES	YES
161	a	1245.62	9.03566	YES	YES
162	a	1248.32	57.21423	YES	YES
163	a	1248.91	109.08260	YES	YES
164	a	1253.36	9.47507	YES	YES
165	a	1261.09	894.74190	YES	YES
166	a	1261.74	867.17914	YES	YES
167	a	1265.05	724.64772	YES	YES
168	a	1338.82	304.48290	YES	YES
169	a	1340.60	293.14444	YES	YES
170	a	1342.64	322.95148	YES	YES
171	a	1368.18	3.96147	YES	YES



Total energy = -4564.4028655710 H = -124203.7921362 eV

HOMO-LUMO Separation

HOMO: 135. 135 a -0.15609578 H = -4.24758 eV

LUMO: 136. 136 a -0.15095521 H = -4.10770 eV

Gap : +0.00514056 H = +0.13988 eV

Number of MOs= 420, Electrons= 270.00, Symmetry: c1

\$coord

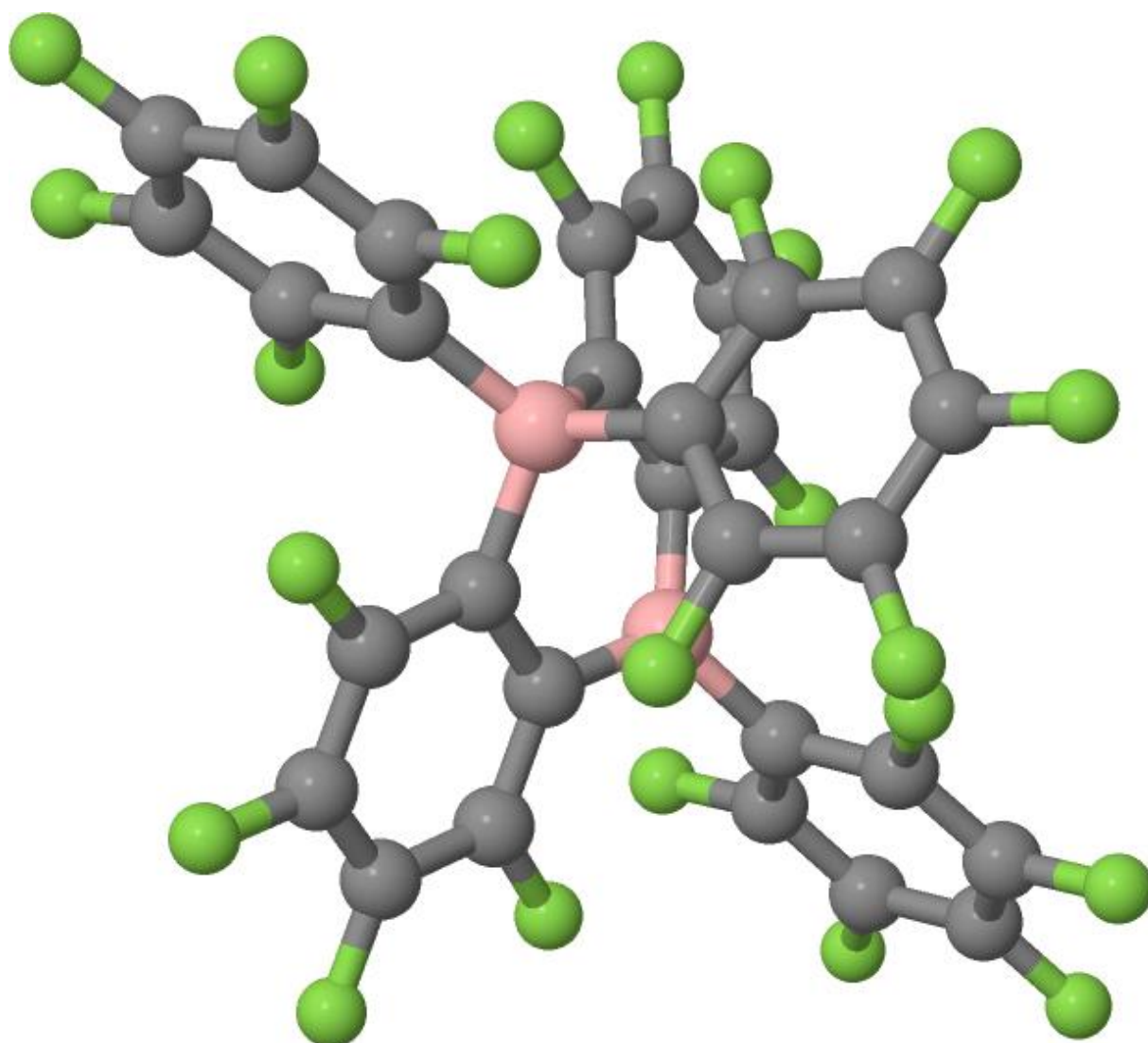
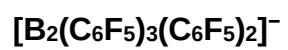
0.02213733224471	-0.01712795048150	0.00142668695017	as
0.68018139323488	1.20089806326207	2.98177522076931	o
2.16956348394957	0.79770721580172	-2.34536928927104	o
0.01258113725816	-3.21978316305546	0.75009117401990	o
-2.73889341433732	1.11902794464824	-1.36190803187585	o
6.12750366541572	0.78413893727533	-2.36342689686501	te
0.71688007223194	4.95028442082260	4.24352189324562	te
-6.53164793440279	0.68398655856462	-0.30680317483580	te
-0.31254186758964	-6.40649332136952	-1.56720223010580	te
2.80567730230855	-5.56049377333972	-3.34357040955005	f
1.62975874463879	-8.33701197548356	0.90602749584568	f
-0.65525295690667	-9.36194970015480	-3.69480806384473	f
-3.43029451078339	-7.38539831524902	0.13525546073908	f
-2.15440333907411	-4.37692835692692	-4.05018273946766	f
6.17288806486050	-2.43903451784137	-0.55640356217856	f
6.10552593448797	-0.92730036806637	-5.62926195941145	f
9.78524519219356	0.78604623694258	-2.40995771179997	f
6.10386980504886	4.04530130474575	-4.08718704631765	f
6.17949580084913	2.49647432087196	0.90758016800217	f
1.65893334633531	6.06542347288242	0.84183014012705	f
4.24993750770932	4.66302517233916	5.25061090301089	f
0.72362185659101	8.42199610892373	5.39867295468387	f
-0.30214029738720	3.77413237911031	7.59050608435087	f
-2.82497458823506	5.33610974902548	3.28433974329070	f
-6.24673505645656	-2.97606005851524	-0.65745090420379	f
-10.03647029262333	0.26189333531762	0.65387218316475	f
-7.48234450806162	0.96784234019229	-3.86169853564624	f
-6.92704090331300	4.32885215551633	0.06207087580957	f
-5.50106097018731	0.32444178424094	3.22764957136386	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		15.41	0.02141	YES	YES
8	a		21.14	0.01901	YES	YES
9	a		25.63	0.00278	YES	YES
10	a		31.46	0.08871	YES	YES
11	a		36.49	0.23152	YES	YES
12	a		38.85	0.19850	YES	YES
13	a		41.38	0.37304	YES	YES
14	a		44.26	0.78268	YES	YES
15	a		46.17	1.14487	YES	YES
16	a		50.64	0.09863	YES	YES
17	a		53.36	0.24461	YES	YES
18	a		61.15	0.64484	YES	YES
19	a		62.41	0.50479	YES	YES
20	a		74.61	0.23411	YES	YES
21	a		78.89	0.01748	YES	YES

22	a	87.74	1.08589	YES	YES
23	a	88.64	1.11731	YES	YES
24	a	101.87	0.04109	YES	YES
25	a	128.12	0.36614	YES	YES
26	a	134.19	0.60753	YES	YES
27	a	137.24	0.78406	YES	YES
28	a	141.11	1.30168	YES	YES
29	a	141.56	1.38359	YES	YES
30	a	146.02	4.85164	YES	YES
31	a	146.53	7.18775	YES	YES
32	a	149.95	1.42911	YES	YES
33	a	169.59	1.35911	YES	YES
34	a	170.42	0.47134	YES	YES
35	a	173.23	1.18810	YES	YES
36	a	178.62	1.06971	YES	YES
37	a	185.59	4.73027	YES	YES
38	a	187.46	6.60222	YES	YES
39	a	189.15	2.70821	YES	YES
40	a	197.97	23.96093	YES	YES
41	a	202.88	5.21560	YES	YES
42	a	203.49	32.03287	YES	YES
43	a	211.04	1.32970	YES	YES
44	a	228.00	2.08062	YES	YES
45	a	228.85	3.19930	YES	YES
46	a	230.92	1.09984	YES	YES
47	a	231.48	0.74523	YES	YES
48	a	233.20	7.05953	YES	YES
49	a	235.25	4.99253	YES	YES
50	a	237.85	7.01966	YES	YES
51	a	238.79	5.70797	YES	YES
52	a	240.23	6.75949	YES	YES
53	a	240.91	15.30713	YES	YES
54	a	243.08	4.05229	YES	YES
55	a	244.43	4.54250	YES	YES
56	a	247.39	0.22601	YES	YES
57	a	276.08	0.18826	YES	YES
58	a	297.69	54.94225	YES	YES
59	a	307.53	52.92410	YES	YES
60	a	323.97	58.47912	YES	YES
61	a	327.16	55.35850	YES	YES
62	a	374.44	0.07499	YES	YES
63	a	448.22	94.67098	YES	YES
64	a	491.58	42.76570	YES	YES
65	a	507.87	568.19309	YES	YES
66	a	508.76	580.00664	YES	YES
67	a	561.52	0.03372	YES	YES
68	a	562.64	0.02671	YES	YES
69	a	563.25	0.18621	YES	YES
70	a	564.70	0.11190	YES	YES
71	a	567.05	0.03778	YES	YES
72	a	590.51	1.53223	YES	YES
73	a	595.28	29.66473	YES	YES
74	a	595.95	15.72276	YES	YES
75	a	598.96	5.54678	YES	YES
76	a	600.55	148.60855	YES	YES
77	a	602.15	401.40231	YES	YES
78	a	602.48	248.03731	YES	YES
79	a	605.41	313.28636	YES	YES
80	a	606.50	140.07052	YES	YES
81	a	607.07	99.56486	YES	YES
82	a	610.86	9.05163	YES	YES
83	a	611.53	4.27152	YES	YES

84	a	646.81	3.40171	YES	YES
85	a	650.97	3.64204	YES	YES
86	a	685.91	13.40975	YES	YES
87	a	690.40	1.73576	YES	YES



Total energy = -3486.8129616230 H = -94881.0622239 eV

HOMO-LUMO Separation

HOMO: 199. 199 a -0.12067534 H = -3.28374 eV

LUMO: 200. 200 a -0.02703969 H = -0.73579 eV

Gap : +0.09363565 H = +2.54796 eV

Number of MOs= 770, Electrons= 398.00, Symmetry: c1

\$coord

-1.74563029657475	2.66947201834482	1.24596970988192	c
0.96140577862830	2.65531085618661	0.95539914951744	c
2.19991008225471	4.98589774371751	1.19947771526559	c
0.91227036599044	7.27052423289360	1.65961582883525	c
-1.72541726302369	7.28753860497826	1.86038620111380	c
-3.01746848184382	4.98945222125809	1.62580823707084	c
-3.19941498781160	0.11540687946994	1.37939429897516	b
-1.67276610945877	-2.29067845792310	2.10447774934174	c
0.98200547276179	-2.38757765297175	1.53685290433880	c
2.40497628474605	-0.00194968240697	0.11041000444855	b
-2.84962919744873	-4.39824619937247	3.24864610823341	c
-1.51194187312783	-6.58580158247885	3.89530618867156	c
1.06612694091883	-6.70528497746304	3.30106293587475	c
2.24634945817408	-4.64634731173170	2.10559827116989	c
5.43120010296752	0.03447648813493	0.91227414819544	c
6.08869654226685	0.45519761151874	3.45354266930833	c
8.58114680271206	0.51607888022798	4.36030735067582	c
10.57889990571688	0.11256821911249	2.66333872597272	c
10.02990792472625	-0.33999870596827	0.11202763586652	c
7.49713228248477	-0.38958589352474	-0.69888110070427	c
-10.65327324433904	0.08150863730892	1.95143921201257	c
-11.36016075906334	-0.42619144183184	-0.55937082970591	c
-9.49338853657261	-0.75669843298570	-2.41458718646406	c
-6.93764178097339	-0.56545902801420	-1.71117904545097	c
-6.15759213256973	-0.06053236753393	0.76852270335197	c
-8.07879050150521	0.25269822357201	2.56491998908037	c
7.16459665933574	-0.91796600245873	-3.17605195801709	f
11.92840008473349	-0.74928956575690	-1.53269149999144	f
12.98792804399669	0.15734611719164	3.47459883469089	f
9.07780625214421	0.94984587419336	6.81828293178789	f
4.25186581933247	0.84868289187236	5.19060765164852	f
4.69521392066197	-5.03325608688954	1.48478106117492	f
2.38281190724849	-8.79579390661015	3.86894107209271	f
-2.65477085710618	-8.54117008459349	5.04609479803636	f
-5.33440570301665	-4.39669859111744	3.83860481907258	f
-5.18539069857387	-0.88207584432833	-3.53786444483787	f
-10.15809163990176	-1.24711011272834	-4.81292961204610	f
-13.81513800280575	-0.59113972861601	-1.17802275180413	f
-12.44501910212703	0.39784796590980	3.72150843976939	f
-7.47016705438754	0.74932205875845	4.98626165058780	f
-5.55687218638709	5.11902958125109	1.86579495492888	f
-2.96652447589618	9.46397904275380	2.28331678551015	f
2.19428000784765	9.44437667673168	1.89625569062302	f
4.73159384721931	5.22751644644208	1.01177215808548	f
1.95354164406249	-0.22287427581357	-3.02774482726596	c
0.88358404397369	-2.30989435677096	-4.28813031644423	c
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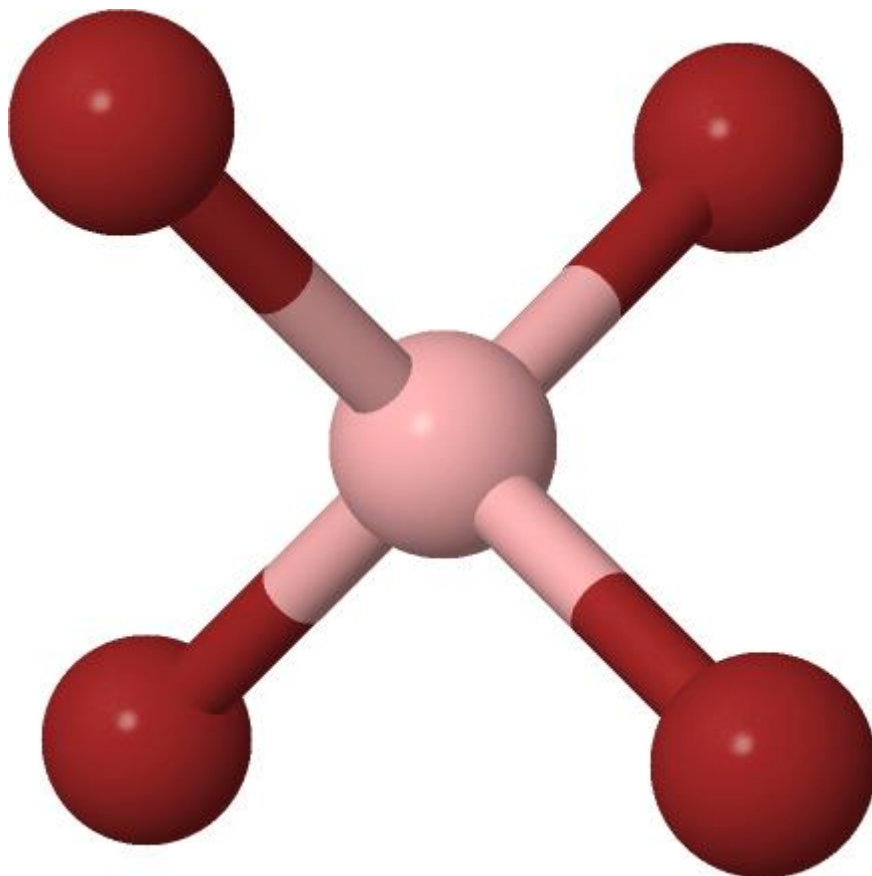
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3.71249691204391	3.88854291010235	-3.72888530965347	f
2.76478333323015	3.83459569100428	-8.68006067338491	f
0.56991859426216	-0.32350752529649	-10.91029633963478	f
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0.25164964242594	-4.45039372466760	-3.04718536935059	f

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		11.33	0.01222	YES	YES
8	a		17.94	0.00455	YES	YES
9	a		20.95	0.01213	YES	YES
10	a		26.89	0.00817	YES	YES
11	a		27.78	0.00795	YES	YES
12	a		29.89	0.00590	YES	YES
13	a		34.52	0.01289	YES	YES
14	a		38.17	0.00018	YES	YES
15	a		42.01	0.01197	YES	YES
16	a		43.33	0.00686	YES	YES
17	a		58.42	0.00412	YES	YES
18	a		81.85	0.03705	YES	YES
19	a		91.35	0.07491	YES	YES
20	a		101.86	0.07257	YES	YES
21	a		109.33	0.11344	YES	YES
22	a		114.74	0.02088	YES	YES
23	a		115.47	0.14086	YES	YES
24	a		119.24	0.03680	YES	YES
25	a		122.27	0.03907	YES	YES
26	a		126.45	0.02231	YES	YES
27	a		129.74	0.00559	YES	YES
28	a		130.47	0.01784	YES	YES
29	a		140.14	0.06395	YES	YES
30	a		146.78	0.05898	YES	YES
31	a		149.50	0.00725	YES	YES
32	a		157.97	0.11532	YES	YES
33	a		161.21	0.00578	YES	YES
34	a		163.73	0.00413	YES	YES
35	a		166.34	0.00979	YES	YES
36	a		188.28	1.07341	YES	YES
37	a		200.33	0.33945	YES	YES
38	a		205.59	0.78664	YES	YES
39	a		220.52	0.32476	YES	YES
40	a		229.07	1.37018	YES	YES
41	a		232.99	1.11585	YES	YES
42	a		236.05	3.22080	YES	YES
43	a		239.80	2.32936	YES	YES
44	a		260.58	0.04035	YES	YES
45	a		261.39	0.05993	YES	YES
46	a		262.89	0.10420	YES	YES

47	a	265.20	0.04329	YES	YES
48	a	269.57	0.06047	YES	YES
49	a	270.61	0.04600	YES	YES
50	a	272.40	0.03072	YES	YES
51	a	278.55	0.05503	YES	YES
52	a	292.36	0.27115	YES	YES
53	a	295.28	0.04730	YES	YES
54	a	298.13	0.41621	YES	YES
55	a	308.13	0.41093	YES	YES
56	a	314.78	0.34551	YES	YES
57	a	326.68	0.89378	YES	YES
58	a	336.64	1.85971	YES	YES
59	a	339.50	1.52321	YES	YES
60	a	345.63	3.59388	YES	YES
61	a	348.49	0.86470	YES	YES
62	a	359.49	1.23574	YES	YES
63	a	363.24	0.68294	YES	YES
64	a	377.69	0.41793	YES	YES
65	a	381.38	0.80327	YES	YES
66	a	385.18	0.11055	YES	YES
67	a	389.15	0.26838	YES	YES
68	a	391.29	0.15934	YES	YES
69	a	396.81	0.10194	YES	YES
70	a	405.76	1.98140	YES	YES
71	a	410.24	1.58596	YES	YES
72	a	431.05	0.14758	YES	YES
73	a	434.11	0.05678	YES	YES
74	a	437.80	0.12225	YES	YES
75	a	451.65	1.43783	YES	YES
76	a	458.45	3.19497	YES	YES
77	a	461.40	0.14341	YES	YES
78	a	464.55	4.13297	YES	YES
79	a	474.26	0.24504	YES	YES
80	a	477.02	2.55178	YES	YES
81	a	500.01	1.50067	YES	YES
82	a	508.02	0.01840	YES	YES
83	a	525.79	0.04296	YES	YES
84	a	526.55	0.07997	YES	YES
85	a	527.58	0.22152	YES	YES
86	a	550.26	0.69947	YES	YES
87	a	554.44	1.38405	YES	YES
88	a	562.43	2.82491	YES	YES
89	a	563.28	0.87480	YES	YES
90	a	565.88	0.73143	YES	YES
91	a	595.26	19.23124	YES	YES
92	a	603.59	13.82707	YES	YES
93	a	607.34	43.78450	YES	YES
94	a	608.55	31.57947	YES	YES
95	a	628.24	1.19371	YES	YES
96	a	630.66	0.15072	YES	YES
97	a	632.55	4.15220	YES	YES
98	a	634.66	2.27620	YES	YES
99	a	639.94	16.87050	YES	YES
100	a	665.64	5.37912	YES	YES
101	a	667.44	4.90786	YES	YES
102	a	676.43	35.01493	YES	YES
103	a	688.93	46.92107	YES	YES
104	a	690.10	10.65595	YES	YES
105	a	727.10	25.83905	YES	YES
106	a	739.28	5.17181	YES	YES
107	a	755.56	46.97694	YES	YES
108	a	760.62	6.09335	YES	YES

109	a	762.45	68.65743	YES	YES
110	a	778.79	12.32204	YES	YES
111	a	808.48	0.25380	YES	YES
112	a	846.55	2.89560	YES	YES
113	a	892.06	1.85754	YES	YES
114	a	922.10	0.69959	YES	YES
115	a	937.73	6.51568	YES	YES
116	a	973.67	52.51110	YES	YES
117	a	976.28	254.22612	YES	YES
118	a	980.26	131.90974	YES	YES
119	a	1002.13	23.31370	YES	YES
120	a	1009.11	222.33969	YES	YES
121	a	1058.56	68.70462	YES	YES
122	a	1083.48	121.87149	YES	YES
123	a	1090.48	182.76761	YES	YES
124	a	1096.89	100.11161	YES	YES
125	a	1108.59	111.46355	YES	YES
126	a	1128.35	3.72081	YES	YES
127	a	1131.43	6.81394	YES	YES
128	a	1144.31	6.69279	YES	YES
129	a	1150.14	133.57023	YES	YES
130	a	1162.42	58.02736	YES	YES
131	a	1253.41	41.96014	YES	YES
132	a	1258.18	27.57675	YES	YES
133	a	1267.18	42.81770	YES	YES
134	a	1268.50	6.70180	YES	YES
135	a	1285.57	20.16655	YES	YES
136	a	1298.51	322.31531	YES	YES
137	a	1314.33	114.69806	YES	YES
138	a	1340.64	7.42932	YES	YES
139	a	1344.05	150.23376	YES	YES
140	a	1346.87	12.31792	YES	YES
141	a	1354.83	13.16985	YES	YES
142	a	1357.54	38.54163	YES	YES
143	a	1368.88	9.88943	YES	YES
144	a	1378.09	21.52895	YES	YES
145	a	1403.59	65.69549	YES	YES
146	a	1416.24	110.70814	YES	YES
147	a	1426.41	484.20478	YES	YES
148	a	1455.55	376.63451	YES	YES
149	a	1463.53	370.51849	YES	YES
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151	a	1478.61	401.48821	YES	YES
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153	a	1510.17	264.29138	YES	YES
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155	a	1514.60	113.17487	YES	YES
156	a	1583.55	133.09882	YES	YES
157	a	1590.29	19.19097	YES	YES
158	a	1606.40	52.17403	YES	YES
159	a	1613.82	71.39057	YES	YES
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161	a	1616.42	9.69341	YES	YES
162	a	1619.37	6.27550	YES	YES
163	a	1625.57	45.59366	YES	YES
164	a	1627.73	15.29672	YES	YES
165	a	1635.76	32.88814	YES	YES



Total energy = -10321.6005131700 H = -280865.2002041 eV

HOMO-LUMO Separation

HOMO: 32. 5 t1 -0.06566804 H = -1.78692 eV

LUMO: 33. 10 a1 +0.14821709 H = +4.03319 eV

Gap : +0.21388513 H = +5.82011 eV

Number of MOs= 61, Electrons= 146.00, Symmetry: td

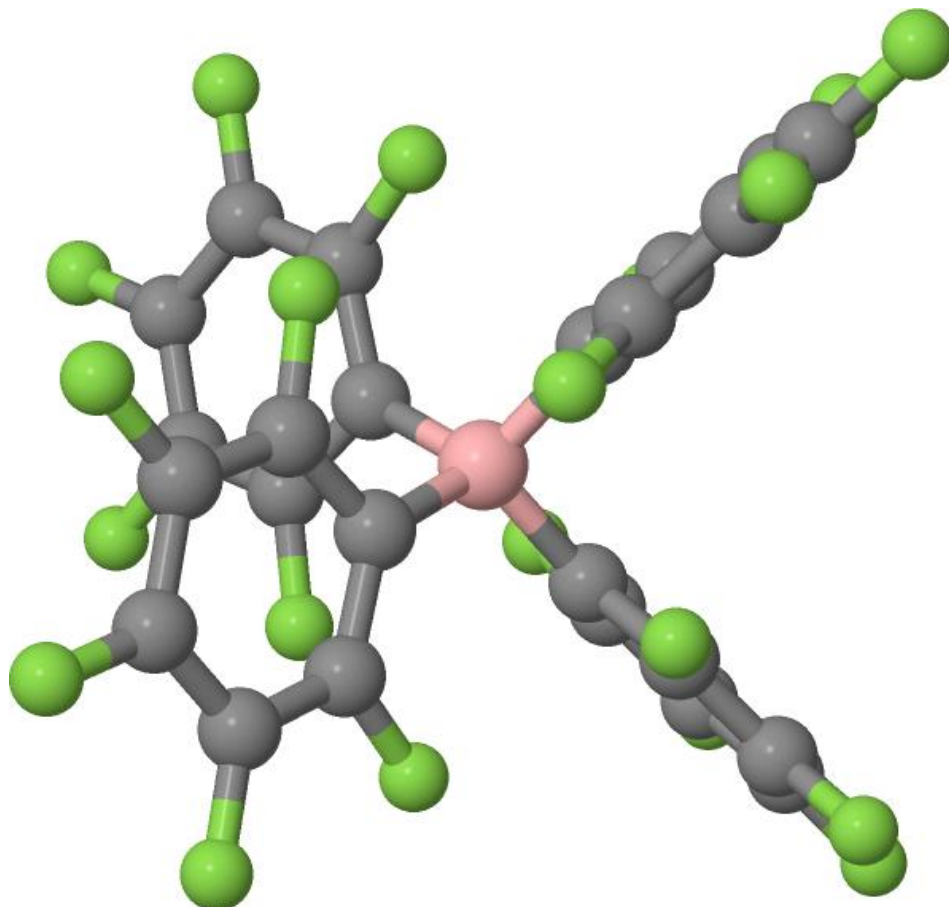
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\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	100.92	0.00000	NO	YES
8		e	100.92	0.00000	NO	YES
9		t2	151.88	0.66435	YES	YES
10		t2	151.88	0.66435	YES	YES
11		t2	151.88	0.66435	YES	YES
12		a1	225.15	0.00000	NO	YES
13		t2	566.50	204.61300	YES	YES
14		t2	566.50	204.61300	YES	YES
15		t2	566.50	204.61300	YES	YES

[B(C₆F₅)₄]⁻



Total energy = -2934.1674363420 H = -79842.8037773 eV

HOMO-LUMO Separation

HOMO: 165. 165 a -0.11464764 H = -3.11972 eV

LUMO: 166. 166 a +0.04023164 H = +1.09476 eV

Gap : +0.15487928 H = +4.21448 eV

Number of MOs= 630, Electrons= 330.00, Symmetry: c1

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0.32531284737299	1.77893593008218	4.87801461545554	c
1.63533316813981	2.21018710331650	7.15552532387486	c
4.17037482592527	1.47991152503592	7.37235846631424	c
5.36277628390194	0.34343463197790	5.29422384654987	c
3.97831274213406	-0.03500079090240	3.06373656851166	c
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-7.40640385510605	1.26636326670534	-1.39905802506566	c
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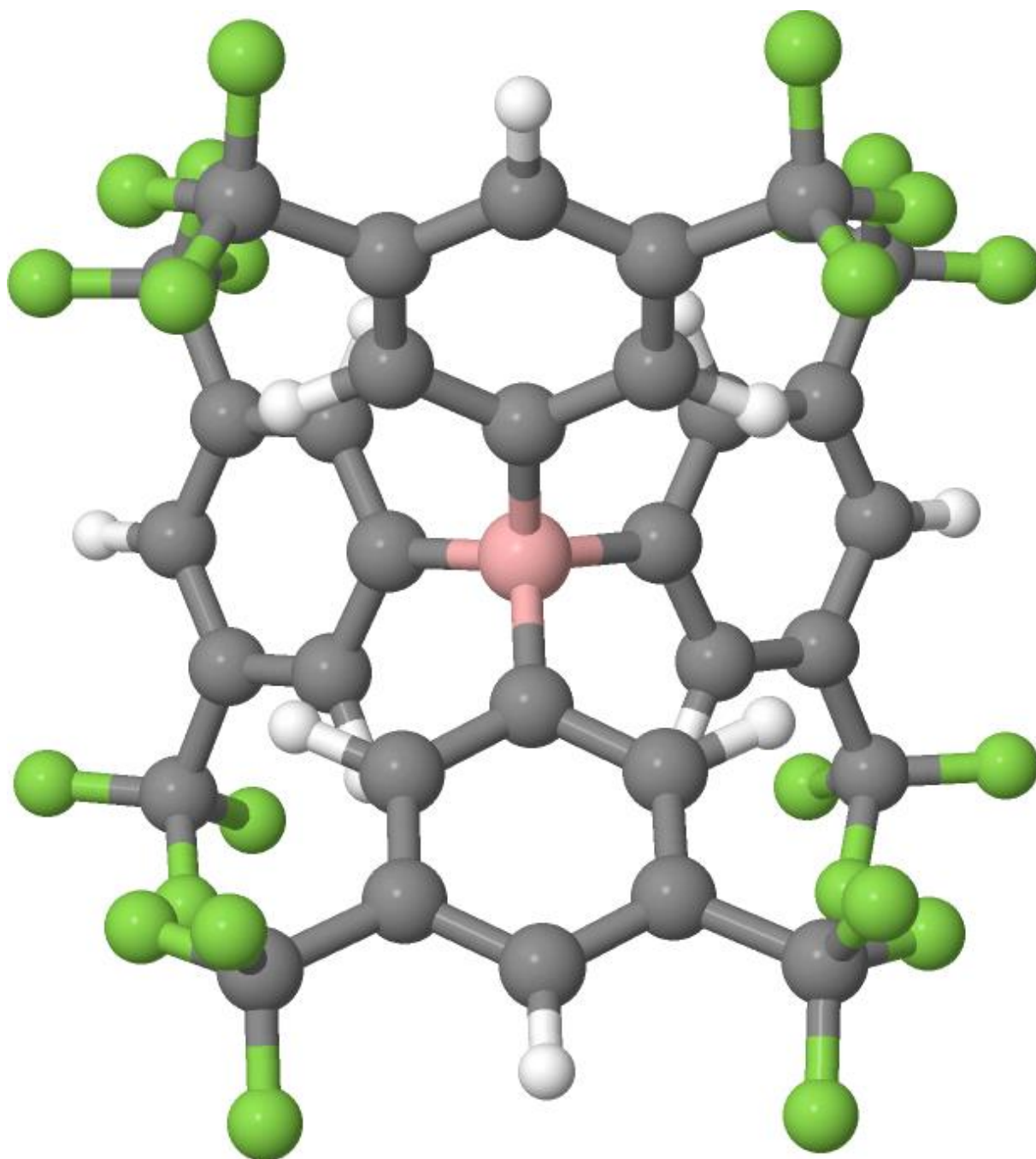
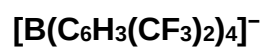
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\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	26.68	0.00028	YES	YES
8		a	26.99	0.00018	YES	YES
9		a	28.54	0.01737	YES	YES
10		a	31.59	0.00556	YES	YES
11		a	41.99	0.01165	YES	YES
12		a	42.43	0.01364	YES	YES
13		a	46.29	0.01091	YES	YES
14		a	47.65	0.00944	YES	YES
15		a	58.15	0.00171	YES	YES
16		a	108.60	0.01571	YES	YES
17		a	108.89	0.01205	YES	YES
18		a	119.78	0.16031	YES	YES
19		a	125.10	0.00110	YES	YES
20		a	125.58	0.00061	YES	YES
21		a	131.29	0.00123	YES	YES
22		a	136.18	0.01223	YES	YES
23		a	137.07	0.01516	YES	YES
24		a	141.52	0.00625	YES	YES
25		a	145.08	0.06297	YES	YES
26		a	145.60	0.07283	YES	YES
27		a	151.84	0.00002	YES	YES
28		a	159.23	0.02429	YES	YES
29		a	164.20	0.09414	YES	YES
30		a	165.13	0.07991	YES	YES
31		a	165.55	0.09528	YES	YES
32		a	174.22	0.00049	YES	YES
33		a	228.17	1.50755	YES	YES
34		a	230.99	1.53701	YES	YES
35		a	237.05	1.12913	YES	YES
36		a	240.65	3.30270	YES	YES
37		a	260.71	0.07915	YES	YES
38		a	261.50	0.07936	YES	YES
39		a	262.24	0.05236	YES	YES
40		a	262.27	0.06046	YES	YES
41		a	272.79	0.03438	YES	YES
42		a	273.33	0.05516	YES	YES
43		a	273.74	0.05325	YES	YES
44		a	274.54	0.00909	YES	YES
45		a	308.96	0.01478	YES	YES
46		a	310.34	0.73608	YES	YES
47		a	310.52	0.16113	YES	YES
48		a	311.11	0.63062	YES	YES
49		a	339.09	1.14391	YES	YES
50		a	339.91	1.09324	YES	YES

51	a	344.77	6.96477	YES	YES
52	a	351.17	0.00840	YES	YES
53	a	366.91	0.44350	YES	YES
54	a	367.48	0.45755	YES	YES
55	a	385.72	0.23946	YES	YES
56	a	386.84	0.29849	YES	YES
57	a	387.96	0.19594	YES	YES
58	a	388.96	0.02279	YES	YES
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60	a	410.05	0.00332	YES	YES
61	a	434.40	0.00005	YES	YES
62	a	435.43	0.02090	YES	YES
63	a	435.71	0.02635	YES	YES
64	a	436.08	0.15030	YES	YES
65	a	461.20	0.94205	YES	YES
66	a	463.21	1.08335	YES	YES
67	a	463.49	1.03468	YES	YES
68	a	477.97	0.00070	YES	YES
69	a	505.77	0.19940	YES	YES
70	a	513.21	0.24057	YES	YES
71	a	514.86	0.06614	YES	YES
72	a	517.41	0.06027	YES	YES
73	a	561.14	4.97183	YES	YES
74	a	563.18	2.37519	YES	YES
75	a	563.48	2.30577	YES	YES
76	a	565.55	0.00918	YES	YES
77	a	597.63	11.96082	YES	YES
78	a	598.50	12.11160	YES	YES
79	a	600.62	23.00116	YES	YES
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81	a	629.10	0.11249	YES	YES
82	a	630.07	0.43492	YES	YES
83	a	632.18	0.05833	YES	YES
84	a	671.14	35.30553	YES	YES
85	a	671.35	35.12167	YES	YES
86	a	673.53	1.71314	YES	YES
87	a	720.82	106.68602	YES	YES
88	a	738.20	0.05261	YES	YES
89	a	755.78	11.04892	YES	YES
90	a	761.99	28.82045	YES	YES
91	a	762.20	29.73812	YES	YES
92	a	809.59	0.00782	YES	YES
93	a	898.67	0.20712	YES	YES
94	a	901.42	0.19989	YES	YES
95	a	944.35	11.47941	YES	YES
96	a	964.24	0.04868	YES	YES
97	a	980.40	30.15139	YES	YES
98	a	984.66	321.33408	YES	YES
99	a	985.02	326.19262	YES	YES
100	a	1083.99	154.32316	YES	YES
101	a	1084.50	155.33454	YES	YES
102	a	1085.13	20.27939	YES	YES
103	a	1098.08	398.73888	YES	YES
104	a	1124.00	0.00458	YES	YES
105	a	1132.57	3.39032	YES	YES
106	a	1134.36	5.02884	YES	YES
107	a	1134.48	5.74578	YES	YES
108	a	1265.10	23.78533	YES	YES
109	a	1265.95	22.69651	YES	YES
110	a	1269.92	70.09062	YES	YES
111	a	1271.38	3.82924	YES	YES
112	a	1341.74	0.00777	YES	YES

113	a	1346.27	7.55894	YES	YES
114	a	1346.39	7.69084	YES	YES
115	a	1347.40	4.43837	YES	YES
116	a	1369.68	15.31421	YES	YES
117	a	1370.59	15.00620	YES	YES
118	a	1379.91	5.46169	YES	YES
119	a	1385.47	0.11390	YES	YES
120	a	1446.76	0.04326	YES	YES
121	a	1464.06	91.85651	YES	YES
122	a	1465.68	685.00912	YES	YES
123	a	1466.19	713.42686	YES	YES
124	a	1509.34	191.68383	YES	YES
125	a	1509.81	190.80509	YES	YES
126	a	1510.83	342.22272	YES	YES
127	a	1514.98	1.86646	YES	YES
128	a	1613.17	0.06154	YES	YES
129	a	1615.34	7.94142	YES	YES
130	a	1615.44	8.18967	YES	YES
131	a	1616.79	12.13179	YES	YES
132	a	1625.77	39.27322	YES	YES
133	a	1626.27	40.32751	YES	YES
134	a	1626.47	57.03128	YES	YES
135	a	1628.94	0.69155	YES	YES



Total energy = -3645.3894886000 H = -99196.1515301 eV

HOMO-LUMO Separation

HOMO: 213. 213 a -0.13958380 H = -3.79827 eV

LUMO: 214. 214 a +0.00485433 H = +0.13209 eV

Gap : +0.14443813 H = +3.93036 eV

Number of MOs= 822, Electrons= 426.00, Symmetry: c1

\$coord

0.00949946454863	0.05208000411949	0.00791569298063	b
-2.27352272352135	-2.01388207528278	-0.51310140957651	c
-1.52923458751667	2.75484414361206	0.27387263175119	c
-2.45846053697878	3.64384935146215	2.61740198371794	c
-3.96540946504930	5.83035437960269	2.81337396021491	c
-4.60260510674203	7.21877335782943	0.64557844016569	c
-3.73634551657094	6.36170847220574	-1.71391623665201	c
-2.23344425420367	4.17582125852767	-1.88193209557080	c
1.69831219010429	-0.64152026721038	2.54155237421017	c
2.13312767047272	0.07327654838892	-2.28145324377434	c
2.13597090030428	-3.16529256644179	3.30560128292653	c
3.72468028571968	-3.78046930555968	5.35142787193098	c
4.94851166439911	-1.86644934739241	6.71997054525174	c
4.57931199891042	0.65865711448210	5.98403042023542	c
2.98995196813182	1.24439201125832	3.93363595187570	c
-3.65243407571229	-3.12318871975693	1.49301409140125	c
-5.69073528785364	-4.77888763847631	1.07365915748082	c
-6.43886622112516	-5.38972955160469	-1.40118331055205	c
-5.13264494586390	-4.28749148771825	-3.42947300484120	c
-3.10077888916954	-2.62694885742202	-2.97848062416241	c
3.48926065914981	2.27480737926232	-2.95706758651341	c
5.43188928801069	2.24446054105798	-4.77924144459030	c
6.08292990770206	-0.01108124332275	-6.01253763371062	c
4.78441038225311	-2.23473608182791	-5.36566562399611	c
2.86398194437746	-2.18032959974356	-3.52747366552007	c
-4.53743700537640	7.77625556898315	-4.05751716524157	c
-6.98730759156725	7.28098956584711	-4.67463906343341	f
-3.12343537318318	7.18104432654811	-6.10559753504327	f
-4.37998288180730	10.32606187411732	-3.74056765947995	f
-5.01800857239239	6.63797554933082	5.33897687771115	c
-7.34169147096821	5.61673079992848	5.76988381874118	f
-5.30926629184952	9.18916590103806	5.49509560593738	f
-3.52949999592934	5.92803190938116	7.29904239136478	f
5.98455231122896	2.71181720486339	7.37999835263957	c
4.94476009582768	5.02636724784286	7.04147760978770	f
8.43750439662906	2.87978743585382	6.61623366618003	f
6.05106322018229	2.27439760940425	9.91569449806130	f
4.19249188710678	-6.51166651560924	6.03264209839345	c
2.20213761151888	-8.01466912180115	5.44646101326159	f
6.23290163135887	-7.47598598392476	4.79468447869040	f
4.66007558584113	-6.81658468807399	8.54381544873684	f
-5.94154277075223	-4.84203137500319	-6.10911425607077	c
-7.07245167811255	-7.14091015565524	-6.32720128782303	f
-7.63459218293072	-3.11370604928684	-6.98487283521230	f
-3.96306002420308	-4.81727609749675	-7.73954353285653	f
-7.14004965757035	-5.87527101497159	3.27289974171490	c
-9.28299009955560	-4.53987256524997	3.77608387605014	f
-5.76706696998067	-5.90304126901080	5.43381368872411	f
-7.88981473678267	-8.29489881186490	2.81844497599463	f
6.89206768581319	4.62972570847819	-5.33912149360534	c

5.39852063370803	6.71346836501651	-5.31519684190779	f
8.04465176220357	4.55279286981872	-7.63647341389768	f
8.74666726140858	5.03934938904061	-3.60397170171531	f
5.53028856341866	-4.69819470481708	-6.59802329365175	c
3.57544332860373	-6.34912832739319	-6.73958774336414	f
7.40954323435455	-5.89071298600560	-5.30680931474707	f
6.40724117366619	-4.35419162333491	-8.99219372449977	f
-1.99587703347341	2.60184215407849	4.36036897018522	h
-5.75235683716743	8.94467314380666	0.79144269298299	h
-1.59249759128600	3.55850609062065	-3.76418841176367	h
1.19776050470350	-4.71822242538457	2.28306870609479	h
6.16023347328548	-2.33225994289184	8.34333469349095	h
2.74706429096875	3.24545603861479	3.41039101380154	h
-3.11126439405504	-2.69914205011434	3.45861415647274	h
-7.99679689257106	-6.72207153791638	-1.74215836221431	h
-2.11416277203886	-1.80680047414731	-4.61876183131826	h
3.01745014948031	4.08563315844700	-2.03987488192404	h
7.56691995690243	-0.03278379431749	-7.46601061203189	h
1.89118480845101	-3.96184871884446	-3.06212182552249	h

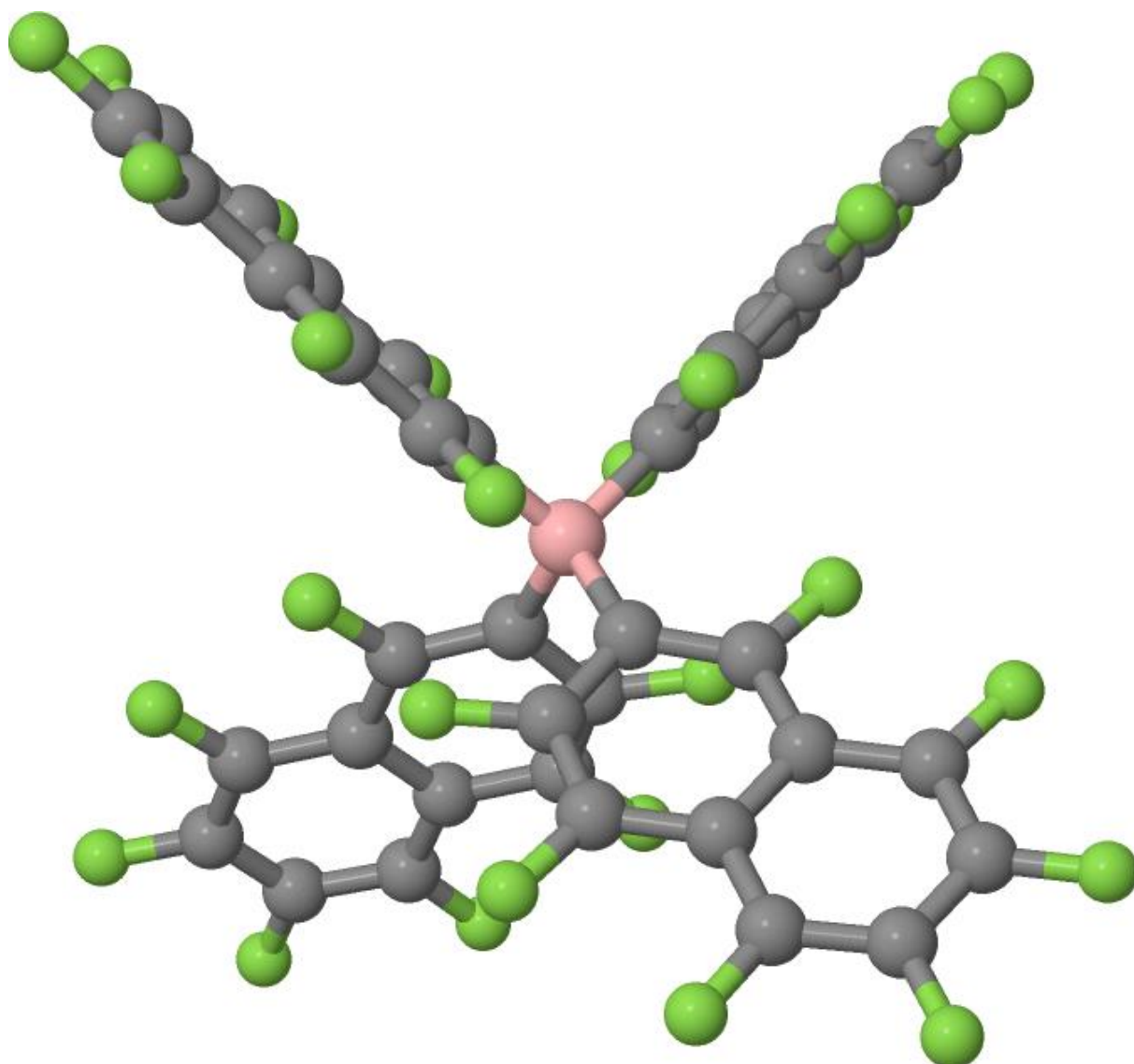
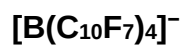
\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	3.73	0.00018	YES	YES
8		a	14.22	0.00098	YES	YES
9		a	16.18	0.00125	YES	YES
10		a	17.08	0.00555	YES	YES
11		a	19.15	0.00115	YES	YES
12		a	20.73	0.01362	YES	YES
13		a	21.79	0.00585	YES	YES
14		a	22.29	0.01848	YES	YES
15		a	23.19	0.04711	YES	YES
16		a	24.86	0.01203	YES	YES
17		a	25.48	0.01880	YES	YES
18		a	26.30	0.01029	YES	YES
19		a	27.43	0.01860	YES	YES
20		a	28.29	0.00643	YES	YES
21		a	30.22	0.00486	YES	YES
22		a	31.48	0.00751	YES	YES
23		a	38.29	0.01938	YES	YES
24		a	82.30	0.00080	YES	YES
25		a	84.68	0.00321	YES	YES
26		a	86.16	0.10796	YES	YES
27		a	87.09	0.05797	YES	YES
28		a	92.17	0.47398	YES	YES
29		a	92.46	0.47136	YES	YES
30		a	95.49	0.69630	YES	YES
31		a	98.86	0.01046	YES	YES
32		a	113.99	0.19268	YES	YES
33		a	117.26	0.15258	YES	YES
34		a	137.53	0.01582	YES	YES
35		a	138.49	0.00826	YES	YES

36	a	139.67	0.00239	YES	YES
37	a	151.23	0.32424	YES	YES
38	a	153.60	0.33232	YES	YES
39	a	163.72	0.00248	YES	YES
40	a	174.62	0.00084	YES	YES
41	a	191.95	0.43173	YES	YES
42	a	193.84	0.45321	YES	YES
43	a	217.97	0.30804	YES	YES
44	a	248.95	0.61593	YES	YES
45	a	250.05	0.66302	YES	YES
46	a	251.58	0.21026	YES	YES
47	a	252.53	0.07849	YES	YES
48	a	259.48	0.10290	YES	YES
49	a	276.76	2.37751	YES	YES
50	a	279.93	2.08731	YES	YES
51	a	281.62	1.78538	YES	YES
52	a	284.19	0.33681	YES	YES
53	a	294.84	0.00476	YES	YES
54	a	310.53	0.20775	YES	YES
55	a	312.92	0.21912	YES	YES
56	a	317.86	0.01730	YES	YES
57	a	335.53	0.08268	YES	YES
58	a	336.51	0.06090	YES	YES
59	a	340.56	0.62373	YES	YES
60	a	348.22	0.05352	YES	YES
61	a	356.25	8.94092	YES	YES
62	a	357.50	9.24687	YES	YES
63	a	361.07	0.33560	YES	YES
64	a	384.54	8.50065	YES	YES
65	a	396.55	0.37763	YES	YES
66	a	397.35	0.25948	YES	YES
67	a	398.90	0.11584	YES	YES
68	a	400.47	0.01100	YES	YES
69	a	435.86	2.74823	YES	YES
70	a	436.12	3.19256	YES	YES
71	a	437.54	0.44911	YES	YES
72	a	449.80	0.04853	YES	YES
73	a	486.96	0.00244	YES	YES
74	a	488.74	0.80349	YES	YES
75	a	488.88	0.76464	YES	YES
76	a	489.40	0.06128	YES	YES
77	a	493.72	0.08070	YES	YES
78	a	494.57	0.02773	YES	YES
79	a	497.50	2.20539	YES	YES
80	a	515.76	0.00347	YES	YES
81	a	551.59	2.35047	YES	YES
82	a	553.85	0.51430	YES	YES
83	a	554.09	0.44380	YES	YES
84	a	555.31	0.08877	YES	YES
85	a	567.80	4.50427	YES	YES
86	a	570.74	2.58628	YES	YES
87	a	571.40	2.33713	YES	YES
88	a	585.86	0.01821	YES	YES
89	a	587.51	0.86533	YES	YES
90	a	587.84	1.03430	YES	YES
91	a	591.78	0.03155	YES	YES
92	a	635.72	0.01328	YES	YES
93	a	647.80	0.00250	YES	YES
94	a	650.24	2.23587	YES	YES
95	a	650.40	1.99732	YES	YES
96	a	650.82	0.18001	YES	YES
97	a	658.63	55.66891	YES	YES

98	a	658.73	58.35798	YES	YES
99	a	659.53	55.12203	YES	YES
100	a	666.40	1.81598	YES	YES
101	a	667.48	15.14255	YES	YES
102	a	667.81	34.28464	YES	YES
103	a	668.22	34.42719	YES	YES
104	a	689.52	0.00865	YES	YES
105	a	703.20	9.90803	YES	YES
106	a	704.19	9.92703	YES	YES
107	a	706.49	38.87861	YES	YES
108	a	720.84	0.02303	YES	YES
109	a	729.15	3.43144	YES	YES
110	a	729.49	0.95467	YES	YES
111	a	730.19	19.67305	YES	YES
112	a	791.09	0.00295	YES	YES
113	a	831.34	31.29983	YES	YES
114	a	831.37	29.69712	YES	YES
115	a	832.50	1.65688	YES	YES
116	a	834.61	0.13091	YES	YES
117	a	867.99	34.00740	YES	YES
118	a	869.14	9.23376	YES	YES
119	a	871.20	25.80111	YES	YES
120	a	874.75	4.80521	YES	YES
121	a	883.27	3.17240	YES	YES
122	a	884.43	5.53801	YES	YES
123	a	885.44	5.66543	YES	YES
124	a	916.98	23.65221	YES	YES
125	a	918.24	25.51615	YES	YES
126	a	919.57	14.17885	YES	YES
127	a	920.82	2.70348	YES	YES
128	a	934.84	0.48834	YES	YES
129	a	939.37	1.92271	YES	YES
130	a	940.62	1.59718	YES	YES
131	a	945.68	24.95633	YES	YES
132	a	983.12	3.67857	YES	YES
133	a	983.30	3.74588	YES	YES
134	a	983.63	4.02362	YES	YES
135	a	984.92	0.15054	YES	YES
136	a	1082.17	0.06951	YES	YES
137	a	1085.93	0.34760	YES	YES
138	a	1086.23	0.66914	YES	YES
139	a	1086.78	0.07023	YES	YES
140	a	1091.94	10.79413	YES	YES
141	a	1092.44	32.54297	YES	YES
142	a	1093.14	39.82475	YES	YES
143	a	1094.19	75.10088	YES	YES
144	a	1119.99	191.75830	YES	YES
145	a	1120.67	142.19082	YES	YES
146	a	1121.90	31.35459	YES	YES
147	a	1123.51	30.71433	YES	YES
148	a	1123.91	8.28958	YES	YES
149	a	1124.94	321.97041	YES	YES
150	a	1125.82	367.34578	YES	YES
151	a	1128.68	92.76094	YES	YES
152	a	1130.15	89.61997	YES	YES
153	a	1132.67	605.21196	YES	YES
154	a	1134.55	115.31928	YES	YES
155	a	1139.73	972.79682	YES	YES
156	a	1154.73	21.57503	YES	YES
157	a	1158.59	63.72709	YES	YES
158	a	1158.99	107.05144	YES	YES
159	a	1159.89	93.72777	YES	YES

160	a	1168.36	112.26941	YES	YES
161	a	1170.02	132.31818	YES	YES
162	a	1173.20	104.08433	YES	YES
163	a	1175.40	18.42544	YES	YES
164	a	1247.43	15.27920	YES	YES
165	a	1250.68	128.33885	YES	YES
166	a	1251.16	970.57856	YES	YES
167	a	1252.60	840.01306	YES	YES
168	a	1256.86	18.75068	YES	YES
169	a	1264.54	71.37845	YES	YES
170	a	1265.42	183.86454	YES	YES
171	a	1267.70	185.16085	YES	YES
172	a	1329.68	381.67842	YES	YES
173	a	1330.94	373.63316	YES	YES
174	a	1335.76	408.71895	YES	YES
175	a	1342.89	2.53606	YES	YES
176	a	1347.26	0.34510	YES	YES
177	a	1359.57	2.79928	YES	YES
178	a	1360.33	2.57757	YES	YES
179	a	1361.28	3.51424	YES	YES
180	a	1415.10	0.27435	YES	YES
181	a	1423.20	13.91803	YES	YES
182	a	1424.43	12.60672	YES	YES
183	a	1426.97	1.72944	YES	YES
184	a	1447.27	0.15061	YES	YES
185	a	1447.43	0.26828	YES	YES
186	a	1450.46	0.14088	YES	YES
187	a	1451.55	1.28700	YES	YES
188	a	1590.88	0.17172	YES	YES
189	a	1591.60	0.28261	YES	YES
190	a	1593.56	0.01718	YES	YES
191	a	1595.01	0.02516	YES	YES
192	a	1603.44	0.58933	YES	YES
193	a	1606.60	15.54140	YES	YES
194	a	1607.17	32.94385	YES	YES
195	a	1607.56	17.40289	YES	YES
196	a	3095.97	3.41272	YES	YES
197	a	3101.67	1.25426	YES	YES
198	a	3102.25	6.33381	YES	YES
199	a	3103.09	3.98344	YES	YES
200	a	3104.86	1.83726	YES	YES
201	a	3105.26	3.79262	YES	YES
202	a	3105.99	1.93775	YES	YES
203	a	3107.55	3.69894	YES	YES
204	a	3129.23	0.68129	YES	YES
205	a	3130.94	0.60879	YES	YES
206	a	3134.16	0.50677	YES	YES
207	a	3138.39	0.23360	YES	YES



Total energy = -4341.6415043440 H = -118142.1436313 eV

HOMO-LUMO Separation

HOMO: 249. 249 a -0.11383554 H = -3.09762 eV

LUMO: 250. 250 a -0.01112785 H = -0.30280 eV

Gap : +0.10270769 H = +2.79482 eV

Number of MOs= 966, Electrons= 498.00, Symmetry: c1

\$coord

3.59798822602528	6.49486840128355	9.47540013316585	c
5.31470955819228	6.75079310862301	7.43054492294407	c
4.88399272760149	5.48614897841209	5.17024395091707	c
2.71135787674286	3.91384976138366	4.83869307881057	c
0.96560999564790	3.65237045717985	6.93813648852796	c
1.46896399649195	4.98123289773067	9.23166106426897	c
2.14433623188607	2.58419154801176	2.56179424048363	c
0.02672650610902	1.06710068523403	2.14962779659904	c
-1.57099943191737	0.82599466660409	4.28733242415614	c
-1.16773780072181	2.06778802522928	6.57553600566375	c
4.06622295658354	7.73928839518546	11.63525964819777	f
7.35527072089330	8.23109158485187	7.71978126192700	f
6.58365530915214	5.80483116632229	3.31870087454855	f
3.79839561667349	2.87341198541018	0.63622469867280	f
-3.62754983599413	-0.66930891818951	4.20909691614230	f
-2.84542348516709	1.71697532287045	8.45712003815523	f
-0.10044369310037	4.80428145671113	11.22000531664635	f
10.36781974723800	-7.69954309980564	-1.14924402931328	c
10.55293988514084	-5.76748936709043	-2.99607166426944	c
8.63054909129640	-3.99555085440044	-3.26628141679746	c
6.41965142443385	-4.07749230556652	-1.71612578869183	c
6.24871485322545	-6.05600942900630	0.17515656798268	c
8.25679206859656	-7.83826970851935	0.40238144965309	c
4.35847619274837	-2.33399822726693	-1.93731769379975	c
2.15229815150381	-2.42315412698546	-0.50593942572207	c
2.13798458573473	-4.34786857779641	1.36542026327309	c
4.04967287407473	-6.10917511363908	1.71473608691069	c
12.24967436823576	-9.38591899750285	-0.93257666052805	f
12.61134910262612	-5.68227300053342	-4.47664958439861	f
8.93691692193957	-2.22580072357727	-5.05304600550608	f
4.63989643311407	-0.50517729631116	-3.69230305072427	f
0.12474965333857	-4.54785678759812	2.91665505665841	f
3.77867396447479	-7.87476941481673	3.52684001112825	f
8.15934004083485	-9.70892433189152	2.11743573633597	f
-1.08180351507241	8.67693034906305	-9.68738164735624	c
-1.31627887242698	9.82602784148775	-7.27790721287501	c
-1.19526405685451	8.36943139628346	-5.09415086324706	c
-0.83510993034270	5.69455659343510	-5.21248697696065	c
-0.62580167491770	4.52735700363205	-7.68379109173583	c
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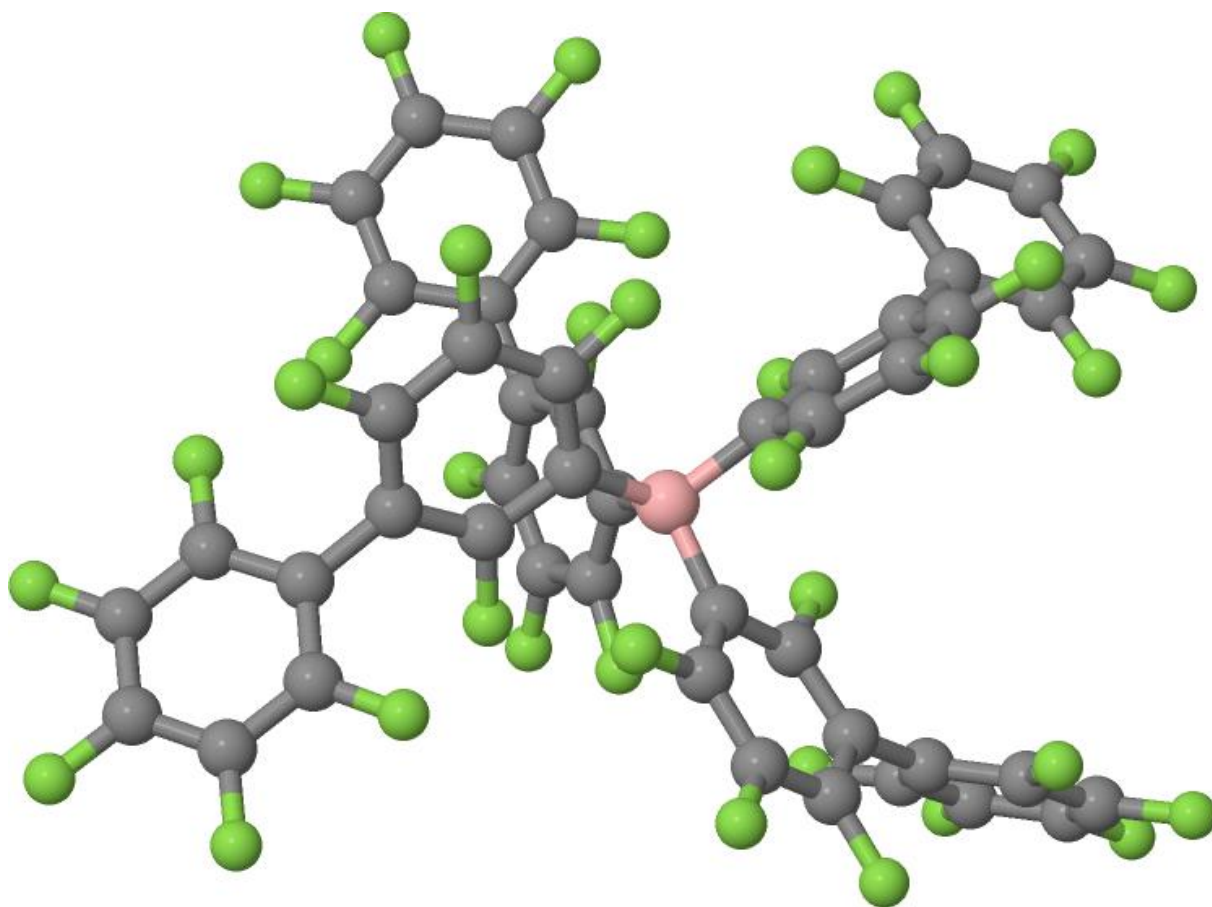
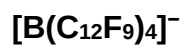
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11		a	21.41	0.00545	YES	YES
12		a	24.44	0.00696	YES	YES
13		a	27.30	0.00316	YES	YES
14		a	30.20	0.00610	YES	YES
15		a	33.66	0.00093	YES	YES
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17		a	64.88	0.02035	YES	YES
18		a	68.32	0.00504	YES	YES
19		a	70.81	0.00232	YES	YES
20		a	75.26	0.04233	YES	YES
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22		a	87.77	0.11680	YES	YES
23		a	91.78	0.05791	YES	YES
24		a	97.39	0.00935	YES	YES
25		a	102.07	0.06268	YES	YES
26		a	108.74	0.04513	YES	YES
27		a	109.68	0.09666	YES	YES
28		a	111.96	0.04420	YES	YES
29		a	117.16	0.06577	YES	YES
30		a	119.02	0.00876	YES	YES
31		a	122.24	0.00871	YES	YES
32		a	125.47	0.18435	YES	YES
33		a	131.92	0.13703	YES	YES
34		a	138.12	0.52061	YES	YES
35		a	141.34	0.12720	YES	YES
36		a	146.81	0.00928	YES	YES
37		a	152.48	0.04346	YES	YES
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39		a	154.21	0.06830	YES	YES
40		a	161.72	0.00474	YES	YES
41		a	180.67	1.51171	YES	YES
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49	a	264.52	0.01130	YES	YES
50	a	266.78	0.02590	YES	YES
51	a	267.01	0.00821	YES	YES
52	a	267.57	0.00582	YES	YES
53	a	274.55	0.29659	YES	YES
54	a	278.04	0.34053	YES	YES
55	a	281.41	0.48291	YES	YES
56	a	282.12	0.08408	YES	YES
57	a	282.85	0.46727	YES	YES
58	a	283.34	0.24224	YES	YES
59	a	289.15	1.25890	YES	YES
60	a	294.68	0.05035	YES	YES
61	a	301.81	0.19584	YES	YES
62	a	305.30	0.22684	YES	YES
63	a	306.38	0.17109	YES	YES
64	a	306.60	0.14113	YES	YES
65	a	311.90	1.21106	YES	YES
66	a	312.99	0.55436	YES	YES
67	a	314.25	1.07248	YES	YES
68	a	318.96	0.82996	YES	YES
69	a	330.99	0.58663	YES	YES
70	a	335.08	0.72362	YES	YES
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72	a	336.49	0.86495	YES	YES
73	a	339.12	7.32542	YES	YES
74	a	342.09	1.17680	YES	YES
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94	a	442.96	0.39795	YES	YES
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HOMO-LUMO Separation

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Gap : +0.12270280 H = +3.33891 eV

Number of MOs= 1190, Electrons= 618.00, Symmetry: c1

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\$vibrational spectrum

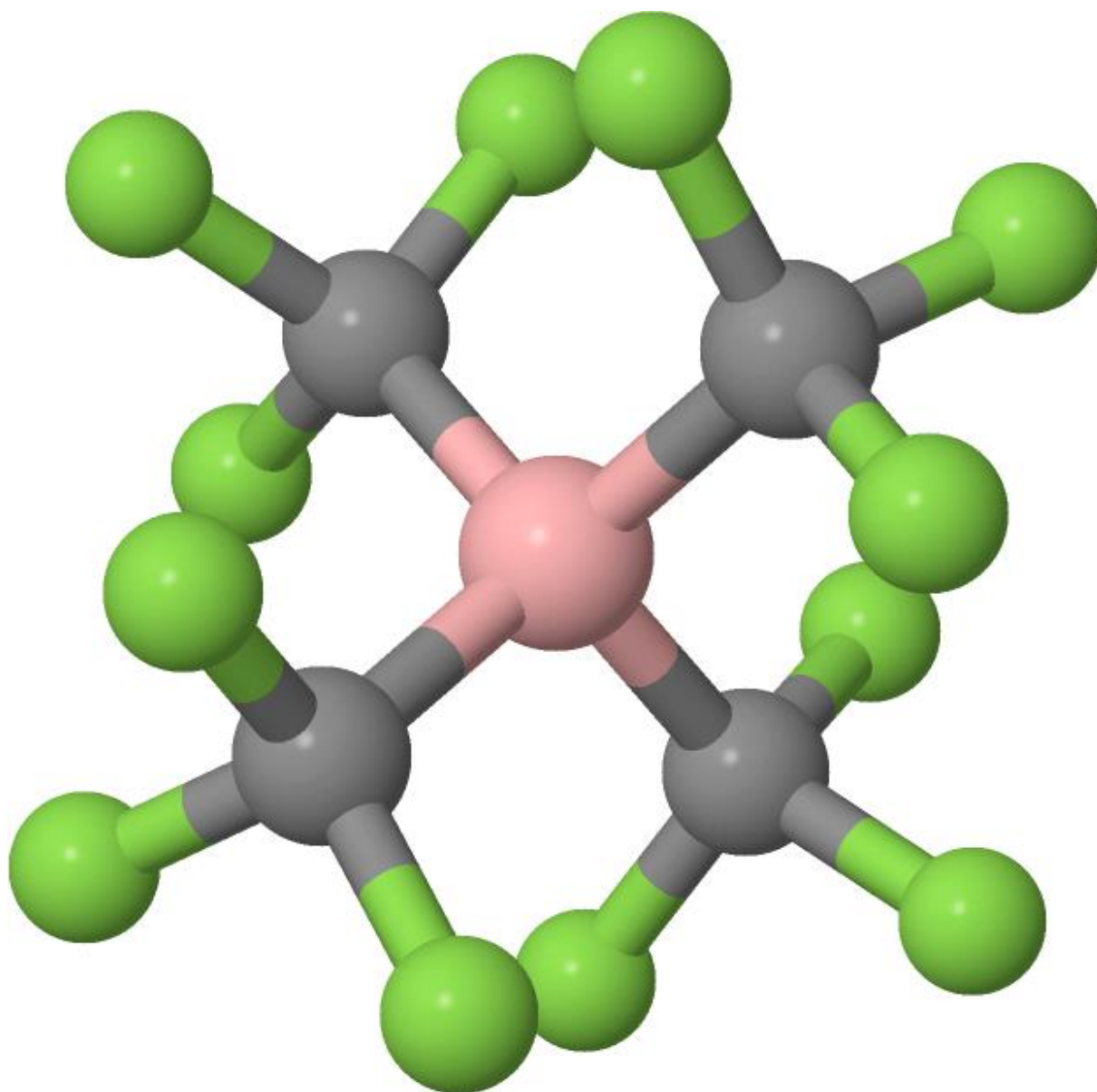
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7		a	9.19	0.01800	YES	YES
8		a	11.37	0.01453	YES	YES
9		a	13.60	0.02095	YES	YES
10		a	16.15	0.02145	YES	YES
11		a	18.26	0.04519	YES	YES
12		a	19.63	0.00666	YES	YES
13		a	21.28	0.00439	YES	YES
14		a	24.08	0.01857	YES	YES
15		a	27.57	0.00651	YES	YES
16		a	31.26	0.02233	YES	YES
17		a	33.02	0.00392	YES	YES
18		a	34.68	0.02414	YES	YES
19		a	37.35	0.01685	YES	YES
20		a	38.20	0.02892	YES	YES
21		a	44.70	0.03475	YES	YES
22		a	48.15	0.00929	YES	YES
23		a	52.11	0.03726	YES	YES
24		a	53.19	0.05209	YES	YES
25		a	58.70	0.02677	YES	YES
26		a	60.89	0.02022	YES	YES
27		a	67.80	0.03161	YES	YES
28		a	91.69	0.01288	YES	YES
29		a	93.73	0.01441	YES	YES
30		a	101.33	0.06062	YES	YES
31		a	102.88	0.11307	YES	YES
32		a	113.67	0.00871	YES	YES
33		a	120.57	0.04888	YES	YES
34		a	123.25	0.01111	YES	YES
35		a	126.07	0.04428	YES	YES
36		a	129.92	0.02589	YES	YES
37		a	131.62	0.05564	YES	YES

38	a	132.68	0.02385	YES	YES
39	a	133.27	0.02567	YES	YES
40	a	134.60	0.09888	YES	YES
41	a	137.21	0.01567	YES	YES
42	a	139.54	0.05752	YES	YES
43	a	139.74	0.02432	YES	YES
44	a	141.37	0.12854	YES	YES
45	a	144.58	0.06547	YES	YES
46	a	146.37	0.11084	YES	YES
47	a	148.52	0.08266	YES	YES
48	a	151.10	0.03290	YES	YES
49	a	164.88	0.35215	YES	YES
50	a	166.05	0.07210	YES	YES
51	a	167.07	0.21549	YES	YES
52	a	169.75	0.00976	YES	YES
53	a	171.00	0.19563	YES	YES
54	a	172.37	0.03792	YES	YES
55	a	173.98	0.11415	YES	YES
56	a	177.70	0.03641	YES	YES
57	a	191.92	0.00404	YES	YES
58	a	198.95	0.11428	YES	YES
59	a	200.42	0.09729	YES	YES
60	a	206.90	0.35831	YES	YES
61	a	236.25	1.10291	YES	YES
62	a	237.94	0.07644	YES	YES
63	a	238.60	2.29552	YES	YES
64	a	240.56	1.25435	YES	YES
65	a	247.24	3.04817	YES	YES
66	a	251.73	2.91187	YES	YES
67	a	255.67	2.49997	YES	YES
68	a	259.47	0.94121	YES	YES
69	a	263.91	0.18705	YES	YES
70	a	265.69	0.17301	YES	YES
71	a	265.98	0.21046	YES	YES
72	a	266.33	0.02162	YES	YES
73	a	267.86	0.02767	YES	YES
74	a	269.66	0.11220	YES	YES
75	a	270.45	0.05198	YES	YES
76	a	270.94	0.09774	YES	YES
77	a	275.02	0.13545	YES	YES
78	a	278.18	0.41000	YES	YES
79	a	278.48	0.23388	YES	YES
80	a	279.28	0.22945	YES	YES
81	a	301.61	0.48715	YES	YES
82	a	303.82	0.72220	YES	YES
83	a	303.89	0.26866	YES	YES
84	a	304.46	0.50147	YES	YES
85	a	317.47	1.32568	YES	YES
86	a	321.05	1.37627	YES	YES
87	a	322.70	1.83643	YES	YES
88	a	323.46	0.57393	YES	YES
89	a	343.31	7.70870	YES	YES
90	a	344.03	3.24409	YES	YES
91	a	344.25	5.41993	YES	YES
92	a	346.57	1.21311	YES	YES
93	a	360.85	0.38305	YES	YES
94	a	363.05	0.79739	YES	YES
95	a	366.54	3.09797	YES	YES
96	a	369.62	0.45793	YES	YES
97	a	370.58	0.49285	YES	YES
98	a	373.62	0.25357	YES	YES
99	a	376.74	0.15108	YES	YES

100	a	378.61	1.25380	YES	YES
101	a	380.84	0.44074	YES	YES
102	a	381.76	0.13483	YES	YES
103	a	382.83	1.37221	YES	YES
104	a	382.96	1.40957	YES	YES
105	a	383.18	0.12081	YES	YES
106	a	384.45	1.20012	YES	YES
107	a	399.31	3.72704	YES	YES
108	a	403.54	0.22605	YES	YES
109	a	405.87	0.74204	YES	YES
110	a	407.16	0.54121	YES	YES
111	a	410.49	1.64822	YES	YES
112	a	423.53	0.11504	YES	YES
113	a	434.73	0.20392	YES	YES
114	a	435.00	0.14102	YES	YES
115	a	436.05	0.04439	YES	YES
116	a	436.77	0.10986	YES	YES
117	a	448.89	0.14553	YES	YES
118	a	449.89	1.04536	YES	YES
119	a	450.59	1.72394	YES	YES
120	a	451.36	0.91240	YES	YES
121	a	473.64	8.84014	YES	YES
122	a	474.10	5.91647	YES	YES
123	a	474.57	2.58619	YES	YES
124	a	477.56	1.05980	YES	YES
125	a	495.21	0.06206	YES	YES
126	a	496.34	0.04222	YES	YES
127	a	497.41	0.02533	YES	YES
128	a	500.08	0.05048	YES	YES
129	a	545.53	61.41403	YES	YES
130	a	554.46	46.72597	YES	YES
131	a	563.03	4.39054	YES	YES
132	a	564.16	1.95329	YES	YES
133	a	564.43	2.80257	YES	YES
134	a	565.15	0.18849	YES	YES
135	a	565.75	1.27976	YES	YES
136	a	568.15	0.39014	YES	YES
137	a	569.48	0.79616	YES	YES
138	a	571.11	3.37535	YES	YES
139	a	577.58	10.99189	YES	YES
140	a	594.78	0.35153	YES	YES
141	a	597.47	0.14889	YES	YES
142	a	600.60	2.15950	YES	YES
143	a	603.47	8.57679	YES	YES
144	a	617.53	0.31815	YES	YES
145	a	618.68	0.18965	YES	YES
146	a	619.53	1.58981	YES	YES
147	a	621.47	1.57852	YES	YES
148	a	624.51	0.07776	YES	YES
149	a	625.07	0.06399	YES	YES
150	a	625.18	0.02876	YES	YES
151	a	626.28	0.11526	YES	YES
152	a	642.85	10.44742	YES	YES
153	a	649.60	15.84523	YES	YES
154	a	653.46	21.67284	YES	YES
155	a	653.80	2.90805	YES	YES
156	a	659.52	8.35336	YES	YES
157	a	671.12	6.92775	YES	YES
158	a	676.90	0.62719	YES	YES
159	a	691.03	60.32832	YES	YES
160	a	703.14	3.21298	YES	YES
161	a	712.71	18.62450	YES	YES

162	a	719.15	16.96657	YES	YES
163	a	744.52	2.23460	YES	YES
164	a	754.19	1.92299	YES	YES
165	a	768.45	28.68008	YES	YES
166	a	770.20	33.70403	YES	YES
167	a	772.19	3.78642	YES	YES
168	a	782.04	3.69101	YES	YES
169	a	784.64	1.36817	YES	YES
170	a	791.93	16.73409	YES	YES
171	a	794.37	24.50666	YES	YES
172	a	834.98	55.15149	YES	YES
173	a	896.25	30.19316	YES	YES
174	a	903.30	26.41694	YES	YES
175	a	935.19	48.76110	YES	YES
176	a	947.46	35.52273	YES	YES
177	a	956.88	39.14902	YES	YES
178	a	960.95	45.07791	YES	YES
179	a	963.74	111.10836	YES	YES
180	a	998.22	128.12929	YES	YES
181	a	1000.26	82.90647	YES	YES
182	a	1000.92	219.83848	YES	YES
183	a	1001.83	176.60022	YES	YES
184	a	1058.12	72.82504	YES	YES
185	a	1065.26	190.68236	YES	YES
186	a	1065.67	339.67878	YES	YES
187	a	1066.17	293.64951	YES	YES
188	a	1080.73	15.19329	YES	YES
189	a	1081.54	105.43219	YES	YES
190	a	1082.69	109.79581	YES	YES
191	a	1095.02	292.81077	YES	YES
192	a	1143.82	1.71619	YES	YES
193	a	1148.79	4.58294	YES	YES
194	a	1149.50	16.34353	YES	YES
195	a	1150.57	13.48193	YES	YES
196	a	1162.64	1.32546	YES	YES
197	a	1164.43	4.63787	YES	YES
198	a	1164.66	8.19683	YES	YES
199	a	1165.43	3.09851	YES	YES
200	a	1249.28	26.32048	YES	YES
201	a	1250.61	4.01559	YES	YES
202	a	1252.44	3.14764	YES	YES
203	a	1254.38	32.76463	YES	YES
204	a	1320.24	14.06247	YES	YES
205	a	1321.38	9.55683	YES	YES
206	a	1322.88	14.55903	YES	YES
207	a	1324.33	1.86369	YES	YES
208	a	1337.37	0.38176	YES	YES
209	a	1339.76	1.13116	YES	YES
210	a	1341.19	1.18046	YES	YES
211	a	1341.89	2.22989	YES	YES
212	a	1345.66	0.27516	YES	YES
213	a	1345.91	0.24268	YES	YES
214	a	1346.07	1.30979	YES	YES
215	a	1347.49	3.43773	YES	YES
216	a	1354.58	5.17658	YES	YES
217	a	1355.00	6.39766	YES	YES
218	a	1361.67	2.31712	YES	YES
219	a	1363.76	13.07279	YES	YES
220	a	1413.87	20.56090	YES	YES
221	a	1421.20	65.62151	YES	YES
222	a	1423.65	41.36772	YES	YES
223	a	1425.23	56.04012	YES	YES

224	a	1444.69	49.76244	YES	YES
225	a	1455.85	635.10645	YES	YES
226	a	1459.19	113.83163	YES	YES
227	a	1459.57	521.27614	YES	YES
228	a	1487.93	125.84406	YES	YES
229	a	1488.73	95.46289	YES	YES
230	a	1489.28	486.80091	YES	YES
231	a	1491.46	37.78178	YES	YES
232	a	1503.36	207.81985	YES	YES
233	a	1505.28	170.37799	YES	YES
234	a	1505.71	559.56681	YES	YES
235	a	1508.02	67.39559	YES	YES
236	a	1519.01	158.31645	YES	YES
237	a	1520.72	351.84033	YES	YES
238	a	1521.04	349.27477	YES	YES
239	a	1521.72	136.50768	YES	YES
240	a	1592.58	61.48085	YES	YES
241	a	1592.85	55.13664	YES	YES
242	a	1594.94	30.47446	YES	YES
243	a	1601.00	63.79443	YES	YES
244	a	1619.95	100.60770	YES	YES
245	a	1622.17	13.71647	YES	YES
246	a	1622.36	12.05589	YES	YES
247	a	1622.68	19.15586	YES	YES
248	a	1623.00	4.26892	YES	YES
249	a	1624.51	116.84473	YES	YES
250	a	1624.64	99.45171	YES	YES
251	a	1626.18	58.95881	YES	YES
252	a	1637.09	7.91091	YES	YES
253	a	1638.04	12.68625	YES	YES
254	a	1638.45	7.55788	YES	YES
255	a	1638.57	9.48411	YES	YES



Total energy = -1374.5730899180 H = -37404.0581790 eV

HOMO-LUMO Separation

HOMO: 69. 34 b -0.12963002 H = -3.52741 eV

LUMO: 70. 36 a +0.20364219 H = +5.54139 eV

Gap : +0.33327221 H = +9.06880 eV

Number of MOs= 238, Electrons= 138.00, Symmetry: c2

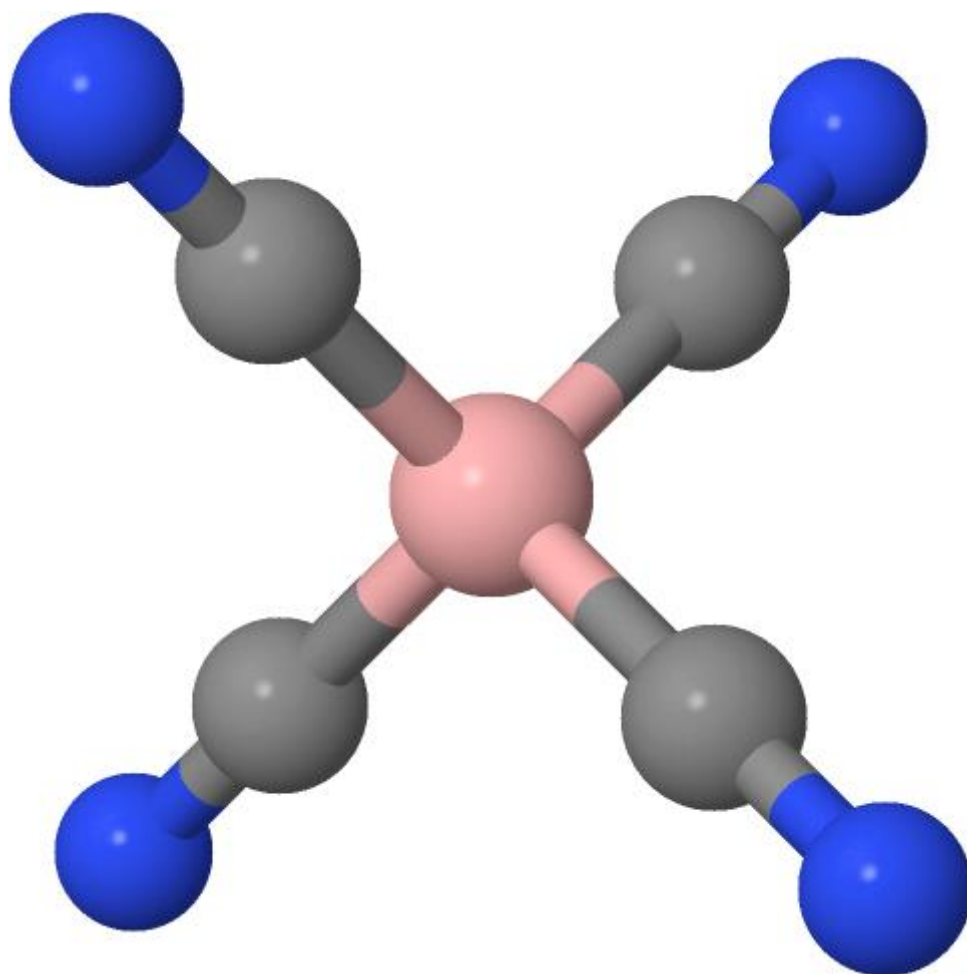
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-1.66449382821996	-1.91546849240542	1.77643414922767	c
-2.84149267877030	-0.71504529426174	3.75325926850585	f
-0.25723244084345	-3.80162020535982	2.87357158317058	f
-3.56477075483680	-3.14413499909254	0.50659789716981	f
2.84149267877030	0.71504529426174	3.75325926850585	f
1.66449382821996	1.91546849240542	1.77643414922767	c
3.56477075483680	3.14413499909254	0.50659789716981	f
0.25723244084345	3.80162020535982	2.87357158317058	f
3.95454177147097	-2.64186811370108	-0.53658425295542	f
1.91844460837758	-1.66449802957596	-1.81712652029033	c
0.77646200592055	-3.71049835791657	-2.93269089883074	f
2.94437861906619	-0.31059174270562	-3.78069751470153	f
-1.91844460837758	1.66449802957596	-1.81712652029033	c
0.00000000000000	0.00000000000000	-0.02181379359863	b
-0.77646200592055	3.71049835791657	-2.93269089883074	f
-2.94437861906619	0.31059174270562	-3.78069751470153	f
-3.95454177147097	2.64186811370108	-0.53658425295542	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
#						
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	49.92	0.00029	YES	YES
8		b	53.62	0.00168	YES	YES
9		a	60.92	0.00102	YES	YES
10		b	62.65	0.00425	YES	YES
11		a	98.96	0.00151	YES	YES
12		a	99.07	0.00207	YES	YES
13		b	138.76	0.07199	YES	YES
14		a	140.78	0.05949	YES	YES
15		b	142.08	0.06262	YES	YES
16		b	244.95	0.05534	YES	YES
17		a	246.96	0.07605	YES	YES
18		b	249.66	0.10793	YES	YES
19		a	264.63	0.00100	YES	YES
20		b	284.85	0.23854	YES	YES
21		a	285.25	0.23825	YES	YES
22		b	285.41	0.25106	YES	YES
23		a	307.73	0.00588	YES	YES
24		a	308.09	0.00052	YES	YES
25		b	502.90	2.38296	YES	YES
26		a	503.64	2.22661	YES	YES
27		b	504.09	2.13992	YES	YES
28		b	509.21	0.39600	YES	YES
29		a	509.21	0.45535	YES	YES
30		b	509.57	0.52779	YES	YES
31		a	531.30	0.00647	YES	YES
32		a	531.57	0.00058	YES	YES
33		b	677.35	31.03098	YES	YES
34		a	677.96	30.75246	YES	YES

35	b	678.65	30.77020	YES	YES
36	a	705.75	0.02919	YES	YES
37	b	901.63	182.07665	YES	YES
38	a	902.02	180.72327	YES	YES
39	b	902.14	179.38094	YES	YES
40	b	1007.69	0.03123	YES	YES
41	a	1009.20	0.01038	YES	YES
42	b	1012.12	0.05255	YES	YES
43	a	1086.68	0.00164	YES	YES
44	a	1087.11	7.58645	YES	YES
45	b	1106.91	325.30136	YES	YES
46	b	1107.35	327.81712	YES	YES
47	a	1108.12	317.99964	YES	YES
48	b	1241.35	334.49422	YES	YES
49	a	1242.30	333.76056	YES	YES
50	b	1243.34	337.60665	YES	YES
51	a	1253.20	2.57559	YES	YES



Total energy = -396.1008307507 H = -10778.4581459 eV

HOMO-LUMO Separation

HOMO: 14. 6 t2 -0.15369905 H = -4.18237 eV

LUMO: 15. 7 t2 +0.09685538 H = +2.63557 eV

Gap : +0.25055444 H = +6.81794 eV

Number of MOs= 55, Electrons= 58.00, Symmetry: td

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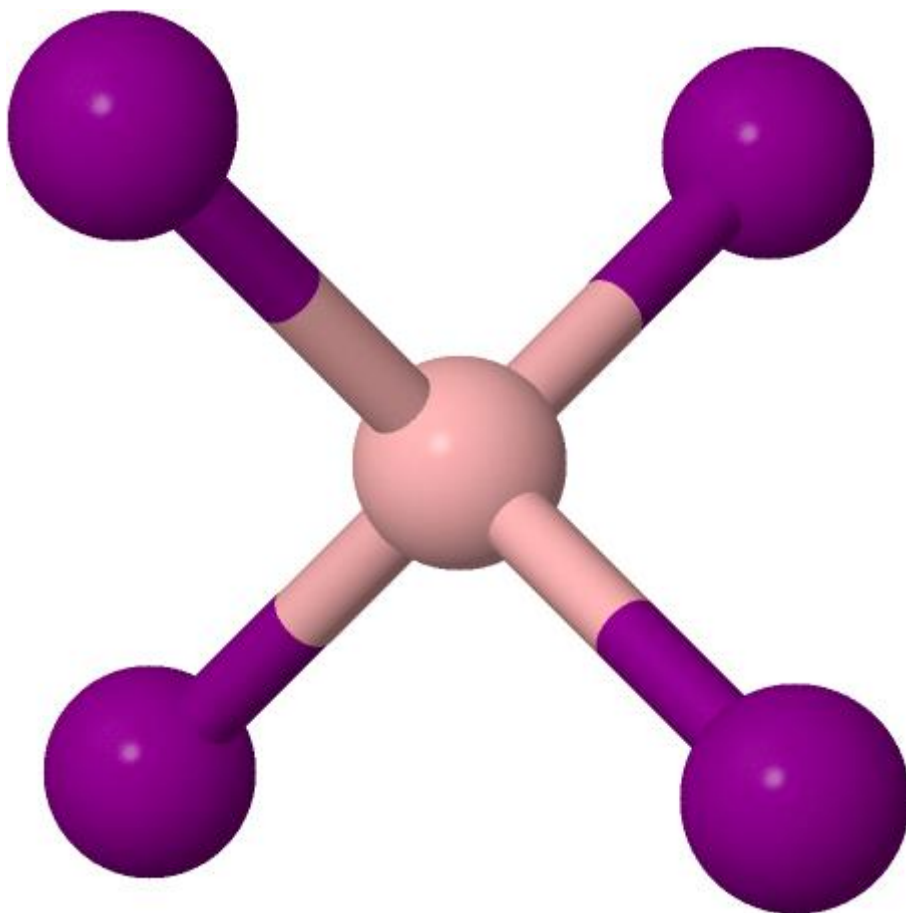
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-1.75177906573481	-1.75177906573481	-1.75177906573481	c
-1.75177906573481	1.75177906573481	1.75177906573480	c
1.75177906573481	-1.75177906573481	1.75177906573481	c
3.03228790065883	-3.03228790065883	3.03228790065883	n
-3.03228790065883	3.03228790065883	3.03228790065883	n
3.03228790065883	3.03228790065883	-3.03228790065883	n
-3.03228790065883	-3.03228790065883	-3.03228790065883	n

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	95.83	0.00000	NO	YES
8		e	95.83	0.00000	NO	YES
9		t2	130.13	8.98026	YES	YES
10		t2	130.13	8.98026	YES	YES
11		t2	130.13	8.98026	YES	YES
12		t1	330.89	0.00000	NO	NO
13		t1	330.89	0.00000	NO	NO
14		t1	330.89	0.00000	NO	NO
15		a1	473.67	0.00000	NO	YES
16		t2	484.86	2.85068	YES	YES
17		t2	484.86	2.85068	YES	YES
18		t2	484.86	2.85068	YES	YES
19		e	513.74	0.00000	NO	YES
20		e	513.74	0.00000	NO	YES
21		t2	933.51	63.85027	YES	YES
22		t2	933.51	63.85027	YES	YES
23		t2	933.51	63.85027	YES	YES

24	t2	2243.45	0.58730	YES	YES
25	t2	2243.45	0.58730	YES	YES
26	t2	2243.45	0.58730	YES	YES
27	a1	2246.55	0.00000	NO	YES

[BI₄]⁻



Total energy = -70.8793558747 H = -1928.7265044 eV

HOMO-LUMO Separation

HOMO: 8. 1 t1 -0.07816006 H = -2.12684 eV

LUMO: 9. 4 a1 +0.05487696 H = +1.49328 eV

Gap : +0.13303702 H = +3.62012 eV

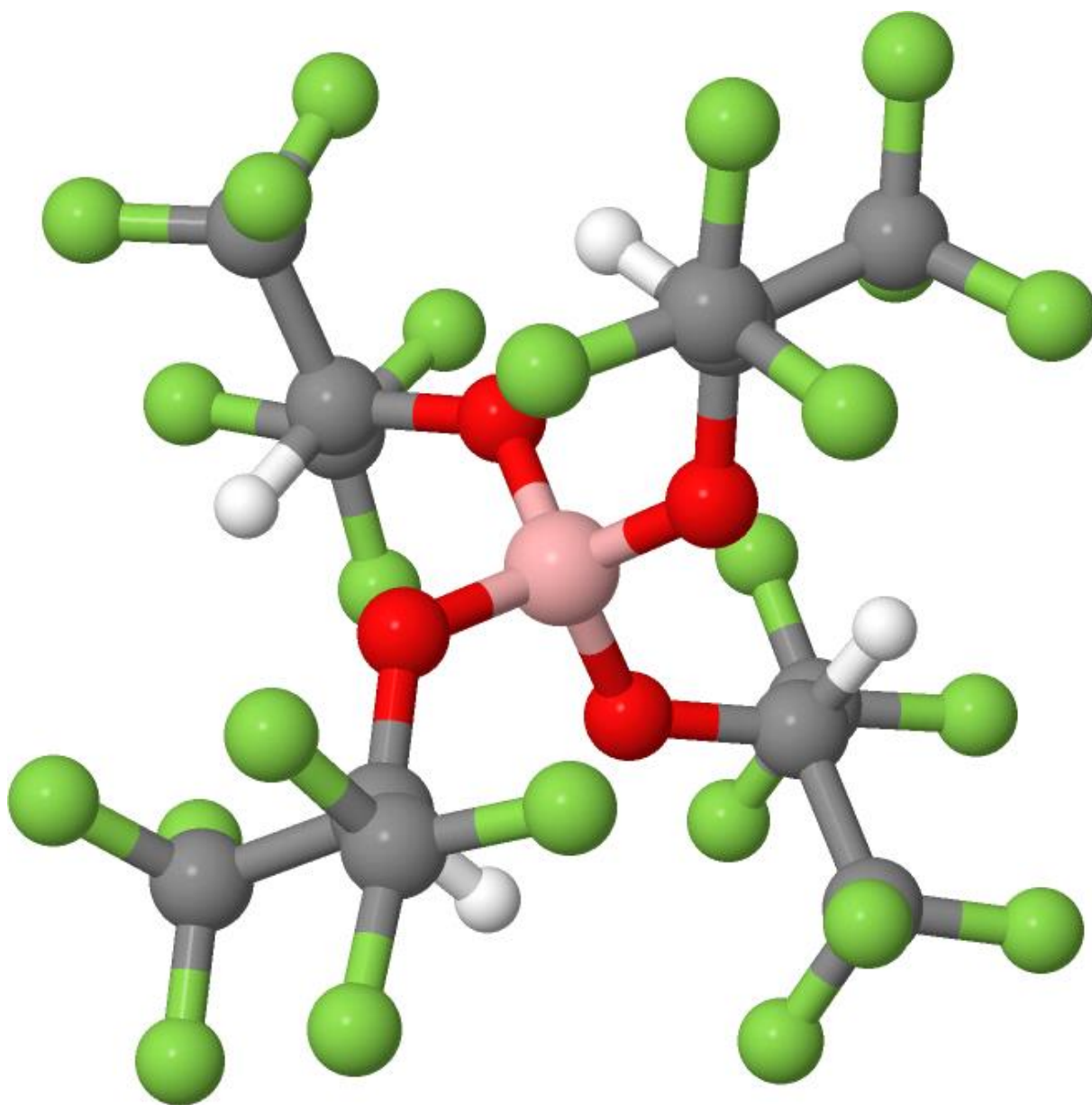
Number of MOs= 29, Electrons= 34.00, Symmetry: td

\$coord

0.0000000000000000	0.0000000000000000	0.0000000000000000	b
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2.49773999034158	-2.49773999034158	2.49773999034158	i
-2.49773999034158	-2.49773999034158	-2.49773999034158	i
2.49773999034158	2.49773999034158	-2.49773999034158	i

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	69.68	0.00000	NO	YES
8		e	69.68	0.00000	NO	YES
9		t2	104.93	0.65430	YES	YES
10		t2	104.93	0.65430	YES	YES
11		t2	104.93	0.65430	YES	YES
12		a1	156.67	0.00000	NO	YES
13		t2	493.57	186.92387	YES	YES
14		t2	493.57	186.92387	YES	YES
15		t2	493.57	186.92387	YES	YES



Total energy = -3179.7470320990 H = -86525.3683893 eV

HOMO-LUMO Separation

HOMO: 165. 165 a -0.12408599 H = -3.37655 eV

LUMO: 166. 166 a +0.13521833 H = +3.67948 eV

Gap : +0.25930432 H = +7.05603 eV

Number of MOs= 582, Electrons= 330.00, Symmetry: c1

\$scoord

-2.55177343441581	1.01975720523768	0.44605525064999	o
-3.27332436819965	3.40699860824867	-0.31577036331818	c
-3.74495635820939	5.12638249918041	1.99988310331344	c
-4.40807429861045	7.50825507614931	1.28119227253016	f
-1.62613104085257	5.32568983380283	3.39385832167902	f
-5.60291905077356	4.25185297726728	3.51979530156884	f
-5.62289154981603	3.17708054053968	-2.03680278296796	c
-7.58569562090643	2.03239432992780	-0.86118631139355	f
-6.45221031280503	5.45847873925016	-2.86924876374908	f
-5.05879264678761	1.78060747031220	-4.09867572967955	f
0.98274084318028	1.25932015292546	-2.32917528259500	o
3.53471083785847	1.57165170496136	-2.76477412619710	c
4.14075817527269	4.42162443572093	-3.03618194960782	c
2.99092428905244	5.48478911196464	-5.06242851669094	f
3.35120375478134	5.69272742222371	-0.96911217123547	f
6.66008261870051	4.85132918113359	-3.27352562420265	f
4.35074223845824	0.03828769333190	-5.11471383315002	c
4.03400987996019	-2.45378966041284	-4.69651596164973	f
6.84192151183718	0.40293002489063	-5.66075046355573	f
3.02018393728943	0.65561310255837	-7.20119025969312	f
-0.22021900951461	-2.77299882258577	-0.23396512115054	o
-2.42037010157815	-3.94808279527673	-0.99187961284075	c
-3.24102849636296	-5.88334136239286	1.04333560475524	c
-5.53758650550295	-6.90720374701391	0.53334615292858	f
-1.58057432660561	-7.81472821716401	1.29569247900338	f
-3.42209569032316	-4.73973878154098	3.32153143641433	f
-2.05728186924400	-5.19482094930120	-3.61105258992687	c
-0.05951039973838	-6.77716718257156	-3.67366330636908	f
-1.69920521325609	-3.41353639599632	-5.39475326727459	f
-4.13276340661583	-6.55466643492634	-4.30670599783844	f
1.84499910875936	0.53263765027408	2.02203958763514	o
2.16757973696518	-1.07336633765371	4.04859164790245	c
4.98914275359534	-1.80789477722306	4.27155031004326	c
5.85191069423456	-2.68557511320445	2.03161350453090	f
5.36029671662901	-3.66493072377275	6.00135727023610	f
6.47897720404928	0.16436274503820	4.93535839010964	f
1.16746421303388	0.16090687633622	6.50290558666999	c
1.69849125654944	-1.28503785045284	8.56966563031361	f
-1.36473854028329	0.41610912796336	6.40075809589990	f
2.17101028915220	2.46712039936754	6.91514031891602	f
0.01241998861697	0.00899060480847	-0.02393183807050	b
-1.79800557660357	4.36247927700463	-1.47683640188466	h
4.71916279602125	0.88566021667135	-1.16477326656381	h
-4.02883980921142	-2.60197953617557	-1.18393780415883	h
1.12025478221969	-2.88517831942535	3.81788108066391	h

\$vibrational spectrum

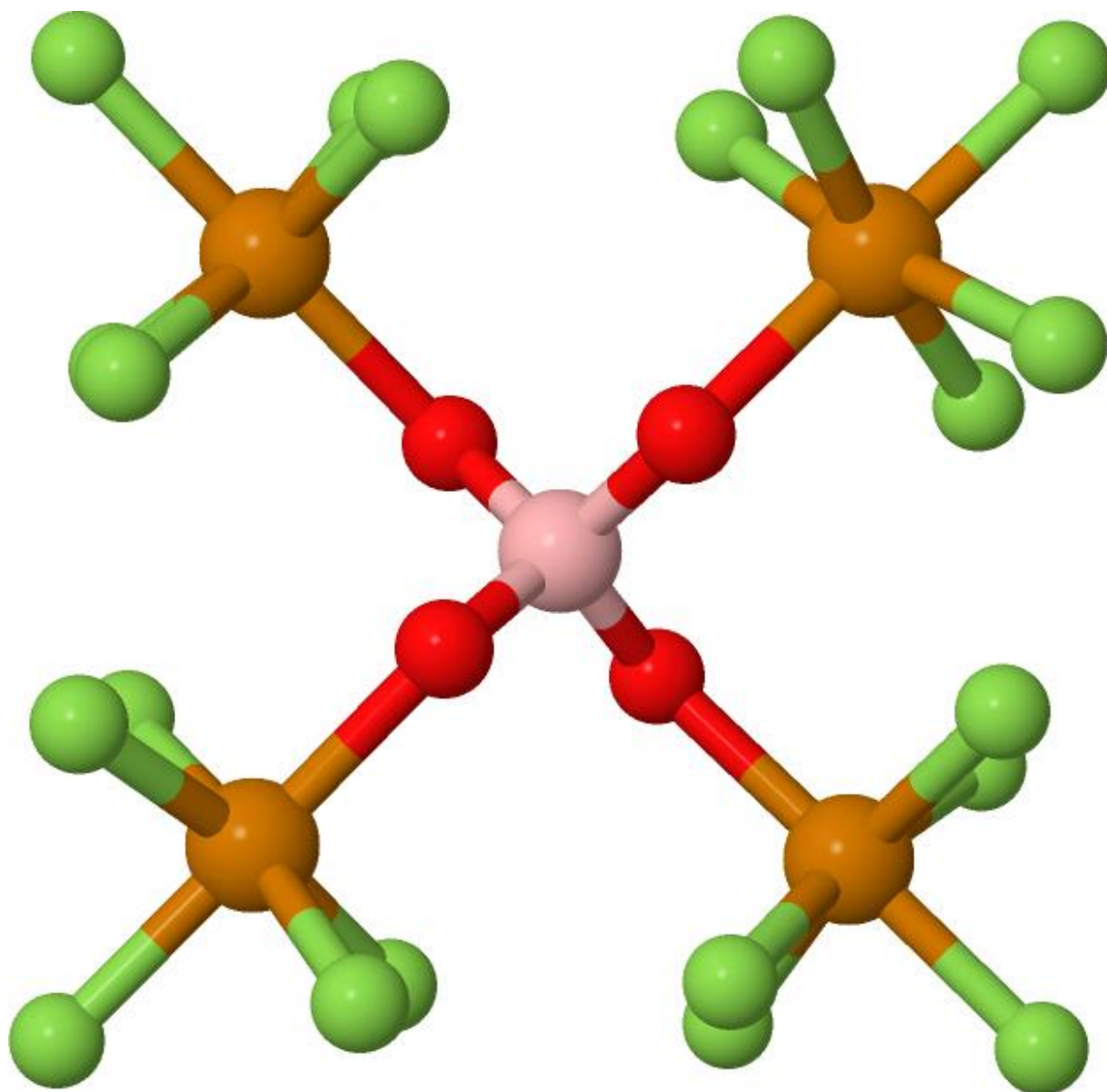
#	mode	symmetry	wave number	IR intensity	selection rules
#			cm** (-1)	km/mol	IR RAMAN
1			0.00	0.00000	- -
2			0.00	0.00000	- -
3			0.00	0.00000	- -
4			0.00	0.00000	- -

5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	14.02	0.05933	YES	YES
8	a	15.71	0.03797	YES	YES
9	a	18.04	0.00075	YES	YES
10	a	20.42	0.05076	YES	YES
11	a	22.37	0.00231	YES	YES
12	a	23.41	0.03621	YES	YES
13	a	26.21	0.07878	YES	YES
14	a	31.03	0.06545	YES	YES
15	a	34.29	0.09644	YES	YES
16	a	39.82	0.23061	YES	YES
17	a	40.68	0.13607	YES	YES
18	a	43.01	0.21292	YES	YES
19	a	48.88	0.07217	YES	YES
20	a	63.33	0.04384	YES	YES
21	a	64.00	0.06166	YES	YES
22	a	69.16	0.01034	YES	YES
23	a	77.91	0.08090	YES	YES
24	a	87.97	0.06860	YES	YES
25	a	88.40	0.08359	YES	YES
26	a	107.41	0.00810	YES	YES
27	a	112.27	0.01943	YES	YES
28	a	113.21	0.38029	YES	YES
29	a	157.39	2.65685	YES	YES
30	a	157.79	2.51208	YES	YES
31	a	170.46	0.01977	YES	YES
32	a	172.42	0.27165	YES	YES
33	a	198.11	0.11103	YES	YES
34	a	198.20	0.11645	YES	YES
35	a	203.17	0.00299	YES	YES
36	a	216.15	0.82496	YES	YES
37	a	256.26	0.83399	YES	YES
38	a	256.86	0.83510	YES	YES
39	a	274.73	2.13519	YES	YES
40	a	283.95	0.01694	YES	YES
41	a	285.42	0.11173	YES	YES
42	a	286.27	0.09428	YES	YES
43	a	286.91	0.19790	YES	YES
44	a	287.36	0.02161	YES	YES
45	a	317.26	1.31337	YES	YES
46	a	317.86	0.92443	YES	YES
47	a	318.45	1.09340	YES	YES
48	a	321.87	0.03587	YES	YES
49	a	338.15	0.01587	YES	YES
50	a	339.88	0.01444	YES	YES
51	a	348.97	0.54969	YES	YES
52	a	375.65	3.27531	YES	YES
53	a	377.28	3.34852	YES	YES
54	a	401.51	0.00099	YES	YES
55	a	420.05	0.00017	YES	YES
56	a	459.88	0.24356	YES	YES
57	a	500.90	0.67695	YES	YES
58	a	501.59	0.70905	YES	YES
59	a	506.42	19.33577	YES	YES
60	a	513.40	0.02851	YES	YES
61	a	518.89	1.54506	YES	YES
62	a	519.18	2.13753	YES	YES
63	a	519.77	4.10153	YES	YES
64	a	520.02	2.64718	YES	YES
65	a	523.44	1.39541	YES	YES
66	a	526.20	10.15894	YES	YES

67	a	526.92	8.60775	YES	YES
68	a	533.43	0.73702	YES	YES
69	a	533.93	0.82508	YES	YES
70	a	534.16	0.87139	YES	YES
71	a	534.69	0.14486	YES	YES
72	a	543.44	0.03171	YES	YES
73	a	614.65	24.99391	YES	YES
74	a	640.46	32.02260	YES	YES
75	a	641.30	30.89456	YES	YES
76	a	667.83	21.02679	YES	YES
77	a	668.46	14.37858	YES	YES
78	a	668.65	19.84546	YES	YES
79	a	672.00	104.61138	YES	YES
80	a	702.13	0.03598	YES	YES
81	a	723.48	6.03919	YES	YES
82	a	726.67	8.09951	YES	YES
83	a	727.00	7.73124	YES	YES
84	a	783.71	0.02399	YES	YES
85	a	847.78	45.45935	YES	YES
86	a	848.05	41.20863	YES	YES
87	a	853.68	49.68964	YES	YES
88	a	861.89	0.41869	YES	YES
89	a	873.51	6.93217	YES	YES
90	a	874.27	10.93865	YES	YES
91	a	875.12	13.93840	YES	YES
92	a	876.95	46.92783	YES	YES
93	a	954.36	234.66162	YES	YES
94	a	1015.32	353.23520	YES	YES
95	a	1016.76	339.68370	YES	YES
96	a	1084.85	216.32202	YES	YES
97	a	1085.63	81.25083	YES	YES
98	a	1087.47	94.90403	YES	YES
99	a	1088.59	97.06923	YES	YES
100	a	1118.62	91.69734	YES	YES
101	a	1118.83	68.76104	YES	YES
102	a	1125.15	4.72048	YES	YES
103	a	1133.42	53.46105	YES	YES
104	a	1158.62	68.65775	YES	YES
105	a	1159.55	49.20985	YES	YES
106	a	1163.34	0.19477	YES	YES
107	a	1165.97	207.99397	YES	YES
108	a	1173.30	84.93469	YES	YES
109	a	1175.46	1171.76655	YES	YES
110	a	1176.99	1198.73710	YES	YES
111	a	1213.22	243.72154	YES	YES
112	a	1214.29	488.64372	YES	YES
113	a	1215.77	532.91368	YES	YES
114	a	1216.40	346.76587	YES	YES
115	a	1223.48	65.83146	YES	YES
116	a	1234.17	68.57656	YES	YES
117	a	1235.49	57.73195	YES	YES
118	a	1236.60	59.69412	YES	YES
119	a	1239.46	245.62088	YES	YES
120	a	1266.57	2.14090	YES	YES
121	a	1272.67	251.53599	YES	YES
122	a	1272.84	255.26167	YES	YES
123	a	1274.80	52.60017	YES	YES
124	a	1320.45	3.31468	YES	YES
125	a	1324.23	7.63320	YES	YES
126	a	1326.82	4.67477	YES	YES
127	a	1334.75	46.06055	YES	YES
128	a	1350.12	11.64733	YES	YES

129	a	1355.49	81.93594	YES	YES
130	a	1356.93	54.02396	YES	YES
131	a	1359.78	188.34832	YES	YES
132	a	2964.47	22.44789	YES	YES
133	a	2965.34	20.69258	YES	YES
134	a	2971.27	20.28997	YES	YES
135	a	2971.58	18.99184	YES	YES

[B(OTeF₅)₄]⁻



Total energy = -2353.4428991050 H = -64040.4761047 eV
644

HOMO-LUMO Separation

HOMO: 121. 121 a -0.20383377 H = -5.54660 eV

LUMO: 122. 122 a -0.12569820 H = -3.42042 eV

Gap : +0.07813558 H = +2.12618 eV

Number of MOs= 402, Electrons= 242.00, Symmetry: c1

\$coord

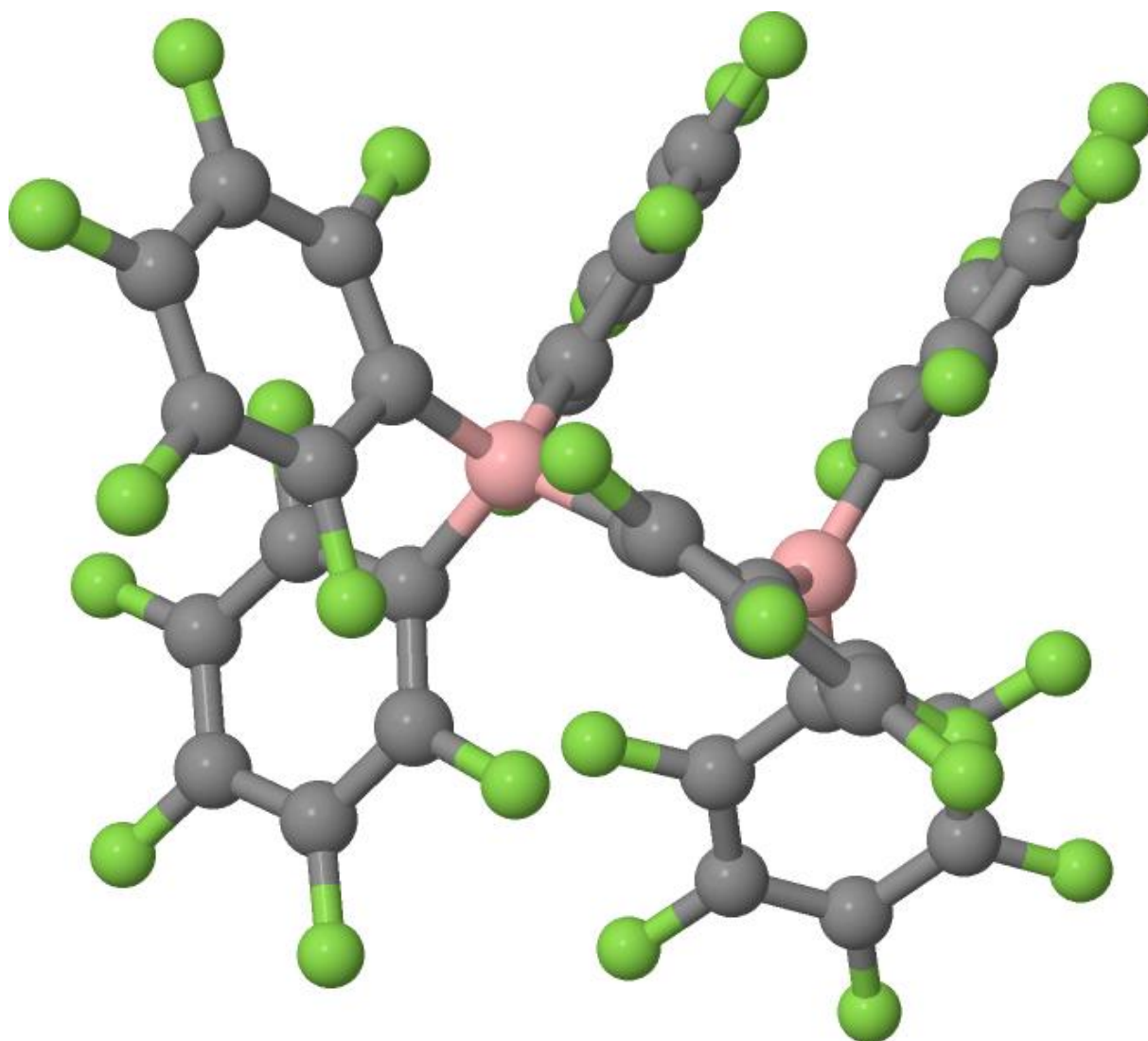
0.01043414505906	0.00213406527618	0.01744854974743	b
0.33632744709943	1.00357762655281	2.62199483664559	o
1.85797305499375	0.95961749367670	-1.86744132321967	o
0.19943683137225	-2.74027661404047	0.59196440931367	o
-2.34903996987424	0.79103061315750	-1.28449771090263	o
5.48084203618486	0.58860316534912	-1.90991332645292	te
0.55700404911781	4.47454953665886	3.71448696805249	te
-5.79633807349264	0.50871866900456	-0.14363267991106	te
-0.24126038908451	-5.57249892209060	-1.66133946845775	te
1.80068143865402	-4.23153858589360	-4.37044105311939	f
2.64078464482584	-7.23374943198435	-0.20467819255577	f
-0.62913788558595	-8.55422096696030	-3.71849369001102	f
-2.32670119951306	-7.25411695368608	0.79096115554545	f
-3.18242687001632	-4.29924888818788	-3.40020749783601	f
5.57764601767492	-2.92287165750788	-0.93443112813582	f
5.38072576291638	-0.32850005118880	-5.42183401971204	f
9.10778577413989	0.35562153488387	-2.16603009185043	f
5.86354633128478	4.05297993926958	-2.92676462496790	f
5.99857036517806	1.47283467425980	1.59245270529290	f
2.83090048161799	5.60896928023400	1.09834511083828	f
3.35955735453153	3.66475683374118	5.87875277534760	f
0.77373261934599	7.86170788605596	5.04275614273465	f
-1.66054903515577	3.77966718271647	6.50470668975882	f
-2.22556689867562	5.69230560324348	1.69418271986148	f
-5.53327275031700	-2.93895785037926	1.02302239821185	f
-9.31576118605576	0.30327780591081	0.77741557632677	f
-6.84005095735874	-0.57535771307223	-3.44945924555807	f
-6.46646268370850	3.92607846569032	-1.17375332183472	f
-5.20938045515856	1.60490725931005	3.28442733684823	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	24.30	0.02040	YES	YES

8	a	35.45	0.02310	YES	YES
9	a	49.75	0.01588	YES	YES
10	a	53.39	0.00743	YES	YES
11	a	56.88	0.09637	YES	YES
12	a	57.50	0.03817	YES	YES
13	a	62.89	0.05346	YES	YES
14	a	67.53	0.17319	YES	YES
15	a	72.72	0.00850	YES	YES
16	a	78.70	0.00912	YES	YES
17	a	86.37	0.00644	YES	YES
18	a	89.03	0.00723	YES	YES
19	a	99.44	0.03153	YES	YES
20	a	116.74	0.06845	YES	YES
21	a	117.35	0.02504	YES	YES
22	a	120.10	0.05446	YES	YES
23	a	120.88	0.02164	YES	YES
24	a	130.45	0.01411	YES	YES
25	a	135.86	0.00034	YES	YES
26	a	170.61	0.41361	YES	YES
27	a	172.65	0.01254	YES	YES
28	a	174.50	0.15622	YES	YES
29	a	177.18	0.32426	YES	YES
30	a	178.65	0.17179	YES	YES
31	a	179.96	0.22656	YES	YES
32	a	181.81	0.53670	YES	YES
33	a	208.83	1.09634	YES	YES
34	a	209.71	0.46487	YES	YES
35	a	211.25	0.20094	YES	YES
36	a	213.45	0.10174	YES	YES
37	a	215.98	0.07756	YES	YES
38	a	247.20	0.80725	YES	YES
39	a	253.25	67.34437	YES	YES
40	a	254.90	83.51178	YES	YES
41	a	255.24	7.27008	YES	YES
42	a	255.73	118.93639	YES	YES
43	a	260.16	0.94737	YES	YES
44	a	261.45	15.68646	YES	YES
45	a	274.02	3.55251	YES	YES
46	a	277.34	1.84530	YES	YES
47	a	277.48	9.78997	YES	YES
48	a	277.98	21.33099	YES	YES
49	a	279.94	104.94247	YES	YES
50	a	280.77	106.20642	YES	YES
51	a	282.96	42.70090	YES	YES
52	a	285.48	19.06803	YES	YES
53	a	288.25	39.33387	YES	YES
54	a	290.14	19.50813	YES	YES
55	a	292.50	37.07156	YES	YES
56	a	312.19	0.29396	YES	YES
57	a	351.56	0.04540	YES	YES
58	a	472.11	13.15195	YES	YES
59	a	473.88	13.45042	YES	YES
60	a	509.35	0.00342	YES	YES
61	a	571.07	0.80913	YES	YES
62	a	574.92	25.73556	YES	YES
63	a	575.70	24.99133	YES	YES
64	a	584.23	0.12262	YES	YES
65	a	585.44	0.04554	YES	YES
66	a	586.56	2.15993	YES	YES
67	a	587.29	1.64887	YES	YES
68	a	588.63	0.23084	YES	YES
69	a	595.41	32.87382	YES	YES

70	a	596.01	39.56656	YES	YES
71	a	609.12	0.03906	YES	YES
72	a	616.27	0.00416	YES	YES
73	a	631.95	0.31043	YES	YES
74	a	638.42	299.29563	YES	YES
75	a	639.43	258.40507	YES	YES
76	a	640.57	56.71878	YES	YES
77	a	641.22	27.58667	YES	YES
78	a	642.51	1.64474	YES	YES
79	a	649.50	212.94205	YES	YES
80	a	650.15	2.12655	YES	YES
81	a	650.17	62.03623	YES	YES
82	a	651.47	11.90776	YES	YES
83	a	698.47	16.53896	YES	YES
84	a	874.09	0.21506	YES	YES
85	a	898.20	854.32626	YES	YES
86	a	899.25	853.21895	YES	YES
87	a	966.46	325.18457	YES	YES



Total energy = -4313.8383935770 H = -117385.5820630 eV

HOMO-LUMO Separation

HOMO: 244. 244 a -0.11784330 H = -3.20668 eV

LUMO: 245. 245 a -0.04546625 H = -1.23720 eV

Gap : +0.07237705 H = +1.96948 eV

Number of MOs= 938, Electrons= 488.00, Symmetry: c1

\$coord

1.40762146008050	5.67906781919646	0.28572983710611	c
0.80471901715921	3.09092975180281	0.35012353463503	c
2.88286007581581	1.43187126757479	0.98126421615820	c
5.15196557881357	2.49618433530202	1.87551906460635	c
5.61212922492316	5.10052596279992	1.99161164391407	c
3.71866406178725	6.70899968017181	1.11816095785679	c
-2.15228552401834	2.02311807653941	-0.06739270210260	b
3.37774293526743	-1.46245796546588	0.34938885088353	b
4.10096262332657	9.21712550421879	1.06989215024633	f
-0.20749663319064	7.43562059482851	-0.62031281558610	f
7.16566211083468	0.99198361535957	2.45694489764742	f
7.83968661999023	6.01017790839191	2.80185599811332	f
-6.69679147778346	8.05212065092353	0.48071606512044	c
-4.82577075126625	6.20743525525045	0.82910663972659	c
-4.28060656936325	4.24618782643899	-0.89928308403605	c
-5.87849213670175	4.23870795838909	-3.02544022225285	c
-7.77660061022079	6.05560341468507	-3.47018551296061	c
-8.20017820893347	7.97516684884881	-1.70074186813519	c
-9.21346578862222	5.93968648023470	-5.56649004818475	f
-5.72292912006999	2.43009844675570	-4.82305711330523	f
-3.48316503677859	6.42906766393604	2.98991259843012	f
-7.06885923811027	9.87752491793330	2.21116069460472	f
-10.00651525357334	9.71947717189150	-2.08399757252361	f
-7.33458383905495	-0.71735805409135	4.67234809322959	c
-5.91755615029981	-0.03651552682484	2.53779075364566	c
-3.48284635131758	1.03987733018900	2.62686894493558	c
-2.58191110148544	1.47967233540279	5.08555783278736	c
-3.92304976086723	0.82379453412088	7.28746517586583	c
-6.32292068374526	-0.27405385257319	7.08324680695560	c
-2.92461926801760	1.25084307702402	9.58803936645105	f
-0.31100869835021	2.56358793906151	5.49292476065178	f
-7.03632825287329	-0.47963566048633	0.28065445239944	f
-9.64191368101495	-1.76238495733599	4.43721353251660	f
-7.63862191272874	-0.90444487200656	9.16353475649604	f
-2.22675127271826	-4.66021476383639	-3.81926407925134	c
-2.38075969417350	-2.86254051447178	-1.86041423692832	c
-1.90918246957477	-0.26463966747580	-2.19875055104049	c
-1.09601639066138	0.38660889790314	-4.65210995487491	c
-0.86053923779052	-1.33466601197450	-6.64704668570461	c
-1.42029215654239	-3.89426621904386	-6.21752372460585	c
-0.04235048565709	-0.59536404361746	-8.93890939820970	f
-0.51172149741472	2.80639856065684	-5.19068982160549	f
-3.03518844709829	-3.82667974008840	0.40697924113733	f
-2.74037312424797	-7.10659841771522	-3.38075181476887	f
-1.14027191342211	-5.59054927215817	-8.08484201728201	f
4.55198158668766	-5.72121342507522	-5.63583866186560	c
3.81835688073521	-4.85936504561333	-3.23834988547836	c
3.99965637282293	-2.30755500878133	-2.45749045420679	c
4.95616578169801	-0.62598508237745	-4.31000355648771	c
5.73013478231686	-1.42102016103147	-6.72256679530071	c
5.51025772749731	-3.97886832899874	-7.39302621442272	c
6.66606206766841	0.23496253543322	-8.38987621875356	f
5.26044026952186	1.83615198740144	-3.81489547621152	f
2.89215587467156	-6.61787634518076	-1.65493685904560	f
4.33370098201155	-8.16205175036298	-6.26618914843100	f
6.22319559121477	-4.75314281224143	-9.68773192113696	f
7.16041004785121	-6.27948792210036	4.56042340138983	c
6.40110469875989	-4.68588837807760	2.58180139430007	c
4.03917005662495	-3.44507635953811	2.53202611430127	c

2.43649096225709	-3.95669330852817	4.59064464594145	c
3.10799606295788	-5.56948207461908	6.59357340667942	c
5.49375094749238	-6.72694307188899	6.57940537194832	c
1.49900012397921	-6.01436950279922	8.49555599563750	f
0.12772218605985	-2.93421109389425	4.68818948848142	f
8.09274379734642	-4.32226885351367	0.71705767597583	f
9.44760711097603	-7.37526533979288	4.54675140481956	f
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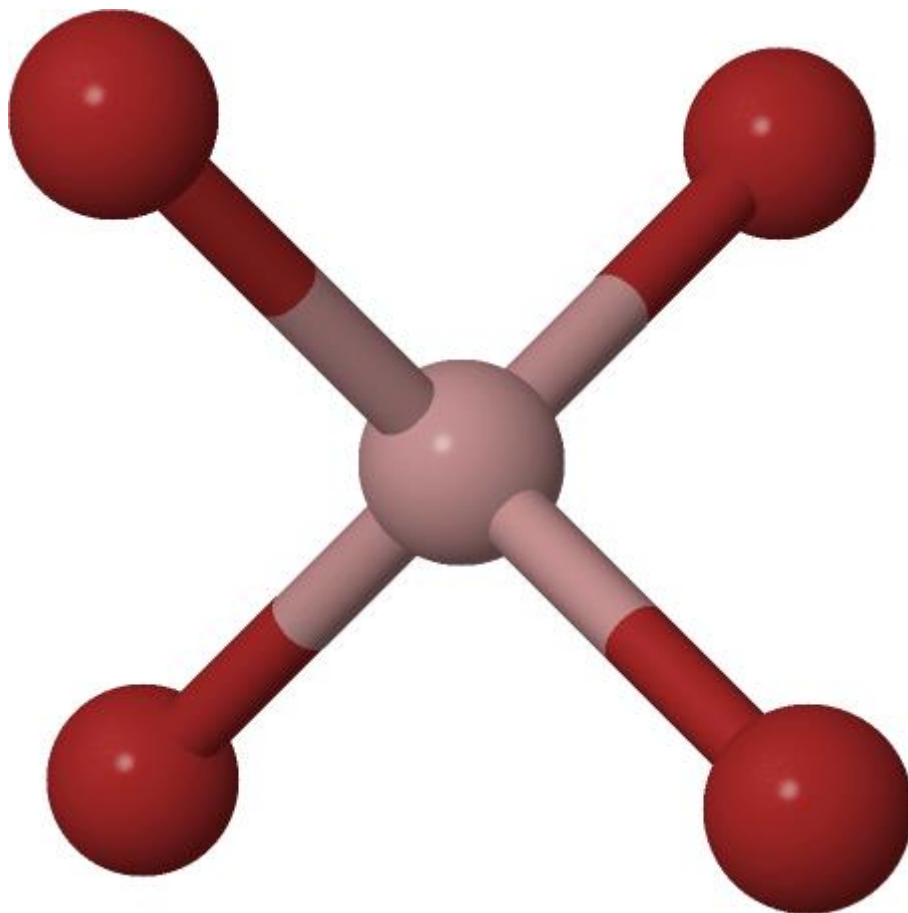
\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
#						
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	10.28	0.00564	YES	YES
8		a	20.70	0.06040	YES	YES
9		a	24.65	0.15124	YES	YES
10		a	26.90	0.18829	YES	YES
11		a	28.01	0.03149	YES	YES
12		a	32.02	0.02368	YES	YES
13		a	32.37	0.02949	YES	YES
14		a	36.48	0.10487	YES	YES
15		a	39.05	0.08768	YES	YES
16		a	42.30	0.00557	YES	YES
17		a	47.29	0.03797	YES	YES
18		a	49.69	0.08356	YES	YES
19		a	53.12	0.14574	YES	YES
20		a	59.40	0.18480	YES	YES
21		a	65.38	0.05444	YES	YES
22		a	80.18	0.74336	YES	YES
23		a	81.50	0.65189	YES	YES
24		a	102.03	0.31755	YES	YES
25		a	106.89	0.03742	YES	YES
26		a	111.96	0.11760	YES	YES
27		a	115.25	0.13614	YES	YES
28		a	118.56	0.08140	YES	YES
29		a	123.28	0.08285	YES	YES
30		a	127.48	0.08292	YES	YES
31		a	132.48	0.17041	YES	YES
32		a	135.05	0.19746	YES	YES
33		a	135.60	0.02764	YES	YES
34		a	139.20	0.03946	YES	YES
35		a	141.37	0.01681	YES	YES
36		a	143.21	0.20442	YES	YES
37		a	147.29	0.03818	YES	YES
38		a	148.70	0.02106	YES	YES
39		a	154.48	0.06602	YES	YES
40		a	155.90	0.20688	YES	YES
41		a	160.40	0.05117	YES	YES
42		a	163.34	0.01327	YES	YES
43		a	164.27	0.31784	YES	YES
44		a	169.04	0.20735	YES	YES
45		a	176.21	0.05752	YES	YES
46		a	188.45	0.33211	YES	YES
47		a	200.57	0.67967	YES	YES
48		a	225.14	5.20184	YES	YES
49		a	229.64	2.71610	YES	YES

50	a	238.65	2.60687	YES	YES
51	a	242.47	1.33243	YES	YES
52	a	245.91	2.29711	YES	YES
53	a	250.72	1.40226	YES	YES
54	a	260.46	0.13389	YES	YES
55	a	262.36	0.10018	YES	YES
56	a	264.08	0.11211	YES	YES
57	a	264.51	0.17547	YES	YES
58	a	264.64	0.14138	YES	YES
59	a	266.99	0.00151	YES	YES
60	a	269.09	0.05203	YES	YES
61	a	272.74	0.03437	YES	YES
62	a	273.78	0.04600	YES	YES
63	a	274.07	0.02645	YES	YES
64	a	277.75	0.04272	YES	YES
65	a	296.87	0.65994	YES	YES
66	a	303.15	0.54675	YES	YES
67	a	309.74	0.22579	YES	YES
68	a	311.02	0.17240	YES	YES
69	a	311.49	0.59444	YES	YES
70	a	313.74	0.38232	YES	YES
71	a	334.93	2.39286	YES	YES
72	a	337.02	1.67307	YES	YES
73	a	343.39	6.07264	YES	YES
74	a	344.32	1.23470	YES	YES
75	a	345.06	0.95867	YES	YES
76	a	348.97	0.58832	YES	YES
77	a	361.67	3.36213	YES	YES
78	a	370.39	0.97106	YES	YES
79	a	377.60	4.70185	YES	YES
80	a	379.86	1.90815	YES	YES
81	a	386.45	0.20845	YES	YES
82	a	387.07	1.14426	YES	YES
83	a	389.26	1.46649	YES	YES
84	a	391.61	0.03922	YES	YES
85	a	393.69	1.09817	YES	YES
86	a	402.68	1.58048	YES	YES
87	a	407.85	2.80804	YES	YES
88	a	414.34	1.43351	YES	YES
89	a	431.41	0.31314	YES	YES
90	a	433.26	0.15000	YES	YES
91	a	434.98	0.31934	YES	YES
92	a	435.86	0.03059	YES	YES
93	a	438.01	0.08907	YES	YES
94	a	453.56	0.90761	YES	YES
95	a	457.40	2.66614	YES	YES
96	a	463.72	3.22854	YES	YES
97	a	464.73	0.84582	YES	YES
98	a	470.91	0.89524	YES	YES
99	a	476.00	0.11477	YES	YES
100	a	493.54	0.47566	YES	YES
101	a	520.24	0.32263	YES	YES
102	a	522.91	0.24186	YES	YES
103	a	524.80	4.94299	YES	YES
104	a	527.72	2.13594	YES	YES
105	a	533.81	6.88984	YES	YES
106	a	553.20	0.44416	YES	YES
107	a	557.27	1.93883	YES	YES
108	a	563.53	2.18173	YES	YES
109	a	564.11	3.68052	YES	YES
110	a	566.16	1.12408	YES	YES
111	a	566.45	0.32801	YES	YES

112	a	568.15	2.71442	YES	YES
113	a	592.87	15.41674	YES	YES
114	a	596.47	15.35392	YES	YES
115	a	609.71	21.66113	YES	YES
116	a	613.18	16.49359	YES	YES
117	a	617.21	31.52938	YES	YES
118	a	630.07	0.28490	YES	YES
119	a	631.22	1.22532	YES	YES
120	a	633.11	0.14853	YES	YES
121	a	634.68	1.00362	YES	YES
122	a	637.30	2.31697	YES	YES
123	a	646.87	9.51432	YES	YES
124	a	659.90	38.82827	YES	YES
125	a	669.62	9.22529	YES	YES
126	a	675.71	14.81921	YES	YES
127	a	676.47	40.29731	YES	YES
128	a	699.62	5.79093	YES	YES
129	a	717.94	85.71197	YES	YES
130	a	739.61	23.86679	YES	YES
131	a	748.49	37.62909	YES	YES
132	a	758.64	19.99858	YES	YES
133	a	759.46	15.69708	YES	YES
134	a	765.84	19.52678	YES	YES
135	a	771.94	10.85334	YES	YES
136	a	804.30	2.55358	YES	YES
137	a	838.79	5.27615	YES	YES
138	a	879.42	3.60521	YES	YES
139	a	901.35	4.81456	YES	YES
140	a	931.37	2.49377	YES	YES
141	a	968.12	22.11106	YES	YES
142	a	973.19	37.76837	YES	YES
143	a	979.30	42.77801	YES	YES
144	a	982.48	214.35974	YES	YES
145	a	983.87	162.47219	YES	YES
146	a	996.24	107.16980	YES	YES
147	a	1002.42	184.38771	YES	YES
148	a	1059.75	26.90086	YES	YES
149	a	1080.83	166.68789	YES	YES
150	a	1086.28	118.72338	YES	YES
151	a	1093.81	227.47614	YES	YES
152	a	1100.99	92.15350	YES	YES
153	a	1126.16	37.04726	YES	YES
154	a	1127.14	155.71822	YES	YES
155	a	1132.24	11.21281	YES	YES
156	a	1134.87	9.55393	YES	YES
157	a	1148.62	103.64717	YES	YES
158	a	1149.95	155.18026	YES	YES
159	a	1152.16	56.74954	YES	YES
160	a	1239.51	18.75325	YES	YES
161	a	1267.26	19.65626	YES	YES
162	a	1269.96	42.58799	YES	YES
163	a	1272.04	17.65637	YES	YES
164	a	1280.04	65.19458	YES	YES
165	a	1296.91	121.64705	YES	YES
166	a	1301.10	140.49274	YES	YES
167	a	1322.67	57.12653	YES	YES
168	a	1337.96	9.68879	YES	YES
169	a	1342.88	2.24340	YES	YES
170	a	1343.73	11.02536	YES	YES
171	a	1344.57	0.61916	YES	YES
172	a	1345.83	3.16526	YES	YES
173	a	1366.46	28.27635	YES	YES

174	a	1369.07	25.38531	YES	YES
175	a	1376.18	61.00776	YES	YES
176	a	1379.07	14.18644	YES	YES
177	a	1391.32	68.40781	YES	YES
178	a	1398.97	216.98965	YES	YES
179	a	1448.64	55.57886	YES	YES
180	a	1458.94	246.08507	YES	YES
181	a	1462.61	354.25497	YES	YES
182	a	1469.08	696.77298	YES	YES
183	a	1472.39	599.90728	YES	YES
184	a	1479.88	196.94784	YES	YES
185	a	1508.77	94.45602	YES	YES
186	a	1512.17	126.63370	YES	YES
187	a	1515.63	296.66655	YES	YES
188	a	1516.81	216.79172	YES	YES
189	a	1520.93	167.24657	YES	YES
190	a	1601.60	70.62445	YES	YES
191	a	1609.35	42.41006	YES	YES
192	a	1610.59	10.30346	YES	YES
193	a	1611.84	4.31178	YES	YES
194	a	1614.36	6.71420	YES	YES
195	a	1615.45	16.76322	YES	YES
196	a	1616.82	4.84415	YES	YES
197	a	1624.78	119.97788	YES	YES
198	a	1626.47	33.28779	YES	YES
199	a	1627.07	32.98828	YES	YES
200	a	1628.88	37.50113	YES	YES
201	a	1629.29	72.77485	YES	YES



Total energy = -12221.7572825800 H = -332571.1261192 eV

HOMO-LUMO Separation

HOMO: 38. 5 t1 -0.09306580 H = -2.53245 eV

LUMO: 39. 12 a1 +0.06747554 H = +1.83610 eV

Gap : +0.16054134 H = +4.36855 eV

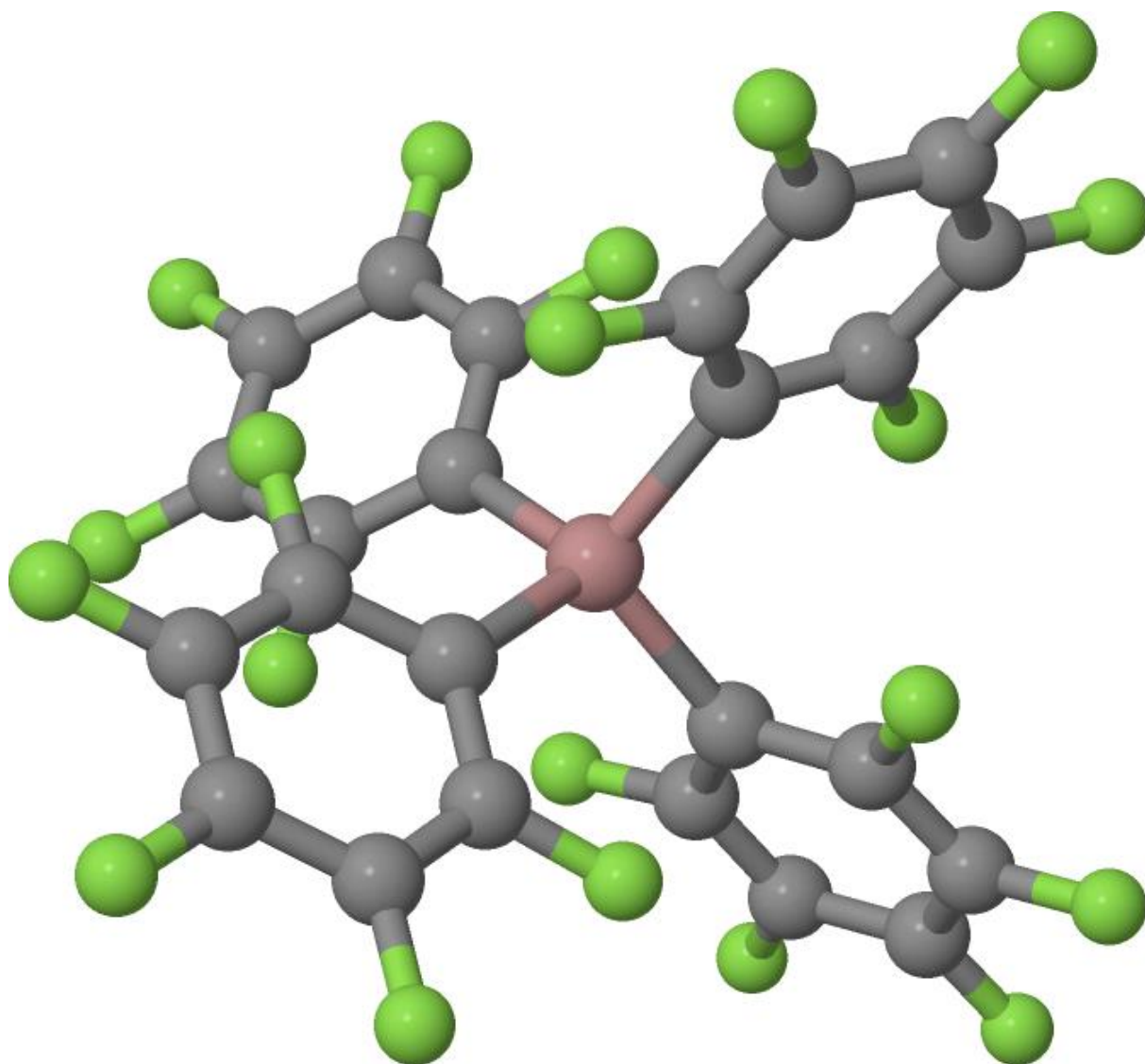
Number of MOs= 69, Electrons= 172.00, Symmetry: td

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  2.60466458735355  -2.60466458735356   2.60466458735356   br
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2.60466458735356	2.60466458735355	-2.60466458735356	br
-2.60466458735356	-2.60466458735355	-2.60466458735356	br

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm**(-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		e	58.09	0.00000	NO	YES
8		e	58.09	0.00000	NO	YES
9		t2	89.41	1.57863	YES	YES
10		t2	89.41	1.57863	YES	YES
11		t2	89.41	1.57863	YES	YES
12		a1	182.85	0.00000	NO	YES
13		t2	256.23	58.98187	YES	YES
14		t2	256.23	58.98187	YES	YES
15		t2	256.23	58.98187	YES	YES



Total energy = -4834.2286697680 H = -131546.1300245 eV

HOMO-LUMO Separation

HOMO: 178. 45 a -0.12155360 H = -3.30764 eV

LUMO: 179. 46 b +0.03764608 H = +1.02440 eV

Gap : +0.15919968 H = +4.33205 eV

Number of MOs= 648, Electrons= 356.00, Symmetry: s4
656

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-5.28683850837430      1.54601376009664      1.72916219231154      c
-2.69930313276216      1.58120134766209      2.27595236757889      c
-2.03509466653947      2.70963326247581      4.57674325414984      c
-3.80258805160291      3.71787935800150      6.28223066411842      c
-6.38163502292272      3.61761412206489      5.66384922889342      c
 3.61761412206489      6.38163502292272      -5.66384922889342      c
 2.53093663605942      7.13927774200653      -3.36637106683425      c
 1.54601376009664      5.28683850837430      -1.72916219231154      c
 1.58120134766209      2.69930313276216      -2.27595236757889      c
 2.70963326247581      2.03509466653947      -4.57674325414984      c
 3.71787935800150      3.80258805160291      -6.28223066411842      c
-3.61761412206489      -6.38163502292272      -5.66384922889342      c
-3.71787935800150      -3.80258805160291      -6.28223066411842      c
-2.70963326247581      -2.03509466653947      -4.57674325414984      c
-1.58120134766209      -2.69930313276216      -2.27595236757889      c
-1.54601376009664      -5.28683850837430      -1.72916219231154      c
-2.53093663605942      -7.13927774200653      -3.36637106683425      c
 6.38163502292272      -3.61761412206489      5.66384922889342      c
 7.13927774200653      -2.53093663605942      3.36637106683425      c
 5.28683850837430      -1.54601376009664      1.72916219231154      c
 2.69930313276216      -1.58120134766209      2.27595236757889      c
 2.03509466653947      -2.70963326247581      4.57674325414984      c
 3.80258805160291      -3.71787935800150      6.28223066411842      c
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-2.87553291397158      0.41960817978160      -5.27329952350269      f
-4.76928244932994      -3.07586117385531      -8.48223613166856      f
-4.56548138406168      -8.11350302627677      -7.26300004070623      f
-2.45264568774661      -9.61136421168048      -2.76573003202198      f
-0.53997281205457      -6.15206369871500      0.45581823334235      f
 2.87553291397158      -0.41960817978160      -5.27329952350269      f
 4.76928244932994      3.07586117385531      -8.48223613166856      f
 4.56548138406168      8.11350302627677      -7.26300004070623      f
 2.45264568774661      9.61136421168048      -2.76573003202198      f
 0.53997281205457      6.15206369871500      0.45581823334235      f
 9.61136421168048      -2.45264568774661      2.76573003202198      f
 6.15206369871500      -0.53997281205457      -0.45581823334235      f
 8.11350302627677      -4.56548138406168      7.26300004070623      f
 3.07586117385531      -4.76928244932994      8.48223613166856      f
-0.41960817978160      -2.87553291397158      5.27329952350269      f
-6.15206369871500      0.53997281205457      -0.45581823334235      f
-9.61136421168048      2.45264568774661      2.76573003202198      f
-8.11350302627677      4.56548138406170      7.26300004070623      f
-3.07586117385531      4.76928244932994      8.48223613166856      f
 0.41960817978160      2.87553291397158      5.27329952350269      f
$

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$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#           #           cm** (-1)      km/mol           IR           RAMAN
    1           0.00           0.00000           -           -
    2           0.00           0.00000           -           -
    3           0.00           0.00000           -           -
    4           0.00           0.00000           -           -
    5           0.00           0.00000           -           -
    6           0.00           0.00000           -           -

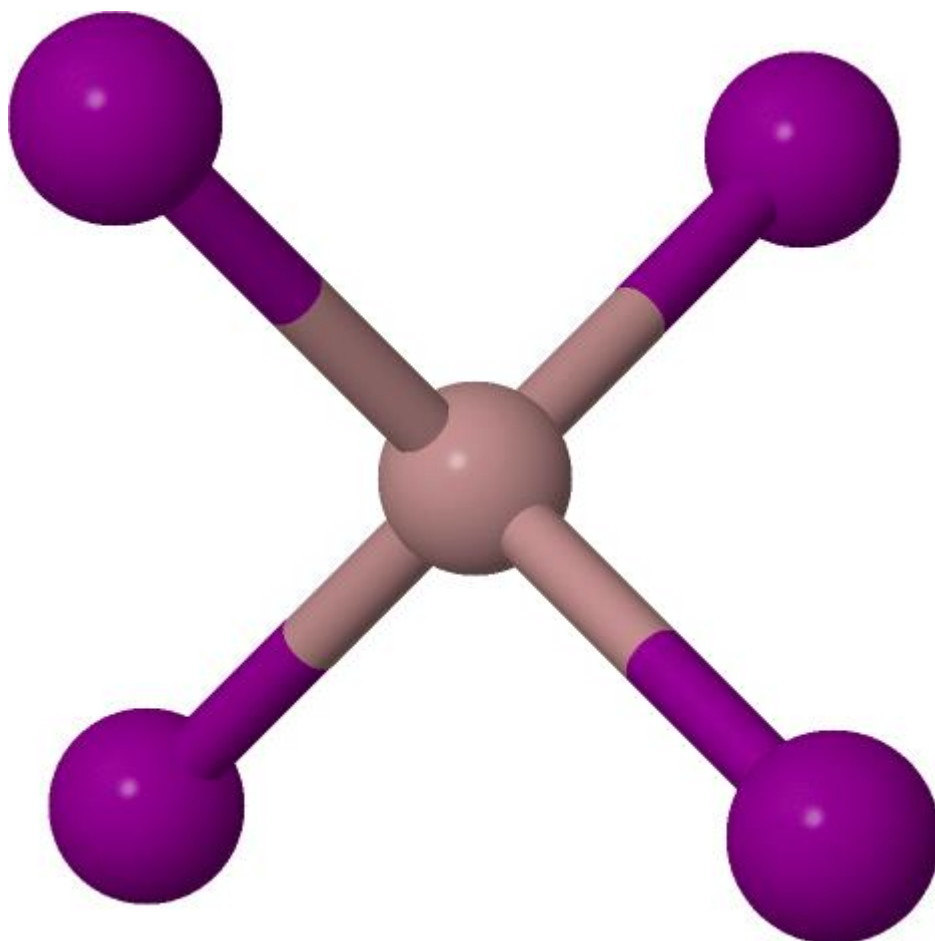
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7	a	12.69	0.00000	NO	YES
8	e	18.81	0.00566	YES	YES
9	e	18.81	0.00566	YES	YES
10	b	20.78	0.00080	YES	YES
11	e	29.52	0.02103	YES	YES
12	e	29.52	0.02103	YES	YES
13	a	29.92	0.00000	NO	YES
14	b	30.65	0.02854	YES	YES
15	b	39.32	0.04764	YES	YES
16	e	86.53	0.05769	YES	YES
17	e	86.53	0.05769	YES	YES
18	a	93.19	0.00000	NO	YES
19	a	103.77	0.00000	NO	YES
20	b	104.76	0.00484	YES	YES
21	e	107.82	0.24260	YES	YES
22	e	107.82	0.24260	YES	YES
23	b	117.36	0.23910	YES	YES
24	e	124.89	0.03024	YES	YES
25	e	124.89	0.03024	YES	YES
26	a	125.25	0.00000	NO	YES
27	b	129.82	0.08543	YES	YES
28	a	130.00	0.00000	NO	YES
29	e	155.14	0.01826	YES	YES
30	e	155.14	0.01826	YES	YES
31	a	156.60	0.00000	NO	YES
32	b	159.86	0.00881	YES	YES
33	a	215.50	0.00000	NO	YES
34	e	216.61	5.65471	YES	YES
35	e	216.61	5.65471	YES	YES
36	b	218.81	1.09873	YES	YES
37	e	236.16	27.58438	YES	YES
38	e	236.16	27.58438	YES	YES
39	b	240.44	34.85312	YES	YES
40	a	261.73	0.00000	NO	YES
41	b	261.86	0.00542	YES	YES
42	e	261.98	0.10914	YES	YES
43	e	261.98	0.10914	YES	YES
44	a	267.47	0.00000	NO	YES
45	e	268.22	2.21781	YES	YES
46	e	268.22	2.21781	YES	YES
47	b	268.49	4.66464	YES	YES
48	a	304.43	0.00000	NO	YES
49	e	304.95	0.14398	YES	YES
50	e	304.95	0.14398	YES	YES
51	b	306.63	0.01250	YES	YES
52	a	341.75	0.00000	NO	YES
53	e	343.44	1.16133	YES	YES
54	e	343.44	1.16133	YES	YES
55	b	346.12	1.62145	YES	YES
56	a	353.73	0.00000	NO	YES
57	e	362.15	9.35033	YES	YES
58	e	362.15	9.35033	YES	YES
59	b	367.27	4.83614	YES	YES
60	a	394.26	0.00000	NO	YES
61	b	394.70	0.01019	YES	YES
62	e	394.73	0.06355	YES	YES
63	e	394.73	0.06355	YES	YES
64	e	432.89	0.03037	YES	YES
65	e	432.89	0.03037	YES	YES
66	a	433.15	0.00000	NO	YES
67	b	433.96	0.00160	YES	YES
68	a	471.70	0.00000	NO	YES

69	e	473.56	4.47674	YES	YES
70	e	473.56	4.47674	YES	YES
71	b	473.90	5.08132	YES	YES
72	e	490.49	1.82701	YES	YES
73	e	490.49	1.82701	YES	YES
74	a	492.10	0.00000	NO	YES
75	b	492.26	1.06362	YES	YES
76	b	563.14	0.00939	YES	YES
77	e	563.20	0.07578	YES	YES
78	e	563.20	0.07578	YES	YES
79	a	563.39	0.00000	NO	YES
80	a	604.62	0.00000	NO	YES
81	e	605.76	13.15838	YES	YES
82	e	605.76	13.15838	YES	YES
83	b	614.11	7.45189	YES	YES
84	e	633.16	0.25440	YES	YES
85	e	633.16	0.25440	YES	YES
86	a	634.28	0.00000	NO	YES
87	b	634.56	0.40258	YES	YES
88	e	729.77	1.14512	YES	YES
89	e	729.77	1.14512	YES	YES
90	a	732.01	0.00000	NO	YES
91	b	735.39	1.09324	YES	YES
92	a	763.49	0.00000	NO	YES
93	e	765.52	15.90622	YES	YES
94	e	765.52	15.90622	YES	YES
95	b	765.62	19.16192	YES	YES
96	e	961.68	201.00791	YES	YES
97	e	961.68	201.00791	YES	YES
98	a	962.75	0.00000	NO	YES
99	b	967.99	217.30438	YES	YES
100	b	1067.84	369.03018	YES	YES
101	e	1068.01	294.28242	YES	YES
102	e	1068.01	294.28242	YES	YES
103	a	1070.98	0.00000	NO	YES
104	a	1124.98	0.00000	NO	YES
105	e	1125.62	1.52839	YES	YES
106	e	1125.62	1.52839	YES	YES
107	b	1130.76	3.06763	YES	YES
108	e	1256.23	39.29124	YES	YES
109	e	1256.23	39.29124	YES	YES
110	b	1256.58	42.00442	YES	YES
111	a	1258.54	0.00000	NO	YES
112	b	1348.54	47.46165	YES	YES
113	e	1353.43	5.18577	YES	YES
114	e	1353.43	5.18577	YES	YES
115	a	1355.15	0.00000	NO	YES
116	e	1360.45	31.53789	YES	YES
117	e	1360.45	31.53789	YES	YES
118	b	1360.91	22.02235	YES	YES
119	a	1370.35	0.00000	NO	YES
120	a	1452.61	0.00000	NO	YES
121	e	1454.77	585.10360	YES	YES
122	e	1454.77	585.10360	YES	YES
123	b	1465.51	667.14216	YES	YES
124	e	1504.53	187.89406	YES	YES
125	e	1504.53	187.89406	YES	YES
126	b	1504.55	283.74349	YES	YES
127	a	1507.52	0.00000	NO	YES
128	e	1614.98	10.41343	YES	YES
129	e	1614.98	10.41343	YES	YES
130	a	1615.47	0.00000	NO	YES

131	b	1616.59	47.53532	YES	YES
132	e	1618.42	54.62573	YES	YES
133	e	1618.42	54.62573	YES	YES
134	b	1618.84	17.35280	YES	YES
135	a	1619.34	0.00000	NO	YES

[GaI₄]⁻



Total energy = -1971.0547911510 H = -53635.1603439 eV

HOMO-LUMO Separation

HOMO: 14. 1 t1 -0.09823146 H = -2.67302 eV

LUMO: 15. 6 a1 +0.01389035 H = +0.37798 eV

Gap : +0.11212181 H = +3.05099 eV

Number of MOs= 37, Electrons= 60.00, Symmetry: td

```
$coord
  0.0000000000000000    0.0000000000000000    0.0000000000000000    ga
-2.85989593215004      2.85989593215004      2.85989593215004    i
  2.85989593215004     -2.85989593215004      2.85989593215004    i
  2.85989593215004      2.85989593215004     -2.85989593215004    i
-2.85989593215004     -2.85989593215004     -2.85989593215004    i
```

vibrational spectrum					selection rules	
#	mode	symmetry	wave number	IR intensity		
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	e		42.84	0.00000	NO	YES
8	e		42.84	0.00000	NO	YES
9	t2		66.87	0.40692	YES	YES
10	t2		66.87	0.40692	YES	YES
11	t2		66.87	0.40692	YES	YES
12	a1		129.62	0.00000	NO	YES
13	t2		213.32	56.44230	YES	YES
14	t2		213.32	56.44230	YES	YES
15	t2		213.32	56.44230	YES	YES

CuL:

CuBr



Total energy = -4214.7135766440 H = -114688.2570195 eV

HOMO-LUMO Separation

HOMO: 23. 7 e1 -0.19660990 H = -5.35003 eV

LUMO: 24. 15 a1 -0.12565440 H = -3.41923 eV

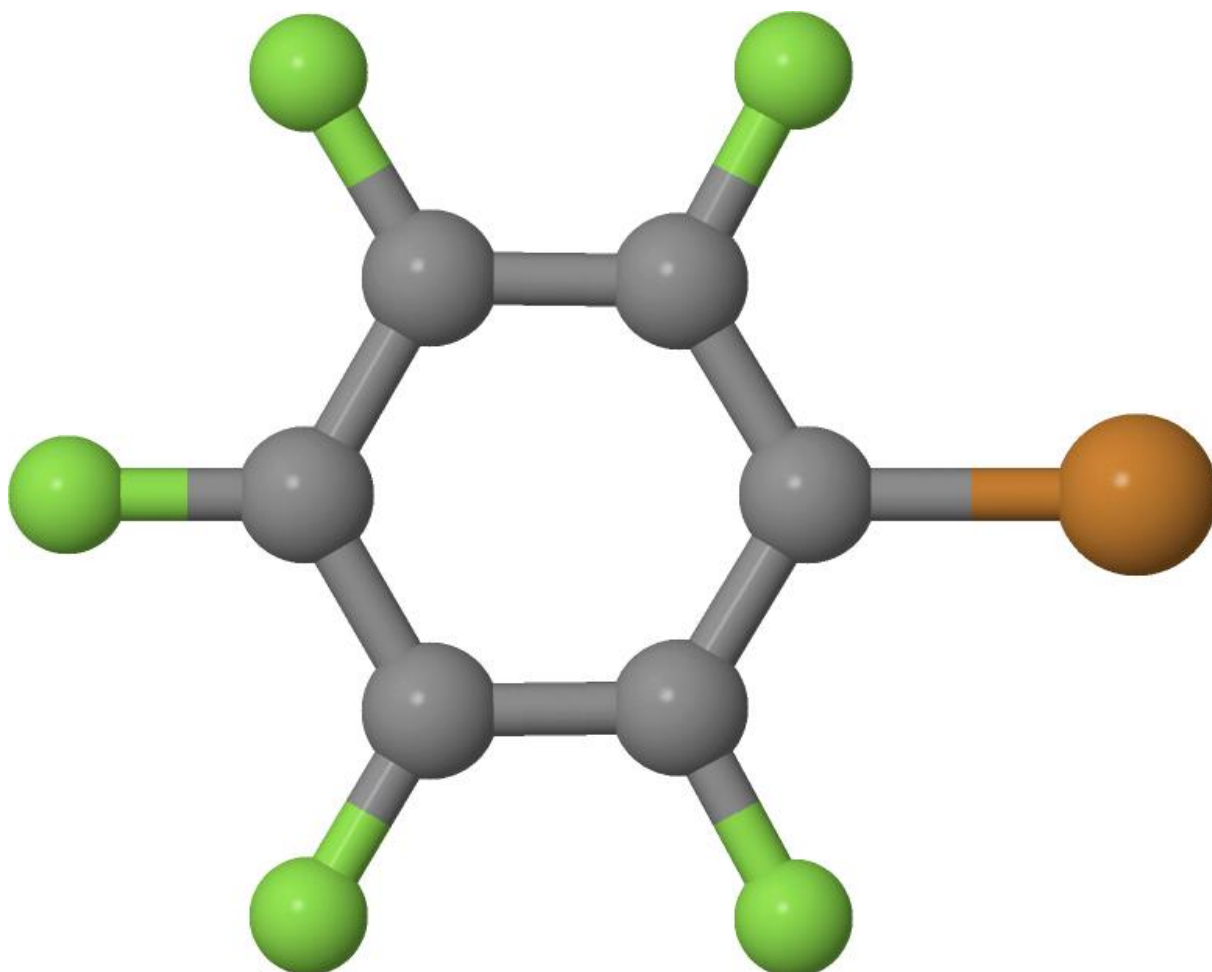
Gap : +0.07095550 H = +1.93080 eV

Number of MOs= 39, Electrons= 64.00, Symmetry: c6v

```
$coord
0.0000000000000000 0.0000000000000000 -2.07725044952114 cu
0.0000000000000000 0.0000000000000000 2.07725044952114 br
```

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm ⁻¹	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6		a1	295.43	9.36835	YES	YES

CuC₆F₅



Total energy = -2367.8345177170 H = -64432.0921954 eV

HOMO-LUMO Separation

HOMO: 55. 8 b2 -0.21202943 H = -5.76962 eV

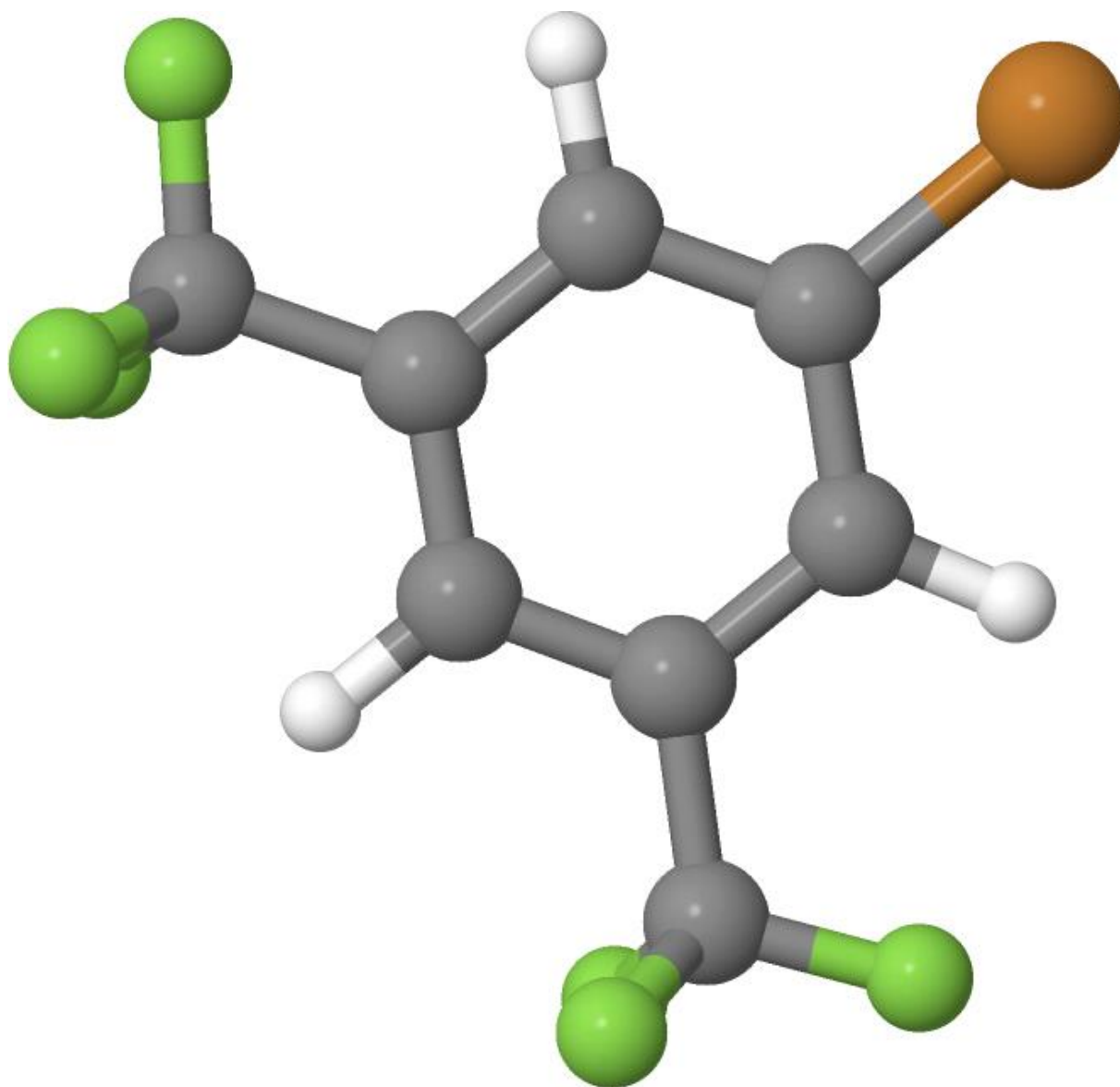
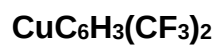
LUMO: 56. 27 a1 -0.11916561 H = -3.24266 eV

Gap : +0.09286382 H = +2.52695 eV

Number of MOs= 178, Electrons= 110.00, Symmetry: c2v

\$coord				
0.0000000000000000	0.0000000000000000	-2.61644010550580	c	
-2.26696549652561	0.0000000000000000	-1.25263235214258	c	
-2.30432271441033	0.0000000000000000	1.40422287382641	c	
0.0000000000000000	0.0000000000000000	2.73005704779434	c	
2.30432271441033	0.0000000000000000	1.40422287382641	c	
2.26696549652561	0.0000000000000000	-1.25263235214258	c	
4.51088562454591	0.0000000000000000	-2.47003575194573	f	
4.48634803856512	0.0000000000000000	2.69216862630672	f	
0.0000000000000000	0.0000000000000000	5.25848397021798	f	
-4.48634803856512	0.0000000000000000	2.69216862630672	f	
-4.51088562454591	0.0000000000000000	-2.47003575194573	f	
0.0000000000000000	0.0000000000000000	-6.11954770459623	cu	

\$vibrational spectrum						
#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		b2	78.11	3.97605	YES	YES
8		b1	84.02	4.69149	YES	YES
9		a2	122.07	0.00000	NO	YES
10		b2	154.38	0.26340	YES	YES
11		b2	200.72	0.01492	YES	YES
12		a1	221.15	5.72785	YES	YES
13		b1	261.72	0.01214	YES	YES
14		a1	267.48	1.60289	YES	YES
15		b1	298.15	0.15398	YES	YES
16		b2	333.00	7.66173	YES	YES
17		a1	342.37	0.37242	YES	YES
18		a2	392.50	0.00000	NO	YES
19		b1	429.10	0.08551	YES	YES
20		b2	477.59	2.92843	YES	YES
21		a1	483.90	0.23957	YES	YES
22		a1	562.61	0.35718	YES	YES
23		b2	571.39	3.55417	YES	YES
24		a2	627.83	0.00000	NO	YES
25		b1	723.11	0.19243	YES	YES
26		a1	794.86	46.83205	YES	YES
27		b1	964.30	159.40135	YES	YES
28		a1	1076.70	96.21662	YES	YES
29		b1	1138.42	2.58749	YES	YES
30		a1	1272.24	0.16484	YES	YES
31		b1	1355.31	0.01371	YES	YES
32		a1	1371.40	26.71766	YES	YES
33		b1	1473.72	481.13153	YES	YES
34		a1	1504.26	229.80236	YES	YES
35		a1	1611.48	7.08410	YES	YES
36		b1	1615.31	0.73602	YES	YES



Total energy = -2545.6322063360 H = -69270.2162195 eV

HOMO-LUMO Separation

HOMO: 67. 28 a1 -0.21055884 H = -5.72960 eV

LUMO: 68. 29 a1 -0.11606653 H = -3.15833 eV

Gap : +0.09449231 H = +2.57127 eV

Number of MOs= 226, Electrons= 134.00, Symmetry: c2v

\$coord

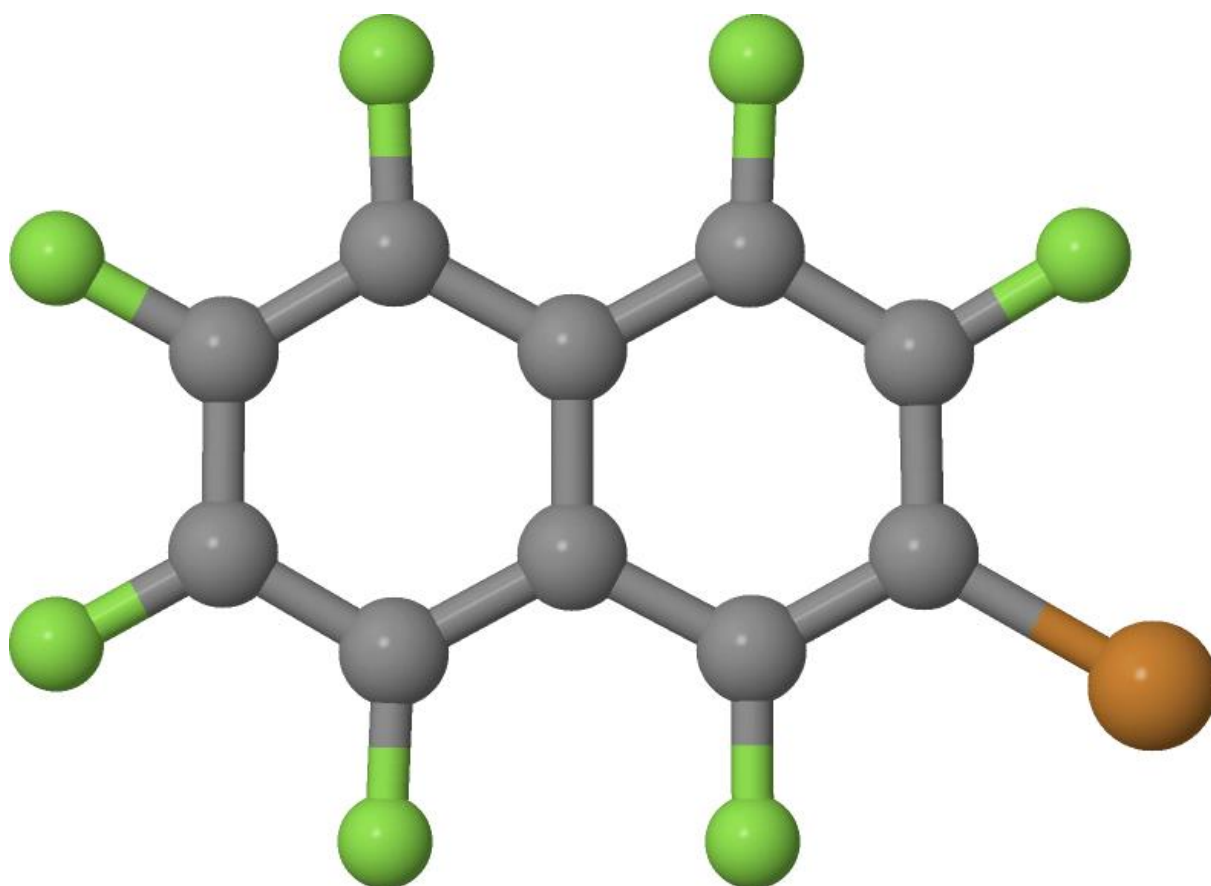
0.0000000000000000	2.29378514385759	-2.41917946859761	c
0.0000000000000000	0.0000000000000000	-3.78391422826311	c
0.0000000000000000	-2.29378514385759	-2.41917946859761	c
0.0000000000000000	-2.28905674384425	0.24186286350256	c
0.0000000000000000	0.0000000000000000	1.58274437719694	c
0.0000000000000000	2.28905674384425	0.24186286350256	c
0.0000000000000000	4.72756832933764	1.73460694795680	c
0.0000000000000000	6.79899273321596	0.23396587589425	f
2.05860759762375	4.88538433558348	3.25812864401264	f
-2.05860759762375	4.88538433558348	3.25812864401264	f
0.0000000000000000	-4.72756832933764	1.73460694795680	c
0.0000000000000000	-6.79899273321596	0.23396587589425	f
2.05860759762375	-4.88538433558348	3.25812864401264	f
-2.05860759762375	-4.88538433558348	3.25812864401264	f
0.0000000000000000	0.0000000000000000	-7.29559408365346	cu
0.0000000000000000	4.12674588517364	-3.40185399049768	h
0.0000000000000000	-4.12674588517364	-3.40185399049768	h
0.0000000000000000	0.0000000000000000	3.66349645321917	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
#						
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		b1	33.09	0.01553	YES	YES
8		a2	34.29	0.00000	NO	YES
9		b1	76.61	0.18185	YES	YES
10		b2	87.76	2.43515	YES	YES
11		a1	105.95	1.25744	YES	YES
12		b1	142.80	6.18805	YES	YES
13		a2	143.94	0.00000	NO	YES
14		a1	235.31	6.86164	YES	YES
15		b2	235.49	4.11421	YES	YES
16		a1	292.06	0.29700	YES	YES
17		a2	299.38	0.00000	NO	YES
18		b1	321.08	0.82434	YES	YES
19		b2	351.92	0.24304	YES	YES
20		a1	395.26	0.37895	YES	YES
21		b2	431.78	2.09395	YES	YES
22		b1	482.63	6.46204	YES	YES
23		a2	487.04	0.00000	NO	YES
24		a1	555.32	0.02858	YES	YES
25		b1	567.38	1.43368	YES	YES
26		b2	583.70	0.15271	YES	YES
27		a2	648.65	0.00000	NO	YES
28		b2	665.88	37.95982	YES	YES
29		a1	686.01	26.82376	YES	YES
30		b1	692.71	10.61944	YES	YES

31	a1	777.26	15.64848	YES	YES
32	b2	832.27	15.38822	YES	YES
33	b1	867.77	23.28269	YES	YES
34	b1	882.97	1.86296	YES	YES
35	a2	913.41	0.00000	NO	YES
36	a1	979.30	3.01899	YES	YES
37	a1	1084.64	50.03615	YES	YES
38	b2	1087.99	30.21671	YES	YES
39	a1	1103.13	29.37123	YES	YES
40	a2	1138.19	0.00000	NO	YES
41	b1	1143.06	501.63411	YES	YES
42	b2	1169.34	28.35153	YES	YES
43	a1	1178.84	286.94288	YES	YES
44	b2	1253.81	569.95965	YES	YES
45	b2	1257.12	129.43655	YES	YES
46	a1	1324.33	307.92653	YES	YES
47	b2	1352.91	0.04856	YES	YES
48	b2	1417.34	1.29320	YES	YES
49	a1	1436.99	0.02584	YES	YES
50	a1	1577.88	6.01916	YES	YES
51	b2	1606.40	15.39160	YES	YES
52	a1	3121.12	0.02902	YES	YES
53	a1	3123.69	0.71049	YES	YES
54	b2	3124.50	0.34711	YES	YES

CuC₁₀F₇



Total energy = -2719.7013956620 H = -74006.8825579 eV

HOMO-LUMO Separation

HOMO: 76. 16 a" -0.19478223 H = -5.30030 eV

LUMO: 77. 61 a' -0.12028215 H = -3.27305 eV

Gap : +0.07450007 H = +2.02725 eV

Number of MOs= 262, Electrons= 152.00, Symmetry: cs

\$coord

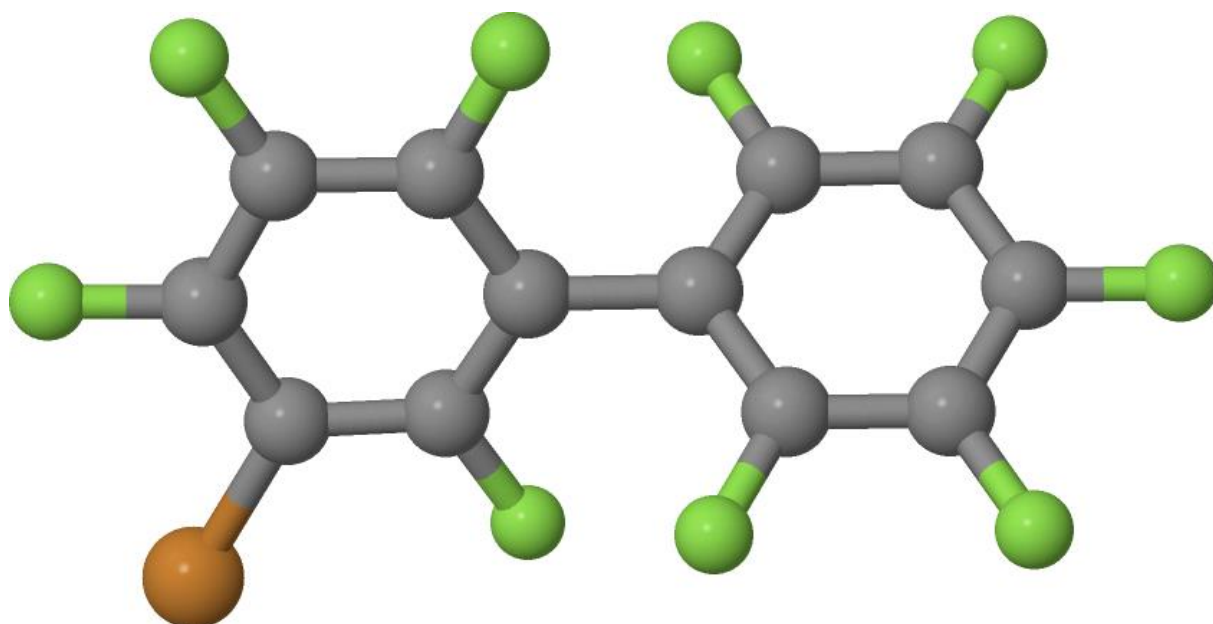
-4.68450121085924	1.30885823363094	0.00000000000000	c
-4.68019053394380	-1.37314539364169	0.00000000000000	c
-2.41026130400278	-2.69638645723881	0.00000000000000	c
-0.04547840565614	-1.40037209451442	0.00000000000000	c
-0.04527634317605	1.34616843487091	0.00000000000000	c
-2.41633809911444	2.63512202355288	0.00000000000000	c
2.32558501499046	-2.68443448042366	0.00000000000000	c
4.57745312473393	-1.32901879888574	0.00000000000000	c
4.63854859349416	1.33692400103154	0.00000000000000	c
2.34682908298944	2.60442489209643	0.00000000000000	c
2.36027895128325	5.16081271709430	0.00000000000000	f
7.67601498086400	3.08496009619907	0.00000000000000	cu
6.76321435286365	-2.64059606780717	0.00000000000000	f
2.41598567657533	-5.22012809128045	0.00000000000000	f
-2.51191449002697	-5.22591229803898	0.00000000000000	f
-6.88467233583392	-2.60555528744861	0.00000000000000	f
-6.89437213088656	2.53471160640984	0.00000000000000	f
-2.53090492429427	5.16356696439360	0.00000000000000	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a"	49.94	1.91352	YES	YES
8		a"	67.63	0.04950	YES	YES
9		a'	77.11	4.36907	YES	YES

10	a"	103.76	1.55171	YES	YES
11	a"	112.14	0.69142	YES	YES
12	a"	147.24	0.11658	YES	YES
13	a"	179.18	0.73287	YES	YES
14	a'	195.52	0.07744	YES	YES
15	a'	210.71	7.47395	YES	YES
16	a"	245.53	4.26702	YES	YES
17	a'	265.84	0.01088	YES	YES
18	a'	278.77	0.33855	YES	YES
19	a'	295.93	0.51150	YES	YES
20	a'	304.63	0.82962	YES	YES
21	a'	323.42	0.27407	YES	YES
22	a'	350.11	0.32333	YES	YES
23	a"	352.32	1.59105	YES	YES
24	a"	371.54	0.15864	YES	YES
25	a"	423.45	0.57205	YES	YES
26	a'	425.90	0.96444	YES	YES
27	a'	442.04	0.09608	YES	YES
28	a"	495.64	0.00006	YES	YES
29	a'	501.89	0.62057	YES	YES
30	a'	507.51	0.27360	YES	YES
31	a"	548.06	5.98113	YES	YES
32	a"	592.43	1.02154	YES	YES
33	a"	632.54	0.08298	YES	YES
34	a'	656.07	21.52544	YES	YES
35	a"	667.45	0.30050	YES	YES
36	a'	722.16	41.03245	YES	YES
37	a'	786.11	5.52829	YES	YES
38	a'	887.10	85.68954	YES	YES
39	a'	944.55	101.06211	YES	YES
40	a'	1038.94	11.47669	YES	YES
41	a'	1114.18	63.63255	YES	YES
42	a'	1153.46	64.37479	YES	YES
43	a'	1233.76	1.53706	YES	YES
44	a'	1258.63	25.60212	YES	YES
45	a'	1332.79	15.73992	YES	YES
46	a'	1373.73	8.13647	YES	YES
47	a'	1395.71	119.41845	YES	YES
48	a'	1407.77	341.63804	YES	YES
49	a'	1459.85	3.15030	YES	YES
50	a'	1489.65	291.90590	YES	YES
51	a'	1528.11	100.71204	YES	YES
52	a'	1595.19	138.38476	YES	YES
53	a'	1615.25	76.10689	YES	YES
54	a'	1646.56	85.07723	YES	YES

CuC₁₂F₉



Total energy = -2995.3854260370 H = -81508.6309821 eV

HOMO-LUMO Separation

HOMO: 91. 91 a -0.21394854 H = -5.82184 eV

LUMO: 92. 92 a -0.12008073 H = -3.26756 eV

Gap : +0.09386780 H = +2.55427 eV

Number of MOs= 318, Electrons= 182.00, Symmetry: c1

\$coord

-5.76643237448327	0.49682145539005	1.18864172913730	c
-6.61256096375133	-1.49699560936825	-0.35035899635481	c
-4.86638268482243	-2.91850351559819	-1.76068529044108	c
-1.37660127078852	-0.34559084976288	-0.08568312454565	c
-3.17212437854501	1.04402419526205	1.31052941627106	c
1.35706988930648	0.25793467450093	0.06300009091902	c
3.12440007254433	-1.55371811773520	0.90010852514380	c
5.71345002767210	-0.99668383255119	1.06776010545558	c
6.54766175503479	1.43495523443700	0.39379802870772	c
4.88084318154830	3.30793056585897	-0.44801290906276	c

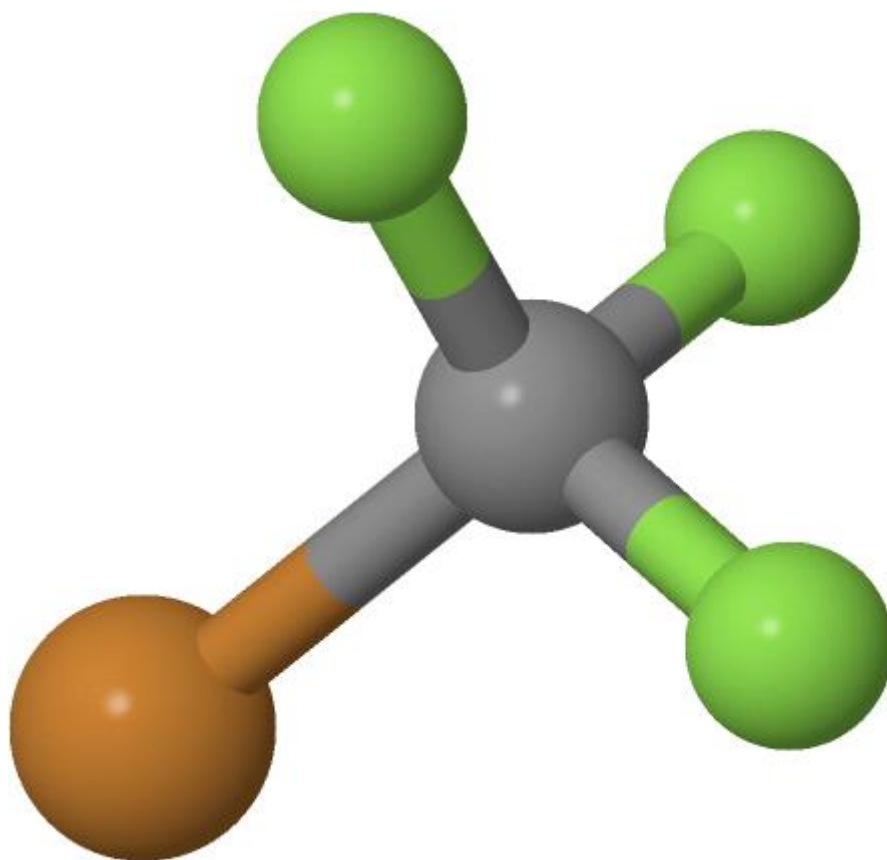
2.32219025940192	2.65734996321438	-0.59724628007572	c
0.65178416419699	4.40096283027737	-1.43950214019505	f
6.01711647395816	6.50462397237668	-1.32294121908737	cu
9.04171302804886	1.91579709446457	0.58614541506702	f
7.34146053469384	-2.75613454264912	1.88785725635236	f
-5.67357307304487	-4.80174151480100	-3.23964221449334	f
-9.07303154719898	-2.04075571663601	-0.46978690704000	f
-2.41866324612209	2.92481243893614	2.82569234773595	f
-7.42702115752132	1.83736993593659	2.54239536445221	f
-2.28241734569610	-2.32521127701322	-1.62259850418465	c
-0.66895341636214	-3.68554315358323	-3.01749238855742	f
2.34007207193040	-3.86170423095655	1.58802169479572	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	28.66	0.64508	YES	YES
8		a	38.72	0.28472	YES	YES
9		a	42.65	0.50368	YES	YES
10		a	81.43	3.17597	YES	YES
11		a	82.50	3.51228	YES	YES
12		a	121.98	0.09754	YES	YES
13		a	130.19	0.07571	YES	YES
14		a	133.79	0.21227	YES	YES
15		a	158.04	0.82342	YES	YES
16		a	163.73	0.20240	YES	YES
17		a	180.11	0.82061	YES	YES
18		a	216.87	0.64335	YES	YES
19		a	226.59	4.75189	YES	YES
20		a	236.97	4.40326	YES	YES
21		a	261.06	0.08220	YES	YES
22		a	266.81	0.06846	YES	YES
23		a	272.15	0.55383	YES	YES
24		a	300.67	1.10100	YES	YES
25		a	317.12	2.19312	YES	YES
26		a	338.26	4.37405	YES	YES
27		a	343.60	2.14340	YES	YES
28		a	363.70	0.25894	YES	YES
29		a	378.80	0.39857	YES	YES
30		a	382.54	0.36849	YES	YES
31		a	405.46	0.01286	YES	YES
32		a	434.14	0.07768	YES	YES
33		a	448.00	1.44541	YES	YES
34		a	477.45	1.91078	YES	YES
35		a	492.75	0.09400	YES	YES
36		a	563.38	2.35207	YES	YES
37		a	566.28	0.15437	YES	YES
38		a	573.87	5.67584	YES	YES
39		a	605.30	1.28071	YES	YES
40		a	619.68	2.73563	YES	YES
41		a	624.85	0.38301	YES	YES
42		a	641.47	29.20235	YES	YES
43		a	668.96	13.83623	YES	YES
44		a	734.53	2.04210	YES	YES
45		a	779.18	1.39265	YES	YES

46	a	826.00	62.54439	YES	YES
47	a	945.21	43.83750	YES	YES
48	a	998.36	165.93136	YES	YES
49	a	1062.44	159.44346	YES	YES
50	a	1073.79	101.32105	YES	YES
51	a	1151.77	8.46366	YES	YES
52	a	1163.41	4.19504	YES	YES
53	a	1252.08	14.91466	YES	YES
54	a	1322.36	0.22948	YES	YES
55	a	1342.96	0.56990	YES	YES
56	a	1352.94	6.68351	YES	YES
57	a	1356.04	3.40032	YES	YES
58	a	1417.68	19.36095	YES	YES
59	a	1465.49	448.98446	YES	YES
60	a	1482.97	180.46872	YES	YES
61	a	1503.89	290.51781	YES	YES
62	a	1521.19	217.65248	YES	YES
63	a	1588.16	29.02219	YES	YES
64	a	1617.89	62.54514	YES	YES
65	a	1619.81	5.57171	YES	YES
66	a	1638.15	14.73083	YES	YES

CuCF₃



Total energy = -1977.9210875740 H = -53822.0018824 eV

HOMO-LUMO Separation

HOMO: 22. 12 a1 -0.20566629 H = -5.59647 eV

LUMO: 23. 13 a1 -0.11662724 H = -3.17359 eV

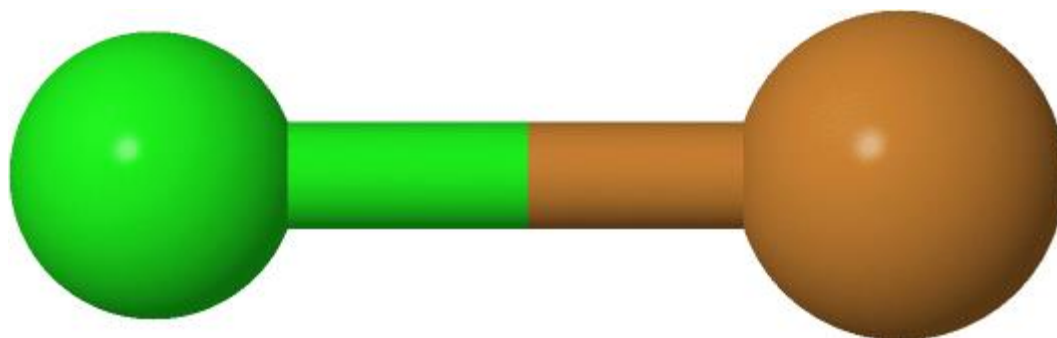
Gap : +0.08903904 H = +2.42288 eV

Number of MOs= 55, Electrons= 62.00, Symmetry: c3v

```
$coord
0.0000000000000000 0.0000000000000000 0.13925891865768 c
0.0000000000000000 0.0000000000000000 -3.47511695844959 cu
1.19168153655590 2.06405296775660 1.11126520149218 f
1.19168153655590 -2.06405296775660 1.11126520149218 f
-2.38336307311183 0.0000000000000000 1.11126520149218 f
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 0.00 0.00000 - -
7 e 189.23 4.16700 YES YES
8 e 189.23 4.16700 YES YES
9 a1 292.29 13.84100 YES YES
10 e 498.01 0.46971 YES YES
11 e 498.01 0.46971 YES YES
12 a1 704.35 9.67660 YES YES
13 e 1075.86 163.99910 YES YES
14 e 1075.86 163.99910 YES YES
15 a1 1084.37 602.74629 YES YES
```

CuCl



Total energy = -2100.6772815750 H = -57162.3697798 eV

HOMO-LUMO Separation

HOMO: 17. 5 e1 -0.19575993 H = -5.32690 eV

LUMO: 18. 12 a1 -0.12443297 H = -3.38600 eV

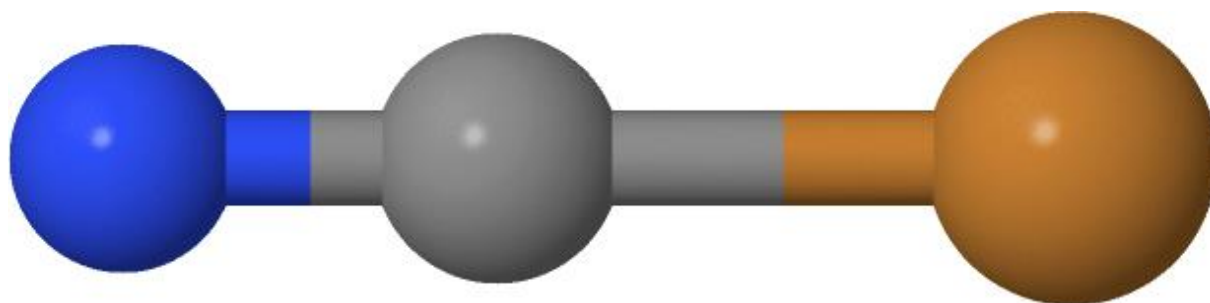
Gap : +0.07132696 H = +1.94091 eV

Number of MOs= 30, Electrons= 46.00, Symmetry: c6v

```
$coord
0.0000000000000000 0.0000000000000000 -1.95894302906375 cu
0.0000000000000000 0.0000000000000000 1.95894302906375 cl
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 a1 413.58 16.32357 YES YES
```

CuCN



Total energy = -1733.3122856080 H = -47165.8539286 eV

HOMO-LUMO Separation

HOMO: 16. 11 a1 -0.23510603 H = -6.39756 eV

LUMO: 17. 12 a1 -0.13345377 H = -3.63146 eV

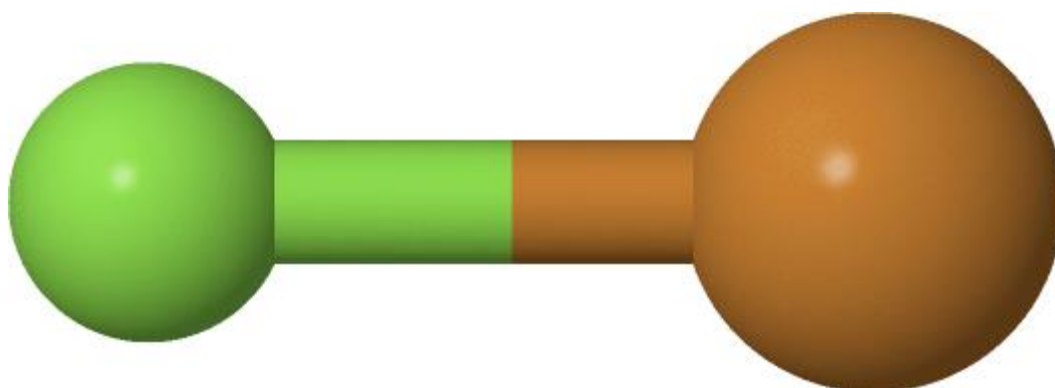
Gap : +0.10165226 H = +2.76610 eV

Number of MOs= 37, Electrons= 42.00, Symmetry: c6v

```
$coord
0.0000000000000000 0.0000000000000000 0.39619188673706 c
0.0000000000000000 0.0000000000000000 2.62364752468635 n
0.0000000000000000 0.0000000000000000 -3.01983941142341 cu
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 e1 256.00 8.30393 YES YES
7 e1 256.00 8.30393 YES YES
8 a1 473.48 10.78687 YES YES
9 a1 2188.33 0.22251 YES YES
```

CuF



Total energy = -1740.2971412270 H = -47355.9216288 eV

HOMO-LUMO Separation

HOMO: 14. 4 e1 -0.19411906 H = -5.28225 eV

LUMO: 15. 10 a1 -0.12923066 H = -3.51655 eV

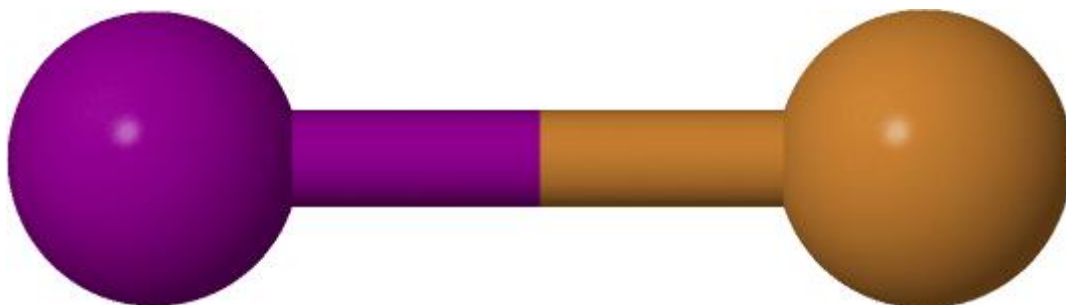
Gap : +0.06488840 H = +1.76570 eV

Number of MOs= 27, Electrons= 38.00, Symmetry: c6v

```
$coord
0.0000000000000000 0.0000000000000000 -1.64596402039690 cu
0.0000000000000000 0.0000000000000000 1.64596402039690 f
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 a1 623.24 39.29300 YES YES
```


CuI



Total energy = -1652.0440561360 H = -44954.4316291 eV

HOMO-LUMO Separation

HOMO: 13. 4 e1 -0.19995035 H = -5.44093 eV

LUMO: 14. 9 a1 -0.12992004 H = -3.53531 eV

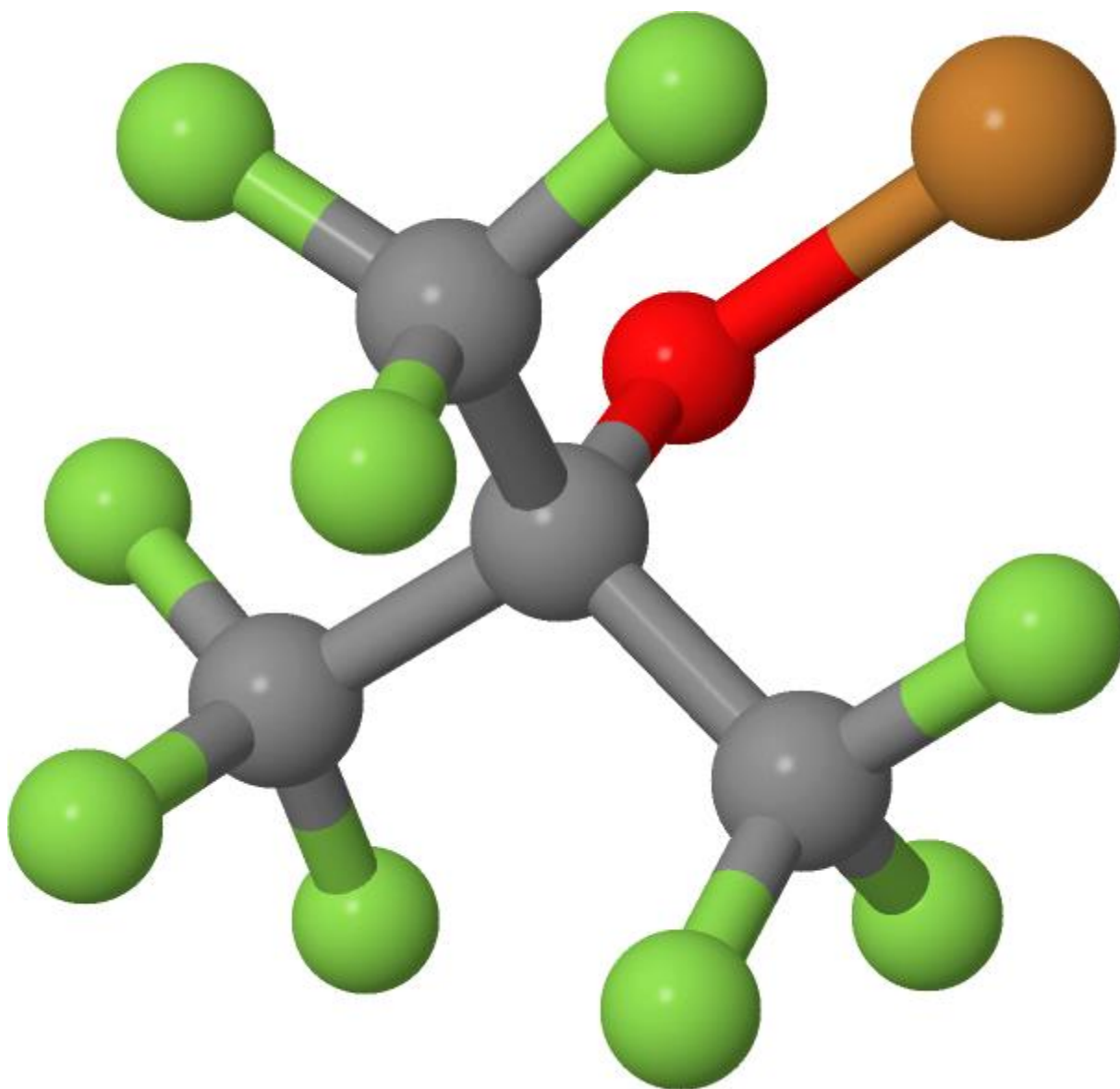
Gap : +0.07003031 H = +1.90562 eV

Number of MOs= 26, Electrons= 36.00, Symmetry: c6v

```
$coord
0.0000000000000000 0.0000000000000000 -2.24951851367393 cu
0.0000000000000000 0.0000000000000000 2.24951851367393 i
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 a1 256.00 7.86802 YES YES
```

CuOCC(CF3)3



Total energy = -2765.9972200930 H = -75266.6567548 eV

HOMO-LUMO Separation

HOMO: 71. 71 a -0.20409535 H = -5.55372 eV

LUMO: 72. 72 a -0.13657736 H = -3.71646 eV

Gap : +0.06751799 H = +1.83726 eV

Number of MOs= 220, Electrons= 142.00, Symmetry: c1

\$vibrational spectrum

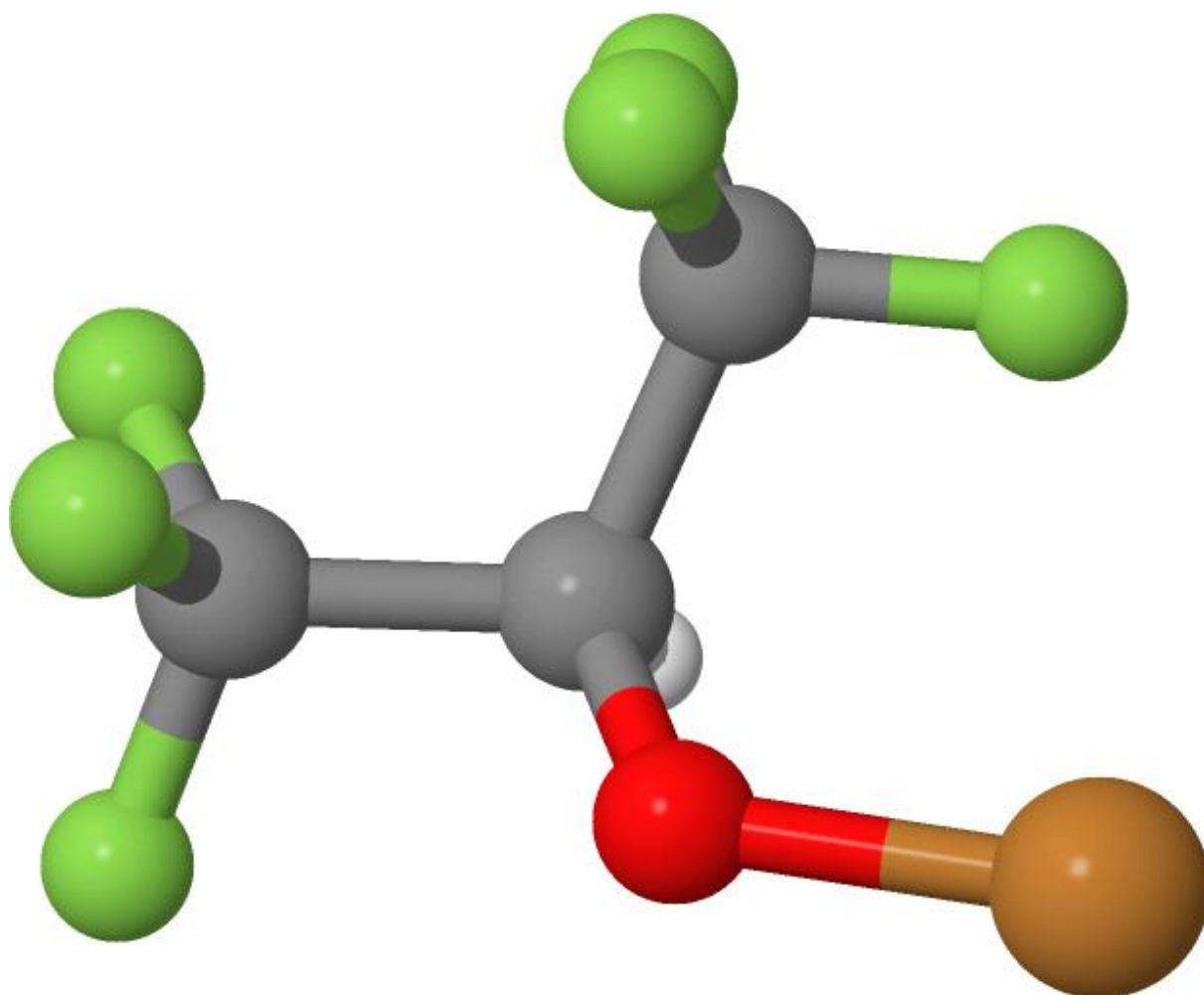
#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	51.63	0.57696	YES	YES
8		a	54.27	5.14472	YES	YES
9		a	67.95	3.62608	YES	YES
10		a	77.44	1.94312	YES	YES
11		a	86.58	3.92146	YES	YES
12		a	145.82	4.01838	YES	YES
13		a	156.15	0.09087	YES	YES
14		a	177.40	0.47719	YES	YES
15		a	220.57	3.71592	YES	YES
16		a	260.36	5.24895	YES	YES
17		a	284.37	0.05382	YES	YES
18		a	291.16	1.39673	YES	YES
19		a	308.38	0.54750	YES	YES
20		a	314.85	0.38955	YES	YES
21		a	326.24	0.28050	YES	YES
22		a	343.74	3.01239	YES	YES
23		a	463.92	2.78824	YES	YES
24		a	514.54	4.28428	YES	YES
25		a	519.20	3.22793	YES	YES
26		a	522.88	1.48199	YES	YES
27		a	535.46	2.55692	YES	YES
28		a	551.88	0.62008	YES	YES
29		a	562.73	2.38906	YES	YES
30		a	678.26	1.08793	YES	YES
31		a	701.88	39.32798	YES	YES
32		a	712.41	33.94623	YES	YES
33		a	747.22	3.96971	YES	YES
34		a	945.93	125.97794	YES	YES
35		a	956.36	144.93064	YES	YES
36		a	1079.05	4.32320	YES	YES
37		a	1131.84	13.74932	YES	YES
38		a	1164.63	3.99511	YES	YES
39		a	1172.99	2.56673	YES	YES
40		a	1182.71	205.40129	YES	YES
41		a	1201.23	192.87489	YES	YES
42		a	1209.85	349.88277	YES	YES
43		a	1249.74	501.14671	YES	YES
44		a	1255.90	523.13948	YES	YES
45		a	1263.50	93.53645	YES	YES

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN

1		0.00	0.00000	-	-
2		0.00	0.00000	-	-
3		0.00	0.00000	-	-
4		0.00	0.00000	-	-
5		0.00	0.00000	-	-
6		0.00	0.00000	-	-
7	a	51.63	0.57696	YES	YES
8	a	54.27	5.14472	YES	YES
9	a	67.95	3.62608	YES	YES
10	a	77.44	1.94312	YES	YES
11	a	86.58	3.92146	YES	YES
12	a	145.82	4.01838	YES	YES
13	a	156.15	0.09087	YES	YES
14	a	177.40	0.47719	YES	YES
15	a	220.57	3.71592	YES	YES
16	a	260.36	5.24895	YES	YES
17	a	284.37	0.05382	YES	YES
18	a	291.16	1.39673	YES	YES
19	a	308.38	0.54750	YES	YES
20	a	314.85	0.38955	YES	YES
21	a	326.24	0.28050	YES	YES
22	a	343.74	3.01239	YES	YES
23	a	463.92	2.78824	YES	YES
24	a	514.54	4.28428	YES	YES
25	a	519.20	3.22793	YES	YES
26	a	522.88	1.48199	YES	YES
27	a	535.46	2.55692	YES	YES
28	a	551.88	0.62008	YES	YES
29	a	562.73	2.38906	YES	YES
30	a	678.26	1.08793	YES	YES
31	a	701.88	39.32798	YES	YES
32	a	712.41	33.94623	YES	YES
33	a	747.22	3.96971	YES	YES
34	a	945.93	125.97794	YES	YES
35	a	956.36	144.93064	YES	YES
36	a	1079.05	4.32320	YES	YES
37	a	1131.84	13.74932	YES	YES
38	a	1164.63	3.99511	YES	YES
39	a	1172.99	2.56673	YES	YES
40	a	1182.71	205.40129	YES	YES
41	a	1201.23	192.87489	YES	YES
42	a	1209.85	349.88277	YES	YES
43	a	1249.74	501.14671	YES	YES
44	a	1255.90	523.13948	YES	YES
45	a	1263.50	93.53645	YES	YES

CuOhfip



Total energy = -2429.1918775470 H = -66101.7118567 eV

HOMO-LUMO Separation

HOMO: 55. 55 a -0.19448917 H = -5.29232 eV

LUMO: 56. 56 a -0.13429806 H = -3.65444 eV

Gap : +0.06019111 H = +1.63788 eV

Number of MOs= 166, Electrons= 110.00, Symmetry: c1

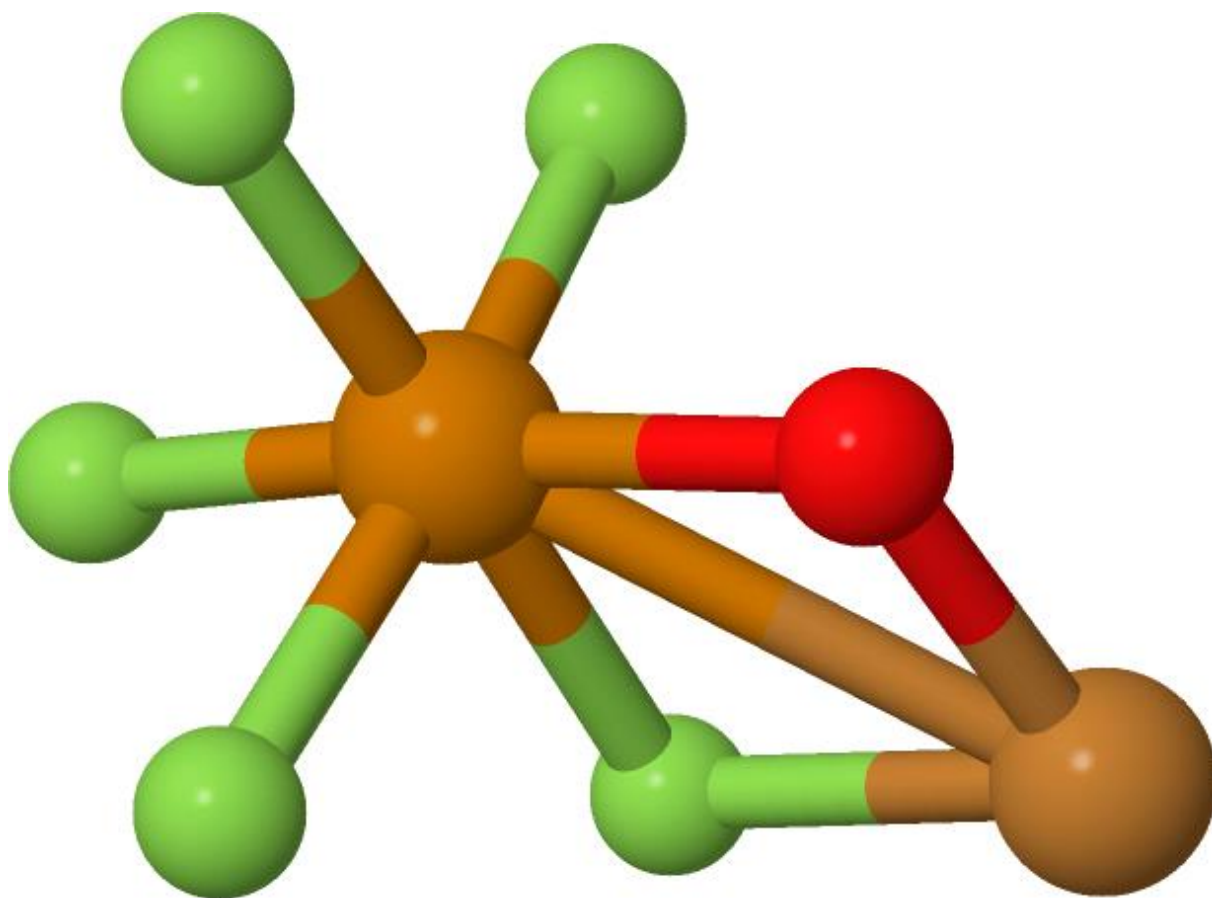
\$coord

-0.26937498906175	0.47790506886453	-0.67567591118717	c
-0.79872578274781	-2.22104483261626	0.34204752202373	c
2.31034996066575	1.51684254498302	0.26745337389752	c
-2.09407281368532	2.19407601890490	0.01389117867122	o
-5.38620522503236	1.51764289982301	-0.64276413152918	cu
4.22919418285168	-0.09588497346962	-0.27014628139114	f
2.32126713792372	1.93814239615639	2.77478159872878	f
2.81261530643206	3.72468979407731	-0.90742808983522	f
0.86931419616524	-3.93966855906190	-0.52497961521432	f
-0.83838767240189	-2.34221002158558	2.87916148090003	f
-3.14079028837149	-2.99069101976556	-0.48564480203654	f
-0.01518401273778	0.22020068368976	-2.77069632302771	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	30.85	0.20582	YES	YES
8		a	53.99	3.23589	YES	YES
9		a	85.18	6.69484	YES	YES
10		a	109.67	4.88840	YES	YES
11		a	151.53	2.43604	YES	YES
12		a	204.24	6.22069	YES	YES
13		a	232.64	5.96622	YES	YES
14		a	287.73	0.37851	YES	YES
15		a	300.76	1.97098	YES	YES
16		a	321.09	0.50426	YES	YES
17		a	432.31	3.29980	YES	YES
18		a	502.30	6.32986	YES	YES
19		a	518.22	2.58732	YES	YES
20		a	529.40	1.62428	YES	YES
21		a	541.72	2.49826	YES	YES
22		a	644.36	2.74229	YES	YES
23		a	679.00	37.03171	YES	YES
24		a	725.63	18.11712	YES	YES
25		a	835.06	27.23296	YES	YES
26		a	877.28	38.19588	YES	YES
27		a	1059.40	138.12943	YES	YES
28		a	1133.54	28.89057	YES	YES
29		a	1155.33	136.82407	YES	YES
30		a	1186.34	138.41232	YES	YES
31		a	1196.42	567.98380	YES	YES
32		a	1237.24	166.62233	YES	YES
33		a	1266.97	316.77874	YES	YES
34		a	1330.93	8.55128	YES	YES
35		a	1341.50	61.61233	YES	YES
36		a	2839.38	76.80402	YES	YES

CuOTeF₅



Total energy = -2222.6405542670 H = -60481.1611784 eV

HOMO-LUMO Separation

HOMO: 44. 44 a -0.22986392 H = -6.25492 eV

LUMO: 45. 45 a -0.20052940 H = -5.45669 eV

Gap : +0.02933452 H = +0.79823 eV

Number of MOs= 121, Electrons= 88.00, Symmetry: c1

\$coord
4.78634357717887 -0.04571584163598 -0.80255813588804 cu
683

1.81571140955328	0.82080910861074	-2.55020227296392	o
-0.71236639252251	0.06698298387618	-0.04350969931305	te
-1.09173431076514	-3.44785408720433	-1.04659214835020	f
-2.86877081340734	-0.82163287807278	2.75761738807500	f
-3.60948719928536	1.01224415340884	-2.02391572381592	f
-0.61117783493831	3.39935248054989	1.50319727786999	f
2.29148156418651	-0.98418591953249	2.20596331438611	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	49.88	2.04905	YES	YES
8		a	108.11	0.07511	YES	YES
9		a	142.86	0.16241	YES	YES
10		a	148.19	6.23040	YES	YES
11		a	190.16	6.93539	YES	YES
12		a	202.48	8.34782	YES	YES
13		a	224.31	0.07828	YES	YES
14		a	255.75	5.38209	YES	YES
15		a	266.15	38.28809	YES	YES
16		a	271.87	3.56593	YES	YES
17		a	274.12	22.70406	YES	YES
18		a	459.87	48.98132	YES	YES
19		a	512.24	5.77355	YES	YES
20		a	554.65	11.99960	YES	YES
21		a	574.59	4.11014	YES	YES
22		a	619.53	80.34442	YES	YES
23		a	621.44	116.50749	YES	YES
24		a	627.10	108.01613	YES	YES

HL:

HBr



Total energy = -2574.7289947850 H = -70061.9805687 eV

HOMO-LUMO Separation

HOMO: 18. 18 a -0.26558829 H = -7.22703 eV

LUMO: 19. 19 a -0.04229846 H = -1.15100 eV

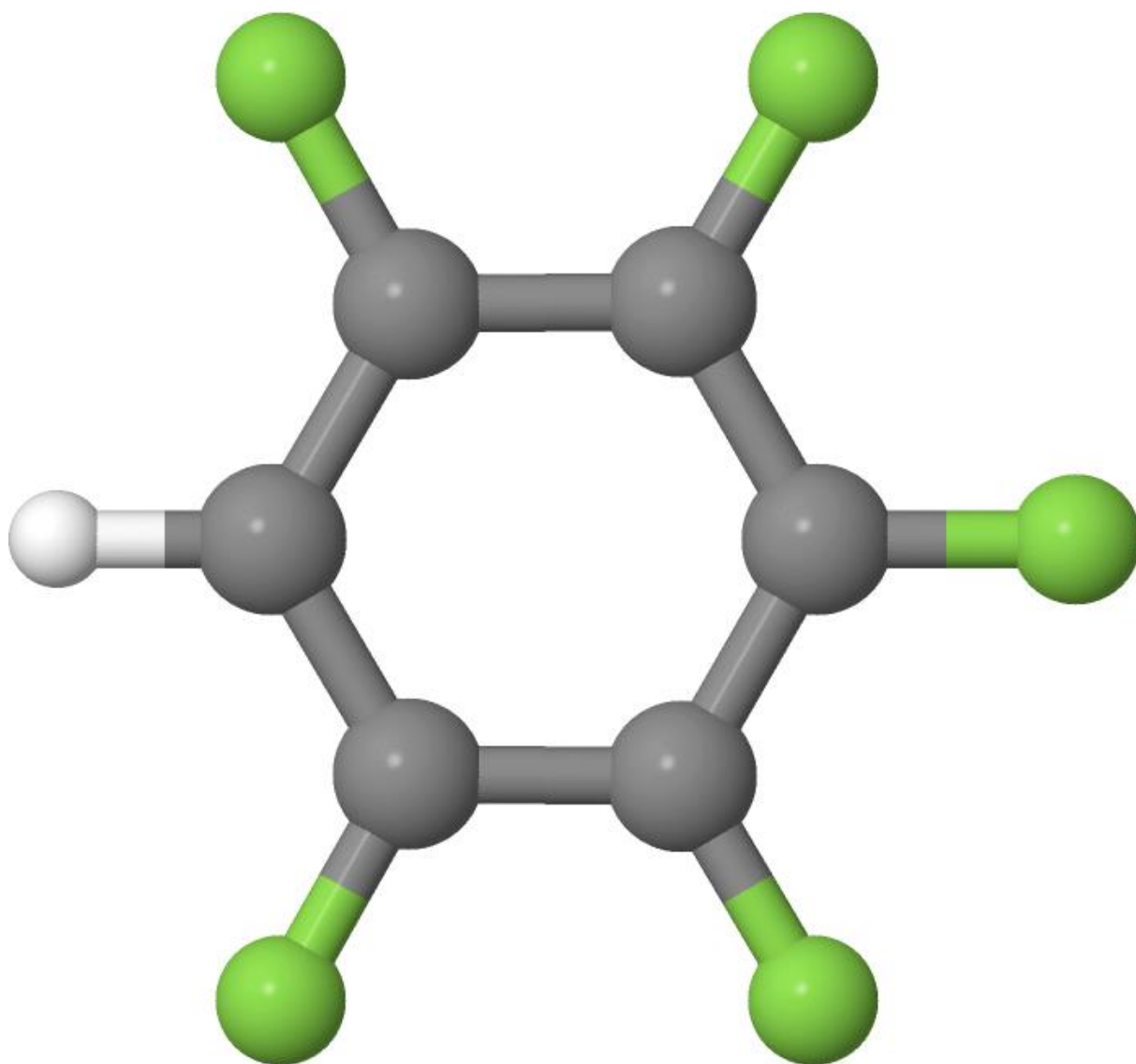
Gap : +0.22328983 H = +6.07603 eV

Number of MOs= 34, Electrons= 36.00, Symmetry: c1

```
$coord
0.0000000000000000 0.0000000000000000 -1.36877186045153 br
0.0000000000000000 0.0000000000000000 1.36877186045153 h
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 a 2514.88 5.17930 YES YES
```

HC₆F₅



Total energy = -727.8926964249 H = -19806.9793195 eV

HOMO-LUMO Separation

HOMO: 41. 3 a2 -0.23411288 H = -6.37054 eV

LUMO: 42. 6 b2 -0.06857740 H = -1.86609 eV

Gap : +0.16553548 H = +4.50445 eV

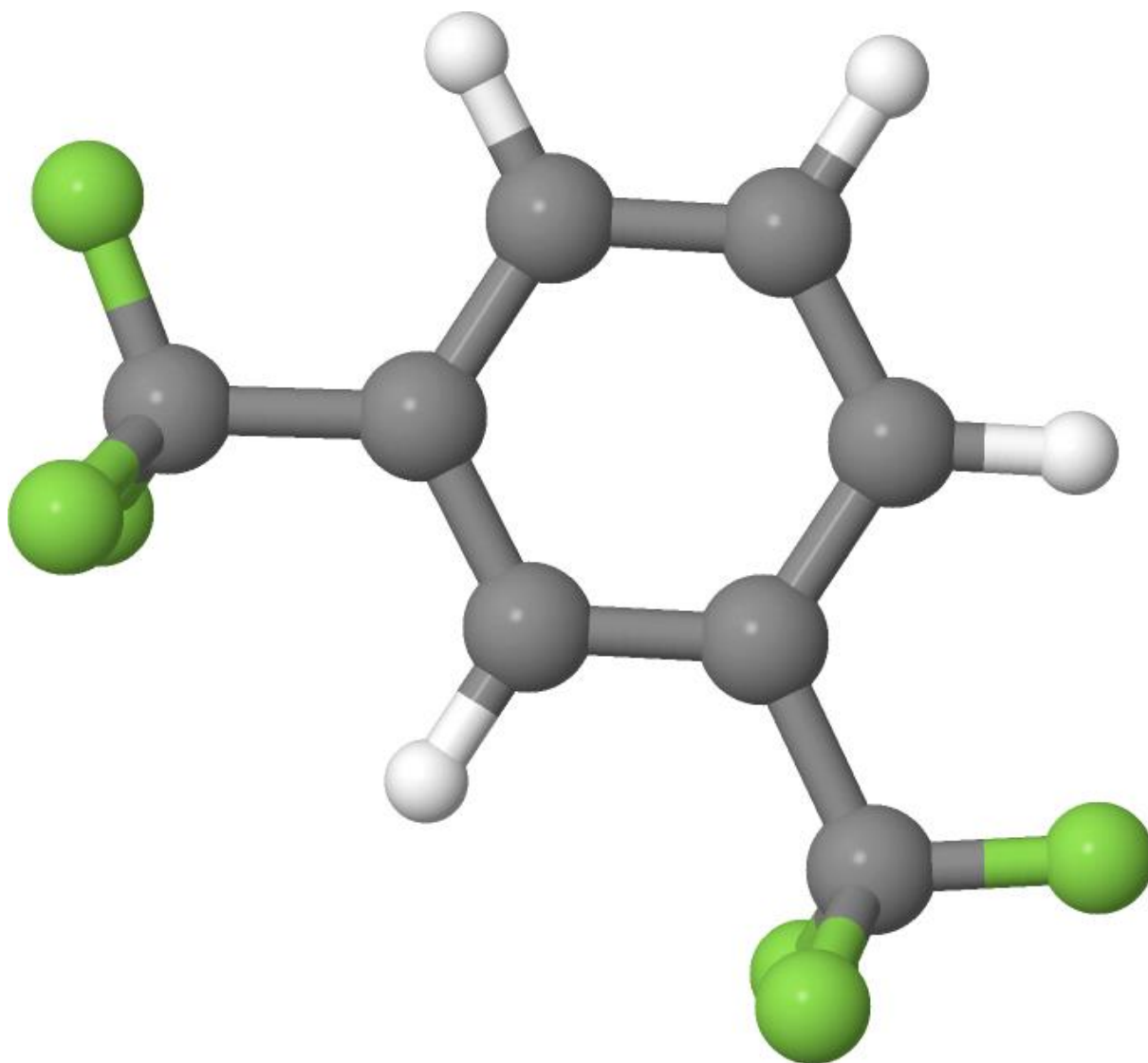
Number of MOs= 156, Electrons= 82.00, Symmetry: c2v

2.30984483596961	0.000000000000000	-1.28939800194865	c
0.000000000000000	0.000000000000000	-2.60710239309042	c
-2.30984483596961	0.000000000000000	-1.28939800194865	c
-2.28262604260381	0.000000000000000	1.36915191182219	c
0.000000000000000	0.000000000000000	2.70731687920671	c
2.28262604260381	0.000000000000000	1.36915191182219	c
4.48755506209259	0.000000000000000	2.61252812001504	f
4.48682161391796	0.000000000000000	-2.56966220891628	f
0.000000000000000	0.000000000000000	-5.12993849763170	f
-4.48682161391796	0.000000000000000	-2.56966220891628	f
-4.48755506209259	0.000000000000000	2.61252812001504	f
0.000000000000000	0.000000000000000	4.78448436957079	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a2	128.37	0.00000	NO	YES
8		b2	147.11	0.11651	YES	YES
9		b2	202.11	1.45522	YES	YES
10		a1	258.34	0.00096	YES	YES
11		b1	261.51	0.02322	YES	YES
12		b1	294.41	0.51795	YES	YES
13		b2	315.35	0.00944	YES	YES
14		a1	321.25	1.42009	YES	YES
15		a2	392.65	0.00000	NO	YES
16		b1	422.22	0.15549	YES	YES
17		a1	459.82	0.41583	YES	YES
18		b2	476.29	0.06932	YES	YES
19		b2	548.23	2.19915	YES	YES
20		a1	564.55	0.00509	YES	YES
21		a2	630.73	0.00000	NO	YES
22		b1	679.08	2.21288	YES	YES
23		a1	702.09	17.67077	YES	YES
24		b2	811.82	26.53749	YES	YES
25		b1	950.62	138.67305	YES	YES
26		a1	1078.85	151.23751	YES	YES
27		b1	1144.33	50.79790	YES	YES
28		b1	1176.08	26.86016	YES	YES
29		a1	1284.68	9.92658	YES	YES
30		b1	1354.67	5.90341	YES	YES
31		a1	1416.14	6.55429	YES	YES
32		a1	1514.57	171.12339	YES	YES
33		b1	1534.29	418.91869	YES	YES
34		a1	1629.78	37.61241	YES	YES
35		b1	1642.68	8.04739	YES	YES
36		a1	3152.17	4.12793	YES	YES

HC₆H₃(CF₃)₃



Total energy = -905.7007711605 H = -24645.3859644 eV

HOMO-LUMO Separation

HOMO: 53. 8 b1 -0.26479238 H = -7.20537 eV

LUMO: 54. 8 a2 -0.08632950 H = -2.34915 eV

Gap : +0.17846288 H = +4.85622 eV

Number of MOs= 204, Electrons= 106.00, Symmetry: c2v

\$coord

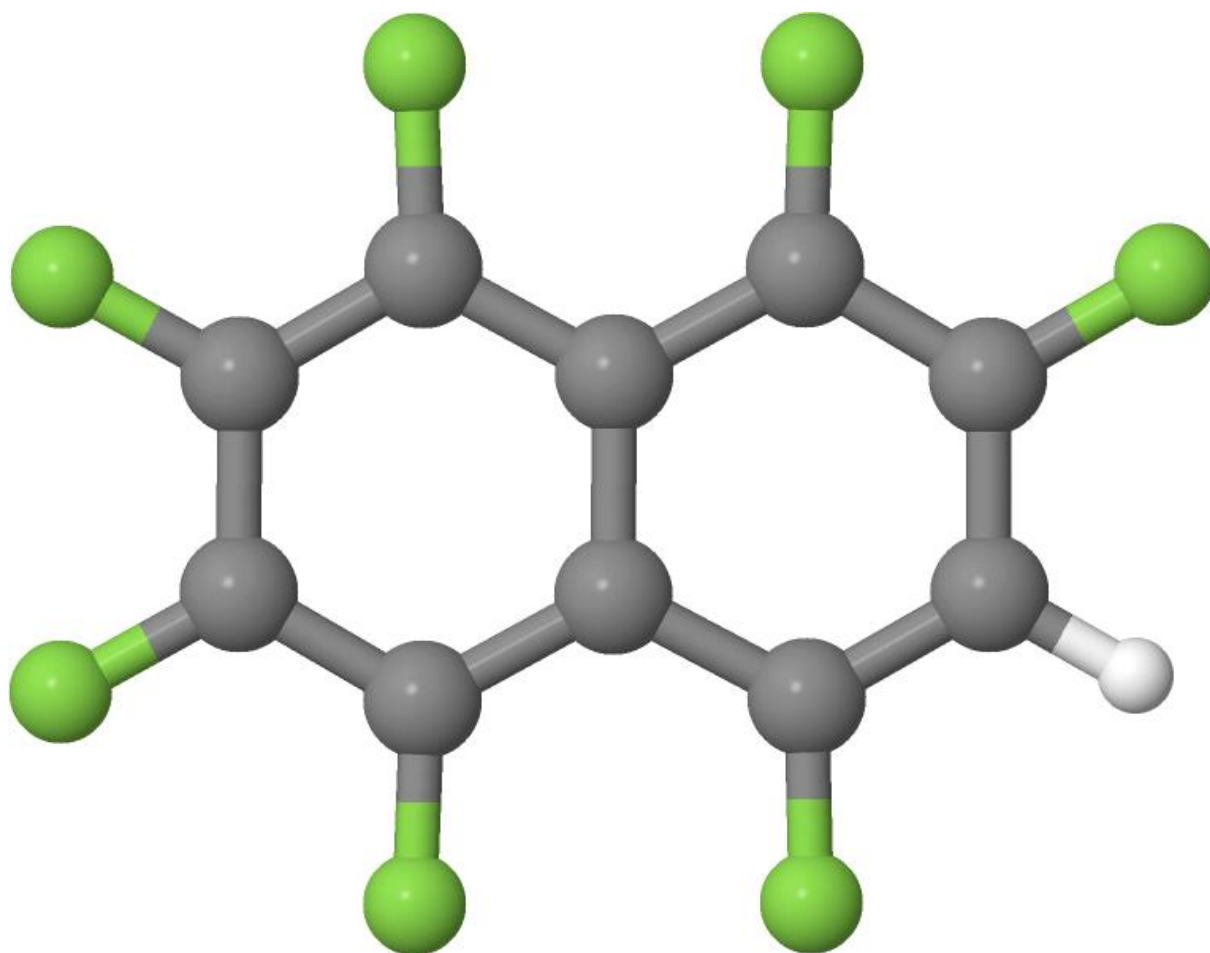
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0.0000000000000000	0.0000000000000000	-3.81638390432651	c
0.0000000000000000	-2.30179715378897	-2.49705412752146	c
0.0000000000000000	-2.29616895378674	0.16045215187503	c
0.0000000000000000	0.0000000000000000	1.49158916863518	c
0.0000000000000000	2.29616895378674	0.16045215187503	c
0.0000000000000000	4.73274886945724	1.65994330044370	c
0.0000000000000000	6.80004121193668	0.15757516996018	f
2.05867823104593	4.88186937074601	3.17992870008976	f
-2.05867823104593	4.88186937074601	3.17992870008976	f
0.0000000000000000	-4.73274886945724	1.65994330044370	c
0.0000000000000000	-6.80004121193668	0.15757516996018	f
2.05867823104593	-4.88186937074601	3.17992870008976	f
-2.05867823104593	-4.88186937074601	3.17992870008976	f
0.0000000000000000	4.10827090948488	-3.52656183316715	h
0.0000000000000000	0.0000000000000000	-5.89851503435978	h
0.0000000000000000	-4.10827090948488	-3.52656183316715	h
0.0000000000000000	0.0000000000000000	3.57247248697478	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		b1	31.98	0.10870	YES	YES
8		a2	35.34	0.00000	NO	YES
9		b1	97.55	0.16637	YES	YES
10		a1	111.65	0.93027	YES	YES
11		a2	144.63	0.00000	NO	YES
12		b2	219.96	0.78523	YES	YES
13		a1	284.58	0.84296	YES	YES
14		a2	305.88	0.00000	NO	YES
15		b1	315.02	0.15242	YES	YES
16		b2	340.70	4.77317	YES	YES
17		a1	375.32	4.50708	YES	YES
18		b2	425.40	0.65046	YES	YES
19		b1	453.12	0.33127	YES	YES
20		a2	489.93	0.00000	NO	YES
21		b1	554.51	2.55612	YES	YES
22		a1	555.18	0.05427	YES	YES
23		b2	579.30	0.27352	YES	YES
24		a1	639.02	5.05752	YES	YES
25		a2	655.38	0.00000	NO	YES
26		b2	664.51	41.48053	YES	YES
27		b1	695.75	22.82882	YES	YES
28		a1	735.22	1.63485	YES	YES
29		b1	799.18	32.22368	YES	YES
30		b2	824.18	15.53752	YES	YES
31		b1	884.43	9.23080	YES	YES
32		a2	923.60	0.00000	NO	YES
33		b1	980.68	1.53158	YES	YES
34		a1	987.53	3.89981	YES	YES

35	a1	1065.70	106.51233	YES	YES
36	b2	1070.49	33.37689	YES	YES
37	a1	1086.65	0.33443	YES	YES
38	a2	1143.61	0.00000	NO	YES
39	b1	1148.25	508.30964	YES	YES
40	b2	1153.43	1.25102	YES	YES
41	b2	1175.88	40.83471	YES	YES
42	a1	1181.03	267.76817	YES	YES
43	b2	1256.65	520.68319	YES	YES
44	b2	1287.19	135.23744	YES	YES
45	a1	1331.30	145.80592	YES	YES
46	b2	1385.71	0.09927	YES	YES
47	a1	1438.84	2.52556	YES	YES
48	b2	1490.08	0.87389	YES	YES
49	a1	1613.52	2.64960	YES	YES
50	b2	1630.14	14.29912	YES	YES
51	a1	3111.90	3.66607	YES	YES
52	a1	3122.48	0.02447	YES	YES
53	b2	3134.53	0.24574	YES	YES
54	a1	3138.22	2.21294	YES	YES

HC₁₀F₇



Total energy = -1079.7599141420 H = -29381.7789277 eV

HOMO-LUMO Separation

HOMO: 62. 12 a" -0.21221123 H = -5.77456 eV

LUMO: 63. 13 a" -0.10081976 H = -2.74345 eV

Gap : +0.11139148 H = +3.03112 eV

Number of MOs= 240, Electrons= 124.00, Symmetry: cs

\$coord

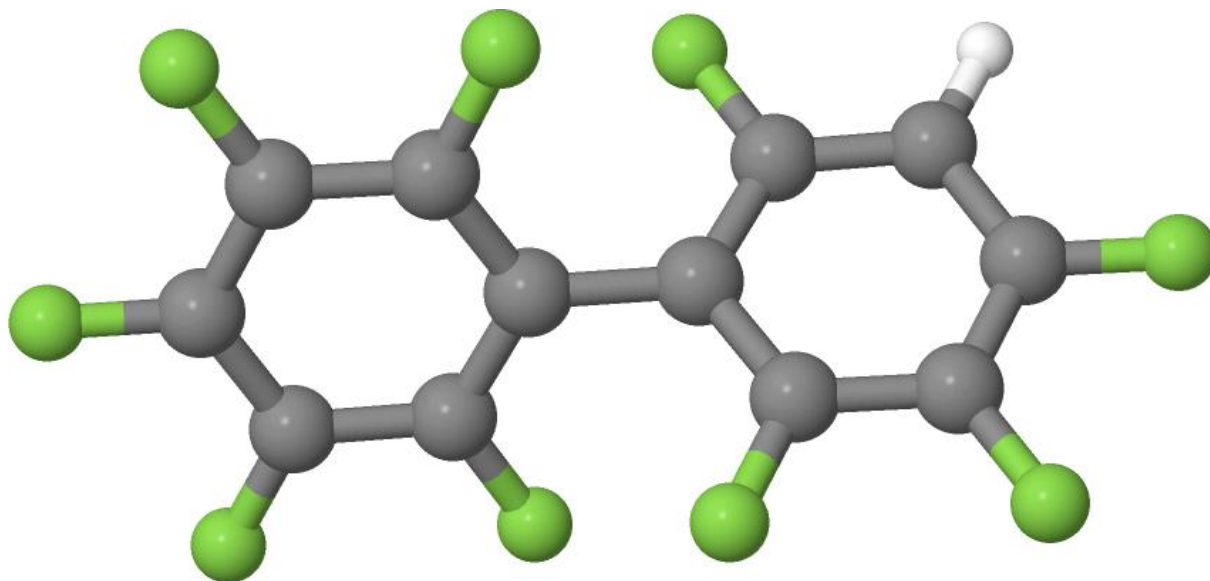
-4.61550337099775	1.35666533960729	0.00000000000000	c
-4.60906389119008	-1.32560996330966	0.00000000000000	c
-2.34026443892761	-2.65249768162202	0.00000000000000	c
0.02642106522598	-1.35879535778205	0.00000000000000	c
0.01923660504671	1.38752725078901	0.00000000000000	c
-2.34647504624394	2.68236572476713	0.00000000000000	c
2.39141288724015	-2.65627112685149	0.00000000000000	c
4.65081722027452	-1.31175634804770	0.00000000000000	c
4.67569377046233	1.35551181980023	0.00000000000000	c
2.40474952477223	2.65605736439622	0.00000000000000	c
2.46321080821900	5.18975321090363	0.00000000000000	f
6.84267613283001	-2.57633698919211	0.00000000000000	f
2.47996160551267	-5.18502583721360	0.00000000000000	f
-2.44333694981939	-5.17849118448071	0.00000000000000	f
-6.80985766639249	-2.55622573784451	0.00000000000000	f
-6.82144006877695	2.58072692089537	0.00000000000000	f
-2.44869952242498	5.20789780254839	0.00000000000000	f
6.48046133518966	2.38450479263662	0.00000000000000	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a"	67.80	0.04224	YES	YES
8		a"	82.52	0.01654	YES	YES
9		a"	112.54	0.00402	YES	YES
10		a"	145.03	0.00985	YES	YES
11		a"	179.64	1.48651	YES	YES
12		a'	192.67	0.09837	YES	YES

13	a"	235.40	0.05709	YES	YES
14	a'	265.88	0.01283	YES	YES
15	a'	275.42	0.02664	YES	YES
16	a'	291.57	0.07029	YES	YES
17	a'	300.92	1.50081	YES	YES
18	a'	321.87	0.97213	YES	YES
19	a'	335.89	0.71744	YES	YES
20	a"	340.72	1.13449	YES	YES
21	a"	370.25	0.18334	YES	YES
22	a'	397.42	0.31815	YES	YES
23	a"	423.99	0.10054	YES	YES
24	a'	438.28	0.27504	YES	YES
25	a"	494.98	0.09245	YES	YES
26	a'	503.25	0.42046	YES	YES
27	a'	505.06	0.26711	YES	YES
28	a"	534.46	0.43024	YES	YES
29	a'	584.58	15.45229	YES	YES
30	a"	592.19	0.01843	YES	YES
31	a"	638.06	0.07958	YES	YES
32	a"	667.87	0.08126	YES	YES
33	a'	689.30	10.27566	YES	YES
34	a'	777.08	20.66330	YES	YES
35	a"	828.41	26.04326	YES	YES
36	a'	850.76	84.83249	YES	YES
37	a'	930.51	111.47773	YES	YES
38	a'	1040.71	28.81681	YES	YES
39	a'	1120.53	30.11923	YES	YES
40	a'	1148.80	73.64883	YES	YES
41	a'	1170.92	32.81003	YES	YES
42	a'	1252.15	1.86523	YES	YES
43	a'	1268.77	28.55611	YES	YES
44	a'	1340.92	12.84794	YES	YES
45	a'	1388.22	15.70306	YES	YES
46	a'	1413.66	207.83830	YES	YES
47	a'	1425.93	345.68836	YES	YES
48	a'	1484.88	147.26916	YES	YES
49	a'	1504.56	189.07517	YES	YES
50	a'	1540.44	23.77341	YES	YES
51	a'	1622.29	8.32443	YES	YES
52	a'	1640.89	265.90516	YES	YES
53	a'	1648.98	47.44078	YES	YES
54	a'	3150.63	3.32455	YES	YES

HC₁₂F₉



Total energy = -1355.4440056010 H = -36883.5290140 eV

HOMO-LUMO Separation

HOMO: 77. 77 a -0.23606153 H = -6.42356 eV

LUMO: 78. 78 a -0.09069939 H = -2.46806 eV

Gap : +0.14536214 H = +3.95551 eV

Number of MOs= 296, Electrons= 154.00, Symmetry: c1

\$coord

-5.24407108382462	2.44727264517405	1.17385051048369	c
-6.73344427524039	0.55194643684384	0.05492186355381	c
-5.57679154052709	-1.5544447597200	-1.08023285001652	c
-2.92895561377784	-1.74163343543083	-1.08935454079349	c
-1.38831952974227	0.12702247764484	0.02273363011815	c
-2.60006905454208	2.21319479722303	1.15551597971175	c
1.40616150869379	-0.09051627565497	-0.01211274000978	c
2.65104900915069	-2.16368730974942	1.11047030392707	c
5.29467268702982	-2.40658919511526	1.07719037068651	c
6.74029352986539	-0.51317900788692	-0.10121189773532	c
5.58530378405335	1.57903669967940	-1.23469395864743	c
2.94821318884602	1.75042368094835	-1.17280334910468	c
1.83187154775010	3.73510105600375	-2.28975031970383	f
9.25637606343066	-0.74836744399273	-0.12552725556296	f

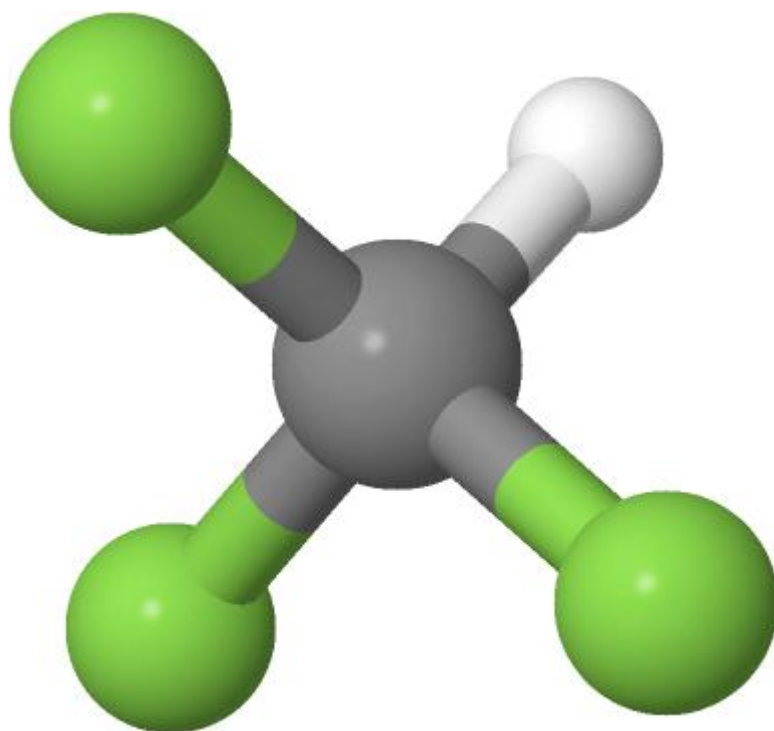
6.41072188518474	-4.39085730715486	2.17162571805816	f
1.30419643538716	-3.96193084577731	2.26890197460616	f
-1.22795182165568	4.02294874969764	2.26821385517195	f
-6.34971162920639	4.43515709215019	2.26890962499182	f
-9.24564829441065	0.75397113090140	0.06917583952379	f
-6.99534694380869	-3.34422211238811	-2.15691857700820	f
-1.86814309607487	-3.74242688269139	-2.21505257347608	f
6.72959324341880	3.04177952554744	-2.16385160877443	h

\$vibrational spectrum

#	mode	symmetry	wave number	IR intensity	selection rules	
#			cm** (-1)	km/mol	IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	35.35	0.07058	YES	YES
8		a	42.33	0.01110	YES	YES
9		a	49.84	0.01933	YES	YES
10		a	124.36	0.00452	YES	YES
11		a	130.19	0.05062	YES	YES
12		a	134.68	0.09322	YES	YES
13		a	152.78	0.02869	YES	YES
14		a	165.01	0.06178	YES	YES
15		a	181.02	0.01503	YES	YES
16		a	216.88	1.07190	YES	YES
17		a	235.35	2.11106	YES	YES
18		a	260.80	0.02860	YES	YES
19		a	266.22	0.07247	YES	YES
20		a	269.27	0.00770	YES	YES
21		a	299.87	0.56945	YES	YES
22		a	306.01	1.21504	YES	YES
23		a	321.38	0.06834	YES	YES
24		a	334.73	4.00578	YES	YES
25		a	359.40	0.10426	YES	YES
26		a	379.64	0.11912	YES	YES
27		a	382.66	0.19170	YES	YES
28		a	406.42	0.03323	YES	YES
29		a	432.71	0.19447	YES	YES
30		a	441.08	1.17926	YES	YES
31		a	472.33	3.90889	YES	YES
32		a	494.07	0.10668	YES	YES
33		a	558.55	9.65390	YES	YES
34		a	562.50	1.31356	YES	YES
35		a	567.00	0.11091	YES	YES
36		a	575.22	7.72610	YES	YES
37		a	605.49	2.82988	YES	YES
38		a	620.10	2.93148	YES	YES
39		a	624.04	0.05450	YES	YES
40		a	660.08	1.73494	YES	YES
41		a	701.26	3.93175	YES	YES
42		a	771.60	36.61743	YES	YES
43		a	785.75	35.14047	YES	YES
44		a	817.59	24.65902	YES	YES
45		a	933.99	30.33611	YES	YES
46		a	999.47	170.48632	YES	YES
47		a	1063.59	90.16441	YES	YES
48		a	1077.21	183.27634	YES	YES

49	a	1145.80	58.31681	YES	YES
50	a	1166.02	2.94317	YES	YES
51	a	1171.11	18.38165	YES	YES
52	a	1260.16	24.45247	YES	YES
53	a	1328.56	3.93734	YES	YES
54	a	1344.33	1.00061	YES	YES
55	a	1357.23	6.22230	YES	YES
56	a	1393.06	17.20059	YES	YES
57	a	1433.34	26.23346	YES	YES
58	a	1486.86	178.79248	YES	YES
59	a	1504.87	375.70426	YES	YES
60	a	1517.47	428.41220	YES	YES
61	a	1530.11	61.07300	YES	YES
62	a	1610.48	53.00722	YES	YES
63	a	1621.64	21.75851	YES	YES
64	a	1638.53	44.24933	YES	YES
65	a	1642.36	56.33415	YES	YES
66	a	3154.46	3.13319	YES	YES

HCF₃



Total energy = -337.9942289580 H = -9197.2961619 eV

HOMO-LUMO Separation

HOMO: 12. 6 a1 -0.33925731 H = -9.23167 eV

LUMO: 13. 7 a1 +0.05813269 H = +1.58187 eV

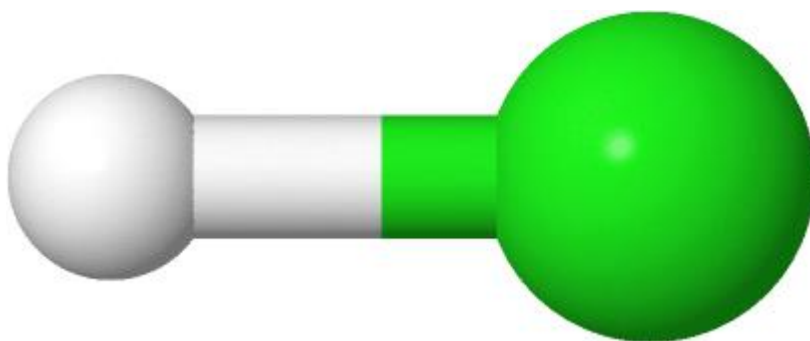
Gap : +0.39739000 H = +10.81354 eV

Number of MOs= 40, Electrons= 34.00, Symmetry: c3v

```
$coord
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-1.19274114649203   -2.06588826600216    0.77140742883769  f
-1.19274114649203    2.06588826600216    0.77140742883769  f
  2.38548229298407    0.0000000000000000    0.77140742883769  f
  0.0000000000000000  0.0000000000000000   -2.20851795028375  h
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#                               cm** (-1)      km/mol              IR      RAMAN
  1              0.00          0.00000
  2              0.00          0.00000
  3              0.00          0.00000
  4              0.00          0.00000
  5              0.00          0.00000
  6              0.00          0.00000
  7              e          493.08          1.98986          YES      YES
  8              e          493.08          1.98986          YES      YES
  9              a1         683.89          12.37593          YES      YES
 10              a1        1120.37          103.39663          YES      YES
 11              e        1141.80          248.91447          YES      YES
 12              e        1141.80          248.91447          YES      YES
 13              e        1371.32          90.20731          YES      YES
 14              e        1371.32          90.20731          YES      YES
 15              a1        3031.85          59.90035          YES      YES
```

HCl



Total energy = -460.6987747911 H = -12536.2586404 eV

HOMO-LUMO Separation

HOMO: 7. 2 e1 -0.27748845 H = -7.55085 eV

LUMO: 8. 6 a1 -0.01526329 H = -0.41534 eV

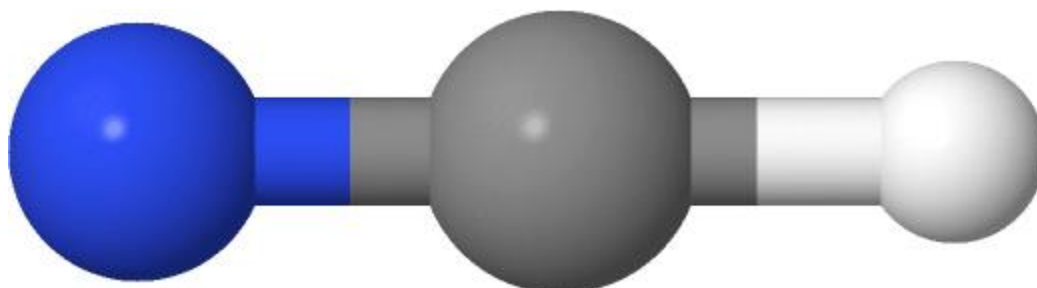
Gap : +0.26222516 H = +7.13551 eV

Number of MOs= 15, Electrons= 18.00, Symmetry: c6v

```
$coord
0.0000000000000000 0.0000000000000000 -1.23773624434614 c1
0.0000000000000000 0.0000000000000000 1.23773624434614 h
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 a1 2781.36 18.09612 YES YES
```

HCN



Total energy = -93.3534378304 H = -2540.2777382 eV

HOMO-LUMO Separation

HOMO: 6. 1 e1 -0.32616177 H = -8.87532 eV

LUMO: 7. 2 e1 -0.02772555 H = -0.75445 eV

Gap : +0.29843622 H = +8.12087 eV

Number of MOs= 22, Electrons= 14.00, Symmetry: c6v

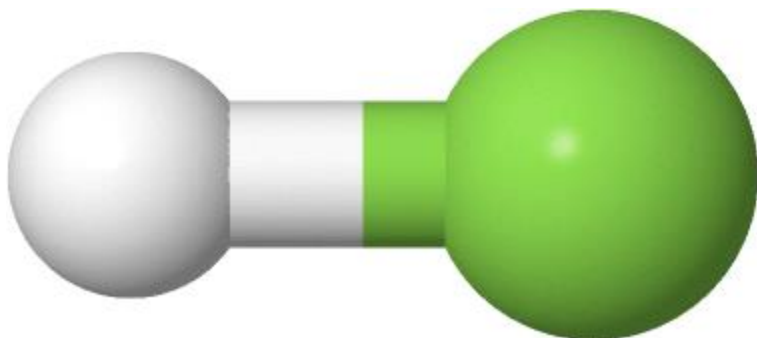
\$coord

0.0000000000000000	0.0000000000000000	-0.04907353480949	c
0.0000000000000000	0.0000000000000000	2.15695118455354	n
0.0000000000000000	0.0000000000000000	-2.10787764974407	h

\$vibrational spectrum

#	mode	symmetry	wave number cm ⁻¹ (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6		e1	718.63	38.26135	YES	YES
7		e1	718.63	38.26135	YES	YES
8		a1	2131.48	1.05662	YES	YES
9		a1	3349.20	52.05016	YES	YES

HF



Total energy = -100.3448514403 H = -2730.5238905 eV

HOMO-LUMO Separation

HOMO: 4. 1 e1 -0.31370154 H = -8.53626 eV

LUMO: 5. 4 a1 +0.01931233 H = +0.52552 eV

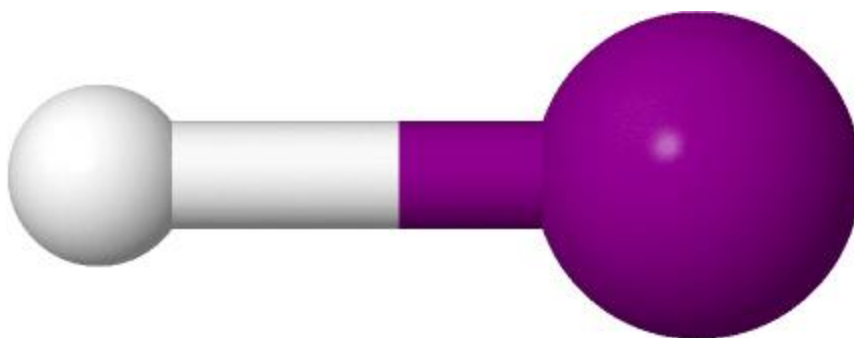
Gap : +0.33301386 H = +9.06177 eV

Number of MOs= 12, Electrons= 10.00, Symmetry: c6v

```
$coord
0.0000000000000000 0.0000000000000000 -0.89252024765708 f
0.0000000000000000 0.0000000000000000 0.89252024765708 h
```

```
$vibrational spectrum
# mode symmetry wave number IR intensity selection rules
# cm** (-1) km/mol IR RAMAN
1 0.00 0.00000 - -
2 0.00 0.00000 - -
3 0.00 0.00000 - -
4 0.00 0.00000 - -
5 0.00 0.00000 - -
6 a1 3749.60 57.43894 YES YES
```

HI



Total energy = -12.0520067910 H = -327.9519776 eV

HOMO-LUMO Separation

HOMO: 3. 1 e1 -0.25320673 H = -6.89011 eV

LUMO: 4. 3 a1 -0.06955029 H = -1.89256 eV

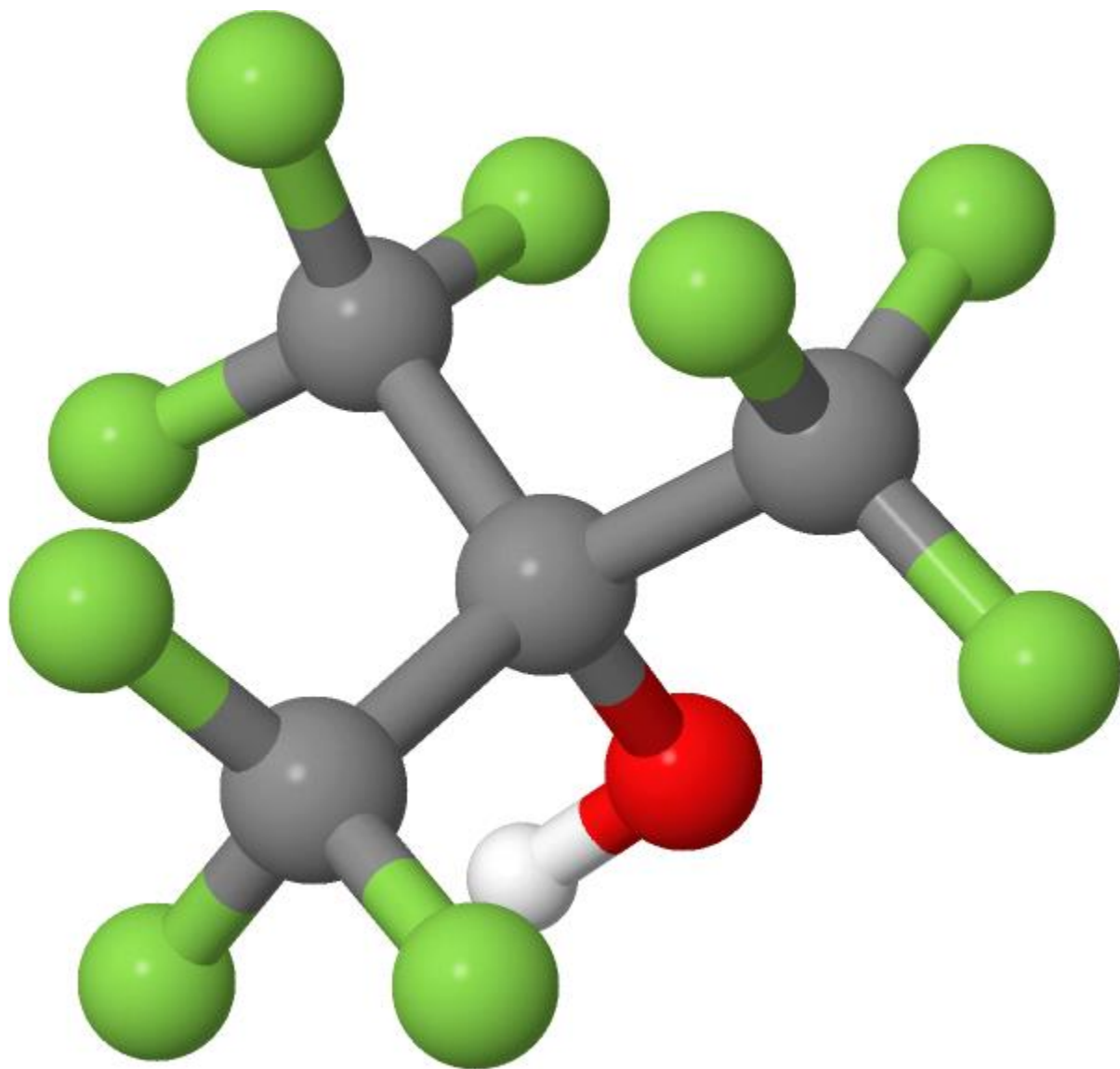
Gap : +0.18365644 H = +4.99755 eV

Number of MOs= 11, Electrons= 8.00, Symmetry: c6v

```
$coord
0.0000000000000000 0.0000000000000000 -1.56383999530885 i
0.0000000000000000 0.0000000000000000 1.56383999530885 h
```

```
$vibrational spectrum
# mode      symmetry      wave number      IR intensity      selection rules
#                               cm** (-1)          km/mol            IR      RAMAN
1                               0.00             0.00000          -      -
2                               0.00             0.00000          -      -
3                               0.00             0.00000          -      -
4                               0.00             0.00000          -      -
5                               0.00             0.00000          -      -
6          a1             2214.77           3.10794          YES     YES
```


HOC(CF₃)₃



Total energy = -1126.0429858370 H = -30641.2061048 eV

HOMO-LUMO Separation

HOMO: 57. 57 a -0.28998693 H = -7.89095 eV

LUMO: 58. 58 a -0.01239268 H = -0.33722 eV

Gap : +0.27759426 H = +7.55373 eV

Number of MOs= 198, Electrons= 114.00, Symmetry: c1

\$coord

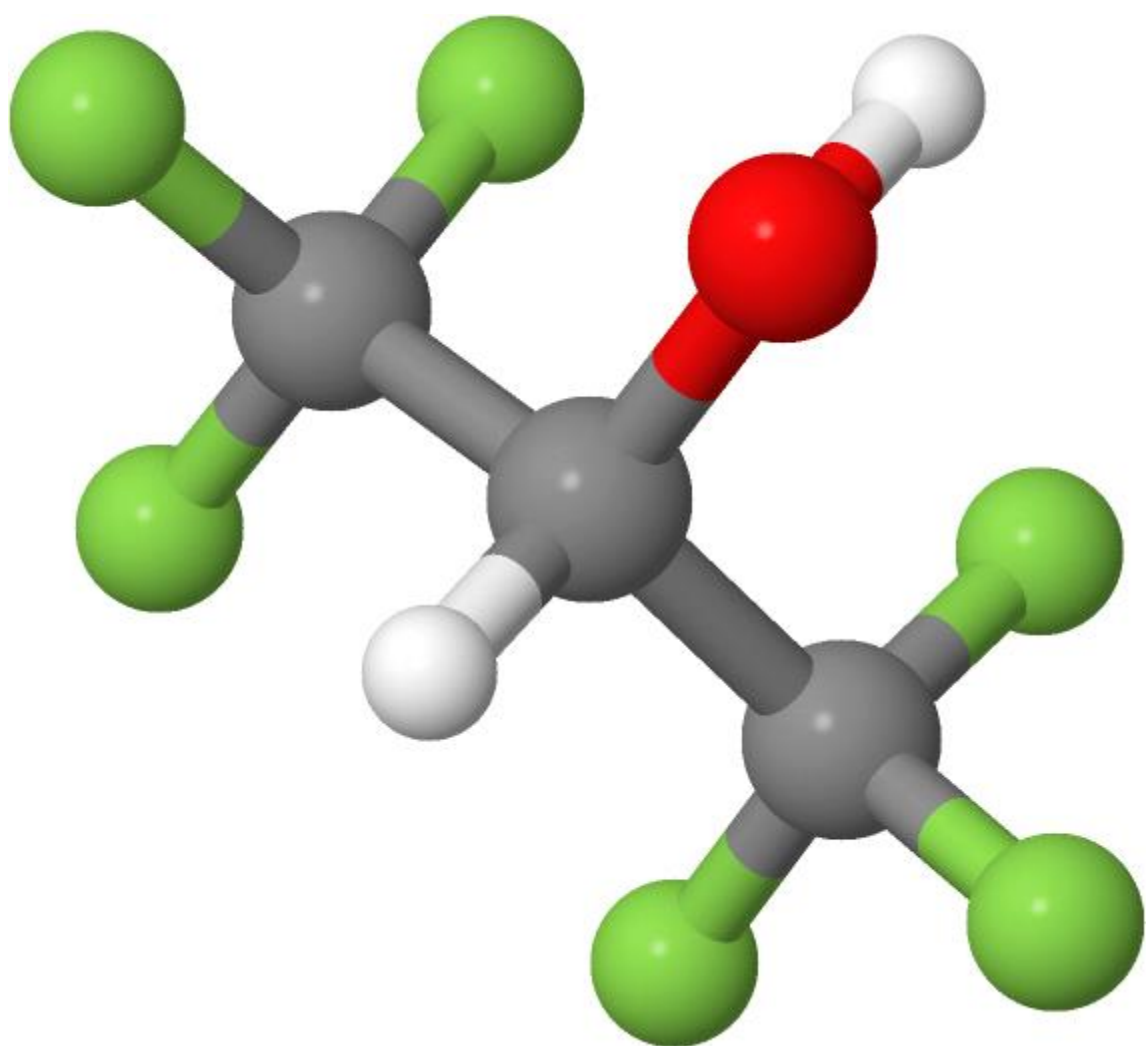
-0.88123482916362	0.26790171126779	3.01622664888316	o
-2.61574935318058	0.94053998798746	2.98775438686975	h
-0.06754634522381	0.00712411415555	0.51514200296535	c
-0.46833968896773	2.57627346793878	-0.92335132586970	c
2.81103223937597	-0.66789283054477	0.65595054694875	c
-1.59700919573943	-2.17223938100441	-0.80823190387143	c
-4.00890877917458	-1.38760917219595	-1.18926965205295	f
-1.69219499580055	-4.21478170306117	0.68307422380308	f
-0.61132684019366	-2.84396123774638	-3.04890583393980	f
3.88898558056237	-0.40019543265458	-1.63829829323198	f
3.14322841211675	-3.07125823700347	1.41395627121484	f
4.00342240481199	0.84471764497686	2.29586780009393	f
1.25990173856057	4.29947959321029	-0.23252598702572	f
-0.38978364053030	2.31400315307834	-3.44279628439288	f
-2.77447670745342	3.50789832159567	-0.28459260039434	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules IR	RAMAN
#						
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7	a		53.50	0.11773	YES	YES
8	a		64.48	0.12380	YES	YES
9	a		72.58	0.12364	YES	YES
10	a		155.95	0.25639	YES	YES
11	a		158.64	0.57616	YES	YES
12	a		179.64	1.94123	YES	YES
13	a		255.72	1.19909	YES	YES
14	a		267.82	3.29650	YES	YES
15	a		280.98	7.35821	YES	YES
16	a		301.79	25.64461	YES	YES
17	a		312.87	7.13618	YES	YES
18	a		318.10	0.10833	YES	YES
19	a		332.05	21.14424	YES	YES
20	a		346.95	3.05716	YES	YES
21	a		378.62	71.30117	YES	YES
22	a		473.16	6.42853	YES	YES
23	a		518.89	7.44751	YES	YES
24	a		521.50	4.59108	YES	YES
25	a		526.66	2.75894	YES	YES
26	a		554.52	0.65837	YES	YES
27	a		556.55	0.30459	YES	YES
28	a		634.46	2.27614	YES	YES
29	a		706.16	45.79825	YES	YES
30	a		708.96	39.84797	YES	YES
31	a		749.99	1.43136	YES	YES
32	a		932.00	127.62003	YES	YES
33	a		965.29	140.93176	YES	YES

34	a	1111.78	2.29548	YES	YES
35	a	1144.30	243.27381	YES	YES
36	a	1159.88	18.74181	YES	YES
37	a	1177.42	3.45066	YES	YES
38	a	1187.75	90.08124	YES	YES
39	a	1189.76	59.46142	YES	YES
40	a	1228.72	331.60950	YES	YES
41	a	1255.21	367.89367	YES	YES
42	a	1265.13	545.33423	YES	YES
43	a	1279.16	212.22580	YES	YES
44	a	1361.17	81.24707	YES	YES
45	a	3529.48	65.97973	YES	YES

HOhfip



Total energy = -789.2461998523 H = -21476.4940427 eV

HOMO-LUMO Separation

HOMO: 41. 18 a" -0.27506701 H = -7.48496 eV

LUMO: 42. 24 a' +0.00588551 H = +0.16015 eV

Gap : +0.28095252 H = +7.64511 eV

Number of MOs= 144, Electrons= 82.00, Symmetry: cs

\$scoord

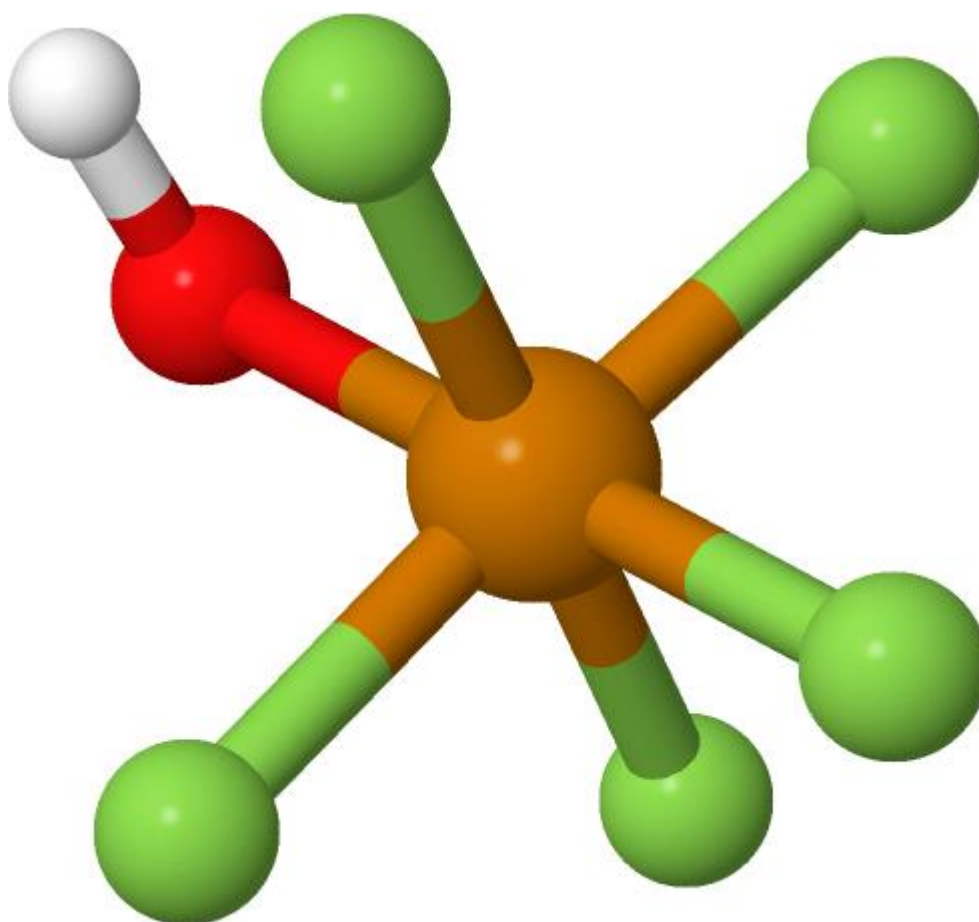
-3.13872330663782	-0.59511252531025	0.0000000000000000	o
-0.81524297125549	0.67946994502898	0.0000000000000000	c
0.66983820524462	0.09996130763327	-2.45082533433549	c
2.91060883243816	1.30236005385483	-2.54112708475070	f
-0.69835455775827	0.81745655807911	-4.47196496525835	f
1.10013121579626	-2.42035459095955	-2.65852685427934	f
0.66983820524462	0.09996130763327	2.45082533433549	c
1.10013121579626	-2.42035459095955	2.65852685427934	f
2.91060883243816	1.30236005385483	2.54112708475070	f
-0.69835455775827	0.81745655807911	4.47196496525835	f
-2.78068889472607	-2.42136749925357	0.0000000000000000	h
-1.22946467417049	2.73568015595539	0.0000000000000000	h

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a"	28.41	0.13524	YES	YES
8		a'	88.32	0.34508	YES	YES
9		a'	160.06	0.80494	YES	YES
10		a'	214.41	8.08583	YES	YES
11		a"	232.60	2.21659	YES	YES
12		a"	279.44	9.85153	YES	YES
13		a'	316.13	0.29663	YES	YES
14		a"	329.00	8.53742	YES	YES
15		a"	411.19	102.94887	YES	YES
16		a'	446.17	8.65320	YES	YES
17		a'	500.57	5.88688	YES	YES
18		a"	517.42	2.62316	YES	YES
19		a"	537.56	5.29026	YES	YES
20		a'	593.90	2.25008	YES	YES
21		a"	671.24	59.27117	YES	YES
22		a'	719.87	11.99386	YES	YES
23		a'	813.89	36.34133	YES	YES
24		a"	880.34	42.92272	YES	YES
25		a"	1095.21	138.92462	YES	YES
26		a'	1098.71	111.49971	YES	YES
27		a"	1169.02	16.34854	YES	YES

28	a'	1191.91	333.29133	YES	YES
29	a''	1223.53	150.36462	YES	YES
30	a'	1232.43	259.84366	YES	YES
31	a'	1247.50	178.32283	YES	YES
32	a'	1283.84	174.00853	YES	YES
33	a''	1347.76	116.54969	YES	YES
34	a'	1391.95	8.52294	YES	YES
35	a'	3032.72	3.55509	YES	YES
36	a'	3519.69	40.72152	YES	YES

HOTeF₅



Total energy = -582.6618379563 H = -15855.0443374 eV

HOMO-LUMO Separation

HOMO: 30. 30 a -0.34108549 H = -9.28141 eV

LUMO: 31. 31 a -0.22791308 H = -6.20183 eV

Gap : +0.11317241 H = +3.07958 eV

Number of MOs= 99, Electrons= 60.00, Symmetry: c1

\$coord

3.73655183150445	0.26527400075999	-1.51058737636527	h
2.10322360424242	0.70742601241210	-2.31912963991699	o
-0.52382037372265	-0.02900557640890	0.19208466055936	te
-0.79364178599170	-3.49910999402051	-0.85182975645218	f
-3.09806481311128	-0.75559504538796	2.62850247227722	f
-3.00763182637239	0.92822571122908	-2.24986423782299	f
-0.46932356900512	3.35784214045717	1.50672382523568	f
2.05270693245622	-0.97505724904101	2.60410005248518	f

\$vibrational spectrum

#	mode	symmetry	wave number cm** (-1)	IR intensity km/mol	selection rules	
#					IR	RAMAN
1			0.00	0.00000	-	-
2			0.00	0.00000	-	-
3			0.00	0.00000	-	-
4			0.00	0.00000	-	-
5			0.00	0.00000	-	-
6			0.00	0.00000	-	-
7		a	148.96	1.02439	YES	YES
8		a	161.67	3.56285	YES	YES
9		a	167.82	2.08462	YES	YES
10		a	200.99	38.42531	YES	YES
11		a	246.00	8.13806	YES	YES
12		a	256.72	2.66178	YES	YES
13		a	264.05	31.24784	YES	YES
14		a	274.62	0.16745	YES	YES
15		a	276.74	56.63659	YES	YES
16		a	288.06	96.69792	YES	YES
17		a	576.28	1.58706	YES	YES
18		a	592.02	3.98125	YES	YES
19		a	594.57	3.28164	YES	YES
20		a	644.60	83.06919	YES	YES
21		a	653.14	113.16406	YES	YES
22		a	657.41	93.38784	YES	YES
23		a	1030.41	104.51633	YES	YES
24		a	3469.78	123.07274	YES	YES

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