Electronic Supplementary Information for Dalton Transactions


Supporting Information to

# Exploring the Chemistry of Free $CI_3^+$: Reactions with the Weak Lewis Bases $PX_3^+$ (X = Cl-I), $AsI_3$ and $Et_2O$

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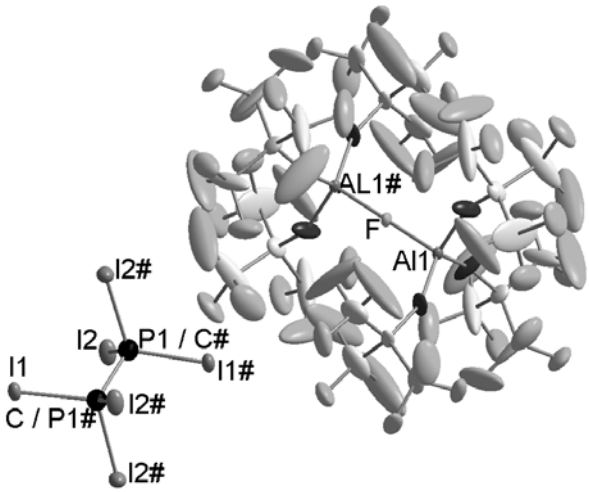
# 1 Solid-state structures

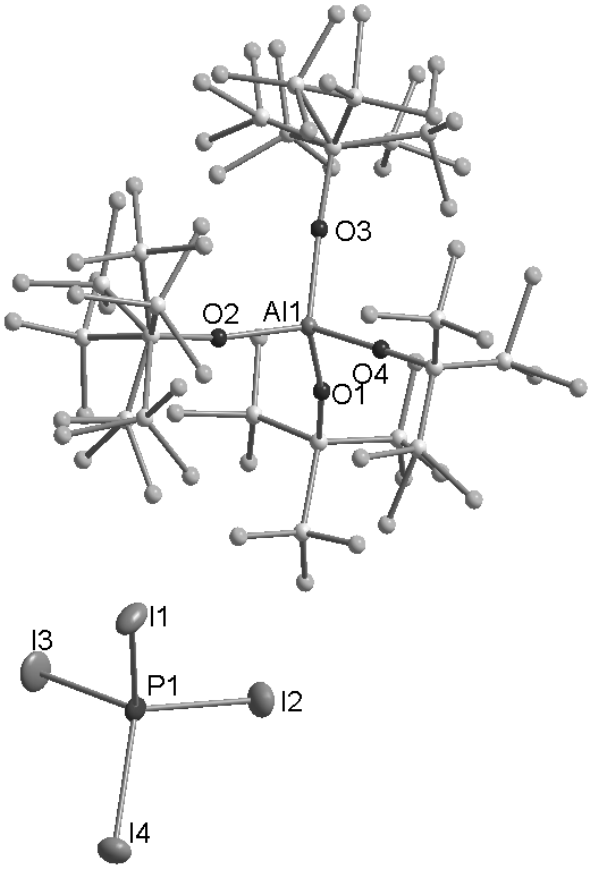
## 1.1 Solid-state structure of $[I_3CPI_3]^+[al\text{-}f\text{-}al]^-$ **5** at 150K

**5** crystallizes in the monoclinic space group C2/m with Z = 2. In this compound, the thermal displacement ellipsoids of the anion are very big, indication motion of the $CF_3$ groups. The iodine positions of the $I_3CPI_3^+$ cation are well defined (small ellipsoids), but the position of phosphorus and carbon are disordered. Therefore, all E-I bond lengths are nearly the same (224.02 and 224.29 pm), which is in between the C-I and the P-I bond lengths of the $I_3CPI_3^+$ cation in **3**




**S_Figure 1:** Section of the solid state structure of $[I_3CPI_3]^+[al\text{-}f\text{-}al]^-$ **5** at 150K, thermal displacement ellipsoids showing 25% probability The disorder of some $CF_3$ groups it not shown for clarity. Selected bond lengths:*d*(I1-P1) = 224(4) pm, *d*(I1-C) = 228(5) ppm, *d*(I2-P1) = 224(2) pm, *d*(I2-C) = 229(3) pm, *d*(P1-C) = 176(4) pm, *d*(Al1-F) = 176.1(3) pm.

## 1.2 Solid-state structure of $[PI_4]^+[pftb]^-$ 6 at 150 K



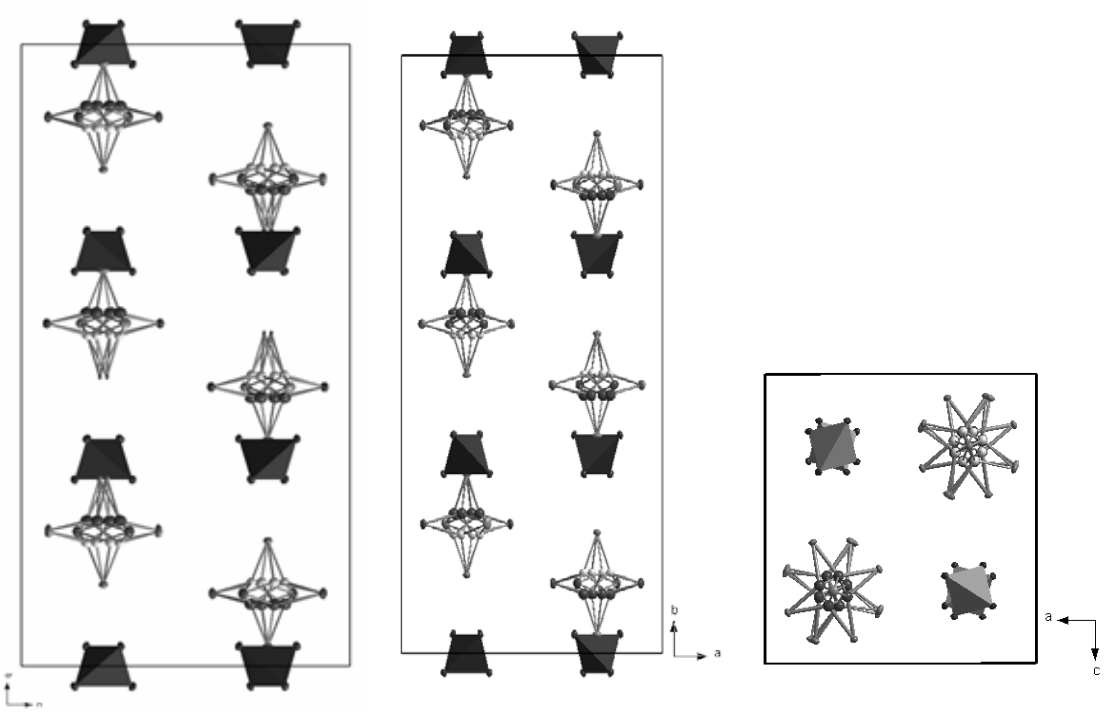

**S_Figure 2:** Section of the solid state structure of $[PI_4]^+[pftb]^-$ **6** at 150K, thermal displacement ellipsoids of the cation showing 25% probability.

**S_Table 1:** Comparison of the geometries of the $PI_4^+$ cations in **6** and in the other modification of $[PI_4]^+[pftb]^-$.

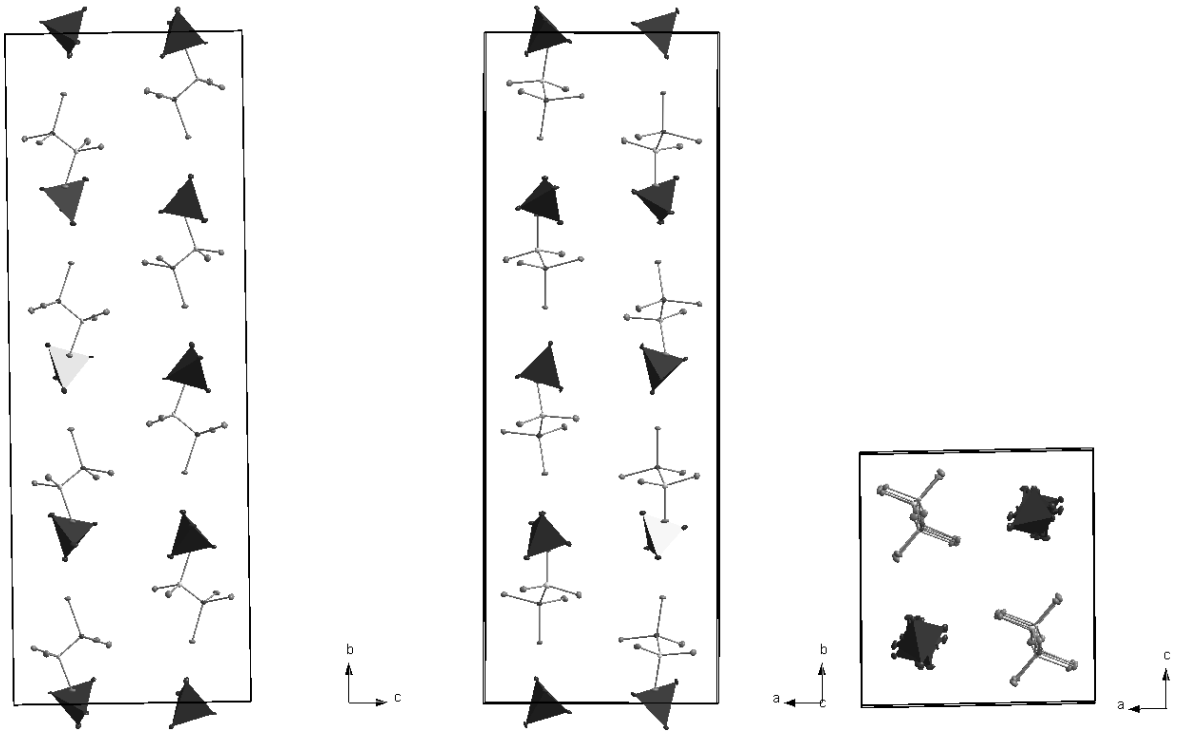
| | **6** | $[PI_4]^+[pftb]^-$ Lit.[1] |
|---|---|---|
| $d_{min}$(P-I) [pm] | 234.4(2) | 237.0(1) |
| $d_{max}$(P-I) [pm] | 236.9(1) | 237.0(1) |
| $d_{av}$(P-I) [pm] | 235.0 | 237.0 |
| $<_{min}$(I-P-I) [°] | 108.8(1) | 109.2(1) |
| $<_{max}$(I-P-I) [°] | 110.4(1) | 109.6(1) |
| $<_{av}$(I-P-I) [°] | 109.5 | 109.4 |

[1] M. Gonsior, I. Krossing, L. Müller, I. Raabe, M. Jansen, L. van Wüllen, *Chem. Eur. J.* **2002**, *8*, 4475.

## 1.3 Packing diagrams of 2 and 3

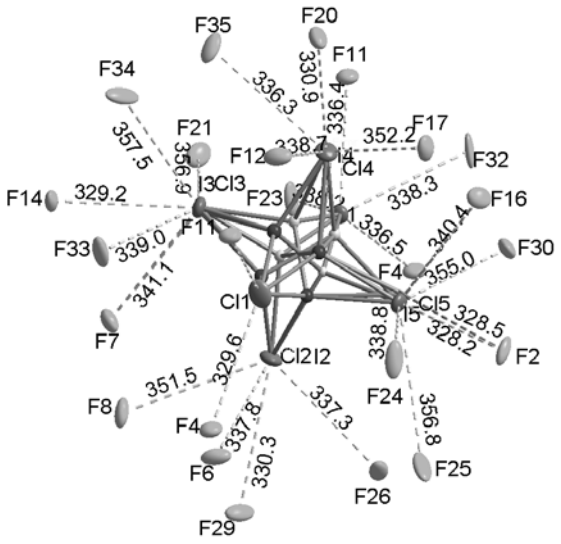



**S_Figure 3:** Packing diagram of $[I_3C\text{-}PBr_3]^+[pftb]^-$ **2** along the crystallographic axes. The $AlO_4$-moieties of the anions are drawn as tetrahedra, the $C(CF_3)_3$ groups have been omitted for clarity.

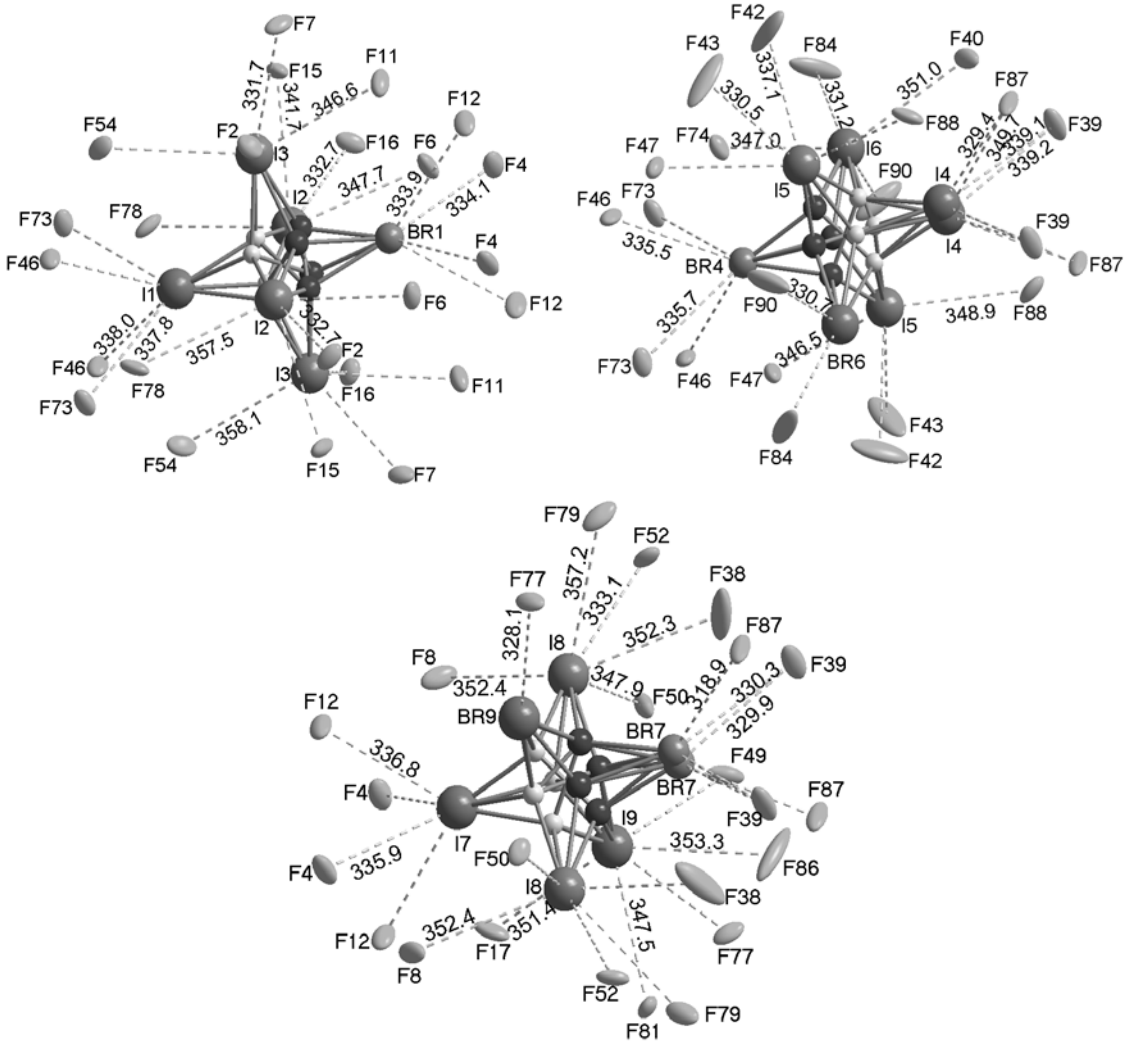



**S_Figure 4:** Packing diagram of $[I_3C\text{-}PI_3]^+[pftb]^-$ **3** along the crystallographic axes. The $AlO_4$-moieties of the anions are drawn as tetrahedra, the $C(CF_3)_3$ groups have been omitted for clarity.

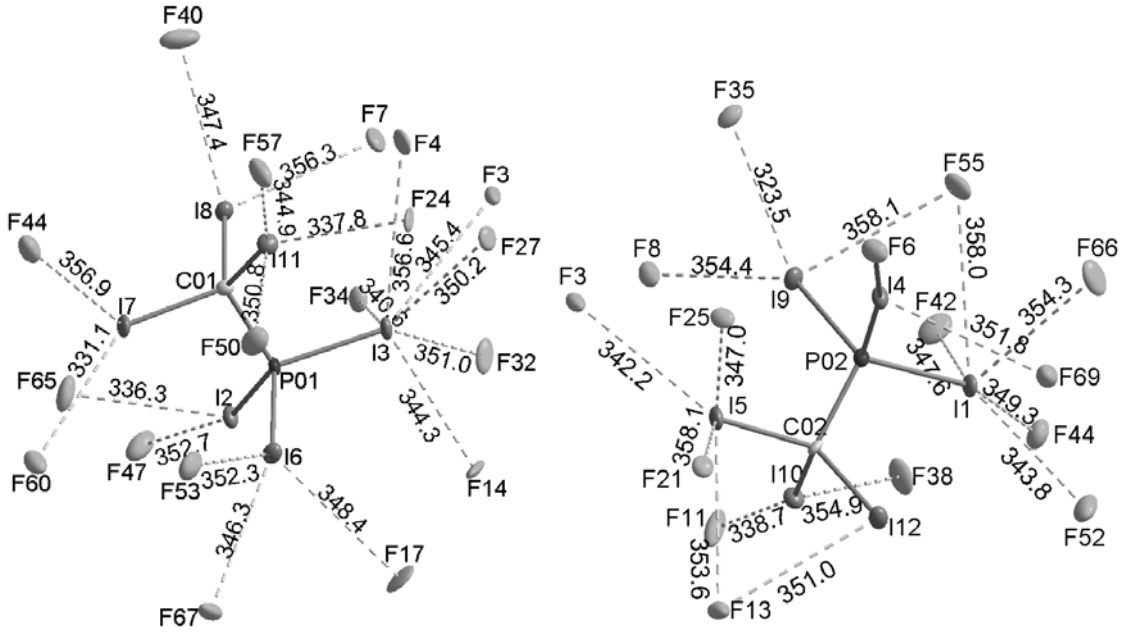
## 1.4 Cation-anion contacts of 1, 2 and 3




**S_Figure 5:** Cation-anion interactions (below the sum of the van-der-Waals radii) of **1**.

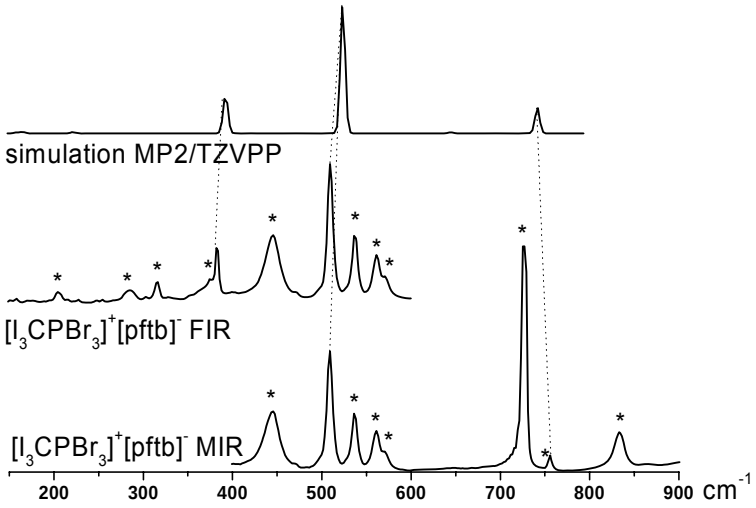



**S_Figure 6:** Cation-anion interactions (below the sum of the van-der-Waals radii) of **2**.

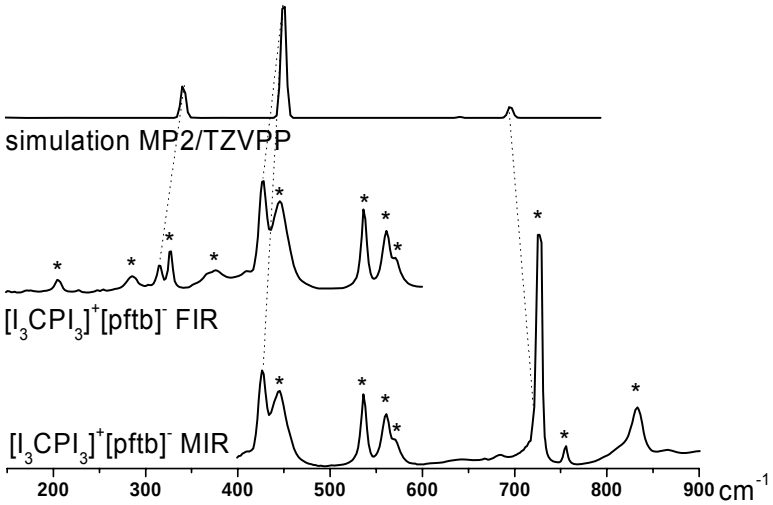



**S_Figure 7:** Cation-anion interactions (below the sum of the van-der-Waals radii) of **3**.

# 2 Experimental and simulated IR spectra of $[I_3CPBr_3]^+[pftb]^-$ 2 and $[I_3CPI_3]^+[pftb]^-$ 3




**S_Figure 8:** Comparison of the experimental and the simulated IR spectrum of $[I_3CPBr_3]^+[pftb]^-$ **2**. Simulation at the MP2/TZVPP level. Bands marked with * can be assigned to the anion.




**S_Figure 9:** Comparison of the experimental and the simulated IR spectrum of $[I_3CPI_3]^+[pftb]^-$ **3**. Simulation at the MP2/TZVPP level. Bands marked with * can be assigned to the anion.

# 3 Calculated structures and properties of all compounds addressed in this study

The calculations were performed with the program package TURBOMOLE with the following methods:

- *geometry optimization and vibrational frequencies:* MP2/TZVPP
- *Zero point energies:* based on (RI)BP86/SV(P) geometries
- *solvation energies:* COSMO model included in TURBOMOLE with ε = 8.93 (for some compounds also with ε = 14.95), based on the (RI)BP86/SV(P) geometry
- *contributions to H° and G°:* module FreeH included in TURBOMOLE (for some compounds also $H^{195}$ and $G^{195}$ contributions)

For the calculated structures, the following information are given:

- picture of converged geometry
- symmetry
- xyz coordinates
- selected distances and angles
- SCF energy U
- ZPE
- vibrational frequencies (symmetry, energy , IR intensity , Raman/IR active)
- contributions to H° and G° (for some also $H^{195}$ and $G^{195}$)
- cosmo solvation energy (if not otherwise mentioned with ε = 8.93)

**$CI_3^+$**

sy d3h

| | | | |
|---|---|---|---|
| c1 | 0.0000 | 0.0000 | 0.0000 |
| i2 | 1.0101 | -1.7496 | 0.0000 |
| i3 | 1.0101 | 1.7496 | 0.0000 |
| i4 | -2.0203 | 0.0000 | 0.0000 |

dist 1 c -- 2 i = 3.8177 au = 202.03 pm
dist 1 c -- 3 i = 3.8177 au = 202.03 pm
dist 1 c -- 4 i = 3.8177 au = 202.03 pm

bend 2 i -> 1 c <- 3 i = 120.00 deg

cycle = 1 SCF+MP2 energy = -71.6559728131 |dE/dxyz| = 0.033253

zero point VIBRATIONAL energy : 0.0050340 Hartree

$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' | 116.19 | 0.01218 | YES | YES |
| 8 | e' | 116.19 | 0.01218 | YES | YES |
| 9 | a1' | 208.51 | 0.00000 | NO | YES |
| 10 | a2'' | 339.77 | 9.88165 | YES | NO |
| 11 | e' | 714.50 | 174.27050 | YES | YES |
| 12 | e' | 714.50 | 174.27050 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.56 | 12.95 | 2.43 | -73.39 | 27.33 | 0.34612 |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 195.15 | 0.1000000 | 18.50 | 12.31 | 1.44 | -39.12 | 21.27 | 0.31777 |

298K
$cosmo_energy
Total energy [a.u.] = -72.1742284258
Total energy + OC corr. [a.u.] = -72.1714229339
Total energy corrected [a.u.] = -72.1728256799 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0698249802
Diel. energy + OC corr. [a.u.] = -0.0670194883

195K
$cosmo_energy
Total energy [a.u.] = -72.1793757731
Total energy + OC corr. [a.u.] = -72.1763563015
Total energy corrected [a.u.] = -72.1778660373 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0749994955
Diel. energy + OC corr. [a.u.] = -0.0719800238

# Electronic excitation spectrum of , IRREP e'

# singlet excitations
#  excitation energy / nm  oscillator strength (length rep.)
 0.38412838743769E+03  0.20180992550491E+00
 0.30837663506003E+03  0.10666537934560E+00
 0.23101293937189E+03  0.10809152654894E+00
 0.19775779887009E+03  0.19690408858264E+00
 0.15311078939159E+03  0.10679609475734E+01
 0.12324570044327E+03  0.12973508634281E+01
 0.11197157625802E+03  0.29461227417360E-01
 0.10435736863926E+03  0.19619970117385E+00
 0.10338123472369E+03  0.85738899362075E-02
 0.98540987195099E+02  0.16249738362241E+00
 0.95737117958991E+02  0.78817574695698E-03
 0.94695951713175E+02  0.17319404445718E-03
 0.91957365598168E+02  0.34623114625005E-04
 0.90941405157512E+02  0.46683146401129E-02
 0.89037575411907E+02  0.13417707823030E+00
 0.86716680921432E+02  0.79446237190817E+00
 0.83403160549061E+02  0.39459194527112E+00
 0.81499088274334E+02  0.48356015338149E-01
 0.80704367565763E+02  0.34939520551010E-02
 0.78732350139171E+02  0.19807648184269E-01
# Electronic excitation spectrum of , IRREP a2"
# singlet excitations
#  excitation energy / nm  oscillator strength (length rep.)
 0.20804309811480E+03  0.26759838044348E-03
 0.19593868052092E+03  0.40385591522528E-02
 0.11997426541686E+03  0.69380892030578E-01
 0.10526418942147E+03  0.76476507126356E-01
 0.94576025790229E+02  0.10354164226493E-03
 0.93428222014711E+02  0.88540596891988E-01
 0.84611578905682E+02  0.94147413141658E-02
 0.81811771050116E+02  0.46917970899482E-01
 0.78897821451943E+02  0.18425608687649E-01
 0.74980971596471E+02  0.14205223442141E-01
 0.74377098279550E+02  0.46320588825558E-01
 0.73807425953477E+02  0.13310147129088E-01
 0.70663059604213E+02  0.45648730941757E-01
 0.68767041198319E+02  0.86209967485961E-02
 0.65939290698903E+02  0.26878773008563E+00
 0.64655164780430E+02  0.24849960553269E-01
 0.59330568687044E+02  0.53223455964031E+00
 0.57455126476470E+02  0.12923445364475E+00
 0.54003867916460E+02  0.16062258508689E+01
 0.51533448049211E+02  0.56768662137405E-01

**$Et_2O$**

sy c1

| | | | |
|---|---|---|---|
| c1 | 2.3689 | -0.3909 | 0.0004 |
| c2 | 1.1703 | 0.5278 | -0.0009 |
| o3 | 0.0000 | -0.2672 | 0.0002 |
| c4 | -1.1703 | 0.5278 | 0.0009 |
| c5 | -2.3689 | -0.3909 | -0.0005 |
| h6 | 2.3554 | -1.0279 | -0.8808 |
| h7 | 2.3570 | -1.0239 | 0.8845 |
| h8 | 3.2905 | 0.1885 | -0.0018 |
| h9 | 1.1778 | 1.1778 | 0.8818 |
| h10 | 1.1778 | 1.1752 | -0.8855 |
| h11 | -1.1776 | 1.1776 | -0.8820 |
| h12 | -1.1779 | 1.1755 | 0.8854 |
| h13 | -3.2905 | 0.1885 | 0.0010 |
| h14 | -2.3558 | -1.0276 | 0.8809 |
| h15 | -2.3566 | -1.0242 | -0.8844 |

dist 2 c -- 3 o = 2.6735 au = 141.47 pm
dist 3 o -- 4 c = 2.6735 au = 141.47 pm
bend 2 c -> 1 c <- 3 o = 34.48 deg

bend 2 c -> 3 o <- 4 c = 111.62 deg

cycle = 6 SCF+MP2 energy = -233.1833760595 |dE/dxyz| = 0.000085

zero point VIBRATIONAL energy : 0.1322514 Hartree

$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 | 96.05 | 0.00019 | YES | YES |
| 8 | a | 109.43 | 3.52783 | YES | YES |
| 9 | a | 187.75 | 0.53375 | YES | YES |
| 10 | a | 256.84 | 0.00031 | YES | YES |
| 11 | a | 262.34 | 1.48381 | YES | YES |
| 12 | a | 423.85 | 3.18453 | YES | YES |
| 13 | a | 433.19 | 0.01988 | YES | YES |
| 14 | a | 799.18 | 0.00016 | YES | YES |
| 15 | a | 809.78 | 1.25530 | YES | YES |
| 16 | a | 842.72 | 6.29955 | YES | YES |
| 17 | a | 932.80 | 5.30150 | YES | YES |
| 18 | a | 1041.95 | 13.56078 | YES | YES |
| 19 | a | 1072.12 | 2.84827 | YES | YES |
| 20 | a | 1137.53 | 0.09689 | YES | YES |
| 21 | a | 1148.62 | 21.54423 | YES | YES |
| 22 | a | 1152.90 | 235.33110 | YES | YES |
| 23 | a | 1169.71 | 14.32227 | YES | YES |
| 24 | a | 1254.18 | 0.00050 | YES | YES |
| 25 | a | 1257.20 | 3.92592 | YES | YES |
| 26 | a | 1334.54 | 35.50492 | YES | YES |
| 27 | a | 1350.31 | 0.44732 | YES | YES |
| 28 | a | 1367.63 | 59.43968 | YES | YES |
| 29 | a | 1408.50 | 4.48769 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 30 | a | 1422.37 | 15.83609 | YES | YES |
| 31 | a | 1422.46 | 0.00647 | YES | YES |
| 32 | a | 1442.32 | 2.51490 | YES | YES |
| 33 | a | 1444.88 | 4.60587 | YES | YES |
| 34 | a | 1462.39 | 5.21375 | YES | YES |
| 35 | a | 1488.93 | 1.65661 | YES | YES |
| 36 | a | 2838.18 | 16.31184 | YES | YES |
| 37 | a | 2852.56 | 125.24295 | YES | YES |
| 38 | a | 2870.41 | 155.91962 | YES | YES |
| 39 | a | 2876.89 | 0.06566 | YES | YES |
| 40 | a | 2952.88 | 25.33710 | YES | YES |
| 41 | a | 2953.35 | 10.36275 | YES | YES |
| 42 | a | 3042.99 | 3.58424 | YES | YES |
| 43 | a | 3043.17 | 37.95169 | YES | YES |
| 44 | a | 3044.33 | 13.87157 | YES | YES |
| 45 | a | 3044.49 | 26.33338 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 17.06 | 11.49 | 3.46 | 267.89 | 365.31 | 0.33509 |

$cosmo_energy
Total energy [a.u.] = -233.4717328131
Total energy corrected [a.u.] = -233.4716866837
Dielectric energy [a.u.] = -0.0029265285
Dielectric energy corr. [a.u.] = -0.0028803992

**$Et_2O^{\cdot\cdot}I\text{-}CI_2^+$**

sy c1

| | | | |
|---|---|---|---|
| o1 | -3.7910 | -0.1324 | 0.0423 |
| c2 | -4.4129 | 0.0175 | 1.3311 |
| i3 | -1.1987 | 0.0532 | -0.0411 |
| c4 | -4.7073 | -0.5770 | -0.9714 |
| c5 | -5.3892 | 1.1722 | 1.3870 |
| c6 | -3.9326 | -0.9444 | -2.2126 |
| c7 | 0.8268 | 0.0517 | 0.0165 |
| i8 | 1.9141 | 0.1443 | -1.6898 |
| i9 | 1.8056 | -0.1488 | 1.7800 |
| h10 | -4.8977 | -0.9263 | 1.5912 |
| h11 | -3.5925 | 0.1793 | 2.0285 |
| h12 | -5.4206 | 0.2184 | -1.1850 |
| h13 | -5.2546 | -1.4388 | -0.5820 |
| h14 | -5.7306 | 1.3028 | 2.4124 |
| h15 | -4.9100 | 2.0941 | 1.0640 |
| h16 | -6.2650 | 0.9953 | 0.7686 |
| h17 | -4.6225 | -1.2802 | -2.9840 |
| h18 | -3.2328 | -1.7536 | -2.0122 |
| h19 | -3.3886 | -0.0858 | -2.6012 |

dist 1 o -- 4 c = 2.7155 au = 143.70 pm
dist 1 o -- 2 c = 2.7191 au = 143.89 pm
dist 1 o -- 3 i = 4.9138 au = 260.03 pm
dist 7 c -- 8 i = 3.8275 au = 202.54 pm
dist 7 c -- 9 i = 3.8301 au = 202.68 pm
bend 8 i -> 7 c <- 9 i = 118.57 deg
bend 9 i -> 7 c <- 3 i = 120.50 deg
bend 3 i -> 7 c <- 8 i = 120.84 deg
bend 2 c -> 1 o <- 4 c = 112.86 deg

cycle = 28 MP2 energy = -304.8678532694 |dE/dxyz| = 0.000213

zero point VIBRATIONAL energy : 0.1386057 Hartree

$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 | 12.56 | 0.27296 | YES | YES |
| 8 | a | 20.58 | 0.82390 | YES | YES |
| 9 | a | 31.55 | 0.42270 | YES | YES |
| 10 | a | 36.83 | 0.23974 | YES | YES |
| 11 | a | 61.40 | 0.81928 | YES | YES |
| 12 | a | 94.53 | 0.93936 | YES | YES |
| 13 | a | 101.26 | 0.23277 | YES | YES |
| 14 | a | 123.03 | 1.83042 | YES | YES |
| 15 | a | 144.16 | 2.81040 | YES | YES |
| 16 | a | 149.87 | 4.45303 | YES | YES |
| 17 | a | 197.50 | 7.81485 | YES | YES |
| 18 | a | 231.59 | 5.90803 | YES | YES |
| 19 | a | 277.74 | 1.29162 | YES | YES |
| 20 | a | 321.09 | 5.73149 | YES | YES |
| 21 | a | 350.46 | 10.85260 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 22 | a | 373.88 | 16.68059 | YES | YES |
| 23 | a | 485.26 | 4.09671 | YES | YES |
| 24 | a | 689.82 | 119.99368 | YES | YES |
| 25 | a | 697.53 | 183.61075 | YES | YES |
| 26 | a | 771.65 | 37.11109 | YES | YES |
| 27 | a | 797.31 | 1.54341 | YES | YES |
| 28 | a | 814.80 | 27.62486 | YES | YES |
| 29 | a | 901.75 | 12.51537 | YES | YES |
| 30 | a | 1009.94 | 85.75394 | YES | YES |
| 31 | a | 1038.05 | 114.69799 | YES | YES |
| 32 | a | 1073.15 | 26.76184 | YES | YES |
| 33 | a | 1090.67 | 18.89334 | YES | YES |
| 34 | a | 1131.18 | 11.34059 | YES | YES |
| 35 | a | 1161.08 | 13.88559 | YES | YES |
| 36 | a | 1264.44 | 2.26053 | YES | YES |
| 37 | a | 1284.10 | 15.23227 | YES | YES |
| 38 | a | 1344.87 | 0.62027 | YES | YES |
| 39 | a | 1354.72 | 41.17077 | YES | YES |
| 40 | a | 1369.32 | 36.37956 | YES | YES |
| 41 | a | 1384.57 | 70.92551 | YES | YES |
| 42 | a | 1426.19 | 15.26041 | YES | YES |
| 43 | a | 1427.52 | 3.81940 | YES | YES |
| 44 | a | 1429.48 | 13.11021 | YES | YES |
| 45 | a | 1439.49 | 4.52234 | YES | YES |
| 46 | a | 1446.00 | 19.08520 | YES | YES |
| 47 | a | 1458.33 | 3.25093 | YES | YES |
| 48 | a | 2933.16 | 17.37348 | YES | YES |
| 49 | a | 2952.30 | 37.03381 | YES | YES |
| 50 | a | 2957.84 | 9.29809 | YES | YES |
| 51 | a | 2960.17 | 7.02673 | YES | YES |
| 52 | a | 2993.15 | 7.70957 | YES | YES |
| 53 | a | 3019.17 | 4.25964 | YES | YES |
| 54 | a | 3046.02 | 17.28173 | YES | YES |
| 55 | a | 3049.45 | 6.85946 | YES | YES |
| 56 | a | 3053.79 | 5.94271 | YES | YES |
| 57 | a | 3056.57 | 12.90854 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.82 | 15.85 | 16.55 | 234.46 | 401.44 | 0.56836 |

$cosmo_energy
Total energy [a.u.] = -305.6631835122
Total energy corrected [a.u.] = -305.6617238228
Dielectric energy [a.u.] = -0.0570968840
Dielectric energy corr. [a.u.] = -0.0556371947

**$Et_2O^{\cdot\cdot}CI_3^+$**

sy c1

| | | | |
|---|---|---|---|
| o1 | -0.2211 | -3.7953 | 0.0465 |
| c2 | -0.0083 | 0.8185 | 0.0094 |
| i3 | -0.0673 | 1.8120 | 1.7766 |
| i4 | 0.1267 | 1.8856 | -1.7100 |
| i5 | -0.0838 | -1.2069 | -0.0388 |
| c6 | -0.1944 | -4.3992 | 1.3520 |
| c7 | 1.1615 | -4.9641 | 1.7158 |
| h8 | -0.9698 | -5.1671 | 1.3887 |
| h9 | -0.4759 | -3.6054 | 2.0420 |
| h10 | 1.9313 | -4.1995 | 1.6288 |
| h11 | 1.1407 | -5.3130 | 2.7469 |
| h12 | 1.4338 | -5.8081 | 1.0879 |
| c13 | -0.1549 | -4.7577 | -1.0190 |
| c14 | -0.3874 | -4.0541 | -2.3329 |
| h15 | -0.9231 | -5.5129 | -0.8387 |
| h16 | 0.8196 | -5.2455 | -1.0082 |
| h17 | 0.3986 | -3.3292 | -2.5351 |
| h18 | -0.3827 | -4.7825 | -3.1410 |
| h19 | -1.3518 | -3.5500 | -2.3363 |

dist 1 o -- 13 c = 2.7161 au = 143.73 pm
dist 1 o -- 6 c = 2.7188 au = 143.87 pm
dist 1 o -- 9 h = 3.8185 au = 202.07 pm
dist 1 o -- 15 h = 3.8850 au = 205.59 pm
dist 1 o -- 8 h = 3.8930 au = 206.01 pm
dist 1 o -- 16 h = 3.9180 au = 207.33 pm
dist 1 o -- 14 c = 4.5338 au = 239.92 pm
dist 1 o -- 7 c = 4.6538 au = 246.27 pm
dist 2 c -- 3 i = 3.8328 au = 202.82 pm
dist 2 c -- 4 i = 3.8326 au = 202.81 pm
dist 2 c -- 5 i = 3.8312 au = 202.74 pm
dist 1 o -- 5 i = 4.9009 au = 259.34 pm
bend 6 c -> 1 o <- 13 c = 113.00 deg
bend 6 c -> 1 o <- 5 i = 116.60 deg
bend 13 c -> 1 o <- 5 i = 129.90 deg
bend 3 i -> 1 o <- 4 i = 34.35 deg
bend 4 i -> 1 o <- 5 i = 15.27 deg
bend 5 i -> 1 o <- 3 i = 19.08 deg

cycle = 11 SCF+MP2 energy = -304.8682630699 |dE/dxyz| = 0.000568

zero point VIBRATIONAL energy : 0.1387550 Hartree

$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 | 16.00 | 0.12206 | YES | YES |
| 8 | a | 28.26 | 0.82039 | YES | YES |
| 9 | a | 33.42 | 0.51873 | YES | YES |
| 10 | a | 44.92 | 0.19593 | YES | YES |
| 11 | a | 55.39 | 0.03909 | YES | YES |
| 12 | a | 93.71 | 1.24061 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 13 | a | 105.67 | 0.18517 | YES | YES |
| 14 | a | 128.52 | 3.55782 | YES | YES |
| 15 | a | 137.91 | 5.10294 | YES | YES |
| 16 | a | 152.53 | 1.87475 | YES | YES |
| 17 | a | 197.98 | 7.95849 | YES | YES |
| 18 | a | 235.73 | 5.45548 | YES | YES |
| 19 | a | 273.49 | 0.11422 | YES | YES |
| 20 | a | 338.47 | 11.58786 | YES | YES |
| 21 | a | 349.87 | 8.97288 | YES | YES |
| 22 | a | 361.77 | 4.71739 | YES | YES |
| 23 | a | 497.43 | 3.22387 | YES | YES |
| 24 | a | 692.65 | 123.73346 | YES | YES |
| 25 | a | 698.21 | 183.34765 | YES | YES |
| 26 | a | 775.61 | 36.28378 | YES | YES |
| 27 | a | 799.76 | 6.65976 | YES | YES |
| 28 | a | 812.48 | 29.61801 | YES | YES |
| 29 | a | 902.55 | 12.45756 | YES | YES |
| 30 | a | 1011.19 | 78.49717 | YES | YES |
| 31 | a | 1043.09 | 109.42981 | YES | YES |
| 32 | a | 1074.90 | 34.34699 | YES | YES |
| 33 | a | 1093.06 | 25.68271 | YES | YES |
| 34 | a | 1129.63 | 17.17081 | YES | YES |
| 35 | a | 1161.13 | 8.71313 | YES | YES |
| 36 | a | 1265.26 | 2.77751 | YES | YES |
| 37 | a | 1286.18 | 14.20714 | YES | YES |
| 38 | a | 1345.85 | 0.68512 | YES | YES |
| 39 | a | 1354.61 | 53.48580 | YES | YES |
| 40 | a | 1371.49 | 35.50172 | YES | YES |
| 41 | a | 1383.27 | 61.16006 | YES | YES |
| 42 | a | 1427.27 | 13.86750 | YES | YES |
| 43 | a | 1427.88 | 3.97303 | YES | YES |
| 44 | a | 1429.61 | 15.11710 | YES | YES |
| 45 | a | 1440.71 | 6.35522 | YES | YES |
| 46 | a | 1444.59 | 8.30007 | YES | YES |
| 47 | a | 1461.04 | 3.05264 | YES | YES |
| 48 | a | 2937.52 | 17.04046 | YES | YES |
| 49 | a | 2948.81 | 37.68500 | YES | YES |
| 50 | a | 2958.41 | 6.70942 | YES | YES |
| 51 | a | 2959.37 | 8.62081 | YES | YES |
| 52 | a | 2990.60 | 12.49549 | YES | YES |
| 53 | a | 3023.20 | 3.45828 | YES | YES |
| 54 | a | 3047.82 | 7.23649 | YES | YES |
| 55 | a | 3048.52 | 13.46728 | YES | YES |
| 56 | a | 3052.46 | 7.15101 | YES | YES |
| 57 | a | 3056.72 | 12.00171 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.82 | 15.84 | 15.81 | 236.70 | 401.66 | 0.56159 |

$cosmo_energy
Total energy [a.u.] = -305.6573033423
Total energy corrected [a.u.] = -305.6558597326
Dielectric energy [a.u.] = -0.0579143595
Dielectric energy corr. [a.u.] = -0.0564707498

**$CI_3OEt$**

sy cs

| | | | |
|---|---|---|---|
| c1 | 1.2958 | 3.8226 | 0.0000 |
| c2 | 1.4512 | 2.3236 | 0.0000 |
| o3 | 0.1205 | 1.7694 | 0.0000 |
| c4 | -0.0024 | 0.4253 | 0.0000 |
| i5 | 0.8936 | -0.5099 | 1.7815 |
| h6 | 0.7562 | 4.1510 | 0.8846 |
| h7 | 0.7562 | 4.1510 | -0.8846 |
| h8 | 2.2805 | 4.2863 | 0.0000 |
| h9 | 1.9729 | 1.9648 | -0.8874 |
| h10 | 1.9729 | 1.9648 | 0.8874 |
| i11 | 0.8936 | -0.5099 | -1.7815 |
| i12 | -2.1236 | 0.0436 | 0.0000 |

dist 3 o -- 4 c = 2.5506 au = 134.97 pm
dist 2 c -- 3 o = 2.7240 au = 144.15 pm
dist 4 c -- 12 i = 4.0729 au = 215.53 pm
dist 4 c -- 5 i = 4.1621 au = 220.25 pm
dist 4 c -- 11 i = 4.1621 au = 220.25 pm
dist 1 c -- 3 o = 4.4707 au = 236.58 pm
bend 4 c -> 3 o <- 2 c = 117.84 deg
bend 5 i -> 4 c <- 11 i = 107.97 deg
bend 5 i -> 4 c <- 12 i = 108.98 deg
bend 11 i -> 4 c <- 12 i = 108.98 deg

cycle = 10 SCF+MP2 energy = -226.1373835945 |dE/dxyz| = 0.000168

zero point VIBRATIONAL energy : 0.0741208 Hartree

$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" | 40.96 | 0.03478 | YES | YES |
| 8 | a' | 79.18 | 0.18285 | YES | YES |
| 9 | a" | 89.31 | 0.01035 | YES | YES |
| 10 | a" | 102.56 | 6.94867 | YES | YES |
| 11 | a' | 112.47 | 1.14276 | YES | YES |
| 12 | a' | 126.62 | 0.53775 | YES | YES |
| 13 | a" | 215.76 | 8.33237 | YES | YES |
| 14 | a' | 225.46 | 7.51051 | YES | YES |
| 15 | a' | 263.17 | 11.77575 | YES | YES |
| 16 | a" | 276.93 | 3.84200 | YES | YES |
| 17 | a' | 445.33 | 22.00627 | YES | YES |
| 18 | a" | 513.99 | 275.47614 | YES | YES |
| 19 | a' | 658.13 | 145.19256 | YES | YES |
| 20 | a" | 800.01 | 0.01063 | YES | YES |
| 21 | a' | 835.91 | 33.46388 | YES | YES |
| 22 | a' | 1001.18 | 58.35690 | YES | YES |
| 23 | a' | 1101.73 | 15.07214 | YES | YES |
| 24 | a" | 1129.56 | 15.22666 | YES | YES |
| 25 | a' | 1189.26 | 530.28985 | YES | YES |
| 26 | a" | 1244.33 | 2.87173 | YES | YES |
| 27 | a' | 1349.99 | 23.47061 | YES | YES |

| | | | | | |
|---|---|---|---|---|---|
| 28 | a' | 1381.43 | 3.22039 | YES | YES |
| 29 | a'' | 1424.45 | 10.06998 | YES | YES |
| 30 | a' | 1441.07 | 1.42840 | YES | YES |
| 31 | a' | 1449.55 | 8.99706 | YES | YES |
| 32 | a' | 2950.05 | 9.25450 | YES | YES |
| 33 | a' | 2963.97 | 10.96520 | YES | YES |
| 34 | a'' | 3007.81 | 5.47369 | YES | YES |
| 35 | a' | 3055.24 | 5.81940 | YES | YES |
| 36 | a'' | 3059.88 | 8.94957 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.73 | 15.26 | 8.31 | 87.28 | 221.46 | 0.45837 |

$cosmo_energy
Total energy [a.u.] = -226.7592369642
Total energy corrected [a.u.] = -226.7595223122
Dielectric energy [a.u.] = -0.0058637315
Dielectric energy corr. [a.u.] = -0.0061490795

**$H(OEt_2)_2^+$**

sy c1

| | | | |
|---|---|---|---|
| h1 | 0.0016 | 0.0017 | -0.2860 |
| o2 | -0.0545 | 1.1936 | -0.3192 |
| o3 | 0.0576 | -1.1912 | -0.3196 |
| c4 | -1.1139 | -1.8055 | -0.9444 |
| h5 | -1.0433 | -1.5328 | -1.9932 |
| h6 | -0.9828 | -2.8803 | -0.8557 |
| c7 | 0.4968 | -1.8061 | 0.9304 |
| h8 | 1.0309 | -1.0179 | 1.4570 |
| h9 | -0.3858 | -2.0766 | 1.5072 |
| c10 | 1.3912 | -2.9869 | 0.6528 |
| h11 | 1.7465 | -3.3903 | 1.5992 |
| h12 | 2.2510 | -2.6868 | 0.0597 |
| h13 | 0.8616 | -3.7802 | 0.1314 |
| c14 | -2.4021 | -1.3264 | -0.3207 |
| h15 | -3.2371 | -1.8159 | -0.8187 |
| h16 | -2.5218 | -0.2525 | -0.4487 |
| h17 | -2.4595 | -1.5730 | 0.7371 |
| c18 | -0.4960 | 1.8067 | 0.9310 |
| h19 | 0.3863 | 2.0880 | 1.5031 |
| h20 | -1.0197 | 1.0150 | 1.4627 |
| c21 | -1.4021 | 2.9782 | 0.6524 |
| h22 | -1.7362 | 3.3993 | 1.5988 |
| h23 | -0.8875 | 3.7622 | 0.1027 |
| h24 | -2.2746 | 2.6641 | 0.0857 |
| c25 | 1.1176 | 1.8093 | -0.9412 |
| h26 | 0.9867 | 2.8839 | -0.8491 |
| h27 | 1.0479 | 1.5401 | -1.9910 |
| c28 | 2.4050 | 1.3280 | -0.3176 |
| h29 | 3.2407 | 1.8211 | -0.8109 |
| h30 | 2.4597 | 1.5690 | 0.7417 |
| h31 | 2.5260 | 0.2550 | -0.4510 |

dist 1 h -- 2 o = 2.2558 au = 119.37 pm
dist 2 o -- 18 c = 2.7604 au = 146.07 pm
dist 2 o -- 25 c = 2.7643 au = 146.28 pm
dist 2 o -- 27 h = 3.8405 au = 203.23 pm
dist 2 o -- 20 h = 3.8444 au = 203.44 pm
dist 2 o -- 26 h = 3.8829 au = 205.47 pm
dist 2 o -- 19 h = 3.9254 au = 207.73 pm
dist 2 o -- 3 o = 4.5118 au = 238.75 pm
dist 2 o -- 21 c = 4.6074 au = 243.81 pm
dist 2 o -- 28 c = 4.6547 au = 246.32 pm
dist 1 h -- 3 o = 2.2578 au = 119.48 pm
dist 3 o -- 7 c = 2.7601 au = 146.06 pm
dist 3 o -- 4 c = 2.7644 au = 146.28 pm
dist 3 o -- 5 h = 3.8402 au = 203.21 pm
dist 3 o -- 8 h = 3.8421 au = 203.32 pm
dist 3 o -- 6 h = 3.8833 au = 205.49 pm
dist 3 o -- 9 h = 3.9267 au = 207.79 pm
dist 2 o -- 3 o = 4.5118 au = 238.75 pm
dist 3 o -- 10 c = 4.6089 au = 243.89 pm
dist 3 o -- 14 c = 4.6551 au = 246.34 pm
bend 2 o -> 1 h <- 3 o = 176.79 deg

cycle = 19 SCF+MP2 energy = -466.7376868073 |dE/dxyz| = 0.000593

zero point VIBRATIONAL energy : 0.2767406 Hartree

$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 | 7.95 | 0.02203 | YES YES |
| 8 | a | 22.53 | 0.22503 | YES YES |
| 9 | a | 38.25 | 0.24366 | YES YES |
| 10 | a | 39.15 | 0.25592 | YES YES |
| 11 | a | 50.07 | 0.47704 | YES YES |
| 12 | a | 70.86 | 0.09046 | YES YES |
| 13 | a | 98.81 | 0.47980 | YES YES |
| 14 | a | 116.89 | 0.80384 | YES YES |
| 15 | a | 125.86 | 12.33801 | YES YES |
| 16 | a | 190.51 | 0.18727 | YES YES |
| 17 | a | 205.11 | 3.15778 | YES YES |
| 18 | a | 254.41 | 0.10078 | YES YES |
| 19 | a | 255.65 | 0.30548 | YES YES |
| 20 | a | 265.89 | 0.20479 | YES YES |
| 21 | a | 299.08 | 19.11484 | YES YES |
| 22 | a | 307.02 | 0.15547 | YES YES |
| 23 | a | 409.64 | 36.11803 | YES YES |
| 24 | a | 438.77 | 3.92916 | YES YES |
| 25 | a | 441.69 | 28.17351 | YES YES |
| 26 | a | 545.55 | 0.57552 | YES YES |
| 27 | a | 725.97 | 341.00329 | YES YES |
| 28 | a | 769.64 | 1.38562 | YES YES |
| 29 | a | 775.48 | 1.57364 | YES YES |
| 30 | a | 776.71 | 7.26823 | YES YES |
| 31 | a | 804.20 | 1.65348 | YES YES |
| 32 | a | 848.91 | 1.09707 | YES YES |
| 33 | a | 879.98 | 51.86624 | YES YES |
| 34 | a | 885.02 | 13.24723 | YES YES |
| 35 | a | 945.50 | 749.44925 | YES YES |
| 36 | a | 991.06 | 1.43144 | YES YES |
| 37 | a | 1005.38 | 166.78267 | YES YES |
| 38 | a | 1006.78 | 126.60643 | YES YES |
| 39 | a | 1067.90 | 259.44102 | YES YES |
| 40 | a | 1078.48 | 10.52604 | YES YES |
| 41 | a | 1079.98 | 2.41600 | YES YES |
| 42 | a | 1081.83 | 19.66600 | YES YES |
| 43 | a | 1107.22 | 357.86009 | YES YES |
| 44 | a | 1113.55 | 1.89644 | YES YES |
| 45 | a | 1128.02 | 366.59797 | YES YES |
| 46 | a | 1180.75 | 2.01604 | YES YES |
| 47 | a | 1211.80 | 887.66733 | YES YES |
| 48 | a | 1268.96 | 0.41727 | YES YES |
| 49 | a | 1270.90 | 24.66598 | YES YES |
| 50 | a | 1311.77 | 257.78724 | YES YES |
| 51 | a | 1318.17 | 2.14456 | YES YES |
| 52 | a | 1338.92 | 0.83871 | YES YES |
| 53 | a | 1340.57 | 29.09837 | YES YES |
| 54 | a | 1361.40 | 1.95784 | YES YES |
| 55 | a | 1365.20 | 73.50697 | YES YES |
| 56 | a | 1372.89 | 112.62894 | YES YES |
| 57 | a | 1373.48 | 4.59999 | YES YES |
| 58 | a | 1377.66 | 0.77928 | YES YES |
| 59 | a | 1390.18 | 59.97368 | YES YES |

| | | | | | |
|---|---|---|---|---|---|
| 60 | a | 1423.19 | 98.92255 | YES | YES |
| 61 | a | 1425.68 | 11.43652 | YES | YES |
| 62 | a | 1425.99 | 5.12975 | YES | YES |
| 63 | a | 1428.87 | 6.89118 | YES | YES |
| 64 | a | 1429.79 | 5.87347 | YES | YES |
| 65 | a | 1430.61 | 2.71453 | YES | YES |
| 66 | a | 1438.29 | 5.22846 | YES | YES |
| 67 | a | 1438.92 | 1.86609 | YES | YES |
| 68 | a | 1441.66 | 2.86067 | YES | YES |
| 69 | a | 1444.56 | 45.03958 | YES | YES |
| 70 | a | 1447.80 | 5.26861 | YES | YES |
| 71 | a | 1449.34 | 0.16814 | YES | YES |
| 72 | a | 1492.84 | 23.21229 | YES | YES |
| 73 | a | 1530.95 | 1719.70082 | YES | YES |
| 74 | a | 2959.57 | 3.14396 | YES | YES |
| 75 | a | 2960.63 | 3.07977 | YES | YES |
| 76 | a | 2963.33 | 1.28775 | YES | YES |
| 77 | a | 2964.30 | 1.29476 | YES | YES |
| 78 | a | 2985.07 | 14.43281 | YES | YES |
| 79 | a | 2987.26 | 18.12771 | YES | YES |
| 80 | a | 3004.82 | 7.25677 | YES | YES |
| 81 | a | 3006.61 | 6.91487 | YES | YES |
| 82 | a | 3039.67 | 1.49711 | YES | YES |
| 83 | a | 3042.02 | 0.81918 | YES | YES |
| 84 | a | 3045.23 | 3.82330 | YES | YES |
| 85 | a | 3047.08 | 3.76347 | YES | YES |
| 86 | a | 3051.23 | 2.67870 | YES | YES |
| 87 | a | 3051.40 | 2.56383 | YES | YES |
| 88 | a | 3054.22 | 3.41770 | YES | YES |
| 89 | a | 3054.74 | 4.35505 | YES | YES |
| 90 | a | 3063.76 | 10.54731 | YES | YES |
| 91 | a | 3065.47 | 10.71284 | YES | YES |
| 92 | a | 3070.16 | 12.83862 | YES | YES |
| 93 | a | 3072.27 | 11.23406 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 18.11 | 14.04 | 17.74 | 602.90 | 767.88 | 0.56166 |

$cosmo_energy
Total energy [a.u.] = -467.3699098684
Total energy corrected [a.u.] = -467.3688339406
Dielectric energy [a.u.] = -0.0585212419
Dielectric energy corr. [a.u.] = -0.0574453141

**$C_2H_4$**

sy d2h

| | | | |
|---|---|---|---|
| c1 | 0.6662 | 0.0000 | 0.0000 |
| h2 | 1.2282 | -0.9227 | 0.0000 |
| c3 | -0.6662 | 0.0000 | 0.0000 |
| h4 | 1.2282 | 0.9227 | 0.0000 |
| h5 | -1.2282 | 0.9227 | 0.0000 |
| h6 | -1.2282 | -0.9227 | 0.0000 |

dist 1 c -- 2 h = 2.0416 au = 108.04 pm
dist 1 c -- 3 c = 2.5177 au = 133.23 pm
dist 2 h -- 4 h = 3.4872 au = 184.53 pm
bend 1 c -> 3 c <- 5 h = 121.35 deg
bend 2 h -> 1 c <- 4 h = 117.30 deg

cycle = 6 MP2 energy = -78.4005771997 |dE/dxyz| = 0.000007

zero point VIBRATIONAL energy : 0.0492616 Hartree

$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 | b2u | 801.34 | 1.36438 | YES | NO |
| 8 | b2g | 913.56 | 0.00000 | NO | YES |
| 9 | b3u | 924.66 | 90.63396 | YES | NO |
| 10 | au | 1025.44 | 0.00000 | NO | NO |
| 11 | b3g | 1190.41 | 0.00000 | NO | YES |
| 12 | ag | 1330.69 | 0.00000 | NO | YES |
| 13 | b1u | 1409.09 | 6.57331 | YES | NO |
| 14 | ag | 1655.65 | 0.00000 | NO | YES |
| 15 | b1u | 3047.70 | 15.74122 | YES | NO |
| 16 | ag | 3061.35 | 0.00000 | NO | YES |
| 17 | b3g | 3119.99 | 0.00000 | NO | YES |
| 18 | b2u | 3143.45 | 20.45002 | YES | NO |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 15.60 | 6.53 | 0.06 | 74.31 | 137.42 | 0.22000 |

**$PCl_3$**

sy c3v

| | | | |
|---|---|---|---|
| p1 | 0.0000 | 0.0000 | 0.7361 |
| cl2 | 0.9087 | 1.5739 | -0.2144 |
| cl3 | 0.9087 | -1.5739 | -0.2144 |
| cl4 | -1.8174 | 0.0000 | -0.2144 |

dist 1 p -- 2 cl = 3.8756 au = 205.09 pm
dist 1 p -- 3 cl = 3.8756 au = 205.09 pm
dist 1 p -- 4 cl = 3.8756 au = 205.09 pm
bend 2 cl -> 1 p <- 3 cl = 100.24 deg

cycle = 3 MP2 energy = -1720.0565832920 |dE/dxyz| = 0.000001

zero point VIBRATIONAL energy : 0.0045334 Hartree

$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 | 164.11 | 0.21469 | YES | YES |
| 8 | e | 164.11 | 0.21469 | YES | YES |
| 9 | a1 | 233.72 | 1.59721 | YES | YES |
| 10 | e | 471.40 | 140.93299 | YES | YES |
| 11 | e | 471.40 | 140.93299 | YES | YES |
| 12 | a1 | 485.21 | 32.49310 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 17.99 | 11.54 | 1.92 | -66.05 | 25.84 | 0.31650 |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 195.15 | 0.1000000 | 16.93 | 10.91 | 1.00 | -34.88 | 19.57 | 0.28732 |

298K
$cosmo_energy
Total energy [a.u.] = -1721.6734122044
Total energy + OC corr. [a.u.] = -1721.6733109472
Total energy corrected [a.u.] = -1721.6733615758 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0022008052
Diel. energy + OC corr. [a.u.] = -0.0020995480

195K
$cosmo_energy
Total energy [a.u.] = -1721.6735775170
Total energy + OC corr. [a.u.] = -1721.6734671157
Total energy corrected [a.u.] = -1721.6735223164 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0024175825
Diel. energy + OC corr. [a.u.] = -0.0023071812

**$PBr_3$**

sy c3v

| | | | |
|---|---|---|---|
| p1 | 0.0000 | 0.0000 | -0.7575 |
| br2 | -0.9913 | 1.7169 | 0.2525 |
| br3 | -0.9913 | -1.7169 | 0.2525 |
| br4 | 1.9825 | 0.0000 | 0.2525 |

dist 1 p -- 2 br = 4.2046 au = 222.50 pm
dist 1 p -- 3 br = 4.2046 au = 222.50 pm
dist 1 p -- 4 br = 4.2046 au = 222.50 pm
bend 2 br -> 1 p <- 3 br = 101.00 deg

cycle = 7 MP2 energy = -8058.6887407425 |dE/dxyz| = 0.000006

zero point VIBRATIONAL energy : 0.0033016 Hartree

$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 | 98.68 | 0.00512 | YES | YES |
| 8 | e | 98.68 | 0.00512 | YES | YES |
| 9 | a1 | 145.34 | 0.07167 | YES | YES |
| 10 | a1 | 368.03 | 11.65804 | YES | YES |
| 11 | e | 369.26 | 104.78010 | YES | YES |
| 12 | e | 369.26 | 104.78010 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.00 | 12.97 | 3.18 | -78.47 | 24.37 | 0.35325 |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 195.15 | 0.1000000 | 17.95 | 12.33 | 1.94 | -43.61 | 17.58 | 0.32188 |

298K
$cosmo_energy
Total energy [a.u.] = -8063.7610118500
Total energy + OC corr. [a.u.] = -8063.7609771901
Total energy corrected [a.u.] = -8063.7609945201 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0024254748
Diel. energy + OC corr. [a.u.] = -0.0023908149

195K
$cosmo_energy
Total energy [a.u.] = -8063.7611920134
Total energy + OC corr. [a.u.] = -8063.7611539653
Total energy corrected [a.u.] = -8063.7611729893 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0026459002
Diel. energy + OC corr. [a.u.] = -0.0026078521

**$PI_3$**

sy c3v

| | | | |
|---|---|---|---|
| p1 | 0.0000 | 0.0000 | -0.9915 |
| i2 | -1.1020 | 1.9088 | 0.0807 |
| i3 | -1.1020 | -1.9088 | 0.0807 |
| i4 | 2.2041 | 0.0000 | 0.0807 |

dist 1 p -- 2 i = 4.6318 au = 245.10 pm
dist 1 p -- 3 i = 4.6318 au = 245.10 pm
dist 1 p -- 4 i = 4.6318 au = 245.10 pm
bend 2 i -> 1 p <- 3 i = 102.30 deg

cycle = 6 MP2 energy = -374.9141282572 |dE/dxyz| = 0.000010

zero point VIBRATIONAL energy : 0.0025413 Hartree

$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 | 66.89 | 0.17340 | YES | YES |
| 8 | e | 66.89 | 0.17340 | YES | YES |
| 9 | a1 | 99.06 | 0.01472 | YES | YES |
| 10 | a1 | 289.87 | 2.68211 | YES | YES |
| 11 | e | 296.40 | 99.41176 | YES | YES |
| 12 | e | 296.40 | 99.41176 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.63 | 13.99 | 4.37 | -87.53 | 23.61 | 0.38108 |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 195.15 | 0.1000000 | 18.57 | 13.36 | 2.91 | -49.86 | 16.51 | 0.34843 |

298K
$cosmo_energy
Total energy [a.u.] = -375.7293156875
Total energy + OC corr. [a.u.] = -375.7295303368
Total energy corrected [a.u.] = -375.7294230121 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0036214258
Diel. energy + OC corr. [a.u.] = -0.0038360751

195K
$cosmo_energy
Total energy [a.u.] = -375.7293156898
Total energy + OC corr. [a.u.] = -375.7295300330
Total energy corrected [a.u.] = -375.7294228614 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0036187456
Diel. energy + OC corr. [a.u.] = -0.0038330888

**$AsI_3$**

sy c3v

| | | | |
|---|---|---|---|
| as1 | 0.0000 | 0.0000 | -0.9591 |
| i2 | -1.1340 | 1.9642 | 0.1887 |
| i3 | -1.1340 | -1.9642 | 0.1887 |
| i4 | 2.2681 | 0.0000 | 0.1887 |

dist 1 as -- 2 i = 4.8036 au = 254.20 pm
dist 1 as -- 3 i = 4.8036 au = 254.20 pm
dist 1 as -- 4 i = 4.8036 au = 254.20 pm
bend 2 i -> 1 as <- 3 i = 101.20 deg

cycle = 7 MP2 energy = -2268.5092000100 |dE/dxyz| = 0.000001

zero point VIBRATIONAL energy : 0.0019050 Hartree

$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 | 58.88 | 0.01721 | YES | YES |
| 8 | e | 58.88 | 0.01721 | YES | YES |
| 9 | a1 | 83.53 | 0.02325 | YES | YES |
| 10 | a1 | 210.14 | 2.18880 | YES | YES |
| 11 | e | 212.39 | 51.00994 | YES | YES |
| 12 | e | 212.39 | 51.00994 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.79 | 14.12 | 5.24 | -92.03 | 23.01 | 0.39417 |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 195.15 | 0.1000000 | 18.73 | 13.49 | 3.57 | -53.06 | 15.65 | 0.36041 |

298K
$cosmo_energy
Total energy [a.u.] = -2270.3646554434
Total energy + OC corr. [a.u.] = -2270.3648911812
Total energy corrected [a.u.] = -2270.3647733123 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0041725633
Diel. energy + OC corr. [a.u.] = -0.0044083011

195K
$cosmo_energy
Total energy [a.u.] = -2270.3649663147
Total energy + OC corr. [a.u.] = -2270.3652246382
Total energy corrected [a.u.] = -2270.3650954765 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0045819239
Diel. energy + OC corr. [a.u.] = -0.0048402474

**$I_3C\text{-}PCl_3^+$**

sy c3v

| | | | |
|---|---|---|---|
| c1 | 0.0000 | 0.0000 | 0.9396 |
| p2 | 0.0000 | 0.0000 | -0.8806 |
| i3 | -1.0288 | -1.7819 | 1.5610 |
| i4 | -1.0288 | 1.7819 | 1.5610 |
| i5 | 2.0576 | 0.0000 | 1.5610 |
| cl6 | 0.9153 | 1.5853 | -1.5901 |
| cl7 | -1.8305 | 0.0000 | -1.5901 |
| cl8 | 0.9153 | -1.5853 | -1.5901 |

dist 1 c -- 2 p = 3.4397 au = 182.02 pm
dist 2 p -- 6 cl = 3.7099 au = 196.32 pm
dist 1 c -- 3 i = 4.0618 au = 214.94 pm
bend 1 c -> 2 p <- 6 cl = 111.18 deg
bend 3 i -> 1 c <- 4 i = 112.00 deg
bend 6 cl -> 2 p <- 7 cl = 107.71 deg

cycle = 20 MP2 energy = -1791.7784401788 |dE/dxyz| = 0.000002

zero point VIBRATIONAL energy : 0.0115859 Hartree

$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 | 48.79 | 0.00000 | NO | NO |
| 8 | e | 71.66 | 0.03289 | YES | YES |
| 9 | e | 71.66 | 0.03289 | YES | YES |
| 10 | e | 105.60 | 0.00026 | YES | YES |
| 11 | e | 105.60 | 0.00026 | YES | YES |
| 12 | a1 | 115.28 | 0.66631 | YES | YES |
| 13 | e | 142.21 | 0.74182 | YES | YES |
| 14 | e | 142.21 | 0.74182 | YES | YES |
| 15 | a1 | 167.58 | 0.22773 | YES | YES |
| 16 | e | 212.85 | 3.70759 | YES | YES |
| 17 | e | 212.85 | 3.70759 | YES | YES |
| 18 | a1 | 283.99 | 20.82548 | YES | YES |
| 19 | a1 | 458.07 | 88.41716 | YES | YES |
| 20 | e | 538.64 | 52.46870 | YES | YES |
| 21 | e | 538.64 | 52.46870 | YES | YES |
| 22 | e | 601.80 | 102.86169 | YES | YES |
| 23 | e | 601.80 | 102.86169 | YES | YES |
| 24 | a1 | 666.39 | 53.83641 | YES | YES |

298K:

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 20.01 | 14.66 | 10.30 | -81.07 | 61.79 | 0.48748 |

195K:

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|

195.15 0.1000000 18.95 14.02 6.67 -33.92 47.42 0.42509

298K:
$cosmo_energy
Total energy [a.u.] = -1793.8598083151
Total energy + OC corr. [a.u.] = -1793.8576237540
Total energy corrected [a.u.] = -1793.8587160346 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0603598277
Diel. energy + OC corr. [a.u.] = -0.0581752666
195K:
$cosmo_energy
Total energy [a.u.] = -1793.8642586034
Total energy + OC corr. [a.u.] = -1793.8619143044
Total energy corrected [a.u.] = -1793.8630864539 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0648568845
Diel. energy + OC corr. [a.u.] = -0.0625125855

| atom | charge |
|---|---|
| 1 c | -0.4766 |
| 2 p | 1.1943 |
| 3 i | 0.1664 |
| 4 i | 0.1664 |
| 5 i | 0.1664 |
| 6 cl | -0.0723 |
| 7 cl | -0.0723 |
| 8 cl | -0.0723 |

**$I_3C\text{-}PBr_3^+$**

sy c3v

| | | | |
|---|---|---|---|
| c1 | 0.0000 | 0.0000 | 0.9670 |
| p2 | 0.0000 | 0.0000 | -0.8735 |
| i3 | -1.0270 | -1.7787 | 1.5982 |
| i4 | -1.0270 | 1.7787 | 1.5982 |
| i5 | 2.0539 | 0.0000 | 1.5982 |
| br6 | 1.0006 | 1.7331 | -1.6293 |
| br7 | -2.0012 | 0.0000 | -1.6293 |
| br8 | 1.0006 | -1.7331 | -1.6293 |

dist 1 c -- 2 p = 3.4780 au = 184.05 pm
dist 2 p -- 6 br = 4.0424 au = 213.91 pm
dist 1 c -- 3 i = 4.0605 au = 214.87 pm
bend 1 c -> 2 p <- 6 br = 110.69 deg
bend 2 p -> 1 c <- 3 i = 107.08 deg
bend 6 br -> 2 p <- 7 br = 108.22 deg
bend 3 i -> 1 c <- 4 i = 111.75 deg

cycle = 3 MP2 energy = -8130.4156727174 |dE/dxyz| = 0.000002

zero point VIBRATIONAL energy : 0.0096701 Hartree

$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 | 33.64 | 0.00000 | NO | NO |
| 8 | e | 61.84 | 0.01593 | YES | YES |
| 9 | e | 61.84 | 0.01593 | YES | YES |
| 10 | e | 87.93 | 0.03865 | YES | YES |
| 11 | e | 87.93 | 0.03865 | YES | YES |
| 12 | a1 | 89.81 | 0.02978 | YES | YES |
| 13 | e | 107.11 | 0.00064 | YES | YES |
| 14 | e | 107.11 | 0.00064 | YES | YES |
| 15 | e | 141.58 | 0.75662 | YES | YES |
| 16 | e | 141.58 | 0.75662 | YES | YES |
| 17 | a1 | 152.48 | 0.81997 | YES | YES |
| 18 | a1 | 195.98 | 0.27371 | YES | YES |
| 19 | a1 | 353.25 | 87.24477 | YES | YES |
| 20 | e | 466.75 | 109.44486 | YES | YES |
| 21 | e | 466.75 | 109.44486 | YES | YES |
| 22 | e | 544.31 | 22.40776 | YES | YES |
| 23 | e | 544.31 | 22.40776 | YES | YES |
| 24 | a1 | 600.50 | 7.25610 | YES | YES |

298K:

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 20.35 | 15.20 | 12.77 | -94.40 | 59.42 | 0.52423 |

195K:

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|

195.15 0.1000000 19.29 14.57 8.66 -43.60 44.30 0.45875

298K:
$cosmo_energy
Total energy [a.u.] = -8135.9433474625
Total energy corrected [a.u.] = -8135.9419983816
Dielectric energy [a.u.] = -0.0597767052
Dielectric energy corr. [a.u.] = -0.0584276242

195K:
$cosmo_energy
Total energy [a.u.] = -8135.9520323391
Total energy + OC corr. [a.u.] = -8135.9492765032
Total energy corrected [a.u.] = -8135.9506544212 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0636095088
Diel. energy + OC corr. [a.u.] = -0.0608536729

| atom | charge |
|---|---|
| 1 c | -0.4669 |
| 2 p | 1.0650 |
| 3 i | 0.1648 |
| 4 i | 0.1648 |
| 5 i | 0.1648 |
| 6 br | -0.0309 |
| 7 br | -0.0309 |
| 8 br | -0.0309 |

**$I_3C\text{-}PI_3^+$**

sy c3v

| | | | |
|---|---|---|---|
| c1 | 0.0000 | 0.0000 | 0.9949 |
| p2 | 0.0000 | 0.0000 | -0.8703 |
| i3 | -1.0244 | -1.7743 | 1.6426 |
| i4 | -1.0244 | 1.7743 | 1.6426 |
| i5 | 2.0488 | 0.0000 | 1.6426 |
| i6 | 1.1142 | 1.9299 | -1.6841 |
| i7 | -2.2284 | 0.0000 | -1.6841 |
| i8 | 1.1142 | -1.9299 | -1.6841 |

dist 1 c -- 2 p = 3.5247 au = 186.52 pm
dist 1 c -- 3 i = 4.0605 au = 214.87 pm
dist 2 p -- 6 i = 4.4832 au = 237.24 pm
bend 1 c -> 2 p <- 6 i = 110.06 deg
bend 2 p -> 1 c <- 3 i = 107.54 deg
bend 3 i -> 1 c <- 4 i = 111.33 deg
bend 6 i -> 2 p <- 7 i = 108.87 deg

cycle = 3 MP2 energy = -446.6542948480 |dE/dxyz| = 0.000010

zero point VIBRATIONAL energy : 0.0085201 Hartree

$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 | 29.94 | 0.00000 | NO | NO |
| 8 | e | 50.68 | 0.04521 | YES | YES |
| 9 | e | 50.68 | 0.04521 | YES | YES |
| 10 | e | 71.49 | 0.00004 | YES | YES |
| 11 | e | 71.49 | 0.00004 | YES | YES |
| 12 | a1 | 71.87 | 0.00609 | YES | YES |
| 13 | e | 90.61 | 0.02290 | YES | YES |
| 14 | e | 90.61 | 0.02290 | YES | YES |
| 15 | e | 118.84 | 0.06260 | YES | YES |
| 16 | e | 118.84 | 0.06260 | YES | YES |
| 17 | a1 | 127.11 | 0.00009 | YES | YES |
| 18 | a1 | 162.06 | 1.09480 | YES | YES |
| 19 | a1 | 302.45 | 62.20298 | YES | YES |
| 20 | e | 378.32 | 93.79270 | YES | YES |
| 21 | e | 378.32 | 93.79270 | YES | YES |
| 22 | a1 | 539.53 | 1.74965 | YES | YES |
| 23 | e | 543.53 | 19.91829 | YES | YES |
| 24 | e | 543.53 | 19.91829 | YES | YES |

298K:

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 20.64 | 15.68 | 14.72 | -104.15 | 58.13 | 0.55263 |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|

195.15 0.1000000 19.58 15.04 10.29 -50.51 42.58 0.48532

298K:
$cosmo_energy
Total energy [a.u.] = -447.9079835744
Total energy corrected [a.u.] = -447.9063569764
Dielectric energy [a.u.] = -0.0592767437
Dielectric energy corr. [a.u.] = -0.0576501456

195K:
$cosmo_energy
Total energy [a.u.] = -447.9194125902
Total energy + OC corr. [a.u.] = -447.9159857291
Total energy corrected [a.u.] = -447.9176991597 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0630273000
Diel. energy + OC corr. [a.u.] = -0.0596004388

| atom | charge |
|---|---|
| 1 c | -0.4541 |
| 2 p | 0.5906 |
| 3 i | 0.1582 |
| 4 i | 0.1582 |
| 5 i | 0.1582 |
| 6 i | 0.1296 |
| 7 i | 0.1296 |
| 8 i | 0.1296 |

**$I_3C\text{-}AsI_3^+$**

sy c3v

| | | | |
|---|---|---|---|
| c1 | 0.0000 | 0.0000 | 1.1721 |
| as2 | 0.0000 | 0.0000 | -0.8171 |
| i3 | -1.0274 | -1.7795 | 1.7771 |
| i4 | -1.0274 | 1.7795 | 1.7771 |
| i5 | 2.0548 | 0.0000 | 1.7771 |
| i6 | 1.1585 | 2.0066 | -1.6532 |
| i7 | -2.3170 | 0.0000 | -1.6532 |
| i8 | 1.1585 | -2.0066 | -1.6532 |

dist 1 c -- 2 as = 3.7591 au = 198.92 pm
dist 1 c -- 3 i = 4.0479 au = 214.20 pm
dist 2 as -- 6 i = 4.6549 au = 246.33 pm
bend 1 c -> 2 as <- 6 i = 109.84 deg
bend 2 as -> 1 c <- 3 i = 106.41 deg
bend 3 i -> 1 c <- 4 i = 112.36 deg
bend 6 i -> 2 as <- 7 i = 109.10 deg

cycle = 7 SCF+MP2 energy = -2340.2318712799 |dE/dxyz| = 0.000165

zero point VIBRATIONAL energy : 0.0073397 Hartree

$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 | 22.69 | 0.00000 | NO | NO |
| 8 | e | 42.53 | 0.04181 | YES | YES |
| 9 | e | 42.53 | 0.04181 | YES | YES |
| 10 | a1 | 59.43 | 0.17425 | YES | YES |
| 11 | e | 61.67 | 0.00745 | YES | YES |
| 12 | e | 61.67 | 0.00745 | YES | YES |
| 13 | e | 80.52 | 0.02472 | YES | YES |
| 14 | e | 80.52 | 0.02472 | YES | YES |
| 15 | a1 | 112.52 | 0.03812 | YES | YES |
| 16 | e | 115.59 | 0.05227 | YES | YES |
| 17 | e | 115.59 | 0.05227 | YES | YES |
| 18 | a1 | 161.75 | 3.44931 | YES | YES |
| 19 | a1 | 213.98 | 26.71502 | YES | YES |
| 20 | e | 256.24 | 37.27007 | YES | YES |
| 21 | e | 256.24 | 37.27007 | YES | YES |
| 22 | a1 | 429.81 | 63.17628 | YES | YES |
| 23 | e | 554.23 | 40.22124 | YES | YES |
| 24 | e | 554.23 | 40.22124 | YES | YES |

298K:

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 20.72 | 15.78 | 16.59 | -112.32 | 56.82 | 0.57563 |

195K:

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|

195.15 0.1000000 19.66 15.14 11.84 -56.40 40.77 0.50625

298K:
$cosmo_energy
Total energy [a.u.] = -2342.5256950902
Total energy corrected [a.u.] = -2342.5240603963
Dielectric energy [a.u.] = -0.0582171525
Dielectric energy corr. [a.u.] = -0.0565824586
195K:
$cosmo_energy
Total energy [a.u.] = -2342.5338124381
Total energy + OC corr. [a.u.] = -2342.5305976665
Total energy corrected [a.u.] = -2342.5322050523 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0574758635
Diel. energy + OC corr. [a.u.] = -0.0542610918

| atom | charge |
|---|---|
| 1 c | -0.4271 |
| 2 as | 0.6265 |
| 3 i | 0.1605 |
| 4 i | 0.1605 |
| 5 i | 0.1605 |
| 6 i | 0.1064 |
| 7 i | 0.1064 |
| 8 i | 0.1064 |

**$BI_3$**

sy d3h

| | | | |
|---|---|---|---|
| b1 | 0.0000 | 0.0000 | 0.0000 |
| i2 | 1.0569 | -1.8306 | 0.0000 |
| i3 | 1.0569 | 1.8306 | 0.0000 |
| i4 | -2.1138 | 0.0000 | 0.0000 |

dist 1 b -- 2 i = 3.9945 au = 211.38 pm
bend 2 i -> 1 b <- 3 i = 120.00 deg

cycle = 5 SCF+MP2 energy = -58.8312373446 |dE/dxyz| = 0.000002

zero point VIBRATIONAL energy : 0.0047376 Hartree

$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' | 98.95 | 0.00038 | YES | YES |
| 8 | e' | 98.95 | 0.00038 | YES | YES |
| 9 | a1' | 187.43 | 0.00000 | NO | YES |
| 10 | a2'' | 308.93 | 1.11979 | YES | NO |
| 11 | e' | 692.66 | 256.25625 | YES | YES |
| 12 | e' | 692.66 | 256.25625 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.56 | 13.07 | 2.78 | -75.34 | 26.95 | 0.35138 |

$cosmo_energy
Total energy [a.u.] = -59.2793453947
Total energy corrected [a.u.] = -59.2793945410
Dielectric energy [a.u.] = -0.0024963906
Dielectric energy corr. [a.u.] = -0.0025455369

**$I_3BPCl_3$**

sy c3v

| | | | |
|---|---|---|---|
| b1 | 0.0000 | 0.0000 | 0.3003 |
| p2 | 0.0000 | 0.0000 | -1.6534 |
| i3 | -1.0697 | -1.8527 | 0.8174 |
| i4 | -1.0697 | 1.8527 | 0.8174 |
| i5 | 2.1393 | 0.0000 | 0.8174 |
| cl6 | 0.9109 | 1.5777 | -2.4748 |
| cl7 | -1.8218 | 0.0000 | -2.4748 |
| cl8 | 0.9109 | -1.5777 | -2.4748 |

dist 1 b -- 2 p = 3.6918 au = 195.36 pm
dist 2 p -- 6 cl = 3.7765 au = 199.84 pm
dist 1 b -- 3 i = 4.1591 au = 220.09 pm
bend 1 b -> 2 p <- 6 cl = 114.27 deg
bend 2 p -> 1 b <- 3 i = 103.59 deg
bend 3 i -> 1 b <- 4 i = 114.66 deg
bend 6 cl -> 2 p <- 7 cl = 104.27 deg

cycle = 8 MP2 energy = -1778.9176480474 |dE/dxyz| = 0.000015

zero point VIBRATIONAL energy : 0.0107921 Hartree

$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 | 41.08 | 0.00000 | NO | NO |
| 8 | e | 58.00 | 0.12243 | YES | YES |
| 9 | e | 58.00 | 0.12243 | YES | YES |
| 10 | e | 92.67 | 0.03921 | YES | YES |
| 11 | e | 92.67 | 0.03921 | YES | YES |
| 12 | a1 | 100.12 | 0.11779 | YES | YES |
| 13 | e | 133.76 | 0.17778 | YES | YES |
| 14 | e | 133.76 | 0.17778 | YES | YES |
| 15 | a1 | 160.33 | 0.18558 | YES | YES |
| 16 | e | 200.36 | 1.30377 | YES | YES |
| 17 | e | 200.36 | 1.30377 | YES | YES |
| 18 | a1 | 264.35 | 15.35806 | YES | YES |
| 19 | a1 | 407.09 | 172.34937 | YES | YES |
| 20 | e | 534.76 | 88.93047 | YES | YES |
| 21 | e | 534.76 | 88.93047 | YES | YES |
| 22 | e | 572.81 | 146.94089 | YES | YES |
| 23 | e | 572.81 | 146.94089 | YES | YES |
| 24 | a1 | 579.46 | 37.37920 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 20.01 | 14.76 | 11.43 | -86.17 | 60.72 | 0.50099 |

$cosmo_energy
Total energy [a.u.] = -1780.9594433020
Total energy + OC corr. [a.u.] = -1780.9600497508

Total energy corrected [a.u.] = -1780.9597465264 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0042401572
Diel. energy + OC corr. [a.u.] = -0.0048466060

| atom | charge |
|---|---|
| 1 b | -0.7539 |
| 2 p | 1.2176 |
| 3 i | -0.0173 |
| 4 i | -0.0173 |
| 5 i | -0.0173 |
| 6 cl | -0.1373 |
| 7 cl | -0.1373 |
| 8 cl | -0.1373 |

**$I_3BPBr_3$**

sy c3v

| | | | |
|---|---|---|---|
| b1 | 0.0000 | 0.0000 | 0.8282 |
| p2 | 0.0000 | 0.0000 | -1.1452 |
| i3 | -1.0688 | -1.8512 | 1.3431 |
| i4 | -1.0688 | 1.8512 | 1.3431 |
| i5 | 2.1376 | 0.0000 | 1.3431 |
| br6 | 0.9953 | 1.7240 | -2.0224 |
| br7 | -1.9907 | 0.0000 | -2.0224 |
| br8 | 0.9953 | -1.7240 | -2.0224 |

dist 1 b -- 2 p = 3.7292 au = 197.34 pm
dist 2 p -- 6 br = 4.1108 au = 217.53 pm
dist 1 b -- 3 i = 4.1550 au = 219.87 pm
bend 1 b -> 2 p <- 6 br = 113.78 deg
bend 2 p -> 1 b <- 3 i = 103.54 deg
bend 6 br -> 2 p <- 7 br = 104.84 deg
bend 3 i -> 1 b <- 4 i = 114.69 deg

cycle = 8 MP2 energy = -8117.5516427889 |dE/dxyz| = 0.000003

zero point VIBRATIONAL energy : 0.0090401 Hartree

$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 | 28.29 | 0.00000 | NO | NO |
| 8 | e | 50.33 | 0.06098 | YES | YES |
| 9 | e | 50.33 | 0.06098 | YES | YES |
| 10 | a1 | 76.80 | 0.00994 | YES | YES |
| 11 | e | 79.74 | 0.00413 | YES | YES |
| 12 | e | 79.74 | 0.00413 | YES | YES |
| 13 | e | 98.30 | 0.07177 | YES | YES |
| 14 | e | 98.30 | 0.07177 | YES | YES |
| 15 | e | 131.54 | 0.11328 | YES | YES |
| 16 | e | 131.54 | 0.11328 | YES | YES |
| 17 | a1 | 148.35 | 0.22944 | YES | YES |
| 18 | a1 | 176.28 | 0.12209 | YES | YES |
| 19 | a1 | 331.06 | 163.52719 | YES | YES |
| 20 | e | 415.15 | 100.15069 | YES | YES |
| 21 | e | 415.15 | 100.15069 | YES | YES |
| 22 | a1 | 505.11 | 0.06538 | YES | YES |
| 23 | e | 576.06 | 96.49117 | YES | YES |
| 24 | e | 576.06 | 96.49117 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 20.35 | 15.29 | 14.00 | -99.32 | 58.71 | 0.53838 |

$cosmo_energy
Total energy [a.u.] = -8123.0454167166
Total energy + OC corr. [a.u.] = -8123.0458996757

Total energy corrected [a.u.] = -8123.0456581961 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0048890949
Diel. energy + OC corr. [a.u.] = -0.0053720540

| atom | charge |
|---|---|
| 1 b | -0.7390 |
| 2 p | 1.0731 |
| 3 i | -0.0130 |
| 4 i | -0.0130 |
| 5 i | -0.0130 |
| 6 br | -0.0984 |
| 7 br | -0.0984 |
| 8 br | -0.0984 |

**$I_3BPI_3$**

sy c3v

| | | | |
|---|---|---|---|
| b1 | 0.0000 | 0.0000 | 1.2175 |
| p2 | 0.0000 | 0.0000 | -0.7740 |
| i3 | -1.0674 | -1.8488 | 1.7406 |
| i4 | -1.0674 | 1.8488 | 1.7406 |
| i5 | 2.1348 | 0.0000 | 1.7406 |
| i6 | 1.1078 | 1.9188 | -1.7122 |
| i7 | -2.2157 | 0.0000 | -1.7122 |
| i8 | 1.1078 | -1.9188 | -1.7122 |

dist 1 b -- 2 p = 3.7634 au = 199.15 pm
dist 1 b -- 3 i = 4.1535 au = 219.79 pm
dist 2 p -- 6 i = 4.5469 au = 240.61 pm
bend 1 b -> 2 p <- 6 i = 112.95 deg
bend 2 p -> 1 b <- 3 i = 103.77 deg
bend 3 i -> 1 b <- 4 i = 114.52 deg
bend 6 i -> 2 p <- 7 i = 105.78 deg

cycle = 9 MP2 energy = -433.7843741267 |dE/dxyz| = 0.000005

zero point VIBRATIONAL energy : 0.0080010 Hartree

$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 | 25.54 | 0.00000 | NO | NO |
| 8 | e | 43.40 | 0.02210 | YES | YES |
| 9 | e | 43.40 | 0.02210 | YES | YES |
| 10 | a1 | 62.14 | 0.03526 | YES | YES |
| 11 | e | 63.07 | 0.09024 | YES | YES |
| 12 | e | 63.07 | 0.09024 | YES | YES |
| 13 | e | 82.96 | 0.05467 | YES | YES |
| 14 | e | 82.96 | 0.05467 | YES | YES |
| 15 | e | 108.06 | 0.01497 | YES | YES |
| 16 | e | 108.06 | 0.01497 | YES | YES |
| 17 | a1 | 114.70 | 0.49978 | YES | YES |
| 18 | a1 | 157.78 | 1.76223 | YES | YES |
| 19 | a1 | 284.88 | 121.80810 | YES | YES |
| 20 | e | 334.32 | 97.69886 | YES | YES |
| 21 | e | 334.32 | 97.69886 | YES | YES |
| 22 | a1 | 444.40 | 26.02664 | YES | YES |
| 23 | e | 579.49 | 71.31014 | YES | YES |
| 24 | e | 579.49 | 71.31014 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 20.64 | 15.76 | 16.00 | -108.88 | 57.66 | 0.56691 |

$cosmo_energy
Total energy [a.u.] = -435.0116723502
Total energy + OC corr. [a.u.] = -435.0120173019

Total energy corrected [a.u.] = -435.0118448261 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0061444311
Diel. energy + OC corr. [a.u.] = -0.0064893827

| atom | charge |
|---|---|
| 1 b | -0.7228 |
| 2 p | 0.6141 |
| 3 i | -0.0117 |
| 4 i | -0.0117 |
| 5 i | -0.0117 |
| 6 i | 0.0479 |
| 7 i | 0.0479 |
| 8 i | 0.0479 |

**$CI_3^{\cdot}$**

sy c1

| | | | |
|---|---|---|---|
| c1 | 0.0000 | 0.0000 | -0.2646 |
| i2 | 1.9875 | -0.5051 | -0.0074 |
| i3 | -0.5563 | 1.9738 | -0.0077 |
| i4 | -1.4310 | -1.4687 | -0.0077 |

dist 1 c -- 2 i = 3.9055 au = 206.67 pm
dist 1 c -- 3 i = 3.9055 au = 206.67 pm
dist 1 c -- 4 i = 3.9055 au = 206.67 pm
bend 2 i -> 1 c <- 3 i = 118.48 deg
bend 2 i -> 1 c <- 4 i = 118.47 deg
bend 3 i -> 1 c <- 4 i = 118.48 deg

cycle = 9 MP2 energy = -71.9206658591 |dE/dxyz| = 0.000078

zero point VIBRATIONAL energy : 0.0041902 Hartree

$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 | 102.31 | 0.10298 | YES | YES |
| 8 | a | 102.50 | 0.10406 | YES | YES |
| 9 | a | 170.49 | 0.86917 | YES | YES |
| 10 | a | 226.61 | 5.88621 | YES | YES |
| 11 | a | 618.36 | 138.38603 | YES | YES |
| 12 | a | 619.03 | 138.43633 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.56 | 14.79 | 2.97 | -81.53 | 26.02 | 0.36903 |

$cosmo_energy
Total energy [a.u.] = -72.3814232843
Total energy + OC corr. [a.u.] = -72.3816676544
Total energy corrected [a.u.] = -72.3815454694 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0031763655
Diel. energy + OC corr. [a.u.] = -0.0034207356

**$PCl_3^{\cdot+}$**

sy c1

| | | | |
|---|---|---|---|
| p1 | 0.0000 | -0.0000 | -0.4443 |
| cl2 | 0.4319 | -1.8131 | 0.1294 |
| cl3 | 1.3542 | 1.2806 | 0.1294 |
| cl4 | -1.7861 | 0.5325 | 0.1294 |

dist 1 p -- 2 cl = 3.6852 au = 195.01 pm
dist 1 p -- 3 cl = 3.6852 au = 195.01 pm
dist 1 p -- 4 cl = 3.6852 au = 195.01 pm
bend 2 cl -> 1 p <- 3 cl = 111.73 deg
bend 3 cl -> 1 p <- 4 cl = 111.72 deg
bend 2 cl -> 1 p <- 4 cl = 111.73 deg

cycle = 8 MP2 energy = -1719.7018556977 |dE/dxyz| = 0.000004

zero point VIBRATIONAL energy : 0.0051169 Hartree

$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 | 175.25 | 1.50293 | YES | YES |
| 8 | a | 175.47 | 1.51223 | YES | YES |
| 9 | a | 244.60 | 3.55011 | YES | YES |
| 10 | a | 455.26 | 5.48497 | YES | YES |
| 11 | a | 597.54 | 113.80743 | YES | YES |
| 12 | a | 597.93 | 113.84365 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 17.99 | 12.63 | 1.72 | -66.74 | 26.85 | 0.32221 |

$cosmo_energy
Total energy [a.u.] = -1721.3929944429
Total energy + OC corr. [a.u.] = -1721.3917110851
Total energy corrected [a.u.] = -1721.3923527640 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0793985897
Diel. energy + OC corr. [a.u.] = -0.0781152318

**$PBr_3^{+}$**

sy c1

| | | | |
|---|---|---|---|
| p1 | 0.0000 | 0.0000 | -0.5309 |
| br2 | -0.7521 | -1.8927 | 0.0686 |
| br3 | 2.0152 | 0.2950 | 0.0686 |
| br4 | -1.2631 | 1.5977 | 0.0686 |

dist 1 p -- 2 br = 4.0120 au = 212.31 pm
dist 1 p -- 3 br = 4.0120 au = 212.31 pm
dist 1 p -- 4 br = 4.0120 au = 212.31 pm
bend 2 br -> 1 p <- 3 br = 112.36 deg
bend 2 br -> 1 p <- 4 br = 112.36 deg
bend 3 br -> 1 p <- 4 br = 112.36 deg

cycle = 8 MP2 energy = -8058.3477228822 |dE/dxyz| = 0.000003

zero point VIBRATIONAL energy : 0.0036372 Hartree

$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 | 104.46 | 0.31491 | YES | YES |
| 8 | a | 105.45 | 0.27268 | YES | YES |
| 9 | a | 163.81 | 0.44946 | YES | YES |
| 10 | a | 308.41 | 2.42707 | YES | YES |
| 11 | a | 457.06 | 87.47550 | YES | YES |
| 12 | a | 457.36 | 87.52518 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.00 | 14.09 | 2.94 | -79.79 | 24.85 | 0.35927 |

$cosmo_energy
Total energy [a.u.] = -8063.4907481176
Total energy + OC corr. [a.u.] = -8063.4886138141
Total energy corrected [a.u.] = -8063.4896809658 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0739528642
Diel. energy + OC corr. [a.u.] = -0.0718185606

**$PI_3^{+}$**

sy c1

| | | | |
|---|---|---|---|
| p1 | 0.0000 | 0.0000 | -0.5704 |
| i2 | -0.7238 | -2.1478 | 0.0464 |
| i3 | 2.2219 | 0.4471 | 0.0464 |
| i4 | -1.4982 | 1.7007 | 0.0464 |

dist 1 p -- 2 i = 4.4387 au = 234.89 pm
dist 1 p -- 3 i = 4.4387 au = 234.89 pm
dist 1 p -- 4 i = 4.4387 au = 234.89 pm
bend 2 i -> 1 p <- 3 i = 113.36 deg
bend 2 i -> 1 p <- 4 i = 113.36 deg
bend 3 i -> 1 p <- 4 i = 113.36 deg

cycle = 8 MP2 energy = -374.5965978030 |dE/dxyz| = 0.000004

zero point VIBRATIONAL energy : 0.0027371 Hartree

$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 | 70.36 | 0.01748 | YES | YES |
| 8 | a | 70.59 | 0.01719 | YES | YES |
| 9 | a | 113.75 | 0.00101 | YES | YES |
| 10 | a | 230.45 | 0.25350 | YES | YES |
| 11 | a | 358.00 | 64.21102 | YES | YES |
| 12 | a | 358.29 | 64.27085 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.63 | 15.13 | 4.14 | -89.25 | 23.85 | 0.38764 |

$cosmo_energy
Total energy [a.u.] = -375.4722286239
Total energy + OC corr. [a.u.] = -375.4690406557
Total energy corrected [a.u.] = -375.4706346398 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0693450001
Diel. energy + OC corr. [a.u.] = -0.0661570319

**$AsI_3^{\cdot+}$**

sy c1

| | | | |
|---|---|---|---|
| as1 | 0.0000 | -0.0000 | -0.6053 |
| i2 | 2.0950 | -1.0438 | 0.1191 |
| i3 | -0.1436 | 2.3362 | 0.1191 |
| i4 | -1.9514 | -1.2924 | 0.1191 |

dist 1 as -- 2 i = 4.6301 au = 245.01 pm
dist 1 as -- 3 i = 4.6301 au = 245.01 pm
dist 1 as -- 4 i = 4.6301 au = 245.01 pm
bend 2 i -> 1 as <- 3 i = 111.65 deg
bend 2 i -> 1 as <- 4 i = 111.65 deg
bend 3 i -> 1 as <- 4 i = 111.65 deg

cycle = 9 MP2 energy = -2268.1827123029 |dE/dxyz| = 0.000002

zero point VIBRATIONAL energy : 0.0019479 Hartree

$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 | 60.57 | 0.05147 | YES | YES |
| 8 | a | 60.99 | 0.04689 | YES | YES |
| 9 | a | 84.89 | 0.01220 | YES | YES |
| 10 | a | 177.81 | 0.34388 | YES | YES |
| 11 | a | 235.10 | 18.40278 | YES | YES |
| 12 | a | 235.67 | 18.45313 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.79 | 15.25 | 5.16 | -94.52 | 23.05 | 0.40264 |

$cosmo_energy
Total energy [a.u.] = -2270.1015226309
Total energy + OC corr. [a.u.] = -2270.0982997399
Total energy corrected [a.u.] = -2270.0999111854 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0694817267
Diel. energy + OC corr. [a.u.] = -0.0662588357

**$PCl_3I^+$**

sy c3v

| | | | |
|---|---|---|---|
| p1 | 0.0000 | 0.0000 | 0.0503 |
| cl2 | -0.9162 | 1.5869 | 0.7526 |
| cl3 | -0.9162 | -1.5869 | 0.7526 |
| cl4 | 1.8324 | 0.0000 | 0.7526 |
| i5 | 0.0000 | 0.0000 | -2.2838 |

dist 1 p -- 2 cl = 3.7083 au = 196.23 pm
dist 1 p -- 5 i = 4.4108 au = 233.41 pm
bend 2 cl -> 1 p <- 3 cl = 107.93 deg
bend 2 cl -> 1 p <- 5 i = 110.97 deg

cycle = 8 MP2 energy = -1731.1076791100 |dE/dxyz| = 0.000001

zero point VIBRATIONAL energy : 0.0065817 Hartree

$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 | 122.88 | 0.21194 | YES | YES |
| 8 | e | 122.88 | 0.21194 | YES | YES |
| 9 | a1 | 170.30 | 0.28119 | YES | YES |
| 10 | e | 203.49 | 2.52720 | YES | YES |
| 11 | e | 203.49 | 2.52720 | YES | YES |
| 12 | a1 | 327.70 | 19.34716 | YES | YES |
| 13 | a1 | 528.92 | 152.51735 | YES | YES |
| 14 | e | 604.67 | 122.07043 | YES | YES |
| 15 | e | 604.67 | 122.07043 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 18.97 | 12.86 | 3.55 | -70.41 | 35.24 | 0.36266 |

$cosmo_energy
Total energy [a.u.] = -1732.9031401040
Total energy + OC corr. [a.u.] = -1732.9015250501
Total energy corrected [a.u.] = -1732.9023325771 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0694019841
Diel. energy + OC corr. [a.u.] = -0.0677869302

**$PBr_3I^+$**

sy c3v

| | | | |
|---|---|---|---|
| p1 | 0.0000 | 0.0000 | -0.3001 |
| i2 | 0.0000 | 0.0000 | 2.0492 |
| br3 | 1.0020 | -1.7355 | -1.0460 |
| br4 | 1.0020 | 1.7355 | -1.0460 |
| br5 | -2.0040 | 0.0000 | -1.0460 |

dist 1 p -- 3 br = 4.0409 au = 213.83 pm
dist 1 p -- 2 i = 4.4395 au = 234.93 pm
bend 2 i -> 1 p <- 3 br = 110.42 deg
bend 3 br -> 1 p <- 4 br = 108.51 deg

cycle = 9 MP2 energy = -8069.7444975526 |dE/dxyz| = 0.000047

zero point VIBRATIONAL energy : 0.0048016 Hartree

$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 | 79.76 | 0.00105 | YES | YES |
| 8 | e | 79.76 | 0.00105 | YES | YES |
| 9 | a1 | 122.26 | 0.45237 | YES | YES |
| 10 | e | 127.48 | 0.47920 | YES | YES |
| 11 | e | 127.48 | 0.47920 | YES | YES |
| 12 | a1 | 218.80 | 0.74512 | YES | YES |
| 13 | a1 | 425.22 | 119.65045 | YES | YES |
| 14 | e | 463.45 | 100.99294 | YES | YES |
| 15 | e | 463.45 | 100.99294 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 19.58 | 13.90 | 5.44 | -83.87 | 32.99 | 0.40027 |

$cosmo_energy
Total energy [a.u.] = -8074.9910309556
Total energy + OC corr. [a.u.] = -8074.9888002790
Total energy corrected [a.u.] = -8074.9899156173 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0662126667
Diel. energy + OC corr. [a.u.] = -0.0639819901

**$PI_4^+$**

sy td

| | | | |
|---|---|---|---|
| p1 | 0.0000 | 0.0000 | 0.0000 |
| i2 | 1.3699 | -1.3699 | 1.3699 |

dist 1 p -- 2 i = 4.4837 au = 237.27 pm

bend 2 i -> 1 p <- 3 i = 109.47 deg

cycle = 7 MP2 energy = -385.9825073972 |dE/dxyz| = 0.000000

zero point VIBRATIONAL energy : 0.0037725 Hartree

$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 | 58.53 | 0.00000 | NO | YES |
| 8 | e | 58.53 | 0.00000 | NO | YES |
| 9 | t2 | 91.35 | 0.05114 | YES | YES |
| 10 | t2 | 91.35 | 0.05114 | YES | YES |
| 11 | t2 | 91.35 | 0.05114 | YES | YES |
| 12 | a1 | 158.93 | 0.00000 | NO | YES |
| 13 | t2 | 368.64 | 91.27787 | YES | YES |
| 14 | t2 | 368.64 | 91.27787 | YES | YES |
| 15 | t2 | 368.64 | 91.27787 | YES | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 20.04 | 13.28 | 7.08 | -90.23 | 31.89 | 0.41787 |

$cosmo_energy

Total energy [a.u.] = -386.9601449132

Total energy + OC corr. [a.u.] = -386.9569902362

Total energy corrected [a.u.] = -386.9585675747 Note: incorrect value contained for downward compatibility

Dielectric energy [a.u.] = -0.0643714261

Diel. energy + OC corr. [a.u.] = -0.0612167492

**$C_2I_4$**

sy d2h

| | | | |
|---|---|---|---|
| c1 | 0.6765 | 0.0000 | 0.0000 |
| c2 | -0.6765 | 0.0000 | 0.0000 |
| i3 | 1.8184 | 1.7486 | 0.0000 |
| i4 | -1.8184 | -1.7486 | 0.0000 |
| i5 | 1.8184 | -1.7486 | 0.0000 |
| i6 | -1.8184 | 1.7486 | 0.0000 |

dist 1 c -- 2 c = 2.5570 au = 135.31 pm
dist 1 c -- 3 i = 3.9465 au = 208.84 pm
bend 1 c -> 2 c <- 3 i = 35.03 deg
bend 2 c -> 1 c <- 3 i = 123.15 deg
bend 3 i -> 2 c <- 5 i = 70.05 deg

cycle = 8 MP2 energy = -121.3128432569 |dE/dxyz| = 0.000004

zero point VIBRATIONAL energy : 0.0105580 Hartree

$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 | au | 35.38 | 0.00000 | NO | NO |
| 8 | b2u | 85.98 | 0.00427 | YES | NO |
| 9 | ag | 101.46 | 0.00000 | NO | YES |
| 10 | b3u | 125.20 | 0.26769 | YES | NO |
| 11 | b1g | 142.52 | 0.00000 | NO | YES |
| 12 | ag | 177.57 | 0.00000 | NO | YES |
| 13 | b1u | 210.02 | 6.70288 | YES | NO |
| 14 | b2g | 422.28 | 0.00000 | NO | YES |
| 15 | b3u | 506.34 | 20.06573 | YES | NO |
| 16 | b2u | 606.21 | 92.82432 | YES | NO |
| 17 | b1g | 730.83 | 0.00000 | NO | YES |
| 18 | ag | 1490.66 | 0.00000 | NO | YES |

| T (K) | p (MPa) | ln(qtrans) | ln(qrot) | ln(qvib) | chem.pot. (kJ/mol) | energy (kJ/mol) | entropy (kJ/mol/K) |
|---|---|---|---|---|---|---|---|
| 298.15 | 0.1000000 | 20.02 | 14.44 | 6.69 | -74.29 | 49.90 | 0.42484 |