Electronic Supplementary Material for Dalton Transactions

Supporting Information

to

Stable CI_3^+ Salts and Attempts to Prepare CHI_2^+ and CH_2I^+

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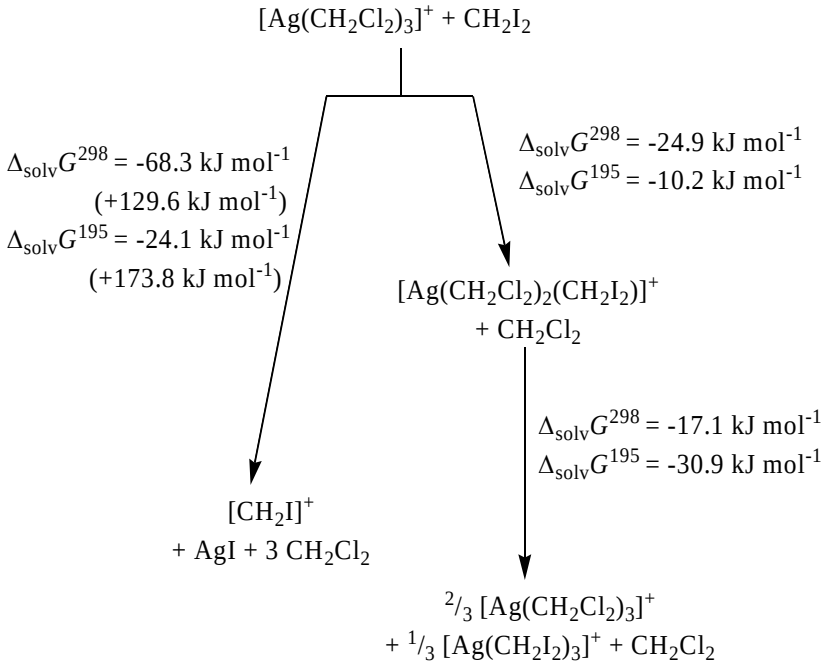
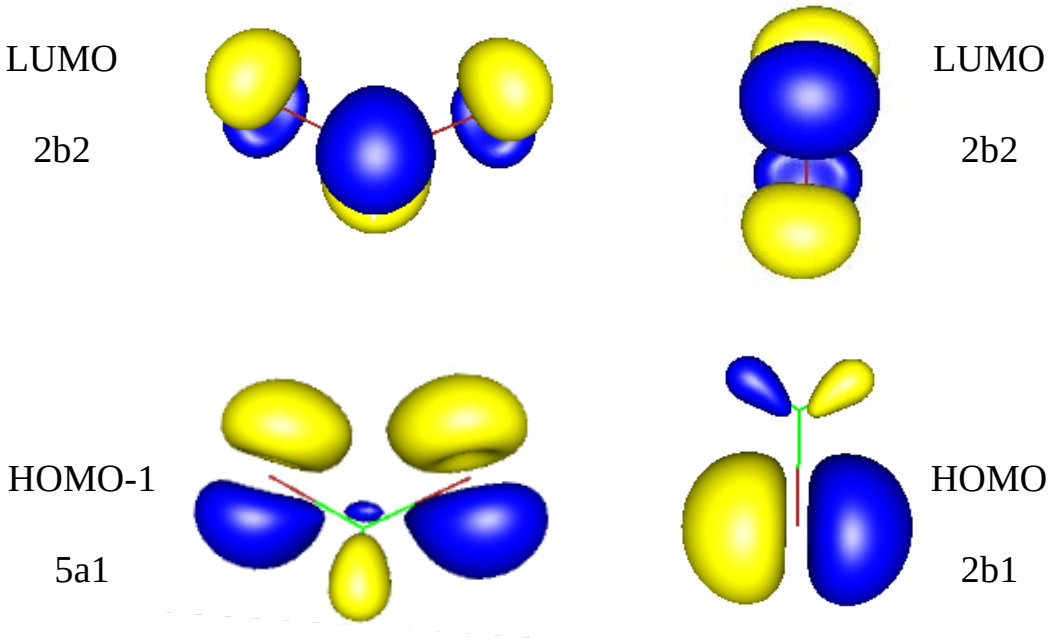
1 Gibbs Free Energies of Ligand Exchange vs. CHI_2^+ Formation.



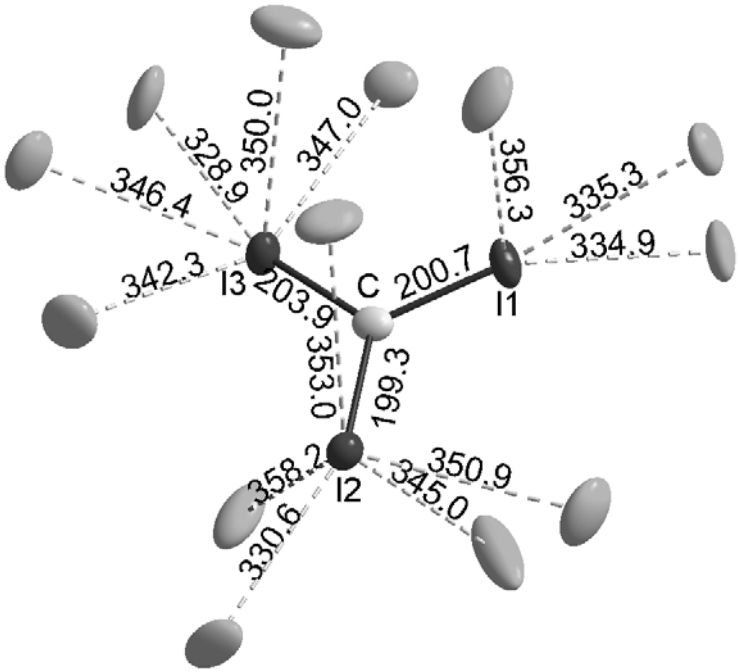
S_Scheme 1: Gibbs free energies $\Delta_r G$ (in kJ mol^{-1}) of ligand exchange vs. CH_2I^+ formation reactions of CH_2I_2 with $[Ag(CH_2Cl_2)_3]^+[pftb]^-$ in CH_2Cl_2 solution. Calculations were done at the MP2/TZVPP level. Values in parenthesis: without consideration of the sublimation enthalpy of AgI (197.9 kJ mol^{-1}).

2 Orbitals Responsible for the Low Field Shift in CHI_2^+ and CH_2I^+

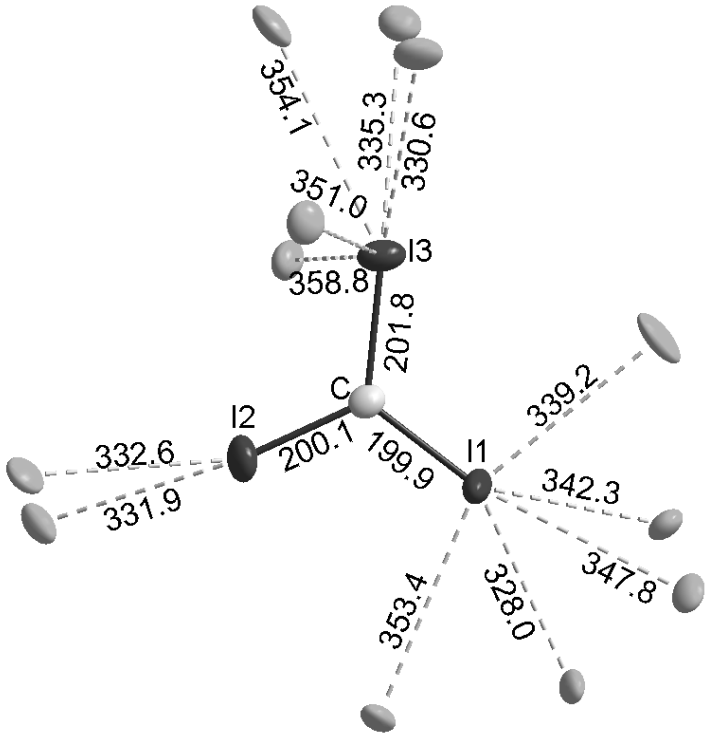


S_Figure 1: Orbitals responsible for the low field shift in CHI_2^+ (left) and CH_2I^+ (right).

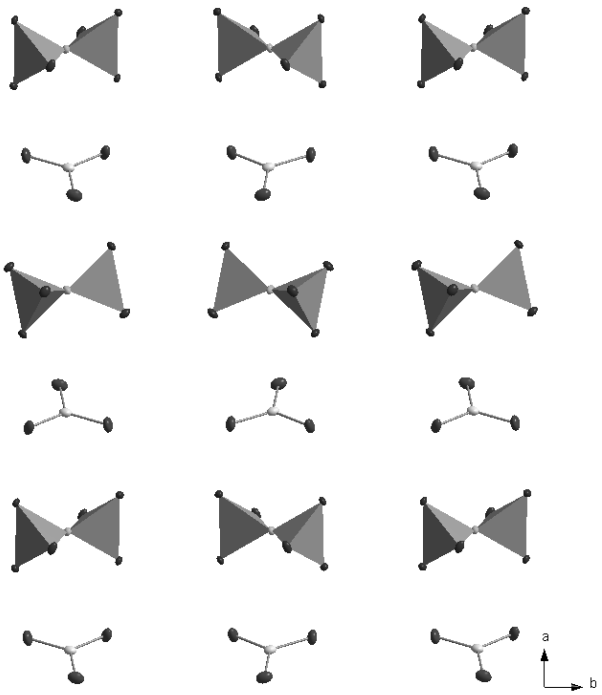
3 Cation-Anion Contacts in $[CI_3]^+[pftb]^-$ 1 and $[CI_3]^+[al\text{-}f\text{-}al]^-$ 2 and packing Diagram of 2



S_Figure 2: Cation-anion contacts in $[CI_3]^+[pftb]^-$ 1

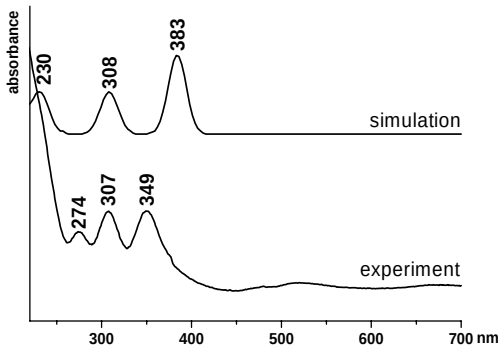


S_Figure 3: Cation-anion contacts in $[CI_3]^+[al\text{-}f\text{-}al]^-$ 2



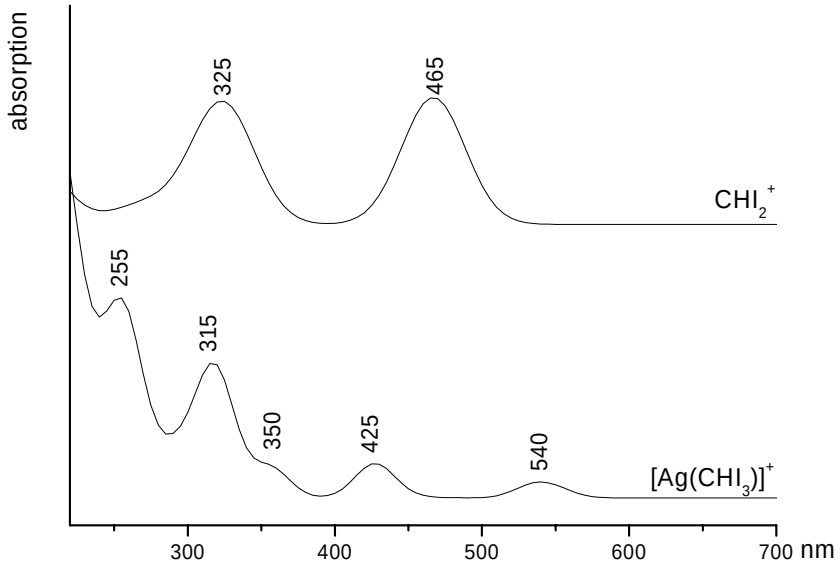
S_Figure 4: Packing diagram of **2**.View along the crystallographic *c* axis. All C and F atoms (except the bridging F's) have been omitted for clarity. The $[al\text{-}f\text{-}al]^-$ anions are drawn as Al_2O_6F polyhedra.

4 Simulated UV-Vis-Spectrum and Structure of CI_3^+

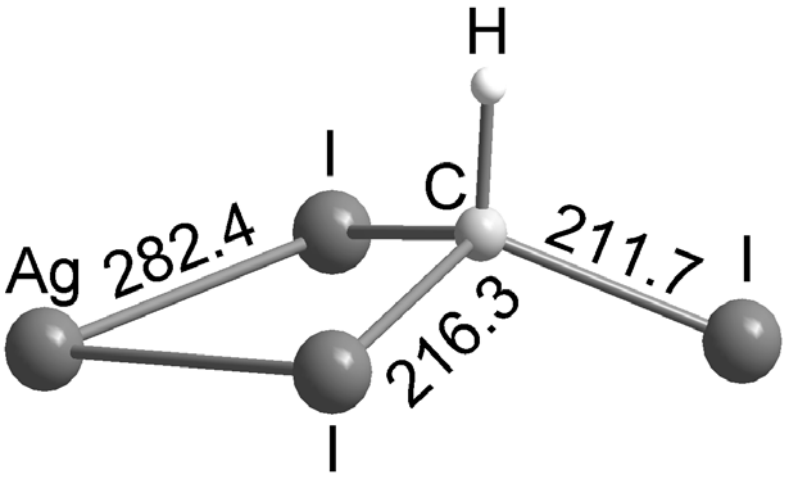


S_Figure 5: UV-VIS spectrum of $[CI_3]^+[pftb]^-$ **1** in Nujol between quartz plates and comparison with the calculated spectrum of the CI_3^+ cation (TD-DFT at the (RI)BP86/SV(P) level).

5 Simulated UV-Vis-Spectrum and Structure of $[Ag(CHI_3)]^+$



S_Figure 6: Simulation of the UV-VIS spectra of $[Ag(CHI_3)]^+$ and $[CHI_2]^+$ (TD-DFT at the (RI-)BP86/SV(P) level).



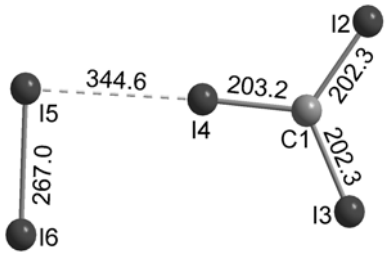
S_Figure 7: C_s symmetric global minimum structure of the $[Ag(CHI_3)]^+$ adduct (MP2/TZVPP). Distances are given in pm.

6 Why are the Bulk Phase and the Solutions of the CI_3^+ Salts 1 and 2 Red-Brown?

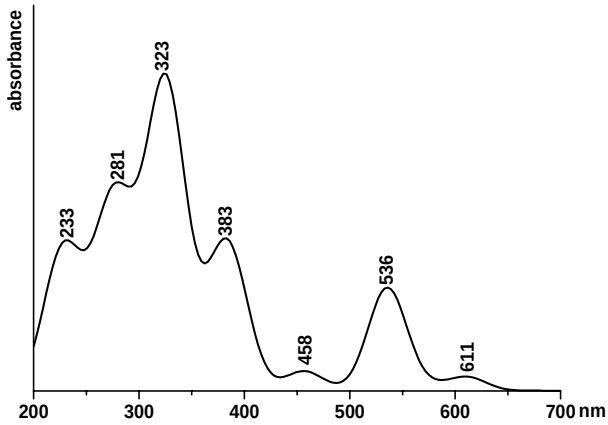
While the single crystals of **1** and **2** are orange-yellow, the colors of the bulk phase of the CI_3^+ salts as well as their solutions in CH_2Cl_2 are red-brown. We assign this to small impurities of I_2 which are – even when the reaction is carried out with the total exclusion of light – probably caused by a partial decomposition of very light sensitive CI_4. These small amounts of I_2 may then form a weak adduct $CI_3^{\cdots}I_2^+$. According to quantum chemical calculations, this complex formation is exergonic by 10 kJ mol^{-1} in the gas phase (MP2/TZVPP) The simulation of the UV-VIS spectrum of this complex by TD-DFT shows absorption maxima up to 611 nm and may be of the reason for the very intense red-brown color (see S_Figure 9).

The minimum geometry (at the MP2/TZVPP level) of that complex is shown in S_Figure 8. This C_s symmetric structure is obtained even when the optimizations were run from very different starting geometries. In this adduct, the C-I bond lengths and the I-C-I bond angles don't change significantly. This indicates – like the structure of the water adduct of the CI_3^+

cation – that the π bonding in CI_3^+ is very strong and remains undisturbed upon complexation with I_2.



S_Figure 8: Calculated geometry of the $[CI_3^{\cdots}I_2]^+$ adduct (MP2/TZVPP). Distances are given in pm. <(I-C-I) = 119.6 – 120.3° (Σ: 360.0°).



S_Figure 9: Simulated UV-VIS spectrum of the $[CI_3^{\cdots}I_2]^+$ adduct (TD-DFT at the (RI)BP86/SV(P) level).

7 Calculated Structures

If not mentioned otherwise, the calculations were performed with the program package TURBOMOLE with the following methods:

- *geometry optimization:* MP2/TZVPP
- *vibrational frequencies:* (RI-)BP86/SV(P)
- *solvation energies:* COSMO model included in TURBOMOLE with ε = 8.93 (for some compounds also with ε = 14.95)
- *thermal contributions to H and G:* module FreeH included in TURBOMOLE
- *electronic excitations:* time-dependent DFT (BP86/SV(P) with MP2/TZVPP geometry)

For some compounds, also ccsd(t) calculations (full geometry optimization) with the aug-cc-pVTZ basis set have been performed with the program package Gaussian03.

For large molecules (e.g. $[X_3C\text{-}(OC(CF_3)_3)]$), the geometry optimizations were only performed at the (RI)BP86/SV(P) level.

For each calculated structure, the following information is given:

- symmetry
- xyz coordinates
- selected distances and angles
- SCF+MP2 energy U
- ZPE
- vibrational frequencies (symmetry, energy , IR intensity , Raman/IR active)
- thermal contributions to $H°$ and $G°$ (for some compounds also H^{195} and G^{195})
- cosmo solvation energy (if not otherwise mentioned with ε = 8.93)

For some compounds, also the following additional information is given:

- electronic excitations
- geometry at the ccsd(t)/aug-ccpVTZ level
- energy at the ccsd(t)/aug-cc-pVTZ level

CF_3^+

sy d3h

c1	0.0000	0.0000	0.0000
f2	0.6163	-1.0674	0.0000
f3	0.6163	1.0674	0.0000

dist 1 c -- 2 f = 2.3292 au = 123.26 pm
dist 1 c -- 3 f = 2.3292 au = 123.26 pm
dist 1 c -- 4 f = 2.3292 au = 123.26 pm

cycle = 6 MP2 energy = -336.8328423407 |dE/dxyz| = 0.000001

zero point VIBRATIONAL energy : 0.0141494 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'	573.35	11.44620	YES	YES
8	e'	573.35	11.44620	YES	YES
9	a2"	765.97	55.73996	YES	NO
10	a1'	1018.80	0.00000	NO	YES
11	e'	1639.69	423.91369	YES	YES
12	e'	1639.69	423.91369	YES	YES

$cosmo_energy
Total energy [a.u.] = -337.0998972373
Total energy + OC corr. [a.u.] = -337.0997320135
Total energy corrected [a.u.] = -337.0998146254 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.1002874126
Diel. energy + OC corr. [a.u.] = -0.1001221887

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	16.95	8.59	0.16	-26.57	45.84	0.25120

Electronic excitation spectrum of , IRREP e'
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.11542631981043E+03 0.25206017438767E+00
0.86478801983258E+02 0.18961608575117E+00
0.68505421260548E+02 0.28119225719507E-02
0.66942965873727E+02 0.18867939566412E+00
0.59550444720775E+02 0.69706849896888E+00
0.56099260189822E+02 0.19186696586566E-01
0.54508803796923E+02 0.27490871567796E-01
0.52983713586697E+02 0.33626391976529E-01
0.52342839367720E+02 0.28909235451824E+00
0.50860973015580E+02 0.54282138059812E+00
Electronic excitation spectrum of , IRREP a2"
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.79404652420443E+02 0.32645244780525E-01

0.68577924345742E+02	0.24906332524596E+00
0.63975386127214E+02	0.10607890504736E+00
0.51509341541807E+02	0.15721544657896E+00
0.49234342915521E+02	0.15603673204796E+00
0.42503138811267E+02	0.39270394525084E-04
0.37436164635993E+02	0.18190838235544E-02
0.31197970907705E+02	0.62152919778170E-01
0.30271566129454E+02	0.39683011490834E-01
0.28606333664534E+02	0.31567363545941E-02

CCl_3^+

sy d3h

c1	0.0000	0.0000	0.0000
cl2	0.8221	-1.4240	0.0000
cl3	0.8221	1.4240	0.0000
cl4	-1.6443	0.0000	0.0000

dist 1 c -- 2 cl = 3.1072 au = 164.43 pm
dist 1 c -- 3 cl = 3.1072 au = 164.43 pm
dist 1 c -- 4 cl = 3.1072 au = 164.43 pm

cycle = 6 MP2 energy = -1416.7678289705 |dE/dxyz| = 0.000001

zero point VIBRATIONAL energy : 0.0083435 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'	303.71	0.33927	YES	YES
8	e'	303.71	0.33927	YES	YES
9	a2"	506.41	0.01578	YES	NO
10	a1'	527.30	0.00000	NO	YES
11	e'	1010.63	254.34729	YES	YES
12	e'	1010.63	254.34729	YES	YES

$cosmo_energy
Total energy [a.u.] = -1418.1229137643
Total energy + OC corr. [a.u.] = -1418.1218688035
Total energy corrected [a.u.] = -1418.1223912839 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0791565674
Diel. energy + OC corr. [a.u.] = -0.0781116066

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	17.76	10.40	0.71	-49.67	32.82	0.28500

Electronic excitation spectrum of , IRREP e'
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.22426354473064E+03 0.27674325533644E+00
0.15097474992901E+03 0.27967466351121E-01
0.13300798826325E+03 0.14080202517113E+00
0.11688770539069E+03 0.38438972770715E+00
0.95698203468527E+02 0.74897407832256E+00
0.83551152086081E+02 0.10222332105612E+01
0.79140507951977E+02 0.33876248831685E+00
0.72757141640941E+02 0.23756001107741E+00
0.70739201080038E+02 0.13354457213772E+01
0.67891541626385E+02 0.84665442273564E+00
Electronic excitation spectrum of , IRREP a2"
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.12308117620135E+03	0.76676531052918E-03
0.11075329764090E+03	0.31371947387937E-02
0.10271449675769E+03	0.91993704322542E-01
0.69373263842230E+02	0.37343868571760E-01
0.65511223950623E+02	0.55062285260542E+00
0.57561065673931E+02	0.28144760449491E-03
0.54317509803551E+02	0.70577886824530E+00
0.50530059229657E+02	0.32153116933269E-02
0.49546206807203E+02	0.20711302123183E-01
0.47377313887954E+02	0.87656734708921E-02

CBr_3^+

sy d3h

c1	0.0000	0.0000	0.0000
br2	0.9038	-1.5654	0.0000
br3	0.9038	1.5654	0.0000
br4	-1.8076	0.0000	0.0000

dist 1 c -- 2 br = 3.4159 au = 180.76 pm
dist 1 c -- 3 br = 3.4159 au = 180.76 pm
dist 1 c -- 4 br = 3.4159 au = 180.76 pm

cycle = 6 MP2 energy = -7755.4100519866 |dE/dxyz| = 0.000000

zero point VIBRATIONAL energy : 0.0063991 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'	177.19	0.02562	YES	YES
8	e'	177.19	0.02562	YES	YES
9	a1'	311.96	0.00000	NO	YES
10	a2''	423.23	3.11996	YES	NO
11	e'	859.66	204.06237	YES	YES
12	e'	859.66	204.06237	YES	YES

$cosmo_energy
Total energy [a.u.] = -7760.2081369589
Total energy + OC corr. [a.u.] = -7760.2062330861
Total energy corrected [a.u.] = -7760.2071850225 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0739831918
Diel. energy + OC corr. [a.u.] = -0.0720793190

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	18.90	11.89	1.53	-63.31	29.52	0.31969

Electronic excitation spectrum of , IRREP e'
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.28419156457596E+03 0.24542553140321E+00
0.20511758834781E+03 0.48268946647018E-01
0.17279559999464E+03 0.13145534162703E+00
0.14916113384580E+03 0.32860094181449E+00
0.11689104990411E+03 0.81736337013470E+00
0.99115848045083E+02 0.10107843659905E+01
0.89580036832981E+02 0.50535712103672E+00
0.82971207030612E+02 0.15421158059817E+01
0.79918779508294E+02 0.30708185854579E+00
0.78385721704828E+02 0.63095914105177E+00
Electronic excitation spectrum of , IRREP a2''
singlet excitations
excitation energy / nm oscillator strength (length rep.)

0.15567952530675E+03	0.25246891818049E-02
0.14193862465522E+03	0.10940129883926E-02
0.10933814258315E+03	0.62603796820695E-01
0.79658660060289E+02	0.16673868132751E+00
0.75253307573883E+02	0.24622369246396E+00
0.70156228619201E+02	0.52114800061894E+00
0.65696602113046E+02	0.32189043363368E-02
0.64069374204663E+02	0.54896391737787E-02
0.62476414915451E+02	0.20100251657358E-02
0.61135229740131E+02	0.27961102785661E-01

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

cycle = 6 SCF+MP2 energy = -71.6583023915 |dE/dxyz| = 0.000001

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

$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

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

Electronic excitation spectrum of , IRREP e'
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.36754756123929E+03 0.24294269495609E+00
0.28447102614405E+03 0.90892197888509E-01
0.22253619224481E+03 0.12013502395032E+00
0.18872164139925E+03 0.23760073079781E+00
0.14568993400956E+03 0.10059054616585E+01
0.11899443098126E+03 0.11344160751817E+01
0.11311206814779E+03 0.43986943309269E-01
0.10459194493027E+03 0.22681481580827E+00
0.10329937640020E+03 0.97213368041639E-03
0.98096447809240E+02 0.13602492221936E+00
Electronic excitation spectrum of , IRREP a2''
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.19551235506096E+03 0.29889174577910E-05

0.18272590582800E+03	0.58380295223589E-02
0.12006985380151E+03	0.68841741309905E-01
0.10563075537468E+03	0.84182402847080E-01
0.93884237755357E+02	0.26958927641256E-01
0.93097963772805E+02	0.71854816026418E-01
0.84633316829274E+02	0.85100243220830E-02
0.80119107806206E+02	0.38478338353259E-01
0.79220151528974E+02	0.26722597102762E-01
0.74523956099446E+02	0.41529774654953E-01

HCF_2^+

sy c2v

c1	0.0000	0.0000	0.4488
f2	1.0562	0.0000	-0.1827
f3	-1.0562	0.0000	-0.1827
h4	0.0000	0.0000	1.5392

dist 1 c -- 4 h = 2.0605 au = 109.04 pm
dist 1 c -- 2 f = 2.3255 au = 123.06 pm
dist 1 c -- 3 f = 2.3255 au = 123.06 pm
bend 2 f -> 1 c <- 3 f = 118.25 deg
bend 4 h -> 1 c <- 2 f = 120.88 deg

cycle = 4 MP2 energy = -237.6976481767 |dE/dxyz| = 0.000411

zero point VIBRATIONAL energy : 0.0205339 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	a1	651.80	30.77510	YES	YES
8	b2	1026.72	0.33686	YES	YES
9	b1	1270.07	53.07972	YES	YES
10	a1	1351.95	120.65855	YES	YES
11	b1	1624.39	326.31756	YES	YES
12	a1	3088.44	31.61000	YES	YES

$cosmo_energy
Total energy [a.u.] = -237.9312797819
Total energy + OC corr. [a.u.] = -237.9310444417
Total energy corrected [a.u.] = -237.9311621118 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.1034819515
Diel. energy + OC corr. [a.u.] = -0.1032466112

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	16.50	8.40	0.06	-7.97	61.85	0.24248

Electronic excitation spectrum of , IRREP a1
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.10098242499114E+03 0.45900250560302E-01
0.88784767387118E+02 0.18737438253393E+00
0.79535004152180E+02 0.22132862417971E-01
0.76049684465250E+02 0.72438946644045E-01
0.66932029608682E+02 0.14775543777001E+00
0.61362383350630E+02 0.65496084851274E-01
0.60372012857534E+02 0.17060099316935E+00
0.58452362309928E+02 0.12749080231332E+00
0.56570912884366E+02 0.16202312511993E-02
0.54709595139088E+02 0.54779139984199E-02

Electronic excitation spectrum of , IRREP b1
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.12409938968803E+03 0.11675702417606E+00
 0.88713595088943E+02 0.48060656314816E-02
 0.78160801301066E+02 0.17807937114106E-03
 0.72807623997621E+02 0.27926460813456E+00
 0.66280497718097E+02 0.28390300831952E+00
 0.61103940605458E+02 0.61808192680041E-01
 0.59881192285602E+02 0.25367118237054E+00
 0.56952052809153E+02 0.72449938262719E-01
 0.53650168800622E+02 0.69014323924484E-03
 0.53149681807300E+02 0.20572931108840E-01
Electronic excitation spectrum of , IRREP b2
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.17181100653354E+03 0.58009413792111E-02
 0.10444199472543E+03 0.34863264425676E-02
 0.82275359616477E+02 0.80515310031578E-01
 0.74060323449538E+02 0.18238206515247E-02
 0.70888723805235E+02 0.10647102591380E+00
 0.64986534108027E+02 0.18693396421227E+00
 0.55974058443430E+02 0.59414503266783E-01
 0.50792575531400E+02 0.25560406125848E-02
 0.50142771542639E+02 0.19920324849645E+00
 0.46314725206426E+02 0.58829410558066E-01

$HCCl_2^+$

sy c2v

c1	0.0000	0.0000	0.6306
cl2	1.4286	0.0000	-0.1312
cl3	-1.4286	0.0000	-0.1312
h4	0.0000	0.0000	1.7176

dist 1 c -- 4 h = 2.0541 au = 108.70 pm
dist 1 c -- 2 cl = 3.0596 au = 161.91 pm
dist 1 c -- 3 cl = 3.0596 au = 161.91 pm
bend 2 cl -> 1 c <- 3 cl = 123.86 deg
bend 4 h -> 1 c <- 2 cl = 118.07 deg

cycle = 5 MP2 energy = -957.6549965965 |dE/dxyz| = 0.000005

zero point VIBRATIONAL energy : 0.0169182 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	a1	349.87	1.82881	YES	YES
8	a1	825.80	19.64840	YES	YES
9	b2	850.61	19.34551	YES	YES
10	b1	1044.23	252.81509	YES	YES
11	b1	1281.80	36.30619	YES	YES
12	a1	3073.93	37.34115	YES	YES

$cosmo_energy
Total energy [a.u.] = -958.6133613506
Total energy + OC corr. [a.u.] = -958.6123639361
Total energy corrected [a.u.] = -958.6128626434 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0866627904
Diel. energy + OC corr. [a.u.] = -0.0856653758

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	17.25	9.80	0.25	-23.24	53.27	0.26495

Electronic excitation spectrum of , IRREP a1
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.16009858121530E+03 0.38757270569608E-01
0.14884344530910E+03 0.32759549733470E-02
0.12224587348747E+03 0.78967243807998E-03
0.10944112924054E+03 0.58842072863596E-01
0.93974919590068E+02 0.40546305377216E-01
0.81124030844127E+02 0.18567876932172E+00
0.77658176485781E+02 0.83525140781679E-01
0.77073038917918E+02 0.17552048425816E+00
0.72399786414850E+02 0.24240615220249E+00
0.69461526307798E+02 0.75481477614780E-01
Electronic excitation spectrum of , IRREP b1

singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.22047342942286E+03   0.16837339931794E+00
 0.14509601063336E+03   0.89281732946176E-01
 0.11892897689896E+03   0.82300083219375E-01
 0.11070792166754E+03   0.11014572472929E+00
 0.91185498006207E+02   0.79871364759965E+00
 0.82115500936828E+02   0.45649676821798E+00
 0.79767079866614E+02   0.11261905125580E+00
 0.77163441366589E+02   0.51755216859656E+00
 0.71863319727511E+02   0.15020670595073E+00
 0.67157252623766E+02   0.12985884918397E-01
Electronic excitation spectrum of , IRREP b2
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.32373423628597E+03   0.25552795165112E-04
 0.14582295032246E+03   0.12414978909065E-02
 0.11780138393999E+03   0.16993737921476E-03
 0.11198426997567E+03   0.24482729317753E-03
 0.98779514021347E+02   0.11483157673744E+00
 0.90250154409387E+02   0.14552949838828E-02
 0.70404864981305E+02   0.40342671544745E-01
 0.65361386723443E+02   0.47244676393715E+00
 0.62034898375692E+02   0.32923331206072E-02
 0.60722179553695E+02   0.14304364265444E-01

$HCBr_2^+$

sy c2v

c1	0.0000	0.0000	0.7488
br2	1.5757	0.0000	-0.0678
br3	-1.5757	0.0000	-0.0678
h4	0.0000	0.0000	1.8349

dist 1 c -- 4 h = 2.0524 au = 108.61 pm
dist 1 c -- 2 br = 3.3537 au = 177.47 pm
dist 1 c -- 3 br = 3.3537 au = 177.47 pm
bend 2 br -> 1 c <- 3 br = 125.21 deg
bend 4 h -> 1 c <- 2 br = 117.40 deg

cycle = 5 MP2 energy = -5183.4162797739 |dE/dxyz| = 0.000005

zero point VIBRATIONAL energy : 0.0156229 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	a1	212.72	0.25914	YES	YES
8	a1	657.77	8.24229	YES	YES
9	b2	777.88	34.15309	YES	YES
10	b1	900.16	224.03128	YES	YES
11	b1	1224.82	29.75887	YES	YES
12	a1	3084.29	43.37211	YES	YES

$cosmo_energy
Total energy [a.u.] = -5186.6702456893
Total energy + OC corr. [a.u.] = -5186.6685582045
Total energy corrected [a.u.] = -5186.6694019469 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0817024891
Diel. energy + OC corr. [a.u.] = -0.0800150043

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	18.33	10.88	0.53	-32.70	50.62	0.28779

Electronic excitation spectrum of , IRREP a1
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.19450487187573E+03 0.19930696494750E-02
0.18869302184793E+03 0.28207216978759E-01
0.15249045499067E+03 0.67783521424367E-05
0.11961938855218E+03 0.20136024157092E-01
0.11018127613934E+03 0.30470034881674E-01
0.92260473171487E+02 0.17591041372404E+00
0.86270449942286E+02 0.14671373272397E+00
0.83978588792132E+02 0.80436235373857E-01
0.79330185920878E+02 0.42370977112391E+00
0.77711748672913E+02 0.45090022550532E-01
Electronic excitation spectrum of , IRREP b1

singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.27264362455317E+03 0.15727776363396E+00
 0.19111712957849E+03 0.11748048927865E+00
 0.14648772272480E+03 0.10696517965104E+00
 0.12292018504497E+03 0.18129821890092E-01
 0.10878078513086E+03 0.96541995182777E+00
 0.94401052856737E+02 0.61899037238923E+00
 0.87328199664797E+02 0.30384466569080E+00
 0.86017237550665E+02 0.28860867940791E+00
 0.79260561849908E+02 0.30476643528067E-01
 0.74414395755383E+02 0.17172660134573E+00
Electronic excitation spectrum of , IRREP b2
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.40606195111276E+03 0.35745378189849E-04
 0.16167084800045E+03 0.23480860768163E-02
 0.14660691291067E+03 0.65822299428769E-03
 0.13998438341422E+03 0.19847163184528E-02
 0.10288177009952E+03 0.79921917453832E-01
 0.98633377137928E+02 0.11711243254191E-03
 0.77858859017313E+02 0.97264378743960E-01
 0.73916000950284E+02 0.38361667505648E+00
 0.68340071328740E+02 0.21178405903381E+00
 0.67319494338003E+02 0.21780518024798E-03

HCI_2^+

sy c2v

c1	0.0000	0.0000	0.8242
i2	1.7731	0.0000	-0.0466
i3	-1.7731	0.0000	-0.0466
h4	0.0000	0.0000	1.9094

dist 1 c -- 4 h = 2.0508 au = 108.52 pm
dist 1 c -- 2 i = 3.7329 au = 197.54 pm
dist 1 c -- 3 i = 3.7329 au = 197.54 pm
bend 2 i -> 1 c <- 3 i = 127.69 deg
bend 4 h -> 1 c <- 2 i = 116.15 deg

cycle = 7 MP2 energy = -60.9166094103 |dE/dxyz| = 0.000006

zero point VIBRATIONAL energy : 0.0145064 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	a1	143.19	0.00007	YES	YES
8	a1	525.94	1.50250	YES	YES
9	b2	685.87	44.75587	YES	YES
10	b1	775.77	197.19009	YES	YES
11	b1	1148.37	38.10927	YES	YES
12	a1	3088.42	40.78640	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	18.98	11.67	0.84	-39.98	48.37	0.30464

$cosmo_energy
Total energy [a.u.] = -61.3148414086
Total energy + OC corr. [a.u.] = -61.3124573593
Total energy corrected [a.u.] = -61.3136493839 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0770750017
Diel. energy + OC corr. [a.u.] = -0.0746909524

Electronic excitation spectrum of , IRREP a1
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.26313573567198E+03 0.31915538280418E-03
0.22976336512909E+03 0.22824950048261E-01
0.19081372011541E+03 0.29355325320501E-03
0.13231171202796E+03 0.57911322464131E-03
0.12954860978548E+03 0.43620716622776E-01
0.10636276120765E+03 0.23504226362090E+00
0.10085315970538E+03 0.25049904228808E-01
0.96658271789794E+02 0.16752339475011E-01
0.95325472382040E+02 0.26134706271742E-01
0.93997510638964E+02 0.35196235614634E-04
Electronic excitation spectrum of , IRREP b1
singlet excitations

excitation energy / nm oscillator strength (length rep.)
0.34810714954161E+03 0.15050086116768E+00
0.26198252749705E+03 0.14484131491710E+00
0.18307393824732E+03 0.77116375427643E-01
0.13833302853253E+03 0.45924446687839E+00
0.13226700847335E+03 0.64149037917222E+00
0.11054708987603E+03 0.49925728972383E+00
0.99518152390670E+02 0.43828194593306E-01
0.99312773031949E+02 0.33540279995575E-01
0.98549314567022E+02 0.27085909478002E-01
0.94929168024781E+02 0.22024315356480E-01
Electronic excitation spectrum of , IRREP b2
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.53658435561031E+03 0.95302491522067E-04
0.18935715517663E+03 0.35100292304532E-02
0.18217134619922E+03 0.30603994035206E-02
0.17643152156145E+03 0.44943083868648E-02
0.11111360560976E+03 0.46935710162356E-01
0.10775583592186E+03 0.27915918388375E-01
0.10172471312252E+03 0.57363480835947E-02
0.97820750390988E+02 0.39231572038472E-01
0.95178623655398E+02 0.12209215532499E-01
0.91176218382988E+02 0.60786363826279E-02

H_2CF^+

sy c2v

c1	0.0000	0.0000	-0.0600
h2	0.9699	0.0000	-0.5557
h3	-0.9699	0.0000	-0.5557
f4	0.0000	0.0000	1.1692

dist 1 c -- 2 h = 2.0583 au = 108.92 pm
dist 1 c -- 3 h = 2.0583 au = 108.92 pm
dist 1 c -- 4 f = 2.3229 au = 122.92 pm
bend 2 h -> 1 c <- 4 f = 117.07 deg
bend 2 h -> 1 c <- 3 h = 125.86 deg

cycle = 6 MP2 energy = -138.5406528653 |dE/dxyz| = 0.000021

zero point VIBRATIONAL energy : 0.0262941 Hartree

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity 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	1209.88	15.19002	YES	YES
8	b2	1224.07	3.70034	YES	YES
9	a1	1402.39	102.00039	YES	YES
10	a1	1574.58	68.41637	YES	YES
11	a1	2985.50	6.15364	YES	YES
12	b1	3145.34	48.04940	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	15.85	6.73	0.01	13.05	76.58	0.22141

$cosmo_energy
Total energy [a.u.] = -138.7382729544
Total energy + OC corr. [a.u.] = -138.7378590251
Total energy corrected [a.u.] = -138.7380659898 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.1048640899
Diel. energy + OC corr. [a.u.] = -0.1044501606

Electronic excitation spectrum of , IRREP a1
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.11301919827636E+03 0.10762098660626E+00
0.84104025182973E+02 0.13710838988683E+00
0.70224669422278E+02 0.78692685093387E-01
0.65275388833018E+02 0.56073858081439E+00
0.63795512973945E+02 0.48676217625041E-02
0.57620904527477E+02 0.57134357249950E-04
0.56169818138365E+02 0.80344536158332E-02
0.49106896862726E+02 0.11489854771917E+00
0.48902670669039E+02 0.71889641966393E-01
0.48773490588902E+02 0.15533273061804E+00
Electronic excitation spectrum of , IRREP b1

singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.96513853210152E+02 0.21545083006866E+00
 0.92662794208035E+02 0.41418396528000E-02
 0.71521836171386E+02 0.19206735372200E+00
 0.68217529270712E+02 0.83626350965511E-01
 0.65576142026895E+02 0.18738366362423E+00
 0.58732978397281E+02 0.18514563968856E+00
 0.55721657312842E+02 0.91351839742591E-03
 0.54378340855507E+02 0.20288793305884E-01
 0.48626338904200E+02 0.40306505681117E-02
 0.46758265986749E+02 0.34468201700541E-02
Electronic excitation spectrum of , IRREP b2
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.12375351706302E+03 0.15346064107094E-01
 0.84750193373370E+02 0.15583778674888E+00
 0.75836077158314E+02 0.29288754175302E-02
 0.71263166014930E+02 0.12186716371617E+00
 0.50994141418498E+02 0.19295054546316E+00
 0.47888405207849E+02 0.43890206847436E-01
 0.47416785179285E+02 0.76782785399332E-01
 0.42072394677209E+02 0.89829791906128E-02
 0.41639709897241E+02 0.18600197160194E-01
 0.41232781452215E+02 0.81140561307670E-02

H_2CCl^+

sy c2v

c1	0.0000	0.0000	-0.1305
h2	0.9482	0.0000	-0.6593
h3	-0.9482	0.0000	-0.6593
cl4	0.0000	0.0000	1.4555

dist 1 c -- 2 h = 2.0517 au = 108.57 pm
dist 1 c -- 3 h = 2.0517 au = 108.57 pm
dist 1 c -- 4 cl = 2.9970 au = 158.59 pm
dist 2 h -- 3 h = 3.5838 au = 189.65 pm
bend 2 h -> 1 c <- 3 h = 121.71 deg
bend 2 h -> 1 c <- 4 cl = 119.15 deg

cycle = 6 MP2 energy = -498.5294537764 |dE/dxyz| = 0.000010

zero point VIBRATIONAL energy : 0.0243892 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	b1	1015.25	0.18998	YES	YES
8	a1	1027.13	80.87827	YES	YES
9	b2	1086.99	27.66850	YES	YES
10	a1	1418.11	0.11826	YES	YES
11	a1	3010.87	21.90029	YES	YES
12	b1	3147.26	59.77072	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	16.46	7.38	0.02	4.89	71.73	0.23251

$cosmo_energy
Total energy [a.u.] = -499.0874812168
Total energy + OC corr. [a.u.] = -499.0865830728
Total energy corrected [a.u.] = -499.0870321448 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0949437693
Diel. energy + OC corr. [a.u.] = -0.0940456253

Electronic excitation spectrum of , IRREP a1
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.17071091975709E+03 0.15324125504287E+00
0.10316399623153E+03 0.99226804688307E-01
0.84676004303693E+02 0.66892648334075E+00
0.77221379923945E+02 0.47728840649026E+00
0.73484799640962E+02 0.29787976755070E-01
0.66181591253775E+02 0.14175100461936E-02
0.60836643241284E+02 0.39252774919010E+00
0.60032023577994E+02 0.22635888174389E+00
0.57241393388355E+02 0.46597825531037E+00
0.54679212752333E+02 0.20630387067373E-02

Electronic excitation spectrum of , IRREP b1
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.13008835388171E+03 0.24410258373716E-02
 0.11125974137412E+03 0.26694175764163E-01
 0.89832659629209E+02 0.19215679449398E-01
 0.78917735514641E+02 0.67026015391961E-01
 0.76955672544104E+02 0.17062473602797E-01
 0.75094660745841E+02 0.54427898682121E+00
 0.63880830206665E+02 0.84752076250373E-01
 0.60244278950632E+02 0.90346797269267E-01
 0.59589838183005E+02 0.29916054064159E-01
 0.53881697630073E+02 0.22444952587539E+00
Electronic excitation spectrum of , IRREP b2
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.16430923139898E+03 0.29007173390318E-04
 0.10570274700837E+03 0.21118865160317E-02
 0.95253944686959E+02 0.12929487606898E+00
 0.91818659090323E+02 0.21823881320666E-01
 0.66076997340788E+02 0.32216509462046E+00
 0.63516616466285E+02 0.84044921369353E-02
 0.57702816451032E+02 0.21765006633942E+00
 0.51386899843366E+02 0.23569936080325E-01
 0.49468741322025E+02 0.20338773145726E-01
 0.46723050697168E+02 0.27863745119300E-06

H_2CBr^+

sy c2v

c1	0.0000	0.0000	-1.4635
h2	0.9461	0.0000	-1.9935
h3	-0.9461	0.0000	-1.9935
br4	0.0000	0.0000	0.2703

dist 1 c -- 2 h = 2.0493 au = 108.44 pm
dist 1 c -- 3 h = 2.0493 au = 108.44 pm
dist 1 c -- 4 br = 3.2763 au = 173.38 pm
bend 2 h -> 1 c <- 3 h = 121.49 deg
bend 2 h -> 1 c <- 4 br = 119.26 deg

cycle = 5 MP2 energy = -2611.4112860208 |dE/dxyz| = 0.000060

zero point VIBRATIONAL energy : 0.0237067 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	a1	854.32	61.94317	YES	YES
8	b1	945.92	1.63871	YES	YES
9	b2	1031.84	38.52486	YES	YES
10	a1	1390.33	0.04375	YES	YES
11	a1	3023.18	30.80922	YES	YES
12	b1	3160.46	62.69936	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	17.42	7.71	0.03	-0.12	70.07	0.24374

$cosmo_energy
Total energy [a.u.] = -2613.1169218942
Total energy + OC corr. [a.u.] = -2613.1155450196
Total energy corrected [a.u.] = -2613.1162334569 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0912898162
Diel. energy + OC corr. [a.u.] = -0.0899129416

Electronic excitation spectrum of , IRREP a1
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.20007263787298E+03 0.14386125237887E+00
0.11086944067541E+03 0.46758447985254E-01
0.94470134986906E+02 0.10205088548450E+01
0.82867048185283E+02 0.17652184719490E+00
0.76666963231655E+02 0.91134793235694E-01
0.71992002827120E+02 0.17290247355745E+00
0.66529385496918E+02 0.92765788929351E+00
0.63737785300511E+02 0.10441541616291E+00
0.61201834900885E+02 0.36391898445580E-01
0.58265098604012E+02 0.16824017926722E+00
Electronic excitation spectrum of , IRREP b1

singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.16040971997330E+03 0.28001774878016E-04
 0.11911544708698E+03 0.66986079582108E-02
 0.10202654575303E+03 0.13504219263192E-01
 0.83227886205361E+02 0.56376011868012E-01
 0.82215908610349E+02 0.14756479934100E-01
 0.78501088307798E+02 0.70063392540666E+00
 0.68014178493183E+02 0.48335042040167E-01
 0.64103472022919E+02 0.92694601864424E-03
 0.62623005118968E+02 0.16112310695320E+00
 0.60590406711855E+02 0.45118013017822E-01
Electronic excitation spectrum of , IRREP b2
singlet excitations
excitation energy / nm oscillator strength (length rep.)
 0.18342243429612E+03 0.82594740362097E-03
 0.12931997733258E+03 0.22093795357767E-02
 0.10140866429415E+03 0.32414559443632E-01
 0.95886193038288E+02 0.79795297658898E-01
 0.72706334801244E+02 0.37651418582407E+00
 0.69122438212433E+02 0.68692303321941E-01
 0.62098016895353E+02 0.79825886031451E-01
 0.60458957080099E+02 0.60518061725239E-01
 0.56896399486292E+02 0.12993226008206E+00
 0.54702720897929E+02 0.28305961838873E-01

H_2ClI^+

sy c2v

c1	0.0000	0.0000	-1.7246
h2	0.9418	0.0000	-2.2595
h3	-0.9418	0.0000	-2.2595
i4	0.0000	0.0000	0.1991

dist 1 c -- 2 h = 2.0468 au = 108.31 pm
dist 1 c -- 3 h = 2.0468 au = 108.31 pm
dist 1 c -- 4 i = 3.6354 au = 192.38 pm
bend 2 h -> 1 c <- 3 h = 120.82 deg
bend 4 i -> 1 c <- 2 h = 119.59 deg

cycle = 6 MP2 energy = -50.1638472978 |dE/dxyz| = 0.000002

zero point VIBRATIONAL energy : 0.0230411 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	a1	725.96	42.35610	YES	YES
8	b1	859.97	5.01476	YES	YES
9	b2	961.74	46.89029	YES	YES
10	a1	1358.68	0.00646	YES	YES
11	a1	3034.20	39.27801	YES	YES
12	b1	3173.33	58.84867	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	18.03	7.97	0.06	-4.09	68.50	0.25178

$cosmo_energy
Total energy [a.u.] = -50.4405132496
Total energy + OC corr. [a.u.] = -50.4387720285
Total energy corrected [a.u.] = -50.4396426391 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0872265500
Diel. energy + OC corr. [a.u.] = -0.0854853289

Electronic excitation spectrum of , IRREP a1
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.24044731499278E+03 0.13563911765616E+00
0.12093636925273E+03 0.10723184242647E-01
0.10927720903030E+03 0.10602113484458E+01
0.89735966601599E+02 0.10665148513388E-03
0.88976019392509E+02 0.33528076327119E-01
0.83921552307889E+02 0.20025419107675E-01
0.81760863908283E+02 0.59727511736455E-02
0.78423418109986E+02 0.65990218989542E+00
0.73282808966439E+02 0.63670270855979E-01
0.69451618979224E+02 0.21938491735372E+00
Electronic excitation spectrum of , IRREP b1
singlet excitations

excitation energy / nm oscillator strength (length rep.)
0.20293574106344E+03 0.64982952029436E-03
0.12690729553535E+03 0.26554209294677E-02
0.11456473382300E+03 0.16742143456419E-01
0.94159919947522E+02 0.17785256492551E-01
0.87522058085087E+02 0.30287022792121E-01
0.81596331595839E+02 0.40700850766147E+00
0.73221052868717E+02 0.49861931962605E-01
0.71254714237654E+02 0.15369750132965E-03
0.68426581567730E+02 0.24422332279815E-02
0.67820342012152E+02 0.84319322029956E-02
Electronic excitation spectrum of , IRREP b2
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.21107655381425E+03 0.29174343618579E-02
0.16218775129495E+03 0.67978228349068E-02
0.10969681653223E+03 0.82813875138949E-02
0.10118994354665E+03 0.99108811243624E-01
0.83994405316404E+02 0.11420597510747E-02
0.78144731940829E+02 0.33411666631751E-01
0.74367025016241E+02 0.35899209901087E-01
0.72480256820409E+02 0.20573927912842E-01
0.65799981114065E+02 0.34385792322331E+00
0.62269276633877E+02 0.55545782063178E-02

CF_4

sy td

c1	0.0000	0.0000	0.0000
f2	0.7618	-0.7618	0.7618
f3	-0.7618	0.7618	0.7618
f4	-0.7618	-0.7618	-0.7618
f5	0.7618	0.7618	-0.7618

dist 1 c -- 2 f = 2.4936 au = 131.95 pm
dist 1 c -- 3 f = 2.4936 au = 131.95 pm
dist 1 c -- 4 f = 2.4936 au = 131.95 pm
dist 1 c -- 5 f = 2.4936 au = 131.95 pm
bend 2 f -> 1 c <- 3 f = 109.47 deg

cycle = 5 MP2 energy = -436.9826160663 |dE/dxyz| = 0.000003

zero point VIBRATIONAL energy : 0.0167135 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	420.46	0.00000	NO	YES
8	e	420.46	0.00000	NO	YES
9	t2	608.87	3.46292	YES	YES
10	t2	608.87	3.46292	YES	YES
11	t2	608.87	3.46292	YES	YES
12	a1	886.32	0.00000	NO	YES
13	t2	1260.84	417.75870	YES	YES
14	t2	1260.84	417.75870	YES	YES
15	t2	1260.84	417.75870	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	17.32	8.62	0.47	-21.56	54.31	0.26281

$cosmo_energy
Total energy [a.u.] = -437.1815213334
Total energy + OC corr. [a.u.] = -437.1815187542
Total energy corrected [a.u.] = -437.1815200438 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0006951062
Diel. energy + OC corr. [a.u.] = -0.0006925270

$FCCl_3$

sy c3v

c1	0.0000	0.0000	0.2467
f2	0.0000	0.0000	1.5874
cl3	-0.8354	1.4470	-0.3114
cl4	-0.8354	-1.4470	-0.3114
cl5	1.6708	0.0000	-0.3114

dist 1 c -- 2 f = 2.5337 au = 134.08 pm
dist 1 c -- 3 cl = 3.3289 au = 176.16 pm
dist 1 c -- 4 cl = 3.3289 au = 176.16 pm
dist 1 c -- 5 cl = 3.3289 au = 176.16 pm
bend 2 f -> 1 c <- 3 cl = 108.47 deg
bend 3 cl -> 1 c <- 4 cl = 110.45 deg

cycle = 7 MP2 energy = -1516.8435205207 |dE/dxyz| = 0.000008

zero point VIBRATIONAL energy : 0.0108603 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	231.72	0.00040	YES	YES
8	e	231.72	0.00040	YES	YES
9	a1	336.98	0.00718	YES	YES
10	e	383.43	1.04547	YES	YES
11	e	383.43	1.04547	YES	YES
12	a1	513.64	4.22248	YES	YES
13	e	786.41	287.89054	YES	YES
14	e	786.41	287.89054	YES	YES
15	a1	1113.36	217.32003	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	11.47	1.49	-48.21	42.40	0.31222

$cosmo_energy
Total energy [a.u.] = -1518.1506935326
Total energy + OC corr. [a.u.] = -1518.1506954676
Total energy corrected [a.u.] = -1518.1506945001 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0008567876
Diel. energy + OC corr. [a.u.] = -0.0008587226

$FCBr_3$

sy c3v

c1	0.0000	0.0000	0.4439
f2	0.0000	0.0000	1.7867
br3	-0.9172	1.5886	-0.1638
br4	-0.9172	-1.5886	-0.1638
br5	1.8344	0.0000	-0.1638

dist 1 c -- 2 f = 2.5375 au = 134.28 pm
dist 1 c -- 3 br = 3.6517 au = 193.24 pm
dist 1 c -- 4 br = 3.6517 au = 193.24 pm
dist 1 c -- 5 br = 3.6517 au = 193.24 pm
bend 2 f -> 1 c <- 3 br = 108.33 deg
bend 3 br -> 1 c <- 4 br = 110.59 deg

cycle = 7 MP2 energy = -7855.4732030456 |dE/dxyz| = 0.000002

zero point VIBRATIONAL energy : 0.0089406 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	140.81	0.06678	YES	YES
8	e	140.81	0.06678	YES	YES
9	a1	205.85	0.30743	YES	YES
10	e	292.81	1.95982	YES	YES
11	e	292.81	1.95982	YES	YES
12	a1	384.20	0.83621	YES	YES
13	e	676.36	233.66049	YES	YES
14	e	676.36	233.66049	YES	YES
15	a1	1114.47	175.35614	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	12.80	2.69	-62.03	39.63	0.34929

$cosmo_energy
Total energy [a.u.] = -7860.2283098208
Total energy + OC corr. [a.u.] = -7860.2283396907
Total energy corrected [a.u.] = -7860.2283247558 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0018207997
Diel. energy + OC corr. [a.u.] = -0.0018506696

FCI_3

sy c3v

c1	0.0000	0.0000	0.1301
f2	0.0000	0.0000	1.4842
i3	-1.0259	1.7770	-0.5261
i4	-1.0259	-1.7770	-0.5261
i5	2.0519	0.0000	-0.5261

dist 1 c -- 2 f = 2.5588 au = 135.41 pm
dist 1 c -- 3 i = 4.0710 au = 215.43 pm
dist 1 c -- 4 i = 4.0710 au = 215.43 pm
dist 1 c -- 5 i = 4.0710 au = 215.43 pm
bend 2 f -> 1 c <- 3 i = 107.74 deg
bend 3 i -> 1 c <- 4 i = 111.15 deg

cycle = 8 MP2 energy = -171.6993534941 |dE/dxyz| = 0.000002

zero point VIBRATIONAL energy : 0.0077735 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	93.17	0.13806	YES	YES
8	e	93.17	0.13806	YES	YES
9	a1	137.17	0.53591	YES	YES
10	e	245.42	2.69345	YES	YES
11	e	245.42	2.69345	YES	YES
12	a1	304.75	0.05472	YES	YES
13	e	584.63	220.83955	YES	YES
14	e	584.63	220.83955	YES	YES
15	a1	1123.82	173.84537	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	13.79	3.88	-72.06	38.14	0.37793

$cosmo_energy
Total energy [a.u.] = -172.1885215968
Total energy + OC corr. [a.u.] = -172.1887719343
Total energy corrected [a.u.] = -172.1886467655 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0034594141
Diel. energy + OC corr. [a.u.] = -0.0037097517

CHF_3

sy c3v

c1	0.0000	0.0000	0.0645
h2	0.0000	0.0000	1.1483
f3	0.6250	-1.0826	-0.4011
f4	0.6250	1.0826	-0.4011
f5	-1.2500	0.0000	-0.4011

dist 1 c -- 2 h = 2.0481 au = 108.38 pm
dist 1 c -- 3 f = 2.5207 au = 133.39 pm
dist 1 c -- 4 f = 2.5207 au = 133.39 pm
dist 1 c -- 5 f = 2.5207 au = 133.39 pm
bend 2 h -> 1 c <- 3 f = 110.43 deg
bend 3 f -> 1 c <- 4 f = 108.50 deg

cycle = 5 MP2 energy = -337.8325587108 |dE/dxyz| = 0.000009

zero point VIBRATIONAL energy : 0.0247482 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	494.18	1.98138	YES	YES
8	e	494.18	1.98138	YES	YES
9	a1	685.84	12.22840	YES	YES
10	a1	1123.65	103.40207	YES	YES
11	e	1144.56	247.07514	YES	YES
12	e	1144.56	247.07514	YES	YES
13	e	1372.13	91.99654	YES	YES
14	e	1372.13	91.99654	YES	YES
15	a1	3031.96	59.94921	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	16.98	9.41	0.25	-1.04	74.14	0.26047

$cosmo_energy
Total energy [a.u.] = -337.9971766200
Total energy + OC corr. [a.u.] = -337.9970971600
Total energy corrected [a.u.] = -337.9971368900 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0032895013
Diel. energy + OC corr. [a.u.] = -0.0032100413

$FCHCl_2$

sy cs

c1	0.4239	-0.3719	0.0000
h2	1.5009	-0.4780	0.0000
f3	-0.1486	-1.5923	0.0000
cl4	-0.0533	0.4964	-1.4545
cl5	-0.0533	0.4964	1.4545

dist 1 c -- 2 h = 2.0450 au = 108.22 pm
dist 1 c -- 3 f = 2.5473 au = 134.80 pm
dist 1 c -- 4 cl = 3.3257 au = 175.99 pm
dist 1 c -- 5 cl = 3.3257 au = 175.99 pm
bend 2 h -> 1 c <- 3 f = 109.50 deg
bend 2 h -> 1 c <- 4 cl = 108.56 deg
bend 4 cl -> 1 c <- 5 cl = 111.47 deg
bend 3 f -> 1 c <- 4 cl = 109.36 deg

cycle = 7 MP2 energy = -1057.7461881142 |dE/dxyz| = 0.000012

zero point VIBRATIONAL energy : 0.0209125 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'	261.92	0.21085	YES	YES
8	a''	349.91	0.22072	YES	YES
9	a'	442.45	2.02832	YES	YES
10	a'	710.61	47.69806	YES	YES
11	a''	744.39	251.94739	YES	YES
12	a'	1107.50	200.48786	YES	YES
13	a''	1204.17	52.63279	YES	YES
14	a'	1300.88	21.60960	YES	YES
15	a'	3057.69	9.71917	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	17.55	11.75	0.73	-19.55	65.91	0.29493

$cosmo_energy
Total energy [a.u.] = -1058.6514414539
Total energy + OC corr. [a.u.] = -1058.6514458707
Total energy corrected [a.u.] = -1058.6514436623 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0031175000
Diel. energy + OC corr. [a.u.] = -0.0031219168

$FCHBr_2$

sy cs

c1	0.4482	-0.6856	0.0000
h2	1.5216	-0.8245	0.0000
f3	-0.1676	-1.8855	0.0000
br4	-0.0234	0.2809	-1.5968
br5	-0.0234	0.2809	1.5968

dist 1 c -- 2 h = 2.0452 au = 108.23 pm
dist 1 c -- 3 f = 2.5487 au = 134.87 pm
dist 1 c -- 4 br = 3.6380 au = 192.52 pm
dist 1 c -- 5 br = 3.6380 au = 192.52 pm
bend 2 h -> 1 c <- 3 f = 109.80 deg
bend 3 f -> 1 c <- 4 br = 109.56 deg
bend 4 br -> 1 c <- 5 br = 112.08 deg
bend 2 h -> 1 c <- 4 br = 107.90 deg

cycle = 7 MP2 energy = -5283.4986023162 |dE/dxyz| = 0.000014

zero point VIBRATIONAL energy : 0.0196652 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'	159.47	0.00133	YES	YES
8	a''	280.48	1.37089	YES	YES
9	a'	343.46	0.86499	YES	YES
10	a'	599.21	25.82670	YES	YES
11	a''	641.32	218.41691	YES	YES
12	a'	1115.25	190.86261	YES	YES
13	a''	1142.52	79.60507	YES	YES
14	a'	1283.24	19.22008	YES	YES
15	a'	3067.08	2.20081	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	18.49	12.77	1.25	-28.94	63.78	0.31931

$cosmo_energy
Total energy [a.u.] = -5286.7039841327
Total energy + OC corr. [a.u.] = -5286.7040680770
Total energy corrected [a.u.] = -5286.7040261048 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0035634511
Diel. energy + OC corr. [a.u.] = -0.0036473955

$FCHI_2$

sy cs

c1	0.4593	-0.8707	0.0000
f2	-0.1814	-2.0658	0.0000
h3	1.5298	-1.0350	0.0000
i4	-0.0142	0.2000	1.7888
i5	-0.0142	0.2000	-1.7888

dist 1 c -- 3 h = 2.0466 au = 108.30 pm
dist 1 c -- 2 f = 2.5625 au = 135.60 pm
dist 1 c -- 4 i = 4.0399 au = 213.78 pm
dist 1 c -- 5 i = 4.0399 au = 213.78 pm
bend 2 f -> 1 c <- 4 i = 109.68 deg
bend 4 i -> 1 c <- 5 i = 113.59 deg
bend 3 h -> 1 c <- 4 i = 107.15 deg
bend 2 f -> 1 c <- 3 h = 109.47 deg

cycle = 7 MP2 energy = -160.9804049510 |dE/dxyz| = 0.000263

zero point VIBRATIONAL energy : 0.0187205 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'	106.88	0.02595	YES	YES
8	a''	241.27	2.75673	YES	YES
9	a'	280.79	0.40421	YES	YES
10	a'	502.34	15.21806	YES	YES
11	a''	563.00	215.35418	YES	YES
12	a''	1061.65	149.95863	YES	YES
13	a'	1127.24	204.44716	YES	YES
14	a'	1269.73	24.02369	YES	YES
15	a'	3064.45	0.20962	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	19.09	13.52	1.76	-36.02	62.19	0.33771

$cosmo_energy
Total energy [a.u.] = -161.3440125058
Total energy + OC corr. [a.u.] = -161.3443693603
Total energy corrected [a.u.] = -161.3441909331 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0044306833
Diel. energy + OC corr. [a.u.] = -0.0047875378

CH_2F_2

sy c2v

c1	0.5553	-0.0000	0.0000
h2	1.1521	-0.9070	0.0000
f3	-0.2367	0.0000	1.1005
f4	-0.2367	0.0000	-1.1005
h5	1.1521	0.9070	0.0000

dist 1 c -- 2 h = 2.0516 au = 108.57 pm
dist 1 c -- 5 h = 2.0516 au = 108.57 pm
dist 1 c -- 3 f = 2.5622 au = 135.59 pm
dist 1 c -- 4 f = 2.5622 au = 135.59 pm
bend 2 h -> 1 c <- 3 f = 108.73 deg
bend 2 h -> 1 c <- 5 h = 113.31 deg
bend 3 f -> 1 c <- 4 f = 108.52 deg

cycle = 7 MP2 energy = -238.6780438599 |dE/dxyz| = 0.000001

zero point VIBRATIONAL energy : 0.0319111 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'	521.73	3.78568	YES	YES
8	a''	1103.93	219.50120	YES	YES
9	a'	1113.02	98.87426	YES	YES
10	a'	1158.38	19.32932	YES	YES
11	a''	1230.60	0.00000	YES	YES
12	a''	1446.60	47.51583	YES	YES
13	a'	1487.80	3.72119	YES	YES
14	a'	2941.15	60.23473	YES	YES
15	a'	3004.11	73.32693	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	16.53	9.46	0.10	19.10	92.01	0.25286

$cosmo_energy
Total energy [a.u.] = -238.8080115865
Total energy + OC corr. [a.u.] = -238.8078696815
Total energy corrected [a.u.] = -238.8079406340 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0038428163
Diel. energy + OC corr. [a.u.] = -0.0037009112

FCH_2Cl

sy cs

c1	-0.6302	-0.5632	0.0000
f2	0.3357	-1.5231	0.0000
h3	-1.2249	-0.6582	0.9007
h4	-1.2249	-0.6582	-0.9007
cl5	0.1033	1.0444	0.0000

dist 1 c -- 3 h = 2.0474 au = 108.34 pm
dist 1 c -- 4 h = 2.0474 au = 108.34 pm
dist 1 c -- 2 f = 2.5734 au = 136.18 pm
dist 1 c -- 5 cl = 3.3394 au = 176.71 pm
bend 3 h -> 1 c <- 4 h = 112.47 deg
bend 3 h -> 1 c <- 2 f = 109.12 deg
bend 3 h -> 1 c <- 5 cl = 107.91 deg
bend 2 f -> 1 c <- 5 cl = 110.29 deg

cycle = 7 MP2 energy = -598.6422805171 |dE/dxyz| = 0.000037

zero point VIBRATIONAL energy : 0.0300722 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'	367.93	1.17986	YES	YES
8	a'	715.45	91.90889	YES	YES
9	a''	970.01	0.55776	YES	YES
10	a'	1095.65	168.78423	YES	YES
11	a''	1217.50	2.18406	YES	YES
12	a'	1332.79	43.28047	YES	YES
13	a'	1459.61	1.99877	YES	YES
14	a'	2982.72	30.92758	YES	YES
15	a''	3058.51	20.50895	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	16.94	10.16	0.24	11.18	87.82	0.26537

$cosmo_energy
Total energy [a.u.] = -599.1436839291
Total energy + OC corr. [a.u.] = -599.1436323247
Total energy corrected [a.u.] = -599.1436581269 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0040830479
Diel. energy + OC corr. [a.u.] = -0.0040314434

FCH_2Br

sy cs

c1	-1.1206	0.6510	0.0000
f2	-2.0233	-0.3676	0.0000
br3	0.6808	-0.0417	0.0000
h4	-1.2393	1.2395	0.9014
h5	-1.2393	1.2395	-0.9014

dist 1 c -- 4 h = 2.0468 au = 108.31 pm
dist 1 c -- 5 h = 2.0468 au = 108.31 pm
dist 1 c -- 2 f = 2.5719 au = 136.10 pm
dist 1 c -- 3 br = 3.6471 au = 193.00 pm
bend 2 f -> 1 c <- 3 br = 110.52 deg
bend 2 f -> 1 c <- 4 h = 109.51 deg
bend 3 br -> 1 c <- 4 h = 107.30 deg
bend 4 h -> 1 c <- 5 h = 112.67 deg

cycle = 8 MP2 energy = -2711.5187859648 |dE/dxyz| = 0.000006

zero point VIBRATIONAL energy : 0.0295052 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'	297.37	0.61454	YES	YES
8	a'	606.36	67.55341	YES	YES
9	a''	909.66	0.01950	YES	YES
10	a'	1104.61	187.68288	YES	YES
11	a''	1213.92	2.29330	YES	YES
12	a'	1294.03	54.73360	YES	YES
13	a'	1454.43	2.05389	YES	YES
14	a'	2994.08	20.80873	YES	YES
15	a''	3076.82	11.22805	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	17.69	10.58	0.35	6.50	86.71	0.27736

$cosmo_energy
Total energy [a.u.] = -2713.1712664820
Total energy + OC corr. [a.u.] = -2713.1713247283
Total energy corrected [a.u.] = -2713.1712956051 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0043232720
Diel. energy + OC corr. [a.u.] = -0.0043815184

FCH_2I

sy cs

c1	-1.5020	0.6602	0.0000
f2	-2.3715	-0.3908	0.0000
i3	0.5232	-0.0238	0.0000
h4	-1.6398	1.2462	0.9005
h5	-1.6398	1.2462	-0.9005

dist 1 c -- 4 h = 2.0469 au = 108.32 pm
dist 1 c -- 5 h = 2.0469 au = 108.32 pm
dist 1 c -- 2 f = 2.5776 au = 136.40 pm
dist 1 c -- 3 i = 4.0395 au = 213.76 pm
bend 2 f -> 1 c <- 3 i = 110.94 deg
bend 2 f -> 1 c <- 4 h = 109.62 deg
bend 3 i -> 1 c <- 4 h = 107.07 deg
bend 4 h -> 1 c <- 5 h = 112.48 deg

cycle = 9 MP2 energy = -150.2588804034 |dE/dxyz| = 0.000006

zero point VIBRATIONAL energy : 0.0289559 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'	250.35	0.70249	YES	YES
8	a'	518.72	53.72636	YES	YES
9	a''	829.07	1.51856	YES	YES
10	a'	1115.38	243.13163	YES	YES
11	a''	1210.06	2.97055	YES	YES
12	a'	1243.27	68.49141	YES	YES
13	a'	1451.69	2.93595	YES	YES
14	a'	3001.76	13.61304	YES	YES
15	a''	3089.85	6.19609	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	18.22	10.88	0.47	2.73	85.63	0.28636

$cosmo_energy
Total energy [a.u.] = -150.4920104066
Total energy + OC corr. [a.u.] = -150.4923945982
Total energy corrected [a.u.] = -150.4922025024 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0046782117
Diel. energy + OC corr. [a.u.] = -0.0050624033

CH_2Cl_2

sy c2v

c1	0.0000	0.0000	-0.8052
cl2	0.0000	1.4688	0.1766
cl3	0.0000	-1.4688	0.1766
h4	0.8945	0.0000	-1.4132
h5	-0.8945	0.0000	-1.4132

dist 1 c -- 4 h = 2.0439 au = 108.16 pm
dist 1 c -- 5 h = 2.0439 au = 108.16 pm
dist 1 c -- 2 cl = 3.3386 au = 176.67 pm
dist 1 c -- 3 cl = 3.3386 au = 176.67 pm
bend 2 cl -> 1 c <- 3 cl = 112.48 deg
bend 2 cl -> 1 c <- 4 h = 108.20 deg
bend 4 h -> 1 c <- 5 h = 111.59 deg

cycle = 6 MP2 energy = -958.6138418440 |dE/dxyz| = 0.000016

zero point VIBRATIONAL energy : 0.0283762 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	a1	270.22	0.57915	YES	YES
8	a1	691.35	13.13523	YES	YES
9	b2	711.21	149.79436	YES	YES
10	b1	872.79	1.69498	YES	YES
11	a2	1127.43	0.00000	NO	YES
12	b2	1244.03	37.77743	YES	YES
13	a1	1407.80	0.15683	YES	YES
14	a1	3023.76	10.08586	YES	YES
15	b1	3107.13	0.75190	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	17.27	10.15	0.41	5.53	84.00	0.27152

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	16.21	9.51	0.16	32.51	80.00	0.25165

$cosmo_energy 298K
Total energy [a.u.] = -959.4843053726
Total energy + OC corr. [a.u.] = -959.4843254241
Total energy corrected [a.u.] = -959.4843153984 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0040086561
Diel. energy + OC corr. [a.u.] = -0.0040287076

$cosmo_energy 195K
Total energy [a.u.] = -959.4846041524
Total energy + OC corr. [a.u.] = -959.4846276423

Total energy corrected [a.u.] = -959.4846158974 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0043927537
Diel. energy + OC corr. [a.u.] = -0.0044162436

CH_2I_2

sy c2v

c1	0.0000	0.0000	-1.0766
i2	0.0000	1.7964	0.0643
i3	0.0000	-1.7964	0.0643
h4	0.8938	0.0000	-1.6850
h5	-0.8938	0.0000	-1.6850

dist 1 c -- 4 h = 2.0432 au = 108.12 pm
dist 1 c -- 5 h = 2.0432 au = 108.12 pm
dist 1 c -- 2 i = 4.0215 au = 212.81 pm
dist 1 c -- 3 i = 4.0215 au = 212.81 pm
bend 2 i -> 1 c <- 3 i = 115.16 deg
bend 2 i -> 1 c <- 4 h = 107.56 deg
bend 4 h -> 1 c <- 5 h = 111.52 deg

cycle = 7 MP2 energy = -61.8577471616 |dE/dxyz| = 0.000001

zero point VIBRATIONAL energy : 0.0261145 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	a1	111.12	0.00046	YES	YES
8	a1	462.61	0.30766	YES	YES
9	b2	522.75	93.27874	YES	YES
10	b1	698.91	13.46720	YES	YES
11	a2	1011.35	0.00000	NO	YES
12	b2	1098.73	113.39990	YES	YES
13	a1	1353.39	0.00581	YES	YES
14	a1	3053.48	0.03178	YES	YES
15	b1	3150.61	5.53623	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	18.99	11.99	1.13	-11.03	79.56	0.31216

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	17.93	11.36	0.64	20.00	74.86	0.28945

$cosmo_energy 298K
Total energy [a.u.] = -62.1852965900
Total energy + OC corr. [a.u.] = -62.1858953845
Total energy corrected [a.u.] = -62.1855959872 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0048595243
Diel. energy + OC corr. [a.u.] = -0.0054583187

$cosmo_energy 195K
Total energy [a.u.] = -62.1856590169
Total energy + OC corr. [a.u.] = -62.1863118369
Total energy corrected [a.u.] = -62.1859854269 Note: incorrect value contained for downward compatibility

Dielectric energy [a.u.] = -0.0053078418
Diel. energy + OC corr. [a.u.] = -0.0059606618

AgI

sy c6v

ag1 0.0000 0.0000 -1.3801
i2 0.0000 0.0000 1.1731

dist 1 ag -- 2 i = 4.8248 au = 255.32 pm

cycle = 8 MP2 energy = -157.8674179846 |dE/dxyz| = 0.000001

zero point VIBRATIONAL energy : 0.0004448 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	a1	195.25	3.78294	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	18.79	8.50	0.49	-67.70	8.86	0.26508

$cosmo_energy
Total energy [a.u.] = -158.5901806032
Total energy + OC corr. [a.u.] = -158.5915644996
Total energy corrected [a.u.] = -158.5908725514 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0135820971
Diel. energy + OC corr. [a.u.] = -0.0149659935

Ag^+

ag1 0.0000 0.0000 0.0000

$energy SCF SCFKIN SCFPOT MP2
1 -145.8506645538 56.62788059784 -202.4785451516 -.36621523393

$cosmo_energy
Total energy [a.u.] = -146.8604665268
Total energy corrected [a.u.] = -146.8600357271
Dielectric energy [a.u.] = -0.1007861834
Dielectric energy corr. [a.u.] = -0.1003553837

CI_4

sy td

c1	0.0000	0.0000	0.0000
i2	1.2466	-1.2466	1.2466
i3	-1.2466	1.2466	1.2466
i4	-1.2466	-1.2466	-1.2466
i5	1.2466	1.2466	-1.2466

dist 1 c -- 2 i = 4.0804 au = 215.92 pm
dist 1 c -- 3 i = 4.0804 au = 215.92 pm
dist 1 c -- 4 i = 4.0804 au = 215.92 pm
dist 1 c -- 5 i = 4.0804 au = 215.92 pm
bend 2 i -> 1 c <- 4 i = 109.47 deg

cycle = 6 MP2 energy = -83.2963786854 |dE/dxyz| = 0.000023

zero point VIBRATIONAL energy : 0.0049998 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	77.90	0.00000	NO	YES
8	e	77.90	0.00000	NO	YES
9	t2	116.16	0.58407	YES	YES
10	t2	116.16	0.58407	YES	YES
11	t2	116.16	0.58407	YES	YES
12	a1	172.55	0.00000	NO	YES
13	t2	505.95	96.06078	YES	YES
14	t2	505.95	96.06078	YES	YES
15	t2	505.95	96.06078	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	19.98	12.98	5.70	-82.72	33.51	0.39815

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	18.92	12.34	3.72	-43.63	24.72	0.35859

$cosmo_energy 298K
Total energy [a.u.] = -83.8690181739
Total energy + OC corr. [a.u.] = -83.8694128290
Total energy corrected [a.u.] = -83.8692155014 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0047605542
Diel. energy + OC corr. [a.u.] = -0.0051552094

$cosmo_energy 195K
Total energy [a.u.] = -83.8693709893
Total energy + OC corr. [a.u.] = -83.8697979761
Total energy corrected [a.u.] = -83.8695844827 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0051540558
Diel. energy + OC corr. [a.u.] = -0.0055810425

HCI_3

sy c3v

c1	0.0000	0.0000	0.5684
h2	0.0000	0.0000	1.6499
i3	-1.0270	1.7788	-0.0223
i4	-1.0270	-1.7788	-0.0223
i5	2.0540	0.0000	-0.0223

dist 1 c -- 2 h = 2.0438 au = 108.16 pm
dist 1 c -- 3 i = 4.0389 au = 213.73 pm
dist 1 c -- 4 i = 4.0389 au = 213.73 pm
dist 1 c -- 5 i = 4.0389 au = 213.73 pm
bend 2 h -> 1 c <- 3 i = 106.04 deg
bend 3 i -> 1 c <- 4 i = 112.67 deg

cycle = 8 MP2 energy = -72.5785939358 |dE/dxyz| = 0.000005

zero point VIBRATIONAL energy : 0.0159298 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	96.34	0.09786	YES	YES
8	e	96.34	0.09786	YES	YES
9	a1	147.22	0.08671	YES	YES
10	a1	414.22	0.56532	YES	YES
11	e	516.38	104.99317	YES	YES
12	e	516.38	104.99317	YES	YES
13	e	1046.29	55.54095	YES	YES
14	e	1046.29	55.54095	YES	YES
15	a1	3112.92	11.39812	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	19.57	13.71	2.99	-48.07	56.91	0.36041

$cosmo_energy
Total energy [a.u.] = -73.0309742385
Total energy + OC corr. [a.u.] = -73.0314560952
Total energy corrected [a.u.] = -73.0312151669 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0050168564
Diel. energy + OC corr. [a.u.] = -0.0054987132

CH_3I

sy c3v

c1	0.0000	0.0000	-1.8977
i2	0.0000	0.0000	0.2328
h3	-0.5150	0.8919	-2.2303
h4	-0.5150	-0.8919	-2.2303
h5	1.0299	0.0000	-2.2303

dist 1 c -- 3 h = 2.0453 au = 108.23 pm
dist 1 c -- 4 h = 2.0453 au = 108.23 pm
dist 1 c -- 5 h = 2.0453 au = 108.23 pm
dist 1 c -- 2 i = 4.0260 au = 213.04 pm
bend 2 i -> 1 c <- 3 h = 107.90 deg
bend 3 h -> 1 c <- 4 h = 111.00 deg

cycle = 7 MP2 energy = -51.1354262919 |dE/dxyz| = 0.000010

zero point VIBRATIONAL energy : 0.0353768 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	a1	504.10	3.38458	YES	YES
8	e	861.77	11.58256	YES	YES
9	e	861.77	11.58256	YES	YES
10	a1	1232.26	30.05275	YES	YES
11	e	1408.00	8.97178	YES	YES
12	e	1408.00	8.97178	YES	YES
13	a1	3000.04	7.47836	YES	YES
14	e	3126.34	0.03793	YES	YES
15	e	3126.34	0.03793	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	18.04	8.10	0.13	27.77	101.30	0.25495

$cosmo_energy
Total energy [a.u.] = -51.3333703848
Total energy + OC corr. [a.u.] = -51.3339416607
Total energy corrected [a.u.] = -51.3336560227 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0035619929
Diel. energy + OC corr. [a.u.] = -0.0041332688

$Ag(CH_2Cl_2)^+$

sy c2v

ag1	0.0000	0.0000	-1.0505
cl2	0.0000	1.4622	1.1522
cl3	0.0000	-1.4622	1.1522
c4	0.0000	0.0000	2.1687
h5	0.9034	0.0000	2.7640
h6	-0.9034	0.0000	2.7640

dist 1 ag -- 2 cl = 4.9962 au = 264.39 pm
dist 4 c -- 5 h = 2.0446 au = 108.19 pm
dist 4 c -- 6 h = 2.0446 au = 108.19 pm
dist 2 cl -- 4 c = 3.3652 au = 178.08 pm
dist 3 cl -- 4 c = 3.3652 au = 178.08 pm
bend 2 cl -> 1 ag <- 3 cl = 67.15 deg
bend 2 cl -> 4 c <- 3 cl = 110.39 deg
bend 5 h -> 4 c <- 6 h = 113.23 deg

cycle = 8 MP2 energy = -1104.8768212189 |dE/dxyz| = 0.000007

zero point VIBRATIONAL energy : 0.0290843 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	b1	54.64	9.04847	YES	YES
8	b2	110.35	0.54880	YES	YES
9	a1	157.84	5.02940	YES	YES
10	a1	319.77	1.82372	YES	YES
11	a1	664.38	20.46586	YES	YES
12	b2	667.86	80.38509	YES	YES
13	b1	878.16	1.55074	YES	YES
14	a2	1101.52	0.00000	NO	YES
15	b2	1230.30	9.01136	YES	YES
16	a1	1397.92	0.77910	YES	YES
17	a1	3042.68	7.16725	YES	YES
18	b1	3141.15	19.52841	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	18.50	12.08	3.32	-7.66	91.48	0.34082

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	17.44	11.44	2.18	25.97	84.99	0.31077

$cosmo_energy 298K
Total energy [a.u.] = -1106.3824678825
Total energy corrected [a.u.] = -1106.3816901823
Dielectric energy [a.u.] = -0.0790376184
Dielectric energy corr. [a.u.] = -0.0782599182

$cosmo_energy 195K
Total energy [a.u.] = -1106.3880826346
Total energy + OC corr. [a.u.] = -1106.3867847453
Total energy corrected [a.u.] = -1106.3874336900 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0847912300
Diel. energy + OC corr. [a.u.] = -0.0834933407

$Ag(CH_2Cl_2)_3^+$

sy c2

ag1	0.0000	0.0000	0.0024
cl2	1.3724	0.5014	2.3689
cl3	-1.4182	2.2402	-0.7965
cl4	1.3709	1.8524	-1.5775
c5	-0.0402	2.9223	-1.6852
h6	0.2162	3.8723	-1.2360
h7	-0.3195	3.0146	-2.7260
c8	0.0000	0.0000	3.3768
h9	-0.3086	0.8458	3.9761
cl10	-1.3724	-0.5014	2.3689
cl11	1.4182	-2.2402	-0.7965
cl12	-1.3709	-1.8524	-1.5775
c13	0.0402	-2.9223	-1.6852
h14	-0.2162	-3.8723	-1.2360
h15	0.3195	-3.0146	-2.7260
h16	0.3086	-0.8458	3.9761

dist 1 ag -- 2 cl = 5.2558 au = 278.12 pm
dist 1 ag -- 3 cl = 5.2328 au = 276.91 pm
dist 1 ag -- 4 cl = 5.2801 au = 279.41 pm
dist 1 ag -- 10 cl = 5.2558 au = 278.12 pm
dist 1 ag -- 11 cl = 5.2328 au = 276.91 pm
dist 1 ag -- 12 cl = 5.2801 au = 279.41 pm
dist 5 c -- 6 h = 2.0439 au = 108.16 pm
dist 5 c -- 7 h = 2.0440 au = 108.16 pm
dist 4 cl -- 5 c = 3.3526 au = 177.41 pm
dist 3 cl -- 5 c = 3.3561 au = 177.60 pm
dist 8 c -- 9 h = 2.0439 au = 108.16 pm
dist 8 c -- 16 h = 2.0439 au = 108.16 pm
dist 2 cl -- 8 c = 3.3544 au = 177.51 pm
dist 8 c -- 10 cl = 3.3544 au = 177.51 pm
dist 13 c -- 14 h = 2.0439 au = 108.16 pm
dist 13 c -- 15 h = 2.0440 au = 108.16 pm
dist 12 cl -- 13 c = 3.3526 au = 177.41 pm
dist 11 cl -- 13 c = 3.3561 au = 177.60 pm
bend 2 cl -> 1 ag <- 10 cl = 63.39 deg
bend 4 cl -> 1 ag <- 3 cl = 63.37 deg
bend 11 cl -> 1 ag <- 12 cl = 63.37 deg
bend 6 h -> 5 c <- 7 h = 112.70 deg
bend 9 h -> 8 c <- 16 h = 112.70 deg
bend 14 h -> 13 c <- 15 h = 112.70 deg

cycle = 7 SCF+MP2 energy = -3022.1668962309 |dE/dxyz| = 0.000226

zero point VIBRATIONAL energy : 0.0871896 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	b	25.13	0.11957	YES	YES
8	a	26.83	0.02027	YES	YES
9	a	28.75	0.05140	YES	YES

10	b	30.36	1.24828	YES	YES
11	b	33.11	2.03438	YES	YES
12	a	34.25	0.93472	YES	YES
13	b	47.15	2.83498	YES	YES
14	b	51.34	7.44695	YES	YES
15	a	51.52	1.44099	YES	YES
16	a	53.26	7.71621	YES	YES
17	b	54.04	0.00036	YES	YES
18	b	91.58	1.86293	YES	YES
19	a	102.97	0.00262	YES	YES
20	a	122.76	9.49820	YES	YES
21	b	125.72	9.29130	YES	YES
22	a	300.36	4.35298	YES	YES
23	b	300.42	4.46870	YES	YES
24	a	301.60	0.02539	YES	YES
25	a	672.40	44.81912	YES	YES
26	b	675.32	17.71876	YES	YES
27	a	676.85	11.22439	YES	YES
28	b	677.78	50.91330	YES	YES
29	a	681.61	0.42120	YES	YES
30	b	688.39	198.08655	YES	YES
31	b	875.22	1.12709	YES	YES
32	b	876.12	1.24688	YES	YES
33	a	876.37	1.86410	YES	YES
34	a	1110.20	0.00200	YES	YES
35	a	1110.77	0.00011	YES	YES
36	b	1110.82	0.00123	YES	YES
37	b	1230.99	3.37758	YES	YES
38	a	1231.24	3.59209	YES	YES
39	b	1236.22	24.54816	YES	YES
40	a	1401.29	0.70103	YES	YES
41	b	1402.00	0.93932	YES	YES
42	a	1402.23	0.16938	YES	YES
43	a	3044.73	0.47477	YES	YES
44	b	3045.77	0.68627	YES	YES
45	a	3045.80	0.23436	YES	YES
46	b	3138.73	7.33863	YES	YES
47	a	3139.93	9.79515	YES	YES
48	b	3139.94	5.02916	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	19.44	14.59	24.35	84.19	274.65	0.64712

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	18.38	13.95	18.31	146.73	255.08	0.56351

$cosmo_energy 298K
Total energy [a.u.] = -3025.4006565338
Total energy corrected [a.u.] = -3025.3999882803
Dielectric energy [a.u.] = -0.0600002844
Dielectric energy corr. [a.u.] = -0.0593320309

$cosmo_energy 195K
Total energy [a.u.] = -3025.4050830128
Total energy corrected [a.u.] = -3025.4043669476
Dielectric energy [a.u.] = -0.0645140300
Dielectric energy corr. [a.u.] = -0.0637979648

$Ag(CH_2I_2)_3^+$

sy c2

ag1	0.0000	0.0000	0.0076
i2	1.5673	0.8434	2.4859
i3	-1.5604	2.5681	-0.5077
i4	1.5677	1.7168	-1.9775
c5	-0.0160	3.1402	-1.8629
h6	0.4007	4.0760	-1.5143
h7	-0.4535	3.2296	-2.8485
c8	0.0000	0.0000	3.6609
h9	-0.4243	0.7915	4.2645
i10	-1.5673	-0.8434	2.4859
i11	1.5604	-2.5681	-0.5077
i12	-1.5677	-1.7168	-1.9775
c13	0.0160	-3.1402	-1.8629
h14	-0.4007	-4.0760	-1.5143
h15	0.4535	-3.2296	-2.8485
h16	0.4243	-0.7915	4.2645

dist 1 ag -- 2 i = 5.7657 au = 305.11 pm
dist 1 ag -- 3 i = 5.7614 au = 304.88 pm
dist 1 ag -- 4 i = 5.7771 au = 305.71 pm
dist 1 ag -- 10 i = 5.7657 au = 305.11 pm
dist 1 ag -- 11 i = 5.7614 au = 304.88 pm
dist 1 ag -- 12 i = 5.7771 au = 305.71 pm
dist 5 c -- 6 h = 2.0449 au = 108.21 pm
dist 5 c -- 7 h = 2.0448 au = 108.21 pm
dist 4 i -- 5 c = 4.0298 au = 213.25 pm
dist 3 i -- 5 c = 4.0303 au = 213.28 pm
dist 8 c -- 9 h = 2.0449 au = 108.21 pm
dist 8 c -- 16 h = 2.0449 au = 108.21 pm
dist 2 i -- 8 c = 4.0301 au = 213.27 pm
dist 8 c -- 10 i = 4.0301 au = 213.27 pm
dist 13 c -- 14 h = 2.0449 au = 108.21 pm
dist 13 c -- 15 h = 2.0448 au = 108.21 pm
dist 12 i -- 13 c = 4.0298 au = 213.25 pm
dist 11 i -- 13 c = 4.0303 au = 213.28 pm
bend 2 i -> 1 ag <- 10 i = 71.37 deg
bend 4 i -> 1 ag <- 3 i = 71.32 deg
bend 11 i -> 1 ag <- 12 i = 71.32 deg
bend 2 i -> 8 c <- 10 i = 113.13 deg
bend 4 i -> 5 c <- 3 i = 113.13 deg
bend 12 i -> 13 c <- 11 i = 113.13 deg
bend 6 h -> 5 c <- 7 h = 112.19 deg
bend 9 h -> 8 c <- 16 h = 112.18 deg
bend 14 h -> 13 c <- 15 h = 112.19 deg

cycle = 10 SCF+MP2 energy = -331.9246822399 |dE/dxyz| = 0.000043

zero point VIBRATIONAL energy : 0.0798041 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	b	16.04	0.01436	YES	YES
8	a	16.35	0.02147	YES	YES
9	a	18.49	0.02984	YES	YES
10	b	19.87	0.08482	YES	YES
11	b	20.77	0.13268	YES	YES
12	a	22.32	0.01967	YES	YES
13	b	22.40	0.09824	YES	YES
14	a	23.45	0.01786	YES	YES
15	b	32.42	3.44945	YES	YES
16	a	33.83	3.16692	YES	YES
17	b	44.40	3.18740	YES	YES
18	b	47.91	0.49637	YES	YES
19	a	52.32	0.00051	YES	YES
20	a	75.98	9.34968	YES	YES
21	b	76.87	9.26770	YES	YES
22	a	126.70	1.01263	YES	YES
23	b	126.91	1.08087	YES	YES
24	a	127.68	0.02050	YES	YES
25	a	470.04	0.09792	YES	YES
26	a	470.53	3.21957	YES	YES
27	b	470.67	3.01303	YES	YES
28	a	519.47	13.84706	YES	YES
29	b	519.72	13.59695	YES	YES
30	b	522.90	73.70579	YES	YES
31	b	712.53	5.50760	YES	YES
32	b	713.89	5.42690	YES	YES
33	a	714.11	6.46111	YES	YES
34	a	1002.59	0.00512	YES	YES
35	b	1003.04	0.01155	YES	YES
36	a	1003.30	0.00072	YES	YES
37	b	1101.37	19.79492	YES	YES
38	a	1101.92	20.67817	YES	YES
39	b	1108.21	90.66139	YES	YES
40	a	1356.94	0.07826	YES	YES
41	a	1357.87	0.08118	YES	YES
42	b	1358.02	0.11916	YES	YES
43	a	3052.31	8.98874	YES	YES
44	b	3052.98	11.78525	YES	YES
45	a	3053.09	3.20301	YES	YES
46	b	3152.63	16.16728	YES	YES
47	b	3153.56	15.00310	YES	YES
48	a	3153.60	18.21226	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	20.83	16.53	33.14	34.77	261.50	0.76878

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	19.77	15.90	26.02	109.43	239.84	0.67654

$cosmo_energy 298K
Total energy [a.u.] = -333.4990428353
Total energy + OC corr. [a.u.] = -333.4967075798
Total energy corrected [a.u.] = -333.4978752076 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0583616298
Diel. energy + OC corr. [a.u.] = -0.0560263742

$cosmo_energy 195K

Total energy [a.u.] = -333.5035600717
Total energy corrected [a.u.] = -333.5021370579
Dielectric energy [a.u.] = -0.0629648557
Dielectric energy corr. [a.u.] = -0.0615418419

$Ag(CH_2Cl_2)_2(CH_2I_2)^+$

sy c2

ag1	0.0000	0.0000	-0.5677
i2	0.3293	1.7481	1.7610
cl3	-2.4299	0.2118	-1.6733
cl4	-0.4232	1.8252	-3.0631
c5	-1.9517	0.9562	-3.2201
h6	-2.7267	1.6583	-3.4974
h7	-1.8289	0.1619	-3.9439
c8	0.0000	0.0000	2.9404
h9	-0.8832	0.1668	3.5434
i10	-0.3293	-1.7481	1.7610
cl11	2.4299	-0.2118	-1.6733
cl12	0.4232	-1.8252	-3.0631
c13	1.9517	-0.9562	-3.2201
h14	2.7267	-1.6583	-3.4974
h15	1.8289	-0.1619	-3.9439
h16	0.8832	-0.1668	3.5434

dist 1 ag -- 2 i = 5.5377 au = 293.04 pm
dist 1 ag -- 3 cl = 5.0606 au = 267.80 pm
dist 1 ag -- 4 cl = 5.8969 au = 312.05 pm
dist 1 ag -- 10 i = 5.5377 au = 293.04 pm
dist 1 ag -- 11 cl = 5.0606 au = 267.80 pm
dist 1 ag -- 12 cl = 5.8969 au = 312.05 pm
dist 5 c -- 7 h = 2.0441 au = 108.17 pm
dist 5 c -- 6 h = 2.0445 au = 108.19 pm
dist 4 cl -- 5 c = 3.3357 au = 176.52 pm
dist 3 cl -- 5 c = 3.3674 au = 178.19 pm
dist 8 c -- 9 h = 2.0452 au = 108.23 pm
dist 8 c -- 16 h = 2.0452 au = 108.23 pm
dist 2 i -- 8 c = 4.0333 au = 213.43 pm
dist 8 c -- 10 i = 4.0333 au = 213.43 pm
dist 13 c -- 15 h = 2.0441 au = 108.17 pm
dist 13 c -- 14 h = 2.0445 au = 108.19 pm
dist 12 cl -- 13 c = 3.3357 au = 176.52 pm
dist 11 cl -- 13 c = 3.3674 au = 178.19 pm
bend 4 cl -> 1 ag <- 3 cl = 60.03 deg
bend 2 i -> 1 ag <- 10 i = 74.75 deg
bend 12 cl -> 1 ag <- 11 cl = 60.03 deg
bend 4 cl -> 5 c <- 3 cl = 111.15 deg
bend 2 i -> 8 c <- 10 i = 112.91 deg
bend 12 cl -> 13 c <- 11 cl = 111.15 deg
bend 7 h -> 5 c <- 6 h = 112.72 deg
bend 9 h -> 8 c <- 16 h = 112.29 deg
bend 14 h -> 13 c <- 15 h = 112.72 deg

cycle = 30 MP2 energy = -2125.4215378371 |dE/dxyz| = 0.000036

zero point VIBRATIONAL energy : 0.0846435 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	b	12.99	0.05660	YES	YES
8	a	14.50	0.02416	YES	YES
9	b	24.93	0.00389	YES	YES
10	a	25.75	0.09433	YES	YES
11	b	29.01	0.21588	YES	YES
12	a	33.54	0.48147	YES	YES
13	b	35.28	0.02068	YES	YES
14	b	43.34	4.18047	YES	YES
15	a	44.68	0.01292	YES	YES
16	b	56.39	5.63945	YES	YES
17	a	57.42	7.03865	YES	YES
18	b	73.35	1.62383	YES	YES
19	a	78.18	1.35101	YES	YES
20	b	105.11	7.53707	YES	YES
21	a	105.52	10.27429	YES	YES
22	a	132.29	1.14315	YES	YES
23	b	296.39	3.99457	YES	YES
24	a	297.27	2.25875	YES	YES
25	a	469.77	2.16961	YES	YES
26	b	515.44	27.76539	YES	YES
27	a	677.47	37.57619	YES	YES
28	b	678.12	28.70878	YES	YES
29	a	681.88	5.93338	YES	YES
30	b	686.33	145.67559	YES	YES
31	b	712.96	8.48266	YES	YES
32	b	877.35	0.83702	YES	YES
33	a	877.65	1.55074	YES	YES
34	a	997.94	0.00040	YES	YES
35	b	1103.55	46.29963	YES	YES
36	a	1113.25	0.00003	YES	YES
37	b	1113.25	0.08028	YES	YES
38	a	1232.80	4.98122	YES	YES
39	b	1235.75	16.67909	YES	YES
40	a	1354.71	0.00219	YES	YES
41	b	1403.56	1.03116	YES	YES
42	a	1403.67	0.19621	YES	YES
43	b	3042.93	0.20410	YES	YES
44	a	3042.95	0.18952	YES	YES
45	a	3046.73	7.80429	YES	YES
46	a	3135.89	6.82193	YES	YES
47	b	3135.90	5.21054	YES	YES
48	b	3148.40	18.50792	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	20.06	15.37	27.72	65.71	270.15	0.69399

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	19.00	14.73	21.30	132.94	249.86	0.60743

$cosmo_energy 298K
Total energy [a.u.] = -2128.1018995185
Total energy corrected [a.u.] = -2128.1009447556
Dielectric energy [a.u.] = -0.0594194342
Dielectric energy corr. [a.u.] = -0.0584646713

$cosmo_energy 195K
Total energy [a.u.] = -2128.1016855330
Total energy + OC corr. [a.u.] = -2128.1001367165

Total energy corrected [a.u.] = -2128.1009111248 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0592283382
Diel. energy + OC corr. [a.u.] = -0.0576795217

$Ag(CH_2Cl_2)(CH_2I_2)^+$

sy c2v

ag1	0.0000	0.0000	-0.8976
i2	0.0000	1.7752	1.3565
cl3	-1.4579	0.0000	-3.1663
i4	0.0000	-1.7752	1.3565
cl5	1.4579	0.0000	-3.1663
c6	0.0000	0.0000	2.5440
c7	0.0000	0.0000	-4.1818
h8	0.8995	0.0000	3.1463
h9	0.0000	0.9013	-4.7801
h10	-0.8995	0.0000	3.1463
h11	0.0000	-0.9013	-4.7801

dist 1 ag -- 2 i = 5.4221 au = 286.92 pm
dist 1 ag -- 3 cl = 5.0960 au = 269.67 pm
dist 1 ag -- 4 i = 5.4221 au = 286.92 pm
dist 1 ag -- 5 cl = 5.0960 au = 269.67 pm
dist 6 c -- 8 h = 2.0457 au = 108.25 pm
dist 6 c -- 10 h = 2.0457 au = 108.25 pm
dist 2 i -- 6 c = 4.0359 au = 213.57 pm
dist 4 i -- 6 c = 4.0359 au = 213.57 pm
dist 7 c -- 9 h = 2.0443 au = 108.18 pm
dist 7 c -- 11 h = 2.0443 au = 108.18 pm
dist 3 cl -- 7 c = 3.3576 au = 177.68 pm
dist 5 cl -- 7 c = 3.3576 au = 177.68 pm
bend 2 i -> 1 ag <- 4 i = 76.44 deg
bend 3 cl -> 1 ag <- 5 cl = 65.45 deg
bend 2 i -> 6 c <- 4 i = 112.44 deg
bend 3 cl -> 7 c <- 5 cl = 110.28 deg
bend 8 h -> 6 c <- 10 h = 112.39 deg
bend 9 h -> 7 c <- 11 h = 112.85 deg

cycle = 9 SCF+MP2 energy = -1166.7871722600 |dE/dxyz| = 0.000012

zero point VIBRATIONAL energy : 0.0558404 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	22.09	0.00000	NO	YES
8	b1	23.54	0.25011	YES	YES
9	b2	27.27	0.53305	YES	YES
10	b1	32.96	3.67677	YES	YES
11	b2	53.80	7.01873	YES	YES
12	b2	68.24	2.31507	YES	YES
13	b1	77.55	0.89769	YES	YES
14	a1	82.00	0.56129	YES	YES
15	a1	133.49	1.73328	YES	YES
16	a1	155.01	13.32311	YES	YES
17	a1	307.16	3.47795	YES	YES
18	a1	473.92	1.73720	YES	YES
19	b2	525.22	22.31551	YES	YES
20	a1	674.61	25.09243	YES	YES

21	b1	679.20	76.12275	YES	YES
22	b1	712.91	9.47611	YES	YES
23	b2	877.38	1.11643	YES	YES
24	a2	998.67	0.00000	NO	YES
25	a2	1106.23	0.00000	NO	YES
26	b2	1108.35	44.72286	YES	YES
27	b1	1232.74	8.64039	YES	YES
28	a1	1354.78	0.01123	YES	YES
29	a1	1402.11	0.37223	YES	YES
30	a1	3044.40	1.71206	YES	YES
31	a1	3048.11	9.90558	YES	YES
32	b2	3139.06	9.72421	YES	YES
33	b1	3150.34	22.32437	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	19.80	14.77	15.54	22.37	178.75	0.53279

$cosmo_energy
Total energy [a.u.] = -1168.6059901122
Total energy + OC corr. [a.u.] = -1168.6038971216
Total energy corrected [a.u.] = -1168.6049436169 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0642528438
Diel. energy + OC corr. [a.u.] = -0.0621598531

$CI_3^{\cdots}I_2^+$

sy cs

c1	1.8782	0.3299	0.0000
i2	3.0701	1.9643	0.0000
i3	2.7108	-1.5141	0.0000
i4	-0.1434	0.5373	0.0000
i5	-3.5831	0.7316	0.0000
i6	-3.6735	-1.9358	0.0000

dist 1 c -- 2 i = 3.8226 au = 202.28 pm
dist 1 c -- 3 i = 3.8234 au = 202.33 pm
dist 1 c -- 4 i = 3.8404 au = 203.22 pm
dist 5 i -- 6 i = 5.0436 au = 266.90 pm
dist 4 i -- 5 i = 6.5104 au = 344.51 pm

cycle = 27 MP2 energy = -94.3224457067 |dE/dxyz| = 0.000056

zero point VIBRATIONAL energy : 0.0056318 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''	10.27	0.00091	YES	YES
8	a'	12.06	0.01700	YES	YES
9	a''	20.55	0.05556	YES	YES
10	a'	35.43	0.12260	YES	YES
11	a'	59.43	4.86712	YES	YES
12	a'	113.49	2.37348	YES	YES
13	a'	121.99	0.31231	YES	YES
14	a'	190.22	10.63765	YES	YES
15	a'	207.24	1.72123	YES	YES
16	a''	336.99	7.10365	YES	YES
17	a'	660.00	91.02548	YES	YES
18	a'	704.41	192.91545	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	20.31	16.73	14.44	-112.84	42.08	0.52789

$cosmo_energy
Total energy [a.u.] = -95.1095698378
Total energy + OC corr. [a.u.] = -95.1064519893
Total energy corrected [a.u.] = -95.1080109135 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0633924847
Diel. energy + OC corr. [a.u.] = -0.0602746362

Electronic excitation spectrum of , IRREP a'
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.16338593976747E+04 0.24170961951988E-01
0.61060861665301E+03 0.16323119519015E-01
0.57253293551548E+03 0.48868996835459E-02
0.53553645985648E+03 0.12222127682976E+00

0.45654754107910E+03 0.23542013645804E-01
0.39298425833271E+03 0.44896980728675E-02
0.39002402572200E+03 0.53080173622547E-01
0.38310073834320E+03 0.82254813598472E-01
0.37505793172544E+03 0.45152621892958E-01
0.35377522561460E+03 0.56968313627159E-02
0.32713286815113E+03 0.26519969043543E+00
0.32275719627431E+03 0.84233262973930E-01
0.30500057959801E+03 0.32730222416474E-01
0.29562707572684E+03 0.17403645982459E-02
0.28848970985445E+03 0.28143635077113E-01
0.27433755903457E+03 0.19992839742757E+00
0.22936402853643E+03 0.31657145238129E-01
0.22902799032012E+03 0.65337064942123E-01
0.22824173643394E+03 0.31096941170812E-01
0.22597568618174E+03 0.39615059510626E-01
Electronic excitation spectrum of , IRREP a"
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.16405099707555E+04 0.18220372618006E-07
0.68704855953391E+03 0.12169856790563E-05
0.67550888492846E+03 0.41266745896117E-03
0.62190724140424E+03 0.29126855441333E-03
0.56440896124495E+03 0.32074602025304E-05
0.48166471351150E+03 0.11112396382447E-08
0.44722880509257E+03 0.19686407049439E-05
0.38341395642604E+03 0.91970429712859E-06
0.36320398187870E+03 0.45597787245827E-08
0.36128024646555E+03 0.16011224193278E-03
0.34567130857785E+03 0.75545681689149E-06
0.31850532470718E+03 0.15837101075294E-07
0.31727182329582E+03 0.76819378044326E-05
0.30246873982562E+03 0.25724411335272E-06
0.30204075618731E+03 0.49375991219378E-05
0.29705110954735E+03 0.44185381507368E-04
0.22793490788896E+03 0.67421195318600E-05
0.22201870549880E+03 0.42767942670546E-04
0.21812192697970E+03 0.11542477318206E-02
0.20940441110675E+03 0.12328332527654E-02

BF_3

sy d3h

b1	0.0000	0.0000	0.0000
f2	0.6581	-1.1399	0.0000
f3	0.6581	1.1399	0.0000
f4	-1.3162	0.0000	0.0000

dist 1 b -- 2 f = 2.4873 au = 131.62 pm
dist 1 b -- 3 f = 2.4873 au = 131.62 pm
dist 1 b -- 4 f = 2.4873 au = 131.62 pm
bend 2 f -> 1 b <- 3 f = 120.00 deg

cycle = 4 SCF+MP2 energy = -324.1775017680 |dE/dxyz| = 0.000003

zero point VIBRATIONAL energy : 0.0121894 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'	462.09	10.34207	YES	YES
8	e'	462.09	10.34207	YES	YES
9	a2"	656.39	82.51553	YES	NO
10	a1'	860.68	0.00000	NO	YES
11	e'	1454.65	388.44752	YES	YES
12	e'	1454.65	388.44752	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	16.93	8.77	0.29	-32.41	41.31	0.25560

$cosmo_energy
Total energy [a.u.] = -324.3236512012
Total energy corrected [a.u.] = -324.3236128702
Dielectric energy [a.u.] = -0.0063884544
Dielectric energy corr. [a.u.] = -0.0063501234

Electronic excitation spectrum of , IRREP e'
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.10743617965519E+03 0.23708210669946E-01
0.10219219179498E+03 0.37437499517477E+00
0.84861961979096E+02 0.45004670205103E-02
0.82064316098608E+02 0.24250322483796E+00
0.76243648863047E+02 0.95295303180165E-01
0.71993536525013E+02 0.35921526187116E-01
0.66376095817029E+02 0.78609175040970E-01
0.63536841561851E+02 0.62759636097479E-02
0.61884541865917E+02 0.37044340965523E-02
0.58338177883373E+02 0.46201791849853E-01
Electronic excitation spectrum of , IRREP a2"
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.89846189197501E+02 0.15716590977316E+00

0.82631871036934E+02	0.12425367682947E+00
0.78727559162883E+02	0.20392109582894E+00
0.58645564788939E+02	0.28327249524457E-01
0.56934006390057E+02	0.17140632632992E-02
0.56026565189953E+02	0.11212330445016E-01
0.39332527262354E+02	0.63414367229071E-02
0.33365734017312E+02	0.11371862406945E-01
0.32813650079619E+02	0.52648820349300E-02
0.32725684378851E+02	0.43452846344202E-01

BCl_3

sy d3h

b1	0.0000	0.0000	0.0000
cl2	0.8697	-1.5063	0.0000
cl3	0.8697	1.5063	0.0000
cl4	-1.7393	0.0000	0.0000

dist 1 b -- 2 cl = 3.2868 au = 173.93 pm
dist 1 b -- 3 cl = 3.2868 au = 173.93 pm
dist 1 b -- 4 cl = 3.2868 au = 173.93 pm
bend 2 cl -> 1 b <- 3 cl = 120.00 deg

cycle = 4 SCF+MP2 energy = -1404.0088931046 |dE/dxyz| = 0.000006

zero point VIBRATIONAL energy : 0.0074971 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'	247.35	0.48718	YES	YES
8	e'	247.35	0.48718	YES	YES
9	a2"	438.40	4.32754	YES	NO
10	a1'	456.52	0.00000	NO	YES
11	e'	950.61	333.00279	YES	YES
12	e'	950.61	333.00279	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	17.75	10.55	0.99	-52.92	31.33	0.29089

$cosmo_energy
Total energy [a.u.] = -1405.2761998688
Total energy corrected [a.u.] = -1405.2761912009
Dielectric energy [a.u.] = -0.0021547392
Dielectric energy corr. [a.u.] = -0.0021460713

Electronic excitation spectrum of , IRREP e'
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.17951986875887E+03 0.26673530911955E+00
0.12952078133648E+03 0.13230377431756E+00
0.11338807206356E+03 0.20325976390297E+00
0.10730127211025E+03 0.17492872948773E-01
0.10483758505496E+03 0.91601948981151E-01
0.97775327157974E+02 0.29701204434664E+00
0.92369241424633E+02 0.65167304929442E+00
0.88170765118416E+02 0.14107712303376E-01
0.86050453562680E+02 0.14238368583116E-02
0.82597130200034E+02 0.20306491856322E+01
Electronic excitation spectrum of , IRREP a2"
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.11332386677191E+03 0.34647727847190E-02

0.10765181720721E+03	0.26427324961007E-02
0.10529331278201E+03	0.18061181875506E+00
0.94623127916113E+02	0.19082266476806E+00
0.87442147265217E+02	0.45405382942729E+00
0.62057499241206E+02	0.42410240730136E-02
0.60499501013573E+02	0.46699165602707E-05
0.54059500407379E+02	0.25289257442498E+00
0.53810803514888E+02	0.68745328978904E-02
0.49943459182662E+02	0.91543098662769E-02

BBr_3

sy d3h

b1	0.0000	0.0000	0.0000
br2	0.9492	-1.6441	0.0000
br3	0.9492	1.6441	0.0000
br4	-1.8985	0.0000	0.0000

dist 1 b -- 2 br = 3.5876 au = 189.85 pm
dist 1 b -- 3 br = 3.5876 au = 189.85 pm
dist 1 b -- 4 br = 3.5876 au = 189.85 pm
bend 2 br -> 1 b <- 3 br = 120.00 deg

cycle = 4 SCF+MP2 energy = -7742.6232030152 |dE/dxyz| = 0.000003

zero point VIBRATIONAL energy : 0.0058584 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'	147.26	0.04892	YES	YES
8	e'	147.26	0.04892	YES	YES
9	a1'	273.64	0.00000	NO	YES
10	a2"	374.98	0.21274	YES	NO
11	e'	814.20	276.71048	YES	YES
12	e'	814.20	276.71048	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	18.89	12.03	1.88	-65.93	28.68	0.32565

$cosmo_energy
Total energy [a.u.] = -7747.3378563568
Total energy corrected [a.u.] = -7747.3378573646
Dielectric energy [a.u.] = -0.0019937987
Dielectric energy corr. [a.u.] = -0.0019948066

Electronic excitation spectrum of , IRREP e'
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.22070356159927E+03 0.25180567660422E+00
0.16185452362514E+03 0.95256058612500E-01
0.14097569544630E+03 0.18154918054831E+00
0.12900095232047E+03 0.18014158164904E+00
0.11635028249482E+03 0.65263260699040E-01
0.11409072734935E+03 0.91026060423720E+00
0.10160650971581E+03 0.67707440332797E-01
0.96447581867191E+02 0.22153214597383E+01
0.93914061695872E+02 0.21300855946438E+00
0.92000784019635E+02 0.50904837334844E+00
Electronic excitation spectrum of , IRREP a2"
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.13731295362342E+03 0.44557364434899E-02

0.13103457376698E+03	0.16055651118376E-01
0.11799760403649E+03	0.50729890660850E-01
0.10155111610209E+03	0.24058544089123E+00
0.93112967005129E+02	0.43361609035894E+00
0.70461221981469E+02	0.45694875637548E+00
0.67495901863859E+02	0.29693955384554E-02
0.67215665871768E+02	0.12764680736163E-02
0.66957636332070E+02	0.25701075444624E-01
0.62557736859885E+02	0.48914176918909E-03

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
dist 1 b -- 3 i = 3.9945 au = 211.38 pm
dist 1 b -- 4 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

Electronic excitation spectrum of , IRREP e'
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.28598881889313E+03 0.27006188126425E+00
0.22255104337988E+03 0.13609078587368E+00
0.19492171382363E+03 0.23452860341097E+00
0.17410563203807E+03 0.32273707239398E+00
0.14750304326575E+03 0.11628200685193E+01
0.12823787508555E+03 0.11558189071969E+01
0.12387516345659E+03 0.29308097795957E-01
0.11539377562215E+03 0.32061224016122E+00
0.11443836552205E+03 0.11996283792240E-01
0.11200987169511E+03 0.20249295845676E+00
Electronic excitation spectrum of , IRREP a2"
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.18242417327509E+03 0.11152802605326E-02

0.17537599446409E+03	0.89323549888027E-02
0.13231824905169E+03	0.56215447937041E-01
0.11643937386879E+03	0.82302682305154E-01
0.10414687531254E+03	0.22134426559248E-02
0.10255233711325E+03	0.44563671141091E-01
0.99083546479608E+02	0.18758602665567E+00
0.94723466106568E+02	0.66737719767169E-01
0.89202440659444E+02	0.31000836529595E+00
0.85327731819008E+02	0.46028109983123E-01

HBF_2

sy c2v

b1	0.0000	0.0000	0.4922
f2	1.1322	0.0000	-0.1845
f3	-1.1322	0.0000	-0.1845
h4	0.0000	0.0000	1.6750

dist 1 b -- 4 h = 2.2351 au = 118.27 pm
dist 1 b -- 2 f = 2.4926 au = 131.90 pm
dist 1 b -- 3 f = 2.4926 au = 131.90 pm
bend 2 f -> 1 b <- 3 f = 118.27 deg
bend 2 f -> 1 b <- 4 h = 120.86 deg

cycle = 5 MP2 energy = -224.9617337977 |dE/dxyz| = 0.000014

zero point VIBRATIONAL energy : 0.0175494 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	a1	532.41	17.69845	YES	YES
8	b2	895.24	63.41645	YES	YES
9	b1	1059.10	0.21502	YES	YES
10	a1	1142.42	101.93619	YES	YES
11	b1	1438.92	353.15466	YES	YES
12	a1	2635.23	116.68914	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	16.47	8.58	0.10	-16.27	54.33	0.24512

$cosmo_energy
Total energy [a.u.] = -225.0817614768
Total energy + OC corr. [a.u.] = -225.0815538860
Total energy corrected [a.u.] = -225.0816576814 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0068683977
Diel. energy + OC corr. [a.u.] = -0.0066608069

$HBCl_2$

sy c2v

b1	0.0000	0.0000	0.7214
cl2	1.5101	0.0000	-0.1370
cl3	-1.5101	0.0000	-0.1370
h4	0.0000	0.0000	1.9014

dist 1 b -- 4 h = 2.2298 au = 117.99 pm
dist 1 b -- 2 cl = 3.2825 au = 173.70 pm
dist 1 b -- 3 cl = 3.2825 au = 173.70 pm
bend 2 cl -> 1 b <- 3 cl = 120.77 deg
bend 2 cl -> 1 b <- 4 h = 119.62 deg

cycle = 5 MP2 energy = -944.8493691030 |dE/dxyz| = 0.000034

zero point VIBRATIONAL energy : 0.0144556 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	a1	285.29	0.68185	YES	YES
8	a1	723.12	30.13211	YES	YES
9	b2	753.02	12.35831	YES	YES
10	b1	880.70	140.04511	YES	YES
11	b1	1067.81	241.19809	YES	YES
12	a1	2635.34	91.13096	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	17.23	9.98	0.37	-30.41	47.29	0.26891

$cosmo_energy
Total energy [a.u.] = -945.7162943085
Total energy + OC corr. [a.u.] = -945.7162041795
Total energy corrected [a.u.] = -945.7162492440 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0035568419
Diel. energy + OC corr. [a.u.] = -0.0034667129

$HBBr_2$

sy c2v

b1	0.0000	0.0000	0.8544
br2	1.6517	0.0000	-0.0706
br3	-1.6517	0.0000	-0.0706
h4	0.0000	0.0000	2.0338

dist 1 b -- 4 h = 2.2287 au = 117.94 pm
dist 1 b -- 2 br = 3.5774 au = 189.31 pm
dist 1 b -- 3 br = 3.5774 au = 189.31 pm
bend 2 br -> 1 b <- 3 br = 121.50 deg
bend 2 br -> 1 b <- 4 h = 119.25 deg

cycle = 5 MP2 energy = -5170.5915907131 |dE/dxyz| = 0.000018

zero point VIBRATIONAL energy : 0.0133904 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	a1	174.02	0.02670	YES	YES
8	a1	590.12	13.06509	YES	YES
9	b2	694.68	3.19659	YES	YES
10	b1	777.15	169.92891	YES	YES
11	b1	1004.59	192.84787	YES	YES
12	a1	2637.16	69.37600	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	18.32	11.05	0.69	-39.37	45.23	0.29206

$cosmo_energy
Total energy [a.u.] = -5173.7576359322
Total energy + OC corr. [a.u.] = -5173.7575842387
Total energy corrected [a.u.] = -5173.7576100855 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0033053237
Diel. energy + OC corr. [a.u.] = -0.0032536302

HBI_2

sy c2v

b1	0.0000	0.0000	0.9535
i2	1.8475	0.0000	-0.0491
i3	-1.8475	0.0000	-0.0491
h4	0.0000	0.0000	2.1337

dist 1 b -- 4 h = 2.2304 au = 118.03 pm
dist 1 b -- 2 i = 3.9722 au = 210.20 pm
dist 1 b -- 3 i = 3.9722 au = 210.20 pm
bend 2 i -> 1 b <- 3 i = 123.03 deg
bend 2 i -> 1 b <- 4 h = 118.49 deg

cycle = 5 MP2 energy = -48.0617650993 |dE/dxyz| = 0.000076

zero point VIBRATIONAL energy : 0.0125030 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	a1	118.00	0.04234	YES	YES
8	a1	486.40	3.25656	YES	YES
9	b2	631.96	0.19611	YES	YES
10	b1	678.88	195.19113	YES	YES
11	b1	934.31	208.60075	YES	YES
12	a1	2638.62	46.55152	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	18.98	11.83	1.03	-46.10	43.54	0.30897

T (K)	P (MPa)	Cv (kJ/mol-K)	Cp (kJ/mol-K)
298.15	0.1000000	0.0479770	0.0562913

$cosmo_energy
Total energy [a.u.] = -48.3855028605
Total energy + OC corr. [a.u.] = -48.3855653269
Total energy corrected [a.u.] = -48.3855340937 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0037448264
Diel. energy + OC corr. [a.u.] = -0.0038072929

H_2BF

sy c2v

b1	0.0000	0.0000	-0.0542
h2	1.0514	0.0000	-0.6098
h3	-1.0514	0.0000	-0.6098
f4	0.0000	0.0000	1.2700

dist 1 b -- 2 h = 2.2472 au = 118.92 pm
dist 1 b -- 3 h = 2.2472 au = 118.92 pm
dist 1 b -- 4 f = 2.5022 au = 132.41 pm
bend 2 h -> 1 b <- 3 h = 124.29 deg
bend 2 h -> 1 b <- 4 f = 117.85 deg

cycle = 7 MP2 energy = -125.7350123900 |dE/dxyz| = 0.000002

zero point VIBRATIONAL energy : 0.0220109 Hartree

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity 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	998.90	52.11917	YES	YES
8	b2	1055.08	80.91363	YES	YES
9	a1	1137.81	8.45555	YES	YES
10	a1	1329.31	165.36496	YES	YES
11	a1	2516.99	72.75603	YES	YES
12	b1	2623.57	197.77517	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	15.79	6.92	0.02	1.43	65.48	0.22316

$cosmo_energy
Total energy [a.u.] = -125.8301669347
Total energy + OC corr. [a.u.] = -125.8299552245
Total energy corrected [a.u.] = -125.8300610796 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0089265810
Diel. energy + OC corr. [a.u.] = -0.0087148708

H_2BCl

sy c2v

b1	0.0000	0.0000	-1.2533
h2	1.0432	0.0000	-1.8117
h3	-1.0432	0.0000	-1.8117
cl4	0.0000	0.0000	0.4852

dist 1 b -- 2 h = 2.2361 au = 118.33 pm
dist 1 b -- 3 h = 2.2361 au = 118.33 pm
dist 1 b -- 4 cl = 3.2853 au = 173.85 pm
bend 2 h -> 1 b <- 3 h = 123.68 deg
bend 2 h -> 1 b <- 4 cl = 118.16 deg

cycle = 5 MP2 energy = -485.6834728809 |dE/dxyz| = 0.000016

zero point VIBRATIONAL energy : 0.0205258 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	a1	817.29	67.67888	YES	YES
8	b1	839.46	9.67164	YES	YES
9	b2	959.30	33.53896	YES	YES
10	a1	1176.75	77.32155	YES	YES
11	a1	2549.76	86.76872	YES	YES
12	b1	2667.24	112.54388	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	16.42	7.59	0.05	-5.75	61.86	0.23508

$cosmo_energy
Total energy [a.u.] = -486.1506292777
Total energy + OC corr. [a.u.] = -486.1504815428
Total energy corrected [a.u.] = -486.1505554102 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0069287542
Diel. energy + OC corr. [a.u.] = -0.0067810193

H_2BBr

sy c2v

b1	0.0000	0.0000	-1.6205
h2	1.0438	0.0000	-2.1755
h3	-1.0438	0.0000	-2.1755
br4	0.0000	0.0000	0.2741

dist 1 b -- 2 h = 2.2339 au = 118.21 pm
dist 1 b -- 3 h = 2.2339 au = 118.21 pm
dist 1 b -- 4 br = 3.5803 au = 189.46 pm
bend 2 h -> 1 b <- 3 h = 124.00 deg
bend 2 h -> 1 b <- 4 br = 118.00 deg

cycle = 5 MP2 energy = -2598.5548155631 |dE/dxyz| = 0.000021

zero point VIBRATIONAL energy : 0.0199939 Hartree

$vibrational spectrum

# mode	symmetry	wave number cm**(-1)	IR intensity 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	a1	691.89	49.80558	YES	YES
8	b1	788.55	3.11078	YES	YES
9	b2	922.51	20.21663	YES	YES
10	a1	1146.62	83.56766	YES	YES
11	a1	2551.46	86.14645	YES	YES
12	b1	2675.26	86.64591	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	17.40	7.90	0.07	-10.40	60.63	0.24657

$cosmo_energy
Total energy [a.u.] = -2600.1720348850
Total energy + OC corr. [a.u.] = -2600.1718947174
Total energy corrected [a.u.] = -2600.1719648012 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0069451327
Diel. energy + OC corr. [a.u.] = -0.0068049650

H_2BI

sy c2v

b1	0.0000	0.0000	-0.2508
h2	1.0432	0.0000	-0.8062
h3	-1.0432	0.0000	-0.8062
i4	0.0000	0.0000	1.8507

dist 1 b -- 2 h = 2.2333 au = 118.18 pm
dist 1 b -- 3 h = 2.2333 au = 118.18 pm
dist 1 b -- 4 i = 3.9712 au = 210.15 pm
bend 2 h -> 1 b <- 3 h = 123.93 deg
bend 2 h -> 1 b <- 4 i = 118.03 deg

cycle = 8 MP2 energy = -37.2893077713 |dE/dxyz| = 0.000001

zero point VIBRATIONAL energy : 0.0194965 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	a1	588.37	35.99293	YES	YES
8	b1	720.20	0.01241	YES	YES
9	b2	883.65	11.75325	YES	YES
10	a1	1111.84	103.75676	YES	YES
11	a1	2561.51	87.62412	YES	YES
12	b1	2692.41	61.15759	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	18.01	8.16	0.11	-13.97	59.55	0.25489

$cosmo_energy
Total energy [a.u.] = -37.4865893736
Total energy + OC corr. [a.u.] = -37.4865628406
Total energy corrected [a.u.] = -37.4865761071 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0076609036
Diel. energy + OC corr. [a.u.] = -0.0076343705

BF_4^-

sy td

b1	0.0000	0.0000	0.0000
f2	0.8131	-0.8131	0.8131
f3	-0.8131	0.8131	0.8131
f4	-0.8131	-0.8131	-0.8131
f5	0.8131	0.8131	-0.8131

dist 1 b -- 2 f = 2.6613 au = 140.83 pm
dist 1 b -- 3 f = 2.6613 au = 140.83 pm
dist 1 b -- 4 f = 2.6613 au = 140.83 pm
dist 1 b -- 5 f = 2.6613 au = 140.83 pm
bend 2 f -> 1 b <- 3 f = 109.47 deg

cycle = 11 MP2 energy = -424.0427677090 |dE/dxyz| = 0.000008

zero point VIBRATIONAL energy : 0.0143580 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	346.20	0.00000	NO	YES
8	e	346.20	0.00000	NO	YES
9	t2	508.86	1.61634	YES	YES
10	t2	508.86	1.61634	YES	YES
11	t2	508.86	1.61634	YES	YES
12	a1	738.27	0.00000	NO	YES
13	t2	1115.05	336.91256	YES	YES
14	t2	1115.05	336.91256	YES	YES
15	t2	1115.05	336.91256	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	17.30	8.80	0.73	-28.80	49.21	0.26995

$cosmo_energy
Total energy [a.u.] = -424.2852407882
Total energy + OC corr. [a.u.] = -424.2859121384
Total energy corrected [a.u.] = -424.2855764633 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0842791131
Diel. energy + OC corr. [a.u.] = -0.0849504633

$FBCl_3^-$

sy c3v

b1	0.0000	0.0000	0.1078
f2	0.0000	0.0000	1.4809
cl3	-0.8832	1.5297	-0.5269
cl4	-0.8832	-1.5297	-0.5269
cl5	1.7664	0.0000	-0.5269

dist 1 b -- 2 f = 2.5949 au = 137.32 pm
dist 1 b -- 3 cl = 3.5469 au = 187.70 pm
dist 1 b -- 4 cl = 3.5469 au = 187.70 pm
dist 1 b -- 5 cl = 3.5469 au = 187.70 pm
bend 2 f -> 1 b <- 3 cl = 109.76 deg
bend 3 cl -> 1 b <- 4 cl = 109.18 deg

cycle = 6 MP2 energy = -1503.8946186630 |dE/dxyz| = 0.000008

zero point VIBRATIONAL energy : 0.0098467 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	192.86	0.04703	YES	YES
8	e	192.86	0.04703	YES	YES
9	a1	282.05	0.04094	YES	YES
10	e	329.98	1.66405	YES	YES
11	e	329.98	1.66405	YES	YES
12	a1	451.19	4.40235	YES	YES
13	e	712.79	348.05671	YES	YES
14	e	712.79	348.05671	YES	YES
15	a1	1117.71	230.47125	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	17.97	11.63	1.94	-52.35	40.79	0.32072

$cosmo_energy
Total energy [a.u.] = -1505.2543475338
Total energy + OC corr. [a.u.] = -1505.2554914354
Total energy corrected [a.u.] = -1505.2549194846 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0723648906
Diel. energy + OC corr. [a.u.] = -0.0735087922

$FBBr_3^-$

sy c3v

b1	0.0000	0.0000	0.1455
f2	0.0000	0.0000	1.5095
br3	-0.9631	1.6682	-0.5480
br4	-0.9631	-1.6682	-0.5480
br5	1.9262	0.0000	-0.5480

dist 1 b -- 2 f = 2.5776 au = 136.40 pm
dist 1 b -- 3 br = 3.8688 au = 204.73 pm
dist 1 b -- 4 br = 3.8688 au = 204.73 pm
dist 1 b -- 5 br = 3.8688 au = 204.73 pm
bend 2 f -> 1 b <- 3 br = 109.80 deg
bend 2 f -> 1 b <- 4 br = 109.80 deg

cycle = 6 MP2 energy = -7842.5194205649 |dE/dxyz| = 0.000022

zero point VIBRATIONAL energy : 0.0081612 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	116.65	0.23488	YES	YES
8	e	116.65	0.23488	YES	YES
9	a1	174.57	0.43648	YES	YES
10	e	254.68	2.77121	YES	YES
11	e	254.68	2.77121	YES	YES
12	a1	340.47	0.64305	YES	YES
13	e	598.22	326.24848	YES	YES
14	e	598.22	326.24848	YES	YES
15	a1	1128.21	200.36068	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	12.94	3.28	-65.87	38.54	0.35850

$cosmo_energy
Total energy [a.u.] = -7847.3254234119
Total energy + OC corr. [a.u.] = -7847.3276265862
Total energy corrected [a.u.] = -7847.3265249990 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0676967158
Diel. energy + OC corr. [a.u.] = -0.0698998901

FBI_3^-

sy c3v

b1	0.0000	0.0000	0.1896
f2	0.0000	0.0000	1.5500
i3	-1.0713	1.8556	-0.5658
i4	-1.0713	-1.8556	-0.5658
i5	2.1427	0.0000	-0.5658

dist 1 b -- 2 f = 2.5708 au = 136.04 pm
dist 1 b -- 3 i = 4.2933 au = 227.19 pm
dist 1 b -- 4 i = 4.2933 au = 227.19 pm
dist 1 b -- 5 i = 4.2933 au = 227.19 pm
bend 2 f -> 1 b <- 3 i = 109.42 deg
bend 2 f -> 1 b <- 4 i = 109.42 deg

cycle = 8 MP2 energy = -158.7334186535 |dE/dxyz| = 0.000003

zero point VIBRATIONAL energy : 0.0072585 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	80.78	0.36669	YES	YES
8	e	80.78	0.36669	YES	YES
9	a1	118.76	0.42277	YES	YES
10	e	216.38	4.04993	YES	YES
11	e	216.38	4.04993	YES	YES
12	a1	278.11	0.02718	YES	YES
13	e	512.69	376.49979	YES	YES
14	e	512.69	376.49979	YES	YES
15	a1	1169.55	194.77130	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	13.91	4.44	-75.10	37.55	0.38613

$cosmo_energy
Total energy [a.u.] = -159.2785579651
Total energy + OC corr. [a.u.] = -159.2844283684
Total energy corrected [a.u.] = -159.2814931667 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0595529857
Diel. energy + OC corr. [a.u.] = -0.0654233890

HBF_3^-

sy c3v

b1	0.0000	0.0000	0.0493
h2	0.0000	0.0000	1.2798
f3	-0.6663	1.1540	-0.4447
f4	-0.6663	-1.1540	-0.4447
f5	1.3325	0.0000	-0.4447

dist 1 b -- 2 h = 2.3252 au = 123.04 pm
dist 1 b -- 3 f = 2.6857 au = 142.12 pm
dist 1 b -- 4 f = 2.6857 au = 142.12 pm
dist 1 b -- 5 f = 2.6857 au = 142.12 pm
bend 2 h -> 1 b <- 3 f = 110.34 deg
bend 2 h -> 1 b <- 4 f = 110.34 deg

cycle = 7 MP2 energy = -324.8114542599 |dE/dxyz| = 0.000001

zero point VIBRATIONAL energy : 0.0199505 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	412.48	0.04924	YES	YES
8	e	412.48	0.04924	YES	YES
9	a1	587.71	3.13676	YES	YES
10	e	935.06	31.46298	YES	YES
11	e	935.06	31.46298	YES	YES
12	a1	940.80	119.20244	YES	YES
13	e	1184.96	324.04778	YES	YES
14	e	1184.96	324.04778	YES	YES
15	a1	2163.73	596.38218	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	16.95	9.59	0.39	-14.38	62.28	0.26543

$cosmo_energy
Total energy [a.u.] = -325.0320804568
Total energy + OC corr. [a.u.] = -325.0338298619
Total energy corrected [a.u.] = -325.0329551593 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0859813823
Diel. energy + OC corr. [a.u.] = -0.0877307874

$FBHCl_2^-$

sy cs

b1	0.1052	-0.1275	0.0000
h2	1.3060	-0.1939	0.0000
f3	-0.5242	-1.3651	0.0000
cl4	-0.4383	0.8450	-1.5479
cl5	-0.4383	0.8450	1.5479

dist 1 b -- 2 h = 2.2726 au = 120.26 pm
dist 1 b -- 3 f = 2.6237 au = 138.84 pm
dist 1 b -- 4 cl = 3.6040 au = 190.71 pm
dist 1 b -- 5 cl = 3.6040 au = 190.71 pm
bend 2 h -> 1 b <- 3 f = 113.80 deg
bend 2 h -> 1 b <- 4 cl = 108.22 deg
bend 3 f -> 1 b <- 4 cl = 108.98 deg

cycle = 8 MP2 energy = -1044.7250651140 |dE/dxyz| = 0.000026

zero point VIBRATIONAL energy : 0.0172233 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'	208.83	0.46976	YES	YES
8	a''	289.56	3.49419	YES	YES
9	a'	370.11	1.80796	YES	YES
10	a''	590.23	210.84664	YES	YES
11	a'	601.08	42.65255	YES	YES
12	a''	986.92	229.15971	YES	YES
13	a'	1001.81	35.18507	YES	YES
14	a'	1126.97	267.72101	YES	YES
15	a'	2384.65	367.61611	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	17.54	11.92	1.06	-30.42	57.23	0.30231

$cosmo_energy
Total energy [a.u.] = -1045.6869224228
Total energy + OC corr. [a.u.] = -1045.6885622327
Total energy corrected [a.u.] = -1045.6877423277 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0761925709
Diel. energy + OC corr. [a.u.] = -0.0778323808

$FBHBr_2^-$

sy cs

b1	0.1167	-0.1761	0.0000
h2	1.3104	-0.2680	0.0000
f3	-0.5667	-1.3724	0.0000
br4	-0.4233	0.9146	-1.6910
br5	-0.4233	0.9146	1.6910

dist 1 b -- 2 h = 2.2624 au = 119.72 pm
dist 1 b -- 3 f = 2.6036 au = 137.77 pm
dist 1 b -- 4 br = 3.9372 au = 208.35 pm
dist 1 b -- 5 br = 3.9372 au = 208.35 pm
bend 2 h -> 1 b <- 3 f = 115.33 deg
bend 2 h -> 1 b <- 4 br = 107.37 deg
bend 3 f -> 1 b <- 4 br = 109.03 deg

cycle = 9 MP2 energy = -5270.4786986365 |dE/dxyz| = 0.000035

zero point VIBRATIONAL energy : 0.0163695 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'	126.60	0.64223	YES	YES
8	a''	233.61	5.43741	YES	YES
9	a'	288.82	0.55362	YES	YES
10	a''	510.94	216.66601	YES	YES
11	a'	517.82	23.88661	YES	YES
12	a''	928.42	264.65065	YES	YES
13	a'	1012.97	22.52527	YES	YES
14	a'	1119.66	277.65603	YES	YES
15	a'	2446.55	272.45542	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	18.48	12.93	1.66	-38.99	56.09	0.32724

$cosmo_energy
Total energy [a.u.] = -5273.7388560925
Total energy + OC corr. [a.u.] = -5273.7413148121
Total energy corrected [a.u.] = -5273.7400854523 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0718505659
Diel. energy + OC corr. [a.u.] = -0.0743092855

$FBHI_2^-$

sy cs

b1	0.2368	-0.1338	0.0000
f2	0.2719	-1.5046	0.0000
h3	1.2909	0.4269	0.0000
i4	-0.8819	0.5916	1.8829
i5	-0.8819	0.5916	-1.8829

dist 1 b -- 3 h = 2.2564 au = 119.40 pm
dist 1 b -- 2 f = 2.5913 au = 137.13 pm
dist 1 b -- 4 i = 4.3599 au = 230.71 pm
dist 1 b -- 5 i = 4.3599 au = 230.71 pm
bend 2 f -> 1 b <- 3 h = 116.54 deg
bend 2 f -> 1 b <- 4 i = 109.07 deg
bend 3 h -> 1 b <- 4 i = 106.29 deg

cycle = 8 MP2 energy = -147.9577583158 |dE/dxyz| = 0.000053

zero point VIBRATIONAL energy : 0.0157457 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'	83.38	0.49043	YES	YES
8	a''	193.62	16.28605	YES	YES
9	a'	235.42	0.37060	YES	YES
10	a''	423.85	296.69260	YES	YES
11	a'	441.76	14.43200	YES	YES
12	a''	871.43	396.87905	YES	YES
13	a'	1002.93	48.16136	YES	YES
14	a'	1144.41	305.76711	YES	YES
15	a'	2514.76	174.69227	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	19.08	13.68	2.28	-45.52	55.39	0.34677

$cosmo_energy
Total energy [a.u.] = -148.3799048627
Total energy + OC corr. [a.u.] = -148.3859256664
Total energy corrected [a.u.] = -148.3829152645 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0638408609
Diel. energy + OC corr. [a.u.] = -0.0698616646

$BH_2F_2^-$

sy c2v

b1	0.0563	-0.0000	0.0000
h2	0.7520	-1.0246	0.0000
f3	-0.7855	0.0000	1.1671
f4	-0.7855	0.0000	-1.1671
h5	0.7520	1.0245	0.0000

dist 1 b -- 2 h = 2.3403 au = 123.84 pm
dist 1 b -- 5 h = 2.3403 au = 123.84 pm
dist 1 b -- 3 f = 2.7195 au = 143.91 pm
dist 1 b -- 4 f = 2.7195 au = 143.91 pm
bend 2 h -> 1 b <- 3 f = 109.19 deg
bend 2 h -> 1 b <- 5 h = 111.65 deg
bend 3 f -> 1 b <- 4 f = 108.39 deg

cycle = 8 MP2 energy = -225.5782790730 |dE/dxyz| = 0.000006

zero point VIBRATIONAL energy : 0.0245251 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'	450.19	0.36920	YES	YES
8	a'	909.46	47.99463	YES	YES
9	a''	915.86	40.86061	YES	YES
10	a''	937.99	0.00000	YES	YES
11	a'	981.22	111.31907	YES	YES
12	a'	1135.82	152.81999	YES	YES
13	a''	1256.40	345.06413	YES	YES
14	a'	2060.26	853.59040	YES	YES
15	a'	2118.06	354.54312	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	16.50	9.64	0.17	-0.81	73.11	0.25625

$cosmo_energy
Total energy [a.u.] = -225.7786581356
Total energy + OC corr. [a.u.] = -225.7819116022
Total energy corrected [a.u.] = -225.7802848689 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0878972167
Diel. energy + OC corr. [a.u.] = -0.0911506833

FBH_2Cl^-

sy cs

b1	-0.1067	-0.1432	0.0000
f2	0.9314	-1.1059	0.0000
h3	-0.7684	-0.1973	1.0195
h4	-0.7684	-0.1973	-1.0195
cl5	0.7144	1.6403	0.0000

dist 1 b -- 3 h = 2.2991 au = 121.66 pm
dist 1 b -- 4 h = 2.2991 au = 121.66 pm
dist 1 b -- 2 f = 2.6755 au = 141.58 pm
dist 1 b -- 5 cl = 3.7103 au = 196.34 pm
bend 2 f -> 1 b <- 3 h = 111.63 deg
bend 2 f -> 1 b <- 5 cl = 108.12 deg
bend 3 h -> 1 b <- 4 h = 113.86 deg
bend 3 h -> 1 b <- 5 cl = 105.53 deg

cycle = 7 MP2 energy = -585.5451467502 |dE/dxyz| = 0.000140

zero point VIBRATIONAL energy : 0.0236088 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'	293.62	4.70020	YES	YES
8	a'	518.29	70.83025	YES	YES
9	a''	792.06	9.78414	YES	YES
10	a'	960.63	58.42299	YES	YES
11	a''	969.67	31.60796	YES	YES
12	a'	1090.88	240.25487	YES	YES
13	a'	1206.68	206.52696	YES	YES
14	a'	2262.40	299.05187	YES	YES
15	a''	2268.84	556.49890	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	16.92	10.36	0.41	-6.66	71.64	0.27093

$cosmo_energy
Total energy [a.u.] = -586.1131301428
Total energy + OC corr. [a.u.] = -586.1158913845
Total energy corrected [a.u.] = -586.1145107636 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0818102666
Diel. energy + OC corr. [a.u.] = -0.0845715083

FBH_2Br^-

sy cs

b1	-0.2125	0.1162	0.0000
f2	-1.0862	-0.9830	0.0000
br3	1.8195	-0.6558	0.0000
h4	-0.2695	0.7603	1.0236
h5	-0.2695	0.7603	-1.0236

dist 1 b -- 4 h = 2.2880 au = 121.07 pm
dist 1 b -- 5 h = 2.2880 au = 121.07 pm
dist 1 b -- 2 f = 2.6534 au = 140.41 pm
dist 1 b -- 3 br = 4.1078 au = 217.37 pm
bend 2 f -> 1 b <- 3 br = 107.68 deg
bend 2 f -> 1 b <- 4 h = 112.78 deg
bend 3 br -> 1 b <- 4 h = 103.47 deg
bend 4 h -> 1 b <- 5 h = 115.43 deg

cycle = 8 MP2 energy = -2698.4256407440 |dE/dxyz| = 0.000074

zero point VIBRATIONAL energy : 0.0234372 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'	224.22	4.86836	YES	YES
8	a'	428.95	52.11569	YES	YES
9	a''	737.40	2.09025	YES	YES
10	a''	973.77	29.52320	YES	YES
11	a'	990.79	80.87433	YES	YES
12	a'	1057.08	309.09826	YES	YES
13	a'	1212.59	169.41027	YES	YES
14	a'	2316.16	255.72423	YES	YES
15	a''	2346.75	451.57917	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	17.68	10.79	0.60	-10.54	71.67	0.28406

$cosmo_energy
Total energy [a.u.] = -2700.1428484337
Total energy + OC corr. [a.u.] = -2700.1460077270
Total energy corrected [a.u.] = -2700.1444280803 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0787022517
Diel. energy + OC corr. [a.u.] = -0.0818615450

FBH_2I^-

sy cs

b1	-0.3239	-0.0477	0.0000
f2	-0.4258	-1.4369	0.0000
i3	2.0507	0.5038	0.0000
h4	-0.6848	0.4689	1.0278
h5	-0.6848	0.4689	-1.0278

dist 1 b -- 4 h = 2.2782 au = 120.56 pm
dist 1 b -- 5 h = 2.2782 au = 120.56 pm
dist 1 b -- 2 f = 2.6323 au = 139.30 pm
dist 1 b -- 3 i = 4.6068 au = 243.78 pm
bend 2 f -> 1 b <- 3 i = 107.27 deg
bend 2 f -> 1 b <- 4 h = 113.92 deg
bend 3 i -> 1 b <- 4 h = 101.22 deg
bend 4 h -> 1 b <- 5 h = 116.98 deg

cycle = 11 MP2 energy = -137.1693062604 |dE/dxyz| = 0.000030

zero point VIBRATIONAL energy : 0.0232552 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'	149.26	10.08525	YES	YES
8	a'	322.74	44.28029	YES	YES
9	a''	648.62	0.75341	YES	YES
10	a''	976.91	34.54662	YES	YES
11	a'	993.47	533.26711	YES	YES
12	a'	1039.64	37.43522	YES	YES
13	a'	1225.91	158.89266	YES	YES
14	a'	2395.70	187.42421	YES	YES
15	a''	2455.63	326.52125	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	18.20	11.14	0.97	-14.10	71.90	0.29674

$cosmo_energy
Total energy [a.u.] = -137.4695252572
Total energy + OC corr. [a.u.] = -137.4757397363
Total energy corrected [a.u.] = -137.4726324967 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0723919069
Diel. energy + OC corr. [a.u.] = -0.0786063859

OCF_2

sy 2v

o1	0.0000	0.0000	1.3383
c2	0.0000	0.0000	0.1621
f3	-1.0612	0.0000	-0.6148
f4	1.0612	0.0000	-0.6148

dist 1 o -- 2 c = 2.2227 au = 117.62 pm
dist 2 c -- 3 f = 2.4853 au = 131.52 pm
dist 2 c -- 4 f = 2.4853 au = 131.52 pm
bend 1 o -> 2 c <- 3 f = 126.20 deg
bend 3 f -> 2 c <- 4 f = 107.59 deg

cycle = 6 MP2 energy = -312.6254593680 |dE/dxyz| = 0.000002

zero point VIBRATIONAL energy : 0.0137934 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	a1	566.97	4.76134	YES	YES
8	b1	601.14	5.15033	YES	YES
9	b2	749.69	28.39992	YES	YES
10	a1	949.99	49.65953	YES	YES
11	b1	1229.74	405.59757	YES	YES
12	a1	1957.09	412.45082	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	16.89	9.67	0.16	-30.03	44.94	0.25979

$cosmo_energy
Total energy [a.u.] = -312.8060260751
Total energy + OC corr. [a.u.] = -312.8060355925
Total energy corrected [a.u.] = -312.8060308338 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0032432575
Diel. energy + OC corr. [a.u.] = -0.0032527749

OCF_3^-

sy c3v

c1	0.0000	0.0000	0.2067
o2	0.0000	0.0000	1.4236
f3	-0.6336	-1.0975	-0.4432
f4	-0.6336	1.0975	-0.4432
f5	1.2673	0.0000	-0.4432

dist 1 c -- 2 o = 2.2996 au = 121.69 pm
dist 1 c -- 3 f = 2.6913 au = 142.42 pm
dist 1 c -- 4 f = 2.6913 au = 142.42 pm
dist 1 c -- 5 f = 2.6913 au = 142.42 pm
bend 2 o -> 1 c <- 3 f = 117.15 deg
bend 3 f -> 1 c <- 4 f = 100.82 deg

cycle = 7 MP2 energy = -412.4365161528 |dE/dxyz| = 0.000009

zero point VIBRATIONAL energy : 0.0154029 Hartree

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	17.27	10.05	0.60	-28.75	51.55	0.27764

$cosmo_energy
Total energy [a.u.] = -412.7232234380
Total energy + OC corr. [a.u.] = -412.7236256774
Total energy corrected [a.u.] = -412.7234245577 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0860596716
Diel. energy + OC corr. [a.u.] = -0.0864619110

$Ag(CHI_3)^+$ (2 contacts)

sy cs

ag1	-2.5042	0.2142	0.0000
i2	-0.3433	-0.1316	1.7842
i3	-0.3433	-0.1316	-1.7842
i4	2.7355	0.1547	0.0000
c5	0.7725	-0.6343	0.0000
h6	0.8310	-1.7161	0.0000

dist 5 c -- 6 h = 2.0473 au = 108.34 pm
dist 4 i -- 5 c = 3.9981 au = 211.57 pm
dist 2 i -- 5 c = 4.0886 au = 216.36 pm
dist 1 ag -- 3 i = 5.3358 au = 282.36 pm
bend 2 i -> 1 ag <- 3 i = 78.38 deg
bend 6 h -> 5 c <- 4 i = 108.80 deg
bend 6 h -> 5 c <- 3 i = 105.06 deg

cycle = 8 SCF+MP2 energy = -218.8574758031 |dE/dxyz| = 0.000285

$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'	8.94	0.37277	YES	YES
8	a''	80.45	0.87598	YES	YES
9	a'	90.58	3.42692	YES	YES
10	a''	97.06	0.34737	YES	YES
11	a'	134.47	5.57238	YES	YES
12	a'	151.11	0.30940	YES	YES
13	a'	404.29	10.76183	YES	YES
14	a''	457.10	45.86863	YES	YES
15	a'	548.02	123.78427	YES	YES
16	a''	1030.06	31.88292	YES	YES
17	a'	1059.56	60.39300	YES	YES
18	a'	3101.23	29.54391	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	19.93	15.39	8.07	-64.73	64.24	0.44089

$cosmo_energy
Total energy [a.u.] = -219.9354594716
Total energy + OC corr. [a.u.] = -219.9329138270
Total energy corrected [a.u.] = -219.9341866493 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0722766493
Diel. energy + OC corr. [a.u.] = -0.0697310047

Electronic excitation spectrum of agi3+, IRREP a'
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.53378709967539E+03 0.67242235729938E-02
0.42672504439133E+03 0.17990573998993E-01
0.41768852289899E+03 0.12806337403327E-02

0.34957216809236E+03 0.40053678759222E-02
0.31732296754704E+03 0.59979077019821E-01
0.30002037736767E+03 0.95118461336367E-02
0.28879475656460E+03 0.18617070022098E-01
0.26401463922307E+03 0.17480662908059E-01
0.26212152036539E+03 0.12275514948244E-02
0.25957287818904E+03 0.55328786476763E-02
0.25513028457617E+03 0.76821453228585E-01
0.24593420388727E+03 0.10110957205129E-01
0.24044516015346E+03 0.18521921965050E-02
0.22871707132103E+03 0.51618471239833E-02
0.22699621967857E+03 0.33411206803985E-02
0.22483407521502E+03 0.29467807289646E-01
0.21171390757949E+03 0.12396491068497E+00
0.19992707656039E+03 0.30770254408394E-02
0.19955237894999E+03 0.51831538121448E-03
0.19545585180722E+03 0.95902218935837E-01
Electronic excitation spectrum of agi3+, IRREP a"
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.55011961303777E+03 0.46596947655391E-02
0.46575084282040E+03 0.20762372427417E-03
0.44040903218750E+03 0.23722712524969E-02
0.39898079217437E+03 0.33531544739546E-04
0.35719394490086E+03 0.14576771793782E-01
0.33700260745901E+03 0.78868215394037E-03
0.32320768143421E+03 0.15874285796649E-01
0.27106184326473E+03 0.18181076125355E-02
0.26369495847915E+03 0.65935704666686E-04
0.25451754538401E+03 0.25127553537674E-02
0.24104024879294E+03 0.26395480669902E-04
0.23642703218767E+03 0.13701773465506E-01
0.23127815510085E+03 0.16662115740418E-03
0.22397013436354E+03 0.30110864858973E-02
0.22072784454348E+03 0.50668888263231E-02
0.21228467686915E+03 0.25548706704022E-01
0.20219883709552E+03 0.87229693763458E-05
0.19995829928338E+03 0.26527624523435E-03
0.19705350592245E+03 0.72677300211147E-04
0.19139864237667E+03 0.14234079823681E-01

$Ag(CHI_3)^+$ (3 contacts)

sy c3v

ag1	0.0000	0.0000	-2.2381
i2	-1.0169	1.7614	-0.0208
i3	-1.0169	-1.7614	-0.0208
i4	2.0339	0.0000	-0.0208
c5	0.0000	0.0000	0.6679
h6	0.0000	0.0000	1.7530

dist 5 c -- 6 h = 2.0506 au = 108.52 pm
dist 2 i -- 5 c = 4.0578 au = 214.73 pm
dist 1 ag -- 2 i = 5.6860 au = 300.89 pm
bend 6 h -> 5 c <- 4 i = 108.70 deg
bend 5 c -> 4 i <- 1 ag = 66.18 deg
bend 2 i -> 1 ag <- 3 i = 71.66 deg

cycle = 9 MP2 energy = -218.8559769201 |dE/dxyz| = 0.000006

zero point VIBRATIONAL energy : 0.0161822 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	31.51	1.91277	YES	YES
8	e	31.51	1.91277	YES	YES
9	a1	101.57	4.44091	YES	YES
10	e	107.50	0.02874	YES	YES
11	e	107.50	0.02874	YES	YES
12	a1	159.94	0.15891	YES	YES
13	a1	458.74	0.33340	YES	YES
14	e	492.45	38.96812	YES	YES
15	e	492.45	38.96812	YES	YES
16	e	1026.42	18.79106	YES	YES
17	e	1026.42	18.79106	YES	YES
18	a1	3067.14	37.24323	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	19.93	14.09	7.62	-60.74	63.91	0.42641

$cosmo_energy
Total energy [a.u.] = -219.9290161388
Total energy + OC corr. [a.u.] = -219.9263211375
Total energy corrected [a.u.] = -219.9276686382 Note: incorrect value contained for downward compatibility
Dielectric energy [a.u.] = -0.0705988394
Diel. energy + OC corr. [a.u.] = -0.0679038381

Electronic excitation spectrum of , IRREP a1
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.31607273053563E+03 0.25005035369239E-01
0.28371591651209E+03 0.61486773451736E-03

0.27189773507663E+03 0.43936509535694E-03
0.25048272003894E+03 0.13045226278892E+00
0.23885029104344E+03 0.36837242578916E-01
0.22936888911294E+03 0.11196330412586E-02
0.19478035173718E+03 0.74917026193838E-03
0.18105693238068E+03 0.14110416818928E-02
0.17439396897676E+03 0.99864927740576E-01
0.16450772377985E+03 0.38195313651121E-02
Electronic excitation spectrum of , IRREP e
singlet excitations
excitation energy / nm oscillator strength (length rep.)
0.50669314772522E+03 0.14855799171806E-04
0.39781311855897E+03 0.14819864859552E-02
0.34099414193848E+03 0.40054764059776E-01
0.30386492351578E+03 0.23544038752032E-03
0.29178899999391E+03 0.37918161145112E-01
0.28198385285014E+03 0.14092425493835E-01
0.27454669979107E+03 0.17424277130110E-01
0.25748636489448E+03 0.13813012650908E-02
0.23792905790829E+03 0.42920063949307E-01
0.22948145805244E+03 0.47642076277666E-03