Electronic Supporting Information

To

Two Synthetic Approaches for the Preparation of Tin(II) Dications

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Contents

Experimental Details Towards Assignment of 1

All manipulations were performed by using Schlenk or dry box techniques and argon atmosphere. $[NO][Al(OR^F)_4]$[1] and $[SnCp][Al(OR^F)_4]$[2] were synthesized according to literature procedures. 1,1,1,3,3,3-Hexafluoro-2-trifluoromethyl-2-propanol was dried with P_4O_{10}. All solvents were distilled prior to use. Pyrazine and PPh_3 were purchased from Acros and used without further purification, dmap was purchased from Sigma-Aldrich and purified by drying the dissolved dmap in toluene over CaH_2, filtration and distillation of dmap after removing toluene *in vacuo*. Tin powder (99.8 %, 2N8) was purchased from ABCR and used without further purification.

NMR spectra were recorded at room temperature on a Bruker Avance III HD 300 and a Bruker DSX500 spectrometer. Chemical shifts are given with respect to TMS for ^1H, $CFCl_3$ for ^{19}F, Me_4Sn for ^{119}Sn and 1.1 M $Al(NO_3)_3$ in D_2O for ^{27}Al.

FT-IR spectra were recorded on a BRUKER Alpha equipped with a Platinum ATR (diamond) unit in a glove box. For measurements and analysis OPUS 7.5 respectively OPUS 7.0 (both BRUKER Optic GmbH) were used. Raman spectra were recorded on a Bruker Vertex70 IR-spectrometer with the RAM II Raman module.

Due to the high fluorine content of the compounds, combustion analyses are notoriously unreliable and, therefore, we refrained using those for assessment of purity issues.

$[Sn(MeCN)_6][Al(OR^F)_4]_2$ (1): An excess of tin (0.358 g, 3.01 mmol, 1.50 eq) and $[NO][Al(OR^F)_4]$ (2.00 g, 2.01 mmol) were filled into a Schlenk flask and while stirring, MeCN (5 mL) was added. The mixture was stirred overnight. After the excess tin powder had completely settled on the bottom of the flask, the solution was transferred into a fresh Schlenk flask. After removing the solvent *in vacuo*, **1** was obtained as off-white solid (1.86 g, 0.809 mmol, 81 %). ^1H-NMR (300.18 MHz, CD_3CN, 298 K): 1.96 ppm (s, 18 H, $[Sn(\boldsymbol{H}_3CCN)_6][Al(OR^F)_4]_2$). ^{19}F-NMR (282.45 MHz, CD_3CN, 298 K) −76.0 ppm (s, 72 F, $[Sn(MeCN)_6][Al\{OC(C\boldsymbol{F}_3)_3\}_4]_2$). ^{119}Sn-NMR (111.94 MHz, CD_3CN, 298 K): −1490 ppm (s, 1 Sn, $[\boldsymbol{Sn}(MeCN)_6][Al(OR^F)_4]_2$). ^{27}Al-NMR (78.22 MHz, CD_3CN, 298 K): 34.5 ppm (s, 2 Al, $[Sn(MeCN)_6][\boldsymbol{Al}(OR^F)_4]_2$). IR (400-4000 cm^{-1}, Diamond ATR, corrected): 2949 (vw), 2320 (vw), 2305 (vw), 2291 (vw), 2272 (vw), 1352 (w), 1297 (w), 1273 (m), 1241 (s), 1211 (vs), 1166 (m), 1035 (vw), 969 (vs), 926 (vw), 831 (vw), 756 (vw), 726 (m), 571 (vw), 560 (vw), 536 (vw), 442 (vw), 402 (vw).

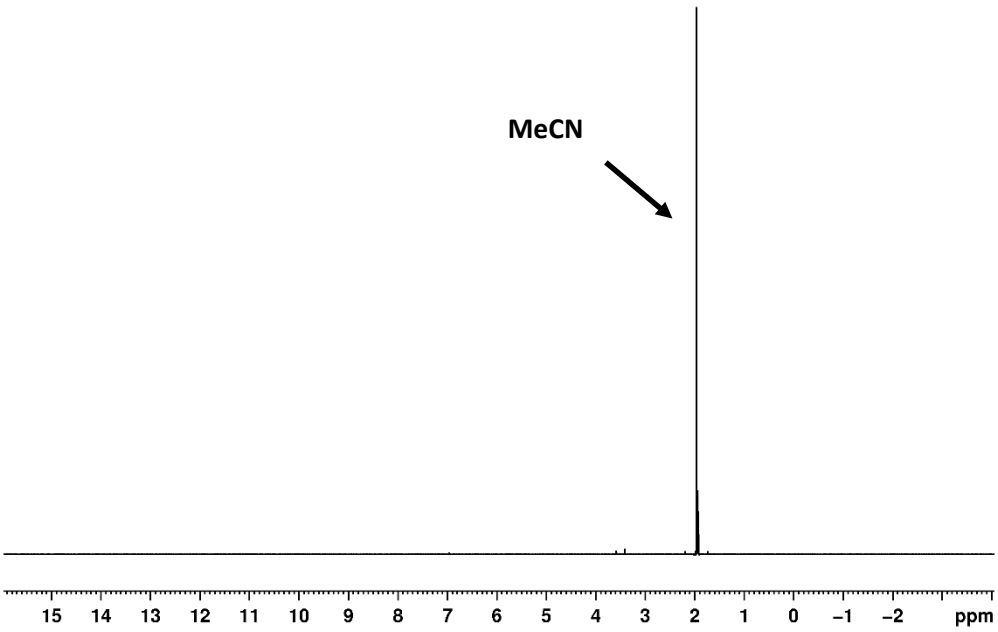


Figure S 1. ^{1}H-NMR spectrum (300.18 MHz) of **1** in CD_3CN at 298 K.

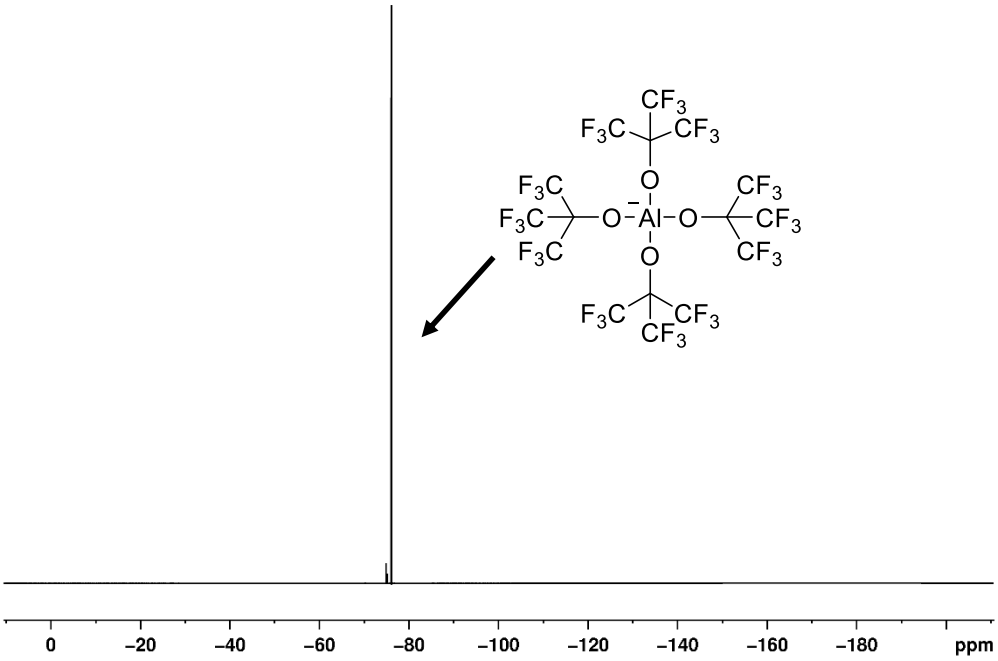


Figure S 2. ^{19}F-NMR spectrum (282.45 MHz) of **1** in CD_3CN at 298 K.

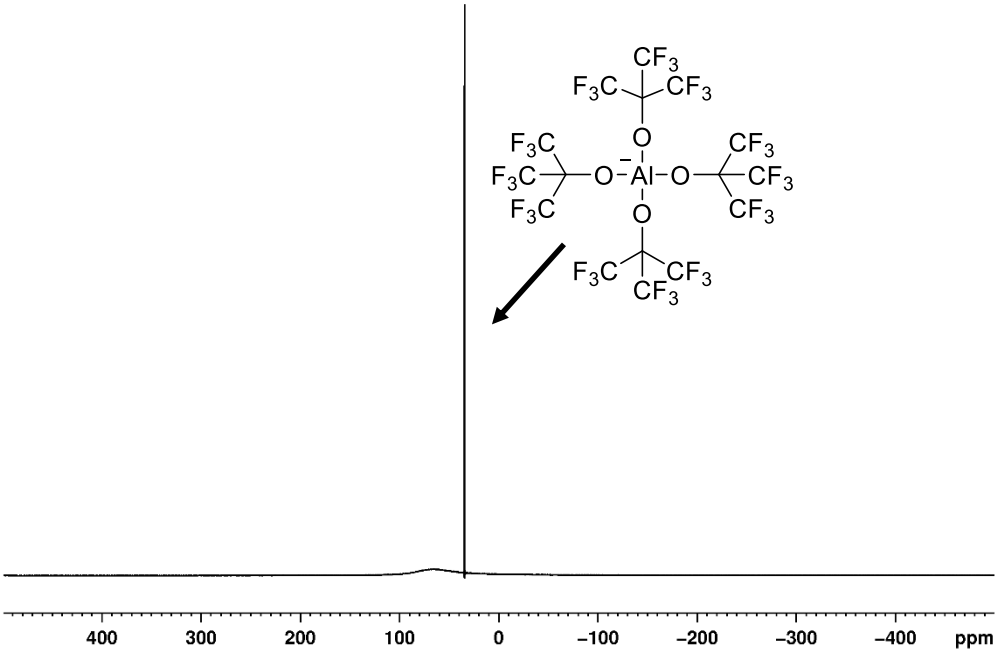


Figure S 3. ^{27}Al-NMR spectrum (78.22 MHz) of **1** in CD_3CN at 298 K.

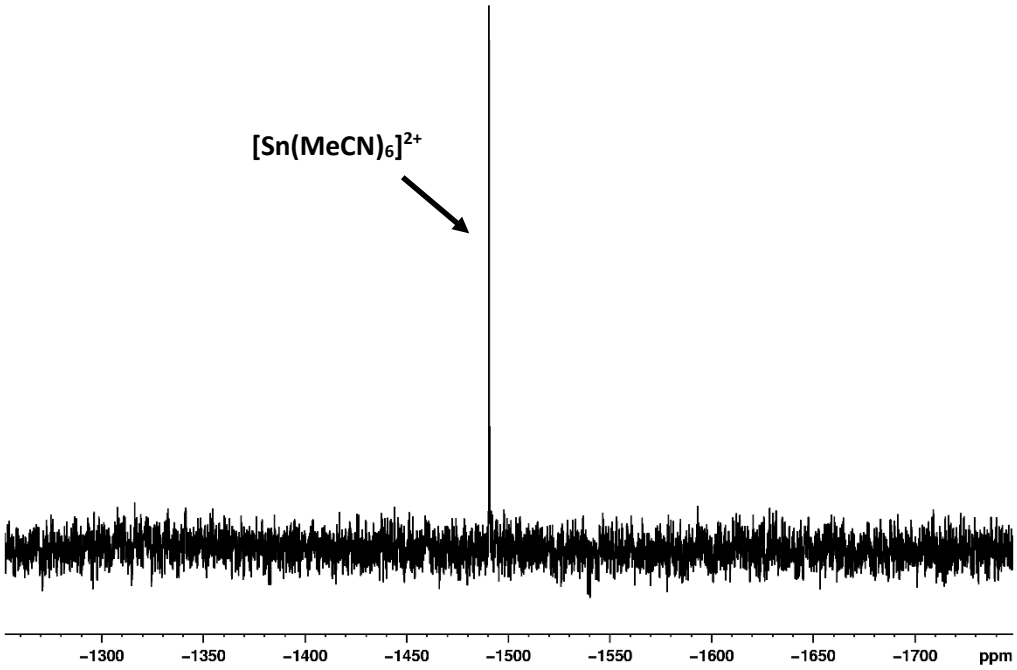


Figure S 4. ^{119}Sn-NMR spectrum (111.94 MHz) of **1** in CD_3CN at 298 K.

In the ^{119}Sn MAS NMR spectrum (Figure S5) two ^{119}Sn resonances are detected at -1270 ppm and -1277 ppm. This compares well to the findings from the crystal data where two different coordination environments of Sn^{2+} with six CH_3CN ligands were obtained. Quantum chemical calculations predict a chemical shift difference for these two coordination environments of 2 ppm in the ^{119}Sn NMR, which is in good accordance with the experimental spectrum. However, the ^{119}Sn chemical shift of -1490 ppm found for **1** in a solution of CD_3CN differs significantly from the chemical shifts detected in the solid state and cannot be explained by an exchange between these two environments in solution. In fact the main species in a solution of acetonitrile must exhibit a quite different coordination sphere for the Sn^{2+} cation. Again in quantum chemical calculations a highfield shift comparable to that observed in experiment could only be produced by a Sn^{2+} cation symmetrically coordinated with eight acetonitrile molecules. The energetics of the formation of such a complex allows for its existence and we therefore consider it to be the species predominant in a solution of **1** in acetonitrile.

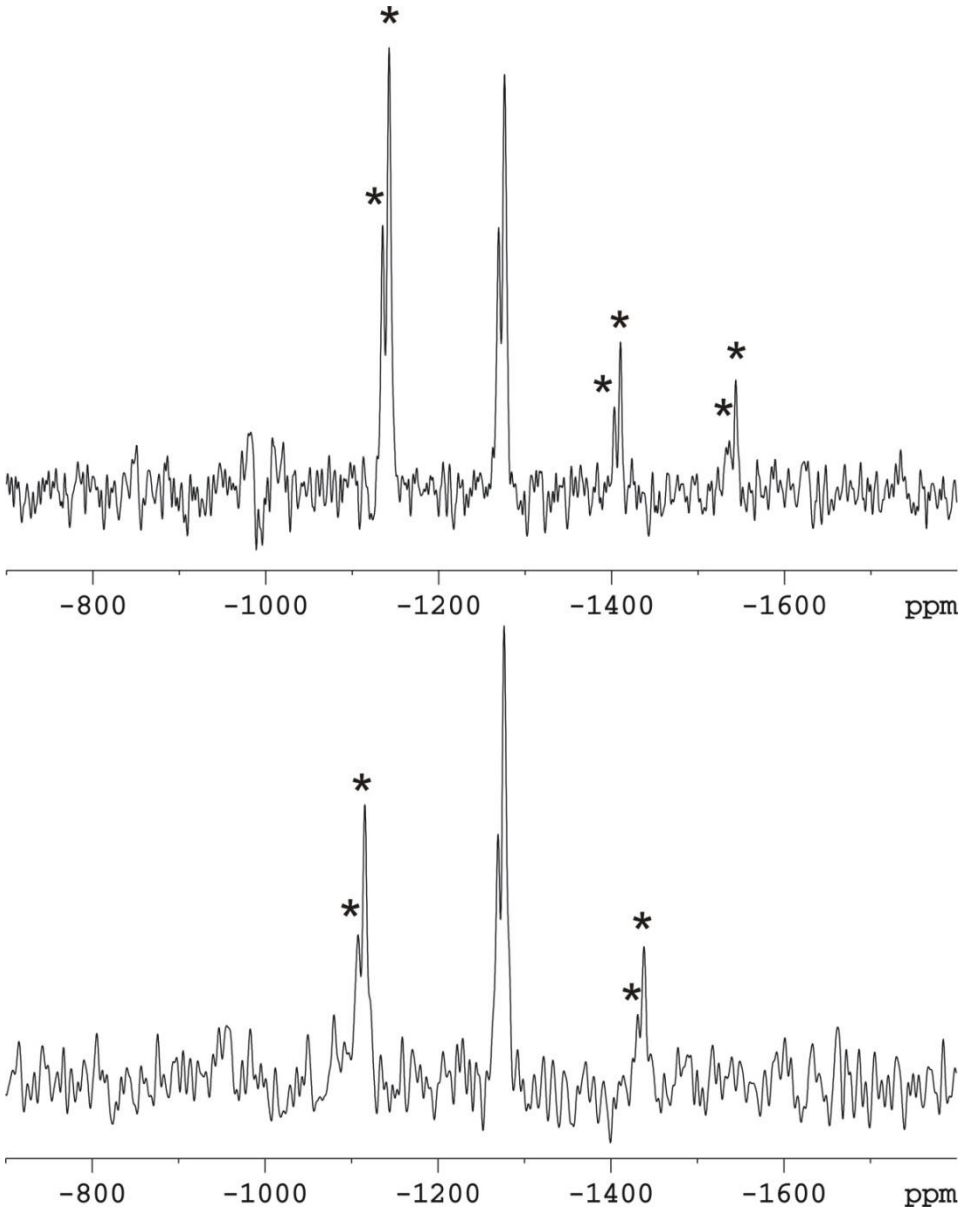


Figure S5. ^{119}Sn MAS NMR (186.5 MHz) spectra (Hahn echo) of **1** at rotation frequencies of 25 kHz (above) and 30 kHz (below). Rotational sidebands are marked by asterisk.

A new batch of material was prepared for the above solid state NMR-spectra, at its purity was investigated by IR and RAMAN spectroscopy in the crystalline state as well as an evacuated powder. The spectra suggest, that some MeCN was lost upon evacuation, but the nature of the anion was unchanged:

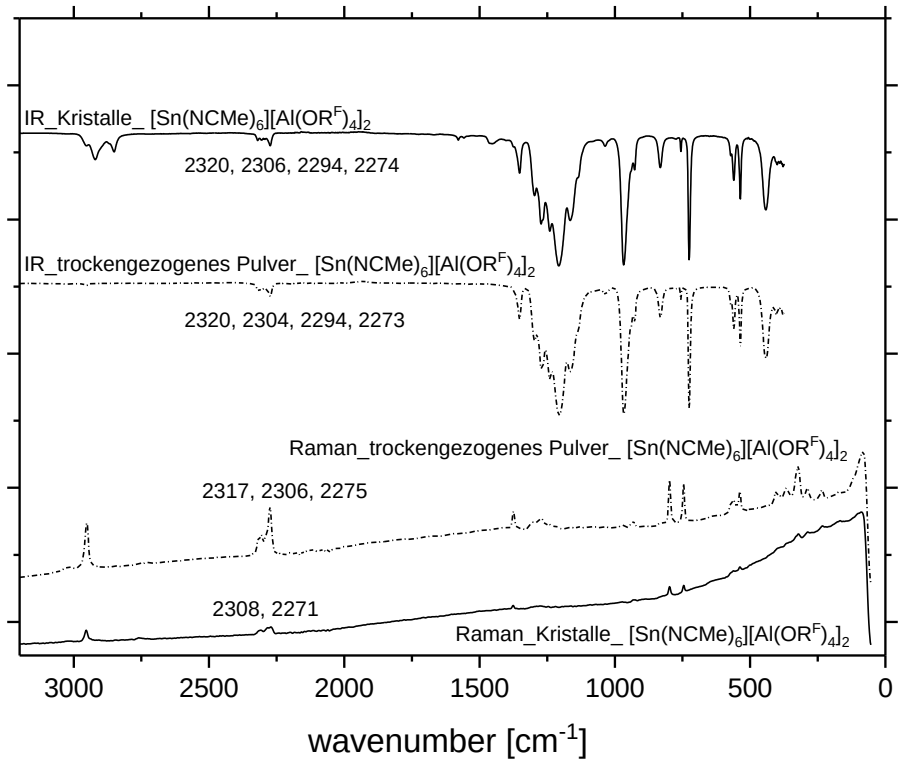


Figure S6. IR and RAMAN spectra in the crystalline state as well as of the evacuated powder of **1**. "trockengezogenes Pulver" indicates "evacuated powder" and "Kristalle" indicates "Crystals", which were isolated and only blown dry by a stream of inert argon gas.

IR_Crystals: ν = 2953 (vw), 2920 (w), 2851 (vw), 2320 (vw), 2306 (vw), 2294 (vw), 2274 (vw), 1579 (vw), 1558 (vw), 1454 (vw), 1352 (w), 1297 (vw), 1273 (vw), 1240 (vw), 1207 (vs), 1165 (vw), 1036 (vw), 967 (vs), 927 (vw), 832 (w), 774 (vw), 756 (vw), 725 (vs), 571 (vw), 560 (w), 536 (m), 442 (m), 400 (vw), 390 (vw), 378 (vw).

IR_evacuated powder: ν = 2951 (vw), 2320 (vw), 2304 (vw), 2273 (vw), 1352 (w), 1296 (vw), 1272 (vw), 1240 (vw), 1206 (vs), 1165 (vw), 1036 (vw), 967 (vs), 927 (vw), 832 (w), 756 (vw), 725 (vs), 571 (vw), 560 (w), 536 (m), 440 (m), 404 (vw), 379 (vw).

FT-Raman_Crystals: ν = 2954 (vw), 2308 (vw), 2271 (vw), 1376 (vw), 1276 (vw), 798 (vw), 746 (vw), 538 (vw), 321 (vw), 88 (vs).

FT-Raman_evacuated powder: ν = 2952 (w), 2317 (vw), 2306 (vw), 2275 (m), 1375 (vw), 1271 (vw), 1244 (vw), 1135 (vw), 973 (vw), 931 (vw), 798 (w), 746 (w), 562 (vw), 538 (vw), 405 (vw), 367 (vw), 322 (w), 288 (vw), 234 (vw), 171 (vw), 82 (vs).

Quantum Chemical Calculations Towards the Coordination Number of Tin in dissolved $[Sn(NC\text{-}Me)_n]^{2+}$ (n = 6, 7, 8).

We have recorded MAS-NMR-spectra and, since they gave at first sight rather unexpected results, we augmented them with extensive DFT-calculations on the chemical shift of $[Sn(MeCN)_x]^{2+}$ (x = 6, 7, 8).

Astonishingly we learned, that most likely in solution an eightfold coordination prevails (calculated shift as well as thermodynamics), while the DFT calculations support two independent but closeby lines for the 3+3 and 2+2+2 coordinated $[Sn(MeCN)_6]^{2+}$ dications in the solid state.

BP86/SVP NMR Calculations	Sn-isotropic (ppm)	δ^{119}Sn = (ppm)	$\Delta(\delta^{119}Sn)$= (ppm)[a)]	$E_{rel.}$ (kJ mol^{-1})
Standard: $SnMe_4$	2994	0	-	-
Octahedral $Sn(NCMe)_6^{2+}$	4223	–1228	78	18.6
2+2+2 $Sn(NCMe)_6^{2+}$	4146	–1152	2	2.3
3+3 $Sn(NCMe)_6^{2+}$	4144	–1150	0	0
C.N. 7: $Sn(NCMe)_7^{2+}$	4227	–1233	83	-
C.N. 8: $Sn(NCMe)_8^{2+}$	4315	–1321	171	-

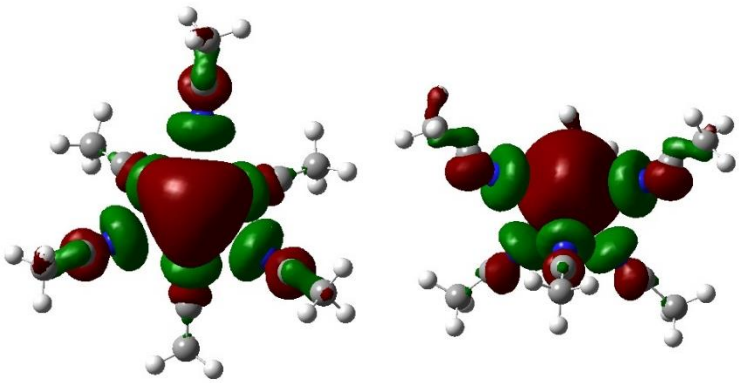
[a)] with respect to the 3+3 $Sn(NCMe)_6^{2+}$ shift.

Also the thermodynamics of this formation is feasible:

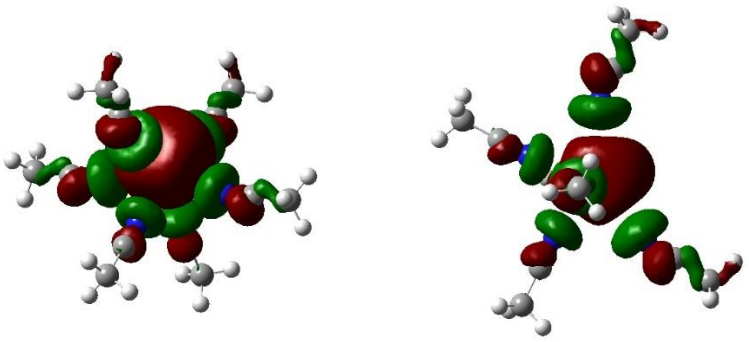
Reactions: in kJ mol^{-1}	BP86/SDD $\Delta_r U$	BP86/SVP $\Delta_r U$
$Sn(NCMe)_7^{2+}$ + MeCN → $Sn(NCMe)_8^{2+}$	–41.4	–40.4
3+3 $Sn(NCMe)_6^{2+}$ + MeCN → $Sn(NCMe)_7^{2+}$	–46.0	–42.0

Bonding within the 3+3 Minimum Structure: Orbitals and NPA / NBO Analyses

Drawings of the orbitals of the 3+3- and 2+2+2-complex are included below. They do **not** suggest heavy s-p-hybridization, but suggest rather s-p-separation.



Two views of the HOMO of 3+3 $Sn(NC\text{-}Me)_6^{2+}$ at a cut off value of 0.02 $e^- Å^3$.



Two views of the HOMO of 2+2+2 $Sn(NC\text{-}Me)_6^{2+}$ at a cut off value of 0.02 $e^- Å^3$.

In addition, we have performed a NPA and NBO analysis. The main information is, that the formal $5s^2$ lone pair exists with a 1.90 e^- population, and that the 5p orbitals are populated by 0.22 to 0.27 e^-:

[3+3]-Complex:

```
NATURAL POPULATIONS:  Natural atomic orbital occupancies

NAO   Atom  #       Type(AO)    Occupancy
-----------------------------------------
    2 sn    1 s    Val(5s)        1.89708
   10 sn    1 p    Val(5px)       0.26155
   11 sn    1 p    Val(5py)       0.21895
   12 sn    1 p    Val(5pz)       0.23487
```

[2+2+2]-Complex:

```
NATURAL POPULATIONS:  Natural atomic orbital occupancies

NAO   Atom  #       Type(AO)    Occupancy
-----------------------------------------
    1 sn    1 s    Val(5s)        1.88702
    3 sn    1 p    Val(5px)       0.22682
    5 sn    1 p    Val(5py)       0.20332
    7 sn    1 p    Val(5pz)       0.27412
```

This is in agreement with the calculated NPA charge of +1.38 residing on Sn and calculated Wiberg / NAO bond orders of 0.23 / 0.26 for the shorter Sn-N-bonds and 0.16 / 0.18 for the longer Sn-N bonds (3+3]-complex; the respective values for the [2+2+2]-complex are: charge +1.40 on Sn, calculated Wiberg / NAO bond orders of 0.23 / 0.25 for the shorter Sn-N-bonds, 0.20 / 0.22 for the middle, and 0.14 / 0.16 for the longer Sn-N bonds).

Moreover, the analysis of the contribution to the individual bonds according to NBO is in agreement with the visualization in the orbitals: One has mainly s-p separation. Interestingly, in the stronger bonds, the orbital contributions are 97 % 5p on Sn, but in the weaker bonds, there is more 5s-contribution (19 %).

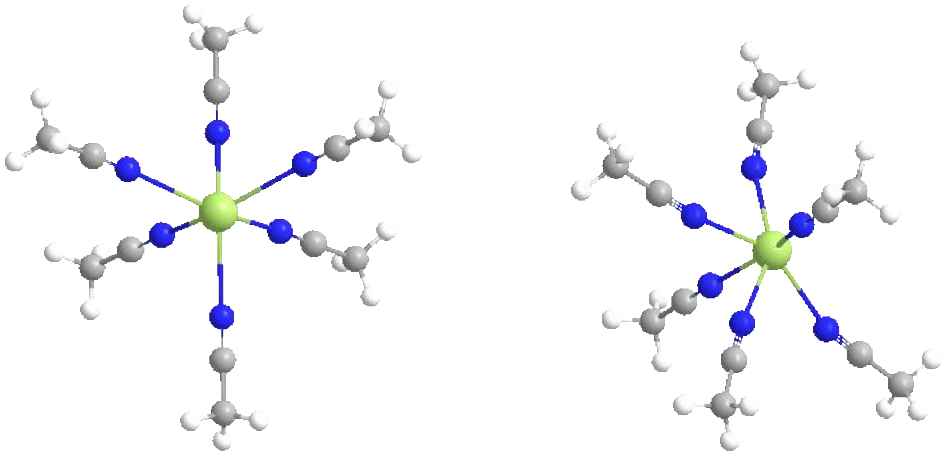
```
      (Occupancy)   Bond orbital/ Coefficients/ Hybrids
-------------------------------------------------------------------------------
    1. (1.93127) BD ( 1)Sn   1 - N   2
               (  4.24%)   0.2059*Sn   1 s(  2.97%)p32.66( 97.03%)
                                        0.1410  0.0991  0.1918  0.4005 -0.3916
                                       -0.4137  0.6645  0.0834
               ( 95.76%)   0.9786* N   2 s( 51.58%)p 0.94( 48.42%)
                                       -0.0004  0.7173 -0.0363 -0.0001 -0.1506
                                       -0.0123  0.5338  0.0439 -0.4160 -0.0370
    4. (1.92998) BD ( 1)Sn   1 - N  26
               (  2.29%)   0.1513*Sn   1 s( 18.64%)p 4.37( 81.36%)
                                        0.0193  0.4313 -0.1423  0.2581  0.6779
                                       -0.3234 -0.0351  0.4017
               ( 97.71%)   0.9885* N  26 s( 51.33%)p 0.95( 48.67%)
                                       -0.0005  0.7155 -0.0374 -0.0001  0.1709
                                        0.0108 -0.6101 -0.0386  0.2886  0.0170
```

However, the contributions of tin orbitals to those bonds is very little (only 2 to 4 %).

Details to the Calculations Summarized above follow here:

A. Optimized Structures of Sn^{2+}-Acetonitrile Complexes

1. (3+3)-$[Sn(NCMe)_6]^{2+}$ at BP86/SDD level:



Sn-N = 242 and 274 pm

```
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 94,-3.0321776589,0.5870200465|C,-1.6040693575,-4.3701573763,0.87429405
 41|H,-2.6956305463,-4.3336856598,1.0379011501|H,-1.1254500626,-4.78025
 24277,1.7810775002|H,-1.3972573795,-5.0500718377,0.0289513555|N,-1.858
 0217582,0.7356557105,-0.6080384659|C,-2.9344052846,1.129186052,-0.9120
 714556|C,-4.2631067701,1.6141253977,-1.2860998319|H,-4.2701332174,2.71
 76068264,-1.3291608956|H,-5.0150903203,1.285748295,-0.5469819839|H,-4.
 5491667596,1.2212800387,-2.2777743643|N,-0.1166424847,-1.0260868148,-2
 .728518974|C,0.0714739308,-1.8486161736,-5.2486563805|H,1.1094715206,-
 1.7418573739,-5.6098116545|H,-0.5895789145,-1.2501218484,-5.8997829506
 |H,-0.221753751,-2.9098640579,-5.3314606646|C,-0.0334226021,-1.3949712
 048,-3.8578603631|N,-0.1783998076,0.6315505722,1.9807441165|C,-0.51390
 5402,1.380435555,4.4991584222|H,-1.5889809299,1.4818953868,4.730437783
 2|H,-0.0219472783,2.3528108254,4.6783358419|H,-0.0753772436,0.63268521
 02,5.1833260999|C,-0.3281783987,0.9671318388,3.1080513537|N,0.61672359
 7,2.8321770955,-0.2849567381|C,1.424787531,5.3279140045,-0.7103857841|
```

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H,1.5276589056,5.5184029512,-1.7931655682|H,2.4039162358,5.5007619896,
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3.9509974907,-0.4752785811|N,2.4006447303,-1.1792286402,1.1556614579|C
,4.7457676836,-2.134658543,1.962131898|H,5.4602121297,-2.1567985292,1.
1204953726|H,4.631316471,-3.1609797218,2.3527951656|H,5.1657144322,-1.
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NMR Calculations at the BP86/SVP level (NMR=GIAO):

```
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65829365,-0.2903196007|N,0,-0.6681992175,-1.947260304,0.3549001769|C,0
,-1.086546394,-3.0321776589,0.5870200465|C,0,-1.6040693575,-4.37015737
63,0.8742940541|H,0,-2.6956305463,-4.3336856598,1.0379011501|H,0,-1.12
54500626,-4.7802524277,1.7810775002|H,0,-1.3972573795,-5.0500718377,0.
0289513555|N,0,-1.8580217582,0.7356557105,-0.6080384659|C,0,-2.9344052
846,1.129186052,-0.9120714556|C,0,-4.2631067701,1.6141253977,-1.286099
8319|H,0,-4.2701332174,2.7176068264,-1.3291608956|H,0,-5.0150903203,1.
285748295,-0.5469819839|H,0,-4.5491667596,1.2212800387,-2.2777743643|N
,0,-0.1166424847,-1.0260868148,-2.728518974|C,0,0.0714739308,-1.848616
1736,-5.2486563805|H,0,1.1094715206,-1.7418573739,-5.6098116545|H,0,-0
.5895789145,-1.2501218484,-5.8997829506|H,0,-0.221753751,-2.9098640579
,-5.3314606646|C,0,-0.0334226021,-1.3949712048,-3.8578603631|N,0,-0.17
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.3528108254,4.6783358419|H,0,-0.0753772436,0.6326852102,5.1833260999|C
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,1.1204953726|H,0,4.631316471,-3.1609797218,2.3527951656|H,0,5.1657144
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6Sn1)]||@
```
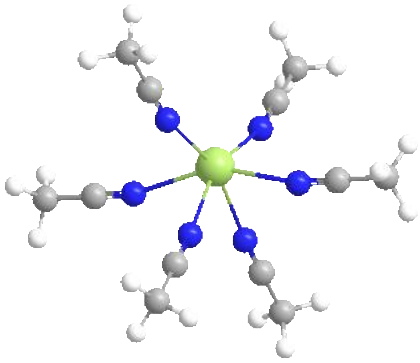

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  Sn   Isotropic =  4144.1560   Anisotropy =   183.2504
   XX=  4083.1458   YX=    -0.0671   ZX=     0.3199
   XY=    -0.1338   YY=  4083.0016   ZY=     0.5319
   XZ=     0.3155   YZ=     0.5944   ZZ=  4266.3207
   Eigenvalues:  4082.9478  4083.1974  4266.3230
  2  N    Isotropic =    38.5651   Anisotropy =   422.1585
   XX=   -98.9055   YX=   -29.0374   ZX=    19.6538
   XY=   -28.9551   YY=   186.5450   ZY=  -196.1784
   XZ=    19.2110   YZ=  -192.3282   ZZ=    28.0559
   Eigenvalues:  -102.4978  -101.8109   320.0042
  3  C    Isotropic =    73.0360   Anisotropy =   306.4370
   XX=   -26.2276   YX=   -20.6504   ZX=    13.9876
   XY=   -20.7564   YY=   178.2513   ZY=  -139.6966
   XZ=    14.5365   YZ=  -144.4890   ZZ=    67.0843
   Eigenvalues:   -29.9168   -28.3026   277.3273
  4  C    Isotropic =   188.0724   Anisotropy =    31.7221
   XX=   177.7766   YX=    -2.1385   ZX=     1.4355
   XY=    -2.1509   YY=   198.9530   ZY=   -14.5900
   XZ=     1.4941   YZ=   -14.8257   ZZ=   187.4876
   Eigenvalues:   177.4347   177.5621   209.2204
  5  H    Isotropic =    28.8155   Anisotropy =    10.0991
   XX=    25.6062   YX=    -0.6337   ZX=    -3.1210
   XY=    -0.0102   YY=    26.8604   ZY=    -2.7149
   XZ=    -3.6985   YZ=    -1.2270   ZZ=    33.9799
   Eigenvalues:    24.0300    26.8683    35.5483
  6  H    Isotropic =    28.8053   Anisotropy =     9.9917
   XX=    32.5134   YX=    -2.6792   ZX=     1.6685
   XY=    -4.1197   YY=    28.0366   ZY=    -2.8119
   XZ=     2.6561   YZ=    -2.8290   ZZ=    25.8658
   Eigenvalues:    23.9257    27.0236    35.4664
  7  H    Isotropic =    28.7856   Anisotropy =     9.9473
   XX=    25.7580   YX=     2.7894   ZX=     1.8520
   XY=     3.5991   YY=    34.1450   ZY=     1.5696
```

```
  XZ=     1.4443   YZ=     0.0778   ZZ=    26.4537
  Eigenvalues:    23.9603    26.9794    35.4171
 8  N    Isotropic =    38.5245   Anisotropy =   422.2027
  XX=   139.8951   YX=  -109.7764   ZX=  -179.5147
  XY=  -109.6678   YY=   -52.1201   ZY=    81.3987
  XZ=  -175.8933   YZ=    79.8102   ZZ=    27.7985
  Eigenvalues:  -102.5122  -101.9073   319.9930
 9  C    Isotropic =    73.0875   Anisotropy =   306.2849
  XX=   144.8267   YX=   -78.5055   ZX=  -127.6689
  XY=   -78.5962   YY=     7.4241   ZY=    57.9972
  XZ=  -132.1379   YZ=    59.9530   ZZ=    67.0117
  Eigenvalues:   -29.7848   -28.2303   277.2774
10  C    Isotropic =   188.0654   Anisotropy =    31.7143
  XX=   195.4856   YX=    -8.1184   ZX=   -13.3340
  XY=    -8.1242   YY=   181.2482   ZY=     6.0683
  XZ=   -13.5672   YZ=     6.1709   ZZ=   187.4624
  Eigenvalues:   177.4186   177.5694   209.2082
11  H    Isotropic =    28.7937   Anisotropy =     9.9698
  XX=    27.1458   YX=    -4.2788   ZX=    -1.4550
  XY=    -3.0276   YY=    33.7911   ZY=    -0.6804
  XZ=    -1.8846   YZ=     0.4544   ZZ=    25.4443
  Eigenvalues:    23.8991    27.0418    35.4402
12  H    Isotropic =    28.8151   Anisotropy =    10.1119
  XX=    26.4764   YX=    -1.1049   ZX=    -1.7838
  XY=    -1.1113   YY=    24.5501   ZY=     0.7797
  XZ=    -0.2182   YZ=     0.0637   ZZ=    35.4188
  Eigenvalues:    24.0449    26.8439    35.5563
13  H    Isotropic =    28.7927   Anisotropy =     9.9684
  XX=    34.5560   YX=     3.4029   ZX=    -0.3986
  XY=     2.1519   YY=    26.3692   ZY=     1.5567
  XZ=    -1.5442   YZ=     1.1463   ZZ=    25.4530
  Eigenvalues:    23.8943    27.0455    35.4383
14  N    Isotropic =    17.9302   Anisotropy =   450.5212
  XX=    89.9733   YX=   158.7628   ZX=   156.8589
  XY=   158.8429   YY=   -19.1432   ZY=   111.8683
  XZ=   162.8380   YZ=   116.1042   ZZ=   -17.0395
  Eigenvalues:  -132.5111  -131.9760   318.2777
15  C    Isotropic =   187.6646   Anisotropy =    30.3955
  XX=   192.5494   YX=    10.7689   ZX=    10.9649
  XY=    10.7949   YY=   185.1744   ZY=     7.8029
  XZ=    10.5034   YZ=     7.5069   ZZ=   185.2702
  Eigenvalues:   177.4655   177.6000   207.9283
16  H    Isotropic =    28.9730   Anisotropy =     9.7832
  XX=    26.5146   YX=     1.5379   ZX=     1.1770
  XY=     1.2261   YY=    25.4606   ZY=     2.7146
  XZ=    -0.4632   YZ=     1.7697   ZZ=    34.9437
  Eigenvalues:    24.2369    27.1869    35.4951
17  H    Isotropic =    29.0177   Anisotropy =     9.8243
  XX=    35.0765   YX=    -2.5477   ZX=     0.9133
  XY=    -1.0006   YY=    26.6436   ZY=     1.2921
  XZ=     1.8942   YZ=     0.9551   ZZ=    25.3330
  Eigenvalues:    24.2701    27.2158    35.5672
18  H    Isotropic =    29.0295   Anisotropy =     9.8438
  XX=    26.7826   YX=     3.8318   ZX=     0.7517
  XY=     2.5992   YY=    34.3159   ZY=    -1.9877
  XZ=     1.3308   YZ=    -0.7429   ZZ=    25.9899
  Eigenvalues:    24.2975    27.1989    35.5920
19  C    Isotropic =    71.8639   Anisotropy =   311.5936
  XX=   123.5325   YX=   110.4534   ZX=   114.9257
  XY=   110.3523   YY=    47.5711   ZY=    81.9382
  XZ=   104.5652   YZ=    74.6082   ZZ=    44.4880
  Eigenvalues:   -32.8002   -31.2012   279.5929
20  N    Isotropic =    38.5955   Anisotropy =   422.1058
  XX=    92.2802   YX=   137.6258   ZX=   160.6706
  XY=   137.5398   YY=    -4.1670   ZY=   114.0540
  XZ=   157.4043   YZ=   111.8161   ZZ=    27.6732
  Eigenvalues:  -102.4946  -101.7183   319.9994
21  C    Isotropic =   188.0442   Anisotropy =    31.7308
  XX=   191.9429   YX=    10.1748   ZX=    11.9656
  XY=    10.1980   YY=   184.8081   ZY=     8.5081
  XZ=    12.1629   YZ=     8.6107   ZZ=   187.3818
  Eigenvalues:   177.3522   177.5825   209.1981
22  H    Isotropic =    28.8158   Anisotropy =    10.0961
  XX=    26.5976   YX=     0.9511   ZX=     0.0616
  XY=     0.3665   YY=    25.7152   ZY=     3.9849
  XZ=    -1.4500   YZ=     3.4074   ZZ=    34.1346
  Eigenvalues:    24.0320    26.8688    35.5466
23  H    Isotropic =    28.7852   Anisotropy =     9.9370
```

```
  XX=    27.2235   YX=     4.8884   ZX=     0.1513
  XY=     4.0497   YY=    32.7461   ZY=    -2.3734
  XZ=     0.9808   YZ=    -1.0819   ZZ=    26.3858
  Eigenvalues:    23.9546    26.9911    35.4098
24  H    Isotropic =    28.8048   Anisotropy =     9.9897
  XX=    33.5194   YX=    -3.3599   ZX=     3.0338
  XY=    -1.9246   YY=    27.1199   ZY=     0.6897
  XZ=     3.7320   YZ=    -0.0084   ZZ=    25.7750
  Eigenvalues:    23.9257    27.0240    35.4646
25  C    Isotropic =    73.0400   Anisotropy =   306.3534
  XX=   110.6040   YX=    98.5417   ZX=   114.3500
  XY=    98.6446   YY=    41.6765   ZY=    81.1692
  XZ=   118.3245   YZ=    83.9150   ZZ=    66.8396
  Eigenvalues:   -29.8530   -28.3026   277.2757
26  N    Isotropic =    18.0439   Anisotropy =   450.4175
  XX=  -129.5189   YX=   -32.5809   ZX=    18.6114
  XY=   -32.5456   YY=   201.2767   ZY=  -191.0507
  XZ=    19.3014   YZ=  -198.2833   ZZ=   -17.6263
  Eigenvalues:  -132.6943  -131.4963   318.3222
27  C    Isotropic =   187.7045   Anisotropy =    30.4253
  XX=   177.7038   YX=    -2.1916   ZX=     1.3709
  XY=    -2.2083   YY=   200.2095   ZY=   -13.3712
  XZ=     1.2654   YZ=   -12.7567   ZZ=   185.2002
  Eigenvalues:   177.4775   177.6481   207.9881
28  H    Isotropic =    28.9826   Anisotropy =     9.7986
  XX=    29.7589   YX=    -0.2867   ZX=     4.7391
  XY=    -1.6616   YY=    27.5305   ZY=    -3.0101
  XZ=     5.3963   YZ=    -1.8803   ZZ=    29.6582
  Eigenvalues:    24.2368    27.1959    35.5150
29  H    Isotropic =    28.9840   Anisotropy =     9.7924
  XX=    30.1098   YX=     1.1308   ZX=    -3.7227
  XY=     2.6210   YY=    28.2779   ZY=    -3.8737
  XZ=    -4.6340   YZ=    -3.1171   ZZ=    28.5644
  Eigenvalues:    24.2359    27.2039    35.5123
30  H    Isotropic =    29.0413   Anisotropy =     9.8714
  XX=    24.5894   YX=    -1.4202   ZX=    -0.6727
  XY=    -1.5313   YY=    34.5289   ZY=     3.4367
  XZ=    -0.4356   YZ=     1.6301   ZZ=    28.0058
  Eigenvalues:    24.3636    27.1382    35.6223
31  C    Isotropic =    71.8940   Anisotropy =   311.5172
  XX=   -28.9073   YX=   -22.5666   ZX=    13.6330
  XY=   -22.5908   YY=   200.7391   ZY=  -140.0321
  XZ=    12.4276   YZ=  -127.5092   ZZ=    43.8502
  Eigenvalues:   -32.7840   -31.1061   279.5721
32  N    Isotropic =    17.9840   Anisotropy =   450.4488
  XX=   144.7411   YX=  -126.6782   ZX=  -175.5984
  XY=  -126.7641   YY=   -74.5754   ZY=    80.1507
  XZ=  -182.2217   YZ=    83.1374   ZZ=   -16.2137
  Eigenvalues:  -132.5135  -131.8177   318.2832
33  C    Isotropic =   187.6747   Anisotropy =    30.4007
  XX=   196.3113   YX=    -8.5899   ZX=   -12.2680
  XY=    -8.6058   YY=   181.4318   ZY=     5.6521
  XZ=   -11.7378   YZ=     5.3802   ZZ=   185.2809
  Eigenvalues:   177.4953   177.5869   207.9418
34  H    Isotropic =    28.9761   Anisotropy =     9.7879
  XX=    27.0771   YX=    -1.1366   ZX=    -1.3165
  XY=    -0.5836   YY=    25.4974   ZY=     3.5264
  XZ=     0.4553   YZ=     3.0674   ZZ=    34.3538
  Eigenvalues:    24.2391    27.1879    35.5014
35  H    Isotropic =    29.0357   Anisotropy =     9.8475
  XX=    28.9351   YX=    -5.3698   ZX=     0.3368
  XY=    -4.3209   YY=    31.6798   ZY=    -2.5905
  XZ=    -0.7018   YZ=    -1.4849   ZZ=    26.4921
  Eigenvalues:    24.3130    27.1934    35.6007
36  H    Isotropic =    29.0111   Anisotropy =     9.8197
  XX=    33.3356   YX=     4.2570   ZX=    -2.1915
  XY=     2.6498   YY=    28.2566   ZY=     0.5129
  XZ=    -2.8508   YZ=    -0.1681   ZZ=    25.4412
  Eigenvalues:    24.2625    27.2133    35.5576
37  C    Isotropic =    71.8621   Anisotropy =   311.5279
  XX=   161.5744   YX=   -88.0975   ZX=  -128.6308
  XY=   -87.9699   YY=     9.0371   ZY=    58.6985
  XZ=  -117.0886   YZ=    53.4973   ZZ=    44.9747
  Eigenvalues:   -32.7902   -31.1709   279.5473
```

2. (2+2+2)-$[Sn(NCMe)_6]^{2+}$ at BP86/SDD level:



Sn-N = 240 (2x), 254 (2x) and 281 (2x) pm

```
1|1|UNPC-UNK|FOpt|RBP86|SDD|C12H18N6Sn1(2+)|PCUSER|27-May-2017|0||# RB
 P86/SDD Opt Test||[No Title]||2,1|Sn,5.9793350413,4.9079787676,4.39745
 48636|N,7.768470247,3.4680462856,5.1091452822|N,3.9571619425,5.6624190
 096,2.5931911079|N,4.6374373415,3.0168558194,5.4619750504|N,6.89152723
 85,6.0031152423,6.8244079612|N,7.8912774672,5.8565241743,3.0063224792|
 N,6.0703036052,3.2785517271,2.6323234146|C,8.6605724506,2.8516457485,5
 .5878312845|C,5.9982448618,2.5535933718,1.6973705407|C,8.6639821741,6.
 5406253601,2.4165842378|C,7.0382510678,6.6866435806,7.7884787598|C,3.8
 536549126,2.3429737133,6.0489636301|C,3.0550184394,6.2259577229,2.0576
 856895|C,9.7612313512,2.0907156761,6.1790706797|C,5.9096552394,1.65876
 1082,0.5435231666|C,9.6159229491,7.3835618284,1.6899719047|C,7.2164930
 454,7.5305648825,8.9751741133|C,2.8876057678,1.5127098409,6.7716671092
 |C,1.9434367186,6.9223137893,1.4006280725|H,9.5939263443,1.955396924,7
 .2622669445|H,9.8393963926,1.0953423579,5.7072862574|H,10.7170743053,2
 .6248319757,6.0350156161|H,5.2754646465,2.1080991533,-0.2409708028|H,6
 .9134627036,1.4734907756,0.1220615699|H,5.4689241956,0.6908558467,0.84
 10987292|H,9.9517758395,8.2199205681,2.328137106|H,10.4995507482,6.794
 6940681,1.3869735178|H,9.1435499319,7.8014389407,0.7834661423|H,6.6801
 733261,8.487565519,8.8500529938|H,6.8213580539,7.022015733,9.872026911
 5|H,8.2869441477,7.7468702123,9.1375759802|H,2.0171422817,1.2903603042
 ,6.129534599|H,3.3519711394,0.5587988414,7.0778795719|H,2.5319974623,2
 .037676139,7.6758239178|H,1.0643254747,6.258683607,1.3243528166|H,1.65
 69641452,7.8188834305,1.9779068285|H,2.2339170005,7.238217981,0.383341
 9533||Version=IA32W-G03RevD.01|State=1-A|HF=-799.4259459|RMSD=6.834e-0
 09|RMSF=2.355e-006|Thermal=0.|Dipole=0.5327957,-0.8609503,-0.3024154|P
 G=C01 [X(C12H18N6Sn1)]||@
```

NMR Calculations at the BP86/SVP level (NMR=GIAO):

```
1|1|UNPC-UNK|SP|RBP86|SVP|C12H18N6Sn1(2+)|PCUSER|27-May-2017|0||# RBP8
 6/SVP NMR=GIAO Test||[No Title]||2,1|Sn,0,0.0001,-0.0025,-0.3362|N,0,1
 .5065,0.0473,1.5371|N,0,-2.5796,-0.0517,-1.4572|N,0,-0.0361,2.4911,0.2
 031|N,0,2.5806,-0.0075,-1.4597|N,0,0.0308,-2.476,0.2733|N,0,-1.5023,0.
 0031,1.5405|C,0,2.3657,0.075,2.3531|C,0,-2.3573,0.0026,2.3613|C,0,0.04
 2,-3.6646,0.284|C,0,3.4994,-0.0161,-2.2173|C,0,-0.0552,3.6794,0.1793|C
 ,0,-3.4947,-0.0708,-2.2191|C,0,3.4264,0.1098,3.36|C,0,-3.4124,0.0019,3
 .3746|C,0,0.0557,-5.1289,0.297|C,0,4.6292,-0.0266,-3.1531|C,0,-0.0793,
 5.1434,0.1499|C,0,-4.6198,-0.094,-3.1602|H,0,4.2041,0.8387,3.071|H,0,3
 .0162,0.4028,4.3426|H,0,3.8956,-0.8852,3.4567|H,0,-4.3847,-0.247,2.913
 9|H,0,-3.1926,-0.7441,4.1587|H,0,-3.4912,0.9967,3.8476|H,0,0.8281,-5.5
 109,-0.3936|H,0,0.2746,-5.5036,1.3125|H,0,-0.9254,-5.5242,-0.0203|H,0,
 4.2867,-0.3032,-4.1657|H,0,5.0977,0.9719,-3.2021|H,0,5.3918,-0.7564,-2
 .8291|H,0,-1.1187,5.5082,0.0715|H,0,0.3698,5.555,1.0709|H,0,0.4909,5.5
 187,-0.7183|H,0,-5.2338,0.8169,-3.0492|H,0,-4.2503,-0.1432,-4.1995|H,0
 ,-5.2603,-0.9738,-2.9737||Version=IA32W-G03RevD.01|State=1-A|HF=-6820.
 7849486|RMSD=1.480e-009|Thermal=0.|Dipole=-0.0016557,0.009973,1.178008
 |PG=C01 [X(C12H18N6Sn1)]||@
```

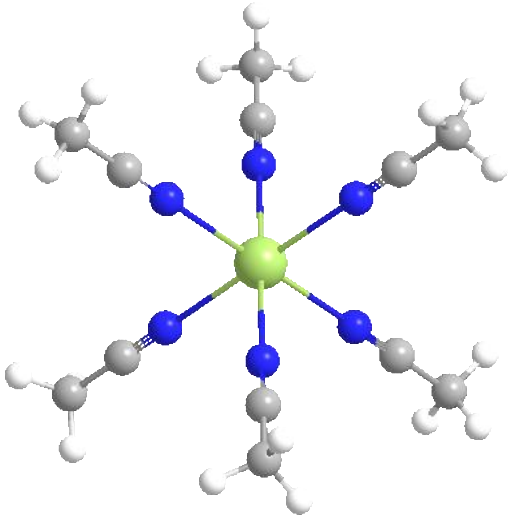
```
SCF GIAO Magnetic shielding tensor (ppm):
  1  Sn   Isotropic =  4146.4616   Anisotropy =   126.5421
   XX=  4094.1156   YX=    -0.2703   ZX=     0.3117
   XY=    -0.1909   YY=  4114.4491   ZY=     0.4209
   XZ=     0.2402   YZ=     0.6094   ZZ=  4230.8201
   Eigenvalues:  4094.1124  4114.4495  4230.8230
```

```
 2  N    Isotropic =    39.3398   Anisotropy =   421.0053
  XX=   121.9558   YX=     7.1063   ZX=   211.5501
  XY=     7.1164   YY=  -102.1400   ZY=     7.0055
  XZ=   207.1716   YZ=     6.8188   ZZ=    98.2036
  Eigenvalues:  -102.3800   -99.6106   320.0100
 3  N    Isotropic =    16.0180   Anisotropy =   452.3684
  XX=   132.9412   YX=     5.5596   ZX=   218.5835
  XY=     5.5967   YY=  -136.4730   ZY=     4.6218
  XZ=   224.4426   YZ=     4.7003   ZZ=    51.5858
  Eigenvalues:  -136.5894  -132.9536   317.5969
 4  N    Isotropic =    30.0601   Anisotropy =   434.3586
  XX=  -115.4423   YX=    -7.0785   ZX=     0.3386
  XY=    -6.9919   YY=   319.2354   ZY=    -7.7995
  XZ=     0.4136   YZ=   -14.3455   ZZ=  -113.6128
  Eigenvalues:  -115.5792  -113.8730   319.6325
 5  N    Isotropic =    15.8795   Anisotropy =   452.5389
  XX=   134.9704   YX=    -2.4602   ZX=  -218.3082
  XY=    -2.5718   YY=  -136.8525   ZY=     2.1031
  XZ=  -224.1219   YZ=     2.0580   ZZ=    49.5207
  Eigenvalues:  -136.8760  -133.0576   317.5721
 6  N    Isotropic =    30.3296   Anisotropy =   433.9939
  XX=  -115.2524   YX=    -4.0856   ZX=     0.0918
  XY=    -4.1412   YY=   319.6151   ZY=    -4.7356
  XZ=     0.0151   YZ=     1.8380   ZZ=  -113.3739
  Eigenvalues:  -115.2921  -113.3779   319.6589
 7  N    Isotropic =    39.3704   Anisotropy =   420.9282
  XX=   119.6657   YX=     0.0738   ZX=  -211.8164
  XY=     0.1497   YY=  -102.0478   ZY=    -0.2036
  XZ=  -207.5649   YZ=    -0.1017   ZZ=   100.4932
  Eigenvalues:  -102.0484   -99.8297   319.9892
 8  C    Isotropic =    72.8438   Anisotropy =   305.4206
  XX=   129.6612   YX=     5.1167   ZX=   149.8261
  XY=     5.1319   YY=   -28.3484   ZY=     4.8444
  XZ=   155.6240   YZ=     5.0182   ZZ=   117.2186
  Eigenvalues:   -29.4120   -28.5142   276.4575
 9  C    Isotropic =    72.8831   Anisotropy =   305.4244
  XX=   128.1803   YX=     0.0938   ZX=  -150.0355
  XY=    -0.0071   YY=   -28.4974   ZY=    -0.0164
  XZ=  -155.6776   YZ=    -0.1143   ZZ=   118.9664
  Eigenvalues:   -29.3529   -28.4971   276.4993
10  C    Isotropic =    72.0102   Anisotropy =   308.9364
  XX=   -29.7878   YX=    -2.9829   ZX=    -0.0123
  XY=    -2.8920   YY=   277.8524   ZY=     0.7013
  XZ=     0.0900   YZ=   -11.1075   ZZ=   -32.0340
  Eigenvalues:   -32.1214   -29.8158   277.9678
11  C    Isotropic =    72.3589   Anisotropy =   313.9912
  XX=   156.1981   YX=    -1.8071   ZX=  -159.5197
  XY=    -1.6290   YY=   -31.2467   ZY=     1.3324
  XZ=  -148.9142   YZ=     1.3768   ZZ=    92.1253
  Eigenvalues:   -33.3482   -31.2615   281.6864
12  C    Isotropic =    72.0380   Anisotropy =   308.9565
  XX=   -29.7395   YX=    -4.9136   ZX=     0.1338
  XY=    -4.9767   YY=   277.8833   ZY=    -9.7171
  XZ=    -0.0639   YZ=     2.1473   ZZ=   -32.0299
  Eigenvalues:   -32.0764   -29.8187   278.0090
13  C    Isotropic =    72.2878   Anisotropy =   313.9638
  XX=   154.6803   YX=     3.9142   ZX=   159.8440
  XY=     3.8533   YY=   -31.2449   ZY=     3.2741
  XZ=   149.0659   YZ=     3.1094   ZZ=    93.4279
  Eigenvalues:   -33.4079   -31.3257   281.5970
14  C    Isotropic =   188.0922   Anisotropy =    31.6601
  XX=   194.0345   YX=     0.5596   ZX=    15.5854
  XY=     0.5913   YY=   177.4120   ZY=     0.5411
  XZ=    15.8860   YZ=     0.5312   ZZ=   192.8301
  Eigenvalues:   177.3920   177.6856   209.1990
15  C    Isotropic =   188.1014   Anisotropy =    31.6661
  XX=   193.9614   YX=     0.0101   ZX=   -15.6558
  XY=     0.0392   YY=   177.4065   ZY=    -0.0193
  XZ=   -15.8539   YZ=    -0.0294   ZZ=   192.9364
  Eigenvalues:   177.4065   177.6857   209.2121
```

```
16  C    Isotropic =   187.9321   Anisotropy =    31.3297
  XX=   177.4926   YX=    -0.3604   ZX=    -0.0445
  XY=    -0.3119   YY=   208.8092   ZY=    -0.1143
  XZ=    -0.0310   YZ=    -0.7340   ZZ=   177.4945
  Eigenvalues:   177.4466   177.5311   208.8186
17  C    Isotropic =   187.6936   Anisotropy =    30.0896
  XX=   195.6136   YX=    -0.1870   ZX=   -14.9685
  XY=    -0.2208   YY=   177.6622   ZY=     0.1405
  XZ=   -14.5495   YZ=     0.1217   ZZ=   189.8051
  Eigenvalues:   177.6353   177.6922   207.7533
18  C    Isotropic =   187.9020   Anisotropy =    31.3118
  XX=   177.4993   YX=    -0.4628   ZX=     0.0065
  XY=    -0.5103   YY=   208.7620   ZY=    -0.7956
  XZ=    -0.0144   YZ=    -0.1395   ZZ=   177.4448
  Eigenvalues:   177.4355   177.4940   208.7765
19  C    Isotropic =   187.7221   Anisotropy =    30.0738
  XX=   195.4954   YX=     0.3721   ZX=    15.0145
  XY=     0.3828   YY=   177.7616   ZY=     0.3094
  XZ=    14.5851   YZ=     0.3072   ZZ=   189.9093
  Eigenvalues:   177.6412   177.7538   207.7713
20  H    Isotropic =    28.7816   Anisotropy =     9.8699
  XX=    32.1440   YX=     5.3250   ZX=     0.4388
  XY=     4.4757   YY=    27.8095   ZY=    -1.1827
  XZ=     1.7028   YZ=    -0.3328   ZZ=    26.3911
  Eigenvalues:    23.9932    26.9900    35.3615
21  H    Isotropic =    28.8179   Anisotropy =    10.1752
  XX=    26.7934   YX=    -0.3600   ZX=     0.6731
  XY=    -0.7198   YY=    24.6196   ZY=     2.3131
  XZ=    -0.9495   YZ=     2.6152   ZZ=    35.0408
  Eigenvalues:    23.9786    26.8738    35.6014
22  H    Isotropic =    28.7919   Anisotropy =     9.9543
  XX=    28.7767   YX=    -4.8265   ZX=     2.8944
  XY=    -3.6165   YY=    31.0773   ZY=    -0.9750
  XZ=     3.3346   YZ=    -2.1281   ZZ=    26.5216
  Eigenvalues:    24.0287    26.9188    35.4281
23  H    Isotropic =    28.7808   Anisotropy =     9.8701
  XX=    34.9523   YX=     2.1426   ZX=     1.3800
  XY=     1.8449   YY=    24.3140   ZY=     0.7376
  XZ=    -0.3252   YZ=     0.4472   ZZ=    27.0761
  Eigenvalues:    23.8771    27.1044    35.3609
24  H    Isotropic =    28.8100   Anisotropy =    10.1192
  XX=    26.2367   YX=    -0.0672   ZX=    -2.1198
  XY=    -0.9403   YY=    28.0231   ZY=    -4.5001
  XZ=    -0.9518   YZ=    -5.3643   ZZ=    32.1702
  Eigenvalues:    23.9974    26.8764    35.5561
25  H    Isotropic =    28.8016   Anisotropy =    10.0549
  XX=    26.4761   YX=    -2.0722   ZX=    -3.2820
  XY=    -0.8955   YY=    31.1626   ZY=     3.7579
  XZ=    -2.8243   YZ=     4.9105   ZZ=    28.7662
  Eigenvalues:    24.0007    26.8992    35.5049
26  H    Isotropic =    28.8577   Anisotropy =     9.9228
  XX=    28.4600   YX=    -2.4815   ZX=    -3.8985
  XY=    -3.8349   YY=    30.6542   ZY=     3.3254
  XZ=    -3.8577   YZ=     2.1114   ZZ=    27.4590
  Eigenvalues:    24.0488    27.0515    35.4729
27  H    Isotropic =    28.9032   Anisotropy =     9.9928
  XX=    24.5363   YX=    -0.7201   ZX=     1.6305
  XY=    -1.0966   YY=    30.5622   ZY=    -4.9999
  XZ=     1.6241   YZ=    -3.2882   ZZ=    31.6112
  Eigenvalues:    24.1800    26.9647    35.5651
28  H    Isotropic =    28.8667   Anisotropy =     9.9132
  XX=    31.0706   YX=     3.1233   ZX=     2.2694
  XY=     4.8438   YY=    30.7660   ZY=     1.5023
  XZ=     2.2290   YZ=     0.9372   ZZ=    24.7634
  Eigenvalues:    24.0429    27.0816    35.4755
29  H    Isotropic =    29.0205   Anisotropy =     9.7364
  XX=    27.1860   YX=     0.1925   ZX=    -1.3546
  XY=     0.5998   YY=    24.8532   ZY=     2.0965
  XZ=     0.5215   YZ=     2.4079   ZZ=    35.0221
  Eigenvalues:    24.2987    27.2513    35.5114
```

```
30  H    Isotropic =    29.0540   Anisotropy =     9.7963
  XX=    29.4816   YX=     4.9832   ZX=    -2.5140
  XY=     3.5432   YY=    31.4801   ZY=    -0.5440
  XZ=    -2.9747   YZ=    -1.6833   ZZ=    26.2003
  Eigenvalues:    24.3521    27.2251    35.5849
31  H    Isotropic =    29.0676   Anisotropy =     9.8061
  XX=    32.6260   YX=    -5.2138   ZX=    -0.0191
  XY=    -4.1824   YY=    28.1955   ZY=    -1.5154
  XZ=    -1.3340   YZ=    -0.6937   ZZ=    26.3812
  Eigenvalues:    24.3789    27.2189    35.6050
32  H    Isotropic =    28.8750   Anisotropy =     9.9159
  XX=    31.9910   YX=    -3.2237   ZX=     0.6250
  XY=    -5.0165   YY=    30.5231   ZY=    -0.4181
  XZ=     0.6238   YZ=    -0.2825   ZZ=    24.1108
  Eigenvalues:    24.0615    27.0779    35.4856
33  H    Isotropic =    28.9058   Anisotropy =     9.9761
  XX=    25.6283   YX=     1.4173   ZX=     2.9541
  XY=     2.1968   YY=    30.8761   ZY=     4.6512
  XZ=     2.9876   YZ=     3.0728   ZZ=    30.2129
  Eigenvalues:    24.1666    26.9942    35.5565
34  H    Isotropic =    28.8481   Anisotropy =     9.9165
  XX=    26.4469   YX=     1.6872   ZX=    -3.5707
  XY=     2.6988   YY=    30.5917   ZY=    -4.3117
  XZ=    -3.6105   YZ=    -2.7954   ZZ=    29.5057
  Eigenvalues:    24.0696    27.0156    35.4590
35  H    Isotropic =    29.0591   Anisotropy =     9.8064
  XX=    30.8655   YX=    -5.4472   ZX=     1.6222
  XY=    -4.1367   YY=    30.2701   ZY=     0.5660
  XZ=     2.4806   YZ=    -0.4610   ZZ=    26.0418
  Eigenvalues:    24.3638    27.2168    35.5967
36  H    Isotropic =    29.0209   Anisotropy =     9.7294
  XX=    27.2584   YX=     0.0068   ZX=     1.1217
  XY=    -0.0757   YY=    24.3200   ZY=     0.4597
  XZ=    -0.8154   YZ=     0.4898   ZZ=    35.4842
  Eigenvalues:    24.2993    27.2562    35.5071
37  H    Isotropic =    29.0605   Anisotropy =     9.8198
  XX=    31.1498   YX=     5.5469   ZX=     1.1335
  XY=     4.3154   YY=    29.9437   ZY=    -0.9451
  XZ=     2.1303   YZ=     0.0593   ZZ=    26.0882
  Eigenvalues:    24.3652    27.2094    35.6071
```

3. (octahedral)-$[Sn(NCMe)_6]^{2+}$ at BP86/SDD level:



Sn-N = 263 pm

```
1|1|UNPC-UNK|FOpt|RBP86|SDD|C12H18N6Sn1(2+)|PCUSER|27-May-2017|0||# RB
 P86/SDD Opt Test||[No Title]||2,1|Sn,5.9793350413,4.9079787676,4.39745
 48636|N,7.768470247,3.4680462856,5.1091452822|N,3.9571619425,5.6624190
 096,2.5931911079|N,4.6374373415,3.0168558194,5.4619750504|N,6.89152723
 85,6.0031152423,6.8244079612|N,7.8912774672,5.8565241743,3.0063224792|
 N,6.0703036052,3.2785517271,2.6323234146|C,8.6605724506,2.8516457485,5
 .5878312845|C,5.9982448618,2.5535933718,1.6973705407|C,8.6639821741,6.
 5406253601,2.4165842378|C,7.0382510678,6.6866435806,7.7884787598|C,3.8
 536549126,2.3429737133,6.0489636301|C,3.0550184394,6.2259577229,2.0576
 856895|C,9.7612313512,2.0907156761,6.1790706797|C,5.9096552394,1.65876
 1082,0.5435231666|C,9.6159229491,7.3835618284,1.6899719047|C,7.2164930
 454,7.5305648825,8.9751741133|C,2.8876057678,1.5127098409,6.7716671092
 |C,1.9434367186,6.9223137893,1.4006280725|H,9.5939263443,1.955396924,7
 .2622669445|H,9.8393963926,1.0953423579,5.7072862574|H,10.7170743053,2
 .6248319757,6.0350156161|H,5.2754646465,2.1080991533,-0.2409708028|H,6
 .9134627036,1.4734907756,0.1220615699|H,5.4689241956,0.6908558467,0.84
 10987292|H,9.9517758395,8.2199205681,2.328137106|H,10.4995507482,6.794
 6940681,1.3869735178|H,9.1435499319,7.8014389407,0.7834661423|H,6.6801
 733261,8.487565519,8.8500529938|H,6.8213580539,7.022015733,9.872026911
 5|H,8.2869441477,7.7468702123,9.1375759802|H,2.0171422817,1.2903603042
 ,6.129534599|H,3.3519711394,0.5587988414,7.0778795719|H,2.5319974623,2
 .037676139,7.6758239178|H,1.0643254747,6.258683607,1.3243528166|H,1.65
 69641452,7.8188834305,1.9779068285|H,2.2339170005,7.238217981,0.383341
 9533||Version=IA32W-G03RevD.01|State=1-A|HF=-799.4259459|RMSD=6.834e-0
 09|RMSF=2.355e-006|Thermal=0.|Dipole=0.5327957,-0.8609503,-0.3024154|P
 G=C01 [X(C12H18N6Sn1)]||@
```

NMR Calculations at the BP86/SVP level (NMR=GIAO):

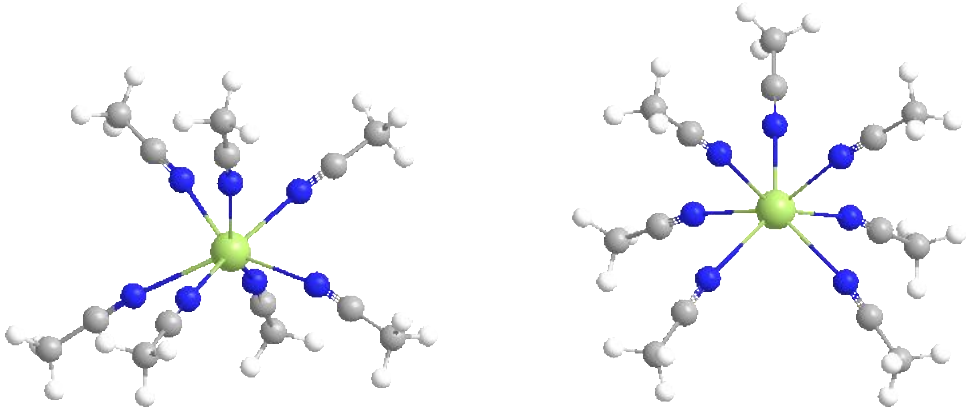
```
1|1|UNPC-UNK|SP|RBP86|SVP|C12H18N6Sn1(2+)|PCUSER|27-May-2017|0||# RBP8
 6/SVP NMR=GIAO Test||[No Title]||2,1|Sn,0,-0.0001,-0.0001,-0.0001|N,0,
 -1.8765,0.0483,-1.8415|N,0,1.875,-0.0521,1.8423|N,0,-1.7822,0.6062,1.8
 356|N,0,-0.4609,-2.5585,0.3943|N,0,1.7883,-0.6025,-1.8311|N,0,0.4563,2
 .5585,-0.3996|C,0,-2.7252,0.0696,-2.6735|C,0,0.662,3.7149,-0.5817|C,0,
 2.5981,-0.8745,-2.6575|C,0,-0.6704,-3.715,0.5716|C,0,-2.5869,0.8812,2.
 666|C,0,2.7226,-0.0761,2.6753|C,0,-3.7714,0.0958,-3.6989|C,0,0.9153,5.
 1405,-0.8061|C,0,3.5966,-1.2098,-3.6761|C,0,-0.9288,-5.1406,0.7898|C,0
 ,-3.5786,1.2206,3.6898|C,0,3.7674,-0.1061,3.702|H,0,-4.6519,-0.4799,-3
 .3636|H,0,-4.086,1.135,-3.8999|H,0,-3.3986,-0.3472,-4.6391|H,0,1.6798,
 5.5103,-0.1004|H,0,1.2762,5.3087,-1.836|H,0,-0.0111,5.7228,-0.6583|H,0
 ,3.8203,-2.2908,-3.6531|H,0,3.2218,-0.9492,-4.6815|H,0,4.5325,-0.6527,
 -3.4941|H,0,-0.1012,-5.5978,1.3602|H,0,-1.8658,-5.2784,1.3574|H,0,-1.0
 224,-5.666,-0.1769|H,0,-3.3461,2.2022,4.1389|H,0,-4.5884,1.2672,3.2456
 |H,0,-3.5807,0.4593,4.4896|H,0,3.321,-0.0078,4.7072|H,0,4.3239,-1.0587
 ,3.6556|H,0,4.4787,0.7247,3.5501||Version=IA32W-G03RevD.01|State=1-A|H
 F=-6820.7787488|RMSD=6.471e-009|Thermal=0.|Dipole=0.0002585,-0.0001909
 ,0.0006879|PG=C01 [X(C12H18N6Sn1)]||@
```

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  Sn   Isotropic =  4222.6031   Anisotropy =     0.4412
   XX=  4222.5060   YX=    -0.0714   ZX=     0.1299
   XY=    -0.1031   YY=  4222.8745   ZY=     0.0671
   XZ=     0.1373   YZ=     0.0663   ZZ=  4222.4286
   Eigenvalues:  4222.3084  4222.6036  4222.8972
  2  N    Isotropic =    27.6073   Anisotropy =   434.9032
   XX=   103.8726   YX=    -9.0257   ZX=   217.2570
   XY=    -9.0393   YY=  -116.9766   ZY=    -8.9270
   XZ=   217.2159   YZ=    -8.9078   ZZ=    95.9260
   Eigenvalues:  -117.3974  -117.3234   317.5428
  3  N    Isotropic =    27.6282   Anisotropy =   434.8614
   XX=   103.3187   YX=    -9.7123   ZX=   217.1860
   XY=    -9.7327   YY=  -116.9110   ZY=    -9.6518
   XZ=   217.1732   YZ=    -9.6251   ZZ=    96.4768
   Eigenvalues:  -117.3768  -117.2745   317.5358
  4  N    Isotropic =    27.6793   Anisotropy =   434.8458
   XX=    80.8613   YX=   -68.9597   ZX=  -205.2585
   XY=   -69.0122   YY=   -93.2487   ZY=    71.5047
   XZ=  -205.3045   YZ=    71.4641   ZZ=    95.4254
   Eigenvalues:  -117.2750  -117.2636   317.5765
  5  N    Isotropic =    27.6516   Anisotropy =   434.8649
   XX=  -102.1359   YX=    78.8928   ZX=   -11.7323
   XY=    78.9072   YY=   293.3919   ZY=   -60.8405
   XZ=   -11.7316   YZ=   -60.8154   ZZ=  -108.3013
   Eigenvalues:  -117.3489  -117.2579   317.5615
  6  N    Isotropic =    27.6777   Anisotropy =   434.8435
   XX=    83.4485   YX=   -68.7044   ZX=  -205.6261
   XY=   -68.6828   YY=   -93.7818   ZY=    70.3523
   XZ=  -205.5777   YZ=    70.3571   ZZ=    93.3664
   Eigenvalues:  -117.2893  -117.2509   317.5734
  7  N    Isotropic =    27.6416   Anisotropy =   434.8792
   XX=  -102.7033   YX=    77.5246   ZX=   -11.8349
   XY=    77.5710   YY=   293.3906   ZY=   -62.5284
   XZ=   -11.8514   YZ=   -62.5757   ZZ=  -107.7626
   Eigenvalues:  -117.3598  -117.2765   317.5610
  8  C    Isotropic =    73.7641   Anisotropy =   316.7247
   XX=   129.2903   YX=    -6.5705   ZX=   158.1839
   XY=    -6.5883   YY=   -31.5397   ZY=    -6.4936
   XZ=   158.2203   YZ=    -6.4786   ZZ=   123.5417
   Eigenvalues:   -31.8287   -31.7928   284.9139
  9  C    Isotropic =    73.8150   Anisotropy =   316.6509
   XX=   -21.0643   YX=    56.5036   ZX=    -8.5975
   XY=    56.4608   YY=   267.3164   ZY=   -45.5542
   XZ=    -8.5823   YZ=   -45.5059   ZZ=   -24.8072
   Eigenvalues:   -31.7451   -31.7256   284.9156
 10  C    Isotropic =    73.8285   Anisotropy =   316.6249
   XX=   114.4149   YX=   -50.0054   ZX=  -149.6599
   XY=   -50.0262   YY=   -14.6132   ZY=    51.2391
   XZ=  -149.7390   YZ=    51.2491   ZZ=   121.6836
   Eigenvalues:   -31.7320   -31.6943   284.9117
 11  C    Isotropic =    73.8009   Anisotropy =   316.6684
   XX=   -20.7159   YX=    57.4366   ZX=    -8.4923
   XY=    57.4842   YY=   267.3077   ZY=   -44.2824
   XZ=    -8.5125   YZ=   -44.3435   ZZ=   -25.1891
   Eigenvalues:   -31.7665   -31.7439   284.9132
 12  C    Isotropic =    73.8243   Anisotropy =   316.6304
   XX=   112.5875   YX=   -50.2575   ZX=  -149.4971
   XY=   -50.2005   YY=   -14.2654   ZY=    52.0132
   XZ=  -149.4370   YZ=    52.0477   ZZ=   123.1509
   Eigenvalues:   -31.7473   -31.6910   284.9113
 13  C    Isotropic =    73.7691   Anisotropy =   316.7155
   XX=   128.8837   YX=    -7.1082   ZX=   158.1784
   XY=    -7.0789   YY=   -31.4924   ZY=    -6.9740
   XZ=   158.1816   YZ=    -7.0036   ZZ=   123.9161
   Eigenvalues:   -31.8078   -31.7976   284.9128
 14  C    Isotropic =   188.0249   Anisotropy =    30.9572
```

```
  XX=   193.4386   YX=    -0.6524   ZX=    15.4756
  XY=    -0.6661   YY=   177.7658   ZY=    -0.6699
  XZ=    15.4807   YZ=    -0.6371   ZZ=   192.8702
  Eigenvalues:   177.6734   177.7382   208.6630
15  C    Isotropic =   188.0026   Anisotropy =    30.9644
  XX=   178.7002   YX=     5.4901   ZX=    -0.8587
  XY=     5.5196   YY=   206.9288   ZY=    -4.4540
  XZ=    -0.8761   YZ=    -4.4606   ZZ=   178.3788
  Eigenvalues:   177.6485   177.7137   208.6455
16  C    Isotropic =   187.9987   Anisotropy =    30.9641
  XX=   191.9747   YX=    -4.8998   ZX=   -14.6448
  XY=    -4.8550   YY=   179.3362   ZY=     4.9823
  XZ=   -14.6451   YZ=     5.0022   ZZ=   192.6854
  Eigenvalues:   177.6726   177.6822   208.6415
17  C    Isotropic =   188.0193   Anisotropy =    30.9489
  XX=   178.7737   YX=     5.5494   ZX=    -0.7770
  XY=     5.6099   YY=   206.9433   ZY=    -4.3416
  XZ=    -0.7955   YZ=    -4.3519   ZZ=   178.3410
  Eigenvalues:   177.6605   177.7456   208.6519
18  C    Isotropic =   188.0011   Anisotropy =    30.9748
  XX=   191.7926   YX=    -4.8975   ZX=   -14.6287
  XY=    -4.8917   YY=   179.3886   ZY=     5.0847
  XZ=   -14.6269   YZ=     5.1107   ZZ=   192.8222
  Eigenvalues:   177.6566   177.6958   208.6510
19  C    Isotropic =   188.0387   Anisotropy =    30.9337
  XX=   193.4172   YX=    -0.7010   ZX=    15.4380
  XY=    -0.7143   YY=   177.7599   ZY=    -0.7056
  XZ=    15.4610   YZ=    -0.6781   ZZ=   192.9390
  Eigenvalues:   177.7239   177.7310   208.6611
20  H    Isotropic =    28.9416   Anisotropy =     9.8693
  XX=    33.7281   YX=     4.3988   ZX=    -0.1912
  XY=     3.6375   YY=    26.5028   ZY=    -1.2809
  XZ=     1.3356   YZ=    -0.5923   ZZ=    26.5938
  Eigenvalues:    24.2139    27.0896    35.5211
21  H    Isotropic =    28.9402   Anisotropy =     9.8815
  XX=    27.6637   YX=    -3.9720   ZX=     3.0207
  XY=    -2.6642   YY=    32.1608   ZY=    -1.8491
  XZ=     3.1553   YZ=    -3.1338   ZZ=    26.9961
  Eigenvalues:    24.1988    27.0940    35.5278
22  H    Isotropic =    28.9420   Anisotropy =     9.8759
  XX=    26.7935   YX=    -0.5930   ZX=     1.0460
  XY=    -1.1341   YY=    25.5832   ZY=     2.9706
  XZ=    -0.6104   YZ=     3.5717   ZZ=    34.4493
  Eigenvalues:    24.2024    27.0977    35.5260
23  H    Isotropic =    28.9415   Anisotropy =     9.8739
  XX=    28.9656   YX=     3.1797   ZX=     4.0550
  XY=     4.3964   YY=    30.1927   ZY=     2.6452
  XZ=     3.6143   YZ=     1.3282   ZZ=    27.6661
  Eigenvalues:    24.2011    27.0992    35.5240
24  H    Isotropic =    28.9413   Anisotropy =     9.8735
  XX=    25.4782   YX=     1.4254   ZX=    -3.2499
  XY=     2.0003   YY=    29.0172   ZY=    -4.0458
  XZ=    -3.0089   YZ=    -2.3162   ZZ=    32.3283
  Eigenvalues:    24.2060    27.0942    35.5236
25  H    Isotropic =    28.9415   Anisotropy =     9.8684
  XX=    30.0528   YX=    -3.2255   ZX=    -1.0166
  XY=    -5.0169   YY=    32.3599   ZY=     0.2856
  XZ=    -0.8227   YZ=    -0.1290   ZZ=    24.4119
  Eigenvalues:    24.2054    27.0987    35.5205
26  H    Isotropic =    28.9415   Anisotropy =     9.8745
  XX=    26.9357   YX=    -3.9499   ZX=    -2.1056
  XY=    -2.7279   YY=    33.5631   ZY=     0.8428
  XZ=    -2.3866   YZ=     2.1911   ZZ=    26.3256
  Eigenvalues:    24.1991    27.1009    35.5244
27  H    Isotropic =    28.9426   Anisotropy =     9.8784
  XX=    26.6266   YX=    -1.0029   ZX=    -0.7686
  XY=    -1.1714   YY=    24.8078   ZY=    -0.8081
  XZ=     0.9136   YZ=    -1.5586   ZZ=    35.3933
  Eigenvalues:    24.2020    27.0976    35.5282
28  H    Isotropic =    28.9398   Anisotropy =     9.8650
```

```
  XX=    34.2525   YX=     3.7309   ZX=    -0.7980
  XY=     2.6811   YY=    26.2789   ZY=     1.2192
  XZ=    -2.1924   YZ=     0.6214   ZZ=    26.2880
  Eigenvalues:    24.2058    27.0971    35.5165
29  H    Isotropic =    28.9428   Anisotropy =     9.8844
  XX=    28.8681   YX=    -2.0802   ZX=     3.0869
  XY=    -3.6614   YY=    31.1225   ZY=    -3.7532
  XZ=     3.4860   YZ=    -2.8910   ZZ=    26.8377
  Eigenvalues:    24.1969    27.0991    35.5324
30  H    Isotropic =    28.9433   Anisotropy =     9.8705
  XX=    31.1669   YX=     2.0696   ZX=    -4.2370
  XY=     3.6501   YY=    28.8402   ZY=    -2.3371
  XZ=    -4.2929   YZ=    -1.3914   ZZ=    26.8229
  Eigenvalues:    24.2061    27.1002    35.5237
31  H    Isotropic =    28.9391   Anisotropy =     9.8698
  XX=    24.4763   YX=     1.4140   ZX=     0.9549
  XY=     1.4105   YY=    31.6061   ZY=     5.0053
  XZ=     0.6044   YZ=     3.1977   ZZ=    30.7348
  Eigenvalues:    24.2068    27.0915    35.5190
32  H    Isotropic =    28.9411   Anisotropy =     9.8665
  XX=    26.2407   YX=    -0.3800   ZX=    -1.8976
  XY=     0.8963   YY=    31.9212   ZY=     4.4046
  XZ=    -1.0479   YZ=     5.4305   ZZ=    28.6614
  Eigenvalues:    24.2050    27.0996    35.5188
33  H    Isotropic =    28.9431   Anisotropy =     9.8715
  XX=    35.2845   YX=    -1.3058   ZX=     1.5452
  XY=    -1.6582   YY=    24.5049   ZY=     0.3296
  XZ=    -0.2531   YZ=     0.5923   ZZ=    27.0398
  Eigenvalues:    24.1999    27.1053    35.5241
34  H    Isotropic =    28.9403   Anisotropy =     9.8711
  XX=    26.2452   YX=     0.4630   ZX=    -3.3145
  XY=    -0.4646   YY=    28.2401   ZY=    -3.4602
  XZ=    -2.3649   YZ=    -4.7534   ZZ=    32.3355
  Eigenvalues:    24.2039    27.0958    35.5210
35  H    Isotropic =    28.9395   Anisotropy =     9.8816
  XX=    27.1032   YX=    -0.2632   ZX=     0.3848
  XY=    -0.3642   YY=    24.2618   ZY=     0.5700
  XZ=    -1.4370   YZ=     0.7474   ZZ=    35.4535
  Eigenvalues:    24.1955    27.0958    35.5273
36  H    Isotropic =    28.9395   Anisotropy =     9.8780
  XX=    29.5840   YX=    -5.3488   ZX=     2.0763
  XY=    -4.1639   YY=    30.9242   ZY=     0.0060
  XZ=     2.8224   YZ=    -1.1843   ZZ=    26.3103
  Eigenvalues:    24.2054    27.0883    35.5248
37  H    Isotropic =    28.9435   Anisotropy =     9.8788
  XX=    31.4901   YX=     5.4330   ZX=     1.4111
  XY=     4.3522   YY=    29.0602   ZY=    -0.7509
  XZ=     2.4927   YZ=     0.2692   ZZ=    26.2800
  Eigenvalues:    24.2113    27.0897    35.5294
```

4. $[Sn(NCMe)_7]^{2+}$ at BP86/SDD level:



Sn-N = 291 (2x), 270 (2x), 251 (2x) and 248 (1x) pm

Sn	0	-0.0043	-0.0232	-0.108
N	0	-1.6027	2.3894	-0.3105
N	0	1.5434	-0.3162	1.8534
N	0	-1.6073	-0.0741	1.8267
N	0	-0.1946	-2.4377	0.4371
N	0	-2.1093	-0.9016	-1.5458
N	0	1.9543	-1.2213	-1.535
N	0	1.9679	2.1071	-0.3015
C	0	-2.1346	3.4321	-0.5281
C	0	2.6632	3.0507	-0.5107
C	0	2.7651	-1.5571	-2.3375
C	0	-2.9557	-1.1204	-2.3519
C	0	-0.2836	-3.6087	0.6021
C	0	-2.4115	0.0616	2.6887
C	0	2.3561	-0.3015	2.7182
C	0	-2.7897	4.718	-0.7996
C	0	3.52	4.2144	-0.7719
C	0	3.7678	-1.9693	-3.3255
C	0	-4.0018	-1.3866	-3.3448
C	0	-0.394	-5.0551	0.8054
C	0	-3.4057	0.2288	3.7515
C	0	3.3605	-0.2841	3.7844
H	0	-3.8871	4.6131	-0.7403
H	0	-2.4708	5.4762	-0.0631
H	0	-2.5271	5.0781	-1.8097
H	0	4.5828	3.9158	-0.7897
H	0	3.268	4.6669	-1.7469
H	0	3.3843	4.9775	0.0143
H	0	4.0924	-1.1028	-3.9279
H	0	4.6518	-2.3977	-2.8214
H	0	3.3482	-2.7311	-4.0056
H	0	-3.966	-0.6334	-4.1513
H	0	-3.8637	-2.3863	-3.7926
H	0	-4.9991	-1.3487	-2.8725
H	0	0.3189	-5.3906	1.579
H	0	-1.4154	-5.3211	1.1296
H	0	-0.172	-5.5924	-0.1333
H	0	-3.294	1.2184	4.2284
H	0	-4.4262	0.1515	3.3369
H	0	-3.2802	-0.5501	4.5239
H	0	3.3668	0.6981	4.2888
H	0	3.1406	-1.0634	4.535
H	0	4.3654	-0.4716	3.367

NMR Calculations at the BP86/SVP level (NMR=GIAO):

```
1|1|UNPC-UNK|SP|RBP86|SVP|C14H21N7Sn1(2+)|PCUSER|27-May-2017|0||# RBP8
 6/SVP NMR=GIAO Test||[No Title]||2,1|Sn,0,-0.0043,-0.0232,-0.108|N,0,-
 1.6027,2.3894,-0.3105|N,0,1.5434,-0.3162,1.8534|N,0,-1.6073,-0.0741,1.
 8267|N,0,-0.1946,-2.4377,0.4371|N,0,-2.1093,-0.9016,-1.5458|N,0,1.9543
 ,-1.2213,-1.535|N,0,1.9679,2.1071,-0.3015|C,0,-2.1346,3.4321,-0.5281|C
```

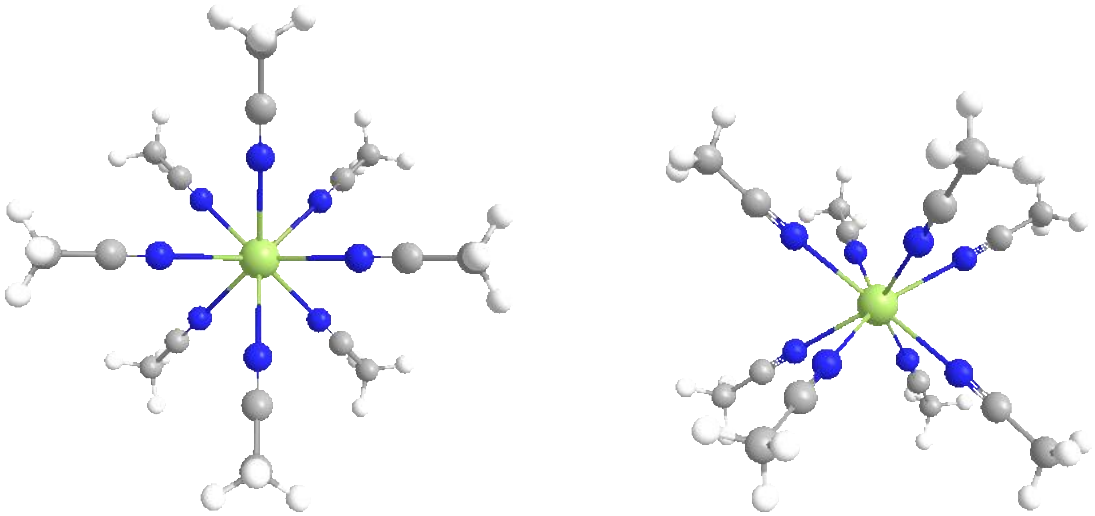
```
,0,2.6632,3.0507,-0.5107|C,0,2.7651,-1.5571,-2.3375|C,0,-2.9557,-1.120
4,-2.3519|C,0,-0.2836,-3.6087,0.6021|C,0,-2.4115,0.0616,2.6887|C,0,2.3
561,-0.3015,2.7182|C,0,-2.7897,4.718,-0.7996|C,0,3.52,4.2144,-0.7719|C
,0,3.7678,-1.9693,-3.3255|C,0,-4.0018,-1.3866,-3.3448|C,0,-0.394,-5.05
51,0.8054|C,0,-3.4057,0.2288,3.7515|C,0,3.3605,-0.2841,3.7844|H,0,-3.8
871,4.6131,-0.7403|H,0,-2.4708,5.4762,-0.0631|H,0,-2.5271,5.0781,-1.80
97|H,0,4.5828,3.9158,-0.7897|H,0,3.268,4.6669,-1.7469|H,0,3.3843,4.977
5,0.0143|H,0,4.0924,-1.1028,-3.9279|H,0,4.6518,-2.3977,-2.8214|H,0,3.3
482,-2.7311,-4.0056|H,0,-3.966,-0.6334,-4.1513|H,0,-3.8637,-2.3863,-3.
7926|H,0,-4.9991,-1.3487,-2.8725|H,0,0.3189,-5.3906,1.579|H,0,-1.4154,
-5.3211,1.1296|H,0,-0.172,-5.5924,-0.1333|H,0,-3.294,1.2184,4.2284|H,0
,-4.4262,0.1515,3.3369|H,0,-3.2802,-0.5501,4.5239|H,0,3.3668,0.6981,4.
2888|H,0,3.1406,-1.0634,4.535|H,0,4.3654,-0.4716,3.367||Version=IA32W-
G03RevD.01|State=1-A|HF=-6953.4525289|RMSD=5.075e-009|Thermal=0.|Dipol
e=-0.0566024,-0.5634615,0.5244016|PG=C01 [X(C14H21N7Sn1)]||@


SCF GIAO Magnetic shielding tensor (ppm):
  1  Sn   Isotropic =  4227.2748   Anisotropy =    58.7576
   XX=  4214.1819   YX=     0.8773   ZX=    -2.6338
   XY=     0.7649   YY=  4216.7249   ZY=   -25.9507
   XZ=    -2.6983   YZ=   -29.2887   ZZ=  4250.9175
   Eigenvalues:  4201.3120  4214.0658  4266.4465
  2  N    Isotropic =     8.9368   Anisotropy =   460.8293
   XX=   -52.2946   YX=  -179.5494   ZX=    36.4359
   XY=  -181.1496   YY=   208.3833   ZY=   -74.3758
   XZ=    37.2220   YZ=   -75.1739   ZZ=  -129.2784
   Eigenvalues:  -145.9053  -143.4407   316.1563
  3  N    Isotropic =    28.6457   Anisotropy =   435.1868
   XX=    88.3753   YX=     4.6169   ZX=   218.2723
   XY=     6.9419   YY=  -115.9240   ZY=     4.5439
   XZ=   216.4994   YZ=     1.9003   ZZ=   113.4858
   Eigenvalues:  -118.4474  -114.3857   318.7703
  4  N    Isotropic =    28.8011   Anisotropy =   435.0223
   XX=    83.6473   YX=   -34.6220   ZX=  -215.0091
   XY=   -36.9378   YY=  -109.3953   ZY=    36.7519
   XZ=  -214.0760   YZ=    33.9753   ZZ=   112.1513
   Eigenvalues:  -118.3572  -114.0555   318.8159
  5  N    Isotropic =    29.4378   Anisotropy =   434.9555
   XX=  -113.1672   YX=    32.1979   ZX=    -4.5279
   XY=    32.2553   YY=   308.7607   ZY=   -59.9532
   XZ=    -4.3715   YZ=   -58.0147   ZZ=  -107.2802
   Eigenvalues:  -115.6205  -115.4743   319.4081
  6  N    Isotropic =    18.5402   Anisotropy =   448.8472
   XX=    94.9152   YX=    58.7898   ZX=   215.9059
   XY=    57.4650   YY=  -114.5355   ZY=    53.5690
   XZ=   219.5127   YZ=    56.0351   ZZ=    75.2410
   Eigenvalues:  -132.9332  -129.2177   317.7717
  7  N    Isotropic =    18.1894   Anisotropy =   449.2749
   XX=    76.1860   YX=   -86.3240   ZX=  -206.3684
   XY=   -84.9288   YY=   -94.5813   ZY=    83.1115
   XZ=  -209.5587   YZ=    86.1784   ZZ=    72.9636
   Eigenvalues:  -133.4080  -129.7297   317.7060
  8  N    Isotropic =     8.6073   Anisotropy =   461.2332
   XX=    12.4685   YX=   212.5771   ZX=   -46.3714
   XY=   214.1629   YY=   144.2357   ZY=   -65.0165
   XZ=   -47.1755   YZ=   -65.5993   ZZ=  -130.8822
   Eigenvalues:  -146.2691  -144.0050   316.0962
  9  C    Isotropic =    74.5470   Anisotropy =   315.3471
   XX=    33.5114   YX=  -125.4110   ZX=    26.9337
   XY=  -121.7833   YY=   210.7940   ZY=   -51.0160
   XZ=    25.4598   YZ=   -49.5763   ZZ=   -20.6645
   Eigenvalues:   -31.2736   -29.8638   284.7784
 10  C    Isotropic =    74.5649   Anisotropy =   315.4895
   XX=    78.0876   YX=   147.6803   ZX=   -33.5694
   XY=   144.1671   YY=   167.0764   ZY=   -44.3033
   XZ=   -31.9983   YZ=   -43.1768   ZZ=   -21.4691
   Eigenvalues:   -31.2950   -29.9014   284.8913
 11  C    Isotropic =    73.9409   Anisotropy =   311.8648
```

```
  XX=   115.9601   YX=   -58.5114   ZX=  -145.1015
  XY=   -62.5243   YY=    -4.5100   ZY=    63.3709
  XZ=  -141.0294   YZ=    57.7361   ZZ=   110.3727
  Eigenvalues:   -30.8436   -29.1845   281.8508
12  C    Isotropic =    73.9552   Anisotropy =   311.8641
  XX=   129.1245   YX=    39.3043   ZX=   152.7478
  XY=    43.0273   YY=   -18.9662   ZY=    42.3713
  XZ=   147.7635   YZ=    37.5627   ZZ=   111.7073
  Eigenvalues:   -30.8036   -29.1954   281.8646
13  C    Isotropic =    74.6012   Anisotropy =   305.5934
  XX=   -25.1838   YX=    22.6565   ZX=    -3.1171
  XY=    22.5888   YY=   270.5580   ZY=   -41.2630
  XZ=    -3.2941   YZ=   -43.6987   ZZ=   -21.5705
  Eigenvalues:   -27.6231   -26.9034   278.3301
14  C    Isotropic =    74.0896   Anisotropy =   307.1255
  XX=   112.4944   YX=   -24.9579   ZX=  -149.5994
  XY=   -20.7738   YY=   -25.0679   ZY=    21.8034
  XZ=  -152.5906   YZ=    26.8056   ZZ=   134.8422
  Eigenvalues:   -28.7801   -27.7911   278.8399
15  C    Isotropic =    74.0086   Anisotropy =   307.1292
  XX=   114.8475   YX=     3.7505   ZX=   150.8384
  XY=    -0.5108   YY=   -28.7925   ZY=    -0.7323
  XZ=   155.1044   YZ=     3.9038   ZZ=   135.9707
  Eigenvalues:   -28.8209   -27.9148   278.7614
16  C    Isotropic =   187.5221   Anisotropy =    29.1872
  XX=   183.8469   YX=   -11.4826   ZX=     2.4378
  XY=   -11.3150   YY=   200.1429   ZY=    -4.7078
  XZ=     2.3511   YZ=    -4.6569   ZZ=   178.5765
  Eigenvalues:   177.6023   177.9837   206.9802
17  C    Isotropic =   187.5269   Anisotropy =    29.1634
  XX=   187.9477   YX=    13.5413   ZX=    -3.0273
  XY=    13.3569   YY=   196.0805   ZY=    -4.0984
  XZ=    -2.9764   YZ=    -4.0739   ZZ=   178.5524
  Eigenvalues:   177.6458   177.9656   206.9692
18  C    Isotropic =   187.6590   Anisotropy =    29.9969
  XX=   191.6095   YX=    -5.6951   ZX=   -13.9669
  XY=    -5.9160   YY=   180.2666   ZY=     5.9654
  XZ=   -13.6998   YZ=     5.6706   ZZ=   191.1009
  Eigenvalues:   177.4979   177.8221   207.6569
19  C    Isotropic =   187.7392   Anisotropy =    29.9798
  XX=   192.9567   YX=     3.8378   ZX=    14.6457
  XY=     4.0190   YY=   178.9202   ZY=     3.9240
  XZ=    14.3746   YZ=     3.7338   ZZ=   191.3405
  Eigenvalues:   177.5929   177.8988   207.7257
20  C    Isotropic =   187.9106   Anisotropy =    30.6874
  XX=   177.8961   YX=     2.2961   ZX=    -0.3450
  XY=     2.2703   YY=   207.5779   ZY=    -4.2296
  XZ=    -0.3692   YZ=    -4.3569   ZZ=   178.2577
  Eigenvalues:   177.6323   177.7305   208.3688
21  C    Isotropic =   187.9332   Anisotropy =    30.6152
  XX=   191.6493   YX=    -2.4671   ZX=   -15.0644
  XY=    -2.2408   YY=   178.1615   ZY=     2.1335
  XZ=   -15.1866   YZ=     2.4120   ZZ=   193.9888
  Eigenvalues:   177.5290   177.9273   208.3434
22  C    Isotropic =   187.9362   Anisotropy =    30.5896
  XX=   191.9486   YX=     0.3932   ZX=    15.1537
  XY=     0.1621   YY=   177.7252   ZY=    -0.1518
  XZ=    15.3413   YZ=     0.1074   ZZ=   194.1347
  Eigenvalues:   177.5207   177.9585   208.3293
23  H    Isotropic =    29.1469   Anisotropy =     9.7793
  XX=    35.1361   YX=    -1.0939   ZX=    -0.0905
  XY=    -2.9692   YY=    27.7746   ZY=    -0.6425
  XZ=     0.3201   YZ=    -0.6922   ZZ=    24.5300
  Eigenvalues:    24.3899    27.3844    35.6665
24  H    Isotropic =    29.1314   Anisotropy =     9.6008
  XX=    25.9140   YX=    -0.7655   ZX=     1.2499
  XY=     0.4350   YY=    33.5096   ZY=     4.6161
  XZ=     1.7662   YZ=     3.1279   ZZ=    27.9705
  Eigenvalues:    24.5159    27.3463    35.5319
25  H    Isotropic =    29.1122   Anisotropy =     9.5393
```

```
  XX=    25.7145   YX=    -1.4103   ZX=    -0.4770
  XY=    -0.6536   YY=    29.5033   ZY=    -5.2542
  XZ=    -1.4392   YZ=    -3.6879   ZZ=    32.1187
  Eigenvalues:    24.5150    27.3498    35.4717
26  H    Isotropic =    29.1459   Anisotropy =     9.7606
  XX=    35.5368   YX=    -0.3309   ZX=    -0.6838
  XY=     1.5692   YY=    27.3663   ZY=    -0.5937
  XZ=    -0.9979   YZ=    -0.4576   ZZ=    24.5347
  Eigenvalues:    24.3932    27.3916    35.6529
27  H    Isotropic =    29.1129   Anisotropy =     9.5383
  XX=    26.2524   YX=     1.7876   ZX=    -0.0129
  XY=     0.8949   YY=    29.5082   ZY=    -5.4637
  XZ=     1.1672   YZ=    -4.1386   ZZ=    31.5781
  Eigenvalues:    24.4965    27.3704    35.4718
28  H    Isotropic =    29.1352   Anisotropy =     9.6082
  XX=    26.1075   YX=     2.2948   ZX=    -0.1572
  XY=     1.2120   YY=    32.7969   ZY=     4.9386
  XZ=    -0.9906   YZ=     3.5054   ZZ=    28.5011
  Eigenvalues:    24.5378    27.3271    35.5407
29  H    Isotropic =    29.0248   Anisotropy =     9.5971
  XX=    27.6269   YX=     2.3557   ZX=    -4.5113
  XY=     1.0622   YY=    29.5504   ZY=    -2.4857
  XZ=    -4.1572   YZ=    -3.8921   ZZ=    29.8971
  Eigenvalues:    24.1918    27.4598    35.4229
30  H    Isotropic =    29.0393   Anisotropy =     9.8320
  XX=    33.4614   YX=    -4.3079   ZX=     1.6532
  XY=    -4.2850   YY=    26.4252   ZY=    -0.8114
  XZ=    -0.0583   YZ=    -0.0415   ZZ=    27.2311
  Eigenvalues:    24.3895    27.1343    35.5939
31  H    Isotropic =    29.0464   Anisotropy =     9.9133
  XX=    26.9793   YX=     0.3443   ZX=    -0.9851
  XY=     1.5085   YY=    29.4364   ZY=     5.2530
  XZ=     0.3811   YZ=     5.7875   ZZ=    30.7234
  Eigenvalues:    24.2309    27.2529    35.6552
32  H    Isotropic =    29.0159   Anisotropy =     9.6435
  XX=    26.4652   YX=    -0.3435   ZX=     3.3035
  XY=     0.6676   YY=    28.2446   ZY=    -3.4704
  XZ=     2.1979   YZ=    -4.7028   ZZ=    32.3380
  Eigenvalues:    24.2643    27.3385    35.4449
33  H    Isotropic =    29.0537   Anisotropy =     9.9418
  XX=    26.5125   YX=     1.1134   ZX=     2.4460
  XY=    -0.2180   YY=    32.1554   ZY=     4.2376
  XZ=     1.7023   YZ=     5.2647   ZZ=    28.4932
  Eigenvalues:    24.2147    27.2648    35.6816
34  H    Isotropic =    29.0358   Anisotropy =     9.7838
  XX=    35.4662   YX=     0.3820   ZX=    -1.6618
  XY=     0.8075   YY=    24.5763   ZY=     0.5947
  XZ=     0.1688   YZ=     0.6929   ZZ=    27.0648
  Eigenvalues:    24.3678    27.1813    35.5583
35  H    Isotropic =    28.9362   Anisotropy =     9.9715
  XX=    27.6747   YX=    -1.5815   ZX=     3.8405
  XY=    -2.8513   YY=    30.3207   ZY=    -4.2082
  XZ=     4.1173   YZ=    -2.9719   ZZ=    28.8132
  Eigenvalues:    24.1121    27.1127    35.5838
36  H    Isotropic =    28.9327   Anisotropy =     9.9368
  XX=    31.8588   YX=     2.7365   ZX=    -2.5390
  XY=     4.4517   YY=    29.8547   ZY=    -2.0260
  XZ=    -2.7498   YZ=    -1.5442   ZZ=    25.0847
  Eigenvalues:    24.1061    27.1348    35.5573
37  H    Isotropic =    28.9223   Anisotropy =     9.8202
  XX=    24.4808   YX=    -0.5006   ZX=    -1.4135
  XY=    -0.9525   YY=    32.1189   ZY=     4.8879
  XZ=    -1.4770   YZ=     3.1381   ZZ=    30.1672
  Eigenvalues:    24.1249    27.1729    35.4691
38  H    Isotropic =    28.9218   Anisotropy =     9.7506
  XX=    26.0119   YX=    -1.0024   ZX=    -2.5694
  XY=     0.2119   YY=    31.4834   ZY=     3.9992
  XZ=    -1.8942   YZ=     5.2056   ZZ=    29.2701
  Eigenvalues:    24.1873    27.1559    35.4222
39  H    Isotropic =    28.9219   Anisotropy =     9.7566
```

```
  XX=    35.4204   YX=     0.3398   ZX=     1.0367
  XY=     0.0795   YY=    24.2180   ZY=     0.3133
  XZ=    -0.7973   YZ=     0.3137   ZZ=    27.1271
  Eigenvalues:    24.1812    27.1581    35.4262
40  H    Isotropic =    28.9661   Anisotropy =    10.1283
  XX=    26.1361   YX=     0.0728   ZX=    -2.6243
  XY=    -0.8037   YY=    28.3915   ZY=    -4.1274
  XZ=    -1.6027   YZ=    -5.2145   ZZ=    32.3708
  Eigenvalues:    24.1103    27.0697    35.7184
41  H    Isotropic =    28.9247   Anisotropy =     9.7516
  XX=    26.1619   YX=     1.5446   ZX=     3.0429
  XY=     0.3494   YY=    31.0593   ZY=     3.7182
  XZ=     2.4890   YZ=     5.0005   ZZ=    29.5530
  Eigenvalues:    24.2095    27.1389    35.4258
42  H    Isotropic =    28.9650   Anisotropy =    10.1495
  XX=    26.2259   YX=     0.1458   ZX=     2.0878
  XY=     1.0479   YY=    28.5462   ZY=    -4.5143
  XZ=     0.9767   YZ=    -5.4815   ZZ=    32.1229
  Eigenvalues:    24.1086    27.0552    35.7314
43  H    Isotropic =    28.9224   Anisotropy =     9.7271
  XX=    35.1924   YX=    -1.6362   ZX=    -1.0137
  XY=    -1.4216   YY=    24.4081   ZY=     0.3459
  XZ=     0.8073   YZ=     0.1257   ZZ=    27.1667
  Eigenvalues:    24.1794    27.1806    35.4071
```

5. $[Sn(NCMe)_8]^{2+}$ at BP86/SDD level:



Sn-N = 272 pm (8x)

Sn	0	0.0009	-0.0009	-0.0016
N	0	2.3103	0.0101	-1.4412
N	0	-2.3124	-0.0106	-1.4401
N	0	0.0107	-2.31	-1.4415
N	0	-1.6195	-1.639	1.4429
N	0	1.6372	-1.623	1.4394
N	0	1.6236	1.6347	1.4432
N	0	-1.6355	1.6211	1.4465
N	0	-0.01	2.3123	-1.4402
C	0	3.2902	0.0175	-2.1135
C	0	-0.0171	3.2944	-2.1093
C	0	-2.3328	2.3103	2.1181
C	0	2.3149	2.3315	2.113
C	0	2.3362	-2.3142	2.1071
C	0	-2.3108	-2.3359	2.1126
C	0	0.0121	-3.2905	-2.1129
C	0	-3.2937	-0.012	-2.1105
C	0	4.5021	0.0261	-2.9415
C	0	-0.0254	4.5091	-2.9332

```
 C                    0    -3.195     3.1631    2.945
 C                    0     3.1696    3.1937    2.938
 C                    0     3.2003   -3.1694    2.9295
 C                    0    -3.1657   -3.1981    2.9373
 C                    0     0.0142   -4.5032   -2.9399
 C                    0    -4.5074   -0.014    -2.9359
 H                    0     5.1082    0.924    -2.7286
 H                    0     4.2365    0.0288   -4.0131
 H                    0     5.1164   -0.8677   -2.7351
 H                    0    -0.0275    4.2472   -4.0057
 H                    0    -0.9235    5.1144   -2.7188
 H                    0     0.8682    5.1229   -2.7243
 H                    0    -2.9979    4.229     2.7358
 H                    0    -4.2587    2.9562    2.7339
 H                    0    -3.0079    2.9762    4.0169
 H                    0     2.9684    4.2573    2.721
 H                    0     2.9788    3.0129    4.0103
 H                    0     4.2352    2.9903    2.7327
 H                    0     4.2634   -2.9676    2.7106
 H                    0     3.0216   -2.9797    4.0023
 H                    0     2.9969   -4.2348    2.7236
 H                    0    -4.2312   -2.9996    2.7269
 H                    0    -2.9596   -4.2618    2.7253
 H                    0    -2.9801   -3.0125    4.0097
 H                    0     0.0126   -4.2386   -4.0117
 H                    0     0.9117   -5.1111   -2.7305
 H                    0    -0.88     -5.1153   -2.729
 H                    0    -5.1193    0.8802   -2.7243
 H                    0    -4.2441   -0.0125   -4.0081
 H                    0    -5.1151   -0.9115   -2.7258
```

NMR Calculations at the BP86/SVP level (NMR=GIAO):

```
1|1|UNPC-UNK|SP|RBP86|SVP|C16H24N8Sn1(2+)|PCUSER|27-May-2017|0||# RBP8
 6/SVP NMR=GIAO Test|||[No Title]||2,1|Sn,0,0.0009,-0.0009,-0.0016|N,0,2
 .3103,0.0101,-1.4412|N,0,-2.3124,-0.0106,-1.4401|N,0,0.0107,-2.31,-1.4
 415|N,0,-1.6195,-1.639,1.4429|N,0,1.6372,-1.623,1.4394|N,0,1.6236,1.63
 47,1.4432|N,0,-1.6355,1.6211,1.4465|N,0,-0.01,2.3123,-1.4402|C,0,3.290
 2,0.0175,-2.1135|C,0,-0.0171,3.2944,-2.1093|C,0,-2.3328,2.3103,2.1181|
 C,0,2.3149,2.3315,2.113|C,0,2.3362,-2.3142,2.1071|C,0,-2.3108,-2.3359,
 2.1126|C,0,0.0121,-3.2905,-2.1129|C,0,-3.2937,-0.012,-2.1105|C,0,4.502
 1,0.0261,-2.9415|C,0,-0.0254,4.5091,-2.9332|C,0,-3.195,3.1631,2.945|C,
 0,3.1696,3.1937,2.938|C,0,3.2003,-3.1694,2.9295|C,0,-3.1657,-3.1981,2.
 9373|C,0,0.0142,-4.5032,-2.9399|C,0,-4.5074,-0.014,-2.9359|H,0,5.1082,
 0.924,-2.7286|H,0,4.2365,0.0288,-4.0131|H,0,5.1164,-0.8677,-2.7351|H,0
 ,-0.0275,4.2472,-4.0057|H,0,-0.9235,5.1144,-2.7188|H,0,0.8682,5.1229,-
 2.7243|H,0,-2.9979,4.229,2.7358|H,0,-4.2587,2.9562,2.7339|H,0,-3.0079,
 2.9762,4.0169|H,0,2.9684,4.2573,2.721|H,0,2.9788,3.0129,4.0103|H,0,4.2
 352,2.9903,2.7327|H,0,4.2634,-2.9676,2.7106|H,0,3.0216,-2.9797,4.0023|
 H,0,2.9969,-4.2348,2.7236|H,0,-4.2312,-2.9996,2.7269|H,0,-2.9596,-4.26
 18,2.7253|H,0,-2.9801,-3.0125,4.0097|H,0,0.0126,-4.2386,-4.0117|H,0,0.
 9117,-5.1111,-2.7305|H,0,-0.88,-5.1153,-2.729|H,0,-5.1193,0.8802,-2.72
 43|H,0,-4.2441,-0.0125,-4.0081|H,0,-5.1151,-0.9115,-2.7258||Version=IA
 32W-G03RevD.01|State=1-A|HF=-7086.1186084|RMSD=8.029e-009|Thermal=0.|D
 ipole=0.0024181,-0.0024803,0.0064329|PG=C01 [X(C16H24N8Sn1)]||@
```

```
SCF GIAO Magnetic shielding tensor (ppm):
  1  Sn   Isotropic =  4314.9967   Anisotropy =    27.6377
   XX=  4305.7114   YX=    -0.0057   ZX=    -0.0155
   XY=    -0.0138   YY=  4305.8569   ZY=     0.0189
   XZ=     0.0377   YZ=    -0.0412   ZZ=  4333.4218
   Eigenvalues:  4305.7107  4305.8575  4333.4218
  2  N    Isotropic =    12.7079   Anisotropy =   456.4133
   XX=   170.6651   YX=     0.9095   ZX=  -212.7022
   XY=     0.9084   YY=  -137.8757   ZY=    -0.6196
   XZ=  -214.3751   YZ=    -0.6220   ZZ=     5.3342
   Eigenvalues:  -140.9814  -137.8784   316.9834
  3  N    Isotropic =    12.5732   Anisotropy =   456.5771
   XX=   171.4518   YX=    -0.9215   ZX=   212.4612
   XY=    -0.9460   YY=  -138.0543   ZY=    -0.6318
   XZ=   214.1026   YZ=    -0.6173   ZZ=     4.3219
   Eigenvalues:  -141.1814  -138.0570   316.9579
  4  N    Isotropic =    12.7226   Anisotropy =   456.4140
```

```
  XX=  -137.8587   YX=     0.9233   ZX=     0.6257
  XY=     0.9113   YY=   171.0500   ZY=   212.5705
  XZ=     0.6197   YZ=   214.2219   ZZ=     4.9764
  Eigenvalues:  -140.9694  -137.8614   316.9985
 5  N    Isotropic =    12.7365   Anisotropy =   456.3980
  XX=    17.1636   YX=   154.7585   ZX=  -150.2231
  XY=   154.7655   YY=    16.9198   ZY=  -150.0976
  XZ=  -151.3320   YZ=  -151.2002   ZZ=     4.1260
  Eigenvalues:  -141.0721  -137.7203   317.0018
 6  N    Isotropic =    12.7988   Anisotropy =   456.3295
  XX=    17.8350   YX=  -155.1497   ZX=   150.0515
  XY=  -155.1665   YY=    17.2189   ZY=  -149.7594
  XZ=   151.1586   YZ=  -150.8530   ZZ=     3.3425
  Eigenvalues:  -140.9906  -137.6315   317.0185
 7  N    Isotropic =    12.7359   Anisotropy =   456.4051
  XX=    17.1241   YX=   154.7296   ZX=   150.2211
  XY=   154.7424   YY=    16.8951   ZY=   150.1217
  XZ=   151.3504   YZ=   151.2327   ZZ=     4.1886
  Eigenvalues:  -141.0718  -137.7264   317.0060
 8  N    Isotropic =    12.6259   Anisotropy =   456.5357
  XX=    16.9239   YX=  -154.4189   ZX=  -150.5994
  XY=  -154.4198   YY=    16.1500   ZY=   150.2266
  XZ=  -151.7226   YZ=   151.3473   ZZ=     4.8038
  Eigenvalues:  -141.2225  -137.8828   316.9830
 9  N    Isotropic =    12.5948   Anisotropy =   456.5545
  XX=  -138.0251   YX=    -0.8166   ZX=     0.5532
  XY=    -0.8194   YY=   172.0002   ZY=  -212.2523
  XZ=     0.5565   YZ=  -213.8712   ZZ=     3.8093
  Eigenvalues:  -141.1528  -138.0272   316.9644
10  C    Isotropic =    75.8902   Anisotropy =   311.4150
  XX=   184.4576   YX=     0.6329   ZX=  -146.0844
  XY=     0.6011   YY=   -27.6925   ZY=    -0.4148
  XZ=  -144.1249   YZ=    -0.4302   ZZ=    70.9056
  Eigenvalues:   -28.1352   -27.6943   283.5002
11  C    Isotropic =    75.9003   Anisotropy =   311.4756
  XX=   -27.7096   YX=    -0.5412   ZX=     0.3707
  XY=    -0.5700   YY=   185.4260   ZY=  -145.7066
  XZ=     0.3849   YZ=  -143.8149   ZZ=    69.9844
  Eigenvalues:   -28.1389   -27.7110   283.5507
12  C    Isotropic =    75.8905   Anisotropy =   311.3829
  XX=    78.7301   YX=  -106.1946   ZX=  -103.3054
  XY=  -106.2037   YY=    78.2017   ZY=   103.0532
  XZ=  -101.9932   YZ=   101.7364   ZZ=    70.7396
  Eigenvalues:   -28.0741   -27.7336   283.4791
13  C    Isotropic =    75.9069   Anisotropy =   311.3198
  XX=    78.8157   YX=   106.4355   ZX=   103.0671
  XY=   106.4160   YY=    78.6413   ZY=   102.9717
  XZ=   101.7410   YZ=   101.6722   ZZ=    70.2636
  Eigenvalues:   -28.0355   -27.6973   283.4535
14  C    Isotropic =    75.8932   Anisotropy =   311.2975
  XX=    79.2350   YX=  -106.7247   ZX=   102.9347
  XY=  -106.7230   YY=    78.8025   ZY=  -102.7276
  XZ=   101.6372   YZ=  -101.4324   ZZ=    69.6420
  Eigenvalues:   -28.0401   -27.7053   283.4249
15  C    Isotropic =    75.9081   Anisotropy =   311.3186
  XX=    78.8295   YX=   106.4373   ZX=  -103.0407
  XY=   106.4494   YY=    78.6648   ZY=  -102.9685
  XZ=  -101.7432   YZ=  -101.6576   ZZ=    70.2299
  Eigenvalues:   -28.0334   -27.6962   283.4538
16  C    Isotropic =    75.8999   Anisotropy =   311.4018
  XX=   -27.6810   YX=     0.5956   ZX=     0.4103
  XY=     0.6391   YY=   184.7107   ZY=   145.9677
  XZ=     0.4335   YZ=   144.0331   ZZ=    70.6700
  Eigenvalues:   -28.1186   -27.6828   283.5011
17  C    Isotropic =    75.8860   Anisotropy =   311.4891
  XX=   185.0576   YX=    -0.6460   ZX=   145.8712
  XY=    -0.5969   YY=   -27.7258   ZY=    -0.4119
  XZ=   143.9489   YZ=    -0.4386   ZZ=    70.3262
  Eigenvalues:   -28.1598   -27.7276   283.5454
18  C    Isotropic =   187.6423   Anisotropy =    29.2325
  XX=   197.8084   YX=     0.0542   ZX=   -13.7180
  XY=     0.0502   YY=   177.9945   ZY=    -0.0350
  XZ=   -13.5952   YZ=    -0.0379   ZZ=   187.1239
  Eigenvalues:   177.8018   177.9943   207.1306
19  C    Isotropic =   187.6401   Anisotropy =    29.2240
  XX=   177.9947   YX=    -0.0447   ZX=     0.0317
  XY=    -0.0484   YY=   197.8921   ZY=   -13.6783
  XZ=     0.0343   YZ=   -13.5566   ZZ=   187.0336
```

```
  Eigenvalues:   177.8030   177.9946   207.1228
20  C    Isotropic =   187.7052   Anisotropy =    29.1937
  XX=   187.9946   YX=    -9.9007   ZX=    -9.6928
  XY=    -9.9042   YY=   187.9501   ZY=     9.6711
  XZ=    -9.6080   YZ=     9.5846   ZZ=   187.1708
  Eigenvalues:   177.8780   178.0699   207.1676
21  C    Isotropic =   187.6988   Anisotropy =    29.1931
  XX=   187.9979   YX=     9.9284   ZX=     9.6689
  XY=     9.9271   YY=   187.9818   ZY=     9.6649
  XZ=     9.5904   YZ=     9.5749   ZZ=   187.1168
  Eigenvalues:   177.8735   178.0621   207.1609
22  C    Isotropic =   187.7067   Anisotropy =    29.2080
  XX=   188.0416   YX=    -9.9572   ZX=     9.6657
  XY=    -9.9644   YY=   188.0117   ZY=    -9.6458
  XZ=     9.5784   YZ=    -9.5656   ZZ=   187.0669
  Eigenvalues:   177.8757   178.0658   207.1787
23  C    Isotropic =   187.7050   Anisotropy =    29.1918
  XX=   188.0034   YX=     9.9275   ZX=    -9.6671
  XY=     9.9295   YY=   187.9941   ZY=    -9.6653
  XZ=    -9.5841   YZ=    -9.5780   ZZ=   187.1174
  Eigenvalues:   177.8785   178.0702   207.1662
24  C    Isotropic =   187.6414   Anisotropy =    29.2423
  XX=   177.9891   YX=     0.0487   ZX=     0.0341
  XY=     0.0523   YY=   197.8363   ZY=    13.7116
  XZ=     0.0367   YZ=    13.5899   ZZ=   187.0987
  Eigenvalues:   177.7989   177.9890   207.1363
25  C    Isotropic =   187.6391   Anisotropy =    29.2273
  XX=   197.8567   YX=    -0.0544   ZX=    13.6952
  XY=    -0.0516   YY=   177.9937   ZY=    -0.0340
  XZ=    13.5717   YZ=    -0.0360   ZZ=   187.0669
  Eigenvalues:   177.7998   177.9936   207.1240
26  H    Isotropic =    29.1089   Anisotropy =     9.7242
  XX=    31.4414   YX=     5.4274   ZX=    -1.0160
  XY=     4.0665   YY=    30.0611   ZY=     1.2281
  XZ=    -2.0011   YZ=     0.2906   ZZ=    25.8241
  Eigenvalues:    24.3073    27.4276    35.5917
27  H    Isotropic =    29.1106   Anisotropy =     9.7233
  XX=    27.4724   YX=     0.0053   ZX=    -2.0858
  XY=    -0.0016   YY=    24.4229   ZY=    -0.0397
  XZ=    -0.1659   YZ=    -0.0391   ZZ=    35.4366
  Eigenvalues:    24.4228    27.3163    35.5929
28  H    Isotropic =    29.1087   Anisotropy =     9.7294
  XX=    31.4422   YX=    -5.4231   ZX=    -1.0551
  XY=    -4.0553   YY=    30.0708   ZY=    -1.1961
  XZ=    -2.0298   YZ=    -0.2589   ZZ=    25.8132
  Eigenvalues:    24.3067    27.4245    35.5950
29  H    Isotropic =    29.1124   Anisotropy =     9.7259
  XX=    24.4254   YX=     0.0010   ZX=     0.0340
  XY=    -0.0050   YY=    27.4792   ZY=    -2.1127
  XZ=     0.0332   YZ=    -0.1926   ZZ=    35.4325
  Eigenvalues:    24.4253    27.3156    35.5963
30  H    Isotropic =    29.1094   Anisotropy =     9.7210
  XX=    30.0638   YX=    -4.0601   ZX=    -1.2396
  XY=    -5.4256   YY=    31.4483   ZY=    -1.0005
  XZ=    -0.3054   YZ=    -1.9866   ZZ=    25.8162
  Eigenvalues:    24.3084    27.4298    35.5901
31  H    Isotropic =    29.1090   Anisotropy =     9.7259
  XX=    30.0686   YX=     4.0507   ZX=     1.2124
  XY=     5.4218   YY=    31.4519   ZY=    -1.0330
  XZ=     0.2791   YZ=    -2.0105   ZZ=    25.8064
  Eigenvalues:    24.3077    27.4264    35.5929
32  H    Isotropic =    29.1102   Anisotropy =     9.7332
  XX=    26.0140   YX=    -1.3703   ZX=    -1.5812
  XY=    -0.0090   YY=    35.5015   ZY=    -0.1124
  XZ=    -1.6173   YZ=     1.2308   ZZ=    25.8149
  Eigenvalues:    24.3117    27.4198    35.5989
33  H    Isotropic =    29.1103   Anisotropy =     9.7315
  XX=    35.5028   YX=    -0.0071   ZX=     0.1265
  XY=    -1.3662   YY=    26.0100   ZY=     1.5798
  XZ=    -1.2194   YZ=     1.6178   ZZ=    25.8180
  Eigenvalues:    24.3118    27.4211    35.5979
34  H    Isotropic =    29.1074   Anisotropy =     9.7411
  XX=    25.9411   YX=    -1.5237   ZX=    -1.4884
  XY=    -1.5253   YY=    25.9387   ZY=     1.4712
  XZ=    -0.1368   YZ=     0.1216   ZZ=    35.4424
  Eigenvalues:    24.4154    27.3053    35.6015
35  H    Isotropic =    29.1085   Anisotropy =     9.7316
  XX=    26.0058   YX=     1.4174   ZX=     1.5728
```

```
  XY=     0.0611   YY=    35.4995   ZY=    -0.1817
  XZ=     1.6234   YZ=     1.1658   ZZ=    25.8204
  Eigenvalues:    24.3102    27.4191    35.5963
36  H    Isotropic =    29.1060   Anisotropy =     9.7421
  XX=    25.9496   YX=     1.5325   ZX=     1.4436
  XY=     1.5190   YY=    25.9308   ZY=     1.5329
  XZ=     0.0876   YZ=     0.1903   ZZ=    35.4376
  Eigenvalues:    24.4139    27.3033    35.6007
37  H    Isotropic =    29.1078   Anisotropy =     9.7335
  XX=    35.5026   YX=    -0.0416   ZX=    -0.0771
  XY=     1.3251   YY=    26.0210   ZY=     1.5854
  XZ=     1.2591   YZ=     1.6116   ZZ=    25.7998
  Eigenvalues:    24.3080    27.4186    35.5968
38  H    Isotropic =    29.1092   Anisotropy =     9.7333
  XX=    35.5035   YX=    -0.0613   ZX=    -0.1995
  XY=    -1.4178   YY=    26.0081   ZY=    -1.5703
  XZ=     1.1474   YZ=    -1.6237   ZZ=    25.8159
  Eigenvalues:    24.3097    27.4197    35.5980
39  H    Isotropic =    29.1063   Anisotropy =     9.7449
  XX=    25.9351   YX=    -1.5209   ZX=     1.5520
  XY=    -1.5346   YY=    25.9490   ZY=    -1.4486
  XZ=     0.2077   YZ=    -0.0948   ZZ=    35.4347
  Eigenvalues:    24.4137    27.3022    35.6029
40  H    Isotropic =    29.1081   Anisotropy =     9.7338
  XX=    26.0277   YX=    -1.3329   ZX=     1.5845
  XY=     0.0374   YY=    35.5038   ZY=     0.0863
  XZ=     1.6118   YZ=    -1.2466   ZZ=    25.7927
  Eigenvalues:    24.3077    27.4192    35.5973
41  H    Isotropic =    29.1079   Anisotropy =     9.7319
  XX=    35.5012   YX=     0.0014   ZX=     0.1236
  XY=     1.3641   YY=    26.0152   ZY=    -1.5800
  XZ=    -1.2180   YZ=    -1.6166   ZZ=    25.8072
  Eigenvalues:    24.3091    27.4188    35.5958
42  H    Isotropic =    29.1086   Anisotropy =     9.7347
  XX=    26.0118   YX=     1.3789   ZX=    -1.5780
  XY=     0.0183   YY=    35.5031   ZY=     0.1374
  XZ=    -1.6187   YZ=    -1.2050   ZZ=    25.8109
  Eigenvalues:    24.3092    27.4182    35.5984
43  H    Isotropic =    29.1061   Anisotropy =     9.7431
  XX=    25.9403   YX=     1.5270   ZX=    -1.4832
  XY=     1.5251   YY=    25.9398   ZY=    -1.4959
  XZ=    -0.1328   YZ=    -0.1474   ZZ=    35.4383
  Eigenvalues:    24.4140    27.3029    35.6015
44  H    Isotropic =    29.1119   Anisotropy =     9.7252
  XX=    24.4240   YX=     0.0047   ZX=     0.0127
  XY=     0.0065   YY=    27.4745   ZY=     2.0924
  XZ=     0.0088   YZ=     0.1733   ZZ=    35.4373
  Eigenvalues:    24.4240    27.3164    35.5954
45  H    Isotropic =    29.1084   Anisotropy =     9.7295
  XX=    30.0471   YX=    -4.0575   ZX=     1.2129
  XY=    -5.4234   YY=    31.4630   ZY=     1.0332
  XZ=     0.2788   YZ=     2.0138   ZZ=    25.8151
  Eigenvalues:    24.3064    27.4240    35.5947
46  H    Isotropic =    29.1109   Anisotropy =     9.7234
  XX=    30.0860   YX=     4.0624   ZX=    -1.2179
  XY=     5.4271   YY=    31.4262   ZY=     1.0295
  XZ=    -0.2797   YZ=     2.0089   ZZ=    25.8203
  Eigenvalues:    24.3089    27.4305    35.5931
47  H    Isotropic =    29.1108   Anisotropy =     9.7214
  XX=    31.4291   YX=    -5.4259   ZX=     1.0215
  XY=    -4.0596   YY=    30.0864   ZY=     1.2232
  XZ=     2.0023   YZ=     0.2857   ZZ=    25.8168
  Eigenvalues:    24.3099    27.4307    35.5917
48  H    Isotropic =    29.1115   Anisotropy =     9.7236
  XX=    27.4769   YX=    -0.0068   ZX=     2.1031
  XY=    -0.0051   YY=    24.4245   ZY=    -0.0121
  XZ=     0.1822   YZ=    -0.0082   ZZ=    35.4330
  Eigenvalues:    24.4245    27.3161    35.5939
49  H    Isotropic =    29.1086   Anisotropy =     9.7272
  XX=    31.4664   YX=     5.4218   ZX=     1.0251
  XY=     4.0544   YY=    30.0475   ZY=    -1.2184
  XZ=     2.0074   YZ=    -0.2849   ZZ=    25.8118
  Eigenvalues:    24.3075    27.4247    35.5934
```

B. Auxilliary Calculations for NMR and Thermodynamics:

1. Me-CN at BP86/SVP level:

```
1|1|UNPC-UNK|SP|RBP86|SVP|C2H3N1|PCUSER|27-May-2017|0||# RBP86/SVP NMR
 =GIAO Test geom=check||[No Title]||0,1|N,0,-6.0821687538,1.0885890472,
 -0.0001081789|C,0,-5.0481441648,0.4915755983,-0.0000831251|C,0,-3.7736
 834727,-0.2442923806,-0.000083893|H,0,-2.9230471494,0.459802467,-0.000
 0075325|H,0,-3.6994337216,-0.8848311736,0.8963048298|H,0,-3.6993227377
 ,-0.8847435583,-0.8965221003||Version=IA32W-G03RevD.01|State=1-A|HF=-1
 32.6506995|RMSD=3.357e-009|Thermal=0.|Dipole=1.2858239,-0.7424027,0.00
 00174|PG=C01 [X(C2H3N1)]||@
```

2. $SnMe_4$ at BP86/SDD level (NMR Standard):

```
C                    0    -0.1888    1.2245   -1.7533
 Sn                   0     0.0039   -0.0244    0.0348
 C                    0    -0.1979    1.2264    1.8206
 C                    0    -1.5688   -1.5476    0.0316
 C                    0     1.9703   -0.9977    0.0403
 H                    0    -0.0929    0.6062   -2.6652
 H                    0     0.6011    1.9983   -1.7673
 H                    0    -1.174     1.7264   -1.7702
 H                    0    -0.1038    0.6097    2.7336
 H                    0     0.59      2.0022    1.8362
 H                    0    -1.1844    1.7259    1.8331
 H                    0    -1.4871   -2.1859    0.931
 H                    0    -1.4806   -2.1888   -0.8651
 H                    0    -2.5667   -1.0714    0.0273
 H                    0     2.5465   -0.7053   -0.8569
 H                    0     2.5431   -0.7018    0.9385
 H                    0     1.8551   -2.0973    0.0422
```

NMR Calculations at the BP86/SVP level (NMR=GIAO):

```
1|1|UNPC-UNK|SP|RBP86|SVP|C4H12Sn1|PCUSER|27-May-2017|0||# RBP86/SVP N
 MR=GIAO Test||[No Title]||0,1|C,0,-0.1888,1.2245,-1.7533|Sn,0,0.0039,-
 0.0244,0.0348|C,0,-0.1979,1.2264,1.8206|C,0,-1.5688,-1.5476,0.0316|C,0
 ,1.9703,-0.9977,0.0403|H,0,-0.0929,0.6062,-2.6652|H,0,0.6011,1.9983,-1
 .7673|H,0,-1.174,1.7264,-1.7702|H,0,-0.1038,0.6097,2.7336|H,0,0.59,2.0
 022,1.8362|H,0,-1.1844,1.7259,1.8331|H,0,-1.4871,-2.1859,0.931|H,0,-1.
 4806,-2.1888,-0.8651|H,0,-2.5667,-1.0714,0.0273|H,0,2.5465,-0.7053,-0.
 8569|H,0,2.5431,-0.7018,0.9385|H,0,1.8551,-2.0973,0.0422||Version=IA32
 W-G03RevD.01|State=1-A|HF=-6184.7891236|RMSD=6.058e-009|Thermal=0.|Dip
 ole=-0.0007217,-0.0005693,-0.0000225|PG=C01 [X(C4H12Sn1)]||@
```

```
Calculating GIAO nuclear magnetic shielding tensors.
 SCF GIAO Magnetic shielding tensor (ppm):
  1  C    Isotropic =   194.2818   Anisotropy =     6.4974
   XX=   194.2665   YX=    -1.0486   ZX=    -1.0078
   XY=    -1.1501   YY=   192.5419   ZY=     3.4106
   XZ=    -1.1626   YZ=     3.3500   ZZ=   196.0369
   Eigenvalues:   190.4443   193.7876   198.6134
  2  Sn   Isotropic =  2994.3842   Anisotropy =     8.3494
   XX=  2983.9395   YX=     0.8887   ZX=     0.0903
   XY=     1.6818   YY=  2999.2637   ZY=     0.0201
   XZ=     0.1329   YZ=    -0.0122   ZZ=  2999.9493
   Eigenvalues:  2983.8317  2999.3704  2999.9504
  3  C    Isotropic =   194.2864   Anisotropy =     6.5010
   XX=   194.2839   YX=    -1.0600   ZX=     1.0309
   XY=    -1.1477   YY=   192.4924   ZY=    -3.3759
   XZ=     1.1909   YZ=    -3.3174   ZZ=   196.0830
   Eigenvalues:   190.4497   193.7891   198.6204
```

```
 4  C    Isotropic =   194.2296   Anisotropy =     6.5431
  XX=   194.7246   YX=     2.0521   ZX=    -0.0197
  XY=     2.1084   YY=   197.4722   ZY=    -0.0483
  XZ=    -0.0216   YZ=    -0.0381   ZZ=   190.4920
  Eigenvalues:   190.4917   193.6054   198.5916
 5  C    Isotropic =   195.9229   Anisotropy =     9.4886
  XX=   202.1329   YX=    -1.0332   ZX=    -0.0252
  XY=    -1.0525   YY=   192.8412   ZY=     0.0046
  XZ=    -0.0261   YZ=     0.0060   ZZ=   192.7945
  Eigenvalues:   192.7255   192.7945   202.2486
 6  H    Isotropic =    31.2077   Anisotropy =    12.9682
  XX=    26.2745   YX=    -1.2391   ZX=     1.1167
  XY=    -1.0443   YY=    27.7945   ZY=    -1.8788
  XZ=     0.8071   YZ=    -1.2843   ZZ=    39.5540
  Eigenvalues:    25.6621    28.1077    39.8531
 7  H    Isotropic =    31.2072   Anisotropy =    12.9593
  XX=    27.0710   YX=     3.0715   ZX=    -0.0209
  XY=     2.6522   YY=    37.3576   ZY=     4.7283
  XZ=    -0.1014   YZ=     4.1734   ZZ=    29.1930
  Eigenvalues:    25.6550    28.1199    39.8468
 8  H    Isotropic =    31.2536   Anisotropy =    13.1012
  XX=    37.1035   YX=    -3.6863   ZX=    -4.0218
  XY=    -3.3135   YY=    27.4507   ZY=     2.6086
  XZ=    -3.3865   YZ=     2.5351   ZZ=    29.2066
  Eigenvalues:    25.5420    28.2310    39.9877
 9  H    Isotropic =    31.2105   Anisotropy =    12.9697
  XX=    26.2741   YX=    -1.2459   ZX=    -1.0456
  XY=    -1.0448   YY=    27.8160   ZY=     1.9735
  XZ=    -0.7361   YZ=     1.3814   ZZ=    39.5414
  Eigenvalues:    25.6644    28.1101    39.8569
10  H    Isotropic =    31.2074   Anisotropy =    12.9594
  XX=    27.0549   YX=     3.0252   ZX=     0.0182
  XY=     2.6050   YY=    37.3030   ZY=    -4.8028
  XZ=     0.0999   YZ=    -4.2490   ZZ=    29.2644
  Eigenvalues:    25.6559    28.1194    39.8471
11  H    Isotropic =    31.2537   Anisotropy =    13.1009
  XX=    37.1571   YX=    -3.6430   ZX=     4.0179
  XY=    -3.2757   YY=    27.3951   ZY=    -2.5711
  XZ=     3.3778   YZ=    -2.4976   ZZ=    29.2089
  Eigenvalues:    25.5405    28.2329    39.9876
12  H    Isotropic =    31.2074   Anisotropy =    12.9649
  XX=    26.5798   YX=     0.5729   ZX=    -1.1742
  XY=     0.7916   YY=    35.2375   ZY=     5.8361
  XZ=    -0.7633   YZ=     6.3482   ZZ=    31.8050
  Eigenvalues:    25.6627    28.1089    39.8507
13  H    Isotropic =    31.2084   Anisotropy =    12.9659
  XX=    26.6012   YX=     0.5230   ZX=     1.2166
  XY=     0.7430   YY=    35.1490   ZY=    -5.8699
  XZ=     0.8057   YZ=    -6.3788   ZZ=    31.8750
  Eigenvalues:    25.6649    28.1080    39.8523
14  H    Isotropic =    31.2532   Anisotropy =    13.0834
  XX=    38.7058   YX=     4.0123   ZX=    -0.0727
  XY=     3.2729   YY=    29.5208   ZY=    -0.0282
  XZ=    -0.0707   YZ=    -0.0312   ZZ=    25.5329
  Eigenvalues:    25.5325    28.2516    39.9754
15  H    Isotropic =    31.1466   Anisotropy =    12.9775
  XX=    34.8367   YX=     1.8328   ZX=     4.9840
  XY=     2.1298   YY=    26.7938   ZY=     3.4131
  XZ=     5.4948   YZ=     3.3568   ZZ=    31.8092
  Eigenvalues:    25.0327    28.6087    39.7983
16  H    Isotropic =    31.1470   Anisotropy =    12.9774
  XX=    34.7744   YX=     1.7864   ZX=    -5.0111
  XY=     2.0808   YY=    26.7551   ZY=    -3.3967
  XZ=    -5.5224   YZ=    -3.3385   ZZ=    31.9114
  Eigenvalues:    25.0334    28.6090    39.7986
17  H    Isotropic =    31.1439   Anisotropy =    12.9820
  XX=    33.0341   YX=    -5.1760   ZX=    -0.0111
  XY=    -5.7720   YY=    35.3689   ZY=    -0.0117
  XZ=    -0.0088   YZ=    -0.0134   ZZ=    25.0287
  Eigenvalues:    25.0287    28.6045    39.7986
```

NPA-Population Analysis of 3+3 $[Sn(NC\text{-}Me)_6]^{2+}$ @ BP86/def2-TZVP Level

```
Nr Atom            Natural Electron Configuration
-------------------------------------------------
   1 sn [ecp-28] [core] 5s( 1.90) 5p( 0.72)
   2 n    [core]        2s( 1.50) 2p( 3.92) 3p( 0.01) 3d( 0.01)
   3 c    [core]        2s( 0.88) 3s( 0.01) 2p( 2.65) 3p( 0.01)
   4 c    [core]        2s( 1.15) 2p( 3.59)
   5 h                  1s( 0.71)
   6 h                  1s( 0.71)
   7 h                  1s( 0.71)
   8 n    [core]        2s( 1.50) 2p( 3.92) 3p( 0.01) 3d( 0.01)
   9 c    [core]        2s( 0.88) 3s( 0.01) 2p( 2.65) 3p( 0.01)
  10 c    [core]        2s( 1.15) 2p( 3.59)
  11 h                  1s( 0.71)
  12 h                  1s( 0.71)
  13 h                  1s( 0.71)
  14 n    [core]        2s( 1.55) 2p( 3.86) 3p( 0.01) 3d( 0.01)
  15 c    [core]        2s( 1.15) 2p( 3.59)
  16 h                  1s( 0.71)
  17 h                  1s( 0.71)
  18 h                  1s( 0.71)
  19 c    [core]        2s( 0.88) 3s( 0.01) 2p( 2.70) 3p( 0.01)
  20 n    [core]        2s( 1.50) 2p( 3.92) 3p( 0.01) 3d( 0.01)
  21 c    [core]        2s( 1.15) 2p( 3.59)
  22 h                  1s( 0.71)
  23 h                  1s( 0.71)
  24 h                  1s( 0.71)
  25 c    [core]        2s( 0.88) 3s( 0.01) 2p( 2.65) 3p( 0.01)
  26 n    [core]        2s( 1.55) 2p( 3.86) 3p( 0.01) 3d( 0.01)
  27 c    [core]        2s( 1.15) 2p( 3.59)
  28 h                  1s( 0.71)
  29 h                  1s( 0.71)
  30 h                  1s( 0.71)
  31 c    [core]        2s( 0.88) 3s( 0.01) 2p( 2.70) 3p( 0.01)
  32 n    [core]        2s( 1.55) 2p( 3.86) 3p( 0.01) 3d( 0.01)
  33 c    [core]        2s( 1.15) 2p( 3.59)
  34 h                  1s( 0.71)
  35 h                  1s( 0.71)
  36 h                  1s( 0.71)
  37 c    [core]        2s( 0.88) 3s( 0.01) 2p( 2.70) 3p( 0.01)

NATURAL POPULATIONS:  Natural atomic orbital occupancies

NAO   Atom  #       Type(AO)    Occupancy
---------------------------------------
    1 sn    1 s    Cor(4s)        1.99948
    2 sn    1 s    Val(5s)        1.89708
    3 sn    1 s    Ryd            0.00098
    4 sn    1 s    Ryd            0.00002
    5 sn    1 s    Ryd            0.00001
    6 sn    1 s    Ryd            0.00000
    7 sn    1 p    Cor(4px)       1.99970
    8 sn    1 p    Cor(4py)       1.99970
    9 sn    1 p    Cor(4pz)       1.99970
   10 sn    1 p    Val(5px)       0.26155
   11 sn    1 p    Val(5py)       0.21895
   12 sn    1 p    Val(5pz)       0.23487
   13 sn    1 p    Ryd            0.00136
   14 sn    1 p    Ryd            0.00161
   15 sn    1 p    Ryd            0.00150
   16 sn    1 p    Ryd            0.00057
   17 sn    1 p    Ryd            0.00056
   18 sn    1 p    Ryd            0.00056
   19 sn    1 p    Ryd            0.00000
   20 sn    1 p    Ryd            0.00000
   21 sn    1 p    Ryd            0.00000
   22 sn    1 d    Cor(4dz2)      1.99925
   23 sn    1 d    Cor(4dxz)      1.99942
```

24	sn	1	d	Cor(4dyz) 1.99944
25	sn	1	d	Cor(4dxy) 1.99935
26	sn	1	d	Cor(4dx2-y2) 1.99932
27	sn	1	d	Ryd 0.00109
28	sn	1	d	Ryd 0.00080
29	sn	1	d	Ryd 0.00088
30	sn	1	d	Ryd 0.00088
31	sn	1	d	Ryd 0.00102
32	sn	1	d	Ryd 0.00011
33	sn	1	d	Ryd 0.00016
34	sn	1	d	Ryd 0.00017
35	sn	1	d	Ryd 0.00015
36	sn	1	d	Ryd 0.00013
37	sn	1	f	Ryd 0.00038
38	sn	1	f	Ryd 0.00027
39	sn	1	f	Ryd 0.00039
40	sn	1	f	Ryd 0.00023
41	sn	1	f	Ryd 0.00021
42	sn	1	f	Ryd 0.00031
43	sn	1	f	Ryd 0.00039
44	sn	1	f	Ryd 0.00006
45	sn	1	f	Ryd 0.00008
46	sn	1	f	Ryd 0.00003
47	sn	1	f	Ryd 0.00004
48	sn	1	f	Ryd 0.00002
49	sn	1	f	Ryd 0.00008
50	sn	1	f	Ryd 0.00004
51	n	2	s	Cor(1s) 1.99914
52	n	2	s	Val(2s) 1.50028
53	n	2	s	Ryd 0.00414
54	n	2	s	Ryd 0.00006
55	n	2	s	Ryd 0.00000
56	n	2	p	Val(2px) 1.24649
57	n	2	p	Val(2py) 1.45073
58	n	2	p	Val(2pz) 1.22253
59	n	2	p	Ryd 0.00258
60	n	2	p	Ryd 0.00677
61	n	2	p	Ryd 0.00182
62	n	2	p	Ryd 0.00004
63	n	2	p	Ryd 0.00016
64	n	2	p	Ryd 0.00003
65	n	2	d	Ryd 0.00142
66	n	2	d	Ryd 0.00029
67	n	2	d	Ryd 0.00231
68	n	2	d	Ryd 0.00297
69	n	2	d	Ryd 0.00349
70	n	2	d	Ryd 0.00002
71	n	2	d	Ryd 0.00001
72	n	2	d	Ryd 0.00002
73	n	2	d	Ryd 0.00004
74	n	2	d	Ryd 0.00003
75	n	2	f	Ryd 0.00012
76	n	2	f	Ryd 0.00004
77	n	2	f	Ryd 0.00017
78	n	2	f	Ryd 0.00012
79	n	2	f	Ryd 0.00015
80	n	2	f	Ryd 0.00027
81	n	2	f	Ryd 0.00029
82	c	3	s	Cor(1s) 1.99934
83	c	3	s	Val(2s) 0.87739
84	c	3	s	Ryd 0.00776
85	c	3	s	Ryd 0.00006
86	c	3	s	Ryd 0.00001
87	c	3	p	Val(2px) 0.84896
88	c	3	p	Val(2py) 0.95884
89	c	3	p	Val(2pz) 0.83776
90	c	3	p	Ryd 0.00096
91	c	3	p	Ryd 0.00798

92	c	3	p	Ryd 0.00040
93	c	3	p	Ryd 0.00008
94	c	3	p	Ryd 0.00012
95	c	3	p	Ryd 0.00006
96	c	3	d	Ryd 0.00020
97	c	3	d	Ryd 0.00010
98	c	3	d	Ryd 0.00079
99	c	3	d	Ryd 0.00069
100	c	3	d	Ryd 0.00064
101	c	3	d	Ryd 0.00005
102	c	3	d	Ryd 0.00004
103	c	3	d	Ryd 0.00003
104	c	3	d	Ryd 0.00002
105	c	3	d	Ryd 0.00006
106	c	3	f	Ryd 0.00031
107	c	3	f	Ryd 0.00010
108	c	3	f	Ryd 0.00057
109	c	3	f	Ryd 0.00026
110	c	3	f	Ryd 0.00036
111	c	3	f	Ryd 0.00098
112	c	3	f	Ryd 0.00073
113	c	4	s	Cor(1s) 1.99923
114	c	4	s	Val(2s) 1.14731
115	c	4	s	Ryd 0.00014
116	c	4	s	Ryd 0.00008
117	c	4	s	Ryd 0.00000
118	c	4	p	Val(2px) 1.24331
119	c	4	p	Val(2py) 1.08969
120	c	4	p	Val(2pz) 1.25858
121	c	4	p	Ryd 0.00039
122	c	4	p	Ryd 0.00046
123	c	4	p	Ryd 0.00038
124	c	4	p	Ryd 0.00005
125	c	4	p	Ryd 0.00024
126	c	4	p	Ryd 0.00002
127	c	4	d	Ryd 0.00125
128	c	4	d	Ryd 0.00105
129	c	4	d	Ryd 0.00050
130	c	4	d	Ryd 0.00070
131	c	4	d	Ryd 0.00115
132	c	4	d	Ryd 0.00001
133	c	4	d	Ryd 0.00001
134	c	4	d	Ryd 0.00003
135	c	4	d	Ryd 0.00002
136	c	4	d	Ryd 0.00002
137	c	4	f	Ryd 0.00002
138	c	4	f	Ryd 0.00017
139	c	4	f	Ryd 0.00028
140	c	4	f	Ryd 0.00004
141	c	4	f	Ryd 0.00016
142	c	4	f	Ryd 0.00023
143	c	4	f	Ryd 0.00005
144	h	5	s	Val(1s) 0.70855
145	h	5	s	Ryd 0.00025
146	h	5	s	Ryd 0.00007
147	h	5	p	Ryd 0.00054
148	h	5	p	Ryd 0.00009
149	h	5	p	Ryd 0.00009
150	h	6	s	Val(1s) 0.70881
151	h	6	s	Ryd 0.00025
152	h	6	s	Ryd 0.00007
153	h	6	p	Ryd 0.00017
154	h	6	p	Ryd 0.00018
155	h	6	p	Ryd 0.00038
156	h	7	s	Val(1s) 0.70878
157	h	7	s	Ryd 0.00025

158	h	7	s	Ryd	0.00007
159	h	7	p	Ryd	0.00009
160	h	7	p	Ryd	0.00028
161	h	7	p	Ryd	0.00036
162	n	8	s	Cor(1s)	1.99914
163	n	8	s	Val(2s)	1.50042
164	n	8	s	Ryd	0.00415
165	n	8	s	Ryd	0.00006
166	n	8	s	Ryd	0.00000
167	n	8	p	Val(2px)	1.44205
168	n	8	p	Val(2py)	1.24325
169	n	8	p	Val(2pz)	1.23465
170	n	8	p	Ryd	0.00749
171	n	8	p	Ryd	0.00204
172	n	8	p	Ryd	0.00163
173	n	8	p	Ryd	0.00016
174	n	8	p	Ryd	0.00004
175	n	8	p	Ryd	0.00003
176	n	8	d	Ryd	0.00140
177	n	8	d	Ryd	0.00258
178	n	8	d	Ryd	0.00069
179	n	8	d	Ryd	0.00284
180	n	8	d	Ryd	0.00296
181	n	8	d	Ryd	0.00002
182	n	8	d	Ryd	0.00002
183	n	8	d	Ryd	0.00000
184	n	8	d	Ryd	0.00002
185	n	8	d	Ryd	0.00005
186	n	8	f	Ryd	0.00010
187	n	8	f	Ryd	0.00020
188	n	8	f	Ryd	0.00004
189	n	8	f	Ryd	0.00012
190	n	8	f	Ryd	0.00015
191	n	8	f	Ryd	0.00029
192	n	8	f	Ryd	0.00025
193	c	9	s	Cor(1s)	1.99934
194	c	9	s	Val(2s)	0.87736
195	c	9	s	Ryd	0.00776
196	c	9	s	Ryd	0.00006
197	c	9	s	Ryd	0.00001
198	c	9	p	Val(2px)	0.95313
199	c	9	p	Val(2py)	0.84931
200	c	9	p	Val(2pz)	0.84295
201	c	9	p	Ryd	0.00699
202	c	9	p	Ryd	0.00128
203	c	9	p	Ryd	0.00110
204	c	9	p	Ryd	0.00014
205	c	9	p	Ryd	0.00006
206	c	9	p	Ryd	0.00006
207	c	9	d	Ryd	0.00030
208	c	9	d	Ryd	0.00070
209	c	9	d	Ryd	0.00014
210	c	9	d	Ryd	0.00064
211	c	9	d	Ryd	0.00065
212	c	9	d	Ryd	0.00004
213	c	9	d	Ryd	0.00004
214	c	9	d	Ryd	0.00004
215	c	9	d	Ryd	0.00003
216	c	9	d	Ryd	0.00004
217	c	9	f	Ryd	0.00034
218	c	9	f	Ryd	0.00050
219	c	9	f	Ryd	0.00009
220	c	9	f	Ryd	0.00039
221	c	9	f	Ryd	0.00046
222	c	9	f	Ryd	0.00064
223	c	9	f	Ryd	0.00089
224	c	10	s	Cor(1s)	1.99923

225	c	10	s	Val(2s) 1.14738
226	c	10	s	Ryd 0.00014
227	c	10	s	Ryd 0.00008
228	c	10	s	Ryd 0.00000
229	c	10	p	Val(2px) 1.10024
230	c	10	p	Val(2py) 1.24234
231	c	10	p	Val(2pz) 1.24931
232	c	10	p	Ryd 0.00047
233	c	10	p	Ryd 0.00038
234	c	10	p	Ryd 0.00037
235	c	10	p	Ryd 0.00023
236	c	10	p	Ryd 0.00004
237	c	10	p	Ryd 0.00003
238	c	10	d	Ryd 0.00112
239	c	10	d	Ryd 0.00071
240	c	10	d	Ryd 0.00100
241	c	10	d	Ryd 0.00074
242	c	10	d	Ryd 0.00109
243	c	10	d	Ryd 0.00001
244	c	10	d	Ryd 0.00003
245	c	10	d	Ryd 0.00001
246	c	10	d	Ryd 0.00002
247	c	10	d	Ryd 0.00003
248	c	10	f	Ryd 0.00011
249	c	10	f	Ryd 0.00017
250	c	10	f	Ryd 0.00022
251	c	10	f	Ryd 0.00002
252	c	10	f	Ryd 0.00012
253	c	10	f	Ryd 0.00005
254	c	10	f	Ryd 0.00027
255	h	11	s	Val(1s) 0.70860
256	h	11	s	Ryd 0.00025
257	h	11	s	Ryd 0.00007
258	h	11	p	Ryd 0.00009
259	h	11	p	Ryd 0.00056
260	h	11	p	Ryd 0.00007
261	h	12	s	Val(1s) 0.70852
262	h	12	s	Ryd 0.00025
263	h	12	s	Ryd 0.00007
264	h	12	p	Ryd 0.00035
265	h	12	p	Ryd 0.00011
266	h	12	p	Ryd 0.00026
267	h	13	s	Val(1s) 0.70858
268	h	13	s	Ryd 0.00025
269	h	13	s	Ryd 0.00007
270	h	13	p	Ryd 0.00013
271	h	13	p	Ryd 0.00013
272	h	13	p	Ryd 0.00047
273	n	14	s	Cor(1s) 1.99929
274	n	14	s	Val(2s) 1.54573
275	n	14	s	Ryd 0.00475
276	n	14	s	Ryd 0.00005
277	n	14	s	Ryd 0.00000
278	n	14	p	Val(2px) 1.18771
279	n	14	p	Val(2py) 1.20960
280	n	14	p	Val(2pz) 1.45991
281	n	14	p	Ryd 0.00098
282	n	14	p	Ryd 0.00155
283	n	14	p	Ryd 0.00494
284	n	14	p	Ryd 0.00002
285	n	14	p	Ryd 0.00003
286	n	14	p	Ryd 0.00015
287	n	14	d	Ryd 0.00629
288	n	14	d	Ryd 0.00299
289	n	14	d	Ryd 0.00362
290	n	14	d	Ryd 0.00037

291	n	14	d	Ryd 0.00031
292	n	14	d	Ryd 0.00002
293	n	14	d	Ryd 0.00001
294	n	14	d	Ryd 0.00001
295	n	14	d	Ryd 0.00000
296	n	14	d	Ryd 0.00000
297	n	14	f	Ryd 0.00027
298	n	14	f	Ryd 0.00022
299	n	14	f	Ryd 0.00024
300	n	14	f	Ryd 0.00006
301	n	14	f	Ryd 0.00006
302	n	14	f	Ryd 0.00000
303	n	14	f	Ryd 0.00000
304	c	15	s	Cor(1s) 1.99923
305	c	15	s	Val(2s) 1.14538
306	c	15	s	Ryd 0.00013
307	c	15	s	Ryd 0.00007
308	c	15	s	Ryd 0.00000
309	c	15	p	Val(2px) 1.25955
310	c	15	p	Val(2py) 1.24533
311	c	15	p	Val(2pz) 1.08734
312	c	15	p	Ryd 0.00041
313	c	15	p	Ryd 0.00041
314	c	15	p	Ryd 0.00045
315	c	15	p	Ryd 0.00002
316	c	15	p	Ryd 0.00003
317	c	15	p	Ryd 0.00023
318	c	15	d	Ryd 0.00149
319	c	15	d	Ryd 0.00032
320	c	15	d	Ryd 0.00061
321	c	15	d	Ryd 0.00101
322	c	15	d	Ryd 0.00119
323	c	15	d	Ryd 0.00002
324	c	15	d	Ryd 0.00003
325	c	15	d	Ryd 0.00003
326	c	15	d	Ryd 0.00001
327	c	15	d	Ryd 0.00001
328	c	15	f	Ryd 0.00022
329	c	15	f	Ryd 0.00009
330	c	15	f	Ryd 0.00019
331	c	15	f	Ryd 0.00004
332	c	15	f	Ryd 0.00005
333	c	15	f	Ryd 0.00019
334	c	15	f	Ryd 0.00017
335	h	16	s	Val(1s) 0.71461
336	h	16	s	Ryd 0.00027
337	h	16	s	Ryd 0.00007
338	h	16	p	Ryd 0.00051
339	h	16	p	Ryd 0.00008
340	h	16	p	Ryd 0.00015
341	h	17	s	Val(1s) 0.71471
342	h	17	s	Ryd 0.00028
343	h	17	s	Ryd 0.00007
344	h	17	p	Ryd 0.00024
345	h	17	p	Ryd 0.00020
346	h	17	p	Ryd 0.00029
347	h	18	s	Val(1s) 0.71492
348	h	18	s	Ryd 0.00028
349	h	18	s	Ryd 0.00007
350	h	18	p	Ryd 0.00009
351	h	18	p	Ryd 0.00053
352	h	18	p	Ryd 0.00010
353	c	19	s	Cor(1s) 1.99936
354	c	19	s	Val(2s) 0.88354
355	c	19	s	Ryd 0.00746

356	c	19	s	Ryd 0.00005
357	c	19	s	Ryd 0.00001
358	c	19	p	Val(2px) 0.85986
359	c	19	p	Val(2py) 0.86827
360	c	19	p	Val(2pz) 0.96693
361	c	19	p	Ryd 0.00068
362	c	19	p	Ryd 0.00119
363	c	19	p	Ryd 0.01061
364	c	19	p	Ryd 0.00010
365	c	19	p	Ryd 0.00010
366	c	19	p	Ryd 0.00019
367	c	19	d	Ryd 0.00069
368	c	19	d	Ryd 0.00074
369	c	19	d	Ryd 0.00070
370	c	19	d	Ryd 0.00006
371	c	19	d	Ryd 0.00012
372	c	19	d	Ryd 0.00005
373	c	19	d	Ryd 0.00003
374	c	19	d	Ryd 0.00002
375	c	19	d	Ryd 0.00003
376	c	19	d	Ryd 0.00004
377	c	19	f	Ryd 0.00128
378	c	19	f	Ryd 0.00065
379	c	19	f	Ryd 0.00105
380	c	19	f	Ryd 0.00019
381	c	19	f	Ryd 0.00018
382	c	19	f	Ryd 0.00001
383	c	19	f	Ryd 0.00001
384	n	20	s	Cor(1s) 1.99914
385	n	20	s	Val(2s) 1.50037
386	n	20	s	Ryd 0.00415
387	n	20	s	Ryd 0.00006
388	n	20	s	Ryd 0.00000
389	n	20	p	Val(2px) 1.21793
390	n	20	p	Val(2py) 1.23517
391	n	20	p	Val(2pz) 1.46694
392	n	20	p	Ryd 0.00165
393	n	20	p	Ryd 0.00185
394	n	20	p	Ryd 0.00766
395	n	20	p	Ryd 0.00002
396	n	20	p	Ryd 0.00003
397	n	20	p	Ryd 0.00017
398	n	20	d	Ryd 0.00483
399	n	20	d	Ryd 0.00217
400	n	20	d	Ryd 0.00297
401	n	20	d	Ryd 0.00026
402	n	20	d	Ryd 0.00025
403	n	20	d	Ryd 0.00006
404	n	20	d	Ryd 0.00002
405	n	20	d	Ryd 0.00002
406	n	20	d	Ryd 0.00000
407	n	20	d	Ryd 0.00000
408	n	20	f	Ryd 0.00038
409	n	20	f	Ryd 0.00030
410	n	20	f	Ryd 0.00030
411	n	20	f	Ryd 0.00008
412	n	20	f	Ryd 0.00008
413	n	20	f	Ryd 0.00000
414	n	20	f	Ryd 0.00000
415	c	21	s	Cor(1s) 1.99923
416	c	21	s	Val(2s) 1.14738
417	c	21	s	Ryd 0.00014
418	c	21	s	Ryd 0.00008
419	c	21	s	Ryd 0.00000
420	c	21	p	Val(2px) 1.26360
421	c	21	p	Val(2py) 1.24842
422	c	21	p	Val(2pz) 1.07981
423	c	21	p	Ryd 0.00038

424	c	21	p	Ryd 0.00038
425	c	21	p	Ryd 0.00048
426	c	21	p	Ryd 0.00002
427	c	21	p	Ryd 0.00003
428	c	21	p	Ryd 0.00025
429	c	21	d	Ryd 0.00152
430	c	21	d	Ryd 0.00021
431	c	21	d	Ryd 0.00064
432	c	21	d	Ryd 0.00112
433	c	21	d	Ryd 0.00117
434	c	21	d	Ryd 0.00002
435	c	21	d	Ryd 0.00003
436	c	21	d	Ryd 0.00003
437	c	21	d	Ryd 0.00001
438	c	21	d	Ryd 0.00001
439	c	21	f	Ryd 0.00023
440	c	21	f	Ryd 0.00007
441	c	21	f	Ryd 0.00021
442	c	21	f	Ryd 0.00004
443	c	21	f	Ryd 0.00002
444	c	21	f	Ryd 0.00037
445	c	21	f	Ryd 0.00000
446	h	22	s	Val(1s) 0.70847
447	h	22	s	Ryd 0.00025
448	h	22	s	Ryd 0.00007
449	h	22	p	Ryd 0.00051
450	h	22	p	Ryd 0.00008
451	h	22	p	Ryd 0.00013
452	h	23	s	Val(1s) 0.70860
453	h	23	s	Ryd 0.00025
454	h	23	s	Ryd 0.00007
455	h	23	p	Ryd 0.00017
456	h	23	p	Ryd 0.00045
457	h	23	p	Ryd 0.00011
458	h	24	s	Val(1s) 0.70869
459	h	24	s	Ryd 0.00025
460	h	24	s	Ryd 0.00007
461	h	24	p	Ryd 0.00015
462	h	24	p	Ryd 0.00028
463	h	24	p	Ryd 0.00030
464	c	25	s	Cor(1s) 1.99934
465	c	25	s	Val(2s) 0.87738
466	c	25	s	Ryd 0.00777
467	c	25	s	Ryd 0.00006
468	c	25	s	Ryd 0.00001
469	c	25	p	Val(2px) 0.83354
470	c	25	p	Val(2py) 0.84469
471	c	25	p	Val(2pz) 0.96709
472	c	25	p	Ryd 0.00025
473	c	25	p	Ryd 0.00100
474	c	25	p	Ryd 0.00813
475	c	25	p	Ryd 0.00007
476	c	25	p	Ryd 0.00005
477	c	25	p	Ryd 0.00013
478	c	25	d	Ryd 0.00069
479	c	25	d	Ryd 0.00079
480	c	25	d	Ryd 0.00076
481	c	25	d	Ryd 0.00008
482	c	25	d	Ryd 0.00010
483	c	25	d	Ryd 0.00006
484	c	25	d	Ryd 0.00001
485	c	25	d	Ryd 0.00003
486	c	25	d	Ryd 0.00004
487	c	25	d	Ryd 0.00004
488	c	25	f	Ryd 0.00132
489	c	25	f	Ryd 0.00060

490	c	25	f	Ryd	0.00105
491	c	25	f	Ryd	0.00016
492	c	25	f	Ryd	0.00017
493	c	25	f	Ryd	0.00001
494	c	25	f	Ryd	0.00001
495	n	26	s	Cor(1s)	1.99929
496	n	26	s	Val(2s)	1.54588
497	n	26	s	Ryd	0.00476
498	n	26	s	Ryd	0.00005
499	n	26	s	Ryd	0.00000
500	n	26	p	Val(2px)	1.21770
501	n	26	p	Val(2py)	1.44677
502	n	26	p	Val(2pz)	1.19220
503	n	26	p	Ryd	0.00113
504	n	26	p	Ryd	0.00535
505	n	26	p	Ryd	0.00097
506	n	26	p	Ryd	0.00003
507	n	26	p	Ryd	0.00014
508	n	26	p	Ryd	0.00002
509	n	26	d	Ryd	0.00181
510	n	26	d	Ryd	0.00066
511	n	26	d	Ryd	0.00290
512	n	26	d	Ryd	0.00412
513	n	26	d	Ryd	0.00410
514	n	26	d	Ryd	0.00001
515	n	26	d	Ryd	0.00000
516	n	26	d	Ryd	0.00001
517	n	26	d	Ryd	0.00001
518	n	26	d	Ryd	0.00002
519	n	26	f	Ryd	0.00009
520	n	26	f	Ryd	0.00003
521	n	26	f	Ryd	0.00013
522	n	26	f	Ryd	0.00008
523	n	26	f	Ryd	0.00011
524	n	26	f	Ryd	0.00019
525	n	26	f	Ryd	0.00024
526	c	27	s	Cor(1s)	1.99923
527	c	27	s	Val(2s)	1.14538
528	c	27	s	Ryd	0.00014
529	c	27	s	Ryd	0.00007
530	c	27	s	Ryd	0.00000
531	c	27	p	Val(2px)	1.23916
532	c	27	p	Val(2py)	1.09748
533	c	27	p	Val(2pz)	1.25596
534	c	27	p	Ryd	0.00041
535	c	27	p	Ryd	0.00045
536	c	27	p	Ryd	0.00041
537	c	27	p	Ryd	0.00004
538	c	27	p	Ryd	0.00022
539	c	27	p	Ryd	0.00002
540	c	27	d	Ryd	0.00134
541	c	27	d	Ryd	0.00103
542	c	27	d	Ryd	0.00035
543	c	27	d	Ryd	0.00088
544	c	27	d	Ryd	0.00103
545	c	27	d	Ryd	0.00001
546	c	27	d	Ryd	0.00001
547	c	27	d	Ryd	0.00002
548	c	27	d	Ryd	0.00002
549	c	27	d	Ryd	0.00002
550	c	27	f	Ryd	0.00040
551	c	27	f	Ryd	0.00005
552	c	27	f	Ryd	0.00005
553	c	27	f	Ryd	0.00003
554	c	27	f	Ryd	0.00005
555	c	27	f	Ryd	0.00024
556	c	27	f	Ryd	0.00013

557	h	28	s	Val(1s) 0.71454
558	h	28	s	Ryd 0.00027
559	h	28	s	Ryd 0.00007
560	h	28	p	Ryd 0.00009
561	h	28	p	Ryd 0.00011
562	h	28	p	Ryd 0.00054
563	h	29	s	Val(1s) 0.71470
564	h	29	s	Ryd 0.00027
565	h	29	s	Ryd 0.00007
566	h	29	p	Ryd 0.00045
567	h	29	p	Ryd 0.00011
568	h	29	p	Ryd 0.00017
569	h	30	s	Val(1s) 0.71485
570	h	30	s	Ryd 0.00029
571	h	30	s	Ryd 0.00007
572	h	30	p	Ryd 0.00026
573	h	30	p	Ryd 0.00034
574	h	30	p	Ryd 0.00012
575	c	31	s	Cor(1s) 1.99937
576	c	31	s	Val(2s) 0.88345
577	c	31	s	Ryd 0.00747
578	c	31	s	Ryd 0.00005
579	c	31	s	Ryd 0.00001
580	c	31	p	Val(2px) 0.87217
581	c	31	p	Val(2py) 0.96208
582	c	31	p	Val(2pz) 0.86143
583	c	31	p	Ryd 0.00197
584	c	31	p	Ryd 0.00974
585	c	31	p	Ryd 0.00080
586	c	31	p	Ryd 0.00010
587	c	31	p	Ryd 0.00020
588	c	31	p	Ryd 0.00009
589	c	31	d	Ryd 0.00025
590	c	31	d	Ryd 0.00012
591	c	31	d	Ryd 0.00066
592	c	31	d	Ryd 0.00067
593	c	31	d	Ryd 0.00062
594	c	31	d	Ryd 0.00005
595	c	31	d	Ryd 0.00004
596	c	31	d	Ryd 0.00002
597	c	31	d	Ryd 0.00004
598	c	31	d	Ryd 0.00003
599	c	31	f	Ryd 0.00031
600	c	31	f	Ryd 0.00011
601	c	31	f	Ryd 0.00057
602	c	31	f	Ryd 0.00030
603	c	31	f	Ryd 0.00036
604	c	31	f	Ryd 0.00098
605	c	31	f	Ryd 0.00074
606	n	32	s	Cor(1s) 1.99929
607	n	32	s	Val(2s) 1.54561
608	n	32	s	Ryd 0.00475
609	n	32	s	Ryd 0.00005
610	n	32	s	Ryd 0.00000
611	n	32	p	Val(2px) 1.43395
612	n	32	p	Val(2py) 1.21816
613	n	32	p	Val(2pz) 1.20505
614	n	32	p	Ryd 0.00401
615	n	32	p	Ryd 0.00175
616	n	32	p	Ryd 0.00173
617	n	32	p	Ryd 0.00014
618	n	32	p	Ryd 0.00003
619	n	32	p	Ryd 0.00003
620	n	32	d	Ryd 0.00181
621	n	32	d	Ryd 0.00316
622	n	32	d	Ryd 0.00047

623	n	32	d	Ryd 0.00381
624	n	32	d	Ryd 0.00433
625	n	32	d	Ryd 0.00001
626	n	32	d	Ryd 0.00001
627	n	32	d	Ryd 0.00001
628	n	32	d	Ryd 0.00001
629	n	32	d	Ryd 0.00001
630	n	32	f	Ryd 0.00008
631	n	32	f	Ryd 0.00014
632	n	32	f	Ryd 0.00003
633	n	32	f	Ryd 0.00011
634	n	32	f	Ryd 0.00011
635	n	32	f	Ryd 0.00021
636	n	32	f	Ryd 0.00018
637	c	33	s	Cor(1s) 1.99923
638	c	33	s	Val(2s) 1.14538
639	c	33	s	Ryd 0.00013
640	c	33	s	Ryd 0.00007
641	c	33	s	Ryd 0.00000
642	c	33	p	Val(2px) 1.10264
643	c	33	p	Val(2py) 1.24038
644	c	33	p	Val(2pz) 1.24942
645	c	33	p	Ryd 0.00044
646	c	33	p	Ryd 0.00040
647	c	33	p	Ryd 0.00041
648	c	33	p	Ryd 0.00021
649	c	33	p	Ryd 0.00004
650	c	33	p	Ryd 0.00003
651	c	33	d	Ryd 0.00104
652	c	33	d	Ryd 0.00072
653	c	33	d	Ryd 0.00106
654	c	33	d	Ryd 0.00072
655	c	33	d	Ryd 0.00110
656	c	33	d	Ryd 0.00001
657	c	33	d	Ryd 0.00003
658	c	33	d	Ryd 0.00001
659	c	33	d	Ryd 0.00002
660	c	33	d	Ryd 0.00002
661	c	33	f	Ryd 0.00003
662	c	33	f	Ryd 0.00024
663	c	33	f	Ryd 0.00008
664	c	33	f	Ryd 0.00009
665	c	33	f	Ryd 0.00029
666	c	33	f	Ryd 0.00004
667	c	33	f	Ryd 0.00017
668	h	34	s	Val(1s) 0.71456
669	h	34	s	Ryd 0.00027
670	h	34	s	Ryd 0.00007
671	h	34	p	Ryd 0.00030
672	h	34	p	Ryd 0.00008
673	h	34	p	Ryd 0.00036
674	h	35	s	Val(1s) 0.71481
675	h	35	s	Ryd 0.00028
676	h	35	s	Ryd 0.00007
677	h	35	p	Ryd 0.00009
678	h	35	p	Ryd 0.00051
679	h	35	p	Ryd 0.00013
680	h	36	s	Val(1s) 0.71466
681	h	36	s	Ryd 0.00028
682	h	36	s	Ryd 0.00007
683	h	36	p	Ryd 0.00017
684	h	36	p	Ryd 0.00022
685	h	36	p	Ryd 0.00033
686	c	37	s	Cor(1s) 1.99937
687	c	37	s	Val(2s) 0.88341

688	c	37	s	Ryd 0.00748
689	c	37	s	Ryd 0.00005
690	c	37	s	Ryd 0.00001
691	c	37	p	Val(2px) 0.95664
692	c	37	p	Val(2py) 0.87165
693	c	37	p	Val(2pz) 0.86707
694	c	37	p	Ryd 0.01006
695	c	37	p	Ryd 0.00148
696	c	37	p	Ryd 0.00095
697	c	37	p	Ryd 0.00017
698	c	37	p	Ryd 0.00010
699	c	37	p	Ryd 0.00011
700	c	37	d	Ryd 0.00023
701	c	37	d	Ryd 0.00070
702	c	37	d	Ryd 0.00014
703	c	37	d	Ryd 0.00063
704	c	37	d	Ryd 0.00062
705	c	37	d	Ryd 0.00004
706	c	37	d	Ryd 0.00003
707	c	37	d	Ryd 0.00004
708	c	37	d	Ryd 0.00002
709	c	37	d	Ryd 0.00005
710	c	37	f	Ryd 0.00034
711	c	37	f	Ryd 0.00053
712	c	37	f	Ryd 0.00009
713	c	37	f	Ryd 0.00036
714	c	37	f	Ryd 0.00044
715	c	37	f	Ryd 0.00070
716	c	37	f	Ryd 0.00091

Summary of Natural Population Analysis:

Atom	No	Natural Charge	Natural Population: Core	Valence	Rydberg	Total
1	sn	1.37710	17.99534	2.61245	0.01511	20.62290
2	n	-0.44651	1.99914	5.42003	0.02734	7.44651
3	c	0.45436	1.99934	3.52295	0.02335	5.54564
4	c	-0.74559	1.99923	4.73890	0.00746	6.74559
5	h	0.29041	0.00000	0.70855	0.00105	0.70959
6	h	0.29015	0.00000	0.70881	0.00105	0.70985
7	h	0.29017	0.00000	0.70878	0.00105	0.70983
8	n	-0.44685	1.99914	5.42037	0.02734	7.44685
9	c	0.45453	1.99934	3.52276	0.02337	5.54547
10	c	-0.74598	1.99923	4.73928	0.00747	6.74598
11	h	0.29034	0.00000	0.70860	0.00105	0.70966
12	h	0.29045	0.00000	0.70852	0.00104	0.70955
13	h	0.29037	0.00000	0.70858	0.00105	0.70963
14	n	-0.42920	1.99929	5.40295	0.02696	7.42920
15	c	-0.74424	1.99923	4.73759	0.00742	6.74424
16	h	0.28431	0.00000	0.71461	0.00108	0.71569
17	h	0.28421	0.00000	0.71471	0.00108	0.71579
18	h	0.28400	0.00000	0.71492	0.00108	0.71600
19	c	0.39580	1.99936	3.57860	0.02624	5.60420
20	n	-0.44688	1.99914	5.42041	0.02733	7.44688
21	c	-0.74593	1.99923	4.73921	0.00749	6.74593
22	h	0.29049	0.00000	0.70847	0.00104	0.70951
23	h	0.29035	0.00000	0.70860	0.00105	0.70965
24	h	0.29026	0.00000	0.70869	0.00105	0.70974
25	c	0.45459	1.99934	3.52270	0.02338	5.54541
26	n	-0.42879	1.99929	5.40255	0.02695	7.42879
27	c	-0.74463	1.99923	4.73797	0.00743	6.74463
28	h	0.28439	0.00000	0.71454	0.00107	0.71561
29	h	0.28422	0.00000	0.71470	0.00108	0.71578
30	h	0.28407	0.00000	0.71485	0.00108	0.71593
31	c	0.39522	1.99937	3.57913	0.02629	5.60478
32	n	-0.42903	1.99929	5.40277	0.02697	7.42903
33	c	-0.74448	1.99923	4.73782	0.00743	6.74448
34	h	0.28436	0.00000	0.71456	0.00108	0.71564
35	h	0.28411	0.00000	0.71481	0.00108	0.71589

36	h	0.28427	0.00000	0.71466	0.00107	0.71573
37	c	0.39559	1.99937	3.57877	0.02628	5.60441
* Total *		2.00000	53.98212	97.62716	0.39072	152.00000

For all atoms:

Core	53.98212	99.9669% of	54)
Valence	97.62716	99.6195% of	98)
Natural Minimal Basis	151.60928	99.7429% of	152)
Natural Rydberg Basis	0.39072	0.2571% of	152)

==========

atomic populations from total density:

atom	charge	n(s)	n(p)	n(d)	n(f)	n(g)
1 sn	1.37710	3.89756	6.72063	10.00217	0.00254	0.00000
2 n	-0.44651	3.50362	3.93116	0.01058	0.00116	0.00000
3 c	0.45436	2.88456	2.65517	0.00261	0.00330	0.00000
4 c	-0.74559	3.14676	3.59312	0.00475	0.00095	0.00000
5 h	0.29041	0.70887	0.00073	0.00000	0.00000	0.00000
6 h	0.29015	0.70913	0.00072	0.00000	0.00000	0.00000
7 h	0.29017	0.70910	0.00073	0.00000	0.00000	0.00000
8 n	-0.44685	3.50377	3.93134	0.01059	0.00115	0.00000
9 c	0.45453	2.88452	2.65502	0.00262	0.00330	0.00000
10 c	-0.74598	3.14684	3.59342	0.00476	0.00095	0.00000
11 h	0.29034	0.70893	0.00073	0.00000	0.00000	0.00000
12 h	0.29045	0.70884	0.00072	0.00000	0.00000	0.00000
13 h	0.29037	0.70890	0.00073	0.00000	0.00000	0.00000
14 n	-0.42920	3.54982	3.86489	0.01363	0.00086	0.00000
15 c	-0.74424	3.14482	3.59375	0.00472	0.00095	0.00000
16 h	0.28431	0.71495	0.00074	0.00000	0.00000	0.00000
17 h	0.28421	0.71506	0.00073	0.00000	0.00000	0.00000
18 h	0.28400	0.71528	0.00073	0.00000	0.00000	0.00000
19 c	0.39580	2.89041	2.70792	0.00250	0.00337	0.00000
20 n	-0.44688	3.50372	3.93143	0.01058	0.00115	0.00000
21 c	-0.74593	3.14684	3.59337	0.00476	0.00095	0.00000
22 h	0.29049	0.70879	0.00072	0.00000	0.00000	0.00000
23 h	0.29035	0.70893	0.00073	0.00000	0.00000	0.00000
24 h	0.29026	0.70902	0.00072	0.00000	0.00000	0.00000
25 c	0.45459	2.88455	2.65494	0.00261	0.00331	0.00000
26 n	-0.42879	3.54997	3.86431	0.01365	0.00086	0.00000
27 c	-0.74463	3.14482	3.59413	0.00472	0.00096	0.00000
28 h	0.28439	0.71488	0.00073	0.00000	0.00000	0.00000
29 h	0.28422	0.71505	0.00073	0.00000	0.00000	0.00000
30 h	0.28407	0.71521	0.00072	0.00000	0.00000	0.00000
31 c	0.39522	2.89034	2.70857	0.00250	0.00337	0.00000
32 n	-0.42903	3.54970	3.86484	0.01363	0.00086	0.00000
33 c	-0.74448	3.14481	3.59398	0.00474	0.00095	0.00000
34 h	0.28436	0.71490	0.00074	0.00000	0.00000	0.00000
35 h	0.28411	0.71517	0.00073	0.00000	0.00000	0.00000
36 h	0.28427	0.71501	0.00072	0.00000	0.00000	0.00000
37 c	0.39559	2.89031	2.70823	0.00250	0.00337	0.00000

==========

moments (from total density versus population analysis)

<charge> =	2.000000	2.000000
<x > =	-0.302396	0.340319
<y > =	-0.071846	0.069733
<z > =	0.198454	-0.214023

```
================================================================================
                        electrostatic moments
================================================================================

reference point for electrostatic moments:    0.00000   0.00000   0.00000


             nuc           elec       ->  total
--------------------------------------------------------------------------------
                          charge
--------------------------------------------------------------------------------
        154.000000    -152.000000       2.000000

--------------------------------------------------------------------------------
                       dipole moment
--------------------------------------------------------------------------------
  x       9.939566     -10.241961      -0.302396
  y       3.163783      -3.235629      -0.071846
  z      -6.832015       7.030469       0.198454

  | dipole moment | =     0.3688 a.u. =     0.9373 debye

--------------------------------------------------------------------------------
                     quadrupole moment
--------------------------------------------------------------------------------
 xx    2364.832474   -2393.289252     -28.456778
 yy    3045.149318   -3059.741347     -14.592029
 zz    2774.404167   -2794.374773     -19.970606
 xy    -157.238497     153.993745      -3.244752
 xz     441.176892    -432.079584       9.097308
 yz     100.368640     -98.305949       2.062691

    1/3  trace=     -21.006471
    anisotropy=      20.957578
```

Experimental Details Towards Assignment of 2-4

Crystals of $[Sn(dmap)_4][Al(OR^F)_4]_2$ (2): $[SnCp][Al(OR^F)_4]$ (0.205 g, 0.178 mmol) and dmap (0.044 g, 0.36 mmol, 2.0 eq) were filled into a Schlenk flask and while stirring CH_2Cl_2 (5 mL) was added. The mixture was stirred overnight and then stored at room temperature. After 8 weeks, crystals of **2** formed.

Crystals of $[Sn(PPh_3)_2(MeCN)_5][Al(OR^F)_4]_2 \bullet MeCN$ (3): **1** (0.049 g, 0.021 mmol) and PPh_3 (0.018 g, 0.069 mmol, 3.3 eq) were filled into a Schlenk flask and while stirring MeCN (1.5 mL) was added. The mixture was stirred for another 1.5 h and then stored at −20 °C. After 4 days, crystals of **3** formed.

$[Sn(pyr)_2(MeCN)_4][Al(OR^F)_4]_2$ (4): **1** (2.222 g, 0.9665 mmol) and pyrazine (0.251 g, 3.13 mmol, 3.2 eq) were filled into a Schlenk flask and while stirring CH_2Cl_2 (20 mL) was added and stirred for about 60 h. The solvent was removed *in vacuo* and the remaining solid was washed twice with CH_2Cl_2 (2x3 mL) and dried *in vacuo* and by that, **4** was obtained as pale brown solid (1.528 g, 0.6427 mmol, 66 %). ^{1}H-NMR (300.18 MHz, CD_3CN, 298 K): 8.75 (s, 8 H, $[Sn(C_4\boldsymbol{H}_4N_2)_2(MeCN)_4][Al(OR^F)_4]_2$), 1.96 ppm (s, 12 H, $[Sn(pyr)_2(\boldsymbol{H}_3CCN)_4][Al(OR^F)_4]_2$). ^{19}F-NMR (282.45 MHz, CD_3CN, 298 K) −76.0 ppm (s, 72 F, $[Sn(pyr)_4(MeCN)_4][Al\{OC(C\boldsymbol{F}_3)_3\}_4]_2$). ^{119}Sn-NMR (111.94 MHz, CD_3CN, 298 K): −1408 ppm (br, 1 Sn, $[\boldsymbol{Sn}(pyr)_2(MeCN)_4][Al(OR^F)_4]_2$). ^{27}Al-NMR (78.22 MHz, CD_3CN, 298 K): 34.5 ppm (s, 2 Al, $[Sn(pyr)_2(MeCN)_4][\boldsymbol{Al}(OR^F)_4]_2$). IR (400-4000 cm^{-1}, Diamond ATR, corrected): 2954 (vw), 2926 (vw), 2855 (vw), 2308 (vw), 2270 (vw), 2263 (vw), 1422 (vw), 1352 (vw), 1297 (w), 1273 (w), 1273 (w), 1266 (w), 1242 (m), 1214 (vs), 1170 (w), 1128 (vw), 1081 (vw), 1054 (vw), 1042 (vw), 969 (s), 832 (vw), 798 (vw), 755 (vw), 726 (w), 599 (vw), 587 (vw), 571 (vw), 560 (vw), 536 (vw), 438 (vw).

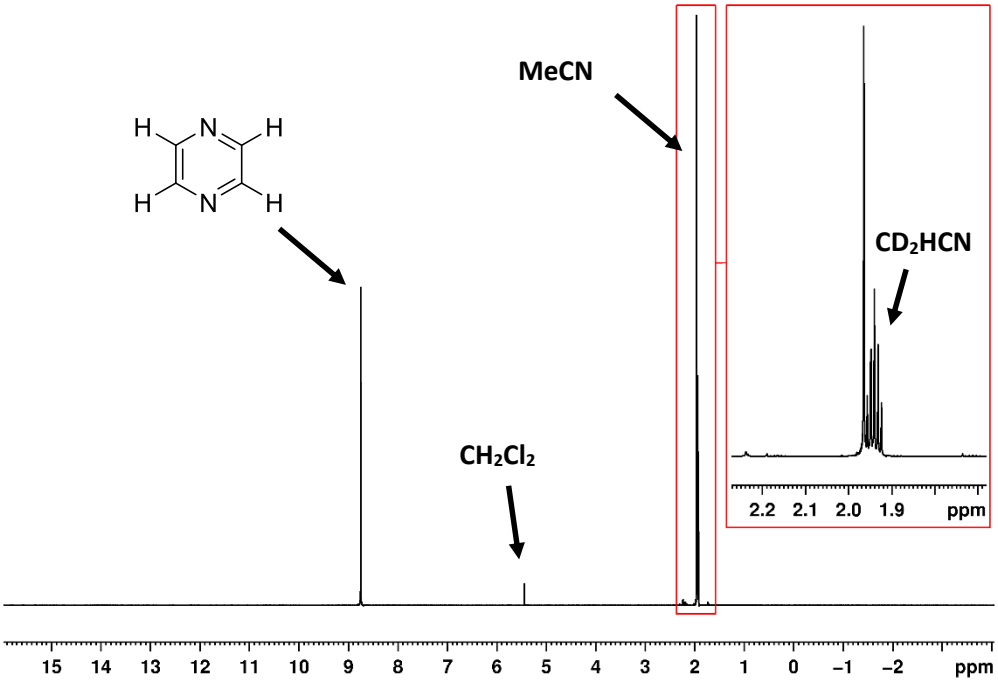


Figure S 7. ^{1}H-NMR spectrum (300.18 MHz) of **4** in CD_3CN at 298 K.

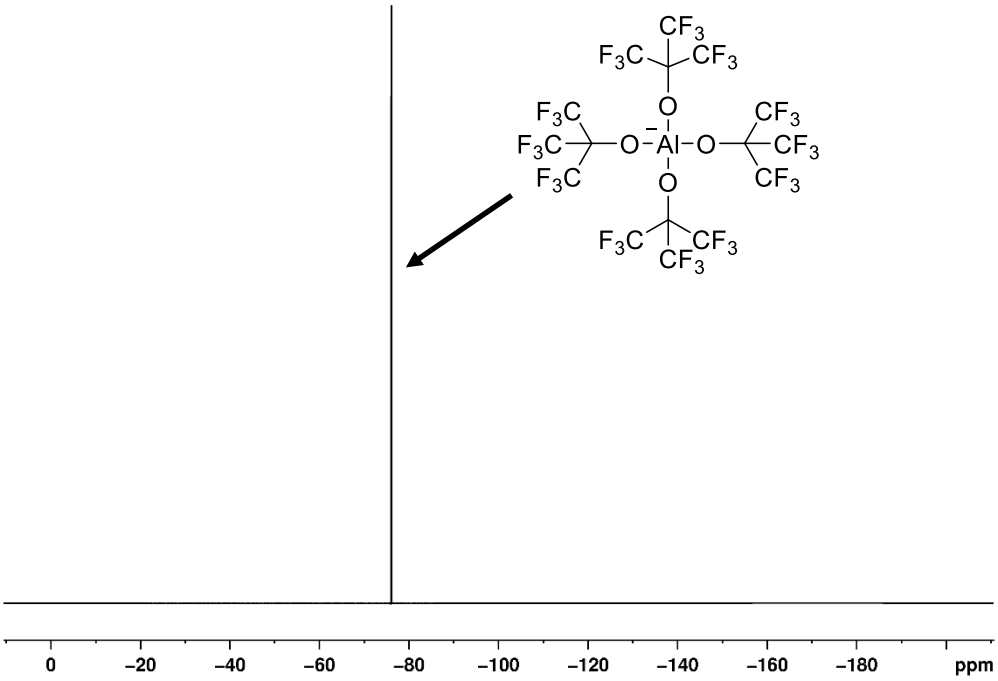


Figure S 8. ^{19}F-NMR spectrum (282.45 MHz) of **4** in CD_3CN at 298 K.

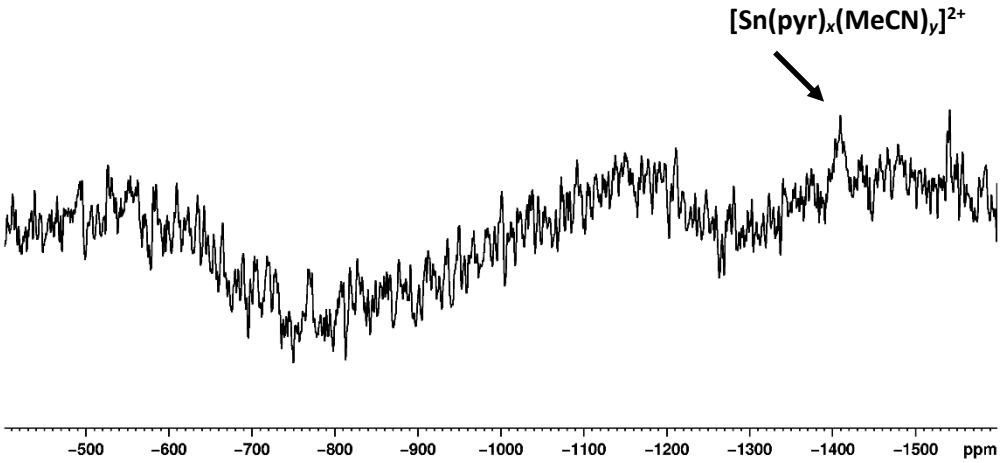


Figure S 9. ^{119}Sn-NMR spectrum (111.94 MHz) of **4** in CD_3CN at 298 K. We have checked the original data together with our NMR spectroscopist Dr. H. Scherer. The signal is real, but we refrained from Baseline and data manipulations.

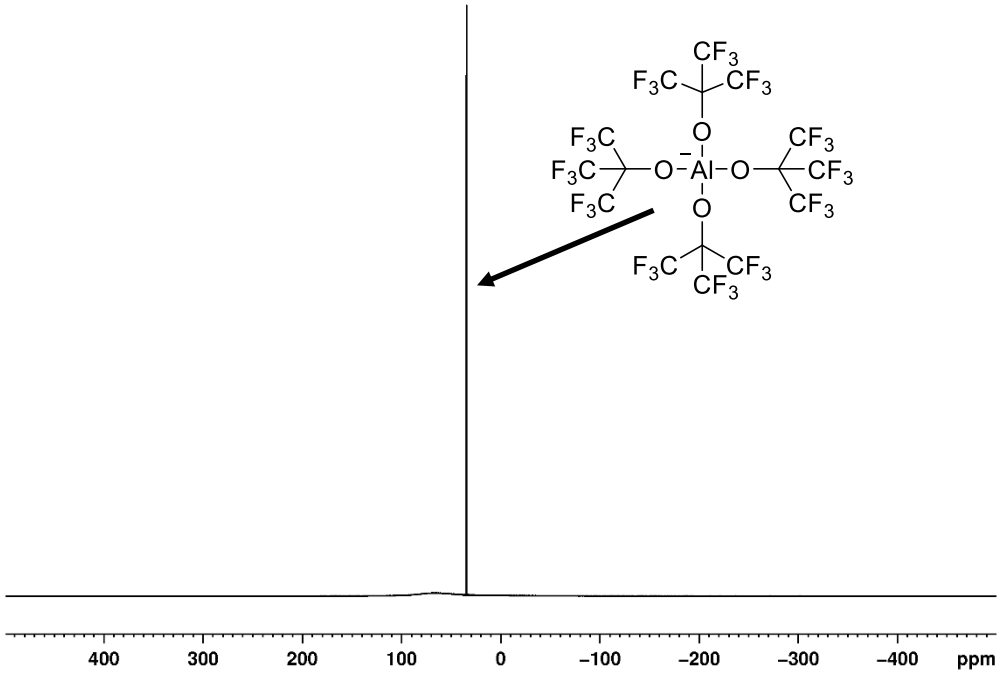


Figure S 10. ^{27}Al-NMR spectrum (78.22 MHz) of **4** in CD_3CN at 298 K.

Crystallographic details

Single crystal X-ray crystallographic data were collected on a Bruker SMART APEXII Quazar with a CCD area detector and an INCOATEC 1st gen. Mo microsource. Structures were solved by SHELXT[3] and refined by using SHELXL,[3] ShelXle,[4] and DSR.[5] Graphics of the crystal structures were produced with Mercury CSD 3.8 and POV-Ray for Windows 3.7.0.

In **1**, six alkoxy-groups are disordered. The disorder was in both cases described by using two different positions and a respective free variable for the occupation. All equal 1,2 and 1,3 distances in the $OC(CF_3)_3$-groups were restrained to be of similar length using SADI. The thermal parameters of the alkoxy-groups were made similar with SIMU and RIGU restraints.

In **4**, two alkoxy-groups are disordered. The disorder was in both cases described by using two different positions and a respective free variable for the occupation. All 1,2 and 1,3 distances in the $OC(CF_3)_3$-groups were restrained using SADI. The thermal parameters of the alkoxy-groups were made similar with SIMU and RIGU.

Crystal data and structure refinement details for 1 and 4

Identification code	**1**	**4**
Empirical formula	$C_{88}H_{36}Al_4F_{144}N_{12}O_{16}Sn_2$	$C_{48}H_{20}Al_2F_{72}N_8O_8Sn$
Formula weight	4598.59	2377.37
Temperature/K	100(2)	100(2)
Wavelength/Å	0.71073	0.71073
Crystal system	Monoclinic	Triclinic
Space group	$P2_1/c$	$P\bar{1}$
a/Å	26.8462(12)	14.2805(6)
b/Å	22.2195(10)	14.2903(6)
c/Å	27.4111(13)	20.9698(10)
α/°	90	82.129(3)
β/°	112.914(2)	83.435(3)
γ/°	90	63.201(2)
Volume/Å^3	15060.7(12)	3777.0(3)
Z	4	2
Density (calculated)/mg m^{-3}	2.028	2.090
Absorption coefficient/mm^{-1}	0.593	0.596
F(000)	8896	2304
Crystal size/mm^3	0.22 x 0.15 x 0.10	0.30 x 0.05 x 0.05
θ range for data collection/°	0.823 to 26.608	0.982 to 28.909
Index ranges	−33≤h≤31, 0≤k≤27, 0≤l≤34	−19≤h≤19, −19≤k≤19, −27≤l≤28
Reflections collected	34439	94441
Independent reflections	34439	18917

	[*R*(int) = 0.0968]	[*R*(int) = 0.0648]
Goodness-of-fit on F^2	1.102	1.021
Final R indices [I>2σ(I)]	R_1 = 0.0667, wR_2 = 0.1456	R_1 = 0.0531, wR_2 = 0.1280
R indices (all data)	R_1 = 0.0976, wR_2 = 0.1628	R_1 = 0.0961, wR_2 = 0.1470
Largest diff. peak and hole/e $Å^{-3}$	1.565 and −1.166	1.130 and −1.393
CCDC	1527811	1527816

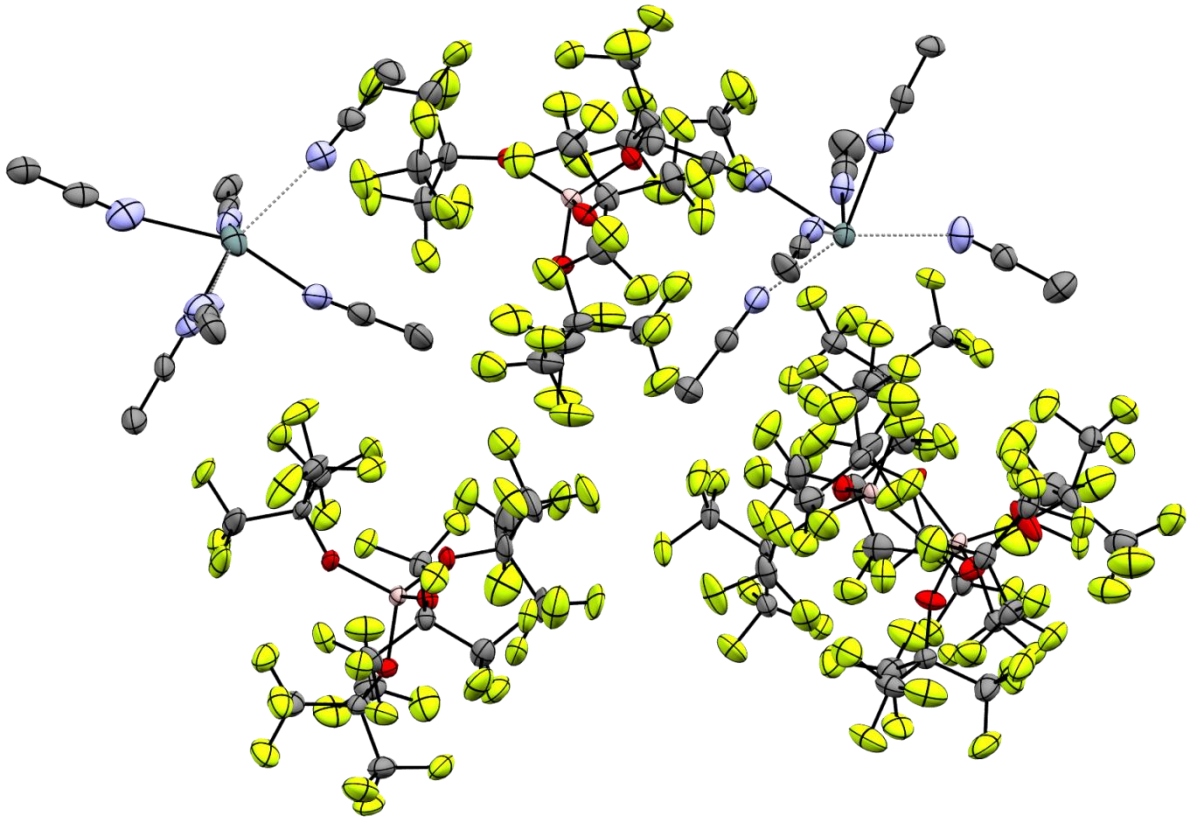


Figure S 11. Molecular structure of **1**. Thermal ellipsoids are drawn at 50 % probability level. H atoms are omitted for clarity and the disorder of the OR^F groups is not shown. Sn, cadet blue; O, red; N, blue; F, green; C, grey; Al, pink.

Crystal data and structure refinement details for 2 and 3

Although the crystal of structure **2** looks like an ordinary single crystal, the reflections have a broad distribution in *c* direction. There is no sign of pseudo tetragonal twinning. Supposedly, this broad distribution is causing the high *R*-values of the refinement. The unusual thermal ellipsoids of some dmap ligands also indicate that there might be a (incommensurable) superstructure. Modelling of additional disorder is possible but has no positive effect on the *R*-value.

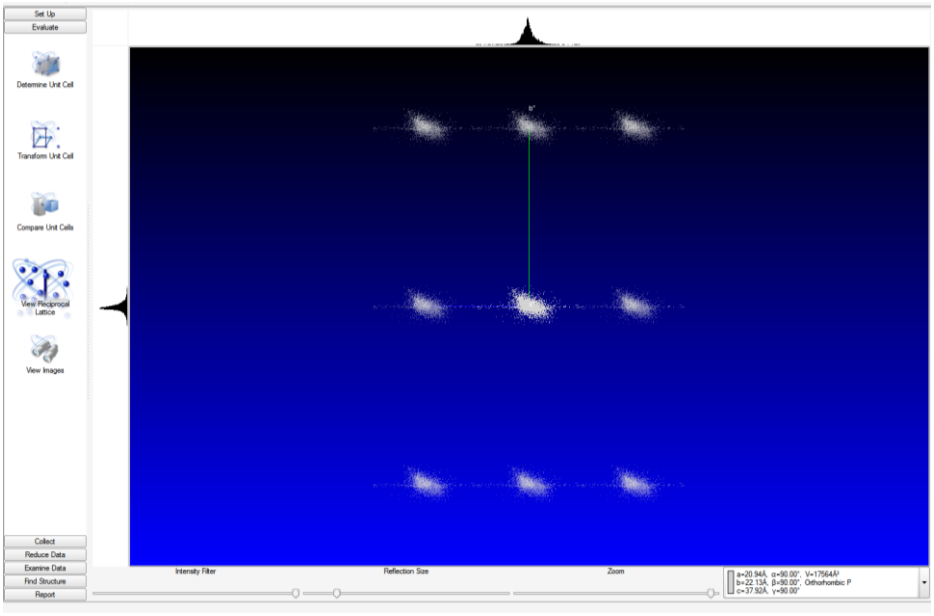


Figure S 12. Reciprocal lattice of **2** in the *b**, *c** plane. The lattice is contracted to a single point with the incommensurate tool of R-Latt in APEX3.

Identification code	**2**
Empirical formula	$C_{60}H_{40}Al_2F_{72}N_8O_8Sn$
Formula weight	2541.65
Temperature/K	100(2)
Wavelength/Å	0.71073
Crystal system	Orthorhombic
Space group	*Pbca*
a/Å	20.8860(6)
b/Å	22.0752(7)
c/Å	37.7998(12)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	17428.1(9)
Z	8
Density (calculated)/mg m^{-3}	1.937
Absorption coefficient/mm^{-1}	0.524
F(000)	9952
Crystal size/mm^3	0.30 x 0.30 x 0.30
θ range for data collection/°	1.077 to 27.103
Index ranges	−26≤h≤26, −28≤k≤28, −48≤l≤48
Reflections collected	580404
Independent reflections	19235 [*R*(int) = 0.0704]
Goodness-of-fit on F^2	1.191
Final R indices [I>2σ(I)]	R_1 = 0.1616, wR_2 = 0.3387
R indices (all data)	R_1 = 0.1659, wR_2 = 0.3403
Largest diff. peak and hole/e Å^{-3}	1.917 and −3.569

Table S 1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$ x 10^3) for **2**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
O114	3244(19)	1620(19)	2551(8)	46(3)
C114	3487(11)	1693(11)	2875(7)	39(2)
C214	2972(12)	1691(13)	3171(8)	57(4)
F114	2736(18)	2259(15)	3183(11)	52(7)
F214	3238(18)	1540(20)	3482(8)	62(7)
F314	2514(17)	1290(20)	3097(13)	69(3)
C314	4004(12)	1205(12)	2952(8)	51(4)
F414	4310(19)	1050(20)	2654(9)	62(3)
F514	3718(19)	722(14)	3096(11)	64(7)
F614	4453(14)	1427(17)	3170(9)	40(6)
C414	3826(14)	2322(12)	2912(8)	59(5)
F714	4419(15)	2250(20)	2789(13)	73(8)
F814	3820(20)	2498(18)	3252(9)	55(7)
F914	3510(20)	2733(16)	2724(13)	65(3)
O113	2237(11)	2443(10)	2335(7)	40(5)
C113	1772(8)	2859(7)	2371(4)	39(4)
C213	2026(10)	3443(8)	2550(5)	49(4)
F113	2059(13)	3374(11)	2900(5)	55(6)
F213	1639(11)	3915(8)	2489(6)	47(5)
F313	2601(10)	3597(11)	2424(7)	60(6)
C313	1494(10)	3029(9)	2003(5)	49(5)
F413	1406(15)	2537(11)	1804(6)	60(6)
F513	1895(11)	3403(9)	1833(6)	50(5)
F613	926(11)	3307(13)	2033(8)	59(7)
C413	1229(9)	2596(8)	2604(5)	44(4)
F713	847(10)	2239(10)	2413(6)	52(5)
F813	868(10)	3040(9)	2736(6)	44(5)
F913	1446(11)	2261(11)	2872(6)	47(5)
O112	4089(10)	3413(16)	4526(9)	20(5)
C112	4681(8)	3440(6)	4384(4)	23(3)
C212	5169(8)	3225(8)	4667(4)	32(4)
F112	5247(8)	3652(8)	4916(4)	37(4)
F212	5750(8)	3116(11)	4535(7)	38(5)
F312	4960(12)	2717(9)	4821(6)	38(5)
C312	4720(9)	3018(7)	4056(4)	31(4)
F412	4220(11)	3104(10)	3845(6)	34(5)
F512	4739(8)	2436(6)	4156(4)	37(4)
F612	5254(12)	3121(14)	3870(9)	37(6)
C412	4855(8)	4094(7)	4272(4)	27(3)
F712	4581(8)	4252(9)	3965(4)	39(4)
F812	5484(8)	4175(13)	4226(6)	32(5)
F912	4667(12)	4494(10)	4517(6)	28(5)
O18	2481(7)	2558(6)	2269(4)	30(3)
C18	2036(6)	2986(5)	2335(3)	35(3)
C28	2374(7)	3600(6)	2264(4)	39(3)
F18	2961(6)	3593(7)	2404(4)	52(3)
F28	2044(7)	4065(6)	2398(4)	48(3)
F38	2440(8)	3681(6)	1915(3)	51(4)
C38	1455(7)	2927(6)	2084(4)	39(3)

F48	1029(6)	2532(6)	2213(3)	46(3)
F58	1638(7)	2719(7)	1766(3)	42(3)
F68	1150(7)	3459(6)	2036(5)	50(4)
C48	1817(6)	2966(6)	2726(3)	37(3)
F78	1692(7)	2400(6)	2831(3)	42(3)
F88	1287(6)	3285(6)	2787(3)	47(3)
F98	2291(6)	3168(7)	2933(3)	47(3)
O111	3134(3)	3902(3)	4098(2)	17(1)
C111	2740(4)	4212(4)	3881(2)	19(2)
C211	2607(5)	4861(4)	4022(2)	30(2)
F111	2179(4)	4848(4)	4285(2)	40(2)
F211	2362(5)	5225(4)	3775(2)	48(2)
F311	3142(4)	5113(3)	4142(2)	37(2)
C311	3065(4)	4258(4)	3513(2)	24(2)
F411	3315(3)	3731(3)	3418(2)	28(1)
F511	3544(3)	4662(3)	3521(2)	30(2)
F611	2660(3)	4437(4)	3260(2)	34(2)
C411	2096(4)	3866(4)	3842(2)	26(2)
F711	2182(3)	3359(3)	3655(2)	32(2)
F811	1649(3)	4195(4)	3680(2)	40(2)
F911	1862(3)	3713(3)	4161(2)	28(2)
O110	2801(3)	3111(3)	4683(2)	17(1)
C110	2678(4)	2509(4)	4707(2)	22(2)
C210	3219(5)	2177(4)	4907(3)	34(2)
F110	3724(4)	2082(3)	4700(2)	43(2)
F210	3029(4)	1635(3)	5033(2)	47(2)
F310	3411(5)	2499(4)	5188(2)	50(2)
C310	2036(5)	2427(4)	4911(3)	36(2)
F410	1599(4)	2825(4)	4794(2)	48(2)
F510	2122(5)	2518(4)	5258(2)	52(2)
F610	1786(4)	1874(3)	4868(2)	43(2)
C410	2607(5)	2219(4)	4334(2)	28(2)
F710	2047(4)	2358(3)	4190(2)	38(2)
F810	2643(4)	1615(3)	4344(2)	39(2)
F910	3063(4)	2426(3)	4119(2)	35(2)
O19	1970(5)	1343(5)	2294(4)	70(3)
C19	1635(5)	824(5)	2261(3)	54(3)
C29	1174(6)	755(7)	2578(3)	88(4)
F19	1481(5)	857(9)	2880(3)	123(5)
F29	932(6)	196(7)	2603(3)	108(4)
F39	688(5)	1150(7)	2547(3)	113(4)
C39	1247(5)	852(5)	1912(3)	45(3)
F49	1634(5)	769(4)	1637(2)	54(2)
F59	950(5)	1380(4)	1872(3)	60(2)
F69	788(5)	432(4)	1894(2)	59(3)
C49	2078(5)	262(5)	2247(3)	49(3)
F79	2590(4)	366(5)	2044(3)	64(3)
F89	1792(5)	-227(4)	2119(2)	60(3)
F99	2302(4)	140(6)	2572(2)	78(3)
O17	3109(7)	1607(5)	1942(3)	77(4)
C17	3409(5)	1737(4)	1637(3)	49(2)
C27	2944(6)	1673(5)	1321(3)	53(3)
F17	2830(4)	1092(4)	1247(3)	56(2)

F27	3176(5)	1924(4)	1026(2)	56(2)
F37	2390(5)	1934(5)	1400(4)	84(3)
C37	3669(6)	2390(5)	1652(3)	60(3)
F47	3920(8)	2517(5)	1969(3)	98(4)
F57	3206(5)	2799(4)	1589(2)	67(3)
F67	4121(5)	2492(4)	1410(2)	59(2)
C47	3970(6)	1286(5)	1601(3)	52(3)
F77	4452(6)	1424(5)	1821(3)	85(3)
F87	4203(4)	1281(4)	1275(2)	50(2)
F97	3782(5)	721(4)	1679(3)	63(3)
O16	2994(6)	1637(6)	2676(3)	46(3)
C16	3448(5)	1600(5)	2923(3)	39(2)
C26	3571(7)	2217(6)	3100(4)	54(3)
F16	3595(7)	2641(6)	2848(3)	65(3)
F26	4119(6)	2196(7)	3292(4)	78(4)
F36	3114(7)	2371(6)	3326(4)	69(4)
C36	3204(6)	1141(5)	3199(3)	43(3)
F46	3284(5)	573(4)	3091(3)	50(3)
F56	2588(5)	1232(7)	3267(4)	69(3)
F66	3518(6)	1171(6)	3509(3)	60(3)
C46	4090(5)	1363(6)	2764(3)	44(3)
F76	3948(6)	907(5)	2534(3)	62(3)
F86	4475(5)	1117(6)	3010(3)	51(3)
F96	4404(5)	1811(5)	2607(3)	57(3)
O15	4065(8)	3378(13)	4537(7)	20(4)
C15	4665(7)	3404(6)	4405(3)	25(3)
C25	5049(7)	2871(6)	4567(4)	32(3)
F15	4916(10)	2819(8)	4911(4)	36(4)
F25	5681(6)	2931(8)	4529(6)	36(4)
F35	4876(7)	2348(6)	4414(4)	40(3)
C35	4655(7)	3355(7)	3995(4)	35(3)
F45	4527(7)	3892(7)	3844(4)	43(3)
F55	4218(10)	2949(9)	3897(5)	42(5)
F65	5223(10)	3173(12)	3870(7)	43(5)
C45	4981(7)	4010(7)	4516(4)	34(3)
F75	4572(10)	4469(9)	4459(6)	42(5)
F85	5514(7)	4132(11)	4331(5)	40(5)
F95	5151(7)	4005(8)	4857(3)	46(4)
N14	5000(5)	861(4)	5307(3)	36(2)
N24	5072(10)	1060(5)	4216(4)	92(5)
C14	4478(8)	766(5)	5104(4)	51(3)
C24	4477(9)	813(6)	4745(4)	67(4)
C34	5040(8)	973(5)	4570(4)	64(3)
C44	5584(9)	1079(6)	4779(3)	58(3)
C54	5539(7)	1019(6)	5134(3)	43(3)
C64	4501(12)	995(9)	3996(6)	116(7)
C74	5667(12)	1251(8)	4046(5)	107(6)
N13	5322(4)	1708(4)	5969(2)	21(2)
N23	5719(4)	3543(4)	6072(2)	25(2)
C13	5172(4)	2108(4)	5711(2)	19(2)
C23	5293(4)	2717(4)	5737(3)	19(2)
C33	5599(5)	2945(4)	6041(2)	21(2)
C43	5754(5)	2529(5)	6311(3)	25(2)

C53	5607(5)	1932(5)	6262(3)	21(2)
C63	5556(6)	3985(6)	5793(3)	33(3)
C73	6028(6)	3781(6)	6388(3)	37(3)
N12	5014(4)	750(4)	6565(2)	23(2)
N22	5013(4)	764(4)	7672(3)	35(2)
C12	4616(5)	1103(4)	6754(3)	27(2)
C22	4594(5)	1128(5)	7116(3)	30(2)
C32	5017(5)	764(5)	7315(3)	28(2)
C42	5438(5)	394(5)	7121(3)	25(2)
C52	5423(5)	413(5)	6762(3)	23(2)
C62	4574(7)	1170(7)	7859(4)	61(5)
C72	5428(5)	352(6)	7871(3)	32(3)
N11	4096(5)	822(4)	5955(2)	29(2)
N21	2143(4)	1018(4)	6129(2)	25(2)
C11	3778(5)	1318(5)	5840(3)	29(3)
C21	3137(5)	1392(5)	5891(3)	26(2)
C31	2773(5)	956(4)	6077(3)	22(2)
C41	3111(5)	441(5)	6189(3)	28(2)
C51	3755(5)	401(5)	6130(3)	31(2)
C61	1819(6)	1567(5)	6001(3)	33(3)
C71	1765(6)	554(6)	6303(3)	31(3)
Sn(01)	5157(1)	691(1)	5938(1)	25(1)
Al(02)	3298(1)	3671(1)	4525(1)	14(1)
Al(03)	2627(2)	1775(1)	2292(1)	16(1)
F(00E)	3831(4)	3754(4)	5318(2)	40(2)
F(00F)	3589(5)	4446(4)	5700(2)	42(2)
F(00L)	3202(5)	5504(4)	5401(2)	47(2)
O(00O)	3209(4)	4304(3)	4786(2)	22(2)
F(00P)	2552(5)	3743(4)	5402(2)	46(2)
F(00S)	3589(5)	5428(4)	4874(2)	50(2)
F(00V)	4249(4)	4639(4)	5270(2)	43(2)
F(00Z)	2315(4)	4652(4)	5558(2)	49(2)
F(011)	2562(5)	5420(4)	4959(2)	56(3)
F(013)	2035(4)	4316(5)	5038(2)	53(2)
C(02L)	3132(6)	4529(5)	5117(3)	22(2)
C(02O)	3710(6)	4341(6)	5353(3)	28(3)
C(031)	2507(7)	4316(7)	5282(3)	40(3)
C(03G)	3115(8)	5230(6)	5085(3)	38(3)

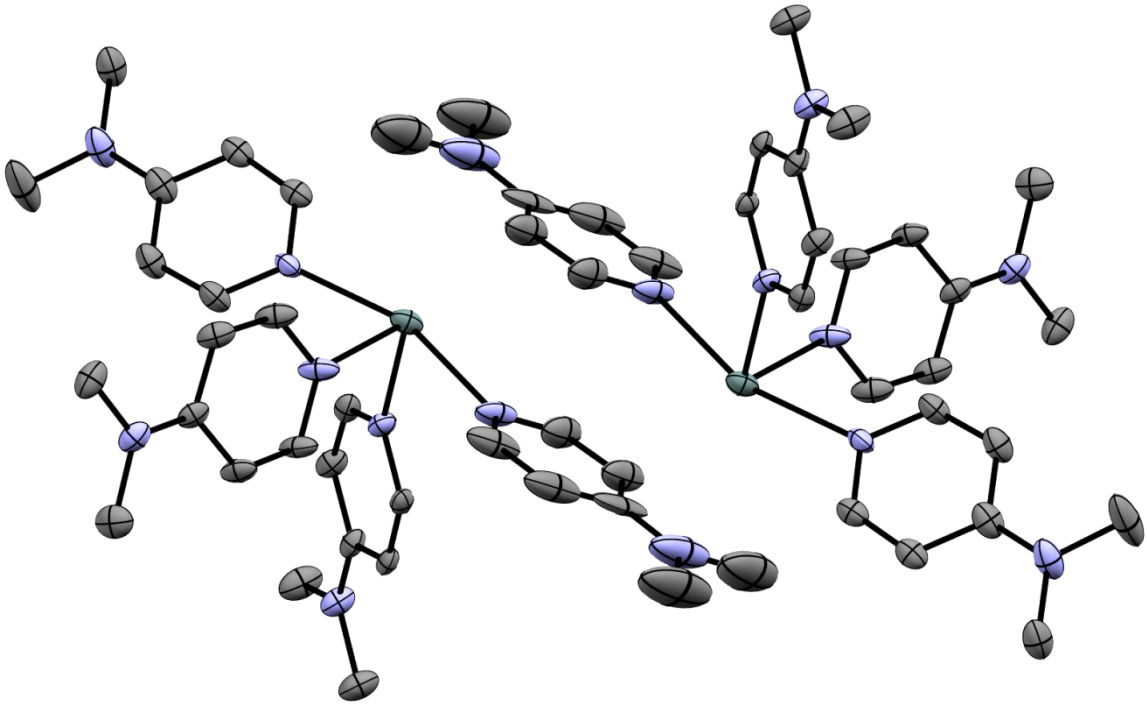


Figure S 13. Dimeric arrangement of the cations in **2**. Thermal ellipsoids are drawn at 50 % probability level, H atoms are omitted for clarity. Sn, cadet blue; N, blue; C, grey.

The structure of **3** could be solved and refined, but not to satisfactory residuals. A very high residual density peak on each Tin atom remains. It is not describable by disorder although the phosphorus ligand would allow this movement, but the acetonitrile molecules also bound to the tin atoms forbid the disorder even if they are on the same occupancy as the second lower occupied part. The reflection images show also very weak reflections between the indexed reflections. Neither a refinement as supercell or as pseudo twin gave improved results.

Identification code	**3**
Empirical formula	$C_{160}H_{96}Al_4F_{144}N_{12}O_{16}P_4Sn_2$
Formula weight	5647.66
Temperature/K	100(2)
Wavelength/Å	0.71073
Crystal system	Triclinic
Space group	$P\bar{1}$
a/Å	19.5545(12)
b/Å	19.9718(12)
c/Å	30.088(2)
α/°	102.847(4)
β/°	102.281(3)
γ/°	109.216(2)
Volume/Å^3	10283.2(12)
Z	2
Density (calculated)/mg m^{-3}	1.824
Absorption coefficient/mm^{-1}	0.483
F(000)	5552
Crystal size/mm^3	0.40 x 0.20 x 0.15
θ range for data collection/°	1.138 to 25.610
Index ranges	−23≤h≤23, −24≤k≤24, −36≤l≤36
Reflections collected	245548
Independent reflections	37768 [*R*(int) = 0.0640]
Goodness-of-fit on F^2	1.834
Final R indices [I>2σ(I)]	R_1 = 0.1441, wR_2 = 0.4086
R indices (all data)	R_1 = 0.1648, wR_2 = 0.4273
Largest diff. peak and hole/e Å^{-3}	16.548 and -2.283

Table S 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

Atom	x	y	z	U(eq)
O118	219(3)	3667(4)	608(2)	24(1)
C118	-454(4)	3715(4)	615(3)	23(2)
C218	-658(4)	4129(4)	262(3)	26(2)
F118	-241(3)	4855(3)	442(2)	35(1)
F218	-1392(3)	4013(4)	141(2)	38(1)
F318	-497(3)	3883(3)	-145(2)	29(1)
C318	-1098(4)	2929(4)	465(3)	30(2)
F418	-858(3)	2491(3)	675(2)	36(1)

F518	-1306(3)	2608(3)	-10(2)	38(1)
F618	-1717(3)	2945(4)	574(2)	39(1)
C418	-394(5)	4163(4)	1125(3)	28(2)
F718	-477(3)	3739(3)	1414(2)	37(1)
F818	-922(3)	4452(4)	1118(2)	40(1)
F918	284(3)	4727(3)	1327(2)	32(1)
O117	759(3)	2494(3)	529(2)	22(1)
C117	770(4)	2032(4)	132(3)	24(2)
C217	342(5)	2135(4)	-329(3)	29(2)
F117	-408(3)	1832(3)	-413(2)	39(1)
F217	482(4)	1818(3)	-718(2)	39(1)
F317	538(3)	2853(3)	-283(2)	31(1)
C317	1598(4)	2155(5)	129(3)	30(2)
F417	2047(3)	2282(4)	566(2)	41(1)
F517	1905(3)	2752(3)	-4(2)	34(1)
F617	1626(4)	1573(4)	-173(2)	48(2)
C417	365(5)	1216(4)	127(3)	32(2)
F717	808(4)	1043(3)	446(2)	40(1)
F817	158(4)	708(3)	-297(2)	47(2)
F917	-265(3)	1135(3)	259(2)	40(1)
O116	4433(4)	1957(4)	-1358(2)	26(1)
C116	4009(5)	1896(4)	-1796(3)	26(2)
C216	4565(5)	2196(5)	-2069(3)	45(2)
F116	5130(4)	2851(4)	-1791(3)	67(2)
F216	4234(4)	2311(5)	-2456(3)	64(2)
F316	4893(4)	1734(5)	-2200(3)	59(2)
C316	3500(5)	1070(5)	-2080(3)	35(2)
F416	2877(3)	834(3)	-1948(2)	44(2)
F516	3859(4)	621(4)	-2005(3)	50(2)
F616	3262(4)	955(4)	-2551(2)	57(2)
C416	3502(5)	2344(5)	-1741(3)	31(2)
F716	3145(3)	2195(4)	-1421(2)	39(1)
F816	2960(4)	2174(4)	-2153(2)	45(2)
F916	3912(4)	3067(3)	-1604(3)	55(2)
O115	3681(4)	995(3)	-924(2)	27(1)
C115	3225(5)	568(4)	-727(3)	26(2)
C215	2684(5)	-182(4)	-1129(3)	35(2)
F115	2115(3)	-110(3)	-1421(2)	41(1)
F215	2373(4)	-719(3)	-953(2)	46(2)
F315	3075(3)	-416(3)	-1401(2)	39(1)
C315	3691(5)	399(5)	-316(3)	34(2)
F415	4293(3)	1024(3)	-32(2)	41(1)
F515	3961(4)	-93(4)	-489(2)	45(2)
F615	3291(4)	135(4)	-43(2)	44(2)
C415	2723(4)	948(4)	-535(3)	28(2)
F715	3118(3)	1476(3)	-116(2)	32(1)
F815	2121(3)	462(3)	-469(2)	40(1)
F915	2465(3)	1276(3)	-834(2)	36(1)
O114	4329(3)	2522(3)	-419(2)	25(1)
C114	4682(5)	3203(5)	-77(3)	29(2)
C214	4062(5)	3452(4)	67(3)	33(2)
F114	3489(4)	3286(4)	-324(2)	50(2)
F214	4323(3)	4172(3)	302(2)	39(1)

F314	3766(4)	3077(4)	338(2)	49(2)
C314	5198(5)	3171(5)	378(3)	37(2)
F414	5851(3)	3141(4)	325(3)	53(2)
F514	4856(4)	2558(4)	485(2)	51(2)
F614	5399(4)	3757(4)	767(2)	51(2)
C414	5173(5)	3788(4)	-267(3)	38(2)
F714	5584(4)	3513(4)	-494(3)	59(2)
F814	5655(4)	4427(4)	83(3)	57(2)
F914	4726(4)	3977(4)	-567(2)	56(2)
O112	5324(3)	1810(4)	-570(2)	26(1)
C112	5893(5)	1599(5)	-650(3)	27(2)
C212	6551(5)	2254(5)	-681(3)	35(2)
F112	6292(4)	2601(4)	-961(2)	46(2)
F212	7064(3)	2052(3)	-837(2)	40(1)
F312	6932(4)	2775(4)	-243(2)	60(2)
C312	6197(5)	1345(6)	-228(3)	52(2)
F412	5684(5)	675(5)	-277(3)	74(2)
F512	6258(5)	1798(5)	186(2)	73(2)
F612	6875(4)	1318(4)	-192(2)	51(2)
C412	5611(5)	940(5)	-1129(3)	36(2)
F712	4902(3)	466(3)	-1203(3)	47(2)
F812	6040(4)	540(3)	-1124(3)	49(2)
F912	5603(4)	1201(4)	-1500(2)	49(2)
O113	4810(4)	6310(4)	4363(2)	31(2)
C113	5456(5)	6237(4)	4322(3)	25(2)
C213	6111(5)	7010(5)	4462(3)	36(2)
F113	5861(3)	7460(3)	4267(2)	44(2)
F213	6698(3)	6980(4)	4319(2)	46(2)
F313	6366(4)	7334(4)	4937(2)	48(2)
C313	5675(5)	5812(5)	4665(3)	31(2)
F413	5224(4)	5090(3)	4492(2)	43(1)
F513	5583(3)	6077(4)	5088(2)	39(1)
F613	6390(3)	5884(4)	4740(2)	44(2)
C413	5336(5)	5784(5)	3801(3)	30(2)
F713	4644(3)	5229(3)	3622(2)	40(1)
F813	5839(4)	5484(4)	3772(2)	45(2)
F913	5377(4)	6210(3)	3514(2)	39(1)
O111	1479(4)	9106(4)	5942(2)	30(1)
C111	1951(5)	9514(5)	5749(3)	31(2)
C211	2462(5)	9136(4)	5572(3)	29(2)
F111	2720(3)	8843(3)	5896(2)	38(1)
F211	3054(3)	9607(3)	5497(2)	43(2)
F311	2062(3)	8574(3)	5170(2)	37(1)
C311	1491(5)	9659(5)	5312(3)	40(2)
F411	1205(5)	10159(4)	5464(3)	57(2)
F511	899(4)	9034(4)	5041(2)	51(2)
F611	1898(4)	9892(4)	5035(2)	50(2)
C411	2465(5)	10285(5)	6128(3)	42(2)
F711	2083(4)	10544(3)	6385(2)	46(2)
F811	2788(4)	10802(4)	5936(3)	57(2)
F911	3035(4)	10226(4)	6425(2)	46(2)
O110	741(3)	8197(4)	6406(2)	25(1)
C110	1187(4)	8241(4)	6831(3)	25(2)

C210	668(5)	7958(5)	7130(3)	39(2)
F110	370(4)	8449(4)	7286(2)	49(2)
F210	1021(4)	7830(4)	7507(2)	49(2)
F310	69(4)	7335(4)	6862(2)	52(2)
C310	1665(4)	7766(4)	6753(3)	29(2)
F410	1977(3)	7886(3)	6411(2)	36(1)
F510	1225(4)	7040(3)	6622(2)	48(2)
F610	2224(3)	7916(4)	7149(2)	42(2)
C410	1742(5)	9067(5)	7115(3)	34(2)
F710	2344(3)	9271(3)	6954(2)	39(1)
F810	2003(4)	9180(4)	7580(2)	51(2)
F910	1400(4)	9533(3)	7061(2)	45(2)
O19	-196(11)	8288(13)	5624(9)	29(4)
C19	-750(9)	8532(8)	5690(5)	32(3)
C29	-966(8)	8880(8)	5300(5)	40(3)
F19	-480(9)	9576(8)	5394(6)	55(4)
F29	-1646(9)	8910(11)	5249(10)	47(5)
F39	-965(18)	8500(13)	4872(8)	52(5)
C39	-1459(7)	7841(7)	5638(5)	39(3)
F49	-1253(15)	7417(10)	5872(8)	49(5)
F59	-1807(8)	7428(9)	5182(4)	50(4)
F69	-1967(8)	8046(9)	5806(5)	45(4)
C49	-508(8)	9110(7)	6187(4)	37(3)
F79	-553(13)	8783(11)	6524(6)	43(5)
F89	-933(9)	9512(9)	6209(5)	46(4)
F99	211(8)	9591(11)	6310(6)	41(4)
O18	-126(12)	8401(14)	5611(10)	15(4)
C18	-688(9)	8630(8)	5680(5)	22(3)
C28	-1293(8)	8393(8)	5190(5)	30(3)
F18	-970(20)	8562(15)	4857(10)	44(6)
F28	-1801(11)	8704(12)	5192(12)	35(5)
F38	-1700(9)	7663(7)	5039(5)	35(3)
C38	-1056(8)	8283(9)	6025(5)	29(3)
F48	-626(13)	8626(13)	6481(6)	34(5)
F58	-1157(17)	7571(10)	5937(9)	41(5)
F68	-1732(8)	8330(11)	6002(6)	38(4)
C48	-372(8)	9488(7)	5895(5)	27(3)
F78	296(9)	9741(14)	6232(8)	38(5)
F88	-840(10)	9736(10)	6075(6)	39(4)
F98	-231(10)	9807(9)	5565(5)	37(4)
O17	900(20)	3370(20)	1416(10)	23(5)
C17	1113(11)	3144(11)	1795(7)	23(4)
C27	1976(10)	3314(10)	1932(7)	29(4)
F17	2210(20)	3176(19)	1551(11)	27(6)
F27	2170(20)	2914(14)	2201(9)	25(5)
F37	2400(13)	4027(10)	2189(9)	35(5)
C37	929(10)	3551(10)	2229(6)	27(4)
F47	183(10)	3288(14)	2165(9)	29(5)
F57	1124(18)	4278(13)	2283(15)	33(6)
F67	1276(11)	3499(12)	2639(6)	31(4)
C47	672(11)	2289(10)	1671(6)	30(4)
F77	-54(15)	2090(20)	1437(12)	39(7)
F87	715(17)	2073(14)	2060(7)	40(5)

F97	975(13)	1936(14)	1397(8)	33(5)
O16	1781(3)	3965(3)	801(2)	24(1)
C16	2257(4)	4658(4)	838(3)	22(2)
C26	2988(4)	4592(4)	734(3)	30(2)
F16	3202(3)	4142(3)	942(2)	34(1)
F26	3579(3)	5254(3)	888(2)	39(1)
F36	2849(3)	4309(3)	262(2)	35(1)
C36	1898(4)	4975(4)	472(3)	25(2)
F46	1401(3)	5225(3)	618(2)	35(1)
F56	1511(3)	4448(3)	50(2)	33(1)
F66	2413(3)	5536(3)	398(2)	36(1)
C46	2504(5)	5204(4)	1349(3)	31(2)
F76	1888(3)	5125(3)	1502(2)	36(1)
F86	2807(4)	5921(3)	1374(2)	38(1)
F96	2994(4)	5076(3)	1661(2)	41(1)
O15	4310(4)	7521(3)	4496(2)	28(1)
C15	4383(5)	8014(4)	4905(3)	29(2)
C25	3583(5)	7931(5)	4953(3)	45(2)
F15	3112(4)	7838(5)	4530(3)	64(2)
F25	3616(5)	8532(4)	5271(3)	67(2)
F35	3265(4)	7337(4)	5087(2)	51(2)
C35	4826(5)	7885(5)	5347(3)	31(2)
F45	5569(3)	8137(4)	5404(2)	51(2)
F55	4608(4)	7170(3)	5310(2)	41(1)
F65	4755(4)	8235(4)	5763(2)	48(2)
C45	4816(6)	8807(5)	4899(3)	49(2)
F75	5429(4)	8841(4)	4757(3)	64(2)
F85	5082(5)	9326(4)	5330(2)	72(2)
F95	4356(5)	8990(4)	4599(3)	65(2)
O14	3268(4)	6074(4)	4267(3)	34(2)
C14	2772(4)	5390(5)	4224(3)	26(2)
C24	3122(5)	5049(5)	4571(3)	31(2)
F14	3587(3)	4775(3)	4413(2)	39(1)
F24	2603(4)	4510(4)	4662(2)	47(2)
F34	3557(3)	5571(3)	4994(2)	42(1)
C34	2076(5)	5498(5)	4355(3)	37(2)
F44	1868(4)	5958(4)	4156(2)	46(2)
F54	2244(3)	5784(4)	4833(2)	46(2)
F64	1472(3)	4859(3)	4228(2)	47(2)
C44	2483(5)	4845(5)	3706(3)	35(2)
F74	2003(4)	5017(4)	3416(2)	52(2)
F84	2139(4)	4138(3)	3683(2)	49(2)
F94	3072(4)	4900(4)	3534(2)	47(2)
O13	3999(18)	6581(18)	3577(9)	25(5)
C13	3780(9)	6841(9)	3220(6)	25(3)
C23	3973(8)	6483(8)	2780(5)	30(3)
F13	4715(7)	6734(10)	2831(6)	35(4)
F23	3630(9)	6584(10)	2383(5)	37(4)
F33	3752(13)	5748(10)	2690(11)	32(4)
C33	2917(8)	6668(8)	3087(5)	27(3)
F43	2673(17)	6773(14)	3472(7)	38(2)
F53	2502(10)	5954(8)	2829(7)	38(4)
F63	2710(12)	7070(10)	2831(6)	29(4)

C43	4224(9)	7698(8)	3368(5)	35(4)
F73	3939(11)	8055(9)	3661(6)	45(4)
F83	4162(14)	7963(14)	2999(7)	40(5)
F93	4962(11)	7933(18)	3603(9)	46(6)
O12	949(11)	3434(10)	1417(5)	20(3)
C12	1148(6)	3187(6)	1786(4)	18(2)
C22	1598(6)	3879(6)	2245(4)	29(2)
F12	2299(6)	4221(6)	2235(5)	35(3)
F22	1650(7)	3713(6)	2649(3)	37(2)
F32	1278(9)	4376(7)	2257(7)	35(3)
C32	424(6)	2677(6)	1866(4)	31(3)
F42	-71(8)	2202(12)	1447(6)	42(4)
F52	65(7)	3065(7)	2057(5)	41(3)
F62	580(7)	2278(7)	2148(4)	37(3)
C42	1653(6)	2745(6)	1706(4)	23(2)
F72	1253(6)	2041(6)	1434(4)	35(3)
F82	2069(10)	2710(7)	2109(4)	29(3)
F92	2133(11)	3049(9)	1483(6)	28(3)
O11	3969(16)	6580(15)	3597(8)	27(4)
C11	3762(8)	6854(8)	3246(6)	27(3)
C21	3333(8)	6205(8)	2774(5)	42(3)
F11	3675(13)	5726(11)	2741(10)	55(6)
F21	3285(9)	6426(10)	2389(5)	55(4)
F31	2628(8)	5816(8)	2765(7)	50(4)
C31	3222(7)	7248(7)	3349(4)	32(3)
F41	3596(8)	7941(7)	3656(5)	44(3)
F51	2760(13)	6901(11)	3568(6)	38(2)
F61	2803(11)	7298(8)	2959(5)	35(4)
C41	4482(8)	7427(8)	3203(5)	42(3)
F71	4947(11)	7846(15)	3646(6)	50(5)
F81	4336(11)	7875(12)	2968(7)	41(4)
F91	4847(8)	7064(8)	2989(6)	49(4)
Sn(1)	2413(1)	5286(1)	-2438(1)	24(1)
Sn(2)	7822(1)	9991(1)	7680(1)	31(1)
P(003)	8866(1)	11270(1)	7524(1)	19(1)
P(004)	1418(1)	3794(1)	-2474(1)	19(1)
P(005)	6330(1)	8789(1)	7454(1)	18(1)
P(006)	3811(1)	6375(1)	-2452(1)	19(1)
Al(07)	931(1)	3397(1)	841(1)	16(1)
Al(08)	703(2)	8299(2)	5848(1)	20(1)
Al(09)	4096(1)	6612(1)	4177(1)	18(1)
Al(0A)	4446(2)	1825(1)	-810(1)	20(1)
F(01A)	1639(4)	6862(4)	5290(3)	53(2)
C(1A)	3915(5)	7866(5)	-2192(3)	22(2)
C(1G)	5329(5)	6730(5)	-1901(3)	21(2)
C(1H)	4812(5)	8425(5)	6896(3)	20(2)
C(1I)	6217(5)	7302(5)	7176(3)	21(2)
C(1J)	4043(5)	7317(6)	-1572(3)	26(2)
C(1L)	7154(5)	8600(5)	8237(3)	25(2)
C(1M)	10392(5)	11644(5)	8082(3)	26(2)
O(01Y)	757(3)	7561(3)	5460(2)	26(1)
N(046)	2715(5)	4631(5)	-3110(3)	34(2)
N(049)	3381(4)	5006(5)	-1991(3)	31(2)

N(04E)	2526(6)	5741(6)	-1470(4)	48(2)
N(04N)	7496(5)	9685(5)	6837(3)	39(2)
C(04P)	8964(5)	12119(5)	7949(3)	19(2)
C(04Q)	11027(6)	11472(6)	8203(4)	30(2)
C(04R)	8936(5)	12746(5)	7825(3)	22(2)
C(04V)	6202(5)	7914(5)	7040(3)	19(2)
C(04W)	1344(5)	2318(5)	-2782(3)	26(2)
C(04X)	1184(5)	2923(5)	-3381(3)	26(2)
C(04Y)	6134(5)	7886(5)	6564(3)	21(2)
C(050)	9759(5)	11148(5)	7682(3)	21(2)
C(052)	8998(5)	12105(5)	8416(3)	24(2)
C(053)	5452(5)	8919(5)	7294(3)	21(2)
C(054)	8739(5)	11418(5)	6942(3)	20(2)
C(055)	-735(5)	3599(5)	-3141(4)	28(2)
C(056)	5962(5)	6566(5)	-1775(3)	26(2)
C(05A)	3657(5)	6449(5)	-3059(3)	22(2)
C(05B)	6478(5)	8681(5)	8047(3)	20(2)
C(05C)	6062(6)	7229(6)	6229(3)	30(2)
C(05D)	1544(5)	3656(5)	-1886(3)	21(2)
C(05E)	1299(5)	2940(5)	-2902(3)	23(2)
C(05F)	-112(5)	3420(5)	-3029(3)	23(2)
C(05G)	2200(5)	3570(5)	-1688(3)	26(2)
C(05H)	4171(6)	8597(6)	6784(4)	29(2)
C(05J)	2965(5)	6503(5)	-3249(3)	27(2)
C(05K)	2599(5)	4511(5)	-3506(3)	28(2)
C(05L)	3953(5)	7257(5)	-2053(3)	20(2)
C(05N)	523(5)	3917(5)	-2633(3)	23(2)
C(05O)	8061(5)	11490(5)	6741(3)	26(2)
C(05Q)	8993(6)	13342(5)	8630(3)	30(2)
C(05R)	4137(5)	6389(5)	-3320(3)	24(2)
C(05T)	4678(5)	6237(5)	-2292(3)	21(2)
C(05U)	6090(6)	6629(6)	6380(4)	31(2)
N(05V)	7511(7)	10559(6)	8553(4)	54(3)
C(05X)	8950(5)	13355(5)	8170(3)	25(2)
C(05Y)	9033(6)	12728(5)	8766(3)	28(2)
C(05Z)	6164(5)	6660(5)	6840(3)	28(2)
C(060)	4141(6)	7977(6)	-1236(4)	33(2)
C(061)	4771(5)	9723(6)	7438(4)	29(2)
C(062)	1109(6)	2277(6)	-3734(4)	35(2)
C(063)	5417(5)	9578(5)	7555(3)	22(2)
C(064)	4712(6)	5573(5)	-2547(3)	27(2)
C(065)	-123(6)	4746(6)	-2483(4)	31(2)
C(066)	5340(6)	5403(6)	-2432(4)	32(2)
C(067)	1180(6)	3600(5)	-1175(3)	30(2)
C(068)	9066(6)	11447(5)	6213(3)	32(2)
C(069)	2537(5)	5642(6)	-1116(4)	34(2)
C(06A)	3941(6)	6405(5)	-3800(3)	29(2)
N(06B)	8194(6)	8800(6)	7323(4)	47(2)
C(06C)	4157(6)	9234(6)	7051(4)	33(2)
C(06E)	7336(5)	8568(5)	8704(3)	27(2)
C(06I)	1031(5)	3668(5)	-1631(3)	25(2)
C(06K)	6186(6)	8712(5)	8785(3)	28(2)
C(06M)	4094(6)	8553(6)	-1391(3)	30(2)

C(06N)	5977(6)	5906(5)	-2046(4)	29(2)
C(06O)	10406(6)	10313(6)	7546(4)	36(2)
C(06P)	9230(5)	11380(5)	6669(3)	26(2)
C(06Q)	398(6)	6878(5)	5127(4)	33(2)
C(06R)	3990(5)	8510(5)	-1868(3)	25(2)
C(06T)	7906(6)	11558(6)	6297(4)	36(2)
C(06U)	7407(6)	9623(6)	6432(4)	38(2)
C(06V)	513(5)	4586(5)	-2361(3)	25(2)
C(06X)	1149(5)	1669(5)	-3599(3)	30(2)
C(071)	1255(5)	1693(6)	-3127(3)	30(2)
C(073)	5993(5)	8738(5)	8319(3)	25(2)
C(077)	7727(6)	10563(6)	8951(4)	39(2)
C(078)	-769(6)	4230(6)	-2878(4)	32(2)
C(079)	9766(6)	10486(5)	7427(4)	28(2)
C(07F)	2778(6)	6510(6)	-3721(3)	34(2)
C(07H)	2355(6)	3492(5)	-1232(4)	34(2)
C(07I)	11034(6)	10823(6)	7936(4)	33(2)
C(07L)	3258(6)	6452(6)	-3995(3)	35(2)
C(07R)	3199(7)	2431(6)	-3331(4)	49(3)
N(07U)	1253(6)	4948(6)	-3340(4)	53(3)
C(07W)	8411(6)	11544(6)	6020(4)	37(2)
C(07X)	6858(6)	8631(5)	8981(3)	31(2)
C(07Y)	3888(6)	4930(6)	-1791(4)	29(2)
C(080)	4568(6)	4843(6)	-1527(4)	35(2)
C(082)	2541(6)	5525(6)	-663(4)	36(2)
C(083)	1836(6)	3515(5)	-976(3)	33(2)
C(084)	8168(6)	8242(6)	7113(4)	37(2)
C(087)	2418(7)	4367(7)	-4021(4)	46(3)
C(088)	7285(6)	9564(6)	5941(4)	41(3)
C(08B)	747(6)	5113(6)	-3440(4)	37(2)
C(08D)	1896(7)	6976(6)	-2020(5)	46(3)
C(08F)	2019(7)	7563(7)	-1597(4)	46(3)
C(08G)	8148(7)	7521(6)	6852(4)	43(3)
C(08N)	3474(7)	3140(6)	-2931(4)	45(3)
C(08Q)	7982(7)	10568(7)	9424(4)	51(3)
C(08U)	4781(6)	10243(7)	6262(5)	46(3)
C(08W)	-374(7)	-47(8)	-1387(5)	53(3)
C(08X)	5549(7)	10232(8)	6359(4)	53(3)
C(08Z)	147(7)	5345(8)	-3551(5)	53(3)
N(091)	3693(9)	3674(7)	-2631(4)	77(4)
N(092)	-883(8)	102(10)	-1446(5)	92(5)
C(094)	931(7)	6436(6)	5194(5)	49(2)
C(096)	147(10)	6920(7)	4632(4)	64(3)
N(098)	1814(11)	6530(8)	-2361(5)	100(6)
C(099)	297(8)	-252(9)	-1305(5)	61(3)
C(09A)	-359(8)	6412(7)	5207(5)	60(3)
N(09B)	6128(7)	10224(9)	6409(5)	79(4)
F(12I)	924(6)	7105(5)	4526(3)	92(3)
F(13I)	-271(5)	6322(4)	4294(2)	65(2)
F(14I)	70(7)	7504(5)	4594(3)	101(3)
F(15I)	727(4)	5857(4)	4796(3)	56(2)
F(16I)	858(6)	6190(5)	5587(3)	84(3)
F(17I)	-613(4)	5698(4)	4987(3)	61(2)

F(18I)	-932(5)	6619(5)	5027(4)	89(3)
F(19I)	-310(5)	6559(5)	5661(3)	76(2)
N(4)	7124(5)	10747(5)	7556(3)	37(2)
C(5)	7011(5)	11283(6)	7718(4)	29(2)
C(6)	6887(7)	11926(7)	7946(5)	46(3)

Quantum chemical calculations

RI-DFT[6] calculations were performed using TURBOMOLE with the def-SV(P) basis set[7] and the BP86 functional.[8] The structure of all compounds was optimized in the highest possible symmetry, and the AOFORCE module[9] was used for frequency analysis to verify that a minimum structure was found.

Table S 3. Summary of calculated thermodynamic data.

Compound	scf energy in Ha	FREEH energy in kJ mol^{-1}	FREEH entropy in kJ mol^{-1} K^{-1}	symmetry	grid
$[Sn(MeCN)_6]^{2+}$	-798.9973673565	788.81	1.06018	C_1	m4
$[Sn(MeCN)_4]^{2+}$	-533.6104126954	525.28	0.74324	C_1	m4
$[SnCp]^+$	-196.5909988394	225.09	0.31142	C_{5v}	m3
$[SnCp]^+$	-196.5910007758	225.06	0.31140	C_{5v}	m4
$[SnCp]^+$	-196.5910019806	225.06	0.31139	C_{5v}	m5
$SnCp_2$	-390.2294453744	446.34	0.46946	C_{2v}	m3
$SnCp_2$	-390.2294375904	446.35	0.46958	C_{2v}	m4
$SnCp_2$	-390.2294404350	446.37	0.46849	C_{2v}	m5
$[SiCp^*]^+$	-679.0522806654	599.51	0.46063	C_{5v}	m4
$SiCp^*_2$	-1069.1118380710	1190.99	0.78479	C_2	m4
$[GeCp^*]^+$	-2466.6703413790	597.82	0.46876	C_{5v}	m3
$GeCp^*_2$	-2856.7327156550	1189.85	0.79912	C_2	m3
$[SnCp^*]^+$	-393.0660474076	596.63	0.47572	C_{5v}	m3
$SnCp^*_2$	-783.1308610327	1188.97	0.79118	C_2	m3
$[PbCp^*]^+$	-393.1223661609	596.14	0.48358	C_{5v}	m3
$PbCp^*_2$	-783.1823255534	1188.12	0.79869	C_2	m3
dmap	-382.0092380830	432.60	0.37746	C_{2v}	m3
dmap	-382.0091908487	432.32	0.37946	C_{2v}	m4
$[Si(dmap)_4]^{2+}$	-1817.1723376240	1774.50	1.06149	C_1	m4
$[Ge(dmap)_4]^{2+}$	-3604.7797763750	1772.47	1.09044	C_1	m3
$[Sn(dmap)_4]^{2+}$	-1531.1823293770	1771.24	1.12262	C_1	m3
$[Pb(dmap)_4]^{2+}$	-1531.2330891060	1771.17	1.13659	C_1	m3
$[Sn(PPh_3)_3]^{2+}$	-3110.5537647700	2242.66	1.30328	C_1	m3
PPh_3	-1035.8150092950	736.42	0.55178	C_3	m3
$[Sn(bipy)_3]^{2+}$	-1488.3292388510	1302.31	0.90234	C_1	m3
bipy	-495.0784117433	423.69	0.38562	C_{2h}	m3
$[Sn(py)_4]^{2+}$	-995.5449933171	983.41	0.75904	C_1	m5
pyridine	-248.1218832667	236.09	0.28393	C_{2v}	m5
$[Sn(pyr)_4]^{2+}$	-1059.5811034010	856.63	0.76905	C_1	m3
$[Sn(pyr)_2(MeCN)_4]^{2+}$	-1061.9922830330	954.56	1.03512	C_1	m4
pyrazine	-264.1472446515	205.45	0.27705	D_{2h}	m3
pyrazine	-264.1472268346	205.42	0.27703	D_{2h}	m4
$[Sn(mes)_3]^{2+}$	-1052.8576457580	1489.15	0.92151	C_1	m4
mesitylene	-349.9612642343	487.82	0.42135	C_{3h}	m4
$[Sn(C_7H_8)_3]^{2+}$	-817.0835292267	1046.69	0.73663	C_1	m3
toluene	-271.3827411380	340.25	0.34513	C_S	m3

acetonitrile	-132.6566392103	123.78	0.24378	C_{3v}	m4

$[Sn(MeCN)_6]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

1.01464751617236	0.22570082077185	-0.66229468620062	sn
-1.20814930441499	-3.63402003371583	0.63339109136137	n
-1.99429626975736	-5.64698564730789	1.07155793166353	c
-2.98121938608327	-8.14814649380564	1.62268255237933	c
-5.04394803776993	-8.04502086597663	2.00854850348129	h
-2.01471742788493	-8.95092760860742	3.30636341780262	h
-2.66132605742326	-9.42410054604859	-0.01555320710428	h
-3.44384315240002	1.39589960955338	-1.17294230488289	n
-5.44822064764128	2.12465673112305	-1.73290835876325	c
-7.94740878751381	3.02697584295513	-2.42086705635341	c
-7.96475892496471	5.12710158775696	-2.47668384246148	h
-9.36661666643855	2.37392310933225	-1.01622044208304	h
-8.48132121867863	2.29347276768403	-4.31574763220341	h
-0.39340275840806	-2.01471771566482	-5.13776928779388	n
0.08511106755887	-3.53316037404832	-9.83823477800267	c
2.06204130329786	-3.25278104094430	-10.49069967950897	h
-1.19816384282801	-2.43908678117267	-11.09097724690770	h
-0.39410439736364	-5.57197497945923	-9.99825729787245	h
-0.17859784817808	-2.69053638133511	-7.23284365950501	c
-0.29652366495133	1.19546012645298	3.67841253123989	n
-0.95478987476114	2.57528907922894	8.38616118215558	c
-3.00533699307479	2.75372663645820	8.80679838848687	h
-0.02860016449941	4.42946353769652	8.73064744482439	h
-0.11761443624709	1.14817002637493	9.68081679352810	h
-0.58551333652286	1.81223069167020	5.77550868926555	c
1.02945105682785	5.41820273851447	-0.44075054973530	n
2.65356045943182	10.03222039273217	-1.27848213505422	c
2.92648520148331	10.34107141493625	-3.33842762828905	h
4.48849785242580	10.34244690184594	-0.30395380642979	h
1.26479178473382	11.43678944570632	-0.56423046097262	h
1.75507903009310	7.47378354315906	-0.81544259855701	c
4.45548516665033	-2.29260450747665	2.30868216082056	n
8.89628465094468	-4.01700121292627	3.69981712030703	c
10.23315777240934	-3.96242083349572	2.08034562486619	h
8.73101398759784	-6.00072788326993	4.37025167428205	h
9.67720121963966	-2.84227222486396	5.25639075395321	h
6.43566512853860	-3.06009987383360	2.92691079826366	c

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules IR	RAMAN
7	a	9.22	0.00472	YES	YES
8	a	10.77	0.06525	YES	YES
9	a	11.25	0.01652	YES	YES

10	a	14.90	0.26427	YES	YES
11	a	16.20	0.36234	YES	YES
12	a	16.54	0.14071	YES	YES
13	a	17.38	0.05505	YES	YES
14	a	18.31	0.05454	YES	YES
15	a	23.27	0.00353	YES	YES
16	a	25.29	2.90538	YES	YES
17	a	27.19	1.49051	YES	YES
18	a	27.32	1.18866	YES	YES
19	a	31.48	6.68598	YES	YES
20	a	31.60	6.46443	YES	YES
21	a	34.12	8.16507	YES	YES
22	a	53.99	0.00358	YES	YES
23	a	57.43	0.39035	YES	YES
24	a	57.63	0.39304	YES	YES
25	a	66.00	1.09592	YES	YES
26	a	66.41	1.01006	YES	YES
27	a	88.31	0.35223	YES	YES
28	a	88.69	0.39600	YES	YES
29	a	90.33	7.79662	YES	YES
30	a	113.15	0.00451	YES	YES
31	a	133.90	1.76874	YES	YES
32	a	140.62	12.47030	YES	YES
33	a	141.19	13.80032	YES	YES
34	a	154.46	16.25246	YES	YES
35	a	154.75	15.51424	YES	YES
36	a	160.64	22.62058	YES	YES
37	a	172.56	109.82646	YES	YES
38	a	172.69	109.41281	YES	YES
39	a	245.84	55.81622	YES	YES
40	a	385.43	0.02681	YES	YES
41	a	385.66	0.16012	YES	YES
42	a	385.86	0.16740	YES	YES
43	a	387.23	0.86528	YES	YES
44	a	387.74	0.51660	YES	YES
45	a	388.32	0.13157	YES	YES
46	a	391.61	0.32831	YES	YES
47	a	391.70	0.48781	YES	YES
48	a	392.19	9.93297	YES	YES
49	a	392.56	11.32973	YES	YES
50	a	393.65	0.83604	YES	YES
51	a	399.81	13.98210	YES	YES
52	a	937.54	12.54935	YES	YES
53	a	937.60	12.66346	YES	YES
54	a	940.04	6.50324	YES	YES
55	a	949.81	13.88432	YES	YES
56	a	949.86	13.90806	YES	YES
57	a	954.51	14.19129	YES	YES
58	a	1010.66	0.13272	YES	YES
59	a	1011.04	13.39278	YES	YES
60	a	1011.47	5.25083	YES	YES
61	a	1011.54	8.64468	YES	YES
62	a	1011.83	1.61073	YES	YES

63	a	1012.21	14.12333	YES	YES
64	a	1013.28	6.42332	YES	YES
65	a	1013.41	9.41827	YES	YES
66	a	1013.66	7.81757	YES	YES
67	a	1014.25	9.49948	YES	YES
68	a	1014.41	3.82740	YES	YES
69	a	1014.59	10.31303	YES	YES
70	a	1346.22	9.08797	YES	YES
71	a	1346.43	8.96790	YES	YES
72	a	1346.94	12.50630	YES	YES
73	a	1348.95	8.16000	YES	YES
74	a	1349.08	8.13085	YES	YES
75	a	1349.46	4.72473	YES	YES
76	a	1390.06	1.05964	YES	YES
77	a	1390.33	33.15513	YES	YES
78	a	1390.44	0.30958	YES	YES
79	a	1390.65	38.58475	YES	YES
80	a	1390.77	29.56713	YES	YES
81	a	1390.95	16.61667	YES	YES
82	a	1394.79	7.46173	YES	YES
83	a	1394.84	26.88086	YES	YES
84	a	1395.02	29.75900	YES	YES
85	a	1395.08	16.73647	YES	YES
86	a	1395.19	18.13211	YES	YES
87	a	1395.35	22.70355	YES	YES
88	a	2294.93	146.06858	YES	YES
89	a	2295.06	147.51970	YES	YES
90	a	2297.35	116.10224	YES	YES
91	a	2323.70	187.81523	YES	YES
92	a	2323.92	187.05952	YES	YES
93	a	2327.91	162.22702	YES	YES
94	a	2960.21	13.44184	YES	YES
95	a	2960.33	13.66006	YES	YES
96	a	2960.48	15.56028	YES	YES
97	a	2960.73	9.39128	YES	YES
98	a	2960.80	9.38044	YES	YES
99	a	2960.88	3.63547	YES	YES
100	a	3057.17	6.25310	YES	YES
101	a	3057.40	6.02327	YES	YES
102	a	3057.46	6.54674	YES	YES
103	a	3057.90	8.77169	YES	YES
104	a	3058.08	8.41867	YES	YES
105	a	3058.22	5.76368	YES	YES
106	a	3058.32	6.88702	YES	YES
107	a	3058.40	6.60340	YES	YES
108	a	3058.52	9.76643	YES	YES
109	a	3058.69	9.82514	YES	YES
110	a	3058.76	5.29582	YES	YES
111	a	3058.84	12.71465	YES	YES

$[Sn(MeCN)_4]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

2.91059351718369	1.20718454951449	-0.22490657491130	sn
1.13670490545037	-2.64841541716135	0.96005616204170	n
0.62010099628725	-4.69391198425105	1.61071412460143	c
-0.03814596068502	-7.22478575128085	2.41569847894480	c
-2.08675170882457	-7.32125711569589	2.88047055430422	h
1.07649519769569	-7.74564359461437	4.12141732096590	h
0.38220118541456	-8.59894949393777	0.88064425270472	h
-1.19929962208343	2.62082785725570	-0.94976611809772	n
-3.08480311505767	3.66903357802580	-1.41942337295454	c
-5.43048725489163	4.95400472849666	-1.99610182740936	c
-5.14241463889745	7.03598734323840	-1.91479357419937	h
-6.90875241736324	4.41297174920790	-0.60195363502347	h
-6.08258864134880	4.42996479963456	-3.92512669740521	h
2.02554114952934	-0.70770754008262	-4.41686451593752	n
2.59706755576893	-2.16289306808312	-9.11648429887510	c
4.58743728140103	-1.86589851355193	-9.72589402767224	h
1.32951621890139	-1.05320333565467	-10.37357779055009	h
2.12560206671524	-4.20281878418894	-9.30217259875521	h
2.28698283596102	-1.35472603287904	-6.51553350713803	c
1.50124309999021	2.17026240965385	4.14544260532426	n
1.47570178467693	3.85497826476620	8.80278799168406	c
-0.50140637456626	4.15092604333943	9.45190416692054	h
2.51147991179119	5.68129931770182	8.91395184788664	h
2.41142297440967	2.46772921415202	10.07527346495314	h
1.49655905254155	2.92504077639469	6.22423756859767	c

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules IR	RAMAN
7	a	7.18	0.01086	YES	YES
8	a	13.08	0.01209	YES	YES
9	a	19.56	0.03973	YES	YES
10	a	21.37	0.01995	YES	YES
11	a	23.35	0.13456	YES	YES
12	a	28.53	4.04288	YES	YES
13	a	35.63	0.01412	YES	YES
14	a	38.04	3.91923	YES	YES
15	a	38.34	11.69687	YES	YES
16	a	79.02	0.00514	YES	YES
17	a	79.47	0.19386	YES	YES
18	a	86.86	7.72226	YES	YES
19	a	105.47	1.67598	YES	YES
20	a	115.00	8.77472	YES	YES
21	a	146.58	9.31282	YES	YES
22	a	149.97	10.83587	YES	YES
23	a	163.30	0.00118	YES	YES
24	a	191.09	3.20096	YES	YES

25	a	191.77	125.59615	YES	YES
26	a	219.06	38.71397	YES	YES
27	a	260.49	52.19242	YES	YES
28	a	394.20	0.24544	YES	YES
29	a	394.68	0.21567	YES	YES
30	a	395.91	0.35290	YES	YES
31	a	398.94	2.37028	YES	YES
32	a	400.89	0.10474	YES	YES
33	a	402.08	0.36669	YES	YES
34	a	404.18	18.02154	YES	YES
35	a	410.56	18.19865	YES	YES
36	a	946.02	29.08291	YES	YES
37	a	949.30	0.01012	YES	YES
38	a	958.36	17.78288	YES	YES
39	a	958.76	14.15519	YES	YES
40	a	1003.88	6.84508	YES	YES
41	a	1004.40	11.97576	YES	YES
42	a	1004.93	3.84375	YES	YES
43	a	1005.29	16.35359	YES	YES
44	a	1006.45	12.15471	YES	YES
45	a	1006.91	13.05670	YES	YES
46	a	1008.25	11.11672	YES	YES
47	a	1008.29	10.12497	YES	YES
48	a	1339.35	20.22016	YES	YES
49	a	1339.61	12.63953	YES	YES
50	a	1342.32	25.61630	YES	YES
51	a	1342.55	0.19412	YES	YES
52	a	1378.19	17.90874	YES	YES
53	a	1378.44	27.59986	YES	YES
54	a	1378.63	9.65406	YES	YES
55	a	1378.89	33.90302	YES	YES
56	a	1383.11	19.72809	YES	YES
57	a	1383.13	28.56138	YES	YES
58	a	1383.21	28.41890	YES	YES
59	a	1383.65	22.54780	YES	YES
60	a	2294.39	533.37507	YES	YES
61	a	2297.54	18.70481	YES	YES
62	a	2312.41	420.71811	YES	YES
63	a	2316.97	184.03909	YES	YES
64	a	2952.78	51.46226	YES	YES
65	a	2953.04	22.55649	YES	YES
66	a	2955.43	55.23632	YES	YES
67	a	2955.65	4.14529	YES	YES
68	a	3051.04	20.16773	YES	YES
69	a	3051.71	20.00335	YES	YES
70	a	3053.07	19.64046	YES	YES
71	a	3053.23	14.45419	YES	YES
72	a	3053.34	16.86452	YES	YES
73	a	3053.61	19.68177	YES	YES
74	a	3055.35	15.35098	YES	YES
75	a	3055.60	14.60699	YES	YES

$[SnCp]^+$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

3.55112979413013	-2.58004681790247	-0.42289127286991	h
3.55112979413013	2.58004681790247	-0.42289127286991	h
1.87086817930654	-1.35926529655815	-0.34872226984974	c
1.87086817930654	1.35926529655815	-0.34872226984974	c
0.00000000000000	0.00000000000000	3.85806771359804	sn
-1.35641088289529	-4.17460344393221	-0.42289127286991	h
-0.71460805602445	-2.19933744955930	-0.34872226984974	c
-0.71460805602445	2.19933744955930	-0.34872226984974	c
-2.31252024656414	0.00000000000000	-0.34872226984974	c
-1.35641088289529	4.17460344393221	-0.42289127286991	h
-4.38943782246968	0.00000000000000	-0.42289127286991	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a1	215.20	12.07641	YES	YES
8	e1	231.92	0.73787	YES	YES
9	e1	231.92	0.73787	YES	YES
10	e2	570.07	0.00000	NO	YES
11	e2	570.07	0.00000	NO	YES
12	e2	817.49	0.00000	NO	YES
13	e2	817.49	0.00000	NO	YES
14	a1	821.71	155.80532	YES	YES
15	e1	830.89	0.36566	YES	YES
16	e1	830.89	0.36566	YES	YES
17	e2	906.46	0.00000	NO	YES
18	e2	906.46	0.00000	NO	YES
19	e1	996.65	10.29031	YES	YES
20	e1	996.65	10.29031	YES	YES
21	e2	1049.47	0.00000	NO	YES
22	e2	1049.47	0.00000	NO	YES
23	a1	1100.11	17.50824	YES	YES
24	a2	1244.41	0.00000	NO	NO
25	e2	1351.65	0.00000	NO	YES
26	e2	1351.65	0.00000	NO	YES
27	e1	1416.50	25.83464	YES	YES
28	e1	1416.50	25.83464	YES	YES
29	e2	3155.45	0.00000	NO	YES
30	e2	3155.45	0.00000	NO	YES
31	e1	3166.80	28.33362	YES	YES
32	e1	3166.80	28.33362	YES	YES
33	a1	3175.55	0.09617	YES	YES

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

3.55132434436863	-2.58018816692456	-0.42300389015083	h
3.55132434436863	2.58018816692456	-0.42300389015083	h
1.87101305252046	-1.35937055310924	-0.34862075722051	c
1.87101305252046	1.35937055310924	-0.34862075722051	c
0.00000000000000	-0.00000000000000	3.85812323685776	sn
-1.35648519447388	-4.17483215145424	-0.42300389015083	h
-0.71466339266813	-2.19950775823650	-0.34862075722051	c
-0.71466339266813	2.19950775823650	-0.34862075722051	c
-2.31269931970468	0.00000000000000	-0.34862075722051	c
-1.35648519447388	4.17483215145424	-0.42300389015083	h
-4.38967829978950	0.00000000000000	-0.42300389015083	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a1	215.50	12.03740	YES	YES
8	e1	232.13	0.73303	YES	YES
9	e1	232.13	0.73303	YES	YES
10	e2	570.05	0.00000	NO	YES
11	e2	570.05	0.00000	NO	YES
12	e2	818.26	0.00000	NO	YES
13	e2	818.26	0.00000	NO	YES
14	a1	821.33	156.09523	YES	YES
15	e1	830.37	0.37163	YES	YES
16	e1	830.37	0.37163	YES	YES
17	e2	905.91	0.00000	NO	YES
18	e2	905.91	0.00000	NO	YES
19	e1	996.37	10.30456	YES	YES
20	e1	996.37	10.30456	YES	YES
21	e2	1049.19	0.00000	NO	YES
22	e2	1049.19	0.00000	NO	YES
23	a1	1100.06	17.64022	YES	YES
24	a2	1243.85	0.00000	NO	NO
25	e2	1351.55	0.00000	NO	YES
26	e2	1351.55	0.00000	NO	YES
27	e1	1416.15	25.83786	YES	YES
28	e1	1416.15	25.83786	YES	YES
29	e2	3155.20	0.00000	NO	YES
30	e2	3155.20	0.00000	NO	YES
31	e1	3166.53	28.30576	YES	YES
32	e1	3166.53	28.30576	YES	YES
33	a1	3175.28	0.09734	YES	YES

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m5).

3.55136871990126	-2.58022040763621	-0.42293165705950	h
3.55136871990126	2.58022040763621	-0.42293165705950	h
1.87106050036550	-1.35940502598652	-0.34874570051491	c
1.87106050036550	1.35940502598652	-0.34874570051491	c
-0.00000000000000	0.00000000000000	3.85838678787199	sn
-1.35650214441908	-4.17488431802151	-0.42293165705950	h
-0.71468151613223	-2.19956353652364	-0.34874570051491	c
-0.71468151613223	2.19956353652364	-0.34874570051491	c
-2.31275796846652	0.00000000000000	-0.34874570051491	c
-1.35650214441908	4.17488431802151	-0.42293165705950	h
-4.38973315096435	0.00000000000000	-0.42293165705950	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m5).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a1	215.62	12.06256	YES	YES
8	e1	232.17	0.73251	YES	YES
9	e1	232.17	0.73251	YES	YES
10	e2	570.08	0.00000	NO	YES
11	e2	570.08	0.00000	NO	YES
12	e2	818.32	0.00000	NO	YES
13	e2	818.32	0.00000	NO	YES
14	a1	821.38	155.93495	YES	YES
15	e1	830.40	0.37041	YES	YES
16	e1	830.40	0.37041	YES	YES
17	e2	905.92	0.00000	NO	YES
18	e2	905.92	0.00000	NO	YES
19	e1	996.34	10.30179	YES	YES
20	e1	996.34	10.30179	YES	YES
21	e2	1049.19	0.00000	NO	YES
22	e2	1049.19	0.00000	NO	YES
23	a1	1099.95	17.52117	YES	YES
24	a2	1243.92	0.00000	NO	NO
25	e2	1351.40	0.00000	NO	YES
26	e2	1351.40	0.00000	NO	YES
27	e1	1416.00	25.82554	YES	YES
28	e1	1416.00	25.82554	YES	YES
29	e2	3155.26	0.00000	NO	YES
30	e2	3155.26	0.00000	NO	YES
31	e1	3166.58	28.31537	YES	YES
32	e1	3166.58	28.31537	YES	YES
33	a1	3175.33	0.09518	YES	YES

$SnCp_2$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

0.00000000000000	0.00000000000000	1.13567940840445	sn
4.00117320281477	1.35748606348403	-1.79173173769937	c
4.00117320281477	-1.35748606348403	-1.79173173769937	c
4.91534655272326	-2.18424490383775	0.62191244057796	c
5.47655338033423	0.00000000000000	2.09713591065016	c
4.91534655272326	2.18424490383775	0.62191244057796	c
-4.00117320281477	1.35748606348403	-1.79173173769937	c
-4.00117320281477	-1.35748606348403	-1.79173173769937	c
-4.91534655272326	-2.18424490383775	0.62191244057796	c
-5.47655338033423	0.00000000000000	2.09713591065016	c
-4.91534655272326	2.18424490383775	0.62191244057796	c
-6.20908177053388	0.00000000000000	4.04119117550216	h
-5.17147826990381	-4.15990675232116	1.21205527595193	h
-3.49522449202987	-2.57825306597651	-3.39531937400778	h
-5.17147826990381	4.15990675232116	1.21205527595193	h
-3.49522449202987	2.57825306597651	-3.39531937400778	h
5.17147826990381	4.15990675232116	1.21205527595193	h
6.20908177053388	0.00000000000000	4.04119117550216	h
5.17147826990381	-4.15990675232116	1.21205527595193	h
3.49522449202987	-2.57825306597651	-3.39531937400778	h
3.49522449202987	2.57825306597651	-3.39531937400778	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number	IR intensity	selection rules	
		[cm^{-1}]	[km mol^{-1}]	IR	RAMAN
7	a2	9.95	0.00000	NO	YES
8	b2	11.08	0.12029	YES	YES
9	a1	33.70	0.36890	YES	YES
10	a1	143.69	3.12841	YES	YES
11	b2	152.69	4.34929	YES	YES
12	b1	196.42	16.94840	YES	YES
13	a2	206.55	0.00000	NO	YES
14	b1	221.98	113.34776	YES	YES
15	a1	326.49	1.59685	YES	YES
16	a2	568.95	0.00000	NO	YES
17	b2	578.69	0.05338	YES	YES
18	b1	590.36	0.05309	YES	YES
19	a1	593.88	0.03652	YES	YES
20	a1	744.67	0.65996	YES	YES
21	b2	747.24	2.34132	YES	YES
22	b1	748.89	147.32406	YES	YES
23	a2	754.80	0.00000	NO	YES
24	b1	758.65	246.95276	YES	YES
25	a1	767.88	34.90111	YES	YES
26	a2	817.61	0.00000	NO	YES
27	b2	821.34	0.10206	YES	YES
28	b1	822.46	0.88125	YES	YES

29	a1	825.33	0.03828	YES	YES
30	a2	843.73	0.00000	NO	YES
31	b2	854.20	0.15225	YES	YES
32	b1	865.62	0.01348	YES	YES
33	a1	869.36	0.17190	YES	YES
34	b2	995.02	25.58128	YES	YES
35	a2	995.06	0.00000	NO	YES
36	b1	996.48	10.78563	YES	YES
37	a1	997.16	22.05067	YES	YES
38	b1	1036.59	1.44544	YES	YES
39	a2	1038.32	0.00000	NO	YES
40	a1	1042.21	0.33095	YES	YES
41	b2	1043.31	0.27510	YES	YES
42	b1	1123.57	19.38402	YES	YES
43	a1	1130.26	0.45805	YES	YES
44	a2	1241.45	0.00000	NO	YES
45	b2	1241.60	0.00206	YES	YES
46	a2	1350.70	0.00000	NO	YES
47	b1	1356.29	1.31805	YES	YES
48	a1	1367.97	0.04960	YES	YES
49	b2	1371.48	0.03962	YES	YES
50	b2	1426.19	10.27891	YES	YES
51	a1	1430.04	7.71023	YES	YES
52	a2	1432.30	0.00000	NO	YES
53	b1	1434.26	1.45739	YES	YES
54	b1	3129.27	0.00041	YES	YES
55	a1	3129.44	0.16787	YES	YES
56	a2	3129.48	0.00000	NO	YES
57	b2	3129.93	0.45507	YES	YES
58	a2	3145.22	0.00000	NO	YES
59	b2	3145.44	12.01070	YES	YES
60	b1	3146.03	1.10893	YES	YES
61	a1	3146.41	10.03264	YES	YES
62	b1	3157.40	18.09795	YES	YES
63	a1	3158.05	0.06088	YES	YES

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

0.00000000000000	0.00000000000000	1.13636630636963	sn
4.00073359299039	1.35762371946920	-1.79168523133046	c
4.00073359299039	-1.35762371946920	-1.79168523133046	c
4.91543056268125	-2.18431648166515	0.62203406942195	c
5.47655121648959	0.00000000000000	2.09728657003280	c
4.91543056268125	2.18431648166515	0.62203406942195	c
-4.00073359299039	1.35762371946920	-1.79168523133046	c
-4.00073359299039	-1.35762371946920	-1.79168523133046	c
-4.91543056268125	-2.18431648166515	0.62203406942195	c
-5.47655121648959	0.00000000000000	2.09728657003280	c
-4.91543056268125	2.18431648166515	0.62203406942195	c
-6.21114054610822	0.00000000000000	4.04075250386233	h
-5.17223774054751	-4.16009943231423	1.21159906987899	h
-3.49357288125337	-2.57820227990279	-3.39505902151045	h
-5.17223774054751	4.16009943231423	1.21159906987899	h

-3.49357288125337	2.57820227990279	-3.39505902151045	h
5.17223774054751	4.16009943231423	1.21159906987899	h
6.21114054610822	0.00000000000000	4.04075250386233	h
5.17223774054751	-4.16009943231423	1.21159906987899	h
3.49357288125337	-2.57820227990279	-3.39505902151045	h
3.49357288125337	2.57820227990279	-3.39505902151045	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a2	9.99	0.00000	NO	YES
8	b2	10.58	0.11991	YES	YES
9	a1	34.61	0.37514	YES	YES
10	a1	143.98	3.12445	YES	YES
11	b2	152.25	4.35606	YES	YES
12	b1	196.63	16.71192	YES	YES
13	a2	206.21	0.00000	NO	YES
14	b1	221.86	113.43112	YES	YES
15	a1	326.54	1.59106	YES	YES
16	a2	568.85	0.00000	NO	YES
17	b2	578.69	0.05321	YES	YES
18	b1	590.15	0.05299	YES	YES
19	a1	593.67	0.03589	YES	YES
20	a1	745.43	0.48322	YES	YES
21	b2	748.03	2.23684	YES	YES
22	b1	749.91	131.91926	YES	YES
23	a2	755.19	0.00000	NO	YES
24	b1	758.11	261.49953	YES	YES
25	a1	768.26	35.53596	YES	YES
26	a2	817.82	0.00000	NO	YES
27	b2	821.48	0.10595	YES	YES
28	b1	822.84	1.07808	YES	YES
29	a1	825.70	0.02292	YES	YES
30	a2	843.69	0.00000	NO	YES
31	b2	854.47	0.14933	YES	YES
32	b1	866.42	0.02947	YES	YES
33	a1	870.16	0.16895	YES	YES
34	b2	995.37	25.64926	YES	YES
35	a2	995.44	0.00000	NO	YES
36	b1	996.54	11.18015	YES	YES
37	a1	997.18	21.86202	YES	YES
38	b1	1037.05	1.28220	YES	YES
39	a2	1038.35	0.00000	NO	YES
40	a1	1042.77	0.31908	YES	YES
41	b2	1043.36	0.26485	YES	YES
42	b1	1123.12	19.43093	YES	YES
43	a1	1129.81	0.44823	YES	YES
44	a2	1241.86	0.00000	NO	YES
45	b2	1242.01	0.00485	YES	YES
46	a2	1350.10	0.00000	NO	YES
47	b1	1356.24	1.39306	YES	YES

48	a1	1367.87	0.03582	YES	YES
49	b2	1370.86	0.04141	YES	YES
50	b2	1425.99	10.41810	YES	YES
51	a1	1429.64	7.66082	YES	YES
52	a2	1432.08	0.00000	NO	YES
53	b1	1433.84	1.39732	YES	YES
54	b1	3128.95	0.00743	YES	YES
55	a1	3129.12	0.22765	YES	YES
56	a2	3129.46	0.00000	NO	YES
57	b2	3129.91	0.44827	YES	YES
58	a2	3145.19	0.00000	NO	YES
59	b2	3145.41	12.04615	YES	YES
60	b1	3145.68	1.29955	YES	YES
61	a1	3146.05	9.96200	YES	YES
62	b1	3157.20	17.96351	YES	YES
63	a1	3157.86	0.08306	YES	YES

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m5).

0.00000000000000	0.00000000000000	1.16471751137363	sn
3.98032941872348	1.35759063747613	-1.78811021903165	c
3.98032941872348	-1.35759063747613	-1.78811021903165	c
4.91277021594499	-2.18422318469052	0.61900456022481	c
5.48462927681130	0.00000000000000	2.09004210993084	c
4.91277021594499	2.18422318469052	0.61900456022481	c
-3.98032941872348	1.35759063747613	-1.78811021903165	c
-3.98032941872348	-1.35759063747613	-1.78811021903165	c
-4.91277021594499	-2.18422318469052	0.61900456022481	c
-5.48462927681130	0.00000000000000	2.09004210993084	c
-4.91277021594499	2.18422318469052	0.61900456022481	c
-6.23298334464205	0.00000000000000	4.02821652508946	h
-5.17362716771443	-4.16012261651534	1.20643060631122	h
-3.46128812518984	-2.57814415283901	-3.38763364285791	h
-5.17362716771443	4.16012261651534	1.20643060631122	h
-3.46128812518984	2.57814415283901	-3.38763364285791	h
5.17362716771443	4.16012261651534	1.20643060631122	h
6.23298334464205	0.00000000000000	4.02821652508946	h
5.17362716771443	-4.16012261651534	1.20643060631122	h
3.46128812518984	-2.57814415283901	-3.38763364285791	h
3.46128812518984	2.57814415283901	-3.38763364285791	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m5).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	b2	10.90	0.12213	YES	YES
8	a2	11.06	0.00000	NO	YES
9	a1	35.22	0.39312	YES	YES
10	a1	143.25	3.09042	YES	YES
11	b2	151.46	4.35890	YES	YES
12	b1	195.63	15.62966	YES	YES

13	a2	205.42	0.00000	NO	YES
14	b1	221.36	114.24608	YES	YES
15	a1	327.16	1.63175	YES	YES
16	a2	568.63	0.00000	NO	YES
17	b2	578.60	0.05594	YES	YES
18	b1	590.19	0.05567	YES	YES
19	a1	593.74	0.03709	YES	YES
20	a1	745.31	0.74626	YES	YES
21	b2	748.37	2.24974	YES	YES
22	b1	749.46	128.90529	YES	YES
23	a2	755.39	0.00000	NO	YES
24	b1	758.82	262.44556	YES	YES
25	a1	769.05	36.74703	YES	YES
26	a2	817.95	0.00000	NO	YES
27	b2	821.57	0.10482	YES	YES
28	b1	822.89	1.20746	YES	YES
29	a1	825.72	0.01673	YES	YES
30	a2	843.96	0.00000	NO	YES
31	b2	855.01	0.14059	YES	YES
32	b1	866.25	0.03216	YES	YES
33	a1	869.99	0.15872	YES	YES
34	b2	995.40	25.65671	YES	YES
35	a2	995.45	0.00000	NO	YES
36	b1	996.65	11.56428	YES	YES
37	a1	997.34	21.67843	YES	YES
38	b1	1037.20	1.32316	YES	YES
39	a2	1038.32	0.00000	NO	YES
40	a1	1042.92	0.32368	YES	YES
41	b2	1043.31	0.26073	YES	YES
42	b1	1123.07	19.39662	YES	YES
43	a1	1129.77	0.46842	YES	YES
44	a2	1241.96	0.00000	NO	YES
45	b2	1242.11	0.00541	YES	YES
46	a2	1350.09	0.00000	NO	YES
47	b1	1356.36	1.52110	YES	YES
48	a1	1367.91	0.02981	YES	YES
49	b2	1370.93	0.03869	YES	YES
50	b2	1425.90	10.43423	YES	YES
51	a1	1429.82	7.55811	YES	YES
52	a2	1431.99	0.00000	NO	YES
53	b1	1433.92	1.41618	YES	YES
54	b1	3128.97	0.00483	YES	YES
55	a1	3129.14	0.22614	YES	YES
56	a2	3129.61	0.00000	NO	YES
57	b2	3130.07	0.49887	YES	YES
58	a2	3145.20	0.00000	NO	YES
59	b2	3145.43	12.01227	YES	YES
60	b1	3145.86	1.43922	YES	YES
61	a1	3146.24	9.86884	YES	YES
62	b1	3157.29	17.78936	YES	YES
63	a1	3157.97	0.10930	YES	YES

$[SiCp^*]^+$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

1.88374005874903	-1.36861726438849	0.03610289782238	c
1.88374005874903	1.36861726438849	0.03610289782238	c
-0.71952467647241	2.21446925137048	0.03610289782238	c
-2.32843076455324	0.00000000000000	0.03610289782238	c
-0.71952467647241	-2.21446925137048	0.03610289782238	c
4.17471724748427	-3.03310962269479	0.11535685153878	c
5.83270876344744	-2.13849600952490	-0.80140503763372	h
3.83623669607477	-4.88640406778232	-0.80140503763372	h
4.69094608045320	-3.40817182402931	2.12045795576977	h
4.17471724748427	3.03310962269479	0.11535685153878	c
4.69094608045320	3.40817182402931	2.12045795576977	h
3.83623669607477	4.88640406778232	-0.80140503763372	h
5.83270876344744	2.13849600952490	-0.80140503763372	h
-1.59460009511857	4.90767446112455	0.11535685153878	c
-3.46178409638362	5.15845980618012	-0.80140503763372	h
-0.23142443378490	6.20806728647473	-0.80140503763372	h
-1.79178196334002	5.51453785077916	2.12045795576977	h
-5.16023430473136	0.00000000000000	0.11535685153878	c
-5.97573692935369	-1.69830057796282	-0.80140503763372	h
-5.97573692935369	1.69830057796282	-0.80140503763372	h
-5.79832823422636	0.00000000000000	2.12045795576977	h
-1.59460009511857	-4.90767446112455	0.11535685153878	c
-1.79178196334002	-5.51453785077916	2.12045795576977	h
-0.23142443378490	-6.20806728647473	-0.80140503763372	h
-3.46178409638362	-5.15845980618012	-0.80140503763372	h
0.00000000000000	0.00000000000000	-3.34553814934719	si

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules IR	RAMAN
7	a2	102.77	0.00000	NO	NO
8	e2	105.62	0.00000	NO	YES
9	e2	105.62	0.00000	NO	YES
10	e1	108.07	0.72035	YES	YES
11	e1	108.07	0.72035	YES	YES
12	e2	146.75	0.00000	NO	YES
13	e2	146.75	0.00000	NO	YES
14	a1	193.37	1.64552	YES	YES
15	e1	210.95	0.00986	YES	YES
16	e1	210.95	0.00986	YES	YES
17	e1	293.81	0.15254	YES	YES
18	e1	293.81	0.15254	YES	YES
19	e2	293.84	0.00000	NO	YES
20	e2	293.84	0.00000	NO	YES
21	e1	425.96	0.03632	YES	YES
22	e1	425.96	0.03632	YES	YES
23	a1	518.52	67.26104	YES	YES

24	e2	537.68	0.00000	NO	YES
25	e2	537.68	0.00000	NO	YES
26	a2	546.28	0.00000	NO	NO
27	e2	569.20	0.00000	NO	YES
28	e2	569.20	0.00000	NO	YES
29	a1	588.65	0.96738	YES	YES
30	e1	799.99	4.06368	YES	YES
31	e1	799.99	4.06368	YES	YES
32	e2	937.04	0.00000	NO	YES
33	e2	937.04	0.00000	NO	YES
34	e2	1005.32	0.00000	NO	YES
35	e2	1005.32	0.00000	NO	YES
36	e1	1006.96	12.83560	YES	YES
37	e1	1006.96	12.83560	YES	YES
38	a1	1013.24	1.03346	YES	YES
39	e1	1059.83	6.86700	YES	YES
40	e1	1059.83	6.86700	YES	YES
41	a2	1086.40	0.00000	NO	NO
42	e2	1164.24	0.00000	NO	YES
43	e2	1164.24	0.00000	NO	YES
44	e2	1355.03	0.00000	NO	YES
45	e2	1355.03	0.00000	NO	YES
46	e1	1368.03	16.45902	YES	YES
47	e1	1368.03	16.45902	YES	YES
48	a1	1371.31	0.00745	YES	YES
49	e2	1391.81	0.00000	NO	YES
50	e2	1391.81	0.00000	NO	YES
51	e1	1402.13	7.85250	YES	YES
52	e1	1402.13	7.85250	YES	YES
53	a2	1410.70	0.00000	NO	NO
54	a1	1415.87	55.39514	YES	YES
55	e2	1416.33	0.00000	NO	YES
56	e2	1416.33	0.00000	NO	YES
57	e1	1425.23	1.33097	YES	YES
58	e1	1425.23	1.33097	YES	YES
59	a1	1446.20	34.45957	YES	YES
60	e2	1455.72	0.00000	NO	YES
61	e2	1455.72	0.00000	NO	YES
62	e1	1475.35	61.33244	YES	YES
63	e1	1475.35	61.33244	YES	YES
64	e2	2960.18	0.00000	NO	YES
65	e2	2960.18	0.00000	NO	YES
66	e1	2960.61	1.11059	YES	YES
67	e1	2960.61	1.11059	YES	YES
68	a1	2960.67	0.19660	YES	YES
69	e1	3043.52	4.10005	YES	YES
70	e1	3043.52	4.10005	YES	YES
71	a1	3043.81	0.85135	YES	YES
72	e2	3043.82	0.00000	NO	YES
73	e2	3043.82	0.00000	NO	YES
74	a2	3073.68	0.00000	NO	NO
75	e1	3074.45	3.18805	YES	YES
76	e1	3074.45	3.18805	YES	YES

77	e2	3074.62	0.00000	NO	YES
78	e2	3074.62	0.00000	NO	YES

$SiCp^*_2$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

-0.00000000000000	0.00000000000000	0.60064159744937	si
3.56997820992079	3.18823435432834	0.18831618040088	c
3.30585374305319	1.67816208652128	-2.06495009779351	c
4.05773106645518	-0.87152105865827	-1.44731875856223	c
4.78797965073809	-0.91015227177953	1.17177062533563	c
4.49311890658113	1.58656315183237	2.16903571158999	c
-4.78797965073809	0.91015227177953	1.17177062533563	c
-4.05773106645518	0.87152105865827	-1.44731875856223	c
-3.30585374305319	-1.67816208652128	-2.06495009779351	c
-3.56997820992079	-3.18823435432834	0.18831618040088	c
-4.49311890658113	-1.58656315183237	2.16903571158999	c
-3.00988274445229	-5.96379205631220	0.39533755701823	c
-2.65659613763779	-2.65841495267709	-4.64935300252049	c
-4.24176562769335	3.05809435697865	-3.25011859639156	c
-4.98285271897739	-2.38013212332523	4.85095836403234	c
-5.68500344830043	3.19826088568097	2.59258525345765	c
4.98285271897739	2.38013212332523	4.85095836403234	c
5.68500344830043	-3.19826088568097	2.59258525345765	c
4.24176562769335	-3.05809435697865	-3.25011859639156	c
2.65659613763779	2.65841495267709	-4.64935300252049	c
3.00988274445229	5.96379205631220	0.39533755701823	c
1.50829164391669	6.55669836246415	-0.94836573165883	h
4.71211817624198	7.13462077199758	-0.02622499457740	h
2.36860910173568	6.48763187462885	2.32586010231297	h
1.33152387971819	4.28309178591585	-4.55954372755029	h
1.76712820857524	1.18493854237001	-5.85034782372405	h
4.38077194901229	3.32245596208046	-5.66499881240090	h
3.10145263346264	-2.73734629703511	-4.98001225049150	h
3.57654909703527	-4.85325572681559	-2.38120235590756	h
6.23231625394301	-3.37662842211189	-3.86673544972429	h
4.84380159433476	-4.96490241264271	1.82863867117654	h
5.19214687265190	-3.09601871576475	4.63206122489258	h
7.77946159846267	-3.41435273581911	2.47654938152817	h
3.70567227701839	3.93778143935784	5.44807820245433	h
6.95765021161332	3.07065556691588	5.11326146147804	h
4.70612064390493	0.79082018223466	6.19639806690046	h
-4.84380159433476	4.96490241264271	1.82863867117654	h
-5.19214687265190	3.09601871576475	4.63206122489258	h
-7.77946159846267	3.41435273581911	2.47654938152817	h
-3.57654909703527	4.85325572681559	-2.38120235590756	h
-6.23231625394301	3.37662842211189	-3.86673544972429	h
-3.10145263346264	2.73734629703511	-4.98001225049150	h
-1.76712820857524	-1.18493854237001	-5.85034782372405	h
-4.38077194901229	-3.32245596208046	-5.66499881240090	h

-1.33152387971819	-4.28309178591585	-4.55954372755029	h
-1.50829164391669	-6.55669836246415	-0.94836573165883	h
-4.71211817624198	-7.13462077199758	-0.02622499457740	h
-2.36860910173568	-6.48763187462885	2.32586010231297	h
-4.70612064390493	-0.79082018223466	6.19639806690046	h
-3.70567227701839	-3.93778143935784	5.44807820245433	h
-6.95765021161332	-3.07065556691588	5.11326146147804	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	b	14.31	0.17740	YES	YES
8	a	19.94	0.00000	YES	YES
9	a	43.30	0.01899	YES	YES
10	b	45.65	0.02664	YES	YES
11	a	55.34	0.15812	YES	YES
12	a	83.17	0.01072	YES	YES
13	b	83.23	0.26077	YES	YES
14	b	87.65	0.83801	YES	YES
15	a	88.58	0.02751	YES	YES
16	b	90.51	0.16110	YES	YES
17	a	92.40	0.04496	YES	YES
18	a	112.61	0.27319	YES	YES
19	b	121.28	0.12280	YES	YES
20	a	130.87	0.00222	YES	YES
21	b	131.89	0.14300	YES	YES
22	a	139.92	0.00119	YES	YES
23	b	141.00	0.00979	YES	YES
24	a	156.50	0.00656	YES	YES
25	b	169.98	1.31971	YES	YES
26	a	176.84	0.01146	YES	YES
27	b	181.80	0.01706	YES	YES
28	b	195.39	0.36934	YES	YES
29	a	212.68	0.00497	YES	YES
30	a	277.36	0.02122	YES	YES
31	b	278.36	2.57728	YES	YES
32	b	280.41	5.35478	YES	YES
33	a	283.84	0.52400	YES	YES
34	a	285.20	1.07619	YES	YES
35	b	288.21	0.20101	YES	YES
36	a	289.06	0.00371	YES	YES
37	b	290.01	0.14890	YES	YES
38	b	309.58	5.36074	YES	YES
39	a	317.94	1.70082	YES	YES
40	b	346.15	620.02148	YES	YES
41	a	386.36	0.01472	YES	YES
42	b	387.33	7.57514	YES	YES
43	a	456.57	3.67539	YES	YES
44	a	517.14	0.31777	YES	YES
45	b	524.19	0.48609	YES	YES

46	b	541.45	0.30603	YES	YES
47	a	542.56	0.00361	YES	YES
48	b	545.09	0.02803	YES	YES
49	a	545.52	0.00937	YES	YES
50	a	558.79	0.16808	YES	YES
51	b	563.96	0.57348	YES	YES
52	b	589.84	0.45201	YES	YES
53	b	592.21	7.42698	YES	YES
54	a	593.05	0.70217	YES	YES
55	a	595.18	0.13074	YES	YES
56	a	802.26	4.12289	YES	YES
57	b	803.52	5.29250	YES	YES
58	b	805.47	1.28847	YES	YES
59	a	807.49	0.00281	YES	YES
60	a	932.30	0.00944	YES	YES
61	b	935.30	0.04883	YES	YES
62	b	937.40	0.43543	YES	YES
63	a	938.34	0.58556	YES	YES
64	b	1005.75	14.94317	YES	YES
65	a	1006.84	9.43352	YES	YES
66	a	1007.87	2.95283	YES	YES
67	b	1008.32	4.89128	YES	YES
68	b	1015.44	0.18195	YES	YES
69	a	1016.32	0.02491	YES	YES
70	b	1017.35	0.16989	YES	YES
71	a	1021.45	0.89504	YES	YES
72	b	1021.74	0.00024	YES	YES
73	a	1022.58	2.46200	YES	YES
74	b	1056.97	6.63631	YES	YES
75	a	1057.12	3.70925	YES	YES
76	b	1058.57	2.37524	YES	YES
77	a	1058.86	0.00499	YES	YES
78	b	1085.44	0.09544	YES	YES
79	a	1086.60	0.09258	YES	YES
80	a	1160.81	0.01152	YES	YES
81	b	1163.60	0.17853	YES	YES
82	b	1172.31	0.15189	YES	YES
83	a	1173.38	0.19991	YES	YES
84	b	1351.91	0.33388	YES	YES
85	a	1352.04	0.02233	YES	YES
86	a	1355.35	0.00403	YES	YES
87	b	1355.67	0.12318	YES	YES
88	b	1360.12	2.16516	YES	YES
89	a	1360.94	0.02039	YES	YES
90	b	1364.45	2.75506	YES	YES
91	b	1365.24	20.62983	YES	YES
92	a	1365.27	1.67076	YES	YES
93	a	1372.55	0.00304	YES	YES
94	a	1395.36	0.17059	YES	YES
95	b	1397.79	0.57010	YES	YES
96	b	1399.44	0.37960	YES	YES
97	a	1401.03	0.89830	YES	YES
98	a	1411.01	0.24882	YES	YES

99	b	1413.30	12.35448	YES	YES
100	b	1413.83	3.98856	YES	YES
101	a	1414.03	16.98177	YES	YES
102	b	1416.24	2.85012	YES	YES
103	a	1417.07	2.45740	YES	YES
104	b	1418.10	5.44236	YES	YES
105	a	1418.60	0.01959	YES	YES
106	b	1421.48	2.00877	YES	YES
107	a	1422.03	1.50258	YES	YES
108	b	1422.66	12.03969	YES	YES
109	a	1423.89	0.02120	YES	YES
110	a	1425.74	0.05556	YES	YES
111	b	1428.15	94.31502	YES	YES
112	b	1429.92	5.10696	YES	YES
113	a	1432.75	5.46974	YES	YES
114	b	1449.99	1.58285	YES	YES
115	a	1451.89	0.02069	YES	YES
116	b	1456.73	0.64486	YES	YES
117	a	1457.78	0.07221	YES	YES
118	b	1459.20	0.10334	YES	YES
119	a	1463.86	0.10182	YES	YES
120	b	1488.83	23.01006	YES	YES
121	a	1493.31	0.01381	YES	YES
122	a	1496.36	21.66162	YES	YES
123	b	1499.43	0.06199	YES	YES
124	a	2922.72	4.36492	YES	YES
125	b	2922.78	75.32633	YES	YES
126	b	2923.21	54.43212	YES	YES
127	a	2923.29	9.01086	YES	YES
128	b	2923.92	96.08734	YES	YES
129	a	2924.46	112.76909	YES	YES
130	b	2925.70	84.54171	YES	YES
131	a	2925.70	5.29375	YES	YES
132	b	2927.10	38.82976	YES	YES
133	a	2928.18	52.74286	YES	YES
134	a	2993.65	2.06496	YES	YES
135	b	2993.70	28.43848	YES	YES
136	b	2995.10	16.93920	YES	YES
137	a	2995.69	11.62215	YES	YES
138	a	2996.21	0.31992	YES	YES
139	b	2996.70	4.90078	YES	YES
140	b	2997.36	2.31117	YES	YES
141	a	2997.68	0.07242	YES	YES
142	b	3003.76	14.22236	YES	YES
143	a	3004.13	0.56859	YES	YES
144	a	3028.02	2.21374	YES	YES
145	b	3028.09	22.99860	YES	YES
146	a	3029.14	0.04902	YES	YES
147	b	3029.23	4.97708	YES	YES
148	b	3029.59	8.10193	YES	YES
149	a	3029.73	44.11218	YES	YES
150	b	3039.98	28.85727	YES	YES
151	a	3041.12	5.08971	YES	YES

152	a	3043.94	15.23864	YES	YES
153	b	3044.43	2.18467	YES	YES

[GeCp*]$^{+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

1.88561667494726	-1.36998070586524	-0.02666191985208	c
1.88561667494726	1.36998070586524	-0.02666191985208	c
-0.72024148007629	2.21667534602153	-0.02666191985208	c
-2.33075038974192	0.00000000000000	-0.02666191985208	c
-0.72024148007629	-2.21667534602153	-0.02666191985208	c
4.17415139259936	-3.03269850505624	0.12972130414793	c
5.85421473893462	-2.15403653813535	-0.76324479695881	h
3.85766232898258	-4.90205517846648	-0.76324479695881	h
4.64873257949892	-3.37750192033002	2.15122868548650	h
4.17415139259936	3.03269850505624	0.12972130414793	c
4.64873257949892	3.37750192033002	2.15122868548650	h
3.85766232898258	4.90205517846648	-0.76324479695881	h
5.85421473893462	2.15403653813535	-0.76324479695881	h
-1.59438395778526	4.90700925881198	0.12972130414793	c
-3.47004830250331	5.18367325315509	-0.76324479695881	h
-0.23955864288039	6.23332297204331	-0.76324479695881	h
-1.77565784075961	5.46491290416202	2.15122868548650	h
-5.15953486962822	0.00000000000000	0.12972130414793	c
-6.00227012253350	-1.69836892144290	-0.76324479695881	h
-6.00227012253350	1.69836892144290	-0.76324479695881	h
-5.74614947747861	0.00000000000000	2.15122868548650	h
-1.59438395778526	-4.90700925881198	0.12972130414793	c
-1.77565784075961	-5.46491290416202	2.15122868548650	h
-0.23955864288039	-6.23332297204331	-0.76324479695881	h
-3.47004830250331	-5.18367325315509	-0.76324479695881	h
0.00000000000000	0.00000000000000	-3.63899237929764	ge

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules IR	RAMAN
7	e2	120.46	0.00000	NO	YES
8	e2	120.46	0.00000	NO	YES
9	a2	120.67	0.00000	NO	NO
10	e1	123.16	0.78480	YES	YES
11	e1	123.16	0.78480	YES	YES
12	e2	144.33	0.00000	NO	YES
13	e2	144.33	0.00000	NO	YES
14	e1	157.93	0.02083	YES	YES
15	e1	157.93	0.02083	YES	YES
16	a1	162.77	1.08474	YES	YES
17	e1	283.79	0.22992	YES	YES
18	e1	283.79	0.22992	YES	YES

19	e2	287.81	0.00000	NO	YES
20	e2	287.81	0.00000	NO	YES
21	a1	394.80	39.86515	YES	YES
22	e1	410.42	0.00407	YES	YES
23	e1	410.42	0.00407	YES	YES
24	e2	534.39	0.00000	NO	YES
25	e2	534.39	0.00000	NO	YES
26	a2	542.06	0.00000	NO	NO
27	e2	585.40	0.00000	NO	YES
28	e2	585.40	0.00000	NO	YES
29	a1	587.36	0.96844	YES	YES
30	e1	796.10	3.65403	YES	YES
31	e1	796.10	3.65403	YES	YES
32	e2	931.40	0.00000	NO	YES
33	e2	931.40	0.00000	NO	YES
34	e1	1003.77	14.57987	YES	YES
35	e1	1003.77	14.57987	YES	YES
36	e2	1005.29	0.00000	NO	YES
37	e2	1005.29	0.00000	NO	YES
38	a1	1008.09	2.95800	YES	YES
39	e1	1057.94	6.65094	YES	YES
40	e1	1057.94	6.65094	YES	YES
41	a2	1084.67	0.00000	NO	NO
42	e2	1161.03	0.00000	NO	YES
43	e2	1161.03	0.00000	NO	YES
44	e2	1350.13	0.00000	NO	YES
45	e2	1350.13	0.00000	NO	YES
46	e1	1364.07	13.94846	YES	YES
47	e1	1364.07	13.94846	YES	YES
48	a1	1367.34	0.41238	YES	YES
49	e2	1389.36	0.00000	NO	YES
50	e2	1389.36	0.00000	NO	YES
51	e1	1400.62	6.10172	YES	YES
52	e1	1400.62	6.10172	YES	YES
53	a2	1409.84	0.00000	NO	NO
54	a1	1413.33	57.86464	YES	YES
55	e2	1415.88	0.00000	NO	YES
56	e2	1415.88	0.00000	NO	YES
57	e1	1424.66	1.53532	YES	YES
58	e1	1424.66	1.53532	YES	YES
59	a1	1443.58	33.87733	YES	YES
60	e2	1451.56	0.00000	NO	YES
61	e2	1451.56	0.00000	NO	YES
62	e1	1470.94	62.20955	YES	YES
63	e1	1470.94	62.20955	YES	YES
64	e2	2956.02	0.00000	NO	YES
65	e2	2956.02	0.00000	NO	YES
66	e1	2956.41	2.07063	YES	YES
67	e1	2956.41	2.07063	YES	YES
68	a1	2956.52	0.05284	YES	YES
69	e1	3038.35	4.41812	YES	YES
70	e1	3038.35	4.41812	YES	YES
71	a1	3038.60	0.62062	YES	YES

72	e2	3038.68	0.00000	NO	YES
73	e2	3038.68	0.00000	NO	YES
74	a2	3068.66	0.00000	NO	NO
75	e1	3069.61	4.39387	YES	YES
76	e1	3069.61	4.39387	YES	YES
77	e2	3070.03	0.00000	NO	YES
78	e2	3070.03	0.00000	NO	YES

$GeCp^*_2$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

0.00000000000000	0.00000000000000	0.68217262847368	ge
3.69409542655607	3.21714732964714	0.16564722047286	c
3.42002042647806	1.69940403483667	-2.08269771341234	c
4.17250421835812	-0.84973342340187	-1.46215738562548	c
4.91339956891145	-0.88409319419050	1.15684668035045	c
4.62227789023659	1.61793298733352	2.15004848099152	c
-4.91339956891145	0.88409319419050	1.15684668035045	c
-4.17250421835812	0.84973342340187	-1.46215738562548	c
-3.42002042647806	-1.69940403483667	-2.08269771341234	c
-3.69409542655607	-3.21714732964714	0.16564722047286	c
-4.62227789023659	-1.61793298733352	2.15004848099152	c
-3.18994366641013	-6.00602877030204	0.34959974773192	c
-2.73790059226558	-2.66688429349701	-4.66500304648269	c
-4.35083132730882	3.03537692035204	-3.26887985788274	c
-5.19012672233202	-2.43342163220483	4.81110115589197	c
-5.87387035288868	3.15391457094756	2.56761051475634	c
5.19012672233202	2.43342163220483	4.81110115589197	c
5.87387035288868	-3.15391457094756	2.56761051475634	c
4.35083132730882	-3.03537692035204	-3.26887985788274	c
2.73790059226558	2.66688429349701	-4.66500304648269	c
3.18994366641013	6.00602877030204	0.34959974773192	c
1.67294176840446	6.61366128658393	-0.97070333961789	h
4.90495773165638	7.13941055775725	-0.12280636911704	h
2.60133589640913	6.56947713924010	2.28569570085201	h
1.39364343245315	4.27619875892335	-4.56721850656509	h
1.85278919589347	1.17882866687478	-5.85238386025599	h
4.44217851137409	3.35089976718799	-5.70174223632974	h
3.13769346378122	-2.75106228223870	-4.95623022327172	h
3.76826145447919	-4.84616527315020	-2.37464644230242	h
6.32439548942789	-3.30236656139041	-3.96155815647164	h
5.06184855349159	-4.93997580092832	1.81657406448482	h
5.40728260997917	-3.06153965394786	4.61378008447036	h
7.97115485406988	-3.32813142860083	2.42589020358794	h
3.95156696492276	4.01530128819635	5.42569129545338	h
7.18024290855093	3.10006496863271	5.01556916520566	h
4.92944334788841	0.86366814722498	6.18267666982003	h
-5.06184855349159	4.93997580092832	1.81657406448482	h
-5.40728260997917	3.06153965394786	4.61378008447036	h
-7.97115485406988	3.32813142860083	2.42589020358794	h

-3.76826145447919	4.84616527315020	-2.37464644230242	h
-6.32439548942789	3.30236656139041	-3.96155815647164	h
-3.13769346378122	2.75106228223870	-4.95623022327172	h
-1.85278919589347	-1.17882866687478	-5.85238386025599	h
-4.44217851137409	-3.35089976718797	-5.70174223632974	h
-1.39364343245315	-4.27619875892335	-4.56721850656509	h
-1.67294176840447	-6.61366128658393	-0.97070333961789	h
-4.90495773165638	-7.13941055775725	-0.12280636911704	h
-2.60133589640913	-6.56947713924010	2.28569570085201	h
-4.92944334788841	-0.86366814722498	6.18267666982003	h
-3.95156696492276	-4.01530128819635	5.42569129545338	h
-7.18024290855093	-3.10006496863271	5.01556916520566	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	b	7.08	0.04810	YES	YES
8	a	24.45	0.00095	YES	YES
9	a	48.08	0.00001	YES	YES
10	b	51.06	0.01539	YES	YES
11	a	51.99	0.09297	YES	YES
12	b	75.42	0.01353	YES	YES
13	a	77.05	0.01284	YES	YES
14	b	87.32	0.52508	YES	YES
15	a	93.14	0.01453	YES	YES
16	a	96.61	0.10842	YES	YES
17	b	100.69	0.02057	YES	YES
18	a	104.66	0.38286	YES	YES
19	b	121.30	0.04466	YES	YES
20	a	127.21	0.04400	YES	YES
21	b	127.77	0.52090	YES	YES
22	b	137.81	0.18692	YES	YES
23	a	141.08	0.00033	YES	YES
24	b	141.98	0.29525	YES	YES
25	a	142.17	0.00025	YES	YES
26	b	149.78	5.78497	YES	YES
27	a	170.15	0.02481	YES	YES
28	b	173.73	0.03942	YES	YES
29	a	174.84	0.02106	YES	YES
30	b	275.77	138.45568	YES	YES
31	b	277.64	2.74330	YES	YES
32	a	279.46	0.13852	YES	YES
33	a	281.32	1.28407	YES	YES
34	b	285.14	116.45834	YES	YES
35	a	286.74	0.30283	YES	YES
36	a	287.01	0.00239	YES	YES
37	b	287.79	101.75620	YES	YES
38	b	290.01	1.82038	YES	YES
39	b	312.41	2.54018	YES	YES
40	a	315.80	0.85916	YES	YES

41	b	383.24	8.61065	YES	YES
42	a	383.49	0.00016	YES	YES
43	a	397.29	3.23935	YES	YES
44	a	528.66	0.03803	YES	YES
45	b	532.33	0.19074	YES	YES
46	b	540.81	0.10371	YES	YES
47	a	541.72	0.00137	YES	YES
48	b	546.52	0.02205	YES	YES
49	a	547.06	0.00888	YES	YES
50	a	573.03	0.14140	YES	YES
51	b	579.92	0.36820	YES	YES
52	b	590.51	6.21684	YES	YES
53	a	592.61	0.00472	YES	YES
54	b	604.23	0.36524	YES	YES
55	a	607.40	0.47901	YES	YES
56	a	802.05	3.86648	YES	YES
57	b	802.61	5.56033	YES	YES
58	b	805.36	0.35284	YES	YES
59	a	806.33	0.09154	YES	YES
60	a	929.93	0.00009	YES	YES
61	b	933.85	0.04751	YES	YES
62	b	936.47	0.29941	YES	YES
63	a	938.55	0.37135	YES	YES
64	b	1005.67	18.24780	YES	YES
65	a	1006.43	12.64014	YES	YES
66	b	1007.55	6.56532	YES	YES
67	a	1007.75	1.29283	YES	YES
68	b	1015.44	1.05365	YES	YES
69	a	1017.93	0.15410	YES	YES
70	b	1018.69	0.03760	YES	YES
71	a	1019.33	3.57886	YES	YES
72	a	1022.60	0.00784	YES	YES
73	b	1022.69	0.01089	YES	YES
74	a	1056.16	4.11562	YES	YES
75	b	1056.92	5.48803	YES	YES
76	b	1057.57	3.49646	YES	YES
77	a	1058.93	0.00519	YES	YES
78	b	1086.04	0.15658	YES	YES
79	a	1087.18	0.00495	YES	YES
80	a	1158.38	0.00551	YES	YES
81	b	1161.11	0.24054	YES	YES
82	b	1170.29	0.10097	YES	YES
83	a	1171.50	0.17145	YES	YES
84	b	1351.11	0.70325	YES	YES
85	a	1352.28	0.00569	YES	YES
86	a	1354.76	0.00017	YES	YES
87	b	1356.57	0.05461	YES	YES
88	b	1360.98	5.42432	YES	YES
89	a	1361.76	0.02826	YES	YES
90	b	1364.12	7.28868	YES	YES
91	a	1365.56	1.09316	YES	YES
92	b	1365.93	24.61327	YES	YES
93	a	1372.24	0.03443	YES	YES

94	a	1392.06	0.11980	YES	YES
95	b	1394.27	0.06153	YES	YES
96	b	1396.74	0.44743	YES	YES
97	a	1397.18	0.39563	YES	YES
98	a	1411.92	1.83224	YES	YES
99	b	1412.61	8.84474	YES	YES
100	a	1413.36	12.93221	YES	YES
101	b	1413.47	10.89951	YES	YES
102	b	1416.06	6.34712	YES	YES
103	a	1417.00	3.48499	YES	YES
104	a	1418.14	0.20868	YES	YES
105	b	1419.32	4.47439	YES	YES
106	b	1421.04	3.32949	YES	YES
107	a	1421.79	1.62724	YES	YES
108	b	1422.70	12.40885	YES	YES
109	a	1423.14	0.53409	YES	YES
110	b	1425.53	67.66128	YES	YES
111	a	1425.58	0.01711	YES	YES
112	b	1428.90	21.55718	YES	YES
113	a	1431.07	5.81212	YES	YES
114	b	1447.79	2.88361	YES	YES
115	a	1450.43	0.03188	YES	YES
116	a	1452.89	0.14254	YES	YES
117	b	1454.09	0.34494	YES	YES
118	b	1456.30	0.20261	YES	YES
119	a	1460.43	0.16067	YES	YES
120	b	1485.27	21.61823	YES	YES
121	a	1489.98	0.14423	YES	YES
122	a	1492.37	20.24407	YES	YES
123	b	1495.73	0.00603	YES	YES
124	a	2919.73	4.37635	YES	YES
125	b	2919.79	90.98434	YES	YES
126	b	2920.21	79.17380	YES	YES
127	a	2920.42	2.34164	YES	YES
128	b	2921.81	75.00907	YES	YES
129	a	2922.22	135.20792	YES	YES
130	b	2923.26	70.62571	YES	YES
131	a	2923.29	5.86851	YES	YES
132	b	2924.22	66.44031	YES	YES
133	a	2925.52	44.65814	YES	YES
134	b	2992.53	34.94925	YES	YES
135	a	2992.70	0.08517	YES	YES
136	a	2993.37	14.16930	YES	YES
137	b	2993.44	8.80579	YES	YES
138	b	2993.88	4.41273	YES	YES
139	a	2994.18	0.00786	YES	YES
140	a	2994.94	0.89946	YES	YES
141	b	2994.97	2.35808	YES	YES
142	b	3000.19	12.60812	YES	YES
143	a	3001.08	0.30167	YES	YES
144	a	3026.77	15.79793	YES	YES
145	b	3026.79	10.68515	YES	YES
146	a	3027.04	0.51512	YES	YES

147	b	3027.11	16.36209	YES	YES
148	b	3028.07	9.87928	YES	YES
149	a	3028.16	32.59178	YES	YES
150	b	3036.29	30.46914	YES	YES
151	a	3037.80	4.84809	YES	YES
152	a	3040.37	15.33959	YES	YES
153	b	3040.65	3.11616	YES	YES

$[SnCp^*]^+$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

1.88779874177138	-1.37156607021192	-0.12758639081768	c
1.88779874177138	1.37156607021192	-0.12758639081768	c
-0.72107495543738	2.21924051941901	-0.12758639081768	c
-2.33344757266800	0.00000000000000	-0.12758639081768	c
-0.72107495543738	-2.21924051941901	-0.12758639081768	c
4.17007745835804	-3.02973861857364	0.15996198251824	c
5.88428755065090	-2.17621118485616	-0.69243384956556	h
3.88804468113190	-4.92380377933160	-0.69243384956556	h
4.57465522677582	-3.32368157321463	2.20562660482398	h
4.17007745835804	3.02973861857364	0.15996198251824	c
4.57465522677582	3.32368157321463	2.20562660482398	h
3.88804468113190	4.92380377933160	-0.69243384956556	h
5.88428755065090	2.17621118485616	-0.69243384956556	h
-1.59282785337299	4.90222006188028	0.15996198251824	c
-3.48134378793314	5.21928927441828	-0.69243384956556	h
-0.25135497525178	6.26877625827038	-0.69243384956556	h
-1.74736280981600	5.37782975324300	2.20562660482398	h
-5.15449920997011	0.00000000000000	0.15996198251824	c
-6.03963346859789	-1.69810561062333	-0.69243384956556	h
-6.03963346859789	1.69810561062333	-0.69243384956556	h
-5.65458483391961	0.00000000000000	2.20562660482398	h
-1.59282785337299	-4.90222006188028	0.15996198251824	c
-1.74736280981600	-5.37782975324300	2.20562660482398	h
-0.25135497525178	-6.26877625827038	-0.69243384956556	h
-3.48134378793314	-5.21928927441828	-0.69243384956556	h
0.00000000000000	0.00000000000000	-4.26567248696892	sn

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules IR	RAMAN
7	e1	126.00	0.21762	YES	YES
8	e1	126.00	0.21762	YES	YES
9	e2	133.85	0.00000	NO	YES
10	e2	133.85	0.00000	NO	YES
11	a2	135.65	0.00000	NO	NO
12	a1	137.72	0.06674	YES	YES
13	e1	143.16	0.40105	YES	YES

14	e1	143.16	0.40105	YES	YES
15	e2	144.89	0.00000	NO	YES
16	e2	144.89	0.00000	NO	YES
17	e1	278.24	0.38314	YES	YES
18	e1	278.24	0.38314	YES	YES
19	e2	283.54	0.00000	NO	YES
20	e2	283.54	0.00000	NO	YES
21	a1	310.64	40.76665	YES	YES
22	e1	388.43	0.02923	YES	YES
23	e1	388.43	0.02923	YES	YES
24	e2	532.59	0.00000	NO	YES
25	e2	532.59	0.00000	NO	YES
26	a2	540.72	0.00000	NO	NO
27	a1	587.39	2.82887	YES	YES
28	e2	600.90	0.00000	NO	YES
29	e2	600.90	0.00000	NO	YES
30	e1	794.49	3.86458	YES	YES
31	e1	794.49	3.86458	YES	YES
32	e2	928.21	0.00000	NO	YES
33	e2	928.21	0.00000	NO	YES
34	e1	1001.32	14.41134	YES	YES
35	e1	1001.32	14.41134	YES	YES
36	a1	1005.17	4.07450	YES	YES
37	e2	1005.45	0.00000	NO	YES
38	e2	1005.45	0.00000	NO	YES
39	e1	1057.24	5.14223	YES	YES
40	e1	1057.24	5.14223	YES	YES
41	a2	1085.03	0.00000	NO	NO
42	e2	1155.96	0.00000	NO	YES
43	e2	1155.96	0.00000	NO	YES
44	e2	1347.85	0.00000	NO	YES
45	e2	1347.85	0.00000	NO	YES
46	e1	1365.02	10.40076	YES	YES
47	e1	1365.02	10.40076	YES	YES
48	a1	1367.59	4.19955	YES	YES
49	e2	1384.96	0.00000	NO	YES
50	e2	1384.96	0.00000	NO	YES
51	e1	1399.66	2.96309	YES	YES
52	e1	1399.66	2.96309	YES	YES
53	a1	1406.27	64.78513	YES	YES
54	a2	1412.36	0.00000	NO	NO
55	e2	1416.75	0.00000	NO	YES
56	e2	1416.75	0.00000	NO	YES
57	e1	1425.35	1.70402	YES	YES
58	e1	1425.35	1.70402	YES	YES
59	a1	1442.17	35.21515	YES	YES
60	e2	1447.02	0.00000	NO	YES
61	e2	1447.02	0.00000	NO	YES
62	e1	1463.98	62.25901	YES	YES
63	e1	1463.98	62.25901	YES	YES
64	e2	2950.79	0.00000	NO	YES
65	e2	2950.79	0.00000	NO	YES
66	e1	2950.95	5.17247	YES	YES

67	e1	2950.95	5.17247	YES	YES
68	a1	2950.98	0.19823	YES	YES
69	e1	3032.54	5.52550	YES	YES
70	e1	3032.54	5.52550	YES	YES
71	a1	3032.63	0.25526	YES	YES
72	e2	3033.12	0.00000	NO	YES
73	e2	3033.12	0.00000	NO	YES
74	a2	3064.72	0.00000	NO	NO
75	e1	3065.62	6.43753	YES	YES
76	e1	3065.62	6.43753	YES	YES
77	e2	3065.95	0.00000	NO	YES
78	e2	3065.95	0.00000	NO	YES

$SnCp^*_2$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

0.00000000000000	-0.00000000000000	1.20854652324380	sn
4.09920355070885	3.32971946347570	0.23857286526907	c
3.61419887626404	1.82541156142356	-1.98766819087465	c
4.40991048880231	-0.73296547063096	-1.45446906782970	c
5.38333616802707	-0.78866241105547	1.09265106632429	c
5.19160472203681	1.71012581266315	2.12561113239194	c
-5.38333616802707	0.78866241105547	1.09265106632429	c
-4.40991048880231	0.73296547063096	-1.45446906782970	c
-3.61419887626404	-1.82541156142356	-1.98766819087465	c
-4.09920355070885	-3.32971946347570	0.23857286526907	c
-5.19160472203681	-1.71012581266315	2.12561113239194	c
-3.71256062481383	-6.13694484890116	0.45495299796115	c
-2.76717652763590	-2.82031174575720	-4.51191738363433	c
-4.49172861031814	2.87758615551648	-3.31793662696154	c
-6.06743100788419	-2.51878019621233	4.70666203552601	c
-6.53800303407269	3.04891583626680	2.37111747296096	c
6.06743100788419	2.51878019621233	4.70666203552601	c
6.53800303407269	-3.04891583626680	2.37111747296096	c
4.49172861031814	-2.87758615551648	-3.31793662696154	c
2.76717652763590	2.82031174575720	-4.51191738363433	c
3.71256062481383	6.13694484890116	0.45495299796115	c
2.12140652245704	6.80474249519657	-0.74340628486552	h
5.42698934672503	7.20460188915413	-0.15588306652526	h
3.30239824258451	6.72525408022873	2.42967107860727	h
1.45539084026209	4.44756591536016	-4.31580477452041	h
1.78191187324625	1.35143590744003	-5.64347705827247	h
4.40406394928960	3.48624803360339	-5.66442984617442	h
3.04992703785419	-2.65654383340134	-4.82649737317533	h
4.15752172920336	-4.73648253615066	-2.39747358206937	h
6.36950061585967	-2.99842545686450	-4.27182618436636	h
5.69854239210084	-4.84993419190683	1.68944970552022	h
6.28852664463745	-2.98731809810627	4.45672549960277	h
8.61327192265394	-3.16929016323487	2.01008253320845	h
4.94223597773774	4.13078449334240	5.44836188972098	h

8.08305221385935	3.14022029353791	4.68867418000715	h
5.92550480852958	0.95903243899403	6.10781884051904	h
-5.69854239210083	4.84993419190683	1.68944970552022	h
-6.28852664463745	2.98731809810627	4.45672549960277	h
-8.61327192265394	3.16929016323487	2.01008253320845	h
-4.15752172920336	4.73648253615066	-2.39747358206937	h
-6.36950061585967	2.99842545686450	-4.27182618436636	h
-3.04992703785419	2.65654383340134	-4.82649737317533	h
-1.78191187324625	-1.35143590744003	-5.64347705827247	h
-4.40406394928960	-3.48624803360339	-5.66442984617442	h
-1.45539084026209	-4.44756591536016	-4.31580477452041	h
-2.12140652245704	-6.80474249519657	-0.74340628486552	h
-5.42698934672503	-7.20460188915413	-0.15588306652526	h
-3.30239824258451	-6.72525408022873	2.42967107860727	h
-5.92550480852958	-0.95903243899403	6.10781884051904	h
-4.94223597773774	-4.13078449334240	5.44836188972098	h
-8.08305221385935	-3.14022029353791	4.68867418000715	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number	IR intensity	selection rules	
		[cm^{-1}]	[km mol^{-1}]	IR	RAMAN
7	b	11.57	0.00516	YES	YES
8	a	19.35	0.00009	YES	YES
9	a	51.88	0.01437	YES	YES
10	b	83.06	0.26066	YES	YES
11	a	84.80	0.15874	YES	YES
12	b	86.15	0.01664	YES	YES
13	a	86.81	0.62334	YES	YES
14	a	88.49	0.00023	YES	YES
15	b	99.86	0.56471	YES	YES
16	a	108.05	0.04537	YES	YES
17	b	108.73	0.13980	YES	YES
18	b	114.59	0.07102	YES	YES
19	a	115.22	0.08943	YES	YES
20	a	117.39	0.19724	YES	YES
21	b	118.93	0.23796	YES	YES
22	b	133.52	0.26491	YES	YES
23	b	135.28	6.23826	YES	YES
24	a	141.34	0.00505	YES	YES
25	b	141.97	0.00170	YES	YES
26	a	142.71	0.00047	YES	YES
27	a	154.34	0.02252	YES	YES
28	a	168.46	0.00011	YES	YES
29	b	171.67	0.12089	YES	YES
30	b	256.18	251.87512	YES	YES
31	b	274.56	4.64528	YES	YES
32	a	275.23	0.72459	YES	YES
33	a	277.78	1.02599	YES	YES
34	b	278.08	15.35633	YES	YES
35	a	281.34	0.06734	YES	YES

36	b	281.77	0.21737	YES	YES
37	a	283.15	0.04667	YES	YES
38	b	286.62	1.26252	YES	YES
39	b	313.92	1.51500	YES	YES
40	a	319.17	0.13243	YES	YES
41	b	362.78	12.69110	YES	YES
42	a	366.94	0.00015	YES	YES
43	a	409.19	5.40835	YES	YES
44	a	533.93	0.00413	YES	YES
45	b	536.03	0.27214	YES	YES
46	b	540.09	0.17486	YES	YES
47	a	540.81	0.00464	YES	YES
48	b	545.94	0.02983	YES	YES
49	a	546.11	0.00221	YES	YES
50	b	589.27	11.33161	YES	YES
51	a	590.74	0.18189	YES	YES
52	a	591.58	0.01819	YES	YES
53	b	598.97	0.64555	YES	YES
54	b	620.93	0.29225	YES	YES
55	a	624.21	0.44383	YES	YES
56	b	799.67	4.85474	YES	YES
57	a	800.27	3.97307	YES	YES
58	b	803.14	1.03026	YES	YES
59	a	803.24	0.33204	YES	YES
60	a	928.47	0.01851	YES	YES
61	b	932.14	0.20387	YES	YES
62	b	934.78	0.31120	YES	YES
63	a	936.75	0.13314	YES	YES
64	b	1006.44	19.78161	YES	YES
65	a	1006.87	8.79713	YES	YES
66	b	1008.24	10.15787	YES	YES
67	a	1008.30	5.93360	YES	YES
68	b	1015.60	2.93708	YES	YES
69	a	1018.49	0.22595	YES	YES
70	b	1019.78	0.08631	YES	YES
71	a	1021.29	3.40757	YES	YES
72	b	1024.31	0.08101	YES	YES
73	a	1024.32	0.01219	YES	YES
74	b	1055.86	4.98649	YES	YES
75	a	1056.14	3.09352	YES	YES
76	b	1057.37	3.58109	YES	YES
77	a	1057.73	0.65462	YES	YES
78	b	1086.06	0.06857	YES	YES
79	a	1086.76	0.00449	YES	YES
80	a	1154.64	0.00536	YES	YES
81	b	1157.27	1.29033	YES	YES
82	b	1166.41	0.15080	YES	YES
83	a	1167.24	0.07828	YES	YES
84	b	1349.72	1.64151	YES	YES
85	a	1351.19	0.00323	YES	YES
86	a	1354.32	0.02574	YES	YES
87	b	1355.83	2.70943	YES	YES
88	b	1362.15	5.06298	YES	YES

89	a	1363.03	0.04504	YES	YES
90	b	1366.54	35.89739	YES	YES
91	a	1367.05	0.61911	YES	YES
92	b	1368.41	16.46785	YES	YES
93	a	1374.66	0.53391	YES	YES
94	a	1386.51	0.01077	YES	YES
95	b	1388.90	0.16351	YES	YES
96	b	1392.22	0.52174	YES	YES
97	a	1392.29	0.43263	YES	YES
98	a	1410.68	1.08474	YES	YES
99	b	1412.88	14.74273	YES	YES
100	b	1414.23	4.43466	YES	YES
101	a	1414.43	6.39342	YES	YES
102	b	1415.80	17.62084	YES	YES
103	a	1416.43	8.04413	YES	YES
104	a	1417.85	0.37189	YES	YES
105	b	1420.69	8.07380	YES	YES
106	b	1420.98	8.80189	YES	YES
107	b	1421.91	39.25641	YES	YES
108	a	1422.25	0.52848	YES	YES
109	b	1423.10	43.70240	YES	YES
110	a	1424.45	1.18535	YES	YES
111	a	1425.48	1.47533	YES	YES
112	b	1428.44	3.43089	YES	YES
113	a	1428.60	6.87376	YES	YES
114	b	1444.33	3.51524	YES	YES
115	a	1448.54	0.00009	YES	YES
116	a	1449.24	0.23424	YES	YES
117	b	1452.16	0.70155	YES	YES
118	b	1453.77	0.30371	YES	YES
119	a	1457.79	0.19116	YES	YES
120	b	1478.28	26.20436	YES	YES
121	a	1483.36	0.05537	YES	YES
122	a	1485.74	20.31020	YES	YES
123	b	1488.52	0.05560	YES	YES
124	a	2916.45	3.20703	YES	YES
125	b	2916.55	115.13839	YES	YES
126	b	2916.76	74.44552	YES	YES
127	a	2917.03	6.16082	YES	YES
128	b	2918.33	29.38402	YES	YES
129	a	2918.55	123.19675	YES	YES
130	b	2918.71	114.84175	YES	YES
131	a	2918.84	39.56889	YES	YES
132	b	2919.89	107.16627	YES	YES
133	a	2921.26	29.83679	YES	YES
134	b	2989.22	17.33603	YES	YES
135	a	2989.55	19.20517	YES	YES
136	a	2990.05	2.32448	YES	YES
137	b	2990.35	9.80452	YES	YES
138	b	2991.19	2.26264	YES	YES
139	a	2991.44	0.01906	YES	YES
140	b	2994.73	18.68164	YES	YES
141	a	2994.85	0.55426	YES	YES

142	b	2996.74	5.59596	YES	YES
143	a	2997.28	0.04110	YES	YES
144	a	3024.30	0.63987	YES	YES
145	b	3024.35	30.81902	YES	YES
146	a	3025.55	0.18256	YES	YES
147	b	3025.66	2.64365	YES	YES
148	b	3026.03	9.06955	YES	YES
149	a	3026.18	44.76923	YES	YES
150	b	3033.75	31.24612	YES	YES
151	a	3034.76	2.58163	YES	YES
152	a	3037.73	14.91904	YES	YES
153	b	3037.97	5.59551	YES	YES

$[PbCp^*]^+$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

1.88816792446246	-1.37183429713759	-0.17034042134697	c
1.88816792446246	1.37183429713759	-0.17034042134697	c
-0.72121597067731	2.21967451970144	-0.17034042134697	c
-2.33390390757029	0.00000000000000	-0.17034042134697	c
-0.72121597067731	-2.21967451970144	-0.17034042134697	c
4.16602105451009	-3.02679146866733	0.17243711001667	c
5.89512854838541	-2.18415128002220	-0.66115543916134	h
3.89894621291553	-4.93166055652688	-0.66115543916134	h
4.54046356758163	-3.29883987870701	2.22735299224324	h
4.16602105451009	3.02679146866733	0.17243711001667	c
4.54046356758163	3.29883987870701	2.22735299224324	h
3.89894621291553	4.93166055652688	-0.66115543916134	h
5.89512854838541	2.18415128002220	-0.66115543916134	h
-1.59127844497517	4.89745147316195	0.17243711001667	c
-3.48544726849592	5.23208512493305	-0.66115543916134	h
-0.25555640196351	6.28154028415219	-0.66115543916134	h
-1.73430275813558	5.33763504719152	2.22735299224324	h
-5.14948521906982	0.00000000000000	0.17243711001667	c
-6.05307109084151	-1.69805411728550	-0.66115543916134	h
-6.05307109084151	1.69805411728550	-0.66115543916134	h
-5.61232161889210	0.00000000000000	2.22735299224324	h
-1.59127844497517	-4.89745147316195	0.17243711001667	c
-1.73430275813558	-5.33763504719152	2.22735299224324	h
-0.25555640196351	-6.28154028415219	-0.66115543916134	h
-3.48544726849592	-5.23208512493305	-0.66115543916134	h
0.00000000000000	0.00000000000000	-4.53569401295223	pb

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	e1	113.55	0.05955	YES	YES
8	e1	113.55	0.05955	YES	YES
9	a1	131.16	0.49690	YES	YES
10	e2	137.41	0.00000	NO	YES
11	e2	137.41	0.00000	NO	YES
12	a2	138.05	0.00000	NO	NO
13	e1	142.87	0.51063	YES	YES
14	e1	142.87	0.51063	YES	YES
15	e2	144.50	0.00000	NO	YES
16	e2	144.50	0.00000	NO	YES
17	e1	275.83	0.46870	YES	YES
18	e1	275.83	0.46870	YES	YES
19	e2	281.76	0.00000	NO	YES
20	e2	281.76	0.00000	NO	YES
21	a1	296.46	28.19857	YES	YES
22	e1	375.73	0.13018	YES	YES
23	e1	375.73	0.13018	YES	YES
24	e2	529.90	0.00000	NO	YES
25	e2	529.90	0.00000	NO	YES
26	a2	541.36	0.00000	NO	NO
27	a1	588.10	2.46894	YES	YES
28	e2	608.12	0.00000	NO	YES
29	e2	608.12	0.00000	NO	YES
30	e1	794.90	3.33255	YES	YES
31	e1	794.90	3.33255	YES	YES
32	e2	927.30	0.00000	NO	YES
33	e2	927.30	0.00000	NO	YES
34	e1	1000.12	15.61629	YES	YES
35	e1	1000.12	15.61629	YES	YES
36	a1	1004.57	6.45452	YES	YES
37	e2	1005.83	0.00000	NO	YES
38	e2	1005.83	0.00000	NO	YES
39	e1	1057.09	5.21260	YES	YES
40	e1	1057.09	5.21260	YES	YES
41	a2	1085.20	0.00000	NO	NO
42	e2	1153.37	0.00000	NO	YES
43	e2	1153.37	0.00000	NO	YES
44	e2	1346.57	0.00000	NO	YES
45	e2	1346.57	0.00000	NO	YES
46	e1	1365.35	8.25819	YES	YES
47	e1	1365.35	8.25819	YES	YES
48	a1	1367.31	9.21019	YES	YES
49	e2	1383.50	0.00000	NO	YES
50	e2	1383.50	0.00000	NO	YES
51	e1	1399.95	2.29487	YES	YES
52	e1	1399.95	2.29487	YES	YES
53	a1	1405.45	71.32890	YES	YES
54	a2	1413.09	0.00000	NO	NO

55	e2	1417.16	0.00000	NO	YES
56	e2	1417.16	0.00000	NO	YES
57	e1	1425.76	1.39181	YES	YES
58	e1	1425.76	1.39181	YES	YES
59	a1	1441.86	31.61357	YES	YES
60	e2	1445.77	0.00000	NO	YES
61	e2	1445.77	0.00000	NO	YES
62	e1	1462.31	61.67713	YES	YES
63	e1	1462.31	61.67713	YES	YES
64	e2	2947.97	0.00000	NO	YES
65	e2	2947.97	0.00000	NO	YES
66	e1	2948.03	7.44728	YES	YES
67	e1	2948.03	7.44728	YES	YES
68	a1	2948.11	0.74382	YES	YES
69	e1	3029.11	6.37369	YES	YES
70	e1	3029.11	6.37369	YES	YES
71	a1	3029.15	0.23874	YES	YES
72	e2	3029.84	0.00000	NO	YES
73	e2	3029.84	0.00000	NO	YES
74	a2	3061.93	0.00000	NO	NO
75	e1	3062.87	8.36499	YES	YES
76	e1	3062.87	8.36499	YES	YES
77	e2	3063.18	0.00000	NO	YES
78	e2	3063.18	0.00000	NO	YES

$PbCp^*_2$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

-0.00000000000000	0.00000000000000	1.34955689358885	pb
4.21274628102858	3.35919514969575	0.29676948084204	c
3.69016344272230	1.85995925909786	-1.92460547857403	c
4.49441290167835	-0.69955830567832	-1.41263309642706	c
5.50947958796139	-0.76382474049137	1.11893164564893	c
5.33444846156177	1.73344275243950	2.16286031407874	c
-5.50947958796139	0.76382474049137	1.11893164564893	c
-4.49441290167835	0.69955830567832	-1.41263309642706	c
-3.69016344272230	-1.85995925909786	-1.92460547857403	c
-4.21274628102858	-3.35919514969573	0.29676948084204	c
-5.33444846156177	-1.73344275243950	2.16286031407874	c
-3.86375079652109	-6.17203404615777	0.51422892889697	c
-2.81347150216372	-2.86118711260346	-4.43740018669911	c
-4.56008993136629	2.83071850106515	-3.29332198854803	c
-6.28698869247574	-2.54215489555919	4.71750242465455	c
-6.71997098408365	3.01680521100618	2.36020355875048	c
6.28698869247574	2.54215489555919	4.71750242465455	c
6.71997098408365	-3.01680521100618	2.36020355875048	c
4.56008993136629	-2.83071850106515	-3.29332198854803	c
2.81347150216372	2.86118711260346	-4.43740018669911	c
3.86375079652109	6.17203404615777	0.51422892889697	c
2.26218256814924	6.86015968081939	-0.65909861905281	h

5.58058961487096	7.21791442424319	-0.12753006368060	h
3.49553488775957	6.77133121473771	2.49422167914947	h
1.50144859567493	4.48685666283175	-4.22448870345223	h
1.81697887998095	1.39388644046306	-5.56178113686021	h
4.43511157203340	3.53266993278450	-5.60870766302990	h
3.04757400343534	-2.64800844667565	-4.73775751141606	h
4.32414373822173	-4.70423259071638	-2.37228594445438	h
6.39647421470651	-2.88992412122907	-4.33087544892795	h
5.88813323871642	-4.82655617874594	1.69159977940088	h
6.52211790028197	-2.96726493187435	4.45185608379940	h
8.78767521134056	-3.11183430040567	1.95010053813072	h
5.19679181387221	4.16548057931703	5.48676515663656	h
8.30610677251334	3.14897711395991	4.64283723220676	h
6.17585535590724	0.98767101918010	6.12783057213248	h
-5.88813323871641	4.82655617874594	1.69159977940088	h
-6.52211790028197	2.96726493187435	4.45185608379940	h
-8.78767521134056	3.11183430040567	1.95010053813072	h
-4.32414373822173	4.70423259071638	-2.37228594445438	h
-6.39647421470651	2.88992412122907	-4.33087544892795	h
-3.04757400343534	2.64800844667565	-4.73775751141606	h
-1.81697887998095	-1.39388644046306	-5.56178113686021	h
-4.43511157203340	-3.53266993278450	-5.60870766302990	h
-1.50144859567493	-4.48685666283175	-4.22448870345223	h
-2.26218256814924	-6.86015968081939	-0.65909861905281	h
-5.58058961487096	-7.21791442424319	-0.12753006368060	h
-3.49553488775957	-6.77133121473771	2.49422167914947	h
-6.17585535590724	-0.98767101918010	6.12783057213248	h
-5.19679181387221	-4.16548057931703	5.48676515663656	h
-8.30610677251334	-3.14897711395991	4.64283723220676	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules IR	RAMAN
7	a	9.62	0.00008	YES	YES
8	b	15.78	0.04243	YES	YES
9	a	47.32	0.12168	YES	YES
10	a	78.46	0.74954	YES	YES
11	b	82.44	0.36416	YES	YES
12	b	84.58	0.72776	YES	YES
13	a	86.87	0.00944	YES	YES
14	a	92.92	0.03991	YES	YES
15	b	93.34	0.04205	YES	YES
16	b	111.18	0.20681	YES	YES
17	a	111.68	0.03091	YES	YES
18	b	117.06	9.56877	YES	YES
19	a	125.65	0.06003	YES	YES
20	b	130.82	0.14154	YES	YES
21	b	132.16	0.34040	YES	YES
22	a	133.67	0.14771	YES	YES
23	a	138.11	0.00136	YES	YES

24	b	139.08	0.09160	YES	YES
25	a	141.55	0.00109	YES	YES
26	b	141.68	0.03394	YES	YES
27	a	153.00	0.00725	YES	YES
28	a	162.73	0.01952	YES	YES
29	b	167.82	0.00559	YES	YES
30	b	239.52	223.91614	YES	YES
31	b	271.82	2.52470	YES	YES
32	a	272.74	0.40767	YES	YES
33	a	274.61	1.41311	YES	YES
34	b	275.80	4.13980	YES	YES
35	a	279.36	0.00184	YES	YES
36	b	280.00	0.03862	YES	YES
37	a	283.91	0.01779	YES	YES
38	b	286.97	0.35796	YES	YES
39	a	309.75	0.27679	YES	YES
40	b	310.21	0.29422	YES	YES
41	b	355.88	16.01935	YES	YES
42	a	358.30	3.45424	YES	YES
43	a	361.31	0.00304	YES	YES
44	a	534.60	0.00027	YES	YES
45	b	536.61	0.36771	YES	YES
46	b	539.79	0.17312	YES	YES
47	a	540.55	0.01254	YES	YES
48	a	544.44	0.00147	YES	YES
49	b	544.49	0.02547	YES	YES
50	b	589.33	12.25612	YES	YES
51	a	590.94	0.08163	YES	YES
52	a	599.65	0.05973	YES	YES
53	b	608.71	0.41113	YES	YES
54	b	626.90	0.30721	YES	YES
55	a	630.92	0.38999	YES	YES
56	b	798.03	4.42598	YES	YES
57	a	799.49	3.08282	YES	YES
58	a	801.35	0.82278	YES	YES
59	b	802.23	0.68956	YES	YES
60	a	926.06	0.01886	YES	YES
61	b	929.65	0.25694	YES	YES
62	b	934.44	0.32997	YES	YES
63	a	935.83	0.04458	YES	YES
64	b	1006.95	20.89730	YES	YES
65	a	1007.03	12.22497	YES	YES
66	b	1008.23	13.48747	YES	YES
67	a	1008.50	3.19326	YES	YES
68	b	1016.42	3.65017	YES	YES
69	a	1019.03	2.69913	YES	YES
70	a	1020.66	1.80941	YES	YES
71	b	1021.04	0.08022	YES	YES
72	b	1024.59	0.06875	YES	YES
73	a	1024.70	0.00451	YES	YES
74	b	1055.04	5.19631	YES	YES
75	a	1055.35	2.77806	YES	YES
76	b	1056.87	3.44549	YES	YES

77	a	1057.01	1.20878	YES	YES
78	b	1085.65	0.04058	YES	YES
79	a	1086.27	0.00005	YES	YES
80	a	1152.24	0.00488	YES	YES
81	b	1155.50	1.80516	YES	YES
82	b	1165.29	0.22493	YES	YES
83	a	1166.55	0.09724	YES	YES
84	b	1348.70	1.64047	YES	YES
85	a	1349.43	0.00017	YES	YES
86	a	1353.73	0.00183	YES	YES
87	b	1355.47	1.02446	YES	YES
88	b	1362.77	0.06234	YES	YES
89	a	1363.48	0.11924	YES	YES
90	a	1365.95	0.36282	YES	YES
91	b	1366.02	50.45289	YES	YES
92	b	1368.22	22.36403	YES	YES
93	a	1374.54	0.87671	YES	YES
94	a	1383.97	0.00488	YES	YES
95	b	1386.15	0.05211	YES	YES
96	a	1390.19	0.32994	YES	YES
97	b	1390.59	0.34247	YES	YES
98	a	1410.96	1.91330	YES	YES
99	b	1413.23	18.65889	YES	YES
100	a	1414.81	4.24016	YES	YES
101	b	1415.01	5.66182	YES	YES
102	b	1416.18	23.29853	YES	YES
103	a	1416.72	8.45179	YES	YES
104	a	1418.12	0.43401	YES	YES
105	b	1420.19	18.46819	YES	YES
106	b	1420.97	20.65820	YES	YES
107	b	1422.26	43.38654	YES	YES
108	a	1423.10	0.00322	YES	YES
109	b	1423.64	3.13847	YES	YES
110	a	1423.70	6.21111	YES	YES
111	a	1424.84	0.61414	YES	YES
112	b	1428.07	2.27173	YES	YES
113	a	1428.14	4.25470	YES	YES
114	b	1443.44	3.88945	YES	YES
115	a	1446.23	0.24073	YES	YES
116	a	1448.66	0.15649	YES	YES
117	b	1451.11	0.53203	YES	YES
118	b	1453.45	0.15743	YES	YES
119	a	1456.81	0.19981	YES	YES
120	b	1476.52	23.35932	YES	YES
121	a	1481.36	0.00011	YES	YES
122	a	1483.28	17.50610	YES	YES
123	b	1486.11	0.11513	YES	YES
124	a	2914.71	1.63914	YES	YES
125	b	2914.77	102.96071	YES	YES
126	b	2915.02	81.07344	YES	YES
127	a	2915.21	11.25805	YES	YES
128	a	2916.04	40.53166	YES	YES
129	b	2916.05	29.13613	YES	YES

130	b	2916.42	109.00450	YES	YES
131	a	2916.49	140.20608	YES	YES
132	b	2917.38	153.88059	YES	YES
133	a	2919.01	19.20279	YES	YES
134	b	2986.69	14.17564	YES	YES
135	a	2987.01	23.98806	YES	YES
136	a	2987.62	0.00000	YES	YES
137	b	2987.90	10.75335	YES	YES
138	b	2988.68	2.83603	YES	YES
139	a	2988.96	0.30634	YES	YES
140	b	2992.19	19.89420	YES	YES
141	a	2992.46	0.27451	YES	YES
142	b	2994.51	3.91781	YES	YES
143	a	2994.55	0.00707	YES	YES
144	a	3021.84	0.65488	YES	YES
145	b	3021.89	33.09600	YES	YES
146	a	3023.18	4.82198	YES	YES
147	b	3023.25	1.77281	YES	YES
148	b	3023.80	10.50910	YES	YES
149	a	3023.92	42.92207	YES	YES
150	b	3030.69	33.87527	YES	YES
151	a	3031.08	1.90886	YES	YES
152	a	3034.01	15.25990	YES	YES
153	b	3034.17	6.63372	YES	YES

dmap

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

0.00000000000000	0.00000000000000	5.89792762479475	n
0.00000000000000	-2.15028204090009	4.54218300667464	c
0.00000000000000	-2.27943016799427	1.89988467859110	c
0.00000000000000	0.00000000000000	0.46910364484354	c
0.00000000000000	2.27943016799427	1.89988467859110	c
0.00000000000000	2.15028204090009	4.54218300667464	c
0.00000000000000	0.00000000000000	-2.13587522635005	n
0.00000000000000	2.38080928104964	-3.50112545412983	c
0.00000000000000	-2.38080928104964	-3.50112545412983	c
0.00000000000000	-1.99852354397876	-5.55942738501177	h
-1.70348540367989	-3.54271967968016	-3.05855782932803	h
1.70348540367989	-3.54271967968016	-3.05855782932803	h
1.70348540367989	3.54271967968016	-3.05855782932803	h
-1.70348540367989	3.54271967968016	-3.05855782932803	h
0.00000000000000	1.99852354397876	-5.55942738501177	h
0.00000000000000	4.14116113248648	0.97865788028414	h
0.00000000000000	3.93026530469192	5.64136491060365	h
0.00000000000000	-3.93026530469192	5.64136491060365	h
0.00000000000000	-4.14116113248648	0.97865788028414	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	b1	70.88	0.53657	YES	YES
8	a2	90.80	0.00000	NO	YES
9	b1	143.25	0.00242	YES	YES
10	a2	204.89	0.00000	NO	YES
11	b2	245.91	0.15965	YES	YES
12	b1	284.75	5.43474	YES	YES
13	a1	378.30	1.06656	YES	YES
14	a2	389.78	0.00000	NO	YES
15	b2	472.10	3.09033	YES	YES
16	b1	534.11	13.24794	YES	YES
17	a1	538.73	2.35162	YES	YES
18	b2	663.79	0.36704	YES	YES
19	b1	735.34	0.41794	YES	YES
20	a1	752.49	6.31606	YES	YES
21	b1	797.85	38.93292	YES	YES
22	a2	807.42	0.00000	NO	YES
23	b1	930.94	0.12392	YES	YES
24	a2	953.85	0.00000	NO	YES
25	a1	959.22	11.16178	YES	YES
26	a1	976.34	35.94850	YES	YES
27	b2	1055.26	21.68037	YES	YES
28	a1	1067.04	0.49812	YES	YES
29	b2	1101.32	2.15470	YES	YES
30	b1	1110.87	0.23327	YES	YES
31	a2	1118.49	0.00000	NO	YES
32	a1	1166.84	0.00168	YES	YES
33	a1	1220.17	19.14186	YES	YES
34	b2	1256.81	42.03177	YES	YES
35	b2	1334.78	15.56656	YES	YES
36	b2	1348.05	2.40777	YES	YES
37	a1	1371.41	59.97813	YES	YES
38	b2	1398.15	0.94125	YES	YES
39	a2	1419.46	0.00000	NO	YES
40	b1	1428.31	14.42949	YES	YES
41	b2	1432.19	0.04115	YES	YES
42	a1	1441.13	12.63110	YES	YES
43	b2	1462.03	4.27798	YES	YES
44	a1	1472.78	61.98874	YES	YES
45	a1	1516.60	99.51850	YES	YES
46	b2	1558.57	42.45154	YES	YES
47	a1	1618.69	297.57535	YES	YES
48	b2	2903.70	93.36678	YES	YES
49	a1	2912.62	52.15441	YES	YES
50	a2	2964.05	0.00000	NO	YES
51	b1	2965.04	64.44986	YES	YES
52	b2	3052.17	51.66993	YES	YES
53	a1	3055.66	24.20147	YES	YES
54	b2	3055.81	0.40954	YES	YES

55	a1	3064.09	21.05970	YES	YES
56	a1	3131.03	3.44113	YES	YES
57	b2	3131.42	16.99924	YES	YES

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

0.00000000000000	0.00000000000000	5.89775017208916	n
0.00000000000000	-2.15040723286183	4.54190943657188	c
0.00000000000000	-2.27942184977459	1.89946130552798	c
0.00000000000000	0.00000000000000	0.46884136975548	c
0.00000000000000	2.27942184977459	1.89946130552798	c
0.00000000000000	2.15040723286183	4.54190943657188	c
0.00000000000000	0.00000000000000	-2.13606113605054	n
0.00000000000000	2.38007574350887	-3.50098407483286	c
0.00000000000000	-2.38007574350887	-3.50098407483286	c
0.00000000000000	-1.99822274031072	-5.55926065109368	h
-1.70331004742666	-3.54237276919379	-3.05801252601572	h
1.70331004742666	-3.54237276919379	-3.05801252601572	h
1.70331004742666	3.54237276919379	-3.05801252601572	h
-1.70331004742666	3.54237276919379	-3.05801252601572	h
0.00000000000000	1.99822274031072	-5.55926065109368	h
0.00000000000000	4.14109216585072	0.97849254438064	h
0.00000000000000	3.93047251243325	5.64114128858042	h
0.00000000000000	-3.93047251243325	5.64114128858042	h
0.00000000000000	-4.14109216585072	0.97849254438064	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	b1	66.73	0.61673	YES	YES
8	a2	78.16	0.00000	NO	YES
9	b1	140.89	0.01018	YES	YES
10	a2	206.45	0.00000	NO	YES
11	b2	245.94	0.15335	YES	YES
12	b1	278.58	5.21054	YES	YES
13	a1	378.38	1.03336	YES	YES
14	a2	389.92	0.00000	NO	YES
15	b2	471.52	3.04606	YES	YES
16	b1	533.94	13.24675	YES	YES
17	a1	537.05	2.41303	YES	YES
18	b2	663.83	0.36815	YES	YES
19	b1	735.51	0.42494	YES	YES
20	a1	752.39	6.32518	YES	YES
21	b1	798.17	38.91798	YES	YES
22	a2	807.87	0.00000	NO	YES
23	b1	931.26	0.11500	YES	YES
24	a2	954.10	0.00000	NO	YES
25	a1	958.59	9.99589	YES	YES
26	a1	976.56	36.53860	YES	YES

27	b2	1051.05	22.03879	YES	YES
28	a1	1067.37	0.43634	YES	YES
29	b2	1101.81	2.08294	YES	YES
30	b1	1106.43	0.16502	YES	YES
31	a2	1112.62	0.00000	NO	YES
32	a1	1165.20	0.01004	YES	YES
33	a1	1220.25	19.28709	YES	YES
34	b2	1257.86	42.15005	YES	YES
35	b2	1334.66	16.41789	YES	YES
36	b2	1347.15	1.59913	YES	YES
37	a1	1370.37	63.19062	YES	YES
38	b2	1392.46	1.03446	YES	YES
39	a2	1416.58	0.00000	NO	YES
40	b1	1425.73	14.52299	YES	YES
41	b2	1430.31	0.02717	YES	YES
42	a1	1435.84	12.64510	YES	YES
43	b2	1461.93	4.04323	YES	YES
44	a1	1472.56	55.44751	YES	YES
45	a1	1515.88	101.69698	YES	YES
46	b2	1557.77	42.33238	YES	YES
47	a1	1617.73	299.21701	YES	YES
48	b2	2902.06	93.69845	YES	YES
49	a1	2910.99	52.15150	YES	YES
50	a2	2962.37	0.00000	NO	YES
51	b1	2963.36	64.86850	YES	YES
52	b2	3051.59	51.61901	YES	YES
53	a1	3055.09	23.83725	YES	YES
54	b2	3055.89	0.53238	YES	YES
55	a1	3064.47	21.45828	YES	YES
56	a1	3131.85	3.46728	YES	YES
57	b2	3132.27	16.87375	YES	YES

$[Si(dmap)_4]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

1.72519823909930	-4.11284126159181	-1.43203597039279	n
1.60646828184185	-12.05580270883545	-2.10550737038344	n
1.05173211435834	-5.61592577341569	0.53599715731615	c
0.98146130092981	-8.23360267315894	0.41352587866297	c
1.63396110181136	-9.49990076630659	-1.89242041862162	c
2.33449064093425	-7.88541861456310	-3.95093724613840	c
2.36086914273450	-5.28683260841473	-3.62406234875143	c
0.91223416054783	-13.62367707413717	0.06168114285140	c
2.31030038355641	-13.25632822994030	-4.49534541949734	c
-1.50373319697021	-0.00458828906198	-2.40220296998231	n
-9.02318440938025	-0.43026188452285	-4.96621708463681	n
-3.31477914152141	-1.23174574298021	-1.03894289755904	c
-5.80826400090409	-1.40840792116029	-1.80147823991036	c
-6.60863437404938	-0.28615530232208	-4.13795704266142	c
-4.67159984973098	0.99188029837718	-5.54447731138742	c

-2.22613429251483	1.07443407423988	-4.63757326817276	c
-10.93107499028164	-1.77074313020803	-3.47441484403581	c
-9.74149396575382	0.72771359903852	-7.37739882547529	c
1.75145872448534	4.08801857389753	-1.48258485129734	n
2.48774479115790	12.02402970101466	-1.29346083959804	n
4.03212069644461	5.23433193605052	-1.74961607974338	c
4.38012988936345	7.82951899087899	-1.68277861460414	c
2.25257584456037	9.47036571205444	-1.34275876973195	c
-0.14425736656717	8.23292932730399	-1.07613399238479	c
-0.28353890311154	5.61625311170067	-1.15327487341485	c
4.97441329703321	13.19419834207307	-1.60249084089186	c
0.25361574778170	13.61977366654151	-0.97894238402210	c
2.09698330283199	0.00277654904039	1.89645198890462	n
3.28669135670232	0.47234125644405	9.74842738141874	n
4.17487386691747	-1.05981213041791	3.00780914645455	c
4.63464016688671	-0.96161139157681	5.57468959836374	c
2.90016568274763	0.31453503078044	7.22596345689099	c
0.73608918194849	1.41928365403828	6.01928445268169	c
0.42820767778293	1.22886991838940	3.43095260185750	c
5.54237720520631	-0.66185590516912	10.88703263870360	c
1.46988654631829	1.80526674281875	11.35621545562569	c
2.12672124214235	-0.01728790435949	-1.78571092896252	si
-0.71672366884109	2.02752127204661	-5.71147758784044	h
1.32147700919633	3.83317033343621	10.82025056902495	h
2.10718232388211	1.70454249243159	13.34335900312310	h
-0.43654884138435	0.92673279306862	11.23936111324895	h
5.59620655380947	-2.73821874603444	10.56265597757447	h
5.51175210456923	-0.32915375021604	12.94939097272069	h
7.29898777775217	0.19573975222459	10.11342928493803	h
0.83508753139085	15.62707013852459	-0.98384443590854	h
-0.71580893887597	13.22983759930152	0.84663294477219	h
-1.11931606381437	13.33756042663535	-2.54798501579942	h
5.82153364135799	12.71401626888483	-3.46698251667838	h
6.29742231024211	12.59022266784396	-0.08348153378601	h
4.77485351318210	15.27174850096501	-1.49767686635800	h
-8.67796599208875	-0.12402622172839	-8.97845272397998	h
-9.39904751436875	2.80170024109129	-7.35677267383048	h
-11.77952223180973	0.41143747694225	-7.71088341964651	h
-12.77126407285288	-1.66612887003315	-4.45823480741943	h
-11.15925767213792	-0.90183173096532	-1.57355640743189	h
-10.42986837227909	-3.79958987777059	-3.24229711523346	h
4.29260746342337	-12.79816061949848	-5.02894360402746	h
1.03459986445499	-12.65739483004607	-6.05624309255406	h
2.15661510446274	-15.33074751473273	-4.29459368962468	h
1.00352155283459	-15.63777229365398	-0.48822750767235	h
-1.04798774393961	-13.21552413204985	0.70677427308728	h
2.23026455057101	-13.33064243594864	1.67508997981215	h
-2.13369617735227	4.67535650114214	-0.96543040745898	h
-1.89741775026158	9.31237402247374	-0.82031007416984	h
6.29925745453638	8.57761354828647	-1.92788321838320	h
5.64857468823065	3.94905968405850	-2.06109679692112	h
-2.69825940529259	-2.11305661433444	0.73794840999648	h
-7.13383752186998	-2.43648089675937	-0.58226096148281	h

-5.07177255260555	1.90677352542849	-7.36173162772384	h
2.94627376778721	-4.02209290882569	-5.17941260497053	h
2.88926443749136	-8.65679259498410	-5.79485025444916	h
0.56322043954499	-4.65266642973226	2.31833889436958	h
0.42974588811109	-9.29133132786803	2.11083200077175	h
-1.21537690920740	2.09752273946828	2.50465196878323	h
-0.70381975307457	2.44527049887610	7.10315020979384	h
6.35706301070069	-1.86417612619198	6.29473869786003	h
5.50326409918559	-2.01320373429601	1.71671717599913	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a	14.28	0.34707	YES	YES
8	a	14.76	0.01545	YES	YES
9	a	19.37	0.01701	YES	YES
10	a	20.29	0.00536	YES	YES
11	a	23.71	0.25093	YES	YES
12	a	29.00	1.72183	YES	YES
13	a	37.42	0.01358	YES	YES
14	a	44.13	1.77513	YES	YES
15	a	51.10	0.02131	YES	YES
16	a	71.35	0.02530	YES	YES
17	a	74.73	7.24679	YES	YES
18	a	79.78	0.18812	YES	YES
19	a	81.53	0.05985	YES	YES
20	a	87.81	0.19721	YES	YES
21	a	97.86	7.95215	YES	YES
22	a	102.54	2.91268	YES	YES
23	a	103.86	52.54489	YES	YES
24	a	108.09	2.39734	YES	YES
25	a	110.32	0.09275	YES	YES
26	a	123.45	0.63278	YES	YES
27	a	126.06	0.94655	YES	YES
28	a	126.27	0.46761	YES	YES
29	a	129.66	0.75952	YES	YES
30	a	137.13	3.87255	YES	YES
31	a	141.36	0.32377	YES	YES
32	a	153.52	0.27468	YES	YES
33	a	171.91	102.54558	YES	YES
34	a	173.33	1.42727	YES	YES
35	a	180.61	7.80007	YES	YES
36	a	185.45	22.41501	YES	YES
37	a	186.50	2.39862	YES	YES
38	a	187.50	1.02452	YES	YES
39	a	193.10	5.55527	YES	YES
40	a	234.69	0.16546	YES	YES
41	a	244.14	69.44754	YES	YES
42	a	256.18	0.00811	YES	YES
43	a	265.77	0.63402	YES	YES

44	a	281.95	35.35375	YES	YES
45	a	284.13	1.33498	YES	YES
46	a	301.51	0.45496	YES	YES
47	a	302.72	2.57376	YES	YES
48	a	326.79	0.62687	YES	YES
49	a	328.30	44.70047	YES	YES
50	a	346.30	184.03949	YES	YES
51	a	389.13	0.84699	YES	YES
52	a	391.52	58.88501	YES	YES
53	a	394.45	3.07932	YES	YES
54	a	414.44	1.41919	YES	YES
55	a	421.30	0.05703	YES	YES
56	a	425.34	2.11399	YES	YES
57	a	426.37	3.54202	YES	YES
58	a	438.17	51.88440	YES	YES
59	a	447.27	28.83070	YES	YES
60	a	480.18	0.35886	YES	YES
61	a	482.15	0.11122	YES	YES
62	a	482.71	0.86352	YES	YES
63	a	489.44	0.82451	YES	YES
64	a	526.78	40.86647	YES	YES
65	a	531.64	13.57167	YES	YES
66	a	535.62	49.50558	YES	YES
67	a	536.73	1.31017	YES	YES
68	a	545.71	0.41628	YES	YES
69	a	546.13	55.85387	YES	YES
70	a	567.61	13.11351	YES	YES
71	a	572.24	34.32870	YES	YES
72	a	653.55	2.63062	YES	YES
73	a	654.71	0.00212	YES	YES
74	a	657.39	0.38717	YES	YES
75	a	658.30	0.05621	YES	YES
76	a	722.07	1.66753	YES	YES
77	a	722.88	0.12066	YES	YES
78	a	727.47	5.64685	YES	YES
79	a	727.77	1.48219	YES	YES
80	a	757.90	0.71484	YES	YES
81	a	758.67	11.61337	YES	YES
82	a	764.46	0.71007	YES	YES
83	a	766.51	1.23197	YES	YES
84	a	796.91	7.54654	YES	YES
85	a	801.98	2.60822	YES	YES
86	a	808.23	5.54716	YES	YES
87	a	808.76	10.17697	YES	YES
88	a	813.86	56.26323	YES	YES
89	a	814.87	32.13764	YES	YES
90	a	816.09	50.77450	YES	YES
91	a	816.90	3.11034	YES	YES
92	a	926.33	3.50128	YES	YES
93	a	935.48	0.02110	YES	YES
94	a	940.24	3.46786	YES	YES
95	a	941.02	0.26612	YES	YES
96	a	944.57	2.84908	YES	YES

97	a	944.78	1.28150	YES	YES
98	a	945.10	0.28964	YES	YES
99	a	947.25	0.06253	YES	YES
100	a	947.39	3.21856	YES	YES
101	a	947.93	0.26082	YES	YES
102	a	953.44	1.52152	YES	YES
103	a	953.83	0.39672	YES	YES
104	a	987.36	320.04388	YES	YES
105	a	988.24	39.68437	YES	YES
106	a	1008.86	37.48313	YES	YES
107	a	1009.74	133.82505	YES	YES
108	a	1045.56	8.05132	YES	YES
109	a	1045.79	14.83709	YES	YES
110	a	1046.99	14.21520	YES	YES
111	a	1047.30	17.09834	YES	YES
112	a	1048.69	167.83388	YES	YES
113	a	1050.75	31.43812	YES	YES
114	a	1052.92	269.75150	YES	YES
115	a	1058.76	18.78636	YES	YES
116	a	1090.52	0.00100	YES	YES
117	a	1090.68	0.00949	YES	YES
118	a	1095.21	0.00293	YES	YES
119	a	1095.41	0.00602	YES	YES
120	a	1108.24	0.15277	YES	YES
121	a	1108.47	0.09312	YES	YES
122	a	1108.51	0.18793	YES	YES
123	a	1108.60	0.10155	YES	YES
124	a	1115.09	1.54204	YES	YES
125	a	1118.21	0.30832	YES	YES
126	a	1119.80	10.28841	YES	YES
127	a	1122.99	2.84086	YES	YES
128	a	1163.52	1.50824	YES	YES
129	a	1163.67	0.63542	YES	YES
130	a	1164.11	0.56032	YES	YES
131	a	1164.26	1.27892	YES	YES
132	a	1206.03	26.27735	YES	YES
133	a	1207.05	141.00594	YES	YES
134	a	1208.44	145.28431	YES	YES
135	a	1218.87	0.35871	YES	YES
136	a	1231.39	16.89423	YES	YES
137	a	1231.52	18.88506	YES	YES
138	a	1236.84	17.82330	YES	YES
139	a	1236.91	28.13166	YES	YES
140	a	1317.28	1.70959	YES	YES
141	a	1318.48	14.06913	YES	YES
142	a	1320.81	14.67236	YES	YES
143	a	1321.81	28.30728	YES	YES
144	a	1339.65	14.77838	YES	YES
145	a	1344.10	35.37687	YES	YES
146	a	1346.33	26.91865	YES	YES
147	a	1346.71	5.78100	YES	YES
148	a	1383.20	130.67296	YES	YES
149	a	1383.88	9.66795	YES	YES

150	a	1387.39	23.02669	YES	YES
151	a	1387.72	93.75718	YES	YES
152	a	1394.53	1.16805	YES	YES
153	a	1394.77	1.50330	YES	YES
154	a	1394.88	1.14249	YES	YES
155	a	1395.34	0.79109	YES	YES
156	a	1423.22	0.01349	YES	YES
157	a	1423.29	0.02512	YES	YES
158	a	1423.65	0.03230	YES	YES
159	a	1423.79	0.04875	YES	YES
160	a	1429.60	42.63690	YES	YES
161	a	1429.90	26.83476	YES	YES
162	a	1431.81	40.66938	YES	YES
163	a	1432.14	24.01813	YES	YES
164	a	1436.78	27.45791	YES	YES
165	a	1436.83	28.09381	YES	YES
166	a	1438.18	29.51746	YES	YES
167	a	1438.34	29.27402	YES	YES
168	a	1442.53	0.56863	YES	YES
169	a	1442.58	0.45134	YES	YES
170	a	1444.15	1.15350	YES	YES
171	a	1444.35	0.61408	YES	YES
172	a	1464.19	73.04457	YES	YES
173	a	1464.44	25.53603	YES	YES
174	a	1465.59	84.93846	YES	YES
175	a	1465.65	20.73994	YES	YES
176	a	1482.43	2.22776	YES	YES
177	a	1482.57	5.07865	YES	YES
178	a	1499.22	12.08497	YES	YES
179	a	1499.87	3.21364	YES	YES
180	a	1518.65	18.11298	YES	YES
181	a	1519.75	6.67136	YES	YES
182	a	1527.81	15.15814	YES	YES
183	a	1529.07	30.42929	YES	YES
184	a	1549.00	285.83809	YES	YES
185	a	1549.30	15.97924	YES	YES
186	a	1558.28	279.81854	YES	YES
187	a	1558.63	66.21124	YES	YES
188	a	1643.59	1073.55625	YES	YES
189	a	1644.87	67.14167	YES	YES
190	a	1654.83	876.34190	YES	YES
191	a	1658.34	218.86549	YES	YES
192	a	2937.40	32.87904	YES	YES
193	a	2937.58	33.58113	YES	YES
194	a	2943.64	53.89125	YES	YES
195	a	2943.77	19.42966	YES	YES
196	a	2944.24	19.49591	YES	YES
197	a	2944.27	28.07043	YES	YES
198	a	2949.50	45.00827	YES	YES
199	a	2949.60	8.77117	YES	YES
200	a	3010.38	8.35846	YES	YES
201	a	3010.76	8.00848	YES	YES
202	a	3015.06	11.41265	YES	YES

203	a	3015.35	11.12007	YES	YES
204	a	3020.73	4.44878	YES	YES
205	a	3020.74	4.74840	YES	YES
206	a	3023.76	8.58556	YES	YES
207	a	3023.83	8.83228	YES	YES
208	a	3079.51	4.09154	YES	YES
209	a	3080.35	3.08029	YES	YES
210	a	3086.46	0.29623	YES	YES
211	a	3086.52	0.31028	YES	YES
212	a	3091.30	0.14951	YES	YES
213	a	3091.32	0.15118	YES	YES
214	a	3094.53	4.50571	YES	YES
215	a	3094.58	3.58920	YES	YES
216	a	3097.77	4.69805	YES	YES
217	a	3099.10	7.22365	YES	YES
218	a	3099.44	2.43465	YES	YES
219	a	3099.46	1.40629	YES	YES
220	a	3113.87	0.50658	YES	YES
221	a	3114.66	0.54564	YES	YES
222	a	3143.05	2.14913	YES	YES
223	a	3145.76	0.80318	YES	YES
224	a	3151.79	1.47595	YES	YES
225	a	3152.28	1.34794	YES	YES
226	a	3156.19	0.95740	YES	YES
227	a	3156.45	0.87997	YES	YES
228	a	3160.37	0.10276	YES	YES
229	a	3160.88	0.10237	YES	YES
230	a	3161.75	0.44970	YES	YES
231	a	3161.79	0.54531	YES	YES

$[Ge(dmap)_4]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

1.87837257187853	-4.43096850929110	-1.60325633342410	n
1.68709881876807	-12.38999551374359	-1.98760673772284	n
1.29306926646222	-5.85423256677447	0.44495593289337	c
1.19809059052563	-8.47623759816496	0.41949034809429	c
1.73783606471035	-9.82705438763916	-1.86697240410415	c
2.34445374258949	-8.29266124633003	-4.01417811816530	c
2.39336947044703	-5.68153372566843	-3.78039209063686	c
1.07848904513511	-13.87422717957612	0.26134424188223	c
2.28286959799913	-13.67904511341912	-4.35982677919416	c
-1.52449722984840	-0.00976056399446	-2.61916046602039	n
-9.14642632022216	-0.34172434510977	-4.85104987327395	n
-3.24018212985292	-1.39300188580047	-1.29025393572106	c
-5.76716779931802	-1.54294412106349	-1.94426640877044	c
-6.69488039166865	-0.22945362003040	-4.12965500792240	c
-4.84902879876803	1.20565329210484	-5.50487283582954	c
-2.36224049404081	1.25355925701316	-4.70538557251119	c
-10.95985252795517	-1.84290734383241	-3.39598122659167	c

-9.99592024824963	1.00809944400527	-7.11448890071420	c
1.92632990242501	4.37164822511692	-1.72130724982031	n
2.58162340717782	12.30030397125161	-1.23432392618095	n
4.18139609373130	5.55175129617725	-2.01803411390024	c
4.50433247168893	8.14979741699307	-1.86861146899005	c
2.37228394707694	9.74673667219781	-1.38349421085411	c
0.00135194546173	8.47023495708490	-1.07785879839990	c
-0.10991459123390	5.85525388697960	-1.26021843294571	c
5.03972339616741	13.51278769946565	-1.59567868900314	c
0.34701056889344	13.85101510296427	-0.75297827617624	c
2.23873972288177	-0.00120286643883	1.83594218001789	n
3.05997003594257	0.46241456707798	9.72671695572947	n
4.27378909040391	-1.03978972568231	3.02860195333523	c
4.62031737257779	-0.93965542314029	5.61681528479415	c
2.79332981432097	0.30690210219933	7.18710414362767	c
0.66851755726165	1.38214926337216	5.88689401610814	c
0.48450728972712	1.19725548339707	3.28489532701034	c
5.27897348840981	-0.63751636783362	10.96461569683023	c
1.14789119276023	1.75759657295292	11.25136336975305	c
2.36291382033291	-0.04538633681518	-2.08427482555341	ge
-0.93076341143193	2.34644271721465	-5.75295436726189	h
0.99183606865311	3.78602058419677	10.71837160917498	h
1.69166951668702	1.65749069055015	13.26602837739763	h
-0.73718199318113	0.84923480536292	11.04218263236925	h
5.37808185445277	-2.71368617359025	10.64748344914005	h
5.15401346311291	-0.30193943767534	13.02302796762241	h
7.05587679603864	0.24293757062217	10.26640703531654	h
0.90714131706938	15.86301280072187	-0.68043407866575	h
-0.54549584844693	13.36015256647892	1.08809525808852	h
-1.08610898308037	13.62948969790128	-2.27749331963236	h
5.81799197448199	13.11487349939371	-3.50939347019053	h
6.43043440446029	12.87158267825126	-0.15354067984819	h
4.82059239579773	15.58247102554805	-1.40567052018016	h
-8.99786824273813	0.32006960557011	-8.83224900806313	h
-9.68458289163500	3.07923793905522	-6.92791633515677	h
-12.04253075967346	0.68287175688003	-7.38076068115696	h
-12.85037432454078	-1.67374988247025	-4.26951820196895	h
-11.09708359888318	-1.15794014567363	-1.41277489749751	h
-10.42875301976970	-3.87766698131309	-3.38068142886495	h
4.23774310140755	-13.24030459192179	-5.00114557739601	h
0.93489375126654	-13.14300154654411	-5.88300967605513	h
2.14569942202192	-15.74473532995006	-4.07384823321970	h
1.11873763023167	-15.90692342563690	-0.22271576800655	h
-0.84453326604703	-13.41902444744787	0.98371846080509	h
2.47408109665179	-13.54490357780809	1.80100275269960	h
-1.94227814797206	4.88165695399799	-1.05114272508891	h
-1.75266631821065	9.51653500993441	-0.71329011096848	h
6.40511568924875	8.93210273802802	-2.14575761881823	h
5.81791162573178	4.31590792224364	-2.41333665637816	h
-2.51684909342468	-2.42465109458474	0.36227741497231	h
-7.01830385384756	-2.70096852883716	-0.76344860153185	h
-5.35229898754147	2.27660173495546	-7.20811468098806	h
2.88760189976391	-4.49428819322540	-5.42578942972169	h

2.79571121532642	-9.13325419980978	-5.85588455437154	h
0.89401241231471	-4.82145600318470	2.21153557847388	h
0.71803462388210	-9.46995920131468	2.17615414018808	h
-1.12713865299950	2.04105805907155	2.27954799651207	h
-0.83461821532512	2.38046192791047	6.90890135666705	h
6.31817189810197	-1.82309123957495	6.41487935059663	h
5.66753769744656	-1.99252905333120	1.80664447335736	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a	12.73	0.24453	YES	YES
8	a	13.43	0.20407	YES	YES
9	a	17.31	0.04221	YES	YES
10	a	19.39	0.00998	YES	YES
11	a	20.92	0.20508	YES	YES
12	a	24.87	1.66368	YES	YES
13	a	34.26	0.04487	YES	YES
14	a	40.54	2.37895	YES	YES
15	a	50.08	0.17948	YES	YES
16	a	68.12	0.15295	YES	YES
17	a	69.61	20.91129	YES	YES
18	a	80.72	34.72471	YES	YES
19	a	81.62	26.65650	YES	YES
20	a	83.03	0.30885	YES	YES
21	a	89.70	2.88180	YES	YES
22	a	91.98	0.62137	YES	YES
23	a	101.09	0.44403	YES	YES
24	a	102.94	1.09343	YES	YES
25	a	106.55	0.13935	YES	YES
26	a	113.28	12.12470	YES	YES
27	a	123.94	1.04664	YES	YES
28	a	127.58	0.36953	YES	YES
29	a	127.82	0.46160	YES	YES
30	a	129.09	0.82977	YES	YES
31	a	129.55	0.74480	YES	YES
32	a	137.19	41.79740	YES	YES
33	a	144.49	5.38680	YES	YES
34	a	162.52	0.35898	YES	YES
35	a	166.99	0.44699	YES	YES
36	a	182.61	0.02257	YES	YES
37	a	186.07	0.05202	YES	YES
38	a	188.12	0.05950	YES	YES
39	a	191.78	0.09308	YES	YES
40	a	203.71	22.80252	YES	YES
41	a	208.40	6.31363	YES	YES
42	a	214.70	18.23903	YES	YES
43	a	236.25	1.33882	YES	YES
44	a	259.44	1.69839	YES	YES
45	a	269.43	1.84450	YES	YES

46	a	271.92	7.33062	YES	YES
47	a	291.13	0.05794	YES	YES
48	a	301.14	10.84831	YES	YES
49	a	307.32	4.93115	YES	YES
50	a	315.95	39.83231	YES	YES
51	a	321.61	12.56556	YES	YES
52	a	387.38	52.06765	YES	YES
53	a	395.43	1.53876	YES	YES
54	a	407.72	25.55797	YES	YES
55	a	412.40	9.20799	YES	YES
56	a	413.07	1.36123	YES	YES
57	a	417.75	0.09321	YES	YES
58	a	423.05	0.79401	YES	YES
59	a	425.93	0.16678	YES	YES
60	a	478.67	1.07137	YES	YES
61	a	479.74	2.88522	YES	YES
62	a	480.88	2.79667	YES	YES
63	a	482.56	3.24623	YES	YES
64	a	524.56	33.16942	YES	YES
65	a	527.06	12.10396	YES	YES
66	a	531.59	19.45627	YES	YES
67	a	534.01	7.30723	YES	YES
68	a	544.30	41.20582	YES	YES
69	a	549.97	0.92896	YES	YES
70	a	557.51	18.42217	YES	YES
71	a	559.55	7.70255	YES	YES
72	a	652.97	1.03962	YES	YES
73	a	654.36	0.06044	YES	YES
74	a	657.29	0.18677	YES	YES
75	a	657.66	0.05424	YES	YES
76	a	719.24	0.73090	YES	YES
77	a	719.84	0.59606	YES	YES
78	a	724.82	1.23617	YES	YES
79	a	724.97	0.65079	YES	YES
80	a	757.27	6.18447	YES	YES
81	a	759.13	0.02651	YES	YES
82	a	761.82	0.63441	YES	YES
83	a	762.35	0.59881	YES	YES
84	a	799.41	6.10775	YES	YES
85	a	803.03	2.37459	YES	YES
86	a	807.92	9.89378	YES	YES
87	a	809.46	15.39159	YES	YES
88	a	812.28	55.36551	YES	YES
89	a	812.85	28.82151	YES	YES
90	a	813.54	50.70522	YES	YES
91	a	814.72	7.90355	YES	YES
92	a	928.56	1.55196	YES	YES
93	a	933.58	0.14031	YES	YES
94	a	936.36	3.19321	YES	YES
95	a	938.31	0.41549	YES	YES
96	a	943.12	0.62409	YES	YES
97	a	944.47	1.25855	YES	YES
98	a	944.74	2.16124	YES	YES

99	a	945.82	0.02443	YES	YES
100	a	947.62	1.20772	YES	YES
101	a	948.50	1.17149	YES	YES
102	a	948.69	0.95349	YES	YES
103	a	950.26	1.13118	YES	YES
104	a	987.04	291.21625	YES	YES
105	a	993.29	15.38901	YES	YES
106	a	1001.29	153.72666	YES	YES
107	a	1004.10	38.88581	YES	YES
108	a	1045.12	13.77495	YES	YES
109	a	1045.46	14.70293	YES	YES
110	a	1047.74	14.53790	YES	YES
111	a	1048.79	13.69429	YES	YES
112	a	1050.88	188.42452	YES	YES
113	a	1053.27	125.53118	YES	YES
114	a	1053.61	99.38213	YES	YES
115	a	1063.58	4.92698	YES	YES
116	a	1091.09	0.03609	YES	YES
117	a	1091.91	0.01485	YES	YES
118	a	1096.06	0.00490	YES	YES
119	a	1096.32	0.01771	YES	YES
120	a	1108.11	0.08788	YES	YES
121	a	1108.35	0.16980	YES	YES
122	a	1108.58	0.15035	YES	YES
123	a	1109.02	0.11492	YES	YES
124	a	1115.01	1.12838	YES	YES
125	a	1117.33	0.71293	YES	YES
126	a	1118.99	7.47347	YES	YES
127	a	1121.30	2.76657	YES	YES
128	a	1162.68	0.30926	YES	YES
129	a	1162.87	0.42704	YES	YES
130	a	1164.09	0.14064	YES	YES
131	a	1164.65	0.11397	YES	YES
132	a	1206.53	50.28621	YES	YES
133	a	1208.19	101.61192	YES	YES
134	a	1209.02	179.25823	YES	YES
135	a	1218.85	1.61515	YES	YES
136	a	1231.25	18.58952	YES	YES
137	a	1231.90	18.44591	YES	YES
138	a	1237.64	18.73103	YES	YES
139	a	1237.71	27.39408	YES	YES
140	a	1319.76	3.73358	YES	YES
141	a	1322.37	0.69583	YES	YES
142	a	1323.29	22.18554	YES	YES
143	a	1323.96	17.54042	YES	YES
144	a	1344.77	14.33388	YES	YES
145	a	1347.82	22.00932	YES	YES
146	a	1349.79	18.59324	YES	YES
147	a	1350.22	16.22182	YES	YES
148	a	1383.99	155.17703	YES	YES
149	a	1385.02	12.86406	YES	YES
150	a	1386.94	38.13344	YES	YES
151	a	1387.30	92.92609	YES	YES

152	a	1394.11	1.30739	YES	YES
153	a	1394.16	1.17689	YES	YES
154	a	1395.30	0.71731	YES	YES
155	a	1396.02	0.70741	YES	YES
156	a	1422.90	0.53168	YES	YES
157	a	1423.09	0.11938	YES	YES
158	a	1423.30	0.02953	YES	YES
159	a	1423.41	0.27218	YES	YES
160	a	1430.11	28.88972	YES	YES
161	a	1430.54	28.19534	YES	YES
162	a	1433.02	53.01388	YES	YES
163	a	1433.19	1.21231	YES	YES
164	a	1436.79	27.20873	YES	YES
165	a	1437.06	28.93216	YES	YES
166	a	1437.56	28.34250	YES	YES
167	a	1437.82	28.75063	YES	YES
168	a	1442.68	0.33253	YES	YES
169	a	1442.70	0.73356	YES	YES
170	a	1444.38	0.96701	YES	YES
171	a	1444.70	0.57199	YES	YES
172	a	1464.04	58.18434	YES	YES
173	a	1464.16	44.02253	YES	YES
174	a	1465.80	125.68930	YES	YES
175	a	1466.44	7.93850	YES	YES
176	a	1478.58	3.56867	YES	YES
177	a	1479.08	3.46345	YES	YES
178	a	1495.86	6.31523	YES	YES
179	a	1496.72	4.96115	YES	YES
180	a	1522.34	26.25484	YES	YES
181	a	1523.35	7.38564	YES	YES
182	a	1531.62	15.82435	YES	YES
183	a	1532.58	33.25219	YES	YES
184	a	1547.89	247.40848	YES	YES
185	a	1548.57	13.36624	YES	YES
186	a	1556.93	202.48013	YES	YES
187	a	1557.66	100.84602	YES	YES
188	a	1640.85	1125.11597	YES	YES
189	a	1642.83	73.89964	YES	YES
190	a	1651.45	843.22028	YES	YES
191	a	1655.22	254.33302	YES	YES
192	a	2935.40	34.59784	YES	YES
193	a	2936.06	34.60988	YES	YES
194	a	2941.59	40.45255	YES	YES
195	a	2942.27	35.99528	YES	YES
196	a	2942.46	22.69371	YES	YES
197	a	2943.07	25.54740	YES	YES
198	a	2948.11	38.12409	YES	YES
199	a	2948.25	15.29476	YES	YES
200	a	3007.84	8.79435	YES	YES
201	a	3008.63	8.73166	YES	YES
202	a	3012.49	11.96795	YES	YES
203	a	3013.41	11.82304	YES	YES
204	a	3018.07	5.32739	YES	YES

205	a	3019.35	4.29631	YES	YES
206	a	3021.71	8.98215	YES	YES
207	a	3021.93	9.88117	YES	YES
208	a	3078.57	3.70896	YES	YES
209	a	3079.77	4.24805	YES	YES
210	a	3085.41	0.33447	YES	YES
211	a	3085.68	0.30097	YES	YES
212	a	3090.40	0.17538	YES	YES
213	a	3091.20	0.14171	YES	YES
214	a	3092.02	6.39080	YES	YES
215	a	3093.66	4.52365	YES	YES
216	a	3093.76	3.82331	YES	YES
217	a	3096.56	5.61687	YES	YES
218	a	3098.41	2.19359	YES	YES
219	a	3099.18	2.12406	YES	YES
220	a	3109.13	0.53537	YES	YES
221	a	3112.76	0.58673	YES	YES
222	a	3137.20	1.32627	YES	YES
223	a	3141.89	1.27837	YES	YES
224	a	3151.70	1.31706	YES	YES
225	a	3152.72	1.23899	YES	YES
226	a	3157.31	0.75774	YES	YES
227	a	3157.44	0.67604	YES	YES
228	a	3159.34	0.20436	YES	YES
229	a	3159.64	0.41280	YES	YES
230	a	3160.20	0.22506	YES	YES
231	a	3160.66	0.35910	YES	YES

$[Sn(dmap)_4]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

1.84055992553369	-5.10904333565865	-1.66659112334970	n
1.76742871800138	-13.07997115223246	-1.44113808863116	n
2.57837535157891	-6.39908818573226	0.42603630772597	c
2.57364869572772	-9.01606536684522	0.60192586896475	c
1.78299858554248	-10.51627230049197	-1.51045213197603	c
1.02139247084989	-9.12729482358973	-3.70927538411374	c
1.09543077093968	-6.50825503985453	-3.68938264117790	c
2.59403915981652	-14.41200276023668	0.83561518874234	c
0.98556493632084	-14.52570352571267	-3.66435449079501	c
-1.37403697361774	-0.15328221517665	-3.21169786771502	n
-9.04560084863006	0.73141044339230	-5.17271495534829	n
-3.15125804634172	-1.86538678495269	-2.48271255174691	c
-5.69409106920120	-1.64687495571432	-3.06671432113612	c
-6.58050774556193	0.44951189508176	-4.53878058787203	c
-4.67748781317305	2.22073779536230	-5.30444991058536	c
-2.18062531378318	1.85103516293572	-4.61563027256488	c
-10.91440872199291	-1.13673191862497	-4.35482394474202	c
-9.84771641341627	2.88308144924154	-6.71645662480186	c
2.66900522473711	4.10231035072058	-1.89383188689385	n

2.61421805749737	12.03076405055684	-1.11481159449034	n
4.21584976273171	5.59546592114235	-3.29201039655755	c
4.27356288921484	8.21180252996369	-3.11065360601794	c
2.63259210583758	9.47656725601387	-1.36712948967489	c
1.01105241318313	7.86853618179956	0.09411658810038	c
1.10435494532830	5.26806139670294	-0.23201401700511	c
4.31182954908195	13.58862043287961	-2.64439825591643	c
0.89575261866638	13.23666361612814	0.68063045790443	c
2.63150756108321	-0.27731707668309	1.84906208121810	n
2.34460499716071	0.89092963302929	9.71476261134395	n
4.59417956047304	0.80248761934482	3.11305083517085	c
4.58941434880702	1.22508615493376	5.69535347804715	c
2.43252717392847	0.52661261151952	7.18095814694840	c
0.37489130169398	-0.58233183844985	5.80680902241626	c
0.56174227653897	-0.93760684929150	3.21847474172968	c
4.50410992478673	2.00999005608198	11.03490442950669	c
0.09890576679272	0.15188760505157	11.14980221084695	c
3.02167609958222	-0.60472493597488	-2.56236540817403	sn
-0.72287047311403	3.21743141616436	-5.19802677004680	h
-1.60596855392263	1.19349042405888	10.49253579395483	h
0.39318082646247	0.60317579621579	13.16872505434992	h
-0.26490757869529	-1.91343674142864	10.99112161199607	h
6.23464086722110	0.83918438824673	10.79688437674341	h
4.07799896539321	2.12356681402545	13.07735942565533	h
4.89981191018976	3.95640171208088	10.34259735950065	h
1.15839769813908	15.30835105519600	0.59995119650405	h
1.28027960736643	12.61006555844818	2.65177208231527	h
-1.11426217337961	12.81897424262869	0.21963327317720	h
3.91706853507859	13.36496947792640	-4.69863104530318	h
6.32665365146905	13.10273547651935	-2.28702566352234	h
4.03523878395418	15.59983198512773	-2.14766772396743	h
-8.90360943330441	2.86990390564484	-8.59536860411351	h
-9.43049204671436	4.70773566547976	-5.75728159922372	h
-11.91107794578725	2.77473533184448	-7.02788665477650	h
-12.80582933527148	-0.55800123797272	-5.02839355678015	h
-10.98627325251805	-1.27590553641699	-2.25795924805561	h
-10.49387940769664	-3.03915577668519	-5.14806075281586	h
2.24110996890109	-14.14453610263657	-5.30851883810833	h
-0.99712939191023	-14.08046860492350	-4.20766522567146	h
1.09128545936023	-16.56710305702549	-3.22993478306790	h
2.43183224533818	-16.47220715128181	0.52503583804366	h
1.39801231376111	-13.90977290978493	2.49144910803049	h
4.60151629216397	-13.97876208789760	1.29262408348433	h
-0.14084948568462	4.02830403975106	0.88988786812924	h
-0.31717263985005	8.64806420388859	1.48425554038696	h
5.59013291084234	9.26239190666256	-4.32103048823156	h
5.48052458211093	4.61681496987746	-4.63477163479834	h
-2.45729347423265	-3.50267984925147	-1.40350768096735	h
-6.98666453281005	-3.12319565574766	-2.39416756947528	h
-5.14338723937571	3.88682171830534	-6.44825509814631	h
0.52729073726362	-5.44614712142058	-5.39458186207909	h
0.39455319186036	-10.08825971234731	-5.43719181432860	h
3.21501222383407	-5.24935761892098	2.04208397801933	h

3.20463372637838	-9.88968606205933	2.37419086532071	h
-1.01247286818082	-1.79848396572466	2.16668858016416	h
-1.37090384408229	-1.17324726713673	6.75778695031732	h
6.26355209811232	2.09761132089732	6.55353932989265	h
6.24683483561174	1.35623595301169	1.96869188011376	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a	8.62	0.18891	YES	YES
8	a	11.90	0.19462	YES	YES
9	a	13.13	0.32205	YES	YES
10	a	15.77	0.56866	YES	YES
11	a	20.81	1.06013	YES	YES
12	a	23.47	0.46462	YES	YES
13	a	28.02	0.01158	YES	YES
14	a	37.58	0.12364	YES	YES
15	a	41.51	0.36475	YES	YES
16	a	63.63	0.88183	YES	YES
17	a	67.06	1.28014	YES	YES
18	a	76.72	0.03509	YES	YES
19	a	79.47	0.01872	YES	YES
20	a	81.74	0.33079	YES	YES
21	a	84.93	0.08448	YES	YES
22	a	87.71	0.97684	YES	YES
23	a	91.42	0.08564	YES	YES
24	a	93.33	9.63975	YES	YES
25	a	99.57	18.68213	YES	YES
26	a	103.68	3.98137	YES	YES
27	a	109.74	5.98109	YES	YES
28	a	114.48	2.23218	YES	YES
29	a	124.06	0.93885	YES	YES
30	a	125.71	0.84532	YES	YES
31	a	129.70	0.91172	YES	YES
32	a	131.70	1.18020	YES	YES
33	a	135.03	36.57358	YES	YES
34	a	148.70	19.30232	YES	YES
35	a	150.42	2.68666	YES	YES
36	a	161.53	1.78862	YES	YES
37	a	179.32	6.70769	YES	YES
38	a	184.57	0.13864	YES	YES
39	a	185.76	0.80379	YES	YES
40	a	185.91	0.15645	YES	YES
41	a	190.19	0.68837	YES	YES
42	a	193.19	8.13765	YES	YES
43	a	198.29	6.17037	YES	YES
44	a	255.79	0.67846	YES	YES
45	a	259.10	1.09555	YES	YES
46	a	262.90	1.27533	YES	YES
47	a	268.36	4.96705	YES	YES

48	a	298.99	8.85393	YES	YES
49	a	302.28	8.85577	YES	YES
50	a	305.80	5.84504	YES	YES
51	a	308.11	19.20400	YES	YES
52	a	388.93	47.16727	YES	YES
53	a	390.97	1.50265	YES	YES
54	a	398.20	21.41326	YES	YES
55	a	398.77	11.89140	YES	YES
56	a	411.60	0.29303	YES	YES
57	a	413.12	0.37313	YES	YES
58	a	416.39	0.40504	YES	YES
59	a	427.65	0.05865	YES	YES
60	a	477.79	3.20427	YES	YES
61	a	478.12	3.76491	YES	YES
62	a	479.29	1.19731	YES	YES
63	a	480.72	2.69365	YES	YES
64	a	524.76	22.60397	YES	YES
65	a	528.23	12.39324	YES	YES
66	a	529.02	12.55710	YES	YES
67	a	531.85	12.49002	YES	YES
68	a	545.11	29.81562	YES	YES
69	a	546.09	7.07131	YES	YES
70	a	550.54	10.60107	YES	YES
71	a	551.52	13.34263	YES	YES
72	a	654.25	0.14341	YES	YES
73	a	655.76	0.08327	YES	YES
74	a	656.26	0.13910	YES	YES
75	a	657.20	1.10169	YES	YES
76	a	720.82	0.51927	YES	YES
77	a	722.10	0.51898	YES	YES
78	a	724.85	0.06022	YES	YES
79	a	725.36	0.19923	YES	YES
80	a	756.13	0.37538	YES	YES
81	a	756.91	3.75373	YES	YES
82	a	759.53	0.74940	YES	YES
83	a	761.04	0.66610	YES	YES
84	a	804.42	18.21946	YES	YES
85	a	806.26	4.29519	YES	YES
86	a	806.71	1.22359	YES	YES
87	a	808.32	1.59195	YES	YES
88	a	810.88	47.82419	YES	YES
89	a	812.09	35.81614	YES	YES
90	a	815.12	16.23996	YES	YES
91	a	815.98	48.94461	YES	YES
92	a	931.41	0.21691	YES	YES
93	a	932.44	0.41543	YES	YES
94	a	933.03	0.27247	YES	YES
95	a	941.36	3.95090	YES	YES
96	a	942.79	0.40075	YES	YES
97	a	945.39	0.25047	YES	YES
98	a	946.16	1.99779	YES	YES
99	a	946.47	2.03606	YES	YES
100	a	946.79	1.70460	YES	YES

101	a	947.34	1.72817	YES	YES
102	a	948.09	1.03180	YES	YES
103	a	958.91	3.48571	YES	YES
104	a	987.10	250.88508	YES	YES
105	a	988.89	35.79005	YES	YES
106	a	993.38	137.97461	YES	YES
107	a	996.72	76.10855	YES	YES
108	a	1046.11	7.55952	YES	YES
109	a	1046.18	22.63030	YES	YES
110	a	1046.80	17.53387	YES	YES
111	a	1047.30	14.37139	YES	YES
112	a	1049.71	105.59641	YES	YES
113	a	1051.44	160.02521	YES	YES
114	a	1054.55	34.47141	YES	YES
115	a	1058.22	48.71519	YES	YES
116	a	1093.57	0.02473	YES	YES
117	a	1093.97	0.03335	YES	YES
118	a	1095.23	0.00452	YES	YES
119	a	1096.58	0.03052	YES	YES
120	a	1108.57	0.35277	YES	YES
121	a	1108.72	0.06147	YES	YES
122	a	1108.77	0.06424	YES	YES
123	a	1109.08	0.18963	YES	YES
124	a	1113.29	2.11181	YES	YES
125	a	1113.83	5.90561	YES	YES
126	a	1115.69	4.61137	YES	YES
127	a	1119.93	5.05923	YES	YES
128	a	1163.25	0.06285	YES	YES
129	a	1163.31	0.16654	YES	YES
130	a	1163.67	0.13820	YES	YES
131	a	1163.79	0.15855	YES	YES
132	a	1207.24	63.65050	YES	YES
133	a	1209.15	154.78057	YES	YES
134	a	1210.43	125.32882	YES	YES
135	a	1220.11	8.92345	YES	YES
136	a	1233.09	19.13969	YES	YES
137	a	1234.30	21.57942	YES	YES
138	a	1236.17	22.10046	YES	YES
139	a	1236.35	23.05614	YES	YES
140	a	1320.73	5.16215	YES	YES
141	a	1322.90	12.24900	YES	YES
142	a	1324.53	7.80460	YES	YES
143	a	1325.83	10.59843	YES	YES
144	a	1341.86	10.41094	YES	YES
145	a	1345.08	11.70999	YES	YES
146	a	1348.06	29.79303	YES	YES
147	a	1349.20	5.07593	YES	YES
148	a	1383.82	133.13497	YES	YES
149	a	1385.12	67.00677	YES	YES
150	a	1385.64	50.20443	YES	YES
151	a	1387.29	53.52254	YES	YES
152	a	1394.48	1.14299	YES	YES
153	a	1394.71	1.01628	YES	YES

154	a	1394.80	0.50193	YES	YES
155	a	1395.11	1.04412	YES	YES
156	a	1423.09	0.04779	YES	YES
157	a	1423.22	0.17450	YES	YES
158	a	1423.77	0.12300	YES	YES
159	a	1423.87	0.02390	YES	YES
160	a	1430.82	39.07967	YES	YES
161	a	1431.89	18.33211	YES	YES
162	a	1432.12	39.00799	YES	YES
163	a	1432.39	12.85075	YES	YES
164	a	1436.63	27.55887	YES	YES
165	a	1436.94	27.89135	YES	YES
166	a	1437.84	16.34132	YES	YES
167	a	1437.87	38.63622	YES	YES
168	a	1443.28	1.04430	YES	YES
169	a	1443.35	0.47587	YES	YES
170	a	1443.95	0.51565	YES	YES
171	a	1444.13	0.43127	YES	YES
172	a	1463.70	56.18805	YES	YES
173	a	1464.71	125.47222	YES	YES
174	a	1465.22	47.75560	YES	YES
175	a	1465.54	19.33193	YES	YES
176	a	1477.83	3.96707	YES	YES
177	a	1481.72	3.06277	YES	YES
178	a	1489.03	1.38677	YES	YES
179	a	1489.59	5.56331	YES	YES
180	a	1521.64	25.21700	YES	YES
181	a	1527.02	26.67217	YES	YES
182	a	1528.12	16.69156	YES	YES
183	a	1530.76	25.61237	YES	YES
184	a	1547.10	148.51406	YES	YES
185	a	1548.40	92.46849	YES	YES
186	a	1552.56	173.32734	YES	YES
187	a	1553.97	106.63853	YES	YES
188	a	1639.58	978.46231	YES	YES
189	a	1643.08	298.10505	YES	YES
190	a	1646.40	718.67556	YES	YES
191	a	1650.97	330.36755	YES	YES
192	a	2936.19	33.64896	YES	YES
193	a	2937.58	32.93487	YES	YES
194	a	2940.37	27.23423	YES	YES
195	a	2940.73	29.79428	YES	YES
196	a	2942.69	43.06495	YES	YES
197	a	2943.07	30.85783	YES	YES
198	a	2945.57	30.31851	YES	YES
199	a	2945.96	26.36801	YES	YES
200	a	3008.61	9.34884	YES	YES
201	a	3011.76	4.72861	YES	YES
202	a	3013.93	14.33308	YES	YES
203	a	3013.99	11.27667	YES	YES
204	a	3015.54	4.03050	YES	YES
205	a	3016.04	4.17896	YES	YES
206	a	3017.60	12.22480	YES	YES

207	a	3018.21	12.42744	YES	YES
208	a	3082.32	4.08095	YES	YES
209	a	3082.58	6.66240	YES	YES
210	a	3085.33	0.23303	YES	YES
211	a	3086.67	0.21195	YES	YES
212	a	3088.58	0.23232	YES	YES
213	a	3088.79	0.24960	YES	YES
214	a	3093.48	4.02438	YES	YES
215	a	3094.64	3.91034	YES	YES
216	a	3096.72	2.87068	YES	YES
217	a	3096.88	2.49606	YES	YES
218	a	3097.49	4.04026	YES	YES
219	a	3100.47	1.88309	YES	YES
220	a	3113.85	3.87798	YES	YES
221	a	3123.63	2.48551	YES	YES
222	a	3128.52	4.13443	YES	YES
223	a	3131.73	2.03405	YES	YES
224	a	3150.39	1.26866	YES	YES
225	a	3155.61	1.52290	YES	YES
226	a	3155.99	0.80970	YES	YES
227	a	3156.27	0.21511	YES	YES
228	a	3156.57	0.63896	YES	YES
229	a	3157.70	0.60132	YES	YES
230	a	3157.97	0.45180	YES	YES
231	a	3159.29	0.19147	YES	YES

$[Pb(dmap)_4]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

1.92363942610325	-5.28751313466393	-1.83471629107714	n
2.02939853603777	-13.24888210375518	-1.31563246751127	n
2.51886998452422	-6.48326358014786	0.35484630633395	c
2.56543755028527	-9.09268543053359	0.63053716215705	c
1.98493799984599	-10.68819784958134	-1.47959898845556	c
1.36174325281633	-9.40023541329846	-3.78001321445451	c
1.36881900082275	-6.77898101877269	-3.85026886770446	c
2.70528289211103	-14.47451361551884	1.06733579768501	c
1.44635490748215	-14.79310358078218	-3.53286865876714	c
-1.53114817128047	-0.09284545533179	-3.31460855496795	n
-9.29146408007077	0.69271382145710	-4.93112495986035	n
-3.20039141042798	-1.98742929267449	-2.82063051206032	c
-5.76872257558501	-1.81047018006428	-3.30268187781676	c
-6.79767886911853	0.44446946146168	-4.39897999852557	c
-5.00869422634910	2.41654647178880	-4.90021317353511	c
-2.47399498421747	2.06940408013228	-4.34407173703939	c
-11.04135142553051	-1.38075656275094	-4.39533231669456	c
-10.23962966110666	3.01813529758491	-6.09146291558822	c
2.80059130170316	4.35185398526623	-2.08116754787262	n
2.96845105612295	12.27693465285669	-1.21144498514548	n
4.17431816631282	5.84743759598613	-3.64775257516041	c

4.29418755701692	8.46112027567714	-3.44817307489265	c
2.91371163163564	9.72547396909787	-1.49242809600441	c
1.47148004416685	8.12046932307696	0.14661832576923	c
1.48329172935267	5.52210976394215	-0.21986719226408	c
4.47673543433177	13.83001951475776	-2.93146496048191	c
1.53064011181610	13.48072870684316	0.81659443540786	c
2.56906472817871	-0.24630842062309	1.76995319344396	n
1.98326311420270	0.78162906825598	9.63950599534858	n
4.52138739287001	0.70796581816952	3.14123173540624	c
4.42117389224190	1.08024680792612	5.73114805799293	c
2.16825572767204	0.46060371611947	7.10386902447542	c
0.12349541570676	-0.51798728195417	5.61683600348522	c
0.41041793509163	-0.83011287847008	3.03093684524159	c
4.13284364001114	1.76522398591609	11.07712940749694	c
-0.35946687143118	0.13047155812669	10.95632133681219	c
3.00301832830901	-0.54384429076963	-2.77438495317434	pb
-1.10182986032851	3.58771675256405	-4.72329505364004	h
-1.97936056519532	1.26822601310915	10.24489598106808	h
-0.13635569742229	0.52973833533895	12.99525980944104	h
-0.81786160025440	-1.91076742111501	10.73972810725946	h
5.81254326458794	0.51341462585919	10.89243668154518	h
3.62013318727099	1.86283733174619	13.10041562726075	h
4.65683914411714	3.70122286173891	10.44359431138088	h
1.80937230966805	15.54997002701479	0.72399057265255	h
2.17213081229307	12.82252008391402	2.70899169195674	h
-0.52963815271707	13.09507134204961	0.63167200032516	h
3.82765081064298	13.62201973702285	-4.92171602140632	h
6.51634772087400	13.32669941455175	-2.83018662652052	h
4.28008132445237	15.84030807463911	-2.39508285383487	h
-9.33892703552108	3.36227520094165	-7.96118462536793	h
-9.89704835219410	4.68407511978859	-4.85442872493461	h
-12.30080831186896	2.84777272314258	-6.38942974549139	h
-12.97612519424141	-0.80544591903374	-4.93631446526259	h
-11.05468547286369	-1.85841450927094	-2.34742401435382	h
-10.54451886779450	-3.10559471944311	-5.49219585808842	h
2.80861898009063	-14.43796985856513	-5.09587650452419	h
-0.50140274123518	-14.42049086853878	-4.23545114376768	h
1.56806397767098	-16.81426240567796	-3.01530699589648	h
2.63948041228290	-16.54844386932648	0.81766566591120	h
1.35980846212359	-13.96233981163069	2.60153711990226	h
4.65209397435711	-13.95484918193426	1.67234731992044	h
0.37227665225357	4.28897226054415	1.04155911135040	h
0.34696930220576	8.89867111014209	1.70679753787120	h
5.46101261961286	9.50909471801775	-4.80561979306162	h
5.24632986950304	4.88178251831119	-5.15678355581605	h
-2.39558499512444	-3.72888222560499	-2.01259839555498	h
-6.96941255780819	-3.43865401614970	-2.84438974553231	h
-5.59234519925279	4.22380769253361	-5.73394703043159	h
0.89818542840099	-5.80056965680959	-5.63410572091272	h
0.89206426188539	-10.43904940261927	-5.51302324306206	h
2.98838229382258	-5.26051044171765	1.97508636917426	h
3.06945064775901	-9.88577755172614	2.47976252979306	h
-1.15660317506110	-1.58819316745585	1.89029630229229	h

-1.68976040228076	-1.04023734089459	6.47737444279760	h
6.09457239212326	1.85351467949945	6.68128211478137	h
6.25159185151169	1.20431396029396	2.08969111277426	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a	10.34	0.50693	YES	YES
8	a	11.16	0.24968	YES	YES
9	a	12.68	0.36597	YES	YES
10	a	14.98	0.69265	YES	YES
11	a	19.99	1.05048	YES	YES
12	a	21.07	0.50925	YES	YES
13	a	29.10	0.11283	YES	YES
14	a	35.03	0.02314	YES	YES
15	a	40.00	0.60418	YES	YES
16	a	61.97	1.91912	YES	YES
17	a	64.67	1.63625	YES	YES
18	a	76.05	1.78521	YES	YES
19	a	78.23	2.21278	YES	YES
20	a	80.31	11.12385	YES	YES
21	a	81.84	8.66342	YES	YES
22	a	84.32	7.24741	YES	YES
23	a	85.58	2.16475	YES	YES
24	a	90.51	6.11846	YES	YES
25	a	93.49	0.17396	YES	YES
26	a	93.80	0.98956	YES	YES
27	a	101.28	1.82321	YES	YES
28	a	108.50	0.54848	YES	YES
29	a	119.08	1.23284	YES	YES
30	a	121.81	11.40821	YES	YES
31	a	124.73	1.18597	YES	YES
32	a	125.72	1.16974	YES	YES
33	a	126.32	2.67631	YES	YES
34	a	128.42	10.60558	YES	YES
35	a	147.62	2.45690	YES	YES
36	a	154.91	0.43383	YES	YES
37	a	168.96	2.34849	YES	YES
38	a	180.47	2.21655	YES	YES
39	a	182.95	0.73415	YES	YES
40	a	184.10	0.12673	YES	YES
41	a	185.47	1.10856	YES	YES
42	a	187.66	0.47748	YES	YES
43	a	188.38	1.12557	YES	YES
44	a	254.10	0.51518	YES	YES
45	a	256.10	0.73460	YES	YES
46	a	260.37	0.22362	YES	YES
47	a	264.03	2.76220	YES	YES
48	a	296.19	7.80413	YES	YES
49	a	298.92	7.97784	YES	YES

50	a	303.58	4.97795	YES	YES
51	a	305.09	13.89097	YES	YES
52	a	387.69	42.88638	YES	YES
53	a	393.36	2.38186	YES	YES
54	a	397.33	17.47379	YES	YES
55	a	405.56	7.49272	YES	YES
56	a	411.33	0.20035	YES	YES
57	a	413.23	0.22600	YES	YES
58	a	415.51	0.35000	YES	YES
59	a	425.76	0.09671	YES	YES
60	a	477.60	3.03684	YES	YES
61	a	477.91	3.97097	YES	YES
62	a	479.37	1.67818	YES	YES
63	a	480.19	2.41796	YES	YES
64	a	525.15	22.16149	YES	YES
65	a	529.60	11.26977	YES	YES
66	a	530.09	15.97848	YES	YES
67	a	531.48	6.72673	YES	YES
68	a	544.36	28.88821	YES	YES
69	a	548.42	1.06187	YES	YES
70	a	550.80	12.88017	YES	YES
71	a	555.09	6.32964	YES	YES
72	a	654.67	0.16268	YES	YES
73	a	656.64	0.29620	YES	YES
74	a	656.79	0.28045	YES	YES
75	a	657.11	0.80810	YES	YES
76	a	720.36	0.39060	YES	YES
77	a	722.07	0.63198	YES	YES
78	a	724.73	0.12813	YES	YES
79	a	725.43	0.33745	YES	YES
80	a	756.97	2.50150	YES	YES
81	a	758.54	0.37816	YES	YES
82	a	759.67	0.52265	YES	YES
83	a	760.62	0.26011	YES	YES
84	a	807.17	1.21750	YES	YES
85	a	809.16	14.51275	YES	YES
86	a	810.04	10.20048	YES	YES
87	a	810.34	24.89087	YES	YES
88	a	811.01	56.84409	YES	YES
89	a	811.55	7.38538	YES	YES
90	a	811.96	12.98571	YES	YES
91	a	816.32	40.97929	YES	YES
92	a	931.05	0.38717	YES	YES
93	a	933.29	0.40513	YES	YES
94	a	934.86	0.22896	YES	YES
95	a	942.81	0.29027	YES	YES
96	a	946.09	3.87041	YES	YES
97	a	946.92	2.61411	YES	YES
98	a	947.21	2.55859	YES	YES
99	a	947.49	0.93341	YES	YES
100	a	947.78	0.23547	YES	YES
101	a	948.73	1.16692	YES	YES
102	a	949.48	1.72677	YES	YES

103	a	961.39	1.79068	YES	YES
104	a	987.36	254.08103	YES	YES
105	a	991.09	45.11014	YES	YES
106	a	993.59	109.57995	YES	YES
107	a	999.32	33.84709	YES	YES
108	a	1046.80	17.64986	YES	YES
109	a	1047.10	16.19039	YES	YES
110	a	1047.41	16.60102	YES	YES
111	a	1047.52	14.95543	YES	YES
112	a	1053.32	98.62614	YES	YES
113	a	1054.29	146.71925	YES	YES
114	a	1057.19	44.56362	YES	YES
115	a	1063.76	19.32460	YES	YES
116	a	1094.20	0.03260	YES	YES
117	a	1094.83	0.06459	YES	YES
118	a	1095.95	0.03711	YES	YES
119	a	1096.39	0.01556	YES	YES
120	a	1108.11	0.07193	YES	YES
121	a	1108.37	0.15222	YES	YES
122	a	1108.78	0.05260	YES	YES
123	a	1109.30	0.14121	YES	YES
124	a	1114.37	6.36474	YES	YES
125	a	1115.13	1.81838	YES	YES
126	a	1115.88	7.71873	YES	YES
127	a	1119.68	3.26894	YES	YES
128	a	1163.35	0.03199	YES	YES
129	a	1163.81	0.02995	YES	YES
130	a	1163.98	0.05007	YES	YES
131	a	1164.07	0.26080	YES	YES
132	a	1209.89	76.68457	YES	YES
133	a	1212.60	125.74123	YES	YES
134	a	1213.20	151.01171	YES	YES
135	a	1222.38	7.44089	YES	YES
136	a	1235.01	14.90326	YES	YES
137	a	1235.08	27.12582	YES	YES
138	a	1237.16	22.05131	YES	YES
139	a	1237.67	24.20620	YES	YES
140	a	1322.72	2.28193	YES	YES
141	a	1326.71	8.97060	YES	YES
142	a	1327.57	6.41332	YES	YES
143	a	1328.05	7.26185	YES	YES
144	a	1344.16	6.97718	YES	YES
145	a	1346.58	13.22013	YES	YES
146	a	1348.38	20.12476	YES	YES
147	a	1349.76	11.68474	YES	YES
148	a	1384.31	164.42661	YES	YES
149	a	1385.25	51.16099	YES	YES
150	a	1385.81	36.42819	YES	YES
151	a	1387.74	62.88257	YES	YES
152	a	1394.78	0.44371	YES	YES
153	a	1395.27	1.08615	YES	YES
154	a	1395.99	0.68068	YES	YES
155	a	1396.04	1.56046	YES	YES

156	a	1422.63	0.05337	YES	YES
157	a	1423.15	0.03444	YES	YES
158	a	1423.62	0.23992	YES	YES
159	a	1424.22	0.09334	YES	YES
160	a	1431.43	37.93238	YES	YES
161	a	1432.75	42.63965	YES	YES
162	a	1432.85	21.24354	YES	YES
163	a	1433.07	9.46900	YES	YES
164	a	1436.06	27.29808	YES	YES
165	a	1436.79	26.94659	YES	YES
166	a	1437.58	27.48015	YES	YES
167	a	1438.14	27.71349	YES	YES
168	a	1442.92	1.52167	YES	YES
169	a	1443.27	0.27314	YES	YES
170	a	1444.00	0.44072	YES	YES
171	a	1444.13	0.48971	YES	YES
172	a	1464.03	52.70261	YES	YES
173	a	1465.31	114.89613	YES	YES
174	a	1465.56	82.83204	YES	YES
175	a	1466.20	3.83735	YES	YES
176	a	1477.02	3.28517	YES	YES
177	a	1478.63	2.98694	YES	YES
178	a	1486.41	3.13348	YES	YES
179	a	1488.34	2.82266	YES	YES
180	a	1522.69	29.61344	YES	YES
181	a	1528.11	24.14657	YES	YES
182	a	1529.75	17.47489	YES	YES
183	a	1531.65	27.66628	YES	YES
184	a	1546.30	189.09805	YES	YES
185	a	1547.24	41.63529	YES	YES
186	a	1551.19	162.01396	YES	YES
187	a	1552.43	113.28457	YES	YES
188	a	1638.95	1185.37049	YES	YES
189	a	1641.29	101.62911	YES	YES
190	a	1644.91	683.13154	YES	YES
191	a	1649.20	335.32422	YES	YES
192	a	2935.53	34.37046	YES	YES
193	a	2936.35	34.78817	YES	YES
194	a	2939.52	26.34764	YES	YES
195	a	2939.64	32.88033	YES	YES
196	a	2941.90	47.92561	YES	YES
197	a	2942.18	28.35662	YES	YES
198	a	2944.70	33.49795	YES	YES
199	a	2945.00	24.73609	YES	YES
200	a	3007.54	9.73805	YES	YES
201	a	3010.09	4.68143	YES	YES
202	a	3012.13	15.87805	YES	YES
203	a	3013.22	11.65572	YES	YES
204	a	3014.17	5.00312	YES	YES
205	a	3014.82	0.88109	YES	YES
206	a	3016.07	16.44876	YES	YES
207	a	3016.64	12.28058	YES	YES
208	a	3077.85	6.44844	YES	YES

209	a	3080.98	7.60492	YES	YES
210	a	3085.13	0.26061	YES	YES
211	a	3085.57	0.28311	YES	YES
212	a	3087.52	0.25768	YES	YES
213	a	3088.48	0.27421	YES	YES
214	a	3093.26	4.25757	YES	YES
215	a	3093.62	4.17582	YES	YES
216	a	3095.70	3.06317	YES	YES
217	a	3096.58	2.67744	YES	YES
218	a	3097.84	3.69125	YES	YES
219	a	3101.65	2.38970	YES	YES
220	a	3109.49	4.07354	YES	YES
221	a	3120.16	6.51070	YES	YES
222	a	3123.16	3.68416	YES	YES
223	a	3123.56	4.35299	YES	YES
224	a	3151.31	1.38178	YES	YES
225	a	3154.57	1.76013	YES	YES
226	a	3155.04	0.16883	YES	YES
227	a	3155.15	1.14559	YES	YES
228	a	3155.89	0.60440	YES	YES
229	a	3157.49	0.59507	YES	YES
230	a	3157.65	0.69366	YES	YES
231	a	3158.60	0.12142	YES	YES

$[Sn(PPh_3)_3]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

2.66295460827596	-1.50727601076275	-0.67070067259323	sn
1.50238165149270	1.39704447042382	-6.64913153251512	c
1.48467402203252	2.66477389935605	-3.44679604019644	p
0.10417675830402	-0.81474908393610	-7.16893845927959	c
-0.96675283223332	-1.77823244439587	-5.66762064746190	h
0.05139664583763	-1.81055960149284	-9.62317675071476	c
-1.03878821380848	-3.54196888301491	-10.00217420246567	h
1.40142559162893	-0.60224317343271	-11.56642719715257	c
1.37444525566975	-1.38606531381089	-13.49486086948970	h
2.79403848703206	1.60320239884231	-11.05405379664358	c
3.84860717778536	2.54825157631314	-12.57974189775008	h
2.85506186479968	2.61123845250325	-8.60077057002997	c
3.95538386360503	4.33335376326236	-8.20665827957045	h
4.25408290690415	4.69655412116768	-3.18048354827283	c
6.67024259567487	3.56153140473400	-3.31012617355114	c
6.86641420244270	1.49511571959192	-3.52506995538788	h
8.84519827393579	5.07103396087526	-3.23691173529187	c
10.72392582265791	4.18348253101154	-3.36487018582852	h
8.62330602929323	7.71221782283074	-3.02383845407729	c
10.33428192772156	8.89742317563529	-2.97780487384565	h
6.22403848454856	8.83808306658508	-2.88470499958951	c
6.04599188696233	10.90631784781500	-2.73233579364281	h
4.03376301803657	7.34176652078304	-2.96605233732327	c

2.16197963571625	8.24508501608723	-2.88537750788547	h
-1.29911494912592	4.66820958747154	-3.15608776286751	c
-1.77031067285231	5.91909143563099	-0.84709173657054	c
-0.44018116705845	5.73115418679646	0.74194829923561	h
-3.91317433060909	7.45605244226273	-0.59503639039325	c
-4.26928757024085	8.44101869624463	1.20395864218076	h
-5.59004367612290	7.74973375653195	-2.63587369590009	c
-7.26901199521656	8.96481333996159	-2.43697350897468	h
-5.11207185384536	6.51445975840673	-4.93903017377653	c
-6.40507926270702	6.77064068071037	-6.55094207399932	h
-2.97287024433987	4.96757523514804	-5.21110692447915	c
-2.60275167731991	4.00757085759413	-7.01978121043812	h
1.76422021290373	0.58493460539274	3.88366727291624	p
5.54949140064867	4.13970750513134	3.04699494488803	c
6.68162233662210	2.53341343527792	2.35171172926600	h
6.62160701145061	6.55859372298091	3.12201950382525	c
8.57522784108311	6.83765335390403	2.46692968807671	h
5.20640902893840	8.61686086566043	4.02995879780546	c
6.05535453732866	10.51694057511407	4.08147359437731	h
2.72424347421394	8.25162122182367	4.89719973983131	c
1.62903012818472	9.85847890969651	5.64046569930578	h
1.64293092058083	5.82715165729485	4.86403794166228	c
-0.28684656367179	5.53072574702538	5.58774513609922	h
3.65878842339534	-1.26459567308241	6.07848400445373	c
4.99271096111822	-0.07085256146213	8.05753327085751	c
4.96646880202508	2.00206891334492	8.24546389596026	h
6.36185543683482	-1.54515886958688	9.78575208124537	c
7.40342177204961	-0.61848054535734	11.33144873035537	h
6.41066741854419	-4.19097693859044	9.54233081983630	c
7.49785276373909	-5.33700639911402	10.89823869105460	h
5.08752585660064	-5.37555026648851	7.56622984543394	c
5.12754425262493	-7.44652380990767	7.36731079532853	h
3.71259516182753	-3.92028709494301	5.83040888711175	c
2.66848091573412	-4.87263553740697	4.29954049287640	h
-1.44042714283142	0.70717820138507	5.10652914759445	c
-1.95508235811790	0.02994412345256	7.63393661920774	c
-0.41042140050941	-0.54674086244513	8.90407249736389	h
-4.46100372707088	0.06042307744087	8.50353909460054	c
-4.87359473519158	-0.46601815938789	10.47517596324156	h
-6.44034015778963	0.75006743893002	6.86715721060866	c
-8.40402673525323	0.74845653251844	7.55815716635402	h
-5.91746710187044	1.44485740325799	4.35592056671399	c
-7.45586526300935	1.98098919284307	3.06211968172671	h
-3.42051094775628	1.42084176103804	3.47326634431378	c
-3.02507941487109	1.94219714750740	1.50059136213583	h
3.05523703396178	3.77139613993000	3.92521170339749	c
-11.70681472677295	0.05945094495071	-1.42601502854748	h
-11.04061992485875	-4.05977945957611	0.82428951478382	h
-9.79242915222308	-0.74474274687704	-1.27445420437829	c
-9.42050127415378	-3.04985178843989	-0.00579034471035	c
-7.72595578645670	0.52588473991023	-2.36028432958657	c
-7.99522517802838	2.32956339991904	-3.36146749904636	h
-3.20802276230607	-6.16347814309833	8.28775175668415	h

-6.98798860293574	-4.08868224994359	0.20061608917291	c
-6.71840573777554	-5.90415039059552	1.18084853518841	h
-2.32487008361858	-6.79505164482003	6.51256107732203	c
-3.81457757282748	-3.63373997006573	4.37425691658009	h
-5.29258903932186	-0.49880113163144	-2.15832620343602	c
-2.66399728884687	-5.36177515993777	4.31054660940188	c
-4.91225383077868	-2.79609286346074	-0.86675300159409	c
-0.62037502361947	-10.14163209778086	8.18938563827312	h
-0.87793641045953	-9.02150310956066	6.45393382898810	c
-3.68529305535631	0.51734199651722	-2.99600174645778	h
-1.55270732317019	-6.17037692015242	2.01980500310279	c
-1.75560594707544	-4.15055325856397	-0.76682409443771	p
0.21921736090057	-9.83192742862534	4.17470835337181	c
-0.10965293596701	-8.41505293568483	1.95489527612839	c
-5.47396109345461	-6.04385516929130	-4.48569932156023	h
1.32306263564068	-11.59574250119559	4.11195989116974	h
-3.59125528689753	-6.72725925621776	-5.04846508695798	c
-1.44330843090194	-6.12571754937075	-3.58556668471133	c
0.72601150304736	-9.08867194001627	0.17184538645357	h
-3.32194595844252	-8.20326779050816	-7.23736263763230	c
-5.00426331114209	-8.67684605912887	-8.36843068551826	h
0.96712702268850	-6.99295186208068	-4.34692207509387	c
2.67428962169520	-6.51298821238249	-3.24870547964562	h
-0.92705861235307	-9.08198793899153	-7.97658949302707	c
1.21684572238996	-8.47510046750666	-6.52971825538371	c
-0.72794594159304	-10.24329471028694	-9.69298382089136	h
3.09805401763060	-9.15274235241439	-7.10702378728825	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a	10.04	0.01763	YES	YES
8	a	18.51	0.03092	YES	YES
9	a	25.39	0.06559	YES	YES
10	a	30.90	0.01266	YES	YES
11	a	32.60	0.07956	YES	YES
12	a	37.28	0.04439	YES	YES
13	a	38.65	0.13956	YES	YES
14	a	42.80	0.00951	YES	YES
15	a	46.57	0.04752	YES	YES
16	a	49.54	0.06607	YES	YES
17	a	50.53	0.03969	YES	YES
18	a	52.35	0.07741	YES	YES
19	a	52.83	0.15279	YES	YES
20	a	56.50	0.03645	YES	YES
21	a	59.02	0.04907	YES	YES
22	a	63.51	0.04443	YES	YES
23	a	64.60	0.27999	YES	YES
24	a	65.83	0.05495	YES	YES
25	a	67.52	0.09241	YES	YES

26	a	73.80	0.07922	YES	YES
27	a	74.91	0.02721	YES	YES
28	a	77.93	0.07409	YES	YES
29	a	79.02	0.13017	YES	YES
30	a	81.33	0.09312	YES	YES
31	a	86.92	0.09428	YES	YES
32	a	93.72	0.10448	YES	YES
33	a	95.99	0.18291	YES	YES
34	a	109.79	0.26287	YES	YES
35	a	114.86	0.06498	YES	YES
36	a	116.01	0.36539	YES	YES
37	a	142.09	3.38511	YES	YES
38	a	150.04	11.74634	YES	YES
39	a	152.93	15.94827	YES	YES
40	a	188.42	0.55664	YES	YES
41	a	190.01	1.57137	YES	YES
42	a	193.10	0.75649	YES	YES
43	a	197.82	0.64535	YES	YES
44	a	206.41	0.57327	YES	YES
45	a	209.91	1.52543	YES	YES
46	a	216.99	4.40382	YES	YES
47	a	222.72	0.62193	YES	YES
48	a	228.94	1.30386	YES	YES
49	a	244.08	3.34126	YES	YES
50	a	248.80	1.38162	YES	YES
51	a	249.29	3.74371	YES	YES
52	a	258.10	1.26782	YES	YES
53	a	259.81	0.30039	YES	YES
54	a	261.01	0.12035	YES	YES
55	a	269.41	0.37029	YES	YES
56	a	270.12	0.93623	YES	YES
57	a	271.81	0.11942	YES	YES
58	a	388.56	0.40041	YES	YES
59	a	392.78	0.13277	YES	YES
60	a	393.19	1.36695	YES	YES
61	a	395.37	2.36112	YES	YES
62	a	396.31	0.14460	YES	YES
63	a	397.08	0.93273	YES	YES
64	a	398.71	1.24580	YES	YES
65	a	401.67	0.81925	YES	YES
66	a	405.79	1.88220	YES	YES
67	a	407.21	0.51688	YES	YES
68	a	410.21	1.42067	YES	YES
69	a	418.01	1.04243	YES	YES
70	a	435.30	3.34531	YES	YES
71	a	436.89	5.01552	YES	YES
72	a	440.15	5.27289	YES	YES
73	a	440.95	2.12821	YES	YES
74	a	445.89	3.43672	YES	YES
75	a	449.44	1.13182	YES	YES
76	a	486.15	22.49324	YES	YES
77	a	487.41	27.26915	YES	YES
78	a	490.58	30.69665	YES	YES

79	a	493.02	20.14995	YES	YES
80	a	496.40	60.48284	YES	YES
81	a	496.76	8.51610	YES	YES
82	a	506.31	60.06113	YES	YES
83	a	507.77	87.19004	YES	YES
84	a	515.09	15.38557	YES	YES
85	a	608.05	0.16513	YES	YES
86	a	608.41	0.20255	YES	YES
87	a	608.68	0.04265	YES	YES
88	a	609.21	0.13182	YES	YES
89	a	609.66	0.00492	YES	YES
90	a	610.04	0.60555	YES	YES
91	a	610.37	0.18571	YES	YES
92	a	610.72	0.10419	YES	YES
93	a	611.48	0.79191	YES	YES
94	a	678.35	0.05453	YES	YES
95	a	680.90	1.64360	YES	YES
96	a	683.20	1.26860	YES	YES
97	a	691.80	38.80582	YES	YES
98	a	692.73	6.78630	YES	YES
99	a	693.31	28.52177	YES	YES
100	a	695.84	24.59788	YES	YES
101	a	696.38	34.75963	YES	YES
102	a	697.13	33.87106	YES	YES
103	a	699.00	20.30634	YES	YES
104	a	700.26	7.53727	YES	YES
105	a	704.42	17.58553	YES	YES
106	a	707.39	7.57431	YES	YES
107	a	707.93	6.14999	YES	YES
108	a	708.84	9.66734	YES	YES
109	a	709.61	11.07809	YES	YES
110	a	712.58	8.22639	YES	YES
111	a	712.85	17.33120	YES	YES
112	a	737.04	9.20819	YES	YES
113	a	737.22	38.12442	YES	YES
114	a	739.09	8.83859	YES	YES
115	a	740.58	5.31183	YES	YES
116	a	741.55	26.49556	YES	YES
117	a	742.17	34.41298	YES	YES
118	a	742.97	6.32658	YES	YES
119	a	745.73	10.81855	YES	YES
120	a	746.00	6.71419	YES	YES
121	a	825.53	0.63650	YES	YES
122	a	831.56	0.76519	YES	YES
123	a	832.45	0.34909	YES	YES
124	a	834.37	0.94318	YES	YES
125	a	834.63	0.39767	YES	YES
126	a	837.44	0.67484	YES	YES
127	a	843.51	0.35249	YES	YES
128	a	848.60	0.05786	YES	YES
129	a	851.53	0.18085	YES	YES
130	a	908.31	0.05423	YES	YES
131	a	910.83	1.54194	YES	YES

132	a	913.16	0.26219	YES	YES
133	a	914.59	0.34062	YES	YES
134	a	914.85	0.16493	YES	YES
135	a	918.74	0.54896	YES	YES
136	a	923.05	0.41037	YES	YES
137	a	928.98	0.29462	YES	YES
138	a	930.50	0.62136	YES	YES
139	a	961.93	0.17788	YES	YES
140	a	963.54	0.33775	YES	YES
141	a	963.67	0.20072	YES	YES
142	a	964.43	1.14964	YES	YES
143	a	966.52	0.21049	YES	YES
144	a	966.67	0.49627	YES	YES
145	a	970.30	0.39740	YES	YES
146	a	974.61	0.58774	YES	YES
147	a	975.92	0.00577	YES	YES
148	a	985.20	9.89081	YES	YES
149	a	985.71	2.57858	YES	YES
150	a	986.29	8.23322	YES	YES
151	a	987.13	5.94887	YES	YES
152	a	987.44	11.99730	YES	YES
153	a	988.10	0.29738	YES	YES
154	a	988.54	6.10481	YES	YES
155	a	989.43	1.42701	YES	YES
156	a	990.05	9.88808	YES	YES
157	a	997.35	0.65721	YES	YES
158	a	999.52	1.29899	YES	YES
159	a	1000.22	0.34922	YES	YES
160	a	1000.79	0.11656	YES	YES
161	a	1002.44	0.27177	YES	YES
162	a	1002.89	0.38235	YES	YES
163	a	1003.41	0.05833	YES	YES
164	a	1003.47	0.12340	YES	YES
165	a	1004.26	0.35742	YES	YES
166	a	1024.00	0.74567	YES	YES
167	a	1024.77	0.34646	YES	YES
168	a	1025.34	0.24487	YES	YES
169	a	1025.95	0.43140	YES	YES
170	a	1026.45	0.42540	YES	YES
171	a	1026.52	0.56122	YES	YES
172	a	1026.83	0.32315	YES	YES
173	a	1027.07	0.59591	YES	YES
174	a	1027.65	0.60798	YES	YES
175	a	1077.85	6.78125	YES	YES
176	a	1079.34	2.49658	YES	YES
177	a	1080.43	2.61962	YES	YES
178	a	1080.71	2.08609	YES	YES
179	a	1081.54	0.47431	YES	YES
180	a	1082.57	3.12676	YES	YES
181	a	1083.21	3.37120	YES	YES
182	a	1084.44	11.25234	YES	YES
183	a	1085.30	37.08430	YES	YES
184	a	1085.39	3.43422	YES	YES

185	a	1088.30	23.27387	YES	YES
186	a	1089.00	28.37281	YES	YES
187	a	1089.61	15.89105	YES	YES
188	a	1090.73	33.96855	YES	YES
189	a	1091.90	31.87639	YES	YES
190	a	1092.83	35.58108	YES	YES
191	a	1093.85	14.44748	YES	YES
192	a	1094.49	26.05628	YES	YES
193	a	1148.58	0.30106	YES	YES
194	a	1149.86	0.78896	YES	YES
195	a	1150.02	0.68146	YES	YES
196	a	1150.27	0.34617	YES	YES
197	a	1150.46	0.44116	YES	YES
198	a	1150.68	0.44125	YES	YES
199	a	1152.15	0.98449	YES	YES
200	a	1152.76	0.02180	YES	YES
201	a	1152.87	0.32204	YES	YES
202	a	1166.82	0.41884	YES	YES
203	a	1167.97	2.09632	YES	YES
204	a	1168.34	0.76646	YES	YES
205	a	1169.58	0.32329	YES	YES
206	a	1170.34	1.06093	YES	YES
207	a	1172.35	1.71118	YES	YES
208	a	1172.77	2.80064	YES	YES
209	a	1175.07	2.99074	YES	YES
210	a	1176.69	0.33163	YES	YES
211	a	1289.90	19.00249	YES	YES
212	a	1290.72	11.58528	YES	YES
213	a	1291.83	2.85952	YES	YES
214	a	1294.70	3.01847	YES	YES
215	a	1294.78	1.01874	YES	YES
216	a	1296.01	5.91435	YES	YES
217	a	1296.44	5.69874	YES	YES
218	a	1300.57	4.12021	YES	YES
219	a	1304.36	4.38566	YES	YES
220	a	1367.16	0.09952	YES	YES
221	a	1367.77	0.17830	YES	YES
222	a	1368.73	0.27248	YES	YES
223	a	1368.99	0.03220	YES	YES
224	a	1370.13	0.05836	YES	YES
225	a	1371.10	0.33996	YES	YES
226	a	1371.87	0.06990	YES	YES
227	a	1372.42	0.01562	YES	YES
228	a	1372.76	0.37440	YES	YES
229	a	1430.35	33.84959	YES	YES
230	a	1431.56	20.63692	YES	YES
231	a	1432.08	28.41472	YES	YES
232	a	1432.87	22.07012	YES	YES
233	a	1434.35	9.40480	YES	YES
234	a	1434.63	14.68479	YES	YES
235	a	1435.48	10.40427	YES	YES
236	a	1436.56	29.53600	YES	YES
237	a	1437.25	18.72152	YES	YES

238	a	1469.26	0.04290	YES	YES
239	a	1470.20	7.68391	YES	YES
240	a	1470.51	7.33108	YES	YES
241	a	1471.36	3.43139	YES	YES
242	a	1471.59	7.12745	YES	YES
243	a	1471.77	8.40617	YES	YES
244	a	1472.07	4.47214	YES	YES
245	a	1472.93	12.79972	YES	YES
246	a	1475.07	7.86307	YES	YES
247	a	1585.20	1.09498	YES	YES
248	a	1586.31	0.55575	YES	YES
249	a	1587.07	0.64549	YES	YES
250	a	1587.25	1.33509	YES	YES
251	a	1588.28	0.17727	YES	YES
252	a	1588.47	0.05162	YES	YES
253	a	1589.26	0.75046	YES	YES
254	a	1589.79	0.20432	YES	YES
255	a	1590.24	0.17928	YES	YES
256	a	1596.68	0.77329	YES	YES
257	a	1597.99	4.53575	YES	YES
258	a	1598.25	4.35847	YES	YES
259	a	1598.46	0.50464	YES	YES
260	a	1598.72	0.73722	YES	YES
261	a	1599.11	1.43182	YES	YES
262	a	1599.89	0.52882	YES	YES
263	a	1600.29	0.18133	YES	YES
264	a	1600.88	2.23442	YES	YES
265	a	3070.73	9.54889	YES	YES
266	a	3071.50	7.69066	YES	YES
267	a	3085.12	2.79803	YES	YES
268	a	3089.17	5.44646	YES	YES
269	a	3100.65	1.42691	YES	YES
270	a	3101.80	5.72717	YES	YES
271	a	3102.02	2.88098	YES	YES
272	a	3107.00	0.20104	YES	YES
273	a	3107.77	0.11251	YES	YES
274	a	3107.86	0.18818	YES	YES
275	a	3108.17	1.53486	YES	YES
276	a	3109.07	0.01164	YES	YES
277	a	3110.06	0.34158	YES	YES
278	a	3110.13	0.39757	YES	YES
279	a	3110.21	0.09462	YES	YES
280	a	3114.27	0.10313	YES	YES
281	a	3114.59	0.49692	YES	YES
282	a	3114.96	0.90097	YES	YES
283	a	3115.24	0.39042	YES	YES
284	a	3116.08	0.06176	YES	YES
285	a	3116.11	0.14456	YES	YES
286	a	3117.14	0.43363	YES	YES
287	a	3117.26	0.02801	YES	YES
288	a	3117.46	0.30901	YES	YES
289	a	3118.75	0.55645	YES	YES
290	a	3121.07	0.16581	YES	YES

291	a	3121.79	0.16349	YES	YES
292	a	3121.99	1.51046	YES	YES
293	a	3123.87	0.33370	YES	YES
294	a	3124.14	1.31085	YES	YES
295	a	3124.21	1.03579	YES	YES
296	a	3124.66	1.10806	YES	YES
297	a	3124.83	1.04994	YES	YES
298	a	3124.88	1.30483	YES	YES
299	a	3126.98	0.10690	YES	YES
300	a	3129.03	1.44436	YES	YES
301	a	3130.14	0.97906	YES	YES
302	a	3131.03	1.26952	YES	YES
303	a	3131.66	1.13517	YES	YES
304	a	3131.89	1.61403	YES	YES
305	a	3132.20	1.69556	YES	YES
306	a	3132.29	1.24526	YES	YES
307	a	3132.35	1.82485	YES	YES
308	a	3135.01	1.05412	YES	YES
309	a	3137.43	1.69741	YES	YES

PPh_3

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

0.00000000000000	-0.00000000000000	2.78176461268879	p
-2.90908504665261	1.12583413907605	1.19607951946434	c
0.47954155843868	-3.08225862170863	1.19607951946434	c
2.42954348821393	1.95642448263259	1.19607951946434	c
1.95008203874038	3.50477812709089	-0.92010525010986	c
3.90768332450714	4.93021853061515	-2.01009574298839	c
6.36522025136688	4.81462129807917	-1.01197998321402	c
6.85916900269885	3.27563512860001	1.09755657300318	c
4.90028814747755	1.87273835509468	2.20457893181640	c
-0.82830508358529	-5.18014319912669	2.20457893181640	c
-0.59280126645310	-7.57803216948799	1.09755657300318	c
0.98697422805473	-7.91975308740649	-1.01197998321402	c
2.31585283146793	-5.84926229427559	-2.01009574298839	c
2.06018587331857	-3.44120964855834	-0.92010525010986	c
-4.07198306389226	3.30740484403198	2.20457893181640	c
-6.26636773624573	4.30239704088798	1.09755657300318	c
-7.35219447942163	3.10513178932730	-1.01197998321402	c
-6.22353615597506	0.91904376366046	-2.01009574298839	c
-4.01026791205893	-0.06356847853253	-0.92010525010986	c
3.09503028626056	-1.82315694504976	-1.72390195252854	h
3.56074421137586	-6.10637513559951	-3.66127268502225	h
1.18901637468973	-9.80639621009223	-1.87212808292069	h
-1.63387224870672	-9.19586513622352	1.89794192553937	h
-2.04886197057401	-4.92244908246645	3.87607187606425	h
0.03138508636883	3.59195332590874	-1.72390195252854	h
3.50790388677887	6.13688251122964	-3.66127268502225	h
7.89808005017045	5.93291649104311	-1.87212808292069	h

8.78078894209856	3.18295769419336	1.89794192553937	h
5.28739693953831	0.68685802586829	3.87607187606425	h
-3.12641537262939	-1.76879638085899	-1.72390195252854	h
-3.23853496896435	4.23559105659816	3.87607187606425	h
-7.14691669339186	6.01290744203017	1.89794192553937	h
-9.08709642486017	3.87347971904912	-1.87212808292069	h
-7.06864809815473	-0.03050737563011	-3.66127268502225	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	e	27.80	0.30662	YES	YES
8	e	27.80	0.30662	YES	YES
9	a	47.06	0.00736	YES	YES
10	e	52.05	0.10494	YES	YES
11	e	52.05	0.10494	YES	YES
12	a	64.78	0.40634	YES	YES
13	a	182.33	0.27891	YES	YES
14	e	198.32	1.12893	YES	YES
15	e	198.32	1.12893	YES	YES
16	a	244.10	0.72097	YES	YES
17	e	256.94	0.44089	YES	YES
18	e	256.94	0.44089	YES	YES
19	e	394.41	1.21812	YES	YES
20	e	394.41	1.21812	YES	YES
21	a	398.05	0.06145	YES	YES
22	a	402.33	0.22712	YES	YES
23	e	423.51	5.59665	YES	YES
24	e	423.51	5.59665	YES	YES
25	e	495.39	23.48600	YES	YES
26	e	495.39	23.48600	YES	YES
27	a	506.51	14.16096	YES	YES
28	e	612.18	0.26943	YES	YES
29	e	612.18	0.26943	YES	YES
30	a	612.25	0.05570	YES	YES
31	a	676.06	0.79936	YES	YES
32	e	690.08	1.45521	YES	YES
33	e	690.08	1.45521	YES	YES
34	e	698.48	34.81876	YES	YES
35	e	698.48	34.81876	YES	YES
36	a	699.13	31.56210	YES	YES
37	a	743.55	13.23311	YES	YES
38	e	743.87	16.00222	YES	YES
39	e	743.87	16.00222	YES	YES
40	e	834.82	0.09105	YES	YES
41	e	834.82	0.09105	YES	YES
42	a	837.18	0.26854	YES	YES
43	e	902.76	1.14820	YES	YES
44	e	902.76	1.14820	YES	YES
45	a	903.32	0.00902	YES	YES

46	e	956.49	0.01130	YES	YES
47	e	956.49	0.01130	YES	YES
48	a	956.98	0.21373	YES	YES
49	e	982.03	0.00233	YES	YES
50	e	982.03	0.00233	YES	YES
51	a	982.14	0.00987	YES	YES
52	e	987.71	4.06230	YES	YES
53	e	987.71	4.06230	YES	YES
54	a	988.15	0.08382	YES	YES
55	e	1025.62	4.98000	YES	YES
56	e	1025.62	4.98000	YES	YES
57	a	1026.10	0.33361	YES	YES
58	e	1072.54	0.91888	YES	YES
59	e	1072.54	0.91888	YES	YES
60	a	1072.68	5.62109	YES	YES
61	e	1080.76	10.10049	YES	YES
62	e	1080.76	10.10049	YES	YES
63	a	1089.31	1.12035	YES	YES
64	a	1140.98	0.01038	YES	YES
65	e	1141.17	0.05808	YES	YES
66	e	1141.17	0.05808	YES	YES
67	e	1164.38	6.10719	YES	YES
68	e	1164.38	6.10719	YES	YES
69	a	1165.72	0.94137	YES	YES
70	a	1288.32	4.82298	YES	YES
71	e	1291.37	1.68664	YES	YES
72	e	1291.37	1.68664	YES	YES
73	a	1360.94	0.04245	YES	YES
74	e	1363.69	0.98235	YES	YES
75	e	1363.69	0.98235	YES	YES
76	a	1430.21	13.51883	YES	YES
77	e	1432.04	7.53654	YES	YES
78	e	1432.04	7.53654	YES	YES
79	a	1472.16	2.01574	YES	YES
80	e	1472.16	12.43694	YES	YES
81	e	1472.16	12.43694	YES	YES
82	a	1588.09	0.29157	YES	YES
83	e	1589.52	0.11213	YES	YES
84	e	1589.52	0.11213	YES	YES
85	e	1602.68	6.37945	YES	YES
86	e	1602.68	6.37945	YES	YES
87	a	1605.13	0.15846	YES	YES
88	a	3079.83	4.34958	YES	YES
89	e	3079.88	1.40196	YES	YES
90	e	3079.88	1.40196	YES	YES
91	e	3089.68	0.25136	YES	YES
92	e	3089.68	0.25136	YES	YES
93	a	3089.72	0.01102	YES	YES
94	e	3099.30	7.73935	YES	YES
95	e	3099.30	7.73935	YES	YES
96	a	3099.59	24.48174	YES	YES
97	e	3107.33	11.17282	YES	YES
98	e	3107.33	11.17282	YES	YES

99	a	3107.81	9.35430	YES	YES
100	e	3114.64	36.07531	YES	YES
101	e	3114.64	36.07531	YES	YES
102	a	3115.26	8.47853	YES	YES

$[Sn(bipy)_3]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

3.33728066673074	-7.71900098407905	7.99201541865177	h
2.13717848633868	-4.82084201232203	11.62793562045221	h
0.93208392069452	-6.52934425206837	-9.51204095729094	h
2.46700833043155	-5.86064729266837	7.65203444003441	c
-11.44675541683879	-0.58661611021561	1.58927644392842	h
1.80304284765820	-4.25284572779297	9.65361283592371	c
5.73152530676078	-6.47875717902847	-9.35952226191709	h
1.95520068789663	-5.58639108628445	-7.96589373735944	c
-12.35587575386052	2.08095311444647	-2.29959946138757	h
2.44101899454928	-6.23671523882495	3.53600258250115	h
4.60533915698889	-5.55163331763563	-7.87475179127492	c
-9.91163136184606	0.09861390494526	0.36451363121170	c
1.97728822258141	-5.03617369008551	5.17985615145959	c
-1.45846560475346	-4.37653106148060	-5.97400401532811	h
-6.89418675783498	-1.67804344939479	2.56028925561458	h
-0.82504766592562	-1.74175364004086	0.01556556651571	sn
0.62889827313410	-4.38651504351501	-6.00832041941003	c
0.70253949122989	-1.90187360418455	9.11848353681418	c
-10.40423580543773	1.57454947271364	-1.78312062200956	c
0.18699202488479	-0.64077095646644	10.68515541137632	h
-7.38633322091609	-0.49997138308614	0.90839310205345	c
5.81858058294626	-4.32136514492924	-5.86512230950733	c
0.93073373424263	-2.78285817286764	4.67126362008157	n
7.89328988624866	-4.29116129781829	-5.79672171718756	h
1.79352126249390	-3.20317547330083	-4.09142004885629	n
0.28839031917313	-1.20335766765622	6.57770834644293	c
4.34760733251424	-3.14098773501948	-3.97888075169225	c
-8.37957172702558	2.40457530753977	-3.27870011895390	c
-5.45078030659229	0.30212001550662	-0.52085843951577	n
-1.40689916235212	2.67348550792804	9.68331703644002	h
-8.76583495550685	3.56232234023692	-4.95834741689756	h
-5.88965040762045	1.74013052806660	-2.58978520063157	c
9.42000469871643	-2.48709240076932	-2.81044369189485	h
-0.81736543488527	1.28210467843980	5.83984722883263	c
5.48358083963862	-1.74045743124207	-1.81269167729635	c
-1.56408165079269	3.08741112132744	7.65553529887373	c
8.12372125122143	-1.54548145066515	-1.49133839110739	c
3.88870226790340	-0.58734027787292	-0.14938952888198	n
-1.04727958165819	1.80286715230298	3.32728053522205	n
-3.62694285361604	2.59797082090760	-4.03505419692466	c
-5.70392011580402	4.68768522430529	-6.92813378822625	h
9.11343379504801	-0.13744220237967	0.51934333384296	c

4.84625380217461	0.77881384891801	1.77487992252895	c
-2.50986312551927	5.43410646410652	6.87900302752597	c
11.17364447883492	0.01990001598622	0.77064657722751	h
-3.83924344917664	4.13291556559690	-6.20545000682993	c
-3.09152466332067	6.84598801167076	8.29347462027321	h
-1.30396719978860	1.90111033366443	-3.16511110138426	n
3.45580794700403	1.68142278458752	3.02896772210192	h
7.44258585834376	1.07162966251182	2.18466222210127	c
-1.94199489532499	4.06870436121388	2.58523459565668	c
-2.68687512676158	5.95255163843015	4.28531001870360	c
-2.05151600287569	4.37464298350551	0.53176750427592	h
8.12730892837407	2.22057177854238	3.77691756251922	h
0.78931912487263	2.72565310418669	-4.35834748887380	c
-1.66090878123458	4.97185914182748	-7.45255200683192	c
-3.39171985326215	7.77781002279615	3.58146979119777	h
2.60174277231691	2.11931379141163	-3.53993372334448	h
-1.82289666496719	6.17312810604387	-9.14469153883321	h
0.71292332436275	4.27266717454710	-6.50176041112359	c
2.47881892918849	4.90756730548143	-7.39777613961241	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a	13.36	0.18716	YES	YES
8	a	13.67	0.18916	YES	YES
9	a	19.96	0.02069	YES	YES
10	a	25.67	0.56771	YES	YES
11	a	26.32	0.48058	YES	YES
12	a	37.25	1.92673	YES	YES
13	a	40.99	0.24725	YES	YES
14	a	42.63	0.40487	YES	YES
15	a	67.68	0.73944	YES	YES
16	a	76.15	1.05928	YES	YES
17	a	77.35	1.19361	YES	YES
18	a	88.24	1.32881	YES	YES
19	a	88.79	1.06698	YES	YES
20	a	96.52	0.03762	YES	YES
21	a	102.13	0.83006	YES	YES
22	a	121.32	4.93437	YES	YES
23	a	122.71	15.92480	YES	YES
24	a	123.35	16.25641	YES	YES
25	a	139.98	21.39408	YES	YES
26	a	140.91	20.50944	YES	YES
27	a	195.25	4.04887	YES	YES
28	a	208.18	17.06186	YES	YES
29	a	208.63	17.09556	YES	YES
30	a	216.33	3.11529	YES	YES
31	a	225.21	1.89717	YES	YES
32	a	225.64	2.49678	YES	YES
33	a	230.14	1.74573	YES	YES

34	a	340.20	0.87232	YES	YES
35	a	340.27	0.87261	YES	YES
36	a	358.10	0.21614	YES	YES
37	a	398.25	2.75797	YES	YES
38	a	398.67	2.58354	YES	YES
39	a	403.03	0.96223	YES	YES
40	a	409.11	6.46502	YES	YES
41	a	409.50	6.63529	YES	YES
42	a	417.21	12.42786	YES	YES
43	a	429.60	0.88871	YES	YES
44	a	429.80	0.86028	YES	YES
45	a	431.66	0.07150	YES	YES
46	a	441.03	0.01184	YES	YES
47	a	441.34	0.01979	YES	YES
48	a	441.87	0.35751	YES	YES
49	a	550.72	0.01193	YES	YES
50	a	551.00	0.01883	YES	YES
51	a	551.49	0.02921	YES	YES
52	a	616.16	11.09923	YES	YES
53	a	617.56	12.27142	YES	YES
54	a	617.66	12.26462	YES	YES
55	a	634.34	18.46293	YES	YES
56	a	634.41	19.04807	YES	YES
57	a	646.78	1.73254	YES	YES
58	a	646.95	4.55172	YES	YES
59	a	647.01	4.94640	YES	YES
60	a	655.33	2.57354	YES	YES
61	a	729.98	0.60704	YES	YES
62	a	730.16	0.27710	YES	YES
63	a	730.95	1.65623	YES	YES
64	a	737.51	4.57008	YES	YES
65	a	737.70	4.62700	YES	YES
66	a	738.56	8.09501	YES	YES
67	a	754.11	114.72418	YES	YES
68	a	754.38	42.58623	YES	YES
69	a	754.74	52.60194	YES	YES
70	a	763.14	8.43610	YES	YES
71	a	763.16	8.09149	YES	YES
72	a	764.48	1.48288	YES	YES
73	a	821.61	0.07660	YES	YES
74	a	821.82	0.06597	YES	YES
75	a	822.87	0.36267	YES	YES
76	a	882.90	0.03307	YES	YES
77	a	883.29	0.09932	YES	YES
78	a	883.42	0.05053	YES	YES
79	a	888.49	0.77423	YES	YES
80	a	888.90	0.71129	YES	YES
81	a	889.58	0.94479	YES	YES
82	a	954.03	0.01696	YES	YES
83	a	955.03	0.00713	YES	YES
84	a	955.94	0.01896	YES	YES
85	a	958.11	0.02134	YES	YES
86	a	958.57	0.02768	YES	YES

87	a	961.79	0.03269	YES	YES
88	a	993.95	37.36077	YES	YES
89	a	994.11	36.18937	YES	YES
90	a	994.91	15.88454	YES	YES
91	a	996.67	35.08634	YES	YES
92	a	996.86	36.28759	YES	YES
93	a	999.48	0.05782	YES	YES
94	a	999.66	0.03266	YES	YES
95	a	999.74	0.01553	YES	YES
96	a	1003.39	0.00165	YES	YES
97	a	1003.44	0.26308	YES	YES
98	a	1003.44	0.33462	YES	YES
99	a	1021.00	1.23637	YES	YES
100	a	1034.12	0.04144	YES	YES
101	a	1035.50	0.86388	YES	YES
102	a	1035.53	0.95132	YES	YES
103	a	1061.81	0.27882	YES	YES
104	a	1062.98	2.99720	YES	YES
105	a	1063.00	3.02999	YES	YES
106	a	1067.77	2.50558	YES	YES
107	a	1067.89	2.58770	YES	YES
108	a	1068.33	5.28473	YES	YES
109	a	1099.36	14.36422	YES	YES
110	a	1099.55	14.13340	YES	YES
111	a	1101.67	0.95871	YES	YES
112	a	1112.29	2.49335	YES	YES
113	a	1112.41	2.36024	YES	YES
114	a	1113.62	0.76837	YES	YES
115	a	1145.92	5.39687	YES	YES
116	a	1145.98	5.39287	YES	YES
117	a	1146.08	5.81652	YES	YES
118	a	1162.50	10.96967	YES	YES
119	a	1162.87	11.17445	YES	YES
120	a	1163.48	1.22241	YES	YES
121	a	1261.49	3.13699	YES	YES
122	a	1261.82	3.15937	YES	YES
123	a	1265.84	0.10364	YES	YES
124	a	1287.50	3.25305	YES	YES
125	a	1288.05	3.09313	YES	YES
126	a	1290.73	1.93317	YES	YES
127	a	1298.56	20.74621	YES	YES
128	a	1298.65	20.33232	YES	YES
129	a	1301.29	1.23127	YES	YES
130	a	1337.31	9.23551	YES	YES
131	a	1337.37	9.09163	YES	YES
132	a	1337.60	13.86372	YES	YES
133	a	1355.14	2.39090	YES	YES
134	a	1355.23	2.60116	YES	YES
135	a	1355.43	3.05021	YES	YES
136	a	1417.77	1.49638	YES	YES
137	a	1418.10	2.61235	YES	YES
138	a	1418.36	3.19894	YES	YES
139	a	1437.28	51.76785	YES	YES

140	a	1437.44	52.30384	YES	YES
141	a	1437.56	56.36693	YES	YES
142	a	1460.16	42.92138	YES	YES
143	a	1462.65	24.48149	YES	YES
144	a	1463.36	24.07757	YES	YES
145	a	1485.46	27.24588	YES	YES
146	a	1485.59	26.62662	YES	YES
147	a	1486.07	1.11295	YES	YES
148	a	1578.70	31.60330	YES	YES
149	a	1578.80	31.43771	YES	YES
150	a	1579.15	1.86137	YES	YES
151	a	1592.04	6.03533	YES	YES
152	a	1592.14	6.81350	YES	YES
153	a	1592.35	4.91708	YES	YES
154	a	1597.13	43.14469	YES	YES
155	a	1597.24	39.85982	YES	YES
156	a	1597.55	5.49778	YES	YES
157	a	1609.60	35.41050	YES	YES
158	a	1610.92	26.34660	YES	YES
159	a	1611.17	25.54526	YES	YES
160	a	3086.42	8.20354	YES	YES
161	a	3087.00	8.19904	YES	YES
162	a	3087.50	8.17815	YES	YES
163	a	3125.29	0.68602	YES	YES
164	a	3125.33	0.70556	YES	YES
165	a	3125.43	0.58377	YES	YES
166	a	3126.13	0.14473	YES	YES
167	a	3126.16	0.06951	YES	YES
168	a	3126.18	0.09759	YES	YES
169	a	3135.60	3.61361	YES	YES
170	a	3136.10	3.33034	YES	YES
171	a	3136.70	3.24147	YES	YES
172	a	3139.21	0.49418	YES	YES
173	a	3139.46	0.40740	YES	YES
174	a	3139.75	0.34667	YES	YES
175	a	3142.99	1.45785	YES	YES
176	a	3143.72	1.44338	YES	YES
177	a	3143.86	1.64074	YES	YES
178	a	3145.62	0.88147	YES	YES
179	a	3146.04	0.93476	YES	YES
180	a	3146.85	0.70885	YES	YES
181	a	3153.06	0.03622	YES	YES
182	a	3153.89	0.03652	YES	YES
183	a	3154.04	0.02419	YES	YES

bipy

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

2.32434388841853	5.36074939867151	0.00000000000000	c
-0.01337212910269	6.61809970887099	0.00000000000000	c
-2.22655747647419	5.14495846964807	0.00000000000000	c
-2.22529619940329	2.61485412880192	0.00000000000000	n
0.02498258742917	1.40835822044668	0.00000000000000	c
2.35234016718551	2.71506437285101	0.00000000000000	c
-0.02498258742917	-1.40835822044668	0.00000000000000	c
2.22529619940329	-2.61485412880192	0.00000000000000	n
2.22655747647419	-5.14495846964807	0.00000000000000	c
0.01337212910269	-6.61809970887099	0.00000000000000	c
-2.32434388841853	-5.36074939867151	0.00000000000000	c
-2.35234016718551	-2.71506437285101	0.00000000000000	c
-4.10444059516458	6.06477287969121	0.00000000000000	h
-0.12891900865240	8.69710890392869	0.00000000000000	h
4.10965276254494	6.43549978210020	0.00000000000000	h
4.11389005255996	1.61191063395858	0.00000000000000	h
-4.11389005255996	-1.61191063395858	0.00000000000000	h
-4.10965276254494	-6.43549978210020	0.00000000000000	h
0.12891900865240	-8.69710890392869	0.00000000000000	h
4.10444059516458	-6.06477287969121	0.00000000000000	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	au	66.80	2.97062	YES	NO
8	au	92.67	2.46120	YES	NO
9	bu	160.25	5.92471	YES	NO
10	bg	216.06	0.00000	NO	YES
11	ag	328.41	0.00000	NO	YES
12	au	395.61	7.06030	YES	NO
13	bg	403.91	0.00000	NO	YES
14	au	430.46	0.00476	YES	NO
15	ag	440.73	0.00000	NO	YES
16	bg	558.99	0.00000	NO	YES
17	ag	608.03	0.00000	NO	YES
18	bu	614.02	11.35670	YES	NO
19	bu	653.08	5.88828	YES	NO
20	bg	737.39	0.00000	NO	YES
21	au	744.21	23.61365	YES	NO
22	au	751.99	60.60203	YES	NO
23	ag	768.48	0.00000	NO	YES
24	bg	836.08	0.00000	NO	YES
25	au	892.89	0.95882	YES	NO
26	bg	903.00	0.00000	NO	YES
27	au	947.58	0.35424	YES	NO
28	bg	955.74	0.00000	NO	YES

29	bu	985.75	8.34893	YES	NO
30	ag	986.12	0.00000	NO	YES
31	au	991.10	0.11076	YES	NO
32	bg	992.01	0.00000	NO	YES
33	bu	1034.54	7.36628	YES	NO
34	ag	1039.72	0.00000	NO	YES
35	bu	1055.05	14.06021	YES	NO
36	ag	1080.84	0.00000	NO	YES
37	bu	1085.33	13.12993	YES	NO
38	bu	1125.56	1.50081	YES	NO
39	ag	1125.90	0.00000	NO	YES
40	bu	1255.73	0.03443	YES	NO
41	ag	1270.36	0.00000	NO	YES
42	ag	1312.87	0.00000	NO	YES
43	ag	1337.78	0.00000	NO	YES
44	bu	1348.93	5.38715	YES	NO
45	bu	1412.36	36.93369	YES	NO
46	ag	1443.01	0.00000	NO	YES
47	bu	1452.84	64.26079	YES	NO
48	ag	1480.78	0.00000	NO	YES
49	bu	1572.69	38.29549	YES	NO
50	ag	1593.08	0.00000	NO	YES
51	ag	1599.15	0.00000	NO	YES
52	bu	1605.51	86.31533	YES	NO
53	bu	3060.66	63.07746	YES	NO
54	ag	3060.96	0.00000	NO	YES
55	ag	3097.81	0.00000	NO	YES
56	bu	3097.85	19.18634	YES	NO
57	bu	3116.56	37.50477	YES	NO
58	ag	3116.83	0.00000	NO	YES
59	bu	3137.53	4.21171	YES	NO
60	ag	3138.33	0.00000	NO	YES

$[Sn(py)_4]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m5).

1.17179360100779	-4.95260665543011	-1.07673217993084	n
1.85948811087978	-6.20214238324531	1.04629192966374	c
1.72703240621567	-8.83848674203585	1.23832015841688	c
0.86382664903660	-10.23226518335743	-0.84980332873138	c
0.16747779412393	-8.93516353989965	-3.06063751487964	c
0.35701517679414	-6.29800994855960	-3.09764276348228	c
-2.10738948574368	-0.02169013210532	-2.71030946862700	n
-3.87684753337884	-1.64892175659748	-1.82235628744553	c
-6.43364890284529	-1.42042442709878	-2.45309164269980	c
-7.18610235811933	0.53918131212205	-4.07962027208334	c
-5.34405065055279	2.20634707312980	-5.01591000097668	c
-2.82650824436375	1.87002754198238	-4.28612173997491	c
1.81397830161322	4.32046021710071	-1.25975468352448	n
3.49224036797945	5.81406902600959	-2.47933308407799	c

3.51290404699178	8.44642389137339	-2.19037713961546	c
1.72595030782910	9.56270819578090	-0.57667295065369	c
-0.01708683173669	8.00526923867551	0.68832302474125	c
0.09301586782261	5.39250736748946	0.29521986485837	c
2.03300236776285	-0.05540801197604	2.51822647197317	n
4.11416249411823	0.87335266975419	3.68856296330641	c
4.18430909658905	1.29053638959393	6.29790650725372	c
2.02359883869240	0.74073977220511	7.73989396710649	c
-0.13244564317071	-0.21280301449667	6.51555007605375	c
-0.05455537843657	-0.58825001144942	3.89996481480963	c
2.34642191793226	-0.41080905520258	-1.97065768889609	sn
-1.32817831077144	3.14309853651933	-4.97209667641910	h
-1.23980770666510	4.10403380774438	1.24798995741377	h
-1.44884648457302	8.80624356919819	1.96778358199750	h
4.91093320144459	9.59327696032669	-3.21907024347795	h
4.86424015100728	4.85983545318810	-3.73079940063057	h
-3.19788154273516	-3.19074943427360	-0.60268632943854	h
-7.81059842406015	-2.77710107408871	-1.68409208529712	h
-5.84269745216628	3.75742241220253	-6.30936318338518	h
-0.15531526079089	-5.21443605987318	-4.80624218084698	h
-0.50296360770077	-9.95141158286096	-4.74745318430557	h
2.54855532650208	-5.04425105971957	2.63416405709429	h
2.30604042626154	-9.77951348293617	3.00099109393483	h
-1.69926582552961	-1.33905850463903	2.87095504302447	h
-1.86478512611193	-0.66729938027349	7.57372483076174	h
5.91556975190654	2.03572901616822	7.17816253969534	h
5.76691270164672	1.29296176951510	2.48714015974271	h
-9.18509399363377	0.75774226977355	-4.62032693582792	h
1.68931546015420	11.62709330306008	-0.30637203950489	h
0.74668557790204	-12.30931491084243	-0.76066453372323	h
2.01959882087195	1.05105655804838	9.79901649660808	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m5).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a	14.82	0.13724	YES	YES
8	a	18.58	0.04494	YES	YES
9	a	24.48	0.20995	YES	YES
10	a	30.12	0.20740	YES	YES
11	a	38.97	0.20325	YES	YES
12	a	41.71	0.66636	YES	YES
13	a	46.21	0.46392	YES	YES
14	a	51.78	0.29578	YES	YES
15	a	68.88	0.19736	YES	YES
16	a	103.12	4.99174	YES	YES
17	a	106.90	2.55299	YES	YES
18	a	110.63	0.22302	YES	YES
19	a	119.24	19.51958	YES	YES
20	a	128.58	12.71113	YES	YES
21	a	137.55	3.54993	YES	YES

22	a	143.89	5.22958	YES	YES
23	a	153.61	0.61705	YES	YES
24	a	160.95	0.48268	YES	YES
25	a	170.73	11.09598	YES	YES
26	a	179.15	27.41190	YES	YES
27	a	228.41	8.84267	YES	YES
28	a	378.05	0.04848	YES	YES
29	a	381.22	0.34107	YES	YES
30	a	382.92	0.04003	YES	YES
31	a	394.25	0.04833	YES	YES
32	a	412.46	3.80616	YES	YES
33	a	415.91	3.56062	YES	YES
34	a	417.95	4.11941	YES	YES
35	a	421.16	8.78427	YES	YES
36	a	614.96	36.00643	YES	YES
37	a	621.95	1.41877	YES	YES
38	a	624.82	15.95335	YES	YES
39	a	632.16	9.07002	YES	YES
40	a	641.38	0.08619	YES	YES
41	a	643.45	0.60561	YES	YES
42	a	643.64	0.17567	YES	YES
43	a	643.92	0.73439	YES	YES
44	a	690.50	54.10182	YES	YES
45	a	695.91	37.74210	YES	YES
46	a	696.63	41.84024	YES	YES
47	a	698.45	40.85182	YES	YES
48	a	746.95	31.36830	YES	YES
49	a	747.52	8.18721	YES	YES
50	a	748.44	4.15613	YES	YES
51	a	748.84	27.98393	YES	YES
52	a	859.89	0.07155	YES	YES
53	a	864.08	0.40273	YES	YES
54	a	865.52	0.17514	YES	YES
55	a	866.48	0.01397	YES	YES
56	a	927.67	0.09913	YES	YES
57	a	929.42	0.39985	YES	YES
58	a	930.07	0.08634	YES	YES
59	a	936.81	1.23201	YES	YES
60	a	967.11	0.02706	YES	YES
61	a	967.76	0.29753	YES	YES
62	a	968.42	0.18108	YES	YES
63	a	970.68	0.25087	YES	YES
64	a	1000.71	107.16053	YES	YES
65	a	1005.31	20.07476	YES	YES
66	a	1007.98	46.92459	YES	YES
67	a	1010.85	0.05675	YES	YES
68	a	1010.88	0.06426	YES	YES
69	a	1012.55	0.06818	YES	YES
70	a	1013.27	0.08541	YES	YES
71	a	1015.38	18.12938	YES	YES
72	a	1023.53	3.73383	YES	YES
73	a	1024.14	8.29938	YES	YES
74	a	1024.56	1.06133	YES	YES

75	a	1027.02	1.21743	YES	YES
76	a	1058.88	49.75017	YES	YES
77	a	1059.21	51.85262	YES	YES
78	a	1059.80	12.21249	YES	YES
79	a	1062.59	11.58370	YES	YES
80	a	1070.58	2.01175	YES	YES
81	a	1070.70	2.75806	YES	YES
82	a	1072.68	0.98821	YES	YES
83	a	1076.54	0.45260	YES	YES
84	a	1145.79	1.78168	YES	YES
85	a	1146.44	2.06718	YES	YES
86	a	1147.39	2.15896	YES	YES
87	a	1147.93	2.34673	YES	YES
88	a	1195.12	21.04731	YES	YES
89	a	1196.76	7.11324	YES	YES
90	a	1197.27	36.96367	YES	YES
91	a	1204.13	0.15214	YES	YES
92	a	1325.67	0.83292	YES	YES
93	a	1328.84	1.34655	YES	YES
94	a	1329.80	3.34379	YES	YES
95	a	1331.21	3.21120	YES	YES
96	a	1344.89	0.99921	YES	YES
97	a	1345.85	0.20612	YES	YES
98	a	1346.44	0.44698	YES	YES
99	a	1347.17	0.32650	YES	YES
100	a	1444.69	29.40551	YES	YES
101	a	1444.97	39.16922	YES	YES
102	a	1446.97	14.87433	YES	YES
103	a	1448.60	58.01639	YES	YES
104	a	1472.03	2.82135	YES	YES
105	a	1473.33	0.19945	YES	YES
106	a	1474.83	0.52496	YES	YES
107	a	1476.03	2.11184	YES	YES
108	a	1582.50	1.35167	YES	YES
109	a	1584.87	0.70186	YES	YES
110	a	1585.06	0.48472	YES	YES
111	a	1586.51	0.52469	YES	YES
112	a	1609.10	78.09658	YES	YES
113	a	1609.89	8.80608	YES	YES
114	a	1613.29	48.61374	YES	YES
115	a	1614.20	33.77054	YES	YES
116	a	3089.05	3.25234	YES	YES
117	a	3090.66	2.56494	YES	YES
118	a	3100.47	1.11374	YES	YES
119	a	3103.89	3.52931	YES	YES
120	a	3118.46	3.53002	YES	YES
121	a	3120.32	2.08691	YES	YES
122	a	3125.63	0.32566	YES	YES
123	a	3125.83	0.46233	YES	YES
124	a	3126.83	0.46669	YES	YES
125	a	3127.40	1.02629	YES	YES
126	a	3131.78	4.67485	YES	YES
127	a	3133.10	3.61492	YES	YES

128	a	3136.65	0.56776	YES	YES
129	a	3138.32	0.88712	YES	YES
130	a	3140.59	2.60073	YES	YES
131	a	3140.88	2.68123	YES	YES
132	a	3141.24	2.73651	YES	YES
133	a	3142.19	2.56598	YES	YES
134	a	3143.73	2.96962	YES	YES
135	a	3144.09	3.33453	YES	YES

Pyridine

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m5).

2.16924098635942	0.00000000000000	1.73806296702269	c
2.27989963654230	0.00000000000000	-0.91759010652283	c
0.00000000000000	0.00000000000000	3.05843375415009	n
-2.16924098635942	0.00000000000000	1.73806296702269	c
-2.27989963654230	0.00000000000000	-0.91759010652283	c
0.00000000000000	0.00000000000000	-2.27427184756308	c
3.93195667794721	0.00000000000000	2.86314042981560	h
-3.93195667794721	0.00000000000000	2.86314042981560	h
-4.11842573851158	0.00000000000000	-1.89655024370362	h
4.11842573851158	0.00000000000000	-1.89655024370362	h
0.00000000000000	0.00000000000000	-4.35828799981069	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m5).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a2	361.42	0.00000	NO	YES
8	b2	407.14	2.96018	YES	YES
9	a1	591.83	4.12945	YES	YES
10	b1	650.64	0.37010	YES	YES
11	b2	694.52	51.29200	YES	YES
12	b2	743.53	4.08266	YES	YES
13	a2	869.49	0.00000	NO	YES
14	b2	922.46	0.01654	YES	YES
15	a2	963.82	0.00000	NO	YES
16	a1	982.44	9.07329	YES	YES
17	b2	984.47	0.00079	YES	YES
18	a1	1024.42	3.22684	YES	YES
19	b1	1050.12	0.00002	YES	YES
20	a1	1063.32	4.59562	YES	YES
21	b1	1130.49	1.34266	YES	YES
22	a1	1206.94	3.20662	YES	YES
23	b1	1326.11	0.83153	YES	YES
24	b1	1338.29	0.09476	YES	YES
25	b1	1437.19	23.88538	YES	YES
26	a1	1471.91	2.81578	YES	YES
27	a1	1593.33	20.16354	YES	YES

28	b1	1594.70	10.51537	YES	YES
29	b1	3060.74	37.33719	YES	YES
30	a1	3063.95	9.42070	YES	YES
31	a1	3095.14	3.79581	YES	YES
32	b1	3109.42	24.92291	YES	YES
33	a1	3117.15	7.56393	YES	YES

$[Sn(pyr)_4]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

1.08609887517428	-4.94419395556063	-1.00641636831141	n
1.74801994272853	-6.21234083050568	1.10863853722365	c
1.56034911944380	-8.86351565381403	1.20864687795216	c
0.73810145741305	-10.22320337983779	-0.76398298375136	n
0.10437930612534	-8.95706727238429	-2.86591141529877	c
0.27781627040969	-6.30891716171623	-3.01185179164378	c
-2.21421716145968	-0.00746330508217	-2.64220986943156	n
-3.99489357004167	-1.60779531545796	-1.74227297590181	c
-6.54598012855955	-1.29069367049789	-2.41658293975802	c
-7.30301989892936	0.55829096986989	-3.97408810106123	n
-5.52380787553003	2.11569777640524	-4.88264171985281	c
-2.96117089698830	1.86049992281083	-4.22404110164927	c
1.70208472116016	4.35051158420210	-1.17169702621194	n
3.37727092857437	5.86597695187954	-2.35953603998733	c
3.31856599997207	8.50101593487321	-1.98289100344580	c
1.62372999563682	9.59100068058290	-0.44985888542924	n
-0.03607653700957	8.07238108933046	0.72068057112059	c
-0.01417826118804	5.43921276309218	0.37225389220623	c
1.95666450533570	-0.02808159530867	2.60902132356199	n
4.02388404103066	0.88797522659434	3.80279287009545	c
3.98206967926542	1.29266748716398	6.43054980280659	c
1.92297103331379	0.80983166941163	7.82504105493202	n
-0.11634829659205	-0.09578246449896	6.62369366812803	c
-0.12533874993300	-0.53146401991728	4.00254278467528	c
2.26980287502725	-0.39229722508023	-1.90671612339094	sn
-1.50773186978807	3.15270131651621	-4.96874908858898	h
-1.38449423115403	4.19881543940723	1.33609952659103	h
-1.43565740588256	8.97124760926337	1.98260617533737	h
4.68534730590321	9.74521707253987	-2.95317665592455	h
4.77958040237320	4.97402409568749	-3.62239686578800	h
-3.37170544202934	-3.16071135315013	-0.50663290823029	h
-8.00712894284421	-2.58206730461726	-1.67097921737663	h
-6.13569447704222	3.62812663844429	-6.18487639224103	h
-0.23054061469715	-5.28206651704153	-4.75595229058672	h
-0.56052995173573	-10.07169203362995	-4.50088719449784	h
2.44249868672682	-5.10799903161216	2.73147714823349	h
2.09787747116387	-9.90248382121746	2.93777849854913	h
-1.80085934706951	-1.28344639295812	3.02450338794351	h
-1.81402585227226	-0.49281336173059	7.77212056900946	h
5.66826064791857	2.02860514604676	7.41698200479202	h
5.71802624604994	1.30229629149751	2.65892026520143	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules IR	RAMAN
7	a	6.66	0.00032	YES	YES
8	a	17.11	0.07262	YES	YES
9	a	23.21	0.19756	YES	YES
10	a	29.25	0.26222	YES	YES
11	a	37.03	0.24502	YES	YES
12	a	41.96	0.15214	YES	YES
13	a	44.95	0.18804	YES	YES
14	a	48.84	0.07618	YES	YES
15	a	66.54	0.42970	YES	YES
16	a	99.67	4.76656	YES	YES
17	a	103.32	0.26616	YES	YES
18	a	108.40	1.40305	YES	YES
19	a	117.39	17.55251	YES	YES
20	a	124.64	12.18705	YES	YES
21	a	133.81	4.17157	YES	YES
22	a	141.50	5.30426	YES	YES
23	a	149.37	1.67217	YES	YES
24	a	157.63	0.50248	YES	YES
25	a	166.53	8.32902	YES	YES
26	a	175.63	14.76257	YES	YES
27	a	225.13	3.13663	YES	YES
28	a	318.29	0.03392	YES	YES
29	a	321.72	0.12402	YES	YES
30	a	323.23	0.02273	YES	YES
31	a	335.14	0.02636	YES	YES
32	a	429.12	26.52701	YES	YES
33	a	433.50	15.54060	YES	YES
34	a	436.73	15.32875	YES	YES
35	a	440.03	33.59581	YES	YES
36	a	606.01	7.20180	YES	YES
37	a	612.46	0.06482	YES	YES
38	a	615.38	1.54085	YES	YES
39	a	624.20	2.44276	YES	YES
40	a	690.77	0.71225	YES	YES
41	a	692.84	1.13647	YES	YES
42	a	693.13	1.16469	YES	YES
43	a	693.47	3.61389	YES	YES
44	a	742.22	1.55241	YES	YES
45	a	745.05	0.97578	YES	YES
46	a	747.12	0.37885	YES	YES
47	a	747.35	0.42324	YES	YES
48	a	776.01	28.83022	YES	YES
49	a	777.86	25.01901	YES	YES
50	a	778.83	6.64296	YES	YES
51	a	782.91	35.11153	YES	YES
52	a	884.06	0.24143	YES	YES
53	a	885.10	0.33183	YES	YES
54	a	887.68	0.24261	YES	YES

55	a	890.86	0.01350	YES	YES
56	a	959.50	0.05022	YES	YES
57	a	959.92	0.22662	YES	YES
58	a	960.38	0.25278	YES	YES
59	a	961.09	0.29178	YES	YES
60	a	969.80	0.03570	YES	YES
61	a	970.65	0.04436	YES	YES
62	a	971.36	0.03479	YES	YES
63	a	971.92	0.04510	YES	YES
64	a	1007.81	49.36307	YES	YES
65	a	1009.14	9.83151	YES	YES
66	a	1009.71	11.17917	YES	YES
67	a	1013.16	9.67357	YES	YES
68	a	1025.62	133.25824	YES	YES
69	a	1028.77	45.54851	YES	YES
70	a	1030.76	62.66495	YES	YES
71	a	1039.91	29.34525	YES	YES
72	a	1074.93	3.83806	YES	YES
73	a	1075.59	2.92484	YES	YES
74	a	1077.13	4.21796	YES	YES
75	a	1081.03	6.89494	YES	YES
76	a	1118.88	31.69192	YES	YES
77	a	1120.38	29.71532	YES	YES
78	a	1121.50	33.38851	YES	YES
79	a	1124.44	6.67250	YES	YES
80	a	1210.21	0.84798	YES	YES
81	a	1211.28	1.73282	YES	YES
82	a	1211.36	1.02704	YES	YES
83	a	1214.59	1.49149	YES	YES
84	a	1274.12	7.02013	YES	YES
85	a	1275.21	4.51252	YES	YES
86	a	1276.53	2.32394	YES	YES
87	a	1277.52	0.28435	YES	YES
88	a	1323.47	1.89715	YES	YES
89	a	1325.97	2.76484	YES	YES
90	a	1326.23	2.67119	YES	YES
91	a	1327.56	4.49628	YES	YES
92	a	1405.61	43.69896	YES	YES
93	a	1406.58	39.80669	YES	YES
94	a	1407.05	33.85963	YES	YES
95	a	1408.99	90.41153	YES	YES
96	a	1463.72	0.08491	YES	YES
97	a	1465.42	2.14507	YES	YES
98	a	1466.46	0.65581	YES	YES
99	a	1466.96	0.46976	YES	YES
100	a	1550.90	4.66565	YES	YES
101	a	1553.49	6.11975	YES	YES
102	a	1554.00	4.47403	YES	YES
103	a	1555.56	5.61099	YES	YES
104	a	1575.01	0.58590	YES	YES
105	a	1575.17	0.70901	YES	YES
106	a	1576.34	0.38615	YES	YES
107	a	1578.08	0.68372	YES	YES

108	a	3092.87	4.03045	YES	YES
109	a	3093.44	3.70771	YES	YES
110	a	3097.60	2.61927	YES	YES
111	a	3101.53	3.16221	YES	YES
112	a	3103.76	2.11658	YES	YES
113	a	3103.89	4.40608	YES	YES
114	a	3104.65	0.69805	YES	YES
115	a	3108.13	6.32346	YES	YES
116	a	3108.25	4.30318	YES	YES
117	a	3110.17	2.82500	YES	YES
118	a	3112.32	1.64563	YES	YES
119	a	3113.64	1.78067	YES	YES
120	a	3125.17	0.33766	YES	YES
121	a	3126.03	2.51661	YES	YES
122	a	3133.13	1.50049	YES	YES
123	a	3136.30	1.23179	YES	YES

$[Sn(pyr)_2(MeCN)_4]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

0.05306037532322	1.61209669094484	-0.04744861901116	sn
-0.10904810779384	-4.50595992696372	-2.02296307365591	c
-0.71956880597778	-4.77965447594111	-0.05285608072204	h
0.07095392369661	-6.52755037911558	-3.73683398011392	c
-0.39756414230739	-8.47219157837236	-3.14031919233963	h
1.37890310414149	-3.82505528605838	-6.84864910470608	c
1.99150885546619	-3.53685275442466	-8.82292195195949	h
0.81032194657800	-6.18952383720375	-6.13713969477866	n
1.21363829698905	-1.77245813689865	-5.17004464153051	c
1.68512711844069	0.16960166513247	-5.75393910672953	h
0.46883526480686	-2.13699706133240	-2.76101994232815	n
2.20061584890577	-1.41010826963590	2.82900665152157	n
4.33694754531081	-2.60529700860716	2.10524764685202	c
5.06814560304318	-2.19170916931910	0.20217805483793	h
4.66367530957479	-4.78951902648257	6.07342669420952	n
5.55507057504157	-4.29501761870533	3.75326090478188	c
7.30211699486783	-5.27479630051064	3.16608918380368	h
2.54912582289786	-3.58341778025852	6.77490259810396	c
1.80987832499764	-3.97612665369045	8.68707718214004	h
1.29426201432893	-1.87943014658635	5.16705352168821	c
-0.42717888618240	-0.86483604242071	5.74374020639374	h
-3.61403156588788	-0.95098933154317	1.39792924923154	n
-8.16327913603720	-2.42934966887778	2.67991951383579	c
-9.55558005244609	-0.90067898265046	2.30501811591703	h
-8.21655670043873	-2.90776400213042	4.72523252143651	h
-8.70735426194907	-4.12897972187017	1.57042995211393	h
-5.64671636520080	-1.60025011142711	1.96721325252982	c
-1.32399063288130	3.56236738994095	4.72937816539927	n
-2.12749509309951	7.22284528271648	7.98467902315138	c
-0.51500964704806	8.56923951152392	7.97794483355621	h

-2.33580888389294	6.43340933679138	9.92042063557809	h
-3.88126858514043	8.26789633415451	7.48992162342281	h
-1.68181074107509	5.19960998633864	6.17550200965037	c
-3.51013202162681	2.06353256688897	-3.90701273510434	n
-6.38984552981966	3.96655330245286	-7.47347682680399	c
-5.57826242319499	3.54129001475842	-9.36383247667532	h
-6.53683246308376	6.05106669111681	-7.25747651423990	h
-8.31801103344158	3.13971084196056	-7.37065264866005	h
-4.79327968502225	2.91603818371436	-5.49464765317665	c
4.93259779285185	1.94365926372833	-1.92234356610887	n
9.12979588328087	4.22768926272184	-3.25993462832398	c
9.74473306636924	3.55875059649772	-5.15429767672996	h
10.65008772628781	3.81110231357775	-1.87082917945684	h
8.83837854237598	6.30700685229259	-3.33833353704814	h
6.80084482797108	2.97104718377276	-2.51859870995195	c

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a	9.38	0.01155	YES	YES
8	a	13.13	0.01735	YES	YES
9	a	14.60	1.06339	YES	YES
10	a	15.27	0.32376	YES	YES
11	a	20.26	0.03521	YES	YES
12	a	22.13	0.31594	YES	YES
13	a	25.77	2.22823	YES	YES
14	a	26.12	0.67393	YES	YES
15	a	30.51	5.57057	YES	YES
16	a	30.97	0.70735	YES	YES
17	a	32.79	2.86408	YES	YES
18	a	37.36	2.21185	YES	YES
19	a	38.73	1.89545	YES	YES
20	a	49.85	0.41139	YES	YES
21	a	56.45	0.05641	YES	YES
22	a	60.70	0.41686	YES	YES
23	a	70.61	5.21582	YES	YES
24	a	72.64	1.51727	YES	YES
25	a	85.01	0.08875	YES	YES
26	a	98.10	7.64570	YES	YES
27	a	102.25	7.36689	YES	YES
28	a	104.71	10.29015	YES	YES
29	a	109.37	18.31255	YES	YES
30	a	126.09	2.58038	YES	YES
31	a	129.72	6.18708	YES	YES
32	a	134.82	13.70454	YES	YES
33	a	142.62	3.47552	YES	YES
34	a	145.84	35.26318	YES	YES
35	a	148.98	8.10748	YES	YES
36	a	159.71	46.67119	YES	YES
37	a	167.27	8.01309	YES	YES

38	a	174.68	38.73073	YES	YES
39	a	237.71	24.18292	YES	YES
40	a	330.25	0.05980	YES	YES
41	a	333.55	0.26919	YES	YES
42	a	387.40	0.23100	YES	YES
43	a	388.30	0.65955	YES	YES
44	a	389.66	1.41362	YES	YES
45	a	391.35	0.34271	YES	YES
46	a	391.94	2.54329	YES	YES
47	a	393.71	6.34751	YES	YES
48	a	395.10	1.37684	YES	YES
49	a	399.86	3.07097	YES	YES
50	a	436.69	30.67363	YES	YES
51	a	441.05	20.44953	YES	YES
52	a	614.40	3.39527	YES	YES
53	a	620.91	5.10245	YES	YES
54	a	695.79	0.75223	YES	YES
55	a	696.10	0.18710	YES	YES
56	a	747.23	3.07188	YES	YES
57	a	748.14	2.82678	YES	YES
58	a	777.32	19.94407	YES	YES
59	a	783.26	38.98815	YES	YES
60	a	888.12	0.04122	YES	YES
61	a	894.88	0.62276	YES	YES
62	a	935.96	8.47465	YES	YES
63	a	937.26	10.60772	YES	YES
64	a	939.61	5.95608	YES	YES
65	a	949.18	7.75614	YES	YES
66	a	957.50	0.28102	YES	YES
67	a	961.91	1.65085	YES	YES
68	a	967.05	0.02478	YES	YES
69	a	969.76	0.52357	YES	YES
70	a	1009.03	6.10165	YES	YES
71	a	1010.33	6.83258	YES	YES
72	a	1011.58	20.39048	YES	YES
73	a	1011.71	1.18056	YES	YES
74	a	1012.30	17.13625	YES	YES
75	a	1012.38	1.61147	YES	YES
76	a	1012.80	6.23982	YES	YES
77	a	1013.05	14.64502	YES	YES
78	a	1013.48	10.92232	YES	YES
79	a	1013.71	6.65824	YES	YES
80	a	1034.23	55.72471	YES	YES
81	a	1040.32	65.78554	YES	YES
82	a	1076.41	11.88316	YES	YES
83	a	1077.50	4.56635	YES	YES
84	a	1128.17	27.90081	YES	YES
85	a	1130.46	29.19046	YES	YES
86	a	1213.27	1.54804	YES	YES
87	a	1214.92	1.55262	YES	YES
88	a	1274.59	6.31514	YES	YES
89	a	1278.23	1.41837	YES	YES
90	a	1327.08	1.38786	YES	YES

91	a	1327.55	0.22568	YES	YES
92	a	1345.20	12.82514	YES	YES
93	a	1347.18	9.31902	YES	YES
94	a	1348.34	8.96987	YES	YES
95	a	1348.96	8.40556	YES	YES
96	a	1388.27	21.34394	YES	YES
97	a	1388.42	19.69897	YES	YES
98	a	1391.75	19.57805	YES	YES
99	a	1391.83	20.36052	YES	YES
100	a	1393.90	20.59029	YES	YES
101	a	1394.05	21.18679	YES	YES
102	a	1394.28	17.78838	YES	YES
103	a	1394.66	21.03771	YES	YES
104	a	1410.34	26.26077	YES	YES
105	a	1410.49	55.03652	YES	YES
106	a	1466.56	0.74793	YES	YES
107	a	1469.31	0.95500	YES	YES
108	a	1553.85	2.08836	YES	YES
109	a	1558.95	2.37825	YES	YES
110	a	1583.60	0.06785	YES	YES
111	a	1585.98	0.32284	YES	YES
112	a	2285.75	178.18884	YES	YES
113	a	2287.83	150.58169	YES	YES
114	a	2294.38	118.67476	YES	YES
115	a	2309.61	177.03214	YES	YES
116	a	2958.62	19.46572	YES	YES
117	a	2959.23	12.84551	YES	YES
118	a	2960.34	10.73315	YES	YES
119	a	2960.64	9.22429	YES	YES
120	a	3056.52	10.02446	YES	YES
121	a	3056.68	8.36566	YES	YES
122	a	3057.10	6.63147	YES	YES
123	a	3057.13	7.35705	YES	YES
124	a	3057.27	6.76933	YES	YES
125	a	3057.29	11.66653	YES	YES
126	a	3058.07	6.50351	YES	YES
127	a	3058.10	6.79185	YES	YES
128	a	3100.46	2.52704	YES	YES
129	a	3100.76	0.96437	YES	YES
130	a	3103.65	2.03836	YES	YES
131	a	3103.80	2.02955	YES	YES
132	a	3125.82	3.48264	YES	YES
133	a	3132.51	1.84667	YES	YES
134	a	3137.07	2.09130	YES	YES
135	a	3142.04	7.05661	YES	YES

Pyrazine

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

-2.15226582852150	1.33020778631456	0.00000000000000	c
-2.15226582852150	-1.33020778631456	0.00000000000000	c
0.00000000000000	2.67552713694526	0.00000000000000	n
2.15226582852150	1.33020778631456	0.00000000000000	c
2.15226582852150	-1.33020778631456	0.00000000000000	c
0.00000000000000	-2.67552713694526	0.00000000000000	n
-3.94594242159110	2.40351081179136	0.00000000000000	h
3.94594242159110	2.40351081179136	0.00000000000000	h
3.94594242159110	-2.40351081179136	0.00000000000000	h
-3.94594242159110	-2.40351081179136	0.00000000000000	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	au	311.17	0.00000	NO	NO
8	b1u	418.98	18.56474	YES	NO
9	ag	586.55	0.00000	NO	YES
10	b1g	703.82	0.00000	NO	YES
11	b3g	761.43	0.00000	NO	YES
12	b1u	771.95	19.70042	YES	NO
13	b2g	912.78	0.00000	NO	YES
14	b3g	957.22	0.00000	NO	YES
15	au	962.54	0.00000	NO	NO
16	b2u	999.72	37.77331	YES	NO
17	ag	1024.27	0.00000	NO	YES
18	b3u	1061.93	8.22918	YES	NO
19	b2u	1139.60	6.52852	YES	NO
20	ag	1215.87	0.00000	NO	YES
21	b3u	1271.86	0.00048	YES	NO
22	b1g	1329.33	0.00000	NO	YES
23	b3u	1408.96	30.05525	YES	NO
24	b2u	1471.12	1.49310	YES	NO
25	b1g	1557.31	0.00000	NO	YES
26	ag	1576.55	0.00000	NO	YES
27	b1g	3063.10	0.00000	NO	YES
28	b2u	3063.64	8.66113	YES	NO
29	b3u	3076.51	85.02470	YES	NO
30	ag	3083.73	0.00000	NO	YES

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

-2.15242982989078	1.33024637701547	0.00000000000000	c
-2.15242982989078	-1.33024637701547	0.00000000000000	c
0.00000000000000	2.67544620812747	0.00000000000000	n
2.15242982989078	1.33024637701547	0.00000000000000	c
2.15242982989078	-1.33024637701547	0.00000000000000	c
0.00000000000000	-2.67544620812747	0.00000000000000	n
-3.94611945824018	2.40349162620061	0.00000000000000	h
3.94611945824018	2.40349162620061	0.00000000000000	h
3.94611945824018	-2.40349162620061	0.00000000000000	h
-3.94611945824018	-2.40349162620061	0.00000000000000	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	au	311.92	0.00000	NO	NO
8	b1u	418.85	18.49629	YES	NO
9	ag	586.86	0.00000	NO	YES
10	b1g	704.11	0.00000	NO	YES
11	b3g	761.62	0.00000	NO	YES
12	b1u	772.62	19.74148	YES	NO
13	b2g	913.20	0.00000	NO	YES
14	b3g	957.58	0.00000	NO	YES
15	au	962.89	0.00000	NO	NO
16	b2u	1000.23	37.80973	YES	NO
17	ag	1023.59	0.00000	NO	YES
18	b3u	1061.40	8.26811	YES	NO
19	b2u	1138.96	6.43577	YES	NO
20	ag	1215.62	0.00000	NO	YES
21	b3u	1269.95	0.00041	YES	NO
22	b1g	1329.14	0.00000	NO	YES
23	b3u	1408.39	29.97130	YES	NO
24	b2u	1470.40	1.51525	YES	NO
25	b1g	1555.96	0.00000	NO	YES
26	ag	1575.68	0.00000	NO	YES
27	b1g	3063.07	0.00000	NO	YES
28	b2u	3063.59	8.65563	YES	NO
29	b3u	3076.47	85.00828	YES	NO
30	ag	3083.70	0.00000	NO	YES

$[Sn(mes)_3]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

-0.00378656044925	0.00053340740711	0.00877738457369	sn
-3.49328516016347	-4.28173299332775	-2.74091421820117	c
-3.98269109717420	-1.93359928673977	-3.93045581437946	c
-3.64015696969247	-1.73628076418546	-5.97692912040614	h
-5.10259856606624	0.11172621051375	-2.60008418252108	c
-5.84681753609666	2.49518714659713	-3.96633476983738	c
-5.62195120125584	-0.21311499840366	0.00887589116283	c
-6.57716483739122	1.31155172304726	1.04534867678560	h
-4.99750943344915	-2.47511222453911	1.30618503888440	c
-5.62774711495647	-2.80913873019535	4.06135518447378	c
-3.88859918537363	-4.47378690013571	-0.09976450202316	c
-3.47127543893157	-6.27280263975105	0.86539747652675	h
-2.77297800170157	-6.56537708962733	-4.27459825821933	c
-1.68897627457074	-7.97649449572676	-3.16504208987048	h
-1.70936191915478	-6.07057466019609	-6.01296880629041	h
-4.53389400758863	-7.53280712276059	-4.91019306074761	h
2.66006707946091	4.23563257607148	2.56838679831855	c
1.27616342573995	5.53066102279158	0.67245255438823	c
2.60385404637826	6.84628296975912	-1.47412634548356	c
-1.39204889722266	5.67425593233378	0.93021820394990	c
-2.48405495172366	6.74385042772770	-0.48616713719517	h
-2.65390860866670	4.65145242077940	3.05850519717824	c
-5.39477874273747	5.23143394082670	3.54438715036219	c
-1.22391118855098	3.22992658269574	4.82020073941960	c
-2.18443421568989	2.37822050218909	6.46150329621967	h
1.44742478630490	3.04478520490119	4.64145557014055	c
2.95334430915096	1.74968099002600	6.67900788277452	c
4.73296031876316	4.19562076259482	2.45187325746967	h
6.14861825952285	-0.37501972129165	-0.30990406223941	c
5.26827538045379	-2.48277037933625	1.08658052260462	c
5.93563864572224	-2.76261076651687	3.04056632699691	h
3.70995809586228	-4.36020547273303	-0.03226180405653	c
3.00671407508366	-6.71236973894939	1.40731685684981	c
2.95677058101387	-4.02137593297041	-2.58204186520658	c
1.83687012912357	-5.50491109757845	-3.50798503681366	h
3.65971238600861	-1.85044125494244	-3.98946963805030	c
2.90605699584731	-1.55785848537102	-6.71839173598807	c
5.21943412151494	-0.02144546760765	-2.79577147680490	c
5.84845554094127	1.63508658318010	-3.89300835880923	h
8.17130161749949	1.32571297183358	0.73959513355679	c
8.12125932331405	1.44909530413075	2.83234847818320	h
8.11048999037670	3.25521759510937	-0.07975515571098	h
10.05399013073440	0.52421010306930	0.23615439919757	h
1.15893086789096	-2.62420086200206	-7.17063418521678	h
4.42832823028156	-2.32066957909980	-7.95764814025913	h
2.63954011114305	0.45369230592120	-7.25124245145967	h
1.29064116620827	-7.62805065060514	0.62626114356273	h
2.71127544272325	-6.32902351458073	3.44870915004389	h

4.56852799220503	-8.11815486306090	1.27226270624432	h
-4.24139291502272	-4.03922215938601	5.04385889687378	h
-7.50781953419146	-3.73861897859809	4.24942206071867	h
-5.75016181313811	-0.97413887113551	5.06766624293168	h
-4.44522411256998	3.03371157031091	-5.43248716840718	h
-6.11575290762959	4.10426469729269	-2.65090930681665	h
-7.67970607861279	2.19875222217483	-4.95942966323893	h
4.46217978993101	5.97445416270949	-1.90081639122829	h
2.97322154755272	8.85294915445356	-0.95293567207663	h
1.44200922158065	6.87568729367602	-3.22064853304586	h
-6.46972521321683	5.59653982313059	1.78136027846567	h
-5.51698772295921	6.99454187503274	4.69201824722139	h
-6.35427404577237	3.73409553474465	4.65568658497111	h
4.79073730830626	1.03620379148134	5.96624865210971	h
1.89522491157767	0.16528917661490	7.55582260057770	h
3.38499842350290	3.12160371622627	8.21711036686569	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules IR	RAMAN
7	a	15.93	0.00326	YES	YES
8	a	22.22	0.00104	YES	YES
9	a	30.65	0.01194	YES	YES
10	a	40.89	0.05660	YES	YES
11	a	45.29	1.90696	YES	YES
12	a	45.61	2.13731	YES	YES
13	a	62.80	0.21582	YES	YES
14	a	70.35	0.00273	YES	YES
15	a	74.47	0.07894	YES	YES
16	a	81.44	0.05461	YES	YES
17	a	84.39	0.21307	YES	YES
18	a	88.67	0.05207	YES	YES
19	a	89.17	0.03014	YES	YES
20	a	91.10	0.24462	YES	YES
21	a	93.67	0.44534	YES	YES
22	a	99.38	0.54005	YES	YES
23	a	109.37	4.56060	YES	YES
24	a	109.94	3.75743	YES	YES
25	a	125.84	19.67364	YES	YES
26	a	126.12	20.03561	YES	YES
27	a	137.31	0.00090	YES	YES
28	a	189.04	2.43456	YES	YES
29	a	194.57	0.58707	YES	YES
30	a	195.39	0.43983	YES	YES
31	a	204.06	52.61734	YES	YES
32	a	204.47	52.92847	YES	YES
33	a	208.64	1.08856	YES	YES
34	a	224.87	0.07102	YES	YES
35	a	225.57	0.01914	YES	YES
36	a	228.57	0.05601	YES	YES

37	a	236.06	13.12949	YES	YES
38	a	237.45	13.15602	YES	YES
39	a	270.22	0.02614	YES	YES
40	a	271.47	0.16480	YES	YES
41	a	272.51	0.49983	YES	YES
42	a	272.89	0.44355	YES	YES
43	a	273.81	0.01703	YES	YES
44	a	274.91	0.00446	YES	YES
45	a	277.66	0.00999	YES	YES
46	a	448.95	0.00066	YES	YES
47	a	449.17	0.00081	YES	YES
48	a	451.11	0.02724	YES	YES
49	a	485.97	3.03350	YES	YES
50	a	486.44	2.99831	YES	YES
51	a	489.91	0.00852	YES	YES
52	a	490.75	0.20585	YES	YES
53	a	493.65	0.00295	YES	YES
54	a	494.00	0.00088	YES	YES
55	a	517.63	2.28511	YES	YES
56	a	519.45	0.00144	YES	YES
57	a	519.56	0.01085	YES	YES
58	a	529.10	0.02328	YES	YES
59	a	530.37	0.75649	YES	YES
60	a	530.76	0.74928	YES	YES
61	a	570.81	2.59299	YES	YES
62	a	570.91	2.63894	YES	YES
63	a	571.59	0.00986	YES	YES
64	a	668.96	10.96040	YES	YES
65	a	669.38	11.06400	YES	YES
66	a	670.58	0.62359	YES	YES
67	a	843.83	11.89880	YES	YES
68	a	846.11	43.85954	YES	YES
69	a	848.12	45.17682	YES	YES
70	a	888.05	4.95460	YES	YES
71	a	889.31	4.59714	YES	YES
72	a	893.24	5.22573	YES	YES
73	a	898.05	0.15479	YES	YES
74	a	900.16	0.03506	YES	YES
75	a	900.90	0.01045	YES	YES
76	a	925.67	0.08548	YES	YES
77	a	926.15	0.22275	YES	YES
78	a	926.51	0.12469	YES	YES
79	a	926.73	0.00600	YES	YES
80	a	927.08	0.09308	YES	YES
81	a	929.20	0.00463	YES	YES
82	a	985.10	32.88163	YES	YES
83	a	985.34	32.96777	YES	YES
84	a	987.96	0.14448	YES	YES
85	a	998.07	18.14144	YES	YES
86	a	999.60	0.76705	YES	YES
87	a	1000.25	4.79520	YES	YES
88	a	1001.46	13.14105	YES	YES
89	a	1002.14	15.92114	YES	YES

90	a	1002.62	1.98555	YES	YES
91	a	1005.27	0.59797	YES	YES
92	a	1005.82	0.32590	YES	YES
93	a	1006.41	0.17650	YES	YES
94	a	1009.25	20.31264	YES	YES
95	a	1009.78	19.69931	YES	YES
96	a	1011.28	0.62810	YES	YES
97	a	1013.28	3.09607	YES	YES
98	a	1013.59	4.45891	YES	YES
99	a	1013.98	3.15972	YES	YES
100	a	1014.27	15.85763	YES	YES
101	a	1014.50	8.50287	YES	YES
102	a	1015.27	14.44249	YES	YES
103	a	1155.57	1.03524	YES	YES
104	a	1156.41	0.21427	YES	YES
105	a	1156.97	0.47445	YES	YES
106	a	1157.21	0.45191	YES	YES
107	a	1157.47	0.29891	YES	YES
108	a	1158.20	0.39556	YES	YES
109	a	1267.49	0.39061	YES	YES
110	a	1268.62	0.05742	YES	YES
111	a	1269.74	0.05922	YES	YES
112	a	1300.33	54.72591	YES	YES
113	a	1300.52	54.33333	YES	YES
114	a	1306.02	0.01818	YES	YES
115	a	1351.59	0.62203	YES	YES
116	a	1351.87	0.05902	YES	YES
117	a	1354.53	1.46670	YES	YES
118	a	1354.81	20.99716	YES	YES
119	a	1356.27	1.94896	YES	YES
120	a	1356.66	14.64660	YES	YES
121	a	1356.88	7.87255	YES	YES
122	a	1357.34	20.62603	YES	YES
123	a	1358.57	54.57221	YES	YES
124	a	1362.43	49.71676	YES	YES
125	a	1362.81	51.32369	YES	YES
126	a	1365.44	0.24983	YES	YES
127	a	1391.96	1.39322	YES	YES
128	a	1392.90	10.23274	YES	YES
129	a	1393.25	11.14054	YES	YES
130	a	1393.37	2.18502	YES	YES
131	a	1393.67	0.51971	YES	YES
132	a	1396.18	14.10368	YES	YES
133	a	1420.35	0.04532	YES	YES
134	a	1420.41	1.58117	YES	YES
135	a	1421.19	7.67712	YES	YES
136	a	1424.45	7.76222	YES	YES
137	a	1424.67	7.48072	YES	YES
138	a	1425.71	3.04475	YES	YES
139	a	1426.55	0.25870	YES	YES
140	a	1426.72	0.10891	YES	YES
141	a	1427.35	0.80137	YES	YES
142	a	1427.77	3.27799	YES	YES

143	a	1430.23	24.51654	YES	YES
144	a	1430.59	24.16365	YES	YES
145	a	1445.48	140.34835	YES	YES
146	a	1451.78	54.01473	YES	YES
147	a	1452.20	52.82005	YES	YES
148	a	1453.34	0.85020	YES	YES
149	a	1453.74	1.58104	YES	YES
150	a	1454.24	1.71532	YES	YES
151	a	1578.26	51.68922	YES	YES
152	a	1578.51	53.39019	YES	YES
153	a	1579.61	81.12215	YES	YES
154	a	1580.93	0.44530	YES	YES
155	a	1581.70	1.36075	YES	YES
156	a	1582.10	0.86558	YES	YES
157	a	2948.46	5.57125	YES	YES
158	a	2948.73	5.80636	YES	YES
159	a	2948.79	4.84577	YES	YES
160	a	2952.81	2.54825	YES	YES
161	a	2953.26	2.34026	YES	YES
162	a	2953.53	1.96571	YES	YES
163	a	2953.84	3.68952	YES	YES
164	a	2953.85	1.98053	YES	YES
165	a	2954.55	2.59223	YES	YES
166	a	3023.39	4.75430	YES	YES
167	a	3023.57	8.20502	YES	YES
168	a	3023.87	8.26058	YES	YES
169	a	3030.75	5.51055	YES	YES
170	a	3031.18	6.69438	YES	YES
171	a	3031.64	8.15785	YES	YES
172	a	3031.85	5.85229	YES	YES
173	a	3032.12	7.32923	YES	YES
174	a	3033.30	7.42037	YES	YES
175	a	3064.38	3.12249	YES	YES
176	a	3064.94	2.41929	YES	YES
177	a	3064.94	1.77699	YES	YES
178	a	3065.28	3.35767	YES	YES
179	a	3065.62	2.40145	YES	YES
180	a	3065.75	2.41824	YES	YES
181	a	3066.12	4.89131	YES	YES
182	a	3066.16	4.64832	YES	YES
183	a	3067.95	3.54124	YES	YES
184	a	3097.44	0.21166	YES	YES
185	a	3097.99	0.21254	YES	YES
186	a	3099.14	0.16961	YES	YES
187	a	3099.82	0.36560	YES	YES
188	a	3100.56	0.46964	YES	YES
189	a	3100.61	0.22092	YES	YES
190	a	3138.37	1.97304	YES	YES
191	a	3138.68	2.28621	YES	YES
192	a	3140.26	2.19959	YES	YES

Mesitylene

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

-2.33543296582383	1.23263062227697	0.00000000000000	c
-2.26626337311887	-1.43602470525704	0.00000000000000	c
-0.11050218865521	2.68065400541567	0.00000000000000	c
2.23520591528640	1.40622896610058	0.00000000000000	c
2.37676556177410	-1.24462930015865	0.00000000000000	c
0.10022705053745	-2.63885958837756	0.00000000000000	c
-0.19802487808249	5.53748616460922	0.00000000000000	c
4.89461613069767	-2.59724850730386	0.00000000000000	c
-4.69659125261521	-2.94023765730536	0.00000000000000	c
-5.87102557054743	-2.49917837379736	1.68957930842969	h
-4.32642740920841	-5.00630594312492	0.00000000000000	h
-5.87102557054743	-2.49917837379736	-1.68957930842969	h
6.49880183046737	-1.24364307244132	0.00000000000000	h
5.09986474557092	-3.83486810346343	-1.68957930842969	h
5.09986474557092	-3.83486810346343	1.68957930842969	h
-2.17237442125898	6.24994901556623	0.00000000000000	h
0.77116082497653	6.33404647726079	-1.68957930842969	h
0.77116082497653	6.33404647726079	1.68957930842969	h
0.18211263842230	-4.72419340933378	0.00000000000000	h
-4.18232782408521	2.20438253344296	0.00000000000000	h
4.00021518566293	2.51981087589082	0.00000000000000	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	e''	27.85	0.00000	NO	YES
8	e''	27.85	0.00000	NO	YES
9	a''	32.65	1.16460	YES	NO
10	a''	171.05	4.66621	YES	NO
11	e''	217.65	0.00000	NO	YES
12	e''	217.65	0.00000	NO	YES
13	e'	267.36	0.46649	YES	YES
14	e'	267.36	0.46649	YES	YES
15	a'	452.04	0.00000	NO	YES
16	e'	508.46	0.66014	YES	YES
17	e'	508.46	0.66014	YES	YES
18	e''	515.15	0.00000	NO	YES
19	e''	515.15	0.00000	NO	YES
20	a'	571.76	0.00000	NO	YES
21	a''	694.86	9.79775	YES	NO
22	a''	834.96	10.78451	YES	NO
23	e''	874.01	0.00000	NO	YES
24	e''	874.01	0.00000	NO	YES
25	e'	929.20	2.92304	YES	YES
26	e'	929.20	2.92304	YES	YES
27	a'	985.34	0.00000	NO	YES

28	e'	1008.41	4.94487	YES	YES
29	e'	1008.41	4.94487	YES	YES
30	a'	1009.06	0.00000	NO	YES
31	e''	1026.71	0.00000	NO	YES
32	e''	1026.71	0.00000	NO	YES
33	a''	1030.50	12.63746	YES	NO
34	e'	1158.93	0.02579	YES	YES
35	e'	1158.93	0.02579	YES	YES
36	a'	1264.90	0.00000	NO	YES
37	a'	1299.61	0.00000	NO	YES
38	e'	1362.17	0.75413	YES	YES
39	e'	1362.17	0.75413	YES	YES
40	a'	1368.73	0.00000	NO	YES
41	a'	1371.21	0.00000	NO	YES
42	e'	1411.21	3.17800	YES	YES
43	e'	1411.21	3.17800	YES	YES
44	a''	1422.62	24.63474	YES	NO
45	e''	1423.65	0.00000	NO	YES
46	e''	1423.65	0.00000	NO	YES
47	a'	1436.65	0.00000	NO	YES
48	e'	1469.31	20.73000	YES	YES
49	e'	1469.31	20.73000	YES	YES
50	e'	1618.06	23.63726	YES	YES
51	e'	1618.06	23.63726	YES	YES
52	e'	2935.86	47.01340	YES	YES
53	e'	2935.86	47.01340	YES	YES
54	a'	2936.64	0.00000	NO	YES
55	e''	3006.14	0.00000	NO	YES
56	e''	3006.14	0.00000	NO	YES
57	a''	3006.23	36.72537	YES	NO
58	a'	3036.87	0.00000	NO	YES
59	e'	3037.13	18.06905	YES	YES
60	e'	3037.13	18.06905	YES	YES
61	e'	3070.88	27.48372	YES	YES
62	e'	3070.88	27.48372	YES	YES
63	a'	3073.57	0.00000	NO	YES

$[Sn(C_7H_8)_3]^{2+}$

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

-0.56880386495871	-0.13236443250343	0.51485517742581	sn
-3.96435354392406	-2.95541587577390	-3.38083918006587	c
-4.97805488832235	-0.46547842361434	-3.23495633282586	c
-4.94433096871256	0.74454992129023	-4.93102473222216	h
-6.13739311294527	0.42533692183807	-1.00522046004545	c
-7.00553896169014	2.31607280067907	-0.98461689827058	h
-6.21602541712079	-1.10604641702167	1.17842038479989	c
-7.13870637047876	-0.42446564579622	2.91556847821064	h
-5.17768638083548	-3.57000170811002	1.08244917691774	c
-5.27923587477794	-4.80414309362399	2.75682570672782	h

-4.08785404221634	-4.47997344423408	-1.17481230765010	c
-3.36442306223273	-6.43035666329767	-1.24595030354235	h
-2.94792619144558	-3.97033437300995	-5.83222407935735	c
-1.65924671310249	-5.59888701607359	-5.54836991409672	h
-1.96512194795925	-2.49538415252435	-6.95468661992946	h
-4.54800218385402	-4.66377466051388	-7.01468562245095	h
1.10242909359649	5.20033783684688	-1.03648926614510	c
-1.55933940799284	5.39770475620984	-0.69522342791995	c
-2.76156526089582	5.83985811968277	-2.33801986067801	h
-2.66815687040138	5.12914799959538	1.71493172282714	c
-4.72242877801284	5.36965614380643	1.94478598218752	h
-1.15235134207288	4.59554754957501	3.84577132846976	c
-2.01282045944280	4.42024955749146	5.73353854885633	h
1.49495364916645	4.39248983789317	3.54390887121687	c
2.70255466355476	4.04727012225323	5.20201340514236	h
2.59901007003621	4.68872615730329	1.13750722653529	c
4.66855349207110	4.58288945151093	0.93717532654939	h
2.30018078188146	5.66152234709391	-3.57197607725036	c
4.10456334497703	4.61616244702412	-3.79569532166164	h
2.75456746046821	7.70981085078809	-3.76759329752042	h
1.01596585541935	5.17147539429622	-5.15545444829478	h
4.64732418491364	-1.75556486414686	2.94257377316692	c
2.88776505792039	-3.70299313765199	3.53466625444896	c
2.43061419921980	-4.09330045425231	5.53033485889059	h
1.83386118573233	-5.24118309453041	1.62364673429472	c
0.56593619710611	-6.80549264740511	2.15107897318724	h
2.44208576059870	-4.80713269533305	-0.93650280644310	c
1.67725912010494	-6.03782287917502	-2.42837562051906	h
4.09751356682904	-2.80772123094392	-1.56961453811344	c
4.60718455636781	-2.46543833977218	-3.55978025547062	h
5.18785475431494	-1.31026614645002	0.35390967852545	c
6.54924817374372	0.17736161724579	-0.16518642300411	h
5.99679853214482	-0.34094541179567	5.00258105612451	c
4.79396638582179	-0.06675213775384	6.69903421275293	h
6.73356290088091	1.51014578511771	4.35144366685198	h
7.66561265652515	-1.46507667223446	5.63027724936764	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	a	13.42	0.01126	YES	YES
8	a	14.93	0.03919	YES	YES
9	a	22.39	0.00571	YES	YES
10	a	38.17	0.03484	YES	YES
11	a	62.56	0.61213	YES	YES
12	a	66.16	0.52291	YES	YES
13	a	76.41	0.69402	YES	YES
14	a	78.88	0.52455	YES	YES
15	a	89.00	0.53755	YES	YES
16	a	93.59	1.48938	YES	YES

17	a	102.17	1.44122	YES	YES
18	a	109.73	4.02358	YES	YES
19	a	117.84	3.93560	YES	YES
20	a	126.97	7.50672	YES	YES
21	a	144.43	37.75380	YES	YES
22	a	151.11	33.30507	YES	YES
23	a	170.61	1.18634	YES	YES
24	a	188.33	3.67374	YES	YES
25	a	217.08	11.40549	YES	YES
26	a	219.64	13.89242	YES	YES
27	a	233.46	0.42117	YES	YES
28	a	333.04	0.20562	YES	YES
29	a	336.82	0.02678	YES	YES
30	a	337.42	0.28563	YES	YES
31	a	382.23	0.03480	YES	YES
32	a	386.12	0.09093	YES	YES
33	a	392.29	0.16007	YES	YES
34	a	452.30	17.43437	YES	YES
35	a	456.42	14.94593	YES	YES
36	a	458.62	2.67108	YES	YES
37	a	511.18	2.74116	YES	YES
38	a	512.12	1.79520	YES	YES
39	a	513.89	2.71304	YES	YES
40	a	608.26	0.09054	YES	YES
41	a	609.61	0.11901	YES	YES
42	a	610.87	0.05266	YES	YES
43	a	671.76	8.63299	YES	YES
44	a	673.89	5.92856	YES	YES
45	a	675.10	0.30328	YES	YES
46	a	757.09	131.79176	YES	YES
47	a	761.17	145.91409	YES	YES
48	a	766.80	1.76148	YES	YES
49	a	780.67	0.19254	YES	YES
50	a	782.36	0.41900	YES	YES
51	a	784.01	0.01610	YES	YES
52	a	866.17	0.07789	YES	YES
53	a	873.41	3.00448	YES	YES
54	a	876.11	1.15136	YES	YES
55	a	907.46	0.77695	YES	YES
56	a	911.93	0.26680	YES	YES
57	a	917.69	0.17040	YES	YES
58	a	966.79	0.59416	YES	YES
59	a	967.12	2.34492	YES	YES
60	a	969.16	1.54016	YES	YES
61	a	976.55	0.21674	YES	YES
62	a	977.45	0.59070	YES	YES
63	a	982.56	5.47410	YES	YES
64	a	983.30	5.83234	YES	YES
65	a	984.24	7.91934	YES	YES
66	a	986.43	1.53144	YES	YES
67	a	993.47	6.20368	YES	YES
68	a	994.91	10.14180	YES	YES
69	a	997.36	0.65728	YES	YES

70	a	1008.73	18.96530	YES	YES
71	a	1010.89	22.31056	YES	YES
72	a	1011.99	11.16346	YES	YES
73	a	1020.85	11.23134	YES	YES
74	a	1022.57	3.88199	YES	YES
75	a	1025.88	4.65674	YES	YES
76	a	1077.32	3.21968	YES	YES
77	a	1078.65	0.67196	YES	YES
78	a	1079.29	3.59648	YES	YES
79	a	1148.15	0.76864	YES	YES
80	a	1148.69	0.62918	YES	YES
81	a	1150.74	0.24803	YES	YES
82	a	1165.09	0.74928	YES	YES
83	a	1166.46	0.47342	YES	YES
84	a	1168.61	1.95780	YES	YES
85	a	1211.60	25.67218	YES	YES
86	a	1211.77	23.25351	YES	YES
87	a	1214.23	1.09705	YES	YES
88	a	1301.83	0.19825	YES	YES
89	a	1303.16	0.35631	YES	YES
90	a	1303.83	0.04282	YES	YES
91	a	1353.91	17.44309	YES	YES
92	a	1355.39	14.73097	YES	YES
93	a	1356.54	12.76018	YES	YES
94	a	1358.09	20.57118	YES	YES
95	a	1360.01	6.04851	YES	YES
96	a	1360.35	5.56749	YES	YES
97	a	1406.36	2.69765	YES	YES
98	a	1408.81	8.39578	YES	YES
99	a	1409.48	4.82494	YES	YES
100	a	1422.99	14.33664	YES	YES
101	a	1425.42	13.60328	YES	YES
102	a	1428.91	19.45848	YES	YES
103	a	1440.26	45.49974	YES	YES
104	a	1441.84	12.88916	YES	YES
105	a	1442.75	39.35939	YES	YES
106	a	1476.70	50.42275	YES	YES
107	a	1477.61	32.68591	YES	YES
108	a	1479.22	31.55133	YES	YES
109	a	1562.55	4.27355	YES	YES
110	a	1563.76	1.19051	YES	YES
111	a	1565.86	1.72520	YES	YES
112	a	1588.54	24.94724	YES	YES
113	a	1591.69	4.31355	YES	YES
114	a	1593.86	22.04852	YES	YES
115	a	2949.84	9.57168	YES	YES
116	a	2950.43	5.79277	YES	YES
117	a	2952.13	7.61431	YES	YES
118	a	3027.60	7.96837	YES	YES
119	a	3030.61	9.33364	YES	YES
120	a	3030.98	9.21203	YES	YES
121	a	3066.78	1.40865	YES	YES
122	a	3069.21	2.11516	YES	YES

123	a	3069.26	1.86068	YES	YES
124	a	3105.95	0.65727	YES	YES
125	a	3106.43	0.34749	YES	YES
126	a	3108.93	0.14034	YES	YES
127	a	3109.77	0.03742	YES	YES
128	a	3113.35	0.12759	YES	YES
129	a	3114.36	0.10058	YES	YES
130	a	3120.90	0.23459	YES	YES
131	a	3121.65	0.09338	YES	YES
132	a	3122.02	1.68948	YES	YES
133	a	3124.83	1.33564	YES	YES
134	a	3127.02	3.58984	YES	YES
135	a	3130.54	0.69299	YES	YES
136	a	3134.95	2.38574	YES	YES
137	a	3137.06	0.61921	YES	YES
138	a	3138.29	1.84218	YES	YES

Toluene

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory.

-1.37693195984459	0.05610887792587	0.00000000000000	c
-0.00547270395296	0.04248475217029	2.28673994657304	c
2.64785499295296	0.00664838859411	2.29251543473111	c
3.98688898782604	-0.01220175761724	0.00000000000000	c
2.64785499295296	0.00664838859411	-2.29251543473111	c
-0.00547270395296	0.04248475217029	-2.28673994657304	c
-4.23418035555670	0.03009512460308	0.00000000000000	c
-1.04012512911134	0.06493279415113	4.09758947884185	h
3.67835972897159	0.00167899070758	4.10383538541379	h
6.06991813199383	-0.03373192736895	0.00000000000000	h
3.67835972897159	0.00167899070758	-4.10383538541379	h
-1.04012512911134	0.06493279415113	-4.09758947884185	h
-5.01516159044126	0.98331391549639	1.70057764327330	h
-5.01516159044126	0.98331391549639	-1.70057764327330	h
-4.97527187498886	-1.94229881715618	0.00000000000000	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory).

mode	symmetry	wave number	IR intensity	selection rules	
		[cm^{-1}]	[km mol^{-1}]	IR	RAMAN
7	a''	12.34	0.51711	YES	YES
8	a'	201.84	2.17470	YES	YES
9	a''	336.78	0.28693	YES	YES
10	a''	402.81	0.00935	YES	YES
11	a'	463.49	7.33612	YES	YES
12	a'	514.82	0.55264	YES	YES
13	a''	616.65	0.11203	YES	YES
14	a'	697.92	28.90365	YES	YES
15	a'	724.98	25.75108	YES	YES

16	a'	785.89	0.88347	YES	YES
17	a"	830.26	0.00563	YES	YES
18	a'	884.52	0.25377	YES	YES
19	a"	951.05	0.00541	YES	YES
20	a"	972.61	0.01290	YES	YES
21	a'	975.92	0.12057	YES	YES
22	a'	989.00	0.10369	YES	YES
23	a'	1027.85	10.44065	YES	YES
24	a'	1030.11	2.86756	YES	YES
25	a"	1081.50	6.60739	YES	YES
26	a"	1140.40	0.04499	YES	YES
27	a'	1162.46	0.26930	YES	YES
28	a'	1211.13	1.09960	YES	YES
29	a"	1302.90	0.00815	YES	YES
30	a'	1362.20	0.79161	YES	YES
31	a"	1368.26	0.01683	YES	YES
32	a"	1419.11	3.19237	YES	YES
33	a'	1427.32	8.20896	YES	YES
34	a"	1455.89	10.57442	YES	YES
35	a'	1494.35	13.93966	YES	YES
36	a"	1601.52	0.29137	YES	YES
37	a'	1624.60	7.05566	YES	YES
38	a'	2934.96	26.18638	YES	YES
39	a'	3009.74	13.29593	YES	YES
40	a"	3039.70	11.23185	YES	YES
41	a'	3078.88	9.33148	YES	YES
42	a"	3080.73	6.72413	YES	YES
43	a'	3093.80	5.77218	YES	YES
44	a"	3101.66	35.56256	YES	YES
45	a'	3113.94	15.13490	YES	YES

Acetonitrile

Optimized atomic coordinates [Bohr units]. (RI-)BP86(D3BJ)/def-SV(P) level of theory (grid m4).

-0.00000000000000	0.00000000000000	-1.84077125441740	c
-0.00000000000000	0.00000000000000	-4.05314605445386	n
-0.00000000000000	0.00000000000000	0.92150614144512	c
-0.98353145203918	-1.70352644577386	1.65747038914204	h
-0.98353145203918	1.70352644577386	1.65747038914204	h
1.96706290407837	0.00000000000000	1.65747038914204	h

List of calculated frequencies ((RI-)BP86(D3BJ)/def-SV(P) level of theory, grid m4).

mode	symmetry	wave number [cm^{-1}]	IR intensity [km mol^{-1}]	selection rules	
				IR	RAMAN
7	e	370.02	0.02656	YES	YES
8	e	370.02	0.02656	YES	YES
9	a1	930.71	0.72428	YES	YES
10	e	1025.11	5.07952	YES	YES
11	e	1025.11	5.07952	YES	YES
12	a1	1357.08	3.40288	YES	YES
13	e	1410.86	13.43006	YES	YES
14	e	1410.86	13.43006	YES	YES
15	a1	2300.22	9.69330	YES	YES
16	a1	2956.35	2.56109	YES	YES
17	e	3047.91	0.11071	YES	YES
18	e	3047.91	0.11071	YES	YES

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