Electronic Supplementary Information for:

Dichlorostannylene complexes of group 10 metals, a unique bonding mode stabilized by bridging 2-pyridyldiphenylphosphine ligands.

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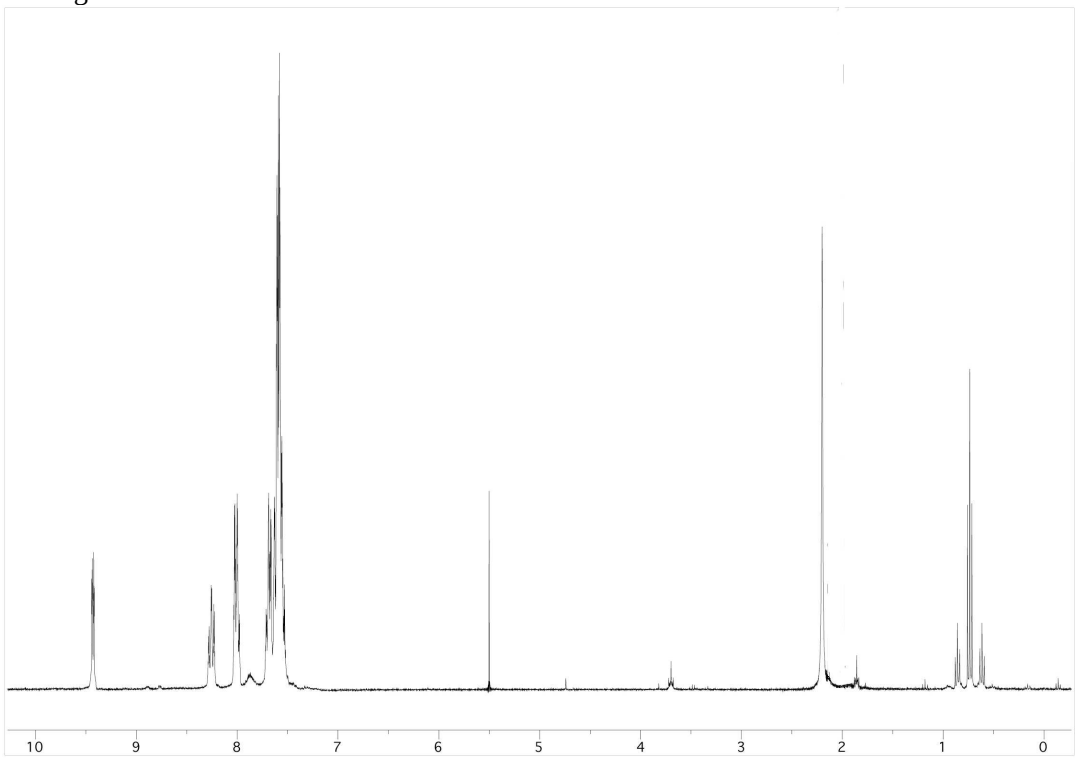
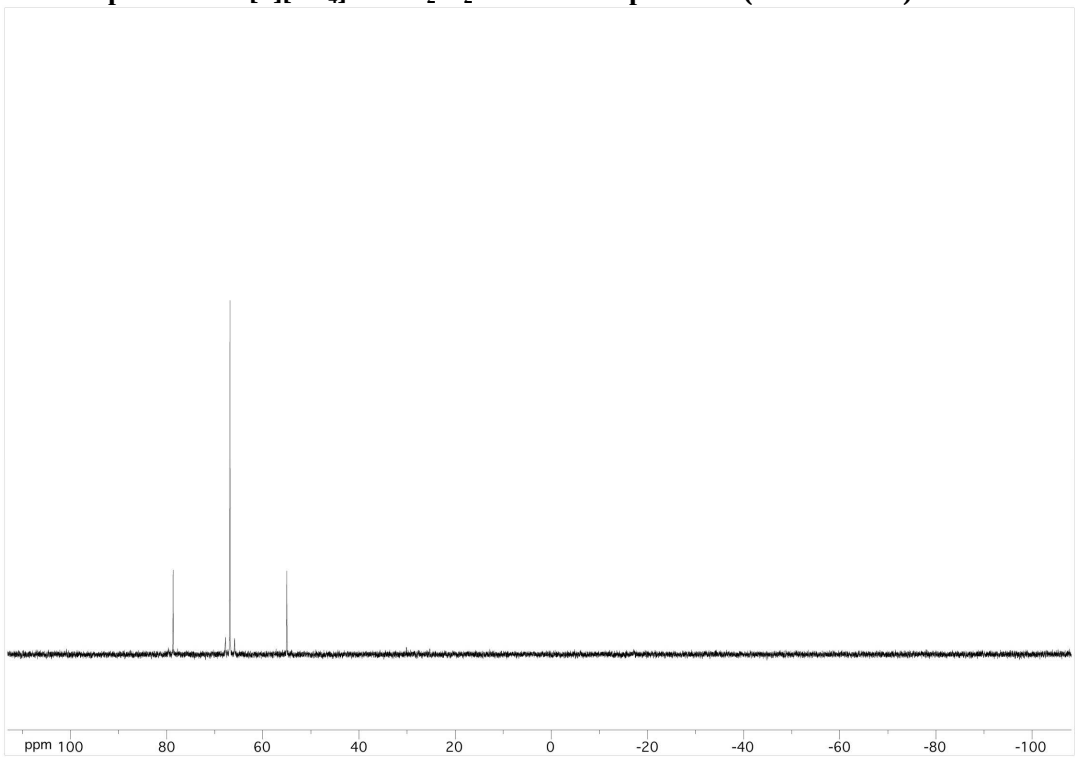
Contents:

^{1}H NMR spectrum of [1][BF_4] in CD_2Cl_2 at room temperature

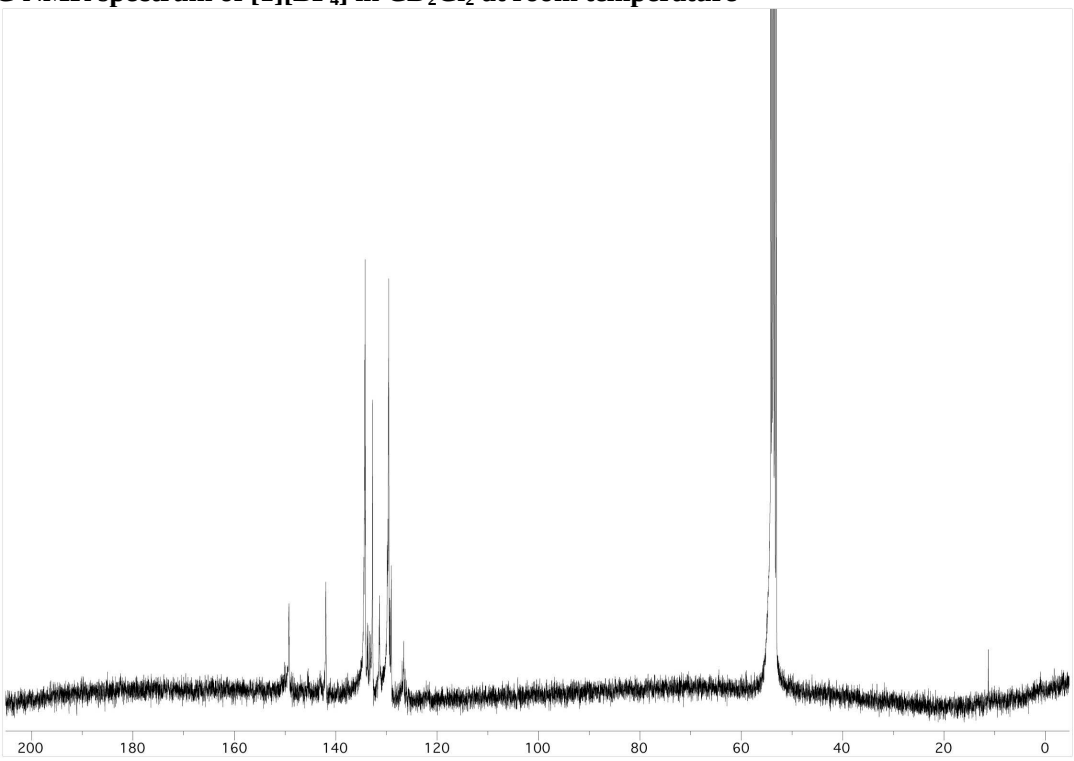
The signal at δ 2.2 is from residual acetone in the NMR tube.



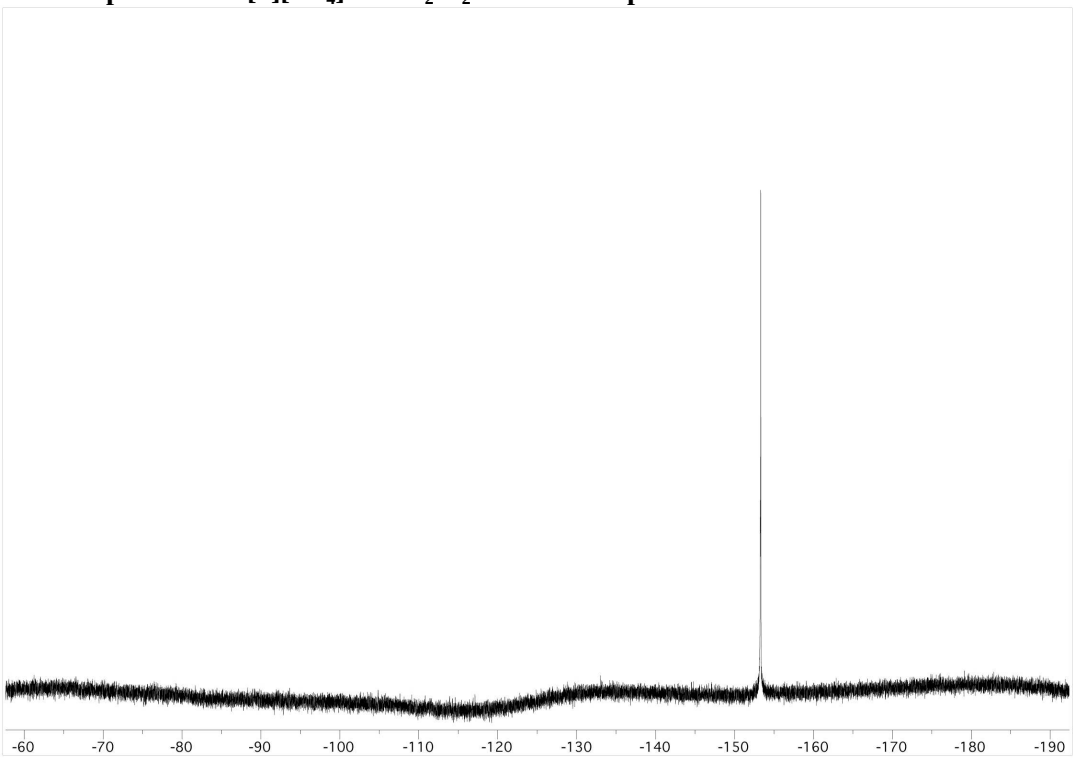
^{31}P NMR spectrum of [1][BF_4] in CD_2Cl_2 at room temperature (32.000 scans)



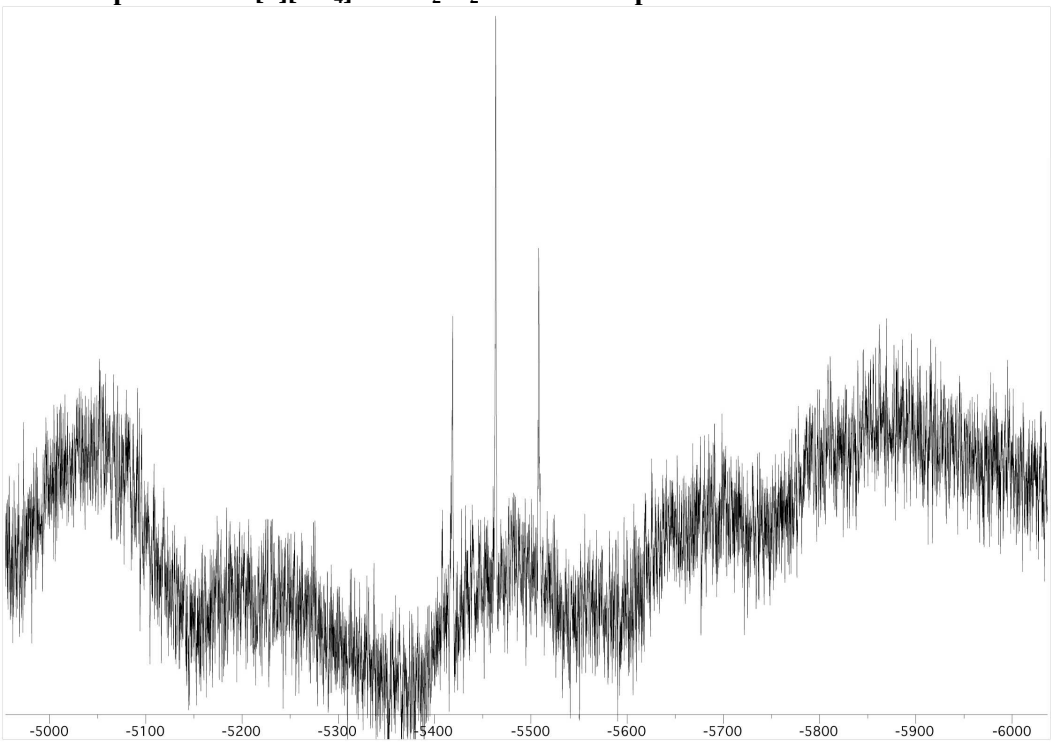
^{13}C NMR spectrum of [1][BF_4] in CD_2Cl_2 at room temperature



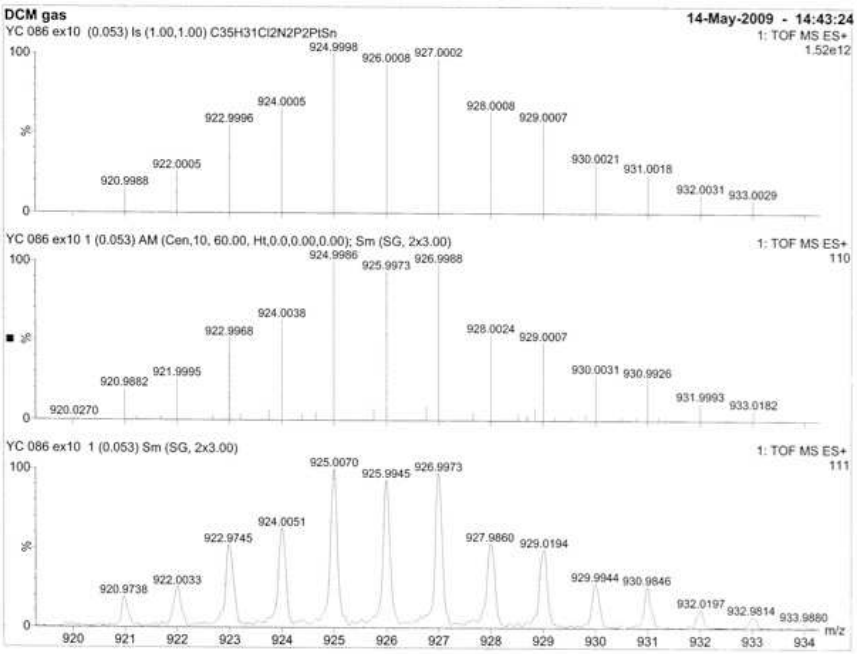
^{19}F NMR spectrum of [1][BF_4] in CD_2Cl_2 at room temperature



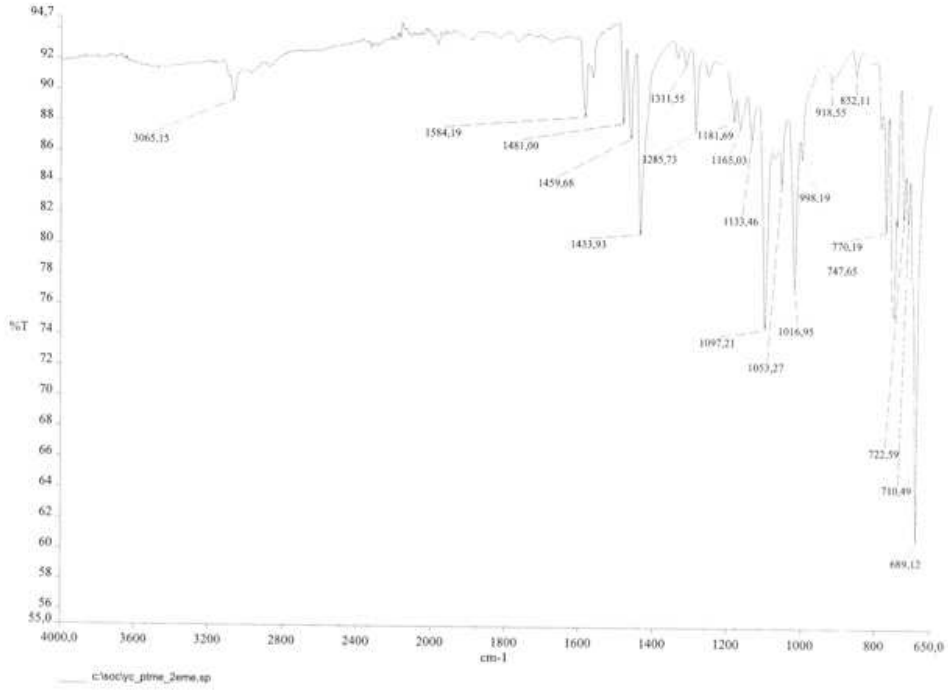
^{195}Pt NMR spectrum of [1][BF_4] in CD_2Cl_2 at room temperature



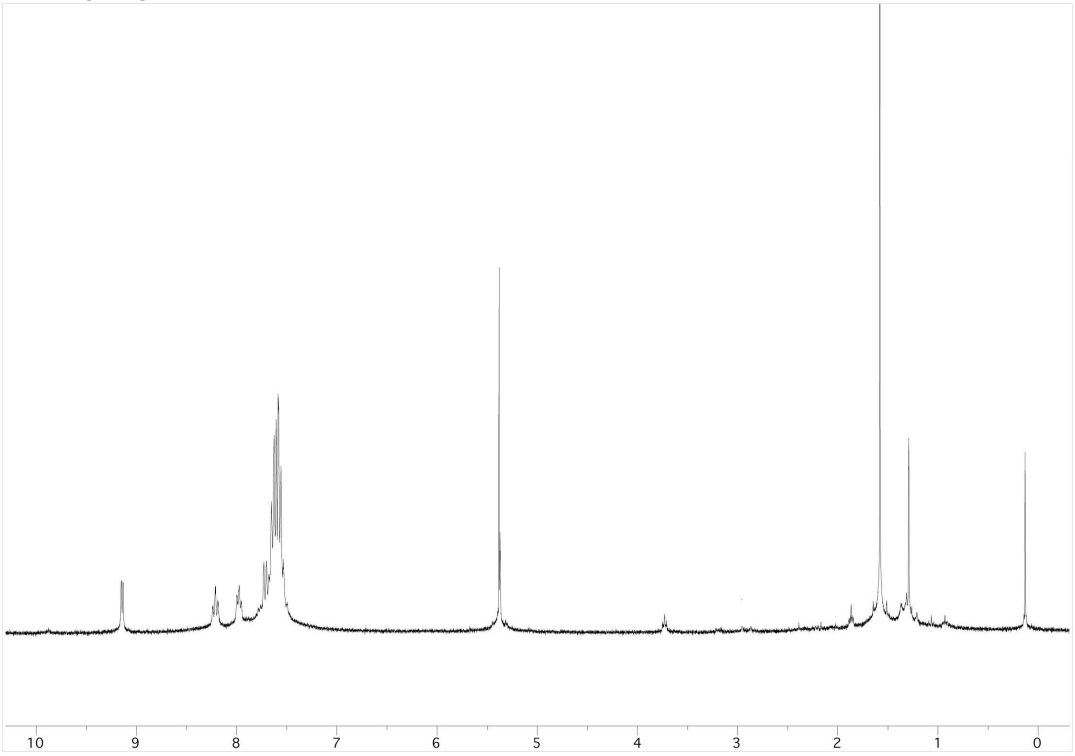
HRMS spectrum of [1][BF_4] (from a CH_2Cl_2 solution with electrospray ionization, positive ion detection mode, top: theoretical spectrum, middle: centered experimental spectra, bottom: original experimental spectrum)



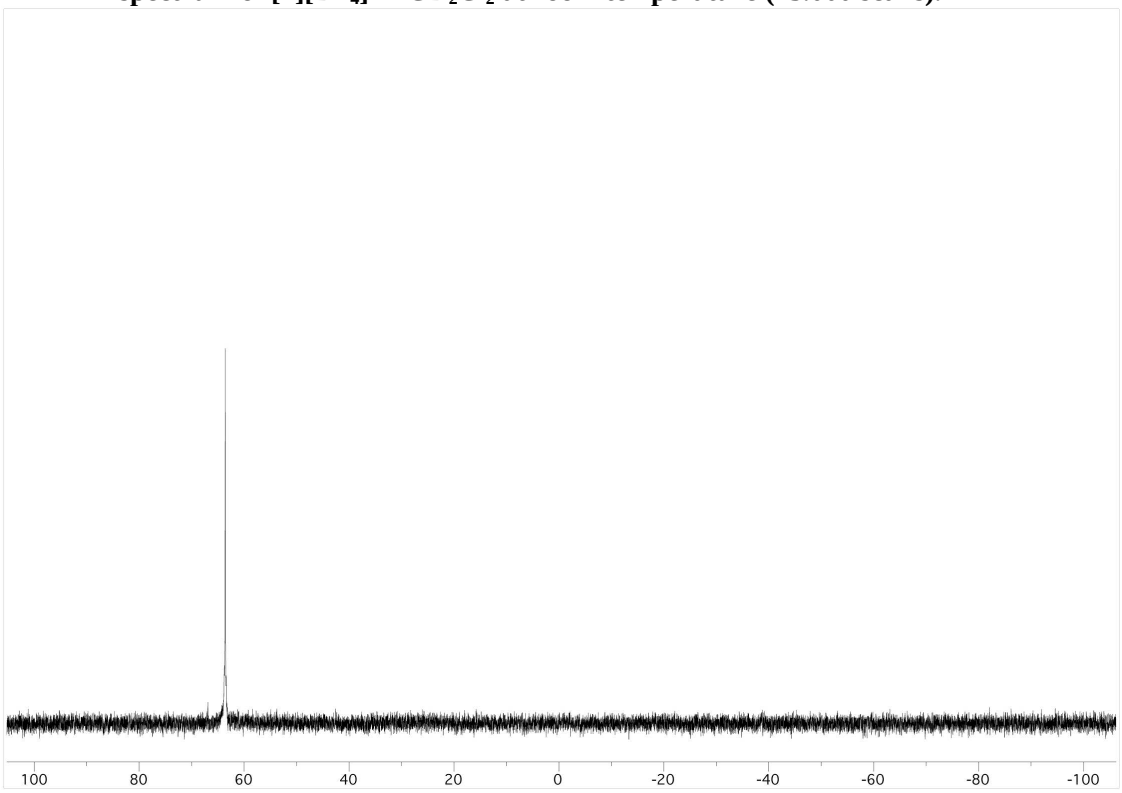
IR spectrum of [1][BF_4] in the solid state



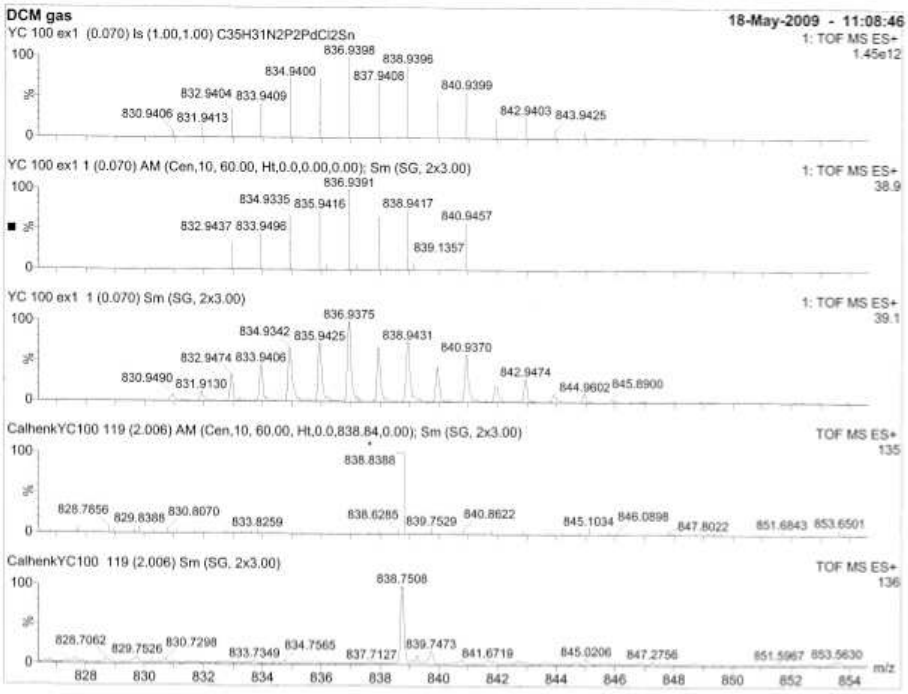
^{1}H NMR spectrum of [2][BF_4] in CD_2Cl_2 at room temperature (128 scans).
The large signal at δ 1.6 is from residual water in the deuterated solvent.



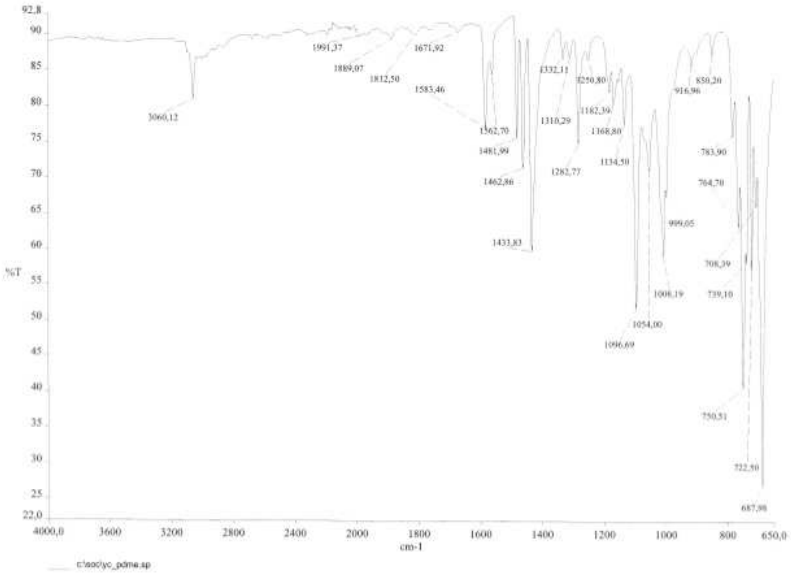
^{31}P NMR spectrum of [2][BF_4] in CD_2Cl_2 at room temperature (25.000 scans).



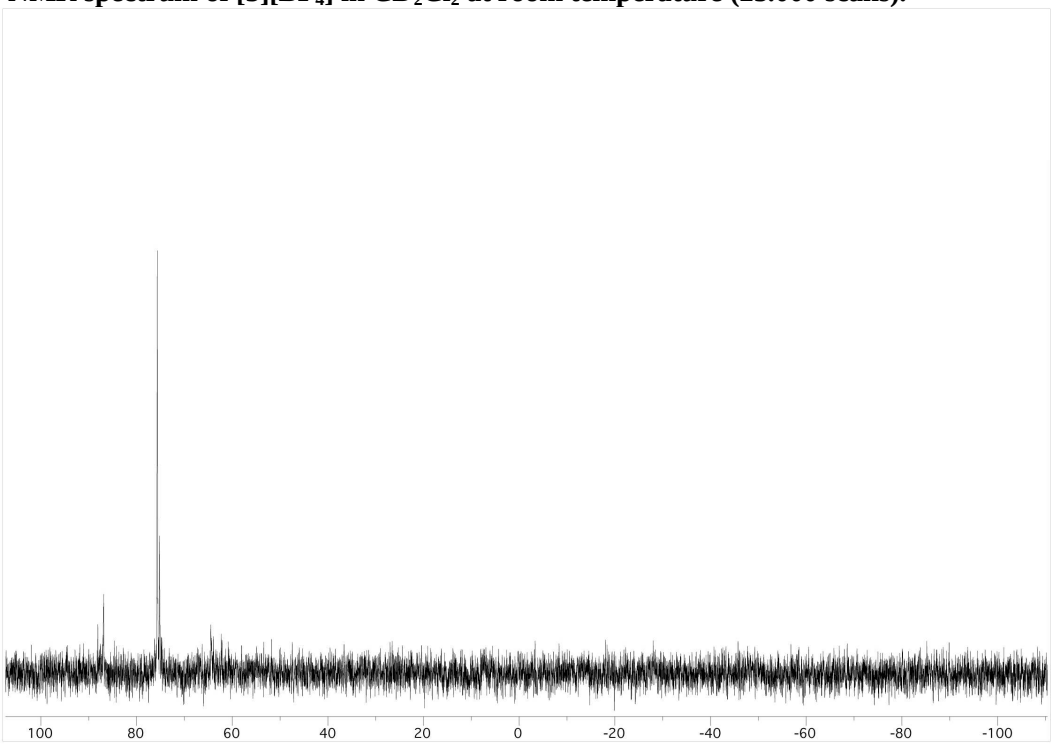
HRMS spectrum of [2][BF_4] (from a CH_2Cl_2 solution with electrospray ionization, positive ion detection mode, top spectrum: theoretical spectrum, 2nd spectrum: centered experimental spectrum, 3rd spectrum: experimental spectrum, 4th and 5th spectrum: calibration spectra)



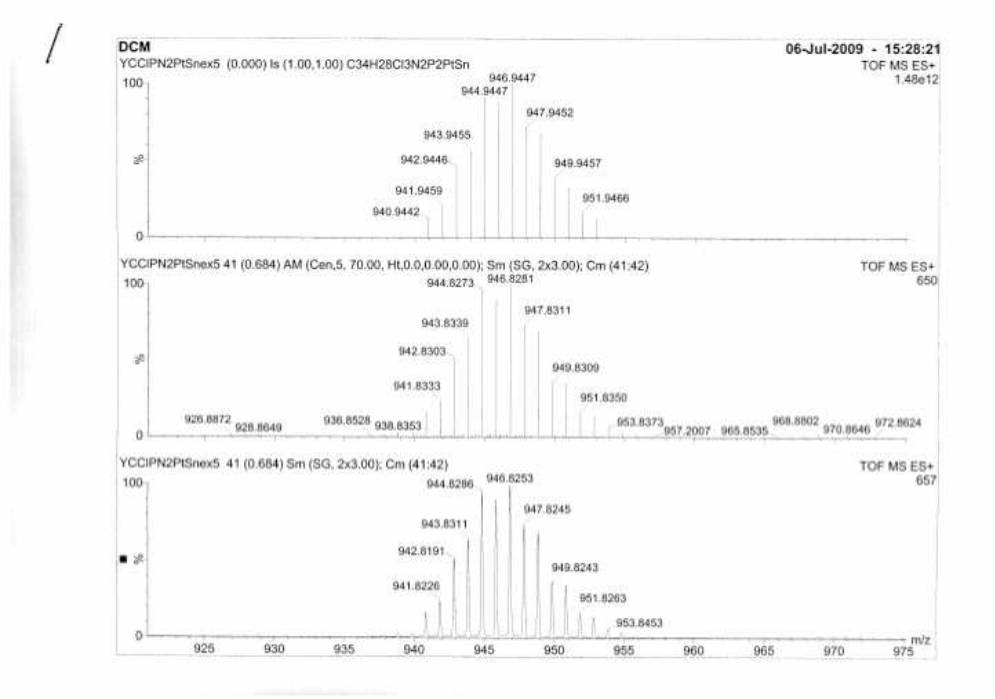
IR spectrum of [2][BF_4] in the solid state



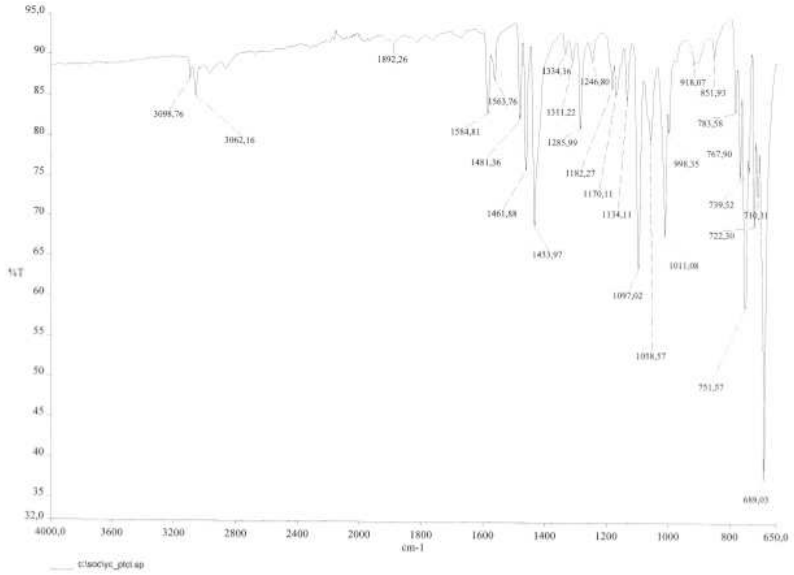
^{31}P NMR spectrum of [3][BF_4] in CD_2Cl_2 at room temperature (25.000 scans).



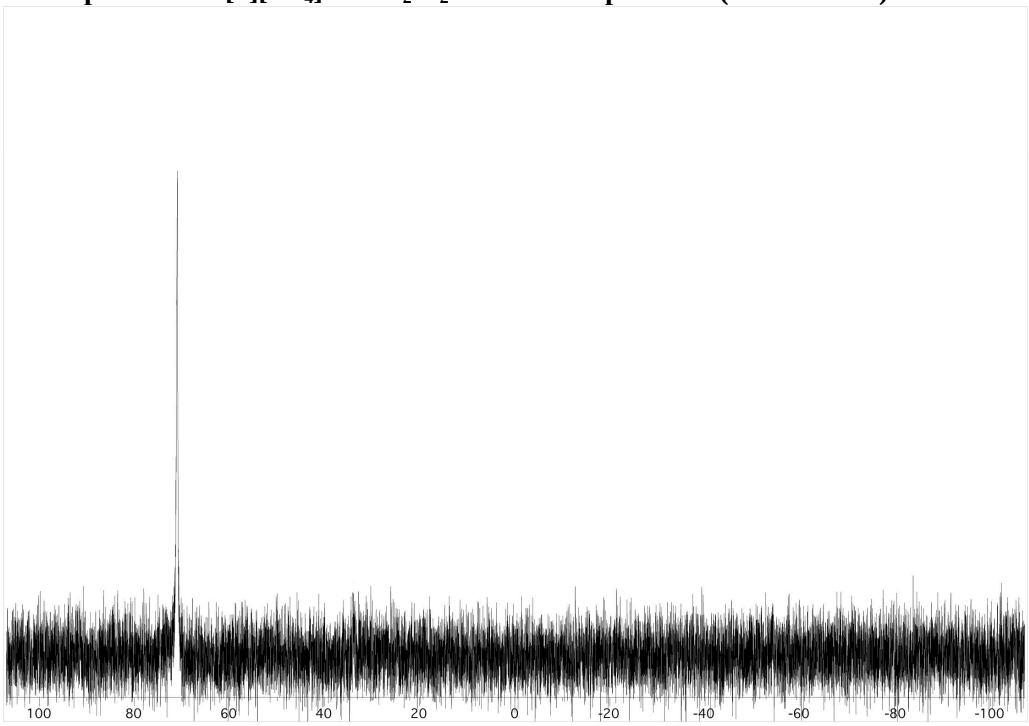
HRMS spectra of [3][BF_4] (from a CH_2Cl_2 solution with electrospray ionization, positive ion detection mode, top: theoretical spectrum, middle: centered experimental spectrum, bottom: original experimental spectrum)



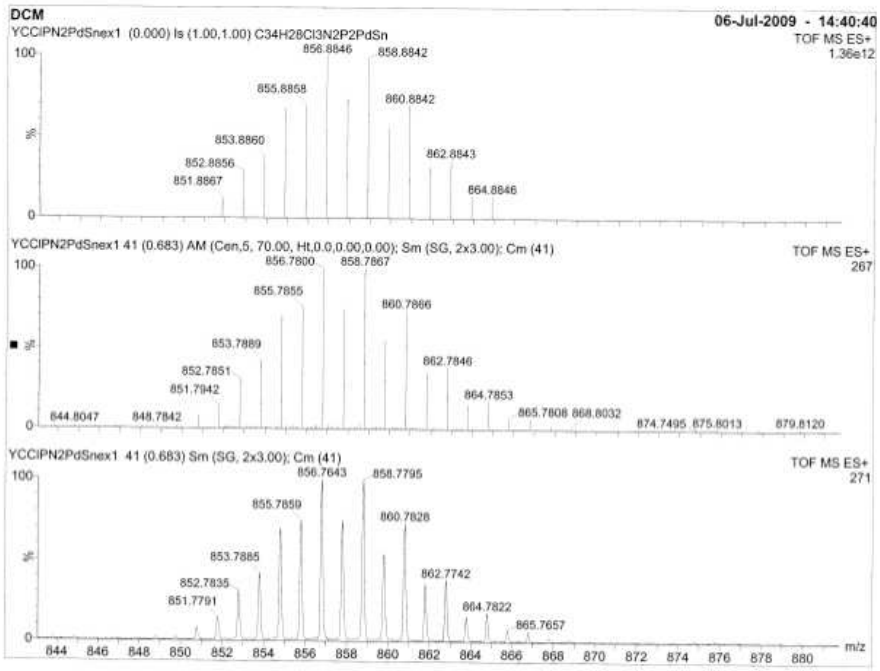
IR spectrum of [3][BF_4] in the solid state



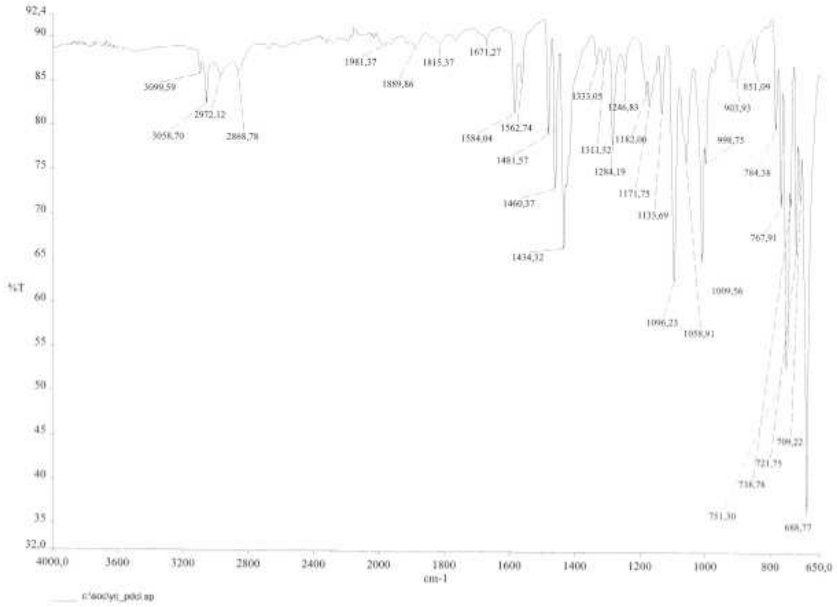
^{31}P NMR spectrum of [4][BF_4] in CD_2Cl_2 at room temperature (25.000 scans)



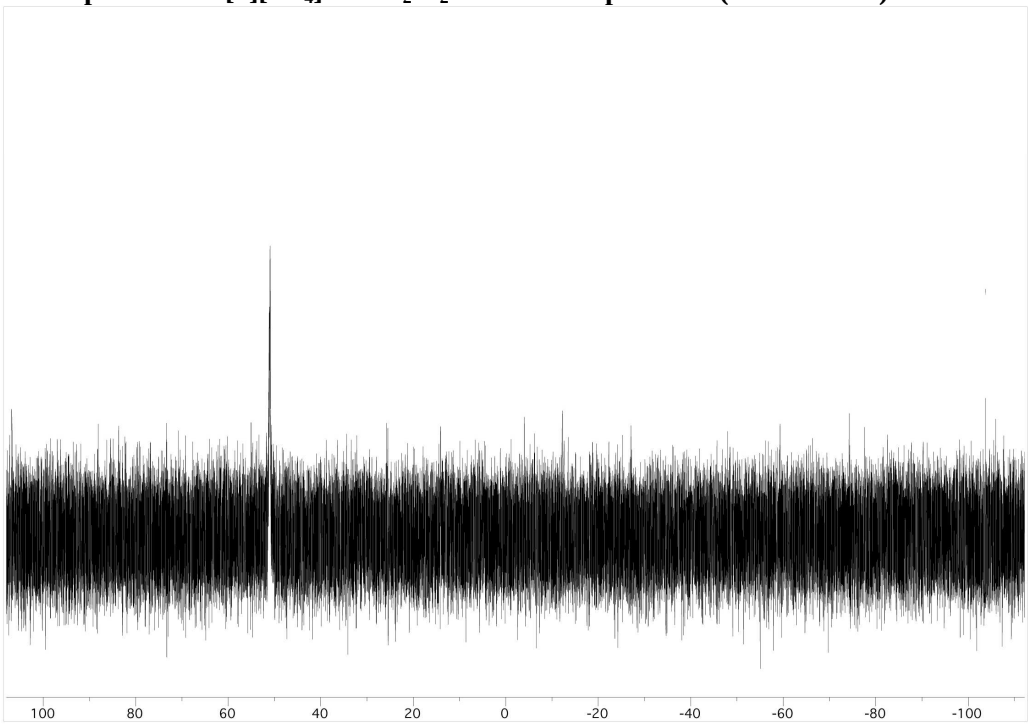
HRMS spectrum of [4][BF_4] (from a CH_2Cl_2 solution with electrospray ionization, positive ion detection mode, top: theoretical spectrum, middle: centered experimental spectrum, bottom: original experimental spectrum)



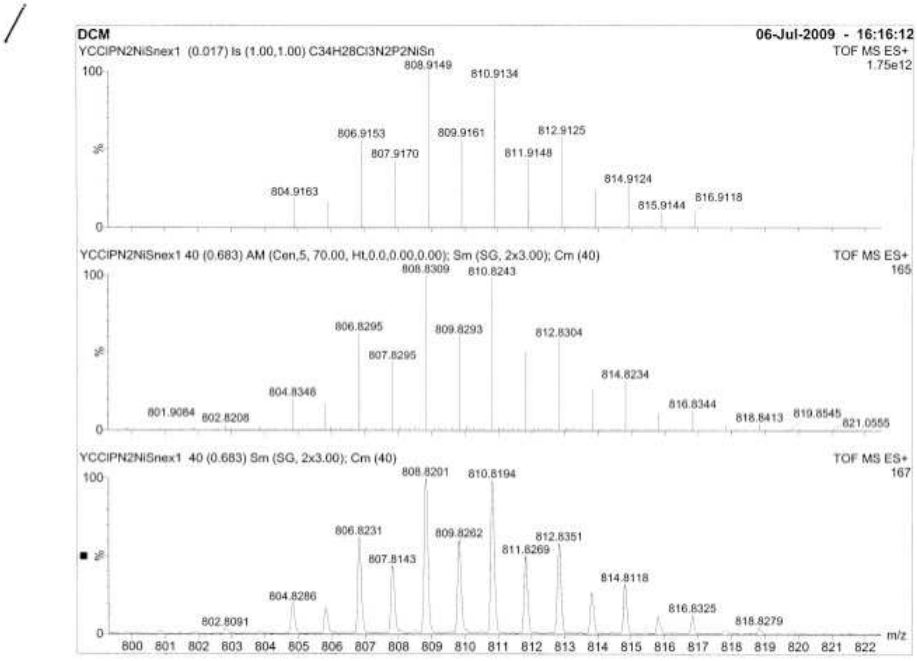
IR spectra of [4][BF_4] in solid state



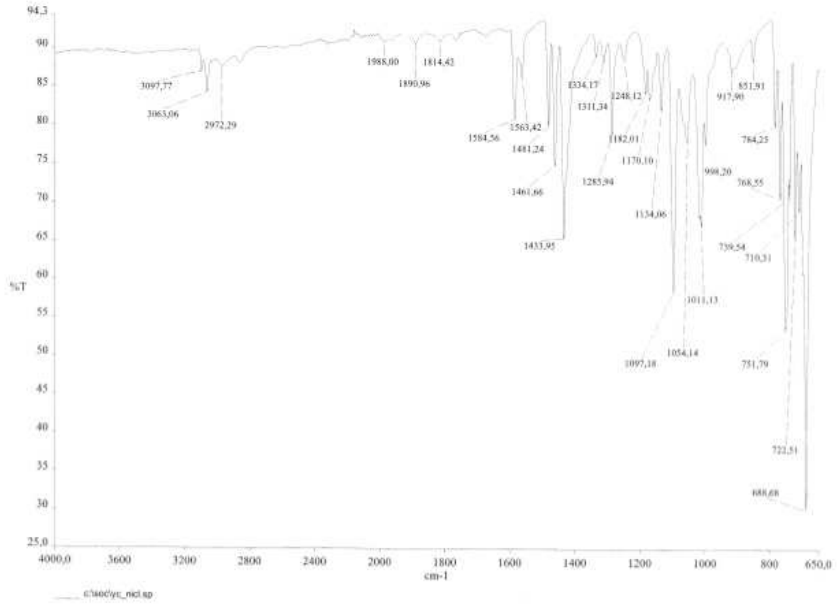
^{31}P NMR spectrum of [5][BF_4] in CD_2Cl_2 at room temperature (25.000 scans).



HRMS spectrum of [5][BF_4] (from a CH_2Cl_2 solution with electrospray ionization, positive ion detection mode, top: theoretical spectrum, middle: centered experimental spectrum, bottom: original experimental spectrum)

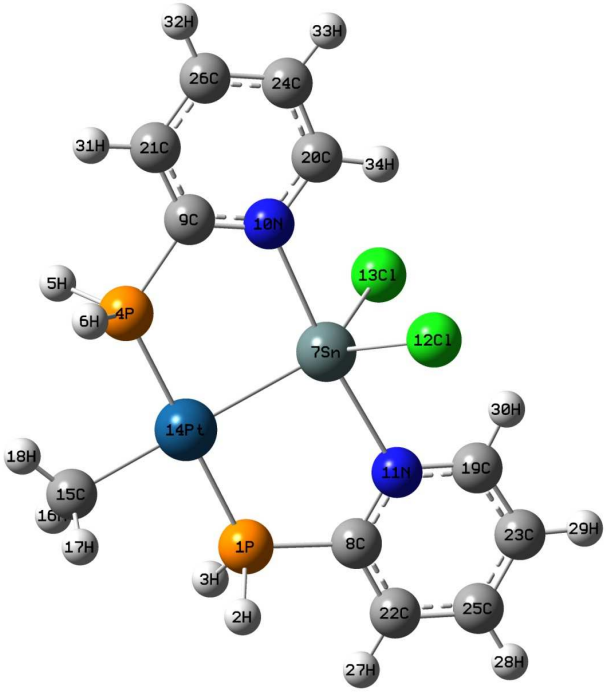


IR spectrum of [5][BF_4] in solid state.



DFT calculations on $[Pt(2\text{-}PyPH_2)_2(Me)(SnCl_2)]^+$

Atom labeling scheme:



Optimization results:

Item	Value	Threshold	Converged?
Maximum Force	0.000057	0.000450	YES
RMS Force	0.000012	0.000300	YES
Maximum Displacement	0.001329	0.001800	YES
RMS Displacement	0.000313	0.001200	YES

Predicted change in Energy=-2.803398D-07
Optimization completed.
-- Stationary point found.

Geometry output:

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.301006	1.689114	0.000313
2	1	0	-2.920346	2.354652	1.077866
3	1	0	-2.921010	2.356042	-1.075990
4	15	0	2.293777	1.690668	0.000047
5	1	0	2.906998	2.362290	-1.077058
6	1	0	2.906561	2.361289	1.078033
7	50	0	0.001904	-0.936363	0.000669
8	6	0	-3.190681	0.058532	-0.000518
9	6	0	3.189492	0.063503	-0.000583
10	7	0	2.448948	-1.059329	-0.000468
11	7	0	-2.446789	-1.062078	-0.000527
12	17	0	0.002065	-2.431023	1.848164
13	17	0	0.002112	-2.432450	-1.845899
14	78	0	0.000810	1.687618	0.000017
15	6	0	-0.016655	3.828704	-0.000690
16	1	0	-0.539664	4.178119	-0.896396
17	1	0	-0.539569	4.178731	0.894834
18	1	0	0.986412	4.263170	-0.000896
19	6	0	-3.058004	-2.259014	-0.000987
20	6	0	3.063482	-2.254512	-0.000801
21	6	0	4.584665	0.024124	-0.001220
22	6	0	-4.585810	0.014947	-0.001162
23	6	0	-4.444944	-2.384169	-0.001201
24	6	0	4.450821	-2.375487	-0.000991
25	6	0	-5.222049	-1.227873	-0.001508
26	6	0	5.224511	-1.216894	-0.001414
27	1	0	-5.166651	0.932133	-0.000788
28	1	0	-6.306089	-1.286817	-0.001314
29	1	0	-4.896889	-3.370039	-0.000781
30	1	0	-2.409596	-3.128811	-0.000272
31	1	0	5.162780	0.943042	-0.000865
32	1	0	6.308716	-1.272726	-0.001174
33	1	0	4.905722	-3.359996	-0.000453
34	1	0	2.417566	-3.126172	0.000005

Selected bond lengths in Angstrom (the related distances in the X-ray structure of $[\mathbf{1}]^{+}[BF_4]^{-}$ *are given in brackets with the deviation between calculated and experimental structure):*

14Pt-7Sn	2.624	[2.5165(6), +4.3%]
14Pt-1P & 14Pt-4P	2.302/2.293	[2.270(1)/2.268(1), +1.1%]
14Pt-15C	2.141	[2.136(5), +0.2%]
7Sn-12Cl & 7Sn-13Cl	2.377/2.376	[2.356(1)/2.352(1), +0.9%]
7Sn-10N & 7Sn-11N	2.452/2.450	[2.348(3)/2.347(3), +4.3%]
1P-8C & 4P-9C	1.857/1.857	[1.862(4)/1.859(4), -0.2%]
10N-9C & 11N-8C	1.345/1.345	[1.344(5)/1.344(5), +0.1%]

Lowest frequencies (showing no negative values):

	1	2	3
	A	A	A
Frequencies --	17.0356	25.2160	33.5168
Red. masses --	3.6683	4.2778	3.9656
Frc consts --	0.0006	0.0016	0.0026
IR Inten --	0.7748	1.7040	2.4138

Thermochemistry:

Zero-point correction=	0.240295 (Hartree/Particule)
Thermal correction to Energy=	0.263684
Thermal correction to Enthalpy=	0.264629
Thermal correction to Gibbs Free Energy=	0.182763
Sum of electronic and zero-point Energies=	-2263.068445
Sum of electronic and thermal Energies=	-2263.045055
Sum of electronic and thermal Enthalpies=	-2263.044111
Sum of electronic and thermal Free Energies=	-2263.125976