Supporting information.

Theoretical calculations

To calculate the structure and energy of the complexes quantum chemical calculations were carried out using the PBE density functional method[1] with SBK pseudopotential[2] and an extended basis set for valence shells implemented in the PRIRODA program package[3]. Atomic charges were determined by Hirshfeld charge analysis[4]. All calculations were performed using the facilities of the Joint Supercomputer Center of RAS.

Cartesian coordinates (in Å), total energies E and zero-point vibration energies ZPVE (a.u.), as well as atomic Hirshfeld charges (q) and spin densities (s) calculated for all model complexes are listed in the Table S1 (see below) together with the data for corresponding subsystem, which are necessary for calculation of dissociation energies. The total number of structures in Table S1 is 20.

According to the DFT calculations under reaction of Cp^*_2Cr and $SnCl_2(Pc^{2-})$, an outer-sphere charge transfer (CT) complex $(Cp^*_2Cr)^+\{Sn^{IV}Cl_2(Pc^{\bullet 3-})\}^{\bullet -}$ (**I**) (see Fig. S1a) with energy gain of 14.5 kcal/mol. It follows from a large dipole moment of this complex (15.5 Debye (D)). The initial components do not have dipole moments and their symmetry persists at the formation of the complex. The calculated charge on the Cp^*_2Cr fragment is equal to +0.40. Assuming the dipole length is equal to

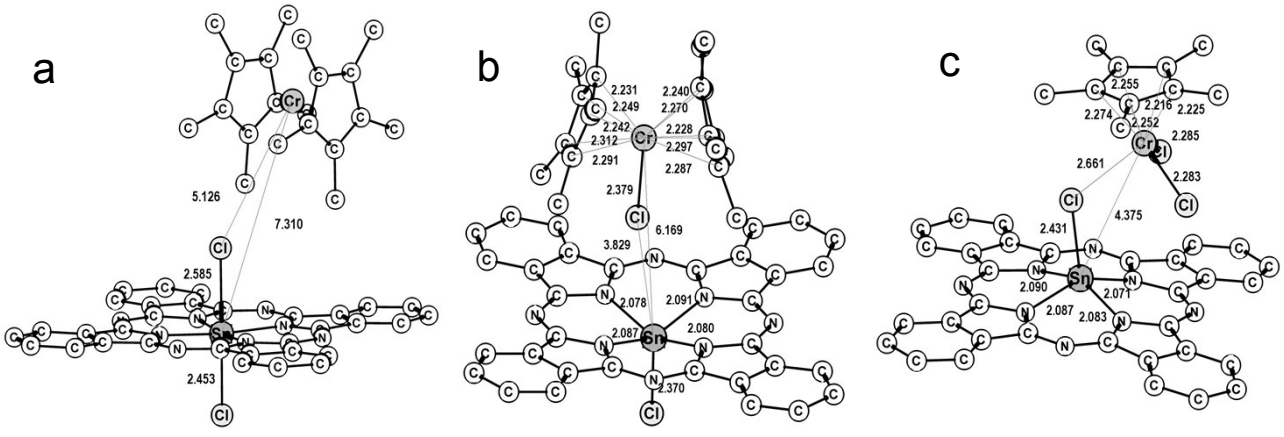

Figure S1. Calculated structures of: (a) CT complex $(Cp^*_2Cr^{III})^+\{Sn^{IV}Cl_2(Pc^{\bullet 3-})\}^{\bullet -}$ (**I**); (b) intermediate van der Waals complex $(Cp^*_2CrCl)\{SnClPc\}$ (**II**); (c) final complex $(Cp^*Cr^{III}Cl_2)\{Sn^{IV}Cl(Pc^{\bullet 3-})\}$ (**III**). The H atoms are omitted for clarity. Interatomic distances are given in Å.

the distance between Sn and Cr atoms of 7.31 Å, we obtain the dipole moment for CT complex of 13.9 D. In the case of the $(Cp^*_2Co)^+\{Sn^{IV}Cl_2(Pc^{\bullet 3-})\}^{\bullet -}$ complex (Fig. S2) the formation energy increases by 6.5 kcal/mol, which correlates well with a smaller value (by 10.2 kcal/mol) of ionization potential of Cp^*_2Co. CT degree increases to +0.58, which fully corresponds to an increase in its dipole moment by about one and half times to 21.4 D.

It is interesting that only in the case of CT complex **I**, chromium atom in the $(Cp^*_2Cr)^+$ cation is able to detach chloride ion from the $\{Sn^{IV}Cl_2(Pc^{\bullet 3-})\}^{\bullet -}$ radical anion to form intermediate van der Waals complex $(Cp_2{*}CrCl)\{SnClPc\}$ (**II**) (Fig. S1b) with the increase of the energy by 7.3 kcal/mol with respect to initial reagents Cp^*_2Cr and $SnCl_2(Pc^{2-})$. For the Co system, such a scenario is impossible since Co-center in the 18e $(Cp^*_2Co)^+$ cation is unable to coordinate additionally Cl^- and gives only contact ion $(Cp^*_2Co)^+(Cl^-)$ pairs. Geometry of the fragments in the complex **II** is very close to the geometry of the corresponding isolated complexes in the doublet state, in which the Sn-Cl and Cr-Cl bond lengths are 2.36 and 2.39 Å, respectively. In this complex, only small transfer of electron density of 0.17 from (Cp^*_2CrCl) to $\{\{Sn^{IV}(Pc^{\bullet 3-})Cl\}$ is realized. The length of the dipole associated with CT we assume to be equal to the distance between the Sn and Cr atoms

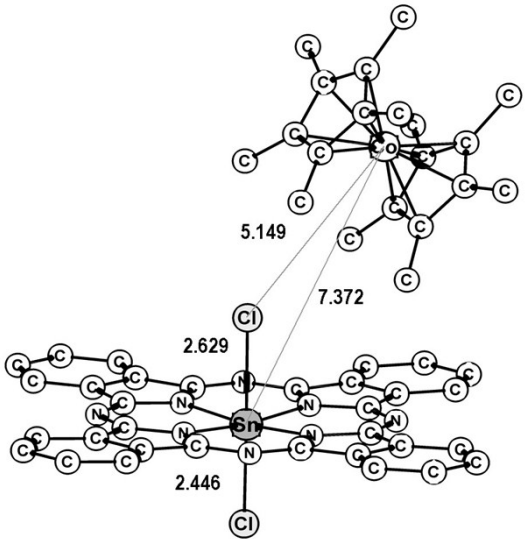

Figure S2. Calculated structure of CT complex $[(Cp^*_2Co)^+\{Sn^{IV}Cl_2(Pc^{\bullet 3-})^{\bullet -}]$ with $S = 1/2$ spin state. The H atoms are omitted for clarity. Interatomic distances are given in Å.

(6.17 Å). Then taking into account the contribution of parallel oriented dipole moments of the Cp^*_2CrCl and SnClPc fragments in **II**, 1.6 and 4.6 D, respectively, we obtain the total dipole moment of 13.9 D, which is close to the calculated dipole moment of 11.8 D.

Under a parallel orientation of spins of the $(Cp^*_2CrCl)^-$ to $\{Sn^{IV}(Pc^{2-})Cl\}^+$ components, the singlet state of the system appears, which is higher in energy than triplet state by 8.2 kcal/mol. Since this state is a state of a system with open shells, the standard calculation in the one-determinant approximation overestimates its energy. The true state should lie slightly below the triplet state and will be the ground state of the van der Waals complex **II**.

The ground state of the (Cp_2*CrCl) species is a triplet state, which is below the singlet state by 4.4 kcal/mol and has much longer Cr-Cl distance, 2.62 Å. So, under interaction of the triplet (Cp_2*CrCl) complex with the coordinatively unsaturated $(Sn^{IV}Cl(Pc^{\bullet 3-})\}$ unit the back transfer of chloride ion is occured. This leads to two possible spin states, S = 1 and S = 2 of the resulting CT complex. The ground triplet complex is shown in Fig. S1b. In the quintet CT complex, there are only small differences in the lengths of the bonds. Only the decrease in the Cl-Cr distance to 4.87 Å is observed at an almost unchanged Sn-Cr distance of 7.25 Å. The quintet complex is located above the triplet charge transfer complex by 3.0 kcal / mol.

The decomposition of the $[(Cp^*_2Cr^{III}Cl)(Sn^{IV}(Pc^{\bullet 3-})Cl)]$ (**II**, S = 1) complex into initial components, namely, $Cp^*_2Cr^{III}Cl$ (S = 3/2) and coordinatively unsaturated $[Sn^{IV}Cl(Pc^{\bullet 3-})]$ units (S = 1/2) requires very low energy expenses of 0.7 kcal/mol. Taking into account entropy increase at the transformation of one particle into two ones, complex **II** is unstable with respect to its decay into the individual $Cp^*_2Cr^{III}Cl$ and $[Sn^{IV}Cl(Pc^{\bullet 3-})]$ components. It is interesting that the latter species show similarity with previously studied $[Sn^{IV}Ph(Pc^{\bullet 3-})]$ species in which negatively charged phenyl substituent is coordinated to tin(IV) atom[5] instead of the Cl^- anion.

The subsequent addition of $(Sn^{IV}Cl(Pc^{\bullet 3-})\}$ to $SnPcCl_2$ leads to the formation of a ClSnPcClSnPcCl dimer with an energy gain of 8.3 kcal / mol. As a result, the total process:

$Cp^*_2Cr + 2SnCl_2Pc = Cp^*_2CrCl + ClSnPcClSnPcCl + 0.3$ kcal/mol

turns out to be thermoneutral. That leads to the formation of a chromium complex with three ligands, as in the isolated product $\{(Cp^*Cr^{II}Cl_2)^-\{Sn^{IV}Cl(Pc^{2-})\}^+$ **2** of the reaction (Fig. 3c).

To answer the question how the Cp* ligand changes to the Cl^- ligand in Cp^*_2CrCl, we consider a formal substitution reaction:

$Cp^*_2CrCl + SnCl_2Pc = Cp^*CrCl_2 + SnPcClCp^*$ -3.8 kcal/mol.

It requires energy costs and, in addition, leads to the formation of the SnCl(Cp*)Pc complex (see Fig. S3) with a weakly bound Cp* ligand. Its decomposition with the dissociation of the Sn-Cp* bond requires a small energy expenses of 5.0 kcal/mol. Therefore, more likely the detachment of an "excess" of Cp* ligand is accompanied by the formation of the $(Cp^*)_2$ dimer. In [$(Cp^*_2CrCl)(SnClPc)$] (**II**), the chloride ligand at the tin(VI) atom is available for coordination. Therefore, the reaction:

$Cp^*CrCl_2 + [(Cp^*_2CrCl)(SnClPc)] = Cp^*_2CrCl + (Cp^*CrCl_2)(SnClPc)$ + 0.1 kcal/mol

can lead to the formation of complex **2** without any kinetic difficulties.

The addition of coordinatively unsaturated SnClPc to $SnCl_2Pc$ can provide the formation of the ClSnPcClSnPcCl dimer with the energy gain of 8.3 kcal/mol. As a result, the total reaction:

$Cp^*_2Cr + 2SnCl_2Pc = Cp^*_2CrCl + ClSnPcClSnPcCl$ + 0.3 kcal/mol (reaction 1) turns out to be thermoneutral.

Then the overall process can be presented as:

$2Cp^*_2CrCl + 4\ SnCl_2Pc = 2Cp^*CrCl_2 + 2ClSnPcClSnPcCl + (Cp^*)_2$ + 13.8 kcal/mol

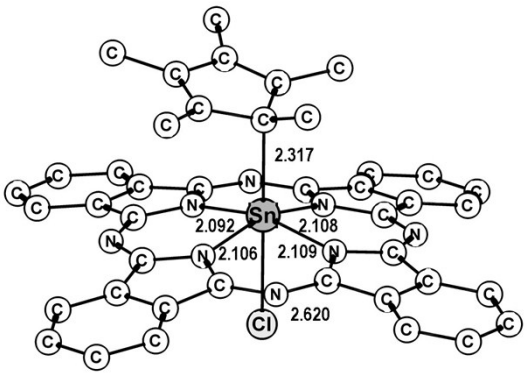

Figure S3. Calculated structure of the SnPcClCp* complex. The H atoms are omitted for clarity. Interatomic distances are given in Å.

which leads to the gain of 6.9 kcal/mole per one Cp^*CrCl_2 complex.

In the structure of the final complex $(Cp^*Cr^{III}Cl_2)^0\{Sn^{IV}(\mu\text{-}Cl)(Pc^{\bullet 3-})\}^0$ (**III**, $S = 1$) (see Fig. S1c) the Cr atom has d^3 electron configuration with effective charge on the Cp^*CrCl_2 fragment of -0.18. Assuming the dipole length to be equal to the distance between the Sn and Cr atoms of 4.38 Å, we obtain the dipole moment of 3.7 D, which, given at the opposite orientation of the dipole moments of Cp^*CrCl_2 and SnClPc and agrees well with the calculated 3.8 D value. This structure is in a rather good agreement with the experimental data, except for the Cl-Cr distance for the μ-bridged Cl atom, which is extended up to 2.66 Å. The difference in the Cl-Cr distance for theoretical and experimental structures can be most probably caused by the absence of electron transfer between the components in the real complex $[(Cp^*Cr^{II}Cl_2)^-\{Sn^{IV}(\mu\text{-}Cl)(Pc^{2-})\}^+]$ (**2**) which results in higher attraction between the ionic components. Optimization of the complex at a fixed experimentally observed Cl-Cr distance of 2.393 Å leads to only a slight increase in energy by 1.1 kcal/mol. The mean values of the Cr-Cl and Cr-C bond lengths of 2.300 and 2.250 Å become much closer to the experimental ones. These data indicate that two states (neutral with CT containing Cr^{III} and $Pc^{\bullet 3-}$ and ionic without CT between the components containing Cr^{II} and Pc^{2-}) are positioned very close to each other in **2**, and in a real system the second ionic case without CT is stabilized as follows from the X-ray diffraction data, green color and UV-vis-NIR solution spectrum of complex **2**.

References:

1. J.P. Perdew, K. Burke and M. Ernzerhof, *Phys. Rev. Lett.,* 1996, **77**, 3865.

2. W.J. Stevens, H. Basch, M. Krauss, *J. Chem. Phys.,* 1984, **81**, 6026.

3. D.N. Laikov, *Chem. Phys. Lett.,* 1997, **281,** 151.

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5. D. V. Konarev, A. V. Kuzmin, S. S. Khasanov, M. Ishikawa, A. Otsuka, H. Yamochi, G. Saito and R. N. Lyubovskaya, *Dalton Trans*. 2016, **45**, 10780.

Table S1

The complex $(Cp^*_2Cr^{III})^+\{Sn^{IV}Cl_2(Pc^{\bullet 3-})\}^{\bullet -}$ (**I**) $S = 1$
E = -522.244590, ZPVE = 0.832570

# / Atom		Coordinates			q	s
1	Sn	2.59843531	7.43016009	7.11311694	0.5084	-0.0045
2	Cl	2.43660610	5.31118424	5.88894820	-0.3212	-0.0025
3	Cl	2.75388470	9.65637976	8.41802084	-0.2831	-0.0024
4	N	3.48179233	8.39459054	5.50407662	-0.1183	0.0007
5	N	1.43624640	9.20933768	4.42693785	-0.1542	-0.0320
6	N	0.74149232	8.06220037	6.46432053	-0.1267	-0.0340
7	N	-0.60220816	7.15734546	8.28915514	-0.1508	-0.0264
8	N	1.73114652	6.63317000	8.81579398	-0.1184	0.0010
9	N	3.77866493	5.87509482	9.92417477	-0.1519	-0.0268
10	N	4.47205233	6.96759918	7.85448091	-0.1266	-0.0337
11	N	5.82199579	7.92287544	6.06033108	-0.1503	-0.0294
12	C	4.84543253	8.43645893	5.28351713	0.0897	-0.0546
13	C	5.04221770	9.16774188	4.04656254	-0.0176	-0.0207
14	C	3.75100065	9.54635425	3.56607240	-0.0156	-0.0209
15	C	2.77301156	9.04433297	4.51264262	0.0926	-0.0523
16	C	0.53142826	8.77482339	5.29493923	0.1024	-0.0100
17	C	-0.91708348	8.98100420	5.19174555	-0.0111	-0.0021
18	C	-1.51601695	8.37778096	6.32783475	-0.0104	-0.0009
19	C	-0.44060965	7.79647933	7.13770363	0.1031	-0.0152
20	C	0.37177693	6.63335551	9.05992751	0.0950	-0.0577
21	C	0.17883185	5.96310453	10.33339591	-0.0153	-0.0187
22	C	1.46820017	5.58556913	10.81481154	-0.0155	-0.0191
23	C	2.44262837	6.02707601	9.83299930	0.0944	-0.0562
24	C	4.68296366	6.29522630	9.04809014	0.1014	-0.0142
25	C	6.13425893	6.13671094	9.18068803	-0.0109	-0.0010
26	C	6.73581513	6.73712942	8.04380362	-0.0113	-0.0016
27	C	5.65802700	7.26961028	7.20443090	0.1023	-0.0112
28	C	6.20114081	9.51888171	3.33633870	-0.0414	-0.0082
29	H	7.18466224	9.22172595	3.70311344	0.0471	-0.0006
30	C	6.05374068	10.24620858	2.15418375	-0.0492	-0.0127
31	H	6.93836887	10.52639755	1.57933129	0.0465	-0.0011
32	C	4.77446849	10.62094962	1.67856921	-0.0485	-0.0138
33	H	4.69682101	11.18428501	0.74694235	0.0472	-0.0011
34	C	3.61524209	10.27649448	2.37516500	-0.0385	-0.0077
35	H	2.62661807	10.55902787	2.01101823	0.0487	-0.0006
36	C	-1.69589363	9.62456583	4.22506192	-0.0352	-0.0007
37	H	-1.22869969	10.08343510	3.35295806	0.0501	0.0000
38	C	-3.08286950	9.65364729	4.41336295	-0.0418	-0.0019
39	H	-3.71673290	10.14556254	3.67351759	0.0497	-0.0002
40	C	-3.67755275	9.05494878	5.54204119	-0.0412	-0.0004
41	H	-4.76207005	9.09348989	5.65789281	0.0501	-0.0000
42	C	-2.90164340	8.41060290	6.51290450	-0.0339	-0.0019
43	H	-3.35446837	7.94326430	7.38800120	0.0510	-0.0001
44	C	-0.97646556	5.67161340	11.07339296	-0.0374	-0.0095
45	H	-1.95960150	5.96123622	10.70059397	0.0487	-0.0007

46	C	-0.82548490	5.00206961	12.28912648	-0.0454	-0.0129
47	H	-1.70785986	4.75993126	12.88407834	0.0479	-0.0010
48	C	0.45201625	4.62788926	12.76609505	-0.0455	-0.0134
49	H	0.53165014	4.10380441	13.72013308	0.0478	-0.0011
50	C	1.60849870	4.91462132	12.03847408	-0.0379	-0.0090
51	H	2.59595621	4.62682860	12.40118900	0.0484	-0.0007
52	C	6.91436065	5.53567280	10.17392830	-0.0344	-0.0018
53	H	6.44399733	5.07450259	11.04308704	0.0510	-0.0001
54	C	8.30448309	5.54311759	10.01076114	-0.0422	-0.0008
55	H	8.93827158	5.07777724	10.76764516	0.0500	-0.0001
56	C	8.90221951	6.13798330	8.88122479	-0.0431	-0.0017
57	H	9.98902663	6.12240237	8.78185040	0.0493	-0.0001
58	C	8.12564868	6.74185698	7.88530245	-0.0366	-0.0011
59	H	8.58126115	7.19997007	7.00651356	0.0493	0.0000
60	Cr	5.45584400	14.01151500	8.50983219	0.2305	2.5746
61	C	4.92888659	15.82182791	7.40052739	-0.0189	-0.0018
62	C	4.09833126	13.73977127	6.75277032	-0.0028	0.0075
63	C	5.08797620	14.74176890	6.45686370	-0.0134	0.0013
64	C	3.83813055	15.47881440	8.28252992	-0.0168	-0.0005
65	C	3.32806494	14.19251664	7.87881327	-0.0062	0.0051
66	C	5.67576916	17.12611455	7.38480034	-0.1017	0.0038
67	H	5.15760610	17.86187308	6.74602699	0.0480	-0.0011
68	H	5.75587006	17.56825262	8.38781950	0.0436	0.0004
69	H	6.69391854	17.01253836	6.98706096	0.0439	0.0005
70	C	6.05516164	14.71268712	5.30687035	-0.1013	0.0041
71	H	5.61826866	15.20826744	4.42328700	0.0485	-0.0002
72	H	6.99309056	15.23590008	5.54182344	0.0424	0.0005
73	H	6.30571393	13.68496412	5.01128504	0.0464	0.0004
74	C	3.87474289	12.46579830	5.99038710	-0.1071	0.0050
75	H	4.79747302	12.10336840	5.51673931	0.0408	0.0007
76	H	3.48374268	11.66364312	6.63269384	0.0329	0.0006
77	H	3.13960330	12.63107129	5.18474260	0.0453	0.0010
78	C	2.15298937	13.47872921	8.48418421	-0.1037	0.0049
79	H	1.21958564	13.80289769	7.99328258	0.0477	0.0007
80	H	2.22549979	12.38898317	8.36450217	0.0364	0.0006
81	H	2.04830927	13.69570301	9.55673578	0.0432	0.0006
82	C	3.26007903	16.36005799	9.35394919	-0.1014	0.0039
83	H	2.47985162	17.01826592	8.93480207	0.0484	-0.0008
84	H	2.79259431	15.77424243	10.15724862	0.0460	0.0004
85	H	4.02078380	17.00910166	9.81032307	0.0429	0.0004
86	C	6.22031918	13.95157074	10.56840974	-0.0167	-0.0006
87	C	6.55643979	12.15987064	9.11628077	-0.0030	0.0074
88	C	5.77027183	12.62598853	10.22583232	-0.0060	0.0054
89	C	7.28943677	14.30613021	9.66468459	-0.0191	-0.0018
90	C	7.49272655	13.19506031	8.76638391	-0.0138	0.0012
91	C	5.74297757	14.77153079	11.73395677	-0.1014	0.0038
92	H	6.33980786	14.54807832	12.63480641	0.0483	-0.0008
93	H	5.83309399	15.85056431	11.54487130	0.0429	0.0004
94	H	4.69333457	14.56029963	11.98011837	0.0460	0.0004
95	C	4.71090260	11.83875001	10.94327857	-0.1036	0.0050

96	H	3.94360936	12.49019670	11.38502950	0.0431	0.0006
97	H	4.20694668	11.12279595	10.27939143	0.0364	0.0007
98	H	5.16205428	11.26077751	11.76768027	0.0482	0.0008
99	C	6.44838506	10.80770715	8.47248255	-0.1076	0.0051
100	H	7.08888347	10.08416784	9.00506279	0.0434	0.0011
101	H	5.42024245	10.41927684	8.49842359	0.0328	0.0008
102	H	6.77695138	10.82141012	7.42412688	0.0405	0.0006
103	C	8.56027958	13.09861633	7.71305303	-0.1010	0.0042
104	H	8.26397137	12.43171185	6.89213589	0.0481	0.0005
105	H	8.80327294	14.07940512	7.28017669	0.0429	0.0005
106	H	9.49159041	12.69281522	8.14350672	0.0490	-0.0002
107	C	8.12714200	15.55233132	9.73340564	-0.1016	0.0039
108	H	8.98634641	15.40537545	10.41018082	0.0479	-0.0010
109	H	8.53297323	15.83051427	8.75072932	0.0440	0.0004
110	H	7.55801876	16.41151330	10.11528048	0.0436	0.0004

The complex $(Cp^*_2Co^{III})^+\{Sn^{IV}Cl_2(Pc^{\bullet 3-})\}^{\bullet -}$ $S = 1/2$
E = -580.894595, ZPVE = 0.834363

# / Atom		Coordinates			q	s
1	Sn	0.68240261	2.75427864	4.90151106	0.5120	0.0062
2	Cl	2.45088266	4.35118041	6.01301346	-0.2914	0.0034
3	N	1.80534157	2.94379375	3.17947917	-0.1303	0.0455
4	N	0.67808805	4.87912812	2.21122121	-0.1579	0.0354
5	N	-0.38418291	4.45795229	4.38523645	-0.1196	-0.0006
6	N	-1.77890254	4.62289414	6.39961118	-0.1587	0.0491
7	N	-0.27473978	2.72987229	6.73344739	-0.1304	0.0448
8	N	0.91434831	0.84649277	7.73647079	-0.1541	0.0262
9	N	1.91618347	1.21389408	5.52866990	-0.1194	-0.0008
10	N	3.36063980	1.10015752	3.55053224	-0.1568	0.0430
11	C	2.85735963	2.10329063	2.84783250	0.1017	0.0141
12	C	3.34359861	2.54874353	1.53633372	-0.0113	0.0027
13	C	2.55569147	3.65943825	1.14133713	-0.0118	0.0014
14	C	1.57693219	3.90897122	2.20554065	0.0978	0.0201
15	C	-0.21499735	5.14094000	3.19313604	0.0833	0.0764
16	C	-1.17347220	6.22345812	3.19796516	-0.0201	0.0268
17	C	-1.89754216	6.14725223	4.43070666	-0.0218	0.0298
18	C	-1.37477624	5.01796476	5.16835290	0.0863	0.0654
19	C	-1.28784630	3.60401805	7.09244374	0.0991	0.0074
20	C	-1.72055626	3.20539567	8.43671645	-0.0134	0.0047
21	C	-0.92716611	2.09688145	8.83067723	-0.0119	-0.0002
22	C	-0.00040562	1.80284712	7.73419186	0.0956	0.0292
23	C	1.79418300	0.57282984	6.75012422	0.0865	0.0846
24	C	2.81590135	-0.45258768	6.78332705	-0.0177	0.0233
25	C	3.53487926	-0.37695880	5.55083384	-0.0179	0.0270
26	C	2.94717683	0.69478422	4.77282915	0.0911	0.0695
27	C	4.37303303	2.06996522	0.72045674	-0.0355	0.0011
28	H	4.97245954	1.21379867	1.03205538	0.0498	-0.0000
29	C	4.59983794	2.71937200	-0.49915128	-0.0442	0.0025
30	H	5.39369785	2.36499831	-1.15904746	0.0483	0.0002
31	C	3.81657817	3.82274241	-0.89238529	-0.0445	0.0008

32	H	4.01602239	4.30485546	-1.85114834	0.0479	0.0001
33	C	2.78634732	4.30640668	-0.07669318	-0.0376	0.0026
34	H	2.17367952	5.15774063	-0.37575895	0.0484	0.0001
35	C	-1.45917350	7.23303437	2.26237806	-0.0429	0.0124
36	H	-0.90827391	7.28375358	1.32217994	0.0460	0.0010
37	C	-2.46122662	8.15250954	2.56938155	-0.0537	0.0168
38	H	-2.70622289	8.94185278	1.85620316	0.0441	0.0014
39	C	-3.17861485	8.07689097	3.78953735	-0.0550	0.0201
40	H	-3.96272678	8.80891636	3.99210497	0.0432	0.0017
41	C	-2.90670427	7.08016143	4.72594950	-0.0453	0.0095
42	H	-3.46177994	7.01308424	5.66286693	0.0446	0.0008
43	C	-2.70749363	3.71970432	9.28422531	-0.0400	-0.0004
44	H	-3.31971187	4.56626109	8.97008420	0.0474	-0.0001
45	C	-2.88785881	3.10912330	10.53113907	-0.0476	0.0050
46	H	-3.65592973	3.48452012	11.20985621	0.0467	0.0004
47	C	-2.09820270	2.00899959	10.92301192	-0.0455	-0.0013
48	H	-2.26652633	1.55141994	11.89960713	0.0479	-0.0001
49	C	-1.10965125	1.49077851	10.07842493	-0.0369	0.0048
50	H	-0.49839918	0.63651234	10.37193395	0.0496	0.0002
51	C	3.16182126	-1.40460538	7.75573407	-0.0414	0.0147
52	H	2.60912177	-1.46096136	8.69438063	0.0461	0.0011
53	C	4.22146441	-2.26946201	7.48141382	-0.0493	0.0152
54	H	4.50800010	-3.02153794	8.21887890	0.0453	0.0012
55	C	4.93378678	-2.19396995	6.26049337	-0.0499	0.0201
56	H	5.75594838	-2.88880606	6.07983107	0.0454	0.0016
57	C	4.60094587	-1.25142129	5.28734615	-0.0401	0.0106
58	H	5.14496112	-1.18941583	4.34402340	0.0468	0.0008
59	Co	2.79130159	8.99336019	8.21336940	0.0735	0.0878
60	C	1.29018518	10.41040648	8.30464022	0.0049	0.0023
61	C	1.35737091	8.67672041	6.73804951	0.0190	-0.0015
62	C	1.58712353	10.09099463	6.93080089	0.0079	0.0042
63	C	0.87330542	9.19162130	8.96165094	0.0083	-0.0005
64	C	0.90469190	8.12224009	7.99301188	0.0179	0.0064
65	C	1.29431598	11.78030896	8.91281267	-0.0989	0.0002
66	H	0.30825423	12.25608824	8.77667045	0.0535	0.0002
67	H	1.49446660	11.75254965	9.99245334	0.0462	-0.0000
68	H	2.03949551	12.43823767	8.44548652	0.0464	0.0001
69	C	1.95861220	11.06960321	5.85892870	-0.0980	0.0004
70	H	1.04690458	11.44815082	5.36641149	0.0545	0.0005
71	H	2.50046803	11.93795380	6.25764025	0.0447	0.0001
72	H	2.57662335	10.60701914	5.07822206	0.0496	0.0001
73	C	1.45449886	7.94009141	5.44029371	-0.1048	0.0000
74	H	2.19925679	8.38591530	4.76704799	0.0437	-0.0001
75	H	1.70227969	6.87790757	5.57983940	0.0344	0.0002
76	H	0.48089337	7.98528512	4.92305891	0.0490	0.0002
77	C	0.46611901	6.71113954	8.21912165	-0.1067	0.0007
78	H	-0.59908887	6.60463545	7.94908512	0.0454	0.0015
79	H	1.02456836	5.99821026	7.59549002	0.0345	0.0002
80	H	0.56860065	6.41128869	9.27095585	0.0416	0.0001
81	C	0.37256395	9.08231817	10.36965254	-0.0980	-0.0001

82	H	-0.71549568	9.26273259	10.39357446	0.0550	-0.0001
83	H	0.54271240	8.08191294	10.78844783	0.0498	-0.0000
84	H	0.84062849	9.81922426	11.03633885	0.0447	-0.0001
85	C	4.04001389	8.54160633	9.80080646	0.0064	-0.0003
86	C	4.52868662	8.04671261	7.57393071	0.0146	-0.0014
87	C	4.09069424	7.47775910	8.82696772	0.0138	0.0068
88	C	4.46292708	9.76512598	9.15682348	0.0035	0.0027
89	C	4.76552635	9.45809013	7.78132856	0.0056	0.0043
90	C	3.72553215	8.38077393	11.25725063	-0.0985	-0.0001
91	H	4.64678165	8.14569759	11.81682982	0.0534	-0.0001
92	H	3.30339191	9.29573348	11.69437778	0.0454	-0.0001
93	H	3.01954214	7.55919638	11.43600484	0.0498	0.0000
94	C	3.82905645	6.02712287	9.08812254	-0.1019	0.0006
95	H	3.12003008	5.87876757	9.91362054	0.0458	0.0002
96	H	3.43946643	5.50438944	8.20320851	0.0374	0.0002
97	H	4.77128945	5.52799489	9.37256287	0.0520	0.0007
98	C	4.80400054	7.28338404	6.31563988	-0.1017	-0.0002
99	H	5.84210614	6.90952767	6.33278553	0.0526	-0.0002
100	H	4.14559174	6.41105575	6.20245888	0.0389	-0.0000
101	H	4.69938421	7.91156574	5.42093103	0.0458	-0.0001
102	C	5.33160113	10.40912137	6.77090198	-0.0986	0.0004
103	H	5.04885587	10.13475987	5.74607915	0.0494	0.0000
104	H	5.00882680	11.44388376	6.94888747	0.0455	0.0001
105	H	6.43380645	10.39709836	6.81789529	0.0531	0.0005
106	C	4.66371496	11.08944074	9.82987283	-0.0992	0.0002
107	H	5.68790004	11.15728035	10.23445452	0.0527	0.0003
108	H	4.53289187	11.93004146	9.13506580	0.0465	0.0001
109	H	3.97263491	11.23428300	10.67123121	0.0464	0.0000
110	Cl	-0.94385083	1.24879133	3.86571787	-0.3180	0.0031

The complex $\{Sn^{IV}Cl_2(Pc^{2-})\}$ $S = 0$
E = -304.143172, ZPVE = 0.404131

# / Atom		Coordinates			q	s
1	Sn	2.60032178	7.58086857	7.18122044	0.4752	0.0000
2	Cl	2.43918433	5.43023587	5.96808089	-0.3295	0.0000
3	Cl	2.76142730	9.73118632	8.39433030	-0.2662	0.0000
4	N	3.46109974	8.45660759	5.51335841	-0.1152	0.0000
5	N	1.41359812	9.21982767	4.43160671	-0.1385	0.0000
6	N	0.72135076	8.11106280	6.48981493	-0.1152	0.0000
7	N	-0.59295862	7.17844530	8.31952454	-0.1385	0.0000
8	N	1.73944201	6.70443523	8.84870462	-0.1152	0.0000
9	N	3.78695979	5.94132172	9.93050843	-0.1385	0.0000
10	N	4.47919818	7.04970425	7.87210246	-0.1152	0.0000
11	N	5.79352836	7.98279153	6.04264569	-0.1385	0.0000
12	C	4.81909104	8.48673075	5.27821718	0.1121	0.0000
13	C	5.00519874	9.18860934	4.00748279	-0.0082	0.0000
14	C	3.71560432	9.55286930	3.53316258	-0.0082	0.0000
15	C	2.74017826	9.07391779	4.51355583	0.1121	0.0000

16	C	0.50216105	8.79210510	5.31147466	0.1121	0.0000
17	C	-0.94636227	8.96645466	5.19567585	-0.0082	0.0000
18	C	-1.53713862	8.36545098	6.34045938	-0.0082	0.0000
19	C	-0.45019928	7.82320790	7.15687703	0.1121	0.0000
20	C	0.38145122	6.67422164	9.08380216	0.1120	0.0000
21	C	0.19534023	5.97221148	10.35446354	-0.0082	0.0000
22	C	1.48494394	5.60799846	10.82880395	-0.0082	0.0000
23	C	2.46036874	6.08711235	9.84848822	0.1120	0.0000
24	C	4.69839834	6.36898508	9.05063716	0.1121	0.0000
25	C	6.14694514	6.19499776	9.16664721	-0.0082	0.0000
26	C	6.73772312	6.79600483	8.02187382	-0.0082	0.0000
27	C	5.65076725	7.33790342	7.20523468	0.1121	0.0000
28	C	6.15628280	9.51067448	3.28147548	-0.0292	0.0000
29	H	7.14287539	9.22849486	3.65004505	0.0541	0.0000
30	C	5.99551921	10.20206014	2.07551455	-0.0340	0.0000
31	H	6.87476422	10.46758703	1.48648488	0.0545	0.0000
32	C	4.71669678	10.56328157	1.60515435	-0.0340	0.0000
33	H	4.62875800	11.10199650	0.66038684	0.0545	0.0000
34	C	3.56128899	10.24366791	2.32701422	-0.0292	0.0000
35	H	2.56962987	10.52028023	1.96794229	0.0541	0.0000
36	C	-1.73528845	9.57812029	4.21625625	-0.0292	0.0000
37	H	-1.27668075	10.03735960	3.34012120	0.0541	0.0000
38	C	-3.12235198	9.57838345	4.40136245	-0.0340	0.0000
39	H	-3.76448219	10.04795411	3.65456637	0.0545	0.0000
40	C	-3.70818660	8.98244052	5.53659147	-0.0340	0.0000
41	H	-4.79339494	9.00128874	5.64839561	0.0545	0.0000
42	C	-2.92407952	8.36877666	6.51985431	-0.0292	0.0000
43	H	-3.37173939	7.90619407	7.39988456	0.0541	0.0000
44	C	-0.95576530	5.64977406	11.08027055	-0.0292	0.0000
45	H	-1.94239490	5.93155036	10.71149226	0.0541	0.0000
46	C	-0.79499248	4.95833374	12.28620008	-0.0340	0.0000
47	H	-1.67424259	4.69268257	12.87516647	0.0545	0.0000
48	C	0.48383821	4.59718266	12.75659027	-0.0340	0.0000
49	H	0.57177636	4.05839707	13.70131817	0.0545	0.0000
50	C	1.63924963	4.91690950	12.03478754	-0.0292	0.0000
51	H	2.63089347	4.64002532	12.39369114	0.0541	0.0000
52	C	6.93590155	5.58376896	10.14631530	-0.0292	0.0000
53	H	6.47727749	5.12433682	11.02234078	0.0541	0.0000
54	C	8.32301608	5.58417652	9.96159364	-0.0340	0.0000
55	H	8.96518259	5.11513010	10.70868777	0.0545	0.0000
56	C	8.90885620	6.18013161	8.82637395	-0.0340	0.0000
57	H	9.99410689	6.16184202	8.71488959	0.0545	0.0000
58	C	8.12470004	6.79314415	7.84274483	-0.0292	0.0000
59	H	8.57234106	7.25552243	6.96259743	0.0541	0.0000

The complex $Sn^{IV}Cl_2(Pc^{\bullet 3-})\}^{\bullet -}$ $S = 1/2$
E = -304.239720, ZPVE = 0.398532

1	Sn	2.60027750	7.58049193	7.18102604	0.4967	0.0063
2	Cl	2.43696226	5.40238595	5.95256714	-0.3714	0.0043
3	Cl	2.76358309	9.75847540	8.40942245	-0.3713	0.0043

4	N	3.46889264	8.45455735	5.51547486	-0.1227	0.0255
5	N	1.41177835	9.22215203	4.42744934	-0.1492	-0.0041
6	N	0.71727835	8.10763885	6.49627723	-0.1227	0.0257
7	N	-0.61156034	7.17611708	8.32613340	-0.1749	0.0975
8	N	1.73164892	6.70623625	8.84646937	-0.1227	0.0255
9	N	3.78878180	5.93888811	9.93463373	-0.1492	-0.0041
10	N	4.48325032	7.05298368	7.86557047	-0.1227	0.0257
11	N	5.81212121	7.98493375	6.03595555	-0.1749	0.0975
12	C	4.81930153	8.48563112	5.27984980	0.0990	0.0081
13	C	5.00167709	9.18724191	4.01030061	-0.0175	0.0272
14	C	3.70915476	9.55325115	3.53328615	-0.0155	0.0081
15	C	2.73617419	9.07949918	4.50393818	0.0805	0.0910
16	C	0.49797982	8.79771895	5.30196739	0.0806	0.0908
17	C	-0.94159151	8.96827566	5.19178277	-0.0154	0.0080
18	C	-1.53248225	8.36515589	6.34030116	-0.0174	0.0271
19	C	-0.44911008	7.82229630	7.15828733	0.0991	0.0079
20	C	0.38124387	6.67520813	9.08211996	0.0990	0.0081
21	C	0.19886903	5.97361007	10.35167625	-0.0175	0.0272
22	C	1.49139450	5.60764345	10.82871478	-0.0155	0.0081
23	C	2.46437576	6.08140447	9.85806781	0.0805	0.0910
24	C	4.70257849	6.36329558	9.06010112	0.0806	0.0908
25	C	6.14218194	6.19316618	9.17052648	-0.0154	0.0080
26	C	6.73307245	6.79628370	8.02200673	-0.0174	0.0271
27	C	5.64966754	7.33870943	7.20377639	0.0991	0.0079
28	C	6.15515266	9.50904294	3.28479486	-0.0437	-0.0038
29	H	7.13801259	9.22250549	3.66189856	0.0427	-0.0003
30	C	6.00602823	10.19984102	2.07839688	-0.0606	0.0245
31	H	6.88882585	10.46342414	1.49240870	0.0375	0.0020
32	C	4.72544754	10.56337210	1.60418831	-0.0566	-0.0014
33	H	4.64057781	11.10262718	0.65814001	0.0381	-0.0001
34	C	3.56917931	10.24628522	2.32161181	-0.0462	0.0176
35	H	2.57900607	10.52529481	1.95841676	0.0423	0.0012
36	C	-1.74518192	9.57841430	4.21712798	-0.0462	0.0175
37	H	-1.29077978	10.03934269	3.33891215	0.0423	0.0012
38	C	-3.12959288	9.57625250	4.40594216	-0.0566	-0.0014
39	H	-3.77494664	10.04547880	3.66005324	0.0382	-0.0001
40	C	-3.71383568	8.97796113	5.54504380	-0.0606	0.0244
41	H	-4.79939134	8.99426548	5.66120161	0.0375	0.0020
42	C	-2.92083382	8.36757774	6.52150064	-0.0437	-0.0038
43	H	-3.35938064	7.90216572	7.40546446	0.0428	-0.0003
44	C	-0.95461728	5.65166773	11.07710219	-0.0437	-0.0038
45	H	-1.93748803	5.93806121	10.69991734	0.0427	-0.0003
46	C	-0.80549773	4.96080522	12.28346395	-0.0606	0.0245
47	H	-1.68830403	4.69710770	12.86938758	0.0375	0.0020
48	C	0.47508688	4.59732679	12.75770225	-0.0566	-0.0014
49	H	0.55995096	4.05799676	13.70370835	0.0381	-0.0001
50	C	1.63136335	4.91452156	12.04033957	-0.0462	0.0176
51	H	2.62153175	4.63544827	12.40349893	0.0423	0.0012
52	C	6.94580841	5.58350537	10.14545051	-0.0462	0.0175
53	H	6.49140527	5.12256306	11.02365851	0.0423	0.0012

54	C	8.33025659	5.58616306	9.95691574	-0.0566	-0.0014
55	H	8.97564033	5.11733489	10.70302904	0.0382	-0.0001
56	C	8.91449966	6.18445906	8.81781664	-0.0606	0.0244
57	H	10.00008645	6.16856946	8.70189249	0.0375	0.0020
58	C	8.12146126	6.79435736	7.84108644	-0.0437	-0.0038
59	H	8.56000629	7.25974546	6.95710914	0.0428	-0.0003

The complex ($Cp^*_2Cr^{II}$) $S = 1$
E = -218.078652, ZPVE = 0.428842

#	Atom	Coordinates			q	s
1	Cr	2.16196173	17.77088003	-5.37239427	0.1399	1.9010
2	C	3.12806992	19.52345040	-4.47103784	-0.0240	0.0087
3	C	1.48557635	19.71705410	-6.10962263	-0.0244	0.0065
4	C	2.89351059	19.82365788	-5.85402786	-0.0172	0.0152
5	C	1.85523941	19.23075835	-3.84870467	-0.0347	-0.0024
6	C	0.82717923	19.34778198	-4.87301443	-0.0353	-0.0036
7	C	4.45271789	19.57727535	-3.76258832	-0.1053	0.0048
8	H	4.60535935	20.55936849	-3.28145624	0.0398	0.0009
9	H	4.52498590	18.81539434	-2.97218944	0.0399	0.0003
10	H	5.29294172	19.41607726	-4.45280903	0.0395	0.0006
11	C	3.94378696	20.19200787	-6.86426933	-0.1047	0.0055
12	H	4.09039747	21.28540718	-6.89937667	0.0414	0.0025
13	H	4.91691371	19.73887103	-6.62640362	0.0404	0.0007
14	H	3.66682850	19.86755951	-7.87789943	0.0406	0.0007
15	C	0.79469839	20.01815367	-7.41001041	-0.1050	0.0044
16	H	1.45254507	19.84671372	-8.27393116	0.0394	0.0007
17	H	-0.10176836	19.39604823	-7.54875592	0.0403	0.0002
18	H	0.46713851	21.07206200	-7.44977650	0.0396	0.0005
19	C	-0.65750136	19.31537163	-4.63873620	-0.1056	0.0029
20	H	-1.03966814	20.31050661	-4.34770933	0.0366	-0.0024
21	H	-1.20692968	19.00500226	-5.53916522	0.0388	0.0004
22	H	-0.92814403	18.61612234	-3.83425699	0.0393	0.0003
23	C	1.61556675	19.03359665	-2.37761443	-0.1058	0.0033
24	H	1.42375734	19.99593670	-1.86950924	0.0368	-0.0020
25	H	0.74516989	18.38860477	-2.18817098	0.0391	0.0001
26	H	2.48046497	18.56933539	-1.88219863	0.0389	0.0005
27	C	2.02751749	15.80690601	-4.53587334	-0.0329	-0.0014
28	C	1.80016335	16.20065138	-6.83380308	-0.0272	0.0048
29	C	1.05681647	15.97779909	-5.60804684	-0.0365	-0.0040
30	C	3.34583554	15.92714588	-5.11313667	-0.0212	0.0104
31	C	3.20202410	16.16763287	-6.51860731	-0.0178	0.0147
32	C	1.71194397	15.39673764	-3.12447490	-0.1055	0.0034
33	H	1.63034885	14.29843123	-3.03561588	0.0372	-0.0017
34	H	2.48906335	15.72461605	-2.41914603	0.0389	0.0005
35	H	0.75743073	15.82091011	-2.78024240	0.0396	0.0002
36	C	-0.42337898	15.73647557	-5.50148272	-0.1058	0.0029
37	H	-0.66705892	14.66667117	-5.63303369	0.0363	-0.0026
38	H	-0.81712277	16.04103665	-4.52095894	0.0389	0.0002
39	H	-0.98320987	16.29515112	-6.26544877	0.0389	0.0005
40	C	1.20315479	16.33520270	-8.20677973	-0.1055	0.0042

41	H	0.23346634	16.85394282	-8.18161357	0.0396	0.0001
42	H	1.85956707	16.89863869	-8.88532467	0.0392	0.0006
43	H	1.02947480	15.34503095	-8.66422554	0.0389	-0.0000
44	C	4.32432718	16.34236624	-7.50307632	-0.1048	0.0054
45	H	4.60382418	15.37596199	-7.95730018	0.0414	0.0024
46	H	4.04671036	17.01965197	-8.32391673	0.0404	0.0006
47	H	5.22617477	16.75243516	-7.02628554	0.0404	0.0007
48	C	4.64267031	15.77438083	-4.36900034	-0.1049	0.0049
49	H	4.94854805	14.71462538	-4.32031424	0.0404	0.0014
50	H	5.46005517	16.33021160	-4.85008145	0.0398	0.0007
51	H	4.56264555	16.13575236	-3.33309740	0.0405	0.0004

The complex ($Cp^*_2Co^{II}$) $S = 1/2$
E = -276.715431, ZPVE = 0.427728

#	Atom	Coordinates			q	s
1	Co	3.09371657	8.23079481	7.94691372	0.0380	0.7714
2	C	1.79869698	9.69540575	8.84482607	-0.0207	0.0510
3	C	1.18251303	8.32710285	7.04752793	-0.0135	0.0063
4	C	1.63238275	9.66511508	7.42901567	-0.0126	0.0051
5	C	1.54046664	8.35632137	9.33268200	-0.0096	-0.0163
6	C	1.07762749	7.53802189	8.22992729	-0.0203	0.0497
7	C	2.16053828	10.88636459	9.68388357	-0.1075	0.0045
8	H	1.26049878	11.39645530	10.07217029	0.0370	0.0055
9	H	2.77002225	10.60311869	10.55486806	0.0388	0.0011
10	H	2.73324699	11.63059878	9.11190963	0.0388	0.0011
11	C	1.75404776	10.83391938	6.49418629	-0.1064	-0.0001
12	H	0.78163442	11.34201762	6.36753061	0.0399	0.0004
13	H	2.46742886	11.58280446	6.86717974	0.0401	0.0002
14	H	2.08883000	10.52677354	5.49319227	0.0391	-0.0004
15	C	0.77620161	7.91544775	5.66187258	-0.1063	-0.0000
16	H	1.39906477	8.39544681	4.89292113	0.0394	-0.0004
17	H	0.85242656	6.82821882	5.51878217	0.0398	0.0003
18	H	-0.27022914	8.20086190	5.45341769	0.0398	0.0005
19	C	0.57146943	6.12827854	8.32883545	-0.1076	0.0044
20	H	-0.51197945	6.10220410	8.54409922	0.0371	0.0054
21	H	0.72987955	5.57142182	7.39370120	0.0392	0.0011
22	H	1.07183654	5.56822092	9.13221285	0.0384	0.0009
23	C	1.54027366	7.94398591	10.77692218	-0.1058	-0.0024
24	H	0.55245529	8.12653305	11.23550082	0.0414	-0.0022
25	H	1.76095126	6.87360219	10.89742775	0.0400	-0.0007
26	H	2.27975777	8.50551990	11.36492129	0.0398	-0.0006
27	C	4.88508106	7.75831696	8.91950913	-0.0104	-0.0102
28	C	4.40785391	7.03006081	6.76331595	-0.0166	0.0299
29	C	4.47475671	6.60949735	8.11932306	-0.0169	0.0286
30	C	5.15162890	8.86080406	8.03886426	-0.0221	0.0583
31	C	4.77487293	8.44072028	6.71785929	-0.0108	-0.0109
32	C	5.17016177	7.72348276	10.39364925	-0.1060	-0.0017
33	H	6.20612397	7.39232970	10.58493899	0.0410	-0.0015
34	H	5.05418982	8.71406464	10.85636216	0.0402	-0.0003
35	H	4.50548481	7.02782660	10.92494787	0.0394	-0.0007

36	C	4.23792210	5.22282075	8.64351318	-0.1069	0.0023
37	H	3.78989128	5.23599621	9.64808068	0.0391	0.0003
38	H	3.56535721	4.64821825	7.99074021	0.0394	0.0007
39	H	5.18292753	4.65571114	8.71998572	0.0384	0.0031
40	C	4.08563174	6.17493368	5.57225486	-0.1070	0.0025
41	H	5.00314982	5.76403371	5.11433469	0.0384	0.0032
42	H	3.44667727	5.32201918	5.84325703	0.0397	0.0007
43	H	3.56281676	6.74217511	4.78866928	0.0386	0.0003
44	C	4.92045886	9.25228384	5.46260668	-0.1059	-0.0019
45	H	4.17061365	8.97647361	4.70702370	0.0397	-0.0007
46	H	4.81785310	10.32935341	5.65612068	0.0399	-0.0002
47	H	5.91353474	9.09480638	5.00592361	0.0411	-0.0016
48	C	5.71102817	10.19920585	8.42497207	-0.1078	0.0052
49	H	6.81359401	10.21446011	8.35230025	0.0366	0.0063
50	H	5.33374496	11.00268989	7.77514787	0.0388	0.0013
51	H	5.45258696	10.46765127	9.45961285	0.0385	0.0012

The complex $(Cp^*_2Cr^{III})^+$ $S = 3/2$
: E = -217.911491:, ZPVE = 0.431754

# / Atom		Coordinates			q	s
1	Cr	2.18870231	17.77662136	-5.38900876	0.2820	2.9551
2	C	3.12378271	19.57435846	-4.45272392	-0.0019	0.0001
3	C	1.47734214	19.77325343	-6.08990657	-0.0018	-0.0010
4	C	2.89608652	19.84175300	-5.84967584	-0.0021	0.0008
5	C	1.84620922	19.34012692	-3.83028418	-0.0016	-0.0020
6	C	0.82890322	19.46306937	-4.84181189	-0.0013	-0.0026
7	C	4.45029544	19.61700277	-3.74921762	-0.0951	0.0048
8	H	4.62318824	20.62080931	-3.32731218	0.0634	0.0002
9	H	4.50158160	18.90419323	-2.91478561	0.0519	0.0006
10	H	5.28534330	19.40296778	-4.42925292	0.0528	0.0006
11	C	3.94428162	20.21027313	-6.86062676	-0.0951	0.0051
12	H	4.08671958	21.30342148	-6.87777876	0.0634	0.0004
13	H	4.91946065	19.76102631	-6.62965876	0.0524	0.0006
14	H	3.66392243	19.90545847	-7.87786264	0.0525	0.0007
15	C	0.78783614	20.06297595	-7.39239953	-0.0950	0.0044
16	H	1.42899656	19.84676481	-8.25721087	0.0525	0.0005
17	H	-0.14160645	19.48877591	-7.50707367	0.0521	0.0006
18	H	0.51695514	21.13028656	-7.44783941	0.0635	-0.0001
19	C	-0.65341406	19.38181218	-4.61617252	-0.0949	0.0038
20	H	-1.04885970	20.37545106	-4.34783274	0.0636	-0.0005
21	H	-1.19245203	19.05194172	-5.51429074	0.0522	0.0004
22	H	-0.91159902	18.70007519	-3.79460498	0.0522	0.0004
23	C	1.61070857	19.10570308	-2.36585004	-0.0950	0.0040
24	H	1.45351787	20.06726877	-1.84969558	0.0635	-0.0003
25	H	0.71890662	18.49164376	-2.18110406	0.0519	0.0004
26	H	2.46654131	18.61593066	-1.88243115	0.0526	0.0005
27	C	2.02492465	15.70678603	-4.56597869	-0.0016	-0.0021
28	C	1.79709625	16.13065009	-6.84598017	-0.0017	-0.0009
29	C	1.07001467	15.85769049	-5.63324638	-0.0013	-0.0026
30	C	3.34280363	15.88591460	-5.11905762	-0.0019	0.0001

31	C	3.20211185	16.14865486	-6.52840701	-0.0021	0.0008
32	C	1.70796060	15.33099658	-3.14702146	-0.0949	0.0040
33	H	1.66358649	14.23374673	-3.04789510	0.0636	-0.0004
34	H	2.47117699	15.68867756	-2.44319249	0.0524	0.0004
35	H	0.73498660	15.72315541	-2.82111203	0.0521	0.0005
36	C	-0.41481957	15.66496005	-5.52024459	-0.0949	0.0038
37	H	-0.66947407	14.60275800	-5.67063245	0.0636	-0.0005
38	H	-0.79695874	15.95040696	-4.53086044	0.0520	0.0004
39	H	-0.96621048	16.23903722	-6.27680824	0.0525	0.0004
40	C	1.20084156	16.27998581	-8.21636265	-0.0950	0.0044
41	H	0.20491915	16.74273046	-8.18841752	0.0519	0.0005
42	H	1.83571687	16.88212476	-8.87974181	0.0527	0.0006
43	H	1.08411581	15.29047964	-8.68844512	0.0635	-0.0001
44	C	4.32521245	16.32571495	-7.51020104	-0.0950	0.0051
45	H	4.60930611	15.35133835	-7.94083190	0.0634	0.0004
46	H	4.04520814	16.97911741	-8.34754084	0.0522	0.0006
47	H	5.22405114	16.74540050	-7.03916901	0.0527	0.0007
48	C	4.63828808	15.73991078	-4.37291918	-0.0950	0.0048
49	H	4.95835823	14.68486580	-4.37233726	0.0634	0.0002
50	H	5.44784942	16.32351131	-4.83091810	0.0526	0.0006
51	H	4.54937419	16.04978418	-3.32278225	0.0522	0.0006

The complex $(Cp^*_2Co^{III})^+$ $S = 0$
E = -276.567127, ZPVE = 0.433230

# / Atom		Coordinates			q	s
1	Co	3.09277474	8.22822330	7.94429102	0.0764	0.0000
2	C	1.88561144	9.64653685	8.84953876	0.0151	0.0000
3	C	1.24046754	8.33678959	7.02473275	0.0151	0.0000
4	C	1.68502027	9.65315113	7.41917515	0.0151	0.0000
5	C	1.56527521	8.32599349	9.33906148	0.0151	0.0000
6	C	1.16653305	7.51649807	8.21127622	0.0151	0.0000
7	C	2.25264537	10.83004974	9.69073630	-0.0935	0.0000
8	H	1.33756782	11.35714762	10.00898722	0.0642	0.0000
9	H	2.79150735	10.53956417	10.60225673	0.0533	0.0000
10	H	2.86867544	11.55484600	9.14308489	0.0528	0.0000
11	C	1.80856915	10.84506895	6.52076121	-0.0935	0.0000
12	H	0.84644436	11.38305226	6.48363412	0.0642	0.0000
13	H	2.56333378	11.55749993	6.87900656	0.0533	0.0000
14	H	2.06160343	10.56486055	5.49010817	0.0528	0.0000
15	C	0.82371374	7.92721891	5.64573724	-0.0935	0.0000
16	H	1.37057860	8.47571984	4.86746824	0.0533	0.0000
17	H	0.96228191	6.85248196	5.47111550	0.0528	0.0000
18	H	-0.24833284	8.14341938	5.50244880	0.0642	0.0000
19	C	0.65922036	6.10881120	8.27514536	-0.0935	0.0000
20	H	-0.43412457	6.11473217	8.42026843	0.0642	0.0000
21	H	0.85904501	5.55390845	7.34901350	0.0533	0.0000
22	H	1.09286599	5.54776900	9.11298009	0.0528	0.0000
23	C	1.54332576	7.90241649	10.77542848	-0.0935	0.0000
24	H	0.54736633	8.10093259	11.20571544	0.0642	0.0000
25	H	1.73780051	6.82826982	10.89369470	0.0533	0.0000

26	H	2.27291837	8.45322911	11.38293562	0.0528	0.0000
27	C	4.85391715	7.77704246	8.93565453	0.0151	0.0000
28	C	4.33457924	7.05409731	6.77483722	0.0151	0.0000
29	C	4.40953280	6.64414929	8.15777615	0.0151	0.0000
30	C	5.05392299	8.88712901	8.03348272	0.0151	0.0000
31	C	4.73291098	8.44031950	6.69802247	0.0151	0.0000
32	C	5.16098605	7.77064852	10.40150841	-0.0935	0.0000
33	H	6.21460959	7.48486983	10.55860672	0.0642	0.0000
34	H	5.02304748	8.75959932	10.85818229	0.0533	0.0000
35	H	4.54512288	7.04819680	10.95248052	0.0528	0.0000
36	C	4.17465678	5.25946303	8.67790560	-0.0935	0.0000
37	H	3.82672005	5.26133535	9.71931991	0.0533	0.0000
38	H	3.44559109	4.70574445	8.07242507	0.0528	0.0000
39	H	5.11790246	4.68834336	8.65204893	0.0642	0.0000
40	C	4.00930427	6.16726568	5.61259631	-0.0935	0.0000
41	H	4.93132931	5.68955480	5.24090760	0.0642	0.0000
42	H	3.31629200	5.36125365	5.88765944	0.0533	0.0000
43	H	3.57349429	6.72432130	4.77322713	0.0528	0.0000
44	C	4.89173373	9.23970314	5.44151908	-0.0935	0.0000
45	H	4.19157728	8.92265563	4.65739421	0.0533	0.0000
46	H	4.75336201	10.31513676	5.61204648	0.0528	0.0000
47	H	5.91039010	9.10332588	5.04123028	0.0642	0.0000
48	C	5.60366694	10.23070792	8.40174432	-0.0936	0.0000
49	H	6.70430039	10.21290505	8.33262776	0.0642	0.0000
50	H	5.25052266	11.02193827	7.72735745	0.0533	0.0000
51	H	5.34954003	10.51659448	9.43057820	0.0527	0.0000

The complex ($Cp^*_2Cr^{III}Cl$) $S = 3/2$
: E = -233.036478, ZPVE = 0.431410

# / Atom		Coordinates			q	s
1	Cl	2.11046538	5.40335851	6.70179094	-0.3168	0.1325
2	Cr	2.92770951	7.66828633	7.73606183	0.2272	2.8834
3	C	1.87738490	9.30178371	8.83430328	-0.0185	-0.0231
4	C	0.64801122	8.26059448	7.15615915	-0.0025	0.0097
5	C	1.48450620	9.38958018	7.45075207	-0.0174	-0.0126
6	C	1.33236270	8.07674466	9.35724908	-0.0150	-0.0100
7	C	0.53413121	7.47100520	8.33815972	0.0028	0.0220
8	C	2.41706305	10.42175402	9.67709262	-0.1017	-0.0011
9	H	1.57796679	10.93326431	10.18076615	0.0457	-0.0041
10	H	3.09420729	10.07302415	10.46959839	0.0404	-0.0006
11	H	2.94595893	11.17912789	9.08668242	0.0411	-0.0001
12	C	1.72212129	10.55953688	6.53642735	-0.1027	0.0021
13	H	0.86513639	11.25447802	6.56650461	0.0454	-0.0016
14	H	2.61325779	11.13490363	6.82199755	0.0396	0.0002
15	H	1.84696524	10.24729853	5.49005358	0.0451	0.0001
16	C	-0.02496583	7.96582905	5.84908985	-0.1112	0.0021
17	H	0.36011459	8.59999533	5.03895938	0.0401	0.0006
18	H	0.13673941	6.91487611	5.56746203	0.0352	0.0004
19	H	-1.11117163	8.14332546	5.92102503	0.0418	0.0009
20	C	-0.33182751	6.26449852	8.52779032	-0.1129	0.0019

21	H	-1.22540506	6.53339175	9.11984073	0.0373	0.0012
22	H	-0.65911519	5.84984655	7.56829510	0.0406	0.0003
23	H	0.19845617	5.46232104	9.05848743	0.0394	0.0010
24	C	1.41506078	7.61042125	10.78385970	-0.1036	0.0028
25	H	0.53794900	7.95598236	11.35846704	0.0450	-0.0008
26	H	1.43314249	6.51323574	10.84954746	0.0480	0.0003
27	H	2.30802055	7.99482623	11.29539140	0.0402	0.0004
28	C	4.94785083	7.54591741	8.75176021	-0.0174	-0.0126
29	C	4.89714513	6.69206350	6.59799179	0.0028	0.0219
30	C	4.94060181	6.33645024	7.97822053	-0.0024	0.0097
31	C	4.92400404	8.65870670	7.83706318	-0.0185	-0.0231
32	C	4.83130336	8.11691306	6.50675506	-0.0150	-0.0100
33	C	5.16322035	7.62693836	10.23782877	-0.1028	0.0021
34	H	6.23561698	7.52772514	10.47939679	0.0455	-0.0016
35	H	4.82685899	8.58629461	10.65407320	0.0396	0.0002
36	H	4.63629089	6.82624681	10.77558728	0.0451	0.0001
37	C	5.00275174	4.93626691	8.51087744	-0.1112	0.0021
38	H	4.84039089	4.90448051	9.59686872	0.0401	0.0006
39	H	4.23349954	4.31331999	8.03105483	0.0352	0.0004
40	H	5.98946027	4.48616229	8.31015342	0.0419	0.0009
41	C	4.99167698	5.75882273	5.43112616	-0.1129	0.0019
42	H	6.00361131	5.81178191	4.99003722	0.0373	0.0012
43	H	4.79249672	4.72339586	5.72762933	0.0405	0.0003
44	H	4.26563141	6.01223912	4.64695122	0.0394	0.0010
45	C	4.86333308	8.90404779	5.22652516	-0.1036	0.0028
46	H	4.26797868	8.41934500	4.43963931	0.0480	0.0003
47	H	4.48272254	9.92615238	5.35759282	0.0402	0.0004
48	H	5.89648597	8.98842864	4.84658576	0.0450	-0.0008
49	C	5.30025555	10.07777546	8.15414421	-0.1016	-0.0011
50	H	6.37587952	10.22191485	7.95001326	0.0457	-0.0041
51	H	4.76206356	10.81113623	7.53710473	0.0404	-0.0006
52	H	5.13680670	10.33420151	9.20745485	0.0411	-0.0001

The complex ($Cp^*_2Cr^{III}Cl$) $S = 1/2$
E = -233.030194, ZPVE = 0.432190

# / Atom		Coordinates			q	s
1	Cl	2.13450612	5.47039512	6.73251275	-0.1849	0.0361
2	Cr	2.87945109	7.53468113	7.67526564	0.1121	1.0988
3	C	2.00117811	9.26502747	8.75579544	-0.0099	-0.0173
4	C	0.76069636	8.21043084	7.11739404	-0.0032	0.0079
5	C	1.57307427	9.34495274	7.37601026	-0.0132	-0.0182
6	C	1.48793454	8.04278202	9.33007360	-0.0263	-0.0092
7	C	0.68632852	7.42508443	8.32823415	0.0038	-0.0167
8	C	2.47479574	10.42209388	9.58811477	-0.1012	-0.0014
9	H	1.59639538	10.87631878	10.08013967	0.0449	-0.0023
10	H	3.16353635	10.12567675	10.39076321	0.0403	-0.0005
11	H	2.95353784	11.21165606	8.99848765	0.0402	-0.0000
12	C	1.75426175	10.52042031	6.46020055	-0.1020	-0.0022
13	H	0.91190390	11.22691812	6.56636225	0.0424	-0.0027
14	H	2.67278075	11.08103660	6.67979432	0.0394	-0.0004

15	H	1.79513068	10.21393976	5.40624897	0.0450	-0.0006
16	C	0.03355998	7.91173721	5.84195251	-0.1090	0.0017
17	H	0.47356163	8.44874249	4.99066337	0.0424	0.0000
18	H	0.06519152	6.83735796	5.61510939	0.0346	0.0011
19	H	-1.02410632	8.21704107	5.92219773	0.0414	0.0014
20	C	-0.20076250	6.24075561	8.56141562	-0.1116	-0.0007
21	H	-1.08770562	6.56171945	9.13662630	0.0402	-0.0012
22	H	-0.54153512	5.79229751	7.62204591	0.0378	-0.0001
23	H	0.30916376	5.45524771	9.13534054	0.0406	-0.0009
24	C	1.50541911	7.66653880	10.78440759	-0.1049	-0.0018
25	H	0.63971171	8.10219071	11.31624214	0.0388	-0.0022
26	H	1.45728211	6.57681052	10.91590378	0.0449	-0.0006
27	H	2.41066141	8.02264492	11.29349258	0.0386	-0.0002
28	C	4.83348071	7.52010669	8.79465179	-0.0133	-0.0182
29	C	4.74785742	6.74420747	6.61066798	0.0039	-0.0167
30	C	4.81283384	6.34564328	7.99827040	-0.0032	0.0079
31	C	4.78516645	8.65304618	7.89590785	-0.0100	-0.0173
32	C	4.68162804	8.16488484	6.54013606	-0.0262	-0.0092
33	C	5.09622899	7.57366106	10.27157604	-0.1020	-0.0022
34	H	6.18194518	7.54424160	10.47247916	0.0424	-0.0027
35	H	4.71012474	8.49413015	10.72965982	0.0394	-0.0004
36	H	4.64166503	6.72354568	10.79796852	0.0450	-0.0006
37	C	4.92323152	4.93584062	8.49322129	-0.1090	0.0017
38	H	4.64853954	4.85737905	9.55391312	0.0424	0.0000
39	H	4.26274583	4.26762177	7.92403685	0.0346	0.0011
40	H	5.95947556	4.57109764	8.38614501	0.0414	0.0014
41	C	4.88127303	5.84001879	5.42384263	-0.1116	-0.0007
42	H	5.91045185	5.91231615	5.02868551	0.0402	-0.0012
43	H	4.68235500	4.79407447	5.68090540	0.0378	-0.0001
44	H	4.18858581	6.11844774	4.61818199	0.0406	-0.0009
45	C	4.82285310	8.98070025	5.28656329	-0.1049	-0.0018
46	H	4.30658545	8.50613407	4.44076261	0.0449	-0.0006
47	H	4.41107620	9.99194518	5.40176609	0.0386	-0.0002
48	H	5.88596344	9.09183720	5.00454743	0.0388	-0.0022
49	C	5.23250094	10.04754757	8.22928978	-0.1012	-0.0014
50	H	6.30576907	10.13416604	7.98306489	0.0449	-0.0023
51	H	4.71503746	10.82047539	7.64511117	0.0403	-0.0005
52	H	5.12885526	10.29245004	9.29210008	0.0402	-0.0000

The complex $\{(Cp^*_2Cr^{III})Sn^{IV}Cl(Pc^{\bullet 3-})\}$ (**II**); $S = 1$
E = -522.210134, ZPVE = 0.832878

# / Atom		Coordinates			q	s
1	Sn	0.29689166	2.96423306	4.85713962	0.5781	0.0071
2	Cl	2.18678342	5.73996297	6.69624937	-0.1503	0.0365
3	N	1.79056632	3.72097722	3.62697886	-0.1415	0.0373
4	N	0.48005663	5.27180131	2.26885889	-0.1606	0.0476
5	N	-0.87259648	4.56804170	4.19962213	-0.1275	0.0004
6	N	-2.69103592	4.42223290	5.85164308	-0.1577	0.0153
7	N	-0.82618965	3.03393691	6.60641908	-0.1422	0.0356
8	N	0.53208313	1.58929853	8.03405283	-0.1599	0.0450

9	N	1.83060039	2.16827458	6.02805763	-0.1267	0.0004
10	N	3.69801146	2.43299617	4.44833682	-0.1548	0.0158
11	C	3.10343484	3.22104368	3.58305623	0.0922	0.0350
12	C	3.73836252	3.78020104	2.39202930	-0.0117	-0.0010
13	C	2.79374792	4.61595389	1.75375206	-0.0130	0.0067
14	C	1.56349371	4.58052696	2.54346728	0.0938	0.0021
15	C	-0.63152890	5.29442209	3.03547655	0.0781	0.0483
16	C	-1.77996637	6.12354981	2.79715689	-0.0213	0.0249
17	C	-2.71348866	5.87410613	3.84944758	-0.0213	0.0171
18	C	-2.12660320	4.89550574	4.72055901	0.0740	0.0808
19	C	-2.11050556	3.60013022	6.69500147	0.0907	0.0340
20	C	-2.69965666	3.13992143	7.95008970	-0.0125	-0.0005
21	C	-1.75192816	2.30988081	8.59126882	-0.0130	0.0065
22	C	-0.56580687	2.24699241	7.73883251	0.0941	0.0037
23	C	1.64958642	1.57947627	7.27520770	0.0786	0.0499
24	C	2.89501246	0.96941857	7.65105183	-0.0209	0.0253
25	C	3.82615480	1.21494500	6.59610113	-0.0206	0.0169
26	C	3.14058213	1.97251652	5.58708104	0.0760	0.0831
27	C	5.02759070	3.62062351	1.87117135	-0.0352	0.0069
28	H	5.75081535	2.97495887	2.37065693	0.0505	0.0003
29	C	5.34777326	4.30954779	0.69598871	-0.0423	-0.0025
30	H	6.34272608	4.19943343	0.26103581	0.0499	-0.0002
31	C	4.40525781	5.14336865	0.05943337	-0.0431	0.0079
32	H	4.68623822	5.66454177	-0.85735124	0.0498	0.0006
33	C	3.11805815	5.30986800	0.58264917	-0.0357	-0.0020
34	H	2.38236340	5.95304115	0.09846757	0.0503	-0.0002
35	C	-2.07145976	7.05565496	1.78261870	-0.0411	0.0067
36	H	-1.35474071	7.24134331	0.98172917	0.0468	0.0005
37	C	-3.29426437	7.71745714	1.83411586	-0.0499	0.0202
38	H	-3.55071686	8.43964899	1.05695102	0.0463	0.0016
39	C	-4.22273469	7.46924992	2.87979745	-0.0490	0.0095
40	H	-5.17289142	8.00653027	2.88378169	0.0464	0.0008
41	C	-3.94524165	6.55598510	3.89212360	-0.0418	0.0157
42	H	-4.65546096	6.36309214	4.69705273	0.0469	0.0011
43	C	-3.94332285	3.40075719	8.53712012	-0.0358	0.0068
44	H	-4.66873886	4.04258020	8.03599235	0.0504	0.0003
45	C	-4.21935862	2.80780700	9.77403226	-0.0418	-0.0017
46	H	-5.18361332	2.98573508	10.25335288	0.0500	-0.0001
47	C	-3.27366611	1.97971453	10.41350457	-0.0424	0.0077
48	H	-3.52158010	1.53093087	11.37692472	0.0500	0.0006
49	C	-2.02717282	1.72346347	9.83180343	-0.0352	-0.0012
50	H	-1.28898953	1.08490398	10.31827096	0.0504	-0.0002
51	C	3.28126897	0.25250481	8.79946860	-0.0408	0.0066
52	H	2.56552150	0.06870561	9.60163621	0.0470	0.0005
53	C	4.59103466	-0.21226605	8.87062770	-0.0499	0.0207
54	H	4.91666749	-0.77762070	9.74563943	0.0463	0.0016
55	C	5.51724236	0.03235560	7.82246893	-0.0492	0.0093
56	H	6.53540999	-0.35026317	7.91440509	0.0463	0.0008
57	C	5.15065520	0.74503434	6.68474117	-0.0417	0.0163
58	H	5.85945031	0.93587736	5.87797177	0.0468	0.0012

59	Cr	2.92017299	7.75782928	7.72106033	0.1390	1.3555
60	C	2.01963177	9.51054725	8.78676477	-0.0040	-0.0243
61	C	0.84155067	8.49373342	7.07592983	0.0024	0.0017
62	C	1.65412984	9.61326474	7.39188598	-0.0071	-0.0180
63	C	1.46234876	8.29156066	9.31905737	-0.0210	-0.0072
64	C	0.70149546	7.69255723	8.27401930	0.0079	-0.0216
65	C	2.48918101	10.64654096	9.64853120	-0.0996	-0.0021
66	H	1.60245808	11.11505555	10.11070038	0.0489	-0.0030
67	H	3.13779180	10.32536843	10.47434778	0.0422	-0.0008
68	H	3.00705254	11.43033158	9.08525836	0.0424	-0.0002
69	C	1.91249836	10.78790956	6.49400905	-0.1002	-0.0015
70	H	1.08060380	11.51037851	6.56158696	0.0472	-0.0024
71	H	2.82934142	11.32767768	6.76534122	0.0405	-0.0003
72	H	1.99816146	10.48577756	5.44183046	0.0482	-0.0005
73	C	0.15800631	8.22558274	5.77076580	-0.1089	0.0011
74	H	0.59575169	8.81114017	4.95172136	0.0427	0.0001
75	H	0.23024332	7.16251857	5.50477653	0.0300	0.0011
76	H	-0.91149708	8.48627553	5.84010761	0.0439	0.0006
77	C	-0.22151808	6.52781178	8.45464326	-0.1119	-0.0009
78	H	-1.12073152	6.86344589	9.00054465	0.0431	-0.0017
79	H	-0.54120407	6.11128883	7.49413324	0.0339	0.0002
80	H	0.24428428	5.72054123	9.03573500	0.0393	-0.0010
81	C	1.42278980	7.88449895	10.76434884	-0.1025	-0.0005
82	H	0.52870270	8.30102806	11.26188075	0.0434	-0.0016
83	H	1.37712477	6.79223478	10.87189570	0.0487	-0.0003
84	H	2.29917793	8.24107299	11.32083349	0.0403	-0.0001
85	C	4.82551148	7.71900399	8.91494612	-0.0105	-0.0195
86	C	4.83732847	6.92404016	6.73471014	0.0118	-0.0226
87	C	4.81503405	6.53579078	8.12686550	-0.0001	0.0040
88	C	4.84720925	8.84483840	8.00676441	-0.0055	-0.0234
89	C	4.80299213	8.34411009	6.65398065	-0.0197	-0.0075
90	C	5.01983160	7.77670217	10.40226176	-0.1005	-0.0019
91	H	6.09352899	7.70851461	10.65018618	0.0463	-0.0028
92	H	4.64911455	8.71477737	10.83586191	0.0405	-0.0004
93	H	4.51303045	6.94734339	10.91329235	0.0473	-0.0005
94	C	4.87006500	5.12710433	8.63438023	-0.1072	0.0019
95	H	4.57052313	5.06357313	9.68891869	0.0434	0.0003
96	H	4.20618969	4.47262194	8.05357727	0.0356	0.0011
97	H	5.89584208	4.73037561	8.54870391	0.0446	0.0011
98	C	5.02547254	6.00926121	5.56549718	-0.1113	-0.0014
99	H	6.07592503	6.07354735	5.22994586	0.0437	-0.0019
100	H	4.81214268	4.96546685	5.81880008	0.0373	0.0001
101	H	4.38605897	6.28986230	4.71793262	0.0389	-0.0011
102	C	4.98773150	9.14925514	5.39967955	-0.1027	-0.0008
103	H	4.49088167	8.67462784	4.54272943	0.0488	-0.0004
104	H	4.58897351	10.16734116	5.49785429	0.0403	-0.0001
105	H	6.05967975	9.24208299	5.14896123	0.0430	-0.0017
106	C	5.29609299	10.23530281	8.35193280	-0.0997	-0.0020
107	H	6.37988459	10.30523020	8.15236313	0.0486	-0.0030
108	H	4.81599036	11.01072719	7.74018576	0.0422	-0.0007

109	H	5.14911825	10.48701846	9.40770051	0.0422	-0.0002
110	Cl	-0.56259410	1.09985186	3.67280465	-0.2239	0.0014

The complex $(Cp^*_2Cr^{III})\{Sn^{IV}Cl_2(Pc^{\bullet 3-})\}^{\bullet -}$; $S = 2$
E = -522.239925, ZPVE = 0.832667

# / Atom		Coordinates			q	s
1	Sn	0.64235619	2.76437326	5.08203748	0.5139	0.0072
2	Cl	1.76378027	4.26405404	6.96537135	-0.2860	0.0036
3	N	2.27102629	3.26050839	3.91134306	-0.1323	0.0507
4	N	1.38131570	5.27125337	2.85109706	-0.1625	0.0515
5	N	-0.32067148	4.48929764	4.44221916	-0.1202	-0.0008
6	N	-2.32638622	4.30550648	5.85088640	-0.1605	0.0427
7	N	-0.86619370	2.44567477	6.45445380	-0.1323	0.0505
8	N	0.06873900	0.49291750	7.58241820	-0.1577	0.0434
9	N	1.72693842	1.21399157	5.92401266	-0.1199	-0.0011
10	N	3.76875732	1.45168615	4.58432146	-0.1566	0.0322
11	C	3.44873342	2.51939056	3.87332600	0.0946	0.0290
12	C	4.31120334	3.16988938	2.88207143	-0.0123	0.0001
13	C	3.60831719	4.29071939	2.37003516	-0.0134	0.0040
14	C	2.30486499	4.34220245	3.04266726	0.0976	0.0109
15	C	0.18496760	5.34865879	3.48448714	0.0797	0.0733
16	C	-0.80436156	6.38378265	3.29310862	-0.0234	0.0325
17	C	-1.89857351	6.09649485	4.17205481	-0.0203	0.0309
18	C	-1.56556854	4.89144911	4.89474076	0.0818	0.0809
19	C	-2.01442146	3.22458110	6.54447391	0.0967	0.0188
20	C	-2.83867868	2.62274336	7.59948303	-0.0125	0.0023
21	C	-2.13347240	1.50307179	8.10797829	-0.0116	0.0021
22	C	-0.86731900	1.40284401	7.37199650	0.0997	0.0194
23	C	1.25615149	0.40387496	6.93857043	0.0881	0.0813
24	C	2.29369700	-0.56743398	7.21075449	-0.0188	0.0291
25	C	3.38290979	-0.28630399	6.32844442	-0.0188	0.0267
26	C	3.00275398	0.85435703	5.52433946	0.0847	0.0908
27	C	5.59774562	2.86038429	2.42779748	-0.0374	0.0048
28	H	6.12958457	1.99465016	2.82437876	0.0494	0.0002
29	C	6.16774173	3.68704091	1.45245810	-0.0462	-0.0007
30	H	7.16770956	3.46506692	1.07528972	0.0476	-0.0001
31	C	5.46871501	4.79958839	0.94179640	-0.0481	0.0049
32	H	5.93785599	5.42022608	0.17608972	0.0464	0.0004
33	C	4.18180046	5.11397619	1.39514316	-0.0405	0.0001
34	H	3.63093736	5.96868689	0.99988551	0.0465	-0.0001
35	C	-0.83679913	7.51485140	2.45767883	-0.0477	0.0111
36	H	-0.00634311	7.72296728	1.78101921	0.0432	0.0009
37	C	-1.95566109	8.34467234	2.51193846	-0.0576	0.0212
38	H	-2.00880137	9.22339693	1.86616299	0.0421	0.0018
39	C	-3.03868146	8.06019868	3.38267247	-0.0562	0.0197
40	H	-3.90338645	8.72655761	3.39149079	0.0431	0.0016
41	C	-3.02191818	6.94149148	4.21383693	-0.0439	0.0125
42	H	-3.85606240	6.71491877	4.87961504	0.0456	0.0010
43	C	-4.09132826	2.97530851	8.11126056	-0.0386	0.0020
44	H	-4.63011780	3.83544568	7.71177746	0.0478	0.0000

45	C	-4.62654394	2.18864991	9.13871996	-0.0456	0.0020
46	H	-5.60519254	2.43693252	9.55356488	0.0473	0.0001
47	C	-3.92482900	1.07636620	9.64457214	-0.0450	0.0018
48	H	-4.37052445	0.48124210	10.44365441	0.0479	0.0001
49	C	-2.66961258	0.72120229	9.13565088	-0.0362	0.0022
50	H	-2.12035898	-0.13956954	9.51888147	0.0495	0.0000
51	C	2.36924630	-1.62902777	8.12719557	-0.0412	0.0129
52	H	1.53442020	-1.83969003	8.79684018	0.0461	0.0010
53	C	3.53236256	-2.39813726	8.14820969	-0.0512	0.0213
54	H	3.61540722	-3.23190468	8.84780878	0.0446	0.0017
55	C	4.61131071	-2.12001913	7.27406058	-0.0508	0.0181
56	H	5.50518317	-2.74517671	7.31668901	0.0445	0.0015
57	C	4.54987552	-1.06748663	6.36133275	-0.0424	0.0156
58	H	5.37772617	-0.85127238	5.68478995	0.0455	0.0012
59	Cr	2.86564742	8.90400277	7.88552935	0.2839	2.9657
60	C	1.52253645	10.35491143	8.91686500	-0.0097	-0.0041
61	C	0.67140202	8.43855300	7.89402934	0.0033	0.0055
62	C	0.85431641	9.85909557	7.74140153	-0.0061	-0.0021
63	C	1.76020992	9.23822057	9.79337323	-0.0083	-0.0024
64	C	1.23493196	8.05395106	9.16242621	0.0002	0.0027
65	C	1.82201921	11.79595581	9.21870713	-0.0996	0.0032
66	H	0.95389248	12.27064967	9.70624856	0.0540	-0.0009
67	H	2.67587112	11.90676571	9.90089442	0.0459	0.0004
68	H	2.03682791	12.37442980	8.30949198	0.0465	0.0003
69	C	0.34913864	10.68964350	6.59582741	-0.0989	0.0042
70	H	-0.67604948	11.03850244	6.80456849	0.0545	-0.0003
71	H	0.96785290	11.58153872	6.42414608	0.0443	0.0005
72	H	0.30747473	10.11445661	5.66128329	0.0507	0.0006
73	C	-0.03424729	7.52753029	6.93565042	-0.1074	0.0060
74	H	-0.00680559	7.90962115	5.90655623	0.0428	0.0012
75	H	0.39441269	6.51397840	6.93932241	0.0321	0.0011
76	H	-1.09646892	7.43642186	7.21843512	0.0501	0.0011
77	C	1.20147602	6.67347823	9.75140004	-0.1033	0.0051
78	H	0.26168796	6.53078914	10.31129082	0.0525	0.0006
79	H	1.24337925	5.89353734	8.97708150	0.0362	0.0007
80	H	2.02916160	6.50498096	10.45433151	0.0447	0.0007
81	C	2.36396845	9.30655351	11.16753459	-0.0993	0.0039
82	H	1.57641443	9.47202805	11.92181581	0.0543	-0.0005
83	H	2.87637966	8.37302311	11.43668832	0.0493	0.0004
84	H	3.08455223	10.13041848	11.26479293	0.0450	0.0005
85	C	5.06888386	8.77401254	8.20829049	-0.0083	-0.0021
86	C	4.08769510	7.95582702	6.25866649	0.0029	0.0055
87	C	4.63513490	7.57590281	7.53553788	0.0002	0.0030
88	C	4.78978300	9.89502212	7.34966325	-0.0098	-0.0037
89	C	4.17846982	9.38900824	6.14778717	-0.0066	-0.0017
90	C	5.77619949	8.83091753	9.53266189	-0.0993	0.0040
91	H	6.86482010	8.72950332	9.38741077	0.0543	-0.0004
92	H	5.60578758	9.78286055	10.05430408	0.0451	0.0005
93	H	5.46332252	8.01647637	10.19996622	0.0493	0.0004
94	C	4.79614991	6.16828537	8.03196259	-0.1030	0.0051

95	H	4.81549634	6.11753819	9.12944173	0.0448	0.0007
96	H	3.99348212	5.50872685	7.67069044	0.0366	0.0007
97	H	5.75076209	5.75216591	7.66779319	0.0533	0.0007
98	C	3.58081806	7.01142793	5.21023803	-0.1077	0.0056
99	H	4.42421434	6.64659050	4.59953473	0.0479	0.0011
100	H	3.08922500	6.13164686	5.65239908	0.0325	0.0009
101	H	2.86814717	7.49011943	4.52543600	0.0423	0.0010
102	C	3.78763599	10.20156252	4.94593174	-0.0985	0.0042
103	H	2.95372002	9.74368863	4.39742265	0.0529	0.0005
104	H	3.49889632	11.22732045	5.21398516	0.0449	0.0006
105	H	4.63564593	10.27365622	4.24451385	0.0549	-0.0003
106	C	5.16369407	11.32595618	7.61465965	-0.0996	0.0033
107	H	6.17767764	11.53200370	7.23250029	0.0538	-0.0009
108	H	4.48272911	12.03029148	7.11737502	0.0466	0.0004
109	H	5.16902399	11.56132625	8.68782031	0.0460	0.0004
110	Cl	-0.38043456	1.36325821	3.36302623	-0.3152	0.0034

The complex $\{ClSn^{IV}(Pc^{2-})(\mu\text{-}Cl)(Sn^{IV}(Pc^{\bullet 3-})Cl\}^{\bullet}$; $S = 1/2$
E = -593.326896, ZPVE = 0.803605

# / Atom		Coordinates			q	s
1	Sn	0.58991408	-2.34776872	1.07141925	0.5319	0.0040
2	Cl	0.17199337	-4.23899823	-0.35663219	-0.2721	0.0010
3	N	0.74452823	-0.93246566	-0.42871471	-0.1238	0.0110
4	N	-1.61839625	-0.32365534	-0.58640509	-0.1391	-0.0015
5	N	-1.38448900	-1.79956274	1.34808115	-0.1243	0.0134
6	N	-1.86314431	-3.11445431	3.34982072	-0.1520	0.0450
7	N	0.52101634	-3.35950573	2.87467381	-0.1226	0.0095
8	N	2.89511022	-3.91101988	3.06997995	-0.1406	-0.0023
9	N	2.65346657	-2.48997070	1.09581531	-0.1232	0.0119
10	N	3.14973088	-1.07519994	-0.83246733	-0.1521	0.0453
11	C	1.91465949	-0.63786271	-1.10031883	0.1051	0.0035
12	C	1.56105557	0.26818191	-2.18667630	-0.0129	0.0133
13	C	0.15746750	0.48407485	-2.12273701	-0.0112	0.0031
14	C	-0.34940438	-0.27839308	-0.99206612	0.0954	0.0470
15	C	-2.09453385	-0.98927336	0.46393000	0.0960	0.0439
16	C	-3.47979772	-0.99682103	0.91194668	-0.0108	0.0019
17	C	-3.54680418	-1.81152490	2.07421167	-0.0126	0.0120
18	C	-2.20228269	-2.31497580	2.33492165	0.1057	0.0010
19	C	-0.63061373	-3.56797262	3.60654217	0.1053	0.0066
20	C	-0.25846111	-4.38297052	4.75648990	-0.0127	0.0143
21	C	1.14015054	-4.62349654	4.67374047	-0.0110	0.0033
22	C	1.62668638	-3.95637152	3.47597165	0.0956	0.0533
23	C	3.37124696	-3.24718289	2.01904628	0.0965	0.0501
24	C	4.77300786	-3.14877667	1.63873367	-0.0107	0.0021
25	C	4.84571464	-2.31004758	0.49402179	-0.0124	0.0131
26	C	3.48566183	-1.89331632	0.16978652	0.1059	0.0032
27	C	2.34217650	0.87681390	-3.17660924	-0.0320	-0.0019
28	H	3.41812143	0.70450166	-3.21718430	0.0503	-0.0001
29	C	1.69546110	1.69751699	-4.10481012	-0.0398	0.0126
30	H	2.27469087	2.18104149	-4.89322210	0.0516	0.0010

31	C	0.30057380	1.90892171	-4.04479659	-0.0374	-0.0014
32	H	-0.17229155	2.55155868	-4.78964985	0.0519	-0.0001
33	C	-0.48400138	1.30941944	-3.05586497	-0.0314	0.0096
34	H	-1.56116860	1.47015427	-3.00665308	0.0492	0.0009
35	C	-4.62888358	-0.37801337	0.40284886	-0.0312	0.0090
36	H	-4.57466839	0.24337274	-0.49124720	0.0493	0.0008
37	C	-5.83603780	-0.58967935	1.07497096	-0.0371	-0.0021
38	H	-6.74937735	-0.12604793	0.69786080	0.0520	-0.0001
39	C	-5.90097170	-1.39584575	2.23204244	-0.0395	0.0118
40	H	-6.86199422	-1.54003996	2.72853127	0.0518	0.0009
41	C	-4.75787177	-2.01482824	2.74625556	-0.0319	-0.0023
42	H	-4.79867059	-2.64182048	3.63739587	0.0505	-0.0002
43	C	-1.01817959	-4.89346964	5.81637277	-0.0323	-0.0013
44	H	-2.09052808	-4.70365463	5.87124538	0.0509	-0.0001
45	C	-0.35743928	-5.65135088	6.78698390	-0.0399	0.0135
46	H	-0.92219850	-6.06834812	7.62232587	0.0516	0.0010
47	C	1.03201263	-5.89015204	6.70588890	-0.0375	-0.0008
48	H	1.51523615	-6.48773747	7.48074836	0.0520	-0.0000
49	C	1.79698816	-5.37906383	5.65411462	-0.0332	0.0108
50	H	2.87010058	-5.56067835	5.58844051	0.0517	0.0007
51	C	5.93231842	-3.70223018	2.19740950	-0.0329	0.0102
52	H	5.87247756	-4.34473189	3.07632641	0.0518	0.0007
53	C	7.15538591	-3.40695777	1.58880027	-0.0372	-0.0017
54	H	8.07490296	-3.82871903	1.99825685	0.0522	-0.0001
55	C	7.22679594	-2.57417357	0.45107324	-0.0395	0.0126
56	H	8.19942093	-2.36755749	0.00166448	0.0517	0.0010
57	C	6.07458133	-2.01377808	-0.10787599	-0.0321	-0.0019
58	H	6.12065319	-1.36986266	-0.98656795	0.0510	-0.0001
59	Sn	0.90615343	2.39350406	3.73519775	0.5326	0.0043
60	Cl	1.15631761	-0.22501519	2.78686500	-0.2825	0.0002
61	Cl	0.76979676	4.62232407	4.62999721	-0.2707	0.0011
62	N	2.41601438	2.75464798	2.37123855	-0.1267	0.0245
63	N	1.04471442	3.44300951	0.47428620	-0.1455	0.0219
64	N	-0.47891376	2.64697084	2.21708422	-0.1218	-0.0001
65	N	-2.49238431	2.02287434	3.46151601	-0.1465	0.0256
66	N	-0.57831957	1.55125622	4.89958228	-0.1266	0.0242
67	N	0.79772234	0.77450552	6.75939529	-0.1459	0.0186
68	N	2.31951441	1.65972443	5.05866666	-0.1202	-0.0004
69	N	4.33278602	2.19722354	3.77443211	-0.1468	0.0225
70	C	3.77019306	2.63571903	2.65677404	0.1041	0.0115
71	C	4.49032333	3.07340696	1.46112346	-0.0100	0.0016
72	C	3.52359451	3.43413062	0.48849727	-0.0101	0.0017
73	C	2.20328285	3.22178520	1.08082357	0.1037	0.0104
74	C	-0.17432160	3.19877712	0.98216198	0.0960	0.0416
75	C	-1.43592996	3.46625142	0.31851615	-0.0137	0.0144
76	C	-2.47632525	3.04788990	1.19730663	-0.0139	0.0152
77	C	-1.84764700	2.52638520	2.39611854	0.0966	0.0380
78	C	-1.92652921	1.56330352	4.57002157	0.1043	0.0072
79	C	-2.63945511	0.96079056	5.69626376	-0.0103	0.0026
80	C	-1.67274347	0.59879474	6.66843164	-0.0099	0.0008

81	C	-0.35995714	0.97560106	6.14577142	0.1033	0.0154
82	C	2.01478588	1.06120333	6.27043407	0.0966	0.0481
83	C	3.27719791	0.75827674	6.91843745	-0.0133	0.0138
84	C	4.31731282	1.17753107	6.04009956	-0.0135	0.0147
85	C	3.68735216	1.73523374	4.85777142	0.0974	0.0444
86	C	5.85875211	3.16351324	1.18516917	-0.0315	0.0014
87	H	6.59632198	2.88563407	1.93857988	0.0522	0.0000
88	C	6.24007489	3.62422781	-0.07983044	-0.0371	0.0014
89	H	7.30014931	3.71053825	-0.32402063	0.0526	0.0001
90	C	5.27864375	3.98122063	-1.04747740	-0.0372	0.0017
91	H	5.61166785	4.33793425	-2.02358944	0.0525	0.0001
92	C	3.90883833	3.88825871	-0.77737597	-0.0310	0.0011
93	H	3.15932169	4.16102245	-1.52087146	0.0502	0.0001
94	C	-1.73329251	4.03578539	-0.92816418	-0.0324	0.0068
95	H	-0.93282529	4.35817929	-1.59452015	0.0489	0.0007
96	C	-3.07742901	4.18034173	-1.27585015	-0.0400	0.0085
97	H	-3.34044750	4.62805240	-2.23587039	0.0509	0.0007
98	C	-4.11014451	3.76466007	-0.40362435	-0.0402	0.0097
99	H	-5.14958155	3.89959127	-0.70794198	0.0509	0.0008
100	C	-3.82398568	3.19430596	0.83788503	-0.0324	0.0058
101	H	-4.61580230	2.87574374	1.51636947	0.0489	0.0006
102	C	-4.00057892	0.71526115	5.90613639	-0.0311	0.0002
103	H	-4.73765966	0.99379837	5.15241941	0.0504	0.0000
104	C	-4.37544383	0.10816932	7.10982848	-0.0374	0.0028
105	H	-5.43020972	-0.09095059	7.30662271	0.0525	0.0002
106	C	-3.41442396	-0.25085157	8.07716294	-0.0370	0.0003
107	H	-3.74204698	-0.72202307	9.00533920	0.0526	0.0000
108	C	-2.05154158	-0.01296816	7.86817174	-0.0315	0.0023
109	H	-1.30274172	-0.28844014	8.61137871	0.0522	0.0001
110	C	3.57500745	0.16181826	8.15237890	-0.0341	0.0084
111	H	2.77499615	-0.15872363	8.82035882	0.0507	0.0006
112	C	4.91933628	-0.00020612	8.49166113	-0.0400	0.0097
113	H	5.18226494	-0.45527480	9.44805842	0.0510	0.0008
114	C	5.95174141	0.41593913	7.61967557	-0.0402	0.0109
115	H	6.99125539	0.27376488	7.91983419	0.0510	0.0009
116	C	5.66517147	1.00460865	6.38682040	-0.0340	0.0074
117	H	6.45711887	1.32585933	5.70962978	0.0507	0.0006

The complex ($Cp^*Cr^{III}Cl_2$); $S = 3/2$
E = -182.313842, ZPVE = 0.217695

# / Atom		Coordinates			q	s
1	Cr	3.11601985	10.81477657	4.74188030	0.2210	2.8976
2	Cl	4.70866614	11.57160164	6.12467747	-0.2402	0.0809
3	Cl	4.18003941	10.77820769	2.76987502	-0.2402	0.0811
4	C	1.20508394	11.45428973	5.66819921	-0.0007	-0.0179
5	C	1.62424641	10.24884241	6.31416143	-0.0013	0.0013
6	C	1.69061068	9.21658896	5.30935676	0.0013	-0.0307
7	C	1.25685040	9.77343283	4.05296824	-0.0014	0.0023
8	C	0.97913779	11.16075397	4.26888798	-0.0006	-0.0196
9	C	1.00854925	12.78493542	6.33291500	-0.0978	0.0022

10	H	-0.03264536	12.88807396	6.68278288	0.0507	-0.0020
11	H	1.20876974	13.61882008	5.64664879	0.0521	0.0007
12	H	1.66955197	12.90031981	7.20133764	0.0519	-0.0002
13	C	1.92920069	10.09994871	7.77517125	-0.1020	0.0020
14	H	2.52502249	10.94434887	8.14758216	0.0452	0.0006
15	H	2.49621149	9.18323218	7.98057110	0.0488	0.0005
16	H	0.99495544	10.05481588	8.35905539	0.0479	-0.0008
17	C	2.10260572	7.79180745	5.54166972	-0.0961	0.0022
18	H	2.83158806	7.70704631	6.35840072	0.0541	0.0003
19	H	2.55188596	7.34688285	4.64405801	0.0543	0.0002
20	H	1.22649818	7.17920805	5.81353816	0.0526	-0.0032
21	C	1.10803661	9.04262653	2.75186744	-0.1022	0.0020
22	H	0.04625521	8.81678729	2.55838625	0.0477	-0.0008
23	H	1.65727020	8.09268883	2.75459392	0.0487	0.0005
24	H	1.49021896	9.63817530	1.91182733	0.0451	0.0006
25	C	0.50809677	12.13474138	3.22929398	-0.0975	0.0022
26	H	0.86013529	13.15478064	3.43446969	0.0523	0.0007
27	H	-0.59442794	12.16502520	3.20455302	0.0509	-0.0022
28	H	0.86007257	11.85391276	2.22843450	0.0523	-0.0002

The complex {$ClSn^{IV}(Pc^{2-})Cp^*$}; $S = 0$
E = -354.858666, ZPVE = 0.616736

# / Atom		Coordinates			q	s
1	Sn	-12.47671976	2.98987918	1.23598470	0.5117	0.0000
2	Cl	-12.29504971	1.04704667	2.98462206	-0.3943	0.0000
3	N	-10.46578233	3.21333248	1.82003627	-0.1118	0.0000
4	N	-9.47389965	1.63980223	0.24317142	-0.1394	0.0000
5	N	-11.89170504	1.46018664	-0.06537580	-0.1088	0.0000
6	N	-14.09104052	0.51458027	-0.54555268	-0.1415	0.0000
7	N	-14.44323250	2.23700322	1.14549609	-0.1109	0.0000
8	N	-15.41770453	3.53997101	2.96361290	-0.1425	0.0000
9	N	-13.03224472	4.06066967	2.96607643	-0.1129	0.0000
10	N	-10.79993890	4.66687648	3.74995264	-0.1428	0.0000
11	C	-10.04735702	3.97313441	2.89091186	0.1071	0.0000
12	C	-8.59164387	3.83482618	2.96803249	-0.0099	0.0000
13	C	-8.20206886	2.93804474	1.93871884	-0.0091	0.0000
14	C	-9.42009374	2.53473436	1.23319332	0.1107	0.0000
15	C	-10.57619855	1.13876006	-0.32420241	0.1113	0.0000
16	C	-10.59334776	0.03350108	-1.28379476	-0.0081	0.0000
17	C	-11.95389715	-0.29977535	-1.51483140	-0.0080	0.0000
18	C	-12.76482426	0.60259737	-0.69567584	0.1111	0.0000
19	C	-14.84085036	1.21983697	0.30422984	0.1106	0.0000
20	C	-16.26655691	0.99454608	0.55243634	-0.0091	0.0000
21	C	-16.65813157	1.88604039	1.58488522	-0.0097	0.0000
22	C	-15.46987185	2.65246406	1.96594143	0.1075	0.0000
23	C	-14.32442696	4.14444942	3.44101449	0.1054	0.0000
24	C	-14.28014074	4.96463427	4.65120323	-0.0107	0.0000
25	C	-12.91884487	5.29710186	4.88231310	-0.0106	0.0000
26	C	-12.13599478	4.67921759	3.81256121	0.1061	0.0000

27	C	-7.64686689	4.38333667	3.84115585	-0.0318	0.0000
28	H	-7.95379160	5.06433532	4.63557779	0.0524	0.0000
29	C	-6.30557887	4.02684810	3.66014647	-0.0371	0.0000
30	H	-5.54426872	4.44149835	4.32286465	0.0529	0.0000
31	C	-5.91883699	3.13540993	2.63900986	-0.0370	0.0000
32	H	-4.86468805	2.87578140	2.52888215	0.0529	0.0000
33	C	-6.86200869	2.57573110	1.76949337	-0.0315	0.0000
34	H	-6.56977632	1.87870353	0.98341958	0.0527	0.0000
35	C	-9.56223874	-0.68015262	-1.90300391	-0.0309	0.0000
36	H	-8.51890446	-0.42641751	-1.71276650	0.0531	0.0000
37	C	-9.91648576	-1.72111438	-2.76871989	-0.0369	0.0000
38	H	-9.13471503	-2.29147001	-3.27300795	0.0532	0.0000
39	C	-11.26754692	-2.05206625	-2.99821162	-0.0369	0.0000
40	H	-11.50773652	-2.87258801	-3.67631800	0.0532	0.0000
41	C	-12.30250269	-1.35136155	-2.36848689	-0.0310	0.0000
42	H	-13.34909603	-1.60953071	-2.53322570	0.0532	0.0000
43	C	-17.18083271	0.09854900	-0.01014333	-0.0315	0.0000
44	H	-16.87111722	-0.59091385	-0.79614059	0.0527	0.0000
45	C	-18.49574303	0.11937397	0.46959317	-0.0372	0.0000
46	H	-19.23369335	-0.56447522	0.04705225	0.0529	0.0000
47	C	-18.88478657	1.00539152	1.49428633	-0.0372	0.0000
48	H	-19.91720563	0.99217933	1.84738316	0.0529	0.0000
49	C	-17.96999163	1.89567272	2.06883045	-0.0318	0.0000
50	H	-18.26259421	2.57690382	2.86846535	0.0524	0.0000
51	C	-15.28337804	5.38528142	5.53115021	-0.0322	0.0000
52	H	-16.32531326	5.11647611	5.35481821	0.0524	0.0000
53	C	-14.90267270	6.15508826	6.63538063	-0.0372	0.0000
54	H	-15.66283380	6.50324685	7.33659923	0.0529	0.0000
55	C	-13.55088608	6.48548766	6.86474288	-0.0372	0.0000
56	H	-13.28933669	7.08334833	7.73932976	0.0528	0.0000
57	C	-12.54212288	6.05525946	5.99630736	-0.0320	0.0000
58	H	-11.49396714	6.29721107	6.17477331	0.0525	0.0000
59	C	-11.32585110	4.60026623	-1.04575610	-0.0257	0.0000
60	C	-13.04819354	3.73345327	-2.32530934	-0.0199	0.0000
61	C	-11.61078374	3.95234212	-2.23201258	-0.0205	0.0000
62	C	-12.59498371	4.74510210	-0.27173601	-0.0610	0.0000
63	C	-13.65776479	4.25511810	-1.19963129	-0.0252	0.0000
64	C	-10.00993084	5.21965957	-0.66535934	-0.1183	0.0000
65	H	-9.84341629	6.15697616	-1.22552131	0.0397	0.0000
66	H	-9.95724408	5.48101372	0.39974870	0.0281	0.0000
67	H	-9.15360037	4.56461671	-0.88859485	0.0333	0.0000
68	C	-10.63897779	3.56640422	-3.31011469	-0.1138	0.0000
69	H	-9.60194369	3.78821044	-3.02457761	0.0390	0.0000
70	H	-10.69933520	2.49229588	-3.55193563	0.0351	0.0000
71	H	-10.84757590	4.10695375	-4.24916361	0.0405	0.0000
72	C	-13.71704612	3.09431063	-3.50846461	-0.1138	0.0000
73	H	-13.57897329	3.69683635	-4.42240127	0.0405	0.0000
74	H	-13.29674430	2.09876097	-3.72676912	0.0356	0.0000
75	H	-14.79751515	2.97364095	-3.35306441	0.0385	0.0000
76	C	-15.12864048	4.48764545	-1.00279888	-0.1176	0.0000

77	H	-15.74430384	3.69795293	-1.45851305	0.0350	0.0000
78	H	-15.41176668	4.56166453	0.05601503	0.0273	0.0000
79	H	-15.43695983	5.43990762	-1.47107122	0.0403	0.0000
80	C	-12.83744652	6.06112441	0.46869127	-0.1159	0.0000
81	H	-12.89768420	6.89419907	-0.25190373	0.0402	0.0000
82	H	-13.77669736	6.05272764	1.03993205	0.0302	0.0000
83	H	-12.02798263	6.29834409	1.17444188	0.0317	0.0000

$(Cp^*)_2$; $S = 0$
E = -131.378961, ZPVE = 0.430433

# / Atom		Coordinates			q	s
1	C	0.20978629	1.60433080	0.37826320	0.0239	0.0000
2	C	0.65916005	2.75593979	-1.64200102	-0.0104	0.0000
3	C	0.98518908	2.73650525	-0.31789078	-0.0061	0.0000
4	C	-0.68379004	1.08510632	-0.76077349	-0.0038	0.0000
5	C	-0.38008131	1.74247570	-1.91358789	-0.0139	0.0000
6	C	-0.73284881	2.16816747	1.46818909	-0.1115	0.0000
7	H	-1.46103475	2.85116104	1.00489528	0.0344	0.0000
8	H	-1.28765440	1.35899948	1.96461014	0.0327	0.0000
9	H	-0.19211923	2.72725901	2.24218131	0.0319	0.0000
10	C	1.88829337	3.71366146	0.37068196	-0.1112	0.0000
11	H	2.19420146	4.51483978	-0.31596449	0.0384	0.0000
12	H	1.38293018	4.19742568	1.22418539	0.0376	0.0000
13	H	2.80924564	3.26237269	0.77223170	0.0351	0.0000
14	C	1.17844433	3.66991803	-2.71465352	-0.1107	0.0000
15	H	1.90653638	4.39577836	-2.33021396	0.0398	0.0000
16	H	1.67557867	3.09771539	-3.51587415	0.0421	0.0000
17	H	0.36289655	4.23526889	-3.19542179	0.0405	0.0000
18	C	-1.04572156	1.59976566	-3.25234129	-0.1112	0.0000
19	H	-1.62388172	2.50193266	-3.51622910	0.0410	0.0000
20	H	-0.30605389	1.45649080	-4.05693231	0.0407	0.0000
21	H	-1.73730983	0.74712579	-3.27761570	0.0404	0.0000
22	C	-1.88999171	0.21823526	-0.53272095	-0.1128	0.0000
23	H	-2.76648056	0.83647075	-0.26770273	0.0391	0.0000
24	H	-2.16290433	-0.35337647	-1.43171639	0.0384	0.0000
25	H	-1.74466922	-0.49339176	0.29040120	0.0325	0.0000
26	C	1.49047276	0.65988339	2.48487005	-0.0060	0.0000
27	C	0.44183047	-1.40058338	2.25193986	-0.0139	0.0000
28	C	0.99321299	-0.39866354	3.18632659	-0.0103	0.0000
29	C	1.20893748	0.45131620	0.98651005	0.0240	0.0000
30	C	0.58151063	-0.95291725	0.97398540	-0.0038	0.0000
31	C	2.27496327	1.79663460	3.06602036	-0.1111	0.0000
32	H	2.48313272	1.62345657	4.13079461	0.0385	0.0000
33	H	3.24990593	1.91239898	2.56260073	0.0378	0.0000
34	H	1.76896776	2.77227629	2.99073274	0.0352	0.0000
35	C	1.01739440	-0.62410220	4.67094215	-0.1106	0.0000
36	H	1.54030692	-1.55946984	4.93082734	0.0405	0.0000
37	H	1.50906796	0.19522396	5.21106214	0.0398	0.0000
38	H	-0.00520495	-0.71661016	5.07381263	0.0421	0.0000
39	C	-0.06092244	-2.74200122	2.70308133	-0.1111	0.0000

40	H	0.74846844	-3.35219176	3.13943375	0.0411	0.0000
41	H	-0.83226055	-2.64206074	3.48411617	0.0407	0.0000
42	H	-0.49566545	-3.31681637	1.87452194	0.0404	0.0000
43	C	0.44781839	-1.78459586	-0.27052369	-0.1128	0.0000
44	H	1.39117868	-2.31948445	-0.48180907	0.0392	0.0000
45	H	-0.33731817	-2.54855028	-0.17377566	0.0384	0.0000
46	H	0.22300365	-1.17778099	-1.15726862	0.0326	0.0000
47	C	2.52673602	0.36187202	0.18085009	-0.1114	0.0000
48	H	3.11904763	-0.49293318	0.54133538	0.0344	0.0000
49	H	2.32331171	0.21234698	-0.88926570	0.0328	0.0000
50	H	3.14299398	1.26401101	0.28168460	0.0318	0.0000

(Cp*)$^{\bullet}$; S = 1/2
E = -65.673201, ZPVE = 0.210369

# / Atom		Coordinates			q	s
1	C	-15.69390697	-3.41454736	1.61919383	0.0055	0.2485
2	C	-17.88248086	-3.38846431	0.83360470	-0.0370	0.0314
3	C	-17.01276941	-4.11177199	1.62464604	-0.0083	0.1791
4	C	-15.79801653	-2.27875010	0.82145566	-0.0435	-0.0027
5	C	-17.14493316	-2.24008165	0.32177776	0.0300	0.3644
6	C	-14.50322268	-3.91139720	2.37169352	-0.1102	0.0229
7	H	-14.20769571	-4.92289781	2.04189210	0.0433	0.0171
8	H	-13.63202635	-3.25380795	2.25186588	0.0419	0.0014
9	H	-14.71382326	-3.99380494	3.45244591	0.0432	0.0169
10	C	-17.27280155	-5.37213708	2.38624384	-0.1115	0.0160
11	H	-17.12718603	-5.23016570	3.47161146	0.0410	0.0123
12	H	-18.29726802	-5.73867975	2.23626918	0.0411	0.0008
13	H	-16.58271314	-6.18006304	2.08726706	0.0409	0.0116
14	C	-19.32275771	-3.66935609	0.52122665	-0.1141	0.0011
15	H	-19.49520828	-3.79099765	-0.56210407	0.0364	0.0004
16	H	-19.67195329	-4.58896103	1.01085330	0.0388	-0.0006
17	H	-19.98516911	-2.85166559	0.85418175	0.0364	0.0004
18	C	-17.72249252	-1.20023371	-0.57910634	-0.1077	0.0338
19	H	-18.59031567	-0.70232781	-0.11138653	0.0472	0.0246
20	H	-16.99100633	-0.42557146	-0.84406081	0.0438	0.0026
21	H	-18.10159803	-1.64545738	-1.51590514	0.0472	0.0245
22	C	-14.73397296	-1.26391885	0.50999135	-0.1150	-0.0016
23	H	-14.52572924	-1.19861027	-0.57159057	0.0352	-0.0021
24	H	-15.01484795	-0.24973328	0.84075782	0.0352	-0.0022
25	H	-13.78442015	-1.51234107	1.00411411	0.0379	-0.0007

The complex {ClSn^{IV}(Pc$^{\bullet 3-}$)}$^{\bullet}$; S = 1/2
E = -289.120104, ZPVE = 0.401028

# / Atom		Coordinates			q	s
1	Sn	7.44177336	14.39488484	14.99113043	0.3641	0.6085
2	Cl	8.49966162	12.38388475	16.17460404	-0.3702	-0.0037
3	N	8.68357543	13.76930999	13.40449656	-0.1207	0.0704
4	N	7.15214084	12.16485507	12.38637268	-0.1436	0.0048
5	N	6.01971507	12.95303337	14.39977044	-0.1207	0.0706
6	N	4.54742422	13.11241949	16.33961803	-0.1436	0.0052

7	N	6.42408494	14.59473347	16.82857896	-0.1208	0.0709
8	N	8.08750873	15.94903362	17.99303009	-0.1436	0.0052
9	N	9.08820578	15.41079412	15.83283568	-0.1207	0.0707
10	N	10.69371759	14.99810425	14.04158793	-0.1435	0.0048
11	C	9.98426032	14.18980669	13.24234643	0.1067	0.0070
12	C	10.48785751	13.52508891	12.03696034	-0.0101	0.0023
13	C	9.44434016	12.69037807	11.54916067	-0.0101	0.0023
14	C	8.30416811	12.84565875	12.45707526	0.1067	0.0070
15	C	6.14162711	12.18159946	13.26613270	0.1069	0.0068
16	C	4.96212049	11.31228531	13.22729013	-0.0101	0.0023
17	C	4.19457460	11.59152662	14.39195775	-0.0100	0.0022
18	C	4.90570225	12.63130824	15.14133629	0.1067	0.0070
19	C	5.23509252	13.96241939	17.11423054	0.1068	0.0068
20	C	4.87843525	14.34837038	18.48250459	-0.0100	0.0022
21	C	5.92131424	15.18409420	18.96966919	-0.0100	0.0022
22	C	6.91443629	15.30822975	17.89884662	0.1068	0.0068
23	C	9.07671805	15.97273651	17.08933786	0.1068	0.0070
24	C	10.40253296	16.56427570	17.29127886	-0.0101	0.0022
25	C	11.17064523	16.28381042	16.12726967	-0.0101	0.0023
26	C	10.31342736	15.52138107	15.21497454	0.1069	0.0067
27	C	11.72804042	13.57560485	11.39287994	-0.0318	0.0014
28	H	12.52726367	14.21054622	11.77647753	0.0526	0.0001
29	C	11.90483917	12.78661337	10.25013716	-0.0366	0.0008
30	H	12.86090779	12.80755763	9.72457528	0.0532	0.0002
31	C	10.87107079	11.95974367	9.76684301	-0.0366	0.0008
32	H	11.04461933	11.35473838	8.87545180	0.0532	0.0002
33	C	9.63038955	11.89776949	10.41222312	-0.0318	0.0014
34	H	8.82993901	11.25305329	10.04797566	0.0526	0.0001
35	C	4.55328779	10.33495808	12.31452398	-0.0318	0.0014
36	H	5.15032838	10.11902221	11.42797339	0.0526	0.0001
37	C	3.36233025	9.64877156	12.57978770	-0.0366	0.0008
38	H	3.01640476	8.88264323	11.88401206	0.0532	0.0002
39	C	2.60199987	9.92528679	13.73366668	-0.0365	0.0007
40	H	1.68055775	9.36840891	13.91132345	0.0532	0.0002
41	C	3.01042071	10.89607647	14.65581950	-0.0318	0.0015
42	H	2.43086224	11.10790087	15.55487346	0.0526	0.0001
43	C	3.78646490	14.01688334	19.29071741	-0.0317	0.0014
44	H	2.99440278	13.36845054	18.91491696	0.0526	0.0001
45	C	3.74949121	14.54081284	20.58827921	-0.0365	0.0007
46	H	2.90838507	14.30200153	21.24114116	0.0532	0.0002
47	C	4.78274039	15.36872627	21.07098425	-0.0365	0.0007
48	H	4.72369425	15.75657349	22.08922568	0.0532	0.0002
49	C	5.88299028	15.69682735	20.27014028	-0.0318	0.0014
50	H	6.68987711	16.32943275	20.64134596	0.0526	0.0001
51	C	10.95801128	17.26334575	18.36747408	-0.0318	0.0015
52	H	10.36721237	17.46766211	19.26092929	0.0526	0.0001
53	C	12.28841593	17.68472927	18.25766556	-0.0365	0.0007
54	H	12.74804071	18.23507121	19.08021634	0.0532	0.0002
55	C	13.04937112	17.40690196	17.10452234	-0.0366	0.0008
56	H	14.08504249	17.74686995	17.05421655	0.0532	0.0002

57	C	12.50205206	16.69960978	16.02758776	-0.0318	0.0013
58	H	13.08881636	16.47390957	15.13662074	0.0526	0.0001

The complex ($Cp^*Cr^{III}Cl_2$){$Sn^{IV}Cl(Pc^{\bullet 3-})$} (**III**); $S = 1$
E = -471.487989, ZPVE = 0.619570

# / Atom		Coordinates			q	s
1	Sn	7.25650344	9.38878720	4.06665179	0.6019	-0.0026
2	Cr	3.28202156	10.63121954	5.40709164	0.1600	2.8478
3	Cl	4.57450013	10.48055432	7.28535450	-0.2490	0.0891
4	Cl	4.86585368	8.94871326	4.08781291	-0.0740	0.0312
5	Cl	4.26881723	12.40937376	4.37037265	-0.2493	0.0892
6	N	7.61752735	11.12923037	2.98156124	-0.1278	0.0007
7	N	7.46848219	10.21187748	0.70587556	-0.1542	-0.0347
8	N	7.69482083	8.37159736	2.29785299	-0.1461	-0.0440
9	N	7.88524657	6.09543042	3.16854646	-0.1568	-0.0423
10	N	7.95895084	7.68094450	5.04532099	-0.1315	0.0005
11	N	8.20712995	8.60308967	7.30889954	-0.1503	-0.0379
12	N	7.92020130	10.44019976	5.72272488	-0.1380	-0.0403
13	N	7.87566562	12.71718711	4.83775221	-0.1464	-0.0379
14	C	1.35229775	10.79931908	6.48423678	0.0018	-0.0268
15	C	1.57061940	9.40416718	6.21494409	-0.0054	0.0034
16	C	1.59706214	9.23445540	4.79060627	-0.0010	-0.0332
17	C	1.40083355	10.52057163	4.17409177	-0.0071	0.0047
18	C	1.23556956	11.48584252	5.22254407	0.0031	-0.0278
19	C	1.20076857	11.41289630	7.84394952	-0.1011	0.0004
20	H	0.14870083	11.35334215	8.17168442	0.0466	-0.0030
21	H	1.49308330	12.47093646	7.84687285	0.0507	-0.0002
22	H	1.82086072	10.89466367	8.58600155	0.0455	-0.0003
23	C	1.69981766	8.32797132	7.25211380	-0.1039	0.0028
24	H	2.34087557	8.65552422	8.08222764	0.0430	0.0010
25	H	2.14004584	7.41312874	6.83457366	0.0460	0.0005
26	H	0.71113435	8.06654106	7.66511096	0.0452	-0.0001
27	C	1.71457278	7.92336705	4.06900510	-0.1062	-0.0011
28	H	2.34190629	7.20580204	4.61391453	0.0433	-0.0009
29	H	2.13447782	8.04125251	3.06175067	0.0414	-0.0006
30	H	0.71508160	7.46971903	3.95777142	0.0499	-0.0041
31	C	1.33323145	10.81191095	2.70322199	-0.1030	0.0034
32	H	0.28547338	10.89912857	2.36980702	0.0455	0.0005
33	H	1.80650672	10.01859672	2.10985869	0.0452	0.0006
34	H	1.84479270	11.75443608	2.46414323	0.0453	0.0009
35	C	0.93322679	12.94174371	5.03374817	-0.1024	-0.0004
36	H	1.30982560	13.54711290	5.86816254	0.0496	-0.0003
37	H	-0.15801929	13.09386312	4.97134724	0.0462	-0.0035
38	H	1.38755183	13.32921663	4.11362775	0.0444	-0.0002
39	C	7.72730716	12.40437723	3.53936455	0.0860	-0.0814
40	C	7.70779632	13.35341384	2.46020604	-0.0157	-0.0269
41	C	7.58352179	12.61902387	1.24519265	-0.0169	-0.0240
42	C	7.53310080	11.22413780	1.58776880	0.0807	-0.0911
43	C	7.55141904	8.93712253	1.01858466	0.0897	-0.0286
44	C	7.53930314	7.84144490	0.05649938	-0.0136	-0.0030

45	C	7.66543475	6.63302014	0.77979900	-0.0140	-0.0049
46	C	7.75453114	6.97095724	2.19610253	0.0900	-0.0200
47	C	8.00557263	6.40735702	4.47212879	0.0771	-0.0812
48	C	8.24023263	5.46353397	5.53038757	-0.0197	-0.0262
49	C	8.33173321	6.20089025	6.74799398	-0.0187	-0.0259
50	C	8.15179449	7.58961523	6.42526385	0.0816	-0.0831
51	C	8.11782154	9.87449220	6.99701891	0.0975	-0.0250
52	C	8.27744248	10.97561220	7.94021663	-0.0098	-0.0048
53	C	8.18382012	12.18246316	7.21395567	-0.0083	-0.0047
54	C	7.96151327	11.84389416	5.81267391	0.1023	-0.0246
55	C	7.79829989	14.75691415	2.44913307	-0.0332	-0.0137
56	H	7.88735240	15.31175488	3.38341714	0.0517	-0.0010
57	C	7.75744957	15.40154006	1.21617852	-0.0425	-0.0213
58	H	7.81707170	16.49039405	1.17449416	0.0498	-0.0017
59	C	7.63681069	14.67065222	0.00604627	-0.0427	-0.0168
60	H	7.60797235	15.21341493	-0.94038206	0.0493	-0.0013
61	C	7.55303582	13.28122839	0.00403045	-0.0380	-0.0174
62	H	7.46083698	12.71541104	-0.92352955	0.0485	-0.0012
63	C	7.44346585	7.84028704	-1.34060610	-0.0340	-0.0047
64	H	7.34897071	8.77701405	-1.89071391	0.0517	-0.0002
65	C	7.47021010	6.60458745	-1.99450270	-0.0391	-0.0027
66	H	7.39342696	6.56932948	-3.08248257	0.0519	-0.0002
67	C	7.59622938	5.39866868	-1.27259105	-0.0395	-0.0053
68	H	7.61480996	4.45185773	-1.81487671	0.0518	-0.0004
69	C	7.69871121	5.39737327	0.12196401	-0.0342	-0.0025
70	H	7.79922609	4.47050755	0.68750139	0.0513	-0.0000
71	C	8.39196107	4.06420739	5.52360045	-0.0392	-0.0145
72	H	8.32495519	3.50503661	4.58979494	0.0484	-0.0011
73	C	8.62396014	3.42818966	6.73958620	-0.0445	-0.0188
74	H	8.74042693	2.34339523	6.76689756	0.0490	-0.0015
75	C	8.71413770	4.16205020	7.95111248	-0.0443	-0.0187
76	H	8.89751553	3.62566821	8.88367132	0.0493	-0.0015
77	C	8.57435258	5.54654543	7.97019447	-0.0372	-0.0146
78	H	8.64420472	6.11609467	8.89742239	0.0501	-0.0011
79	C	8.50684821	10.97800365	9.32012492	-0.0299	-0.0035
80	H	8.57499008	10.04110003	9.87343315	0.0527	-0.0001
81	C	8.62965709	12.21775637	9.95598170	-0.0361	-0.0046
82	H	8.79900682	12.25561338	11.03336588	0.0523	-0.0004
83	C	8.53406501	13.42346885	9.23071013	-0.0361	-0.0046
84	H	8.63058193	14.37313897	9.75947853	0.0524	-0.0003
85	C	8.31358927	13.42183448	7.84940634	-0.0282	-0.0034
86	H	8.23357096	14.34813031	7.28014317	0.0541	-0.0000

The complex $(Cp^*Cr^{III}Cl_2)\{Sn^{IV}Cl(Pc^{\bullet 3-})\}$ (**III**); $S = 1$
Optimization at fixed Sn(1)-Cl(4) distance equal to 2.393 A
E = -471.486207, ZPVE = 0.619782

# / Atom		Coordinates			q	s
1	Sn	7.16399338	9.56186477	4.09852949	0.6036	0.0052
2	Cr	3.36626804	10.25582152	5.43582085	0.1403	2.8033
3	Cl	4.60957829	9.42083733	7.18154855	-0.2499	0.0872

4	Cl	4.74134935	9.17565493	3.80216221	-0.0442	0.0464
5	Cl	4.46769713	12.25475300	5.15975178	-0.2490	0.0863
6	N	7.60012995	11.23544552	2.93129583	-0.1279	0.0024
7	N	7.47503524	10.20801115	0.70166899	-0.1560	-0.0394
8	N	7.62810424	8.44640921	2.38903552	-0.1472	-0.0438
9	N	7.71444360	6.21169514	3.37556941	-0.1560	-0.0394
10	N	7.80011354	7.88808249	5.17130047	-0.1283	0.0022
11	N	8.09711724	8.91530319	7.38224745	-0.1474	-0.0365
12	N	7.84642282	10.67579790	5.70485505	-0.1352	-0.0381
13	N	7.86942056	12.90826323	4.70962834	-0.1473	-0.0363
14	C	1.44132632	10.20491681	6.56894126	0.0010	-0.0185
15	C	1.55600849	8.97292027	5.83325249	-0.0063	0.0018
16	C	1.56934038	9.29838895	4.43636120	-0.0030	-0.0312
17	C	1.48084346	10.72904622	4.30301164	-0.0089	0.0055
18	C	1.38273731	11.28537034	5.62386350	0.0029	-0.0239
19	C	1.33128474	10.31993371	8.05980810	-0.1024	0.0009
20	H	0.28271922	10.18481701	8.37583400	0.0456	-0.0021
21	H	1.66519382	11.30284844	8.41634110	0.0496	0.0000
22	H	1.94159131	9.55950628	8.56354756	0.0438	0.0000
23	C	1.59507315	7.60101231	6.43945652	-0.1043	0.0028
24	H	2.25631656	7.57666602	7.31667437	0.0424	0.0008
25	H	1.96244566	6.85180181	5.72601497	0.0454	0.0005
26	H	0.58706242	7.29067051	6.76227327	0.0449	-0.0001
27	C	1.58794640	8.31017290	3.30592134	-0.1062	-0.0012
28	H	2.14345090	7.39864295	3.56344659	0.0435	-0.0008
29	H	2.03531536	8.73116334	2.39590994	0.0415	-0.0006
30	H	0.55683161	8.00867917	3.05581406	0.0494	-0.0040
31	C	1.43663625	11.51189303	3.02283692	-0.1032	0.0036
32	H	0.39825766	11.77751920	2.76207628	0.0453	0.0008
33	H	1.85429665	10.94149036	2.18263969	0.0446	0.0005
34	H	2.01203777	12.44391114	3.10942541	0.0454	0.0008
35	C	1.19192798	12.73611473	5.94831073	-0.1037	-0.0003
36	H	1.59872644	12.98866062	6.93580039	0.0485	-0.0003
37	H	0.11636911	12.98296034	5.95160587	0.0453	-0.0030
38	H	1.68989510	13.38028040	5.21314875	0.0430	-0.0001
39	C	7.73283252	12.53503059	3.42652920	0.0843	-0.0804
40	C	7.75407651	13.42855287	2.30129434	-0.0167	-0.0266
41	C	7.63354208	12.63610718	1.12235415	-0.0181	-0.0247
42	C	7.54491181	11.26203969	1.53389308	0.0788	-0.0868
43	C	7.52280321	8.94949651	1.08094257	0.0887	-0.0238
44	C	7.49577784	7.80767564	0.17389784	-0.0141	-0.0038
45	C	7.56662705	6.63419083	0.95916769	-0.0141	-0.0038
46	C	7.63771769	7.04132135	2.35784682	0.0887	-0.0239
47	C	7.82289476	6.58533602	4.66288789	0.0785	-0.0867
48	C	8.03903974	5.69200829	5.76771122	-0.0182	-0.0247
49	C	8.15458276	6.48807149	6.94474478	-0.0168	-0.0266
50	C	8.00354711	7.86250443	6.55301348	0.0845	-0.0802
51	C	8.02463666	10.16976983	7.00750488	0.0993	-0.0253
52	C	8.19295632	11.31278942	7.89751415	-0.0079	-0.0048
53	C	8.12679007	12.48455615	7.11307427	-0.0078	-0.0048

54	C	7.91606866	12.08256397	5.72711164	0.0994	-0.0254
55	C	7.87909314	14.82757228	2.22044452	-0.0349	-0.0136
56	H	7.96890875	15.42711129	3.12672227	0.0511	-0.0010
57	C	7.87536761	15.40928208	0.95607564	-0.0435	-0.0206
58	H	7.96368717	16.49279586	0.86055592	0.0496	-0.0016
59	C	7.75841038	14.62058455	-0.21792239	-0.0435	-0.0171
60	H	7.76035952	15.11487307	-1.19096283	0.0492	-0.0014
61	C	7.64169565	13.23527379	-0.15117753	-0.0388	-0.0164
62	H	7.55425078	12.62503927	-1.05064784	0.0484	-0.0012
63	C	7.42805463	7.73925747	-1.22313136	-0.0342	-0.0034
64	H	7.37612464	8.64963434	-1.82108135	0.0515	-0.0001
65	C	7.42661927	6.47188900	-1.81400718	-0.0394	-0.0038
66	H	7.37091081	6.38406266	-2.90030313	0.0519	-0.0003
67	C	7.49735131	5.30061691	-1.03007328	-0.0394	-0.0038
68	H	7.49508415	4.32751777	-1.52399356	0.0518	-0.0003
69	C	7.57133786	5.36631610	0.36469156	-0.0342	-0.0034
70	H	7.62869512	4.46643918	0.97783230	0.0515	-0.0001
71	C	8.16207760	4.29140546	5.83144959	-0.0388	-0.0164
72	H	8.07775083	3.68662116	4.92799963	0.0484	-0.0012
73	C	8.38699754	3.71388119	7.07767103	-0.0436	-0.0171
74	H	8.47960595	2.62956296	7.16022104	0.0492	-0.0013
75	C	8.49903846	4.50647024	8.24950183	-0.0435	-0.0206
76	H	8.67436119	4.01461443	9.20776182	0.0496	-0.0016
77	C	8.38944724	5.89298699	8.19779544	-0.0349	-0.0135
78	H	8.47469327	6.50822759	9.09393458	0.0511	-0.0010
79	C	8.40453192	11.37782130	9.27886016	-0.0290	-0.0037
80	H	8.44984231	10.46726706	9.87668492	0.0536	-0.0001
81	C	8.54086386	12.64461499	9.85621220	-0.0363	-0.0049
82	H	8.69761309	12.73152388	10.93264969	0.0524	-0.0004
83	C	8.47470481	13.81530193	9.07250150	-0.0364	-0.0049
84	H	8.58146422	14.78767273	9.55617052	0.0523	-0.0004
85	C	8.27040580	13.75084311	7.69019270	-0.0290	-0.0037
86	H	8.21351142	14.64987634	7.07614702	0.0535	-0.0001

IR- spectra.

Table S2. IR-spectra (cm^{-1} in KBr) of starting compounds and complex **1**.

Components	Cp^*_2Co	$Sn^{IV}Cl_2(Pc^{2-})$	$(Cp^*_2Co^+)\{Sn^{IV}Cl_2(Pc^{\bullet 3-})\}^{\bullet -}\cdot 2C_6H_4Cl_2$ (**1**)
Cp*Co	445w		436w*
	717w		-
	1024s		1021m
	1078m		1091s*
	1260w		1262w
	1314m		1319s*
	1376s		1381m
	1425m		1434m
	1452m		1457s*
	1474m		-
	1612s		1615w
	2850w		-
	2904w		2919w
	2960w		2965w
$Sn^{IV}Cl_2Pc$		434w	436w*
		444w	-
		497m	494w
		573m	572w
		723s	705s
		749m	745s*
		779m	767m
		890m	888w
		960w	948w
		1059m	1051m
		1084s	1091s*
		1120s	1118s
		1171w	1171m
		1288m	1286m
		1339s	1319s*
		1409w	1414m
		1467m	1457s*
		1605w	-
		3051w	3056w
$C_6H_4Cl_2$			658w
			745s*
			1033m
			1457s*

* Bands are overlapped, w - weak intensity, m – middle intensity, s – strong intensity.

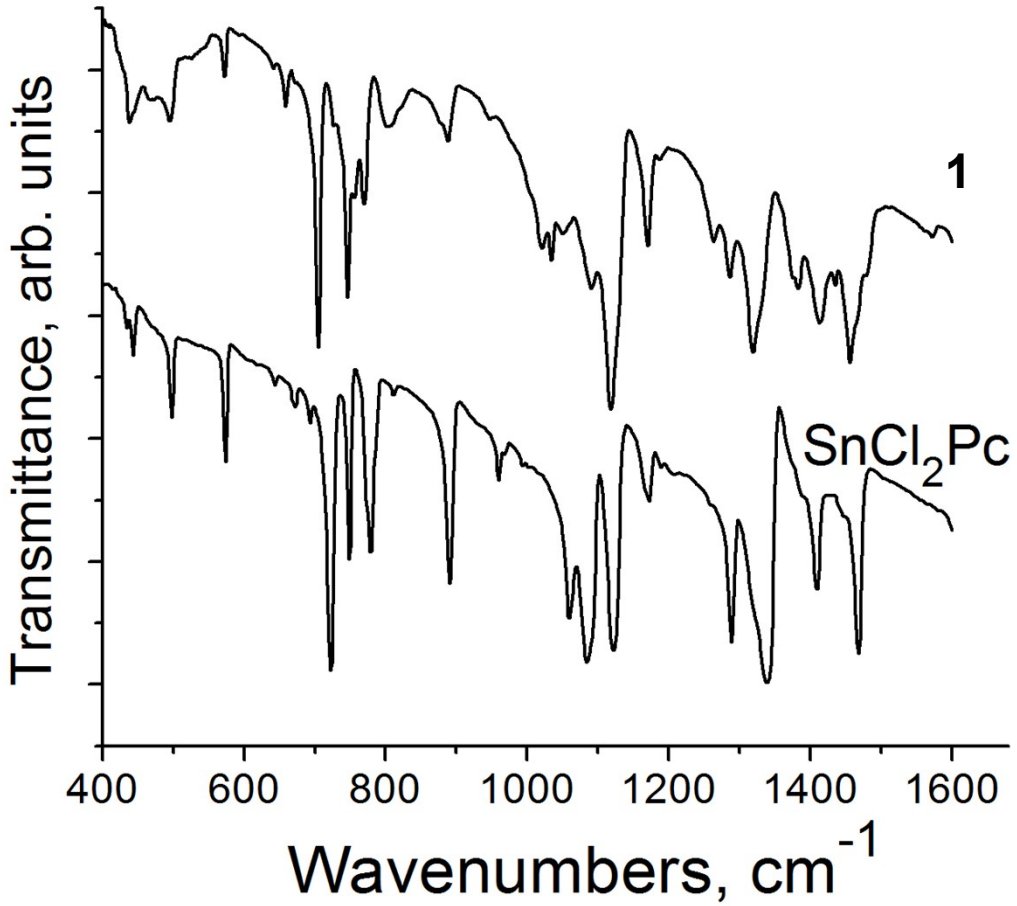

Fig. S4. IR spectrum of starting $Sn^{IV}Cl_2(Pc^{2-})$ and complex $(Cp^*_2Co^+)\{Sn^{IV}Cl_2(Pc^{\bullet 3-})\}\cdot 2C_6H_4Cl_2$ (**1**) measure in KBr pellets. The pellet for **1** was prepared in anaerobic conditions.

Crystal structure of complex **2**.

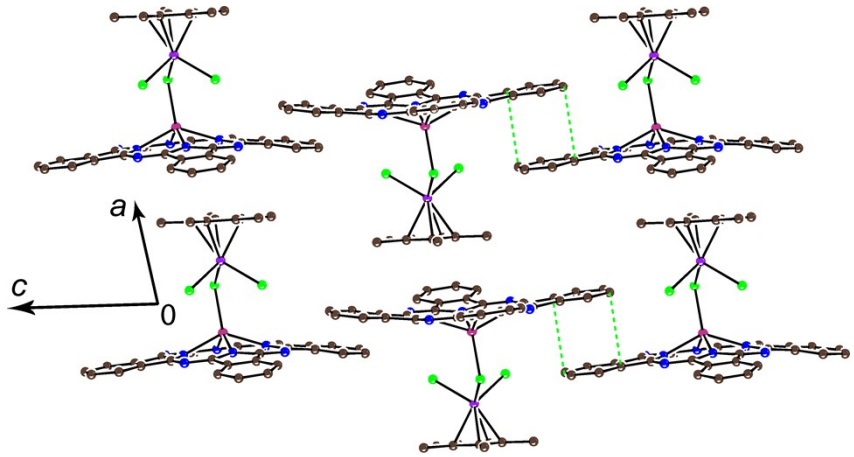

Fig. S5. View along the *b* axis on the packing of the coordination **{**$(Cp^*Cr^{II}Cl_2)^-(Sn^{IV}Cl(Pc^{2-})^+$**}** units in **2**. Short van der Waals C···C contacts between the Pc planes are shown by green dashed lines. Solvent $C_6H_4Cl_2$ molecules are not shown.

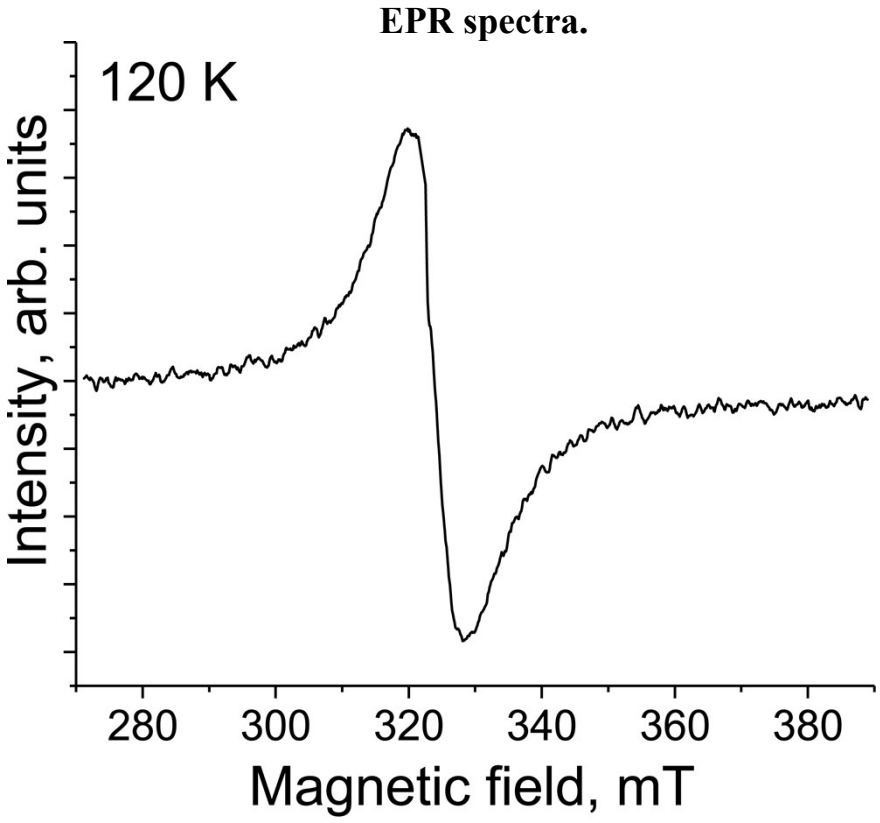

Fig. S6. EPR spectrum of polycrystalline **1** at 120 K.

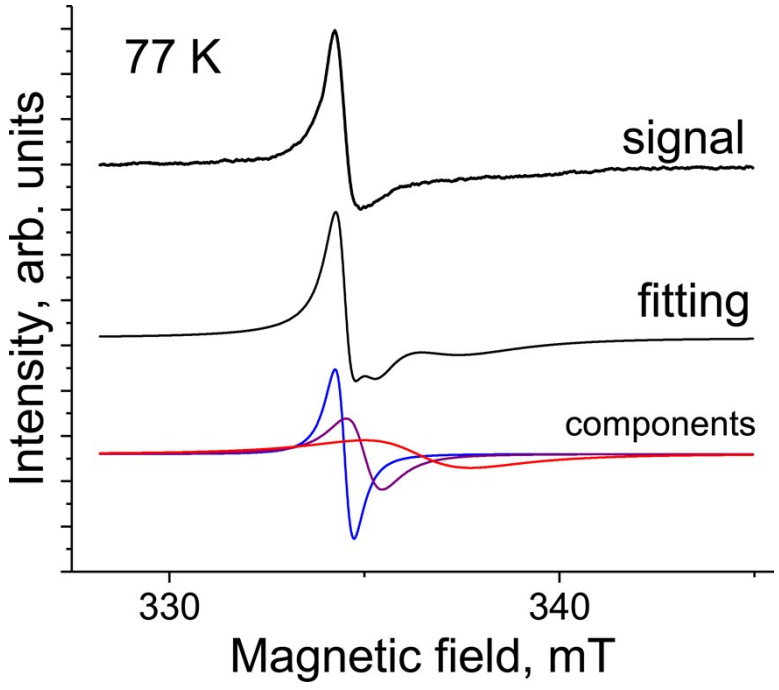

Fig. S7. EPR spectrum of $Sn^{IV}Cl_2Pc$ (14.2 mg) by one equivalent of Cp^*_2Co (7 mg) in *o*-dichlorobenzene (10 mL) in anaerobic conditions. The fitting of the spectrum by three Lorentzian lines is shown below: g_1 = 2.0050 and the linewidth (ΔH) of 0.482 mT (blue curve); g_2 = 2.0021 and ΔH = 0.924 mT (violet curve) and g_3 =1.9942 and ΔH = 2.704 mT (red curve).