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Easy Activation of the Aryl-Sulfur Bond by Platinum(II)

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Supporting Information

Experimental

Reagents and General Procedures. All reactions were carried out in an inert atmosphere of dry nitrogen using standard Schlenk techniques, unless otherwise specified. NMR spectra were recorded at ambient temperature, unless otherwise noted (ca. 25°C), on Varian Mercury 400 or Varian Inova 600 spectrometers. ^{1}H chemical shifts are reported relative to TMS (^{1}H). Complete assignment of each compound was aided by the use of ^{1}H-^{1}H NOESY and ^{1}H-^{1}H gCOSY experiments. Commonly practiced labeling schemes for pyridyl rings are utilized when labeling signals in NMR analysis. Elemental analyses were performed by Laboratoire d'Analyse Élémentaire de l'Université de Montréal. The complex $[Pt_2Me_4(\mu\text{-}SMe_2)_2]$ was prepared from $K_2[PtCl_4]$ according to the literature.[1] Mass spectrometric analysis was carried out using an electrospray PE-Sciex Mass Spectrometer (ESI-MS) coupled with a TOF detector.

X-ray Crystallography. A suitable crystal of each compound was coated in Paratone oil and mounted on a glass fibre loop. X-ray data for compounds **1**, **2** were collected at 150K with ω and φ scans on a Bruker Smart Apex II diffractometer using graphite-monochromated $Mo_{K\alpha}$ radiation (λ = 0.71073 Å) and Bruker SMART software.[4] Unit cell parameters were calculated and refined from the full data set. Cell refinement and data reduction were performed using the Bruker APEX2 and SAINT programs respectively.[5] Reflections were scaled and corrected for absorption effects using SADABS.[6] All structures were solved by either Patterson or direct methods with SHELXS[7] and refined by full-matrix least-squares techniques against F^2 using SHELXL.[8] All non-hydrogen atoms were refined anisotropically. The hydrogen atoms were placed in calculated positions and refined using the riding model.

DFT Calculations

DFT calculations were carried out by using the Amsterdam Density Functional program based on the BLYP functional, with double-zeta basis set and first-order scalar relativistic

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corrections.[7] The reported results are from gas phase calculations. The energy minima were confirmed by vibrational frequency analysis in each case

(*E*)-*N*^{1},*N*^{1}-dimethyl-*N*^{2}-(2-(methylthio)benzylidene)ethane-1,2-diamine, ***NNS***

To a solution of 2-(methylthio)benzaldehyde (1.99g, 13.1mmol) in CH_2Cl_2 (10mL) was added an equimolar amount of $Me_2NCH_2CH_2NH_2$ (1.16g, 13.1mmol). The reaction mixture was allowed to stir for 12h., then the solvent was removed under reduced pressure. The resultant oil was extracted with hot hexanes and filtered to remove insoluble byproducts. Upon cooling the solvent to room temperature, the solvent was again removed *in vacuo* yielding the product as a colourless oil. Yield, 2.65g, 91%. NMR in acetone-d_6: δ(^{1}H) 2.22 (s, 6H, MeN); 2.48 (s, 3H, MeS); 2.66 (t, 2H, J = 7 Hz,CH_2); 3.71 (t, 2H, J = 7 Hz,CH_2); 7.22-7.87 (m, 4H, C_6H_4); 8.74 (s, 1H, CH=N). EI-MS: *m/z* 222.1199; calc. for $C_{12}H_{18}N_2S$: m/z = 222.1191.

(*E*)-*N*-(2-(methylthio)benzylidene)aniline, *NS*

To a solution of 2-(methylthio)benzaldehyde (0.50 g, 3.3 mmol) in toluene (10 mL) was added an equimolar amount of aniline (0.31g, 3.3mmol). The reaction mixture was allowed to stir under reflux for 24 h. The solvent was then removed under reduced pressure yielding the product as an oil. Yield, 0.71g, 95%. NMR in acetone-d_6: δ(^{1}H) 2.53 (s, 3H, MeS); 7.24-8.08 (m, 9H, Ph and C_6H_4); 8.96 (s, 1H, CH=N). EI-MS: *m/z* 227.0762; calc. for $C_{14}H_{13}NS$: m/z = 227.0769.

[{Pt(μ-SMe)Me$_2$(κ^2-*C*,*N*-C$_6$H$_4$-2-CH=NCH$_2$CH$_2$NMe$_2$)}$_2$], 6

To a solution of ***NNS*** (15.9 mg, 0.072 mmol) in acetone-d_6 (0.5 mL) was added a solution of $[Pt_2Me_4(\mu\text{-}SMe_2)_2]$ (14.0 mg, 0.024 mmol) in acetone-d_6 (0.5 mL). The ^{1}H NMR spectrum

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indicated formation of 3 isomers of complex **6**. After allowing the NMR tube to stand for 2 days, a yellow crystalline solid product was formed, and was determined to be complex **6a**. ESI-MS: *m/z* = 895.3; calc. for $C_{28}H_{49}N_4Pt_2S_2$ (M + H^+): m/z = 895.3. Anal. Calc. for $C_{28}H_{48}N_4Pt_2S_2$: C, 37.58; H, 5.41; N, 6.26. Found: C, 37.29; H, 5.22; N, 6.01%. The crystals were not soluble in acetone, so NMR data were obtained in $CDCl_3$. In a similar experiment, the reagents were mixed at -30°C and ^{1}H NMR spectra were recorded at -20, -10, 0, 10 and 20°C.

3a: NMR in acetone-d_6: δ(^{1}H) = 0.27 [s, 3H, ^2J(PtH) = 85 Hz, MePt]; 0.33 [s, 3H, ^2J(PtH) = 85 Hz, MePt]; 2.23 [s, 6H, Me_2N]; 2.66 [s, 3H, ^3J(PtH) = 24 Hz, MeS]; 8.55 [s, 1H, ^3J(PtH) = 36 Hz, N=CH].

4a: NMR in acetone-d_6: δ(^{1}H) = 0.37 [s, 3H, ^2J(PtH) = 85 Hz, MePt]; 0.54 [s, 3H, ^2J(PtH) = 86 Hz, MePt]; 1.96 [s, 6H, ^3J(PtH) = 22 Hz, Me_2S]; 2.24 [s, 6H, Me_2N]; 2.50 [s, 3H, MeS]; 9.28 [s, 1H, ^3J(PtH) = 43 Hz, N=CH].

5: NMR in acetone-d_6: δ(^{1}H) = -0.12 [s, 3H, ^2J(PtH) = 91 Hz, MePt]; 0.53 [s, 3H, ^2J(PtH) = 85 Hz, MePt]; 2.52 [s, 3H, MeS]; 2.75 [s, 6H, ^3J(PtH) = 21 Hz, Me_2N]; 3.2, 4.1 [m, each 2H, CH_2CH_2]; 7.27, 7.45, 7.92, 9.99 [m, each 1H, C_6H_4]; 9.18 [s, 1H, ^3J(PtH) = 40 Hz, N=CH].

6a: NMR in $CDCl_3$: δ(^{1}H) = 0.30 [s, 6H, ^2J(PtH) = 65 Hz, MePt]; 1.23 [s, 6H, ^3J(PtH) = 20 Hz, MeS]; 1.51 [s, 6H, ^2J(PtH) = 70 Hz, MePt]; 2.31 [s, 12H, Me_2N]; 2.68, 2.77, 4.06, 4.80 [m, each 2H, CH_2CH_2]; 7.11 [t, 2H, ^3J(HH) = 7 Hz, H^5]; 7.25 [t, 2H, ^3J(HH) = 7 Hz, H^4]; 7.45 [d, 2H, ^3J(HH) = 7 Hz, H^6]; 7.52 [d, 2H, ^3J(HH) = 7 Hz, ^3J(PtH) = 39 Hz, H^3]; 8.65 [s, 2H, ^3J(PtH) = 46 Hz, N=CH].

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6c: NMR in $CDCl_3$: $\delta(^1H)$ = 0.36 [s, 6H, ^2J(PtH) = 66 Hz, MePt]; 0.87 [s, 3H, ^3J(PtH) = 20 Hz, MeS]; 1.49 [s, 6H, ^2J(PtH) = 70 Hz, MePt]; 2.51 [s, 3H, ^3J(PtH) = 20 Hz, MeS]; 2.27 [s, 12H, Me_2N]; 2.5-4.9 [m, 4H, CH_2CH_2]; 7.1-7.6[m, 8H, C_6H_4]; 8.76 [s, 2H, ^3J(PtH) = 46 Hz, N=CH].

6d: NMR in $CDCl_3$: $\delta(^1H)$ = 0.28 [s, 6H, ^2J(PtH) = 66 Hz, MePt]; 1.53 [s, 6H, ^2J(PtH) = 70 Hz, MePt]; 1.55 [s, 6H, ^3J(PtH) = 21 Hz, MeS]; 2.19 [s, 12H, Me_2N]; 2.5-4.9 [m, 4H, CH_2CH_2]; 7.1-7.6[m, 8H, C_6H_4]; 8.74 [s, 2H, ^3J(PtH) = 45 Hz, N=CH].

[{Pt(μ-SMe)Me_2(κ^2-*C*,*N*-C_6H_4-2-CH=NPh)}$_2$], 7

To a solution of ***NS*** (19.8 mg, 0.087 mmol) in acetone-d_6 (0.5 mL) was added a solution of [Pt_2Me_4(μ-SMe_2)$_2$] (24.8mg, 0.043mmol) in acetone-d_6 (0.5 mL). The ^{1}H NMR spectrum indicated formation of 4 isomers of complex **7**. The mixture was allowed to stand for 24 h., to give a yellow crystalline solid product, identified as a mixture of **7a** and **7b**. Anal. Calc. for $C_{32}H_{38}N_2Pt_2S_2$: C, 42.47; H, 4.23; N, 3.10. Found: C, 42.04; H, 4.11; N, 2.98%.The crystals were isolated, but were insoluble in acetone so NMR data were recorded using dmso-d_6 or $CDCl_3$. In a similar experiment, the reagents were mixed at -30^{o}C and ^{1}H NMR spectra were recorded at ten degree intervals at -20, -10, 0, 10 and 20^{o}C.

3b: NMR in acetone-d_6: $\delta(^1H)$ = 0.46 [s, 3H, ^2J(PtH) = 84 Hz, MePt]; 0.61 [s, 3H, ^2J(PtH) = 87 Hz, MePt]; 2.11 [s, 3H, ^3J(PtH) = 24 Hz, MeS]; 9.10 [s, 1H, ^3J(PtH) = 39 Hz, N=CH].

4b: NMR in acetone-d_6: $\delta(^1H)$ = 0.47 [s, 3H, ^2J(PtH) = 84 Hz, MePt]; 0.48 [s, 3H, ^2J(PtH) = 85 Hz, MePt]; 2.31 [s, 3H, MeS]; 2.33 [s, 6H, ^3J(PtH) = 18 Hz, Me_2S]; 9.51 [s, 1H, ^3J(PtH) = 40 Hz, N=CH].

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7a: NMR in dmso-d_6: δ(^{1}H) = 0.26 [s, 6H, ^2J(PtH) = 63 Hz, MePt]; 0.72 [s, 6H, ^2J(PtH) = 71 Hz, MePt]; 1.19 [s, 6H, ^3J(PtH) = 19 Hz, MeS]; 7.13 [d, 2H, ^3J(HH) = 7 Hz, H^5]; 7.14 [t, 2H, ^3J(HH) = 7 Hz, H^3]; 7.24 [t, 2H, ^3J(HH) = 7 Hz, H^4]; 7.42 [t, 2H, ^3J(HH) = 7 Hz, H^p]; 7.50 [d, 4H, ^3J(HH) = 7 Hz, H^o]; 7.55 [t, 4H, ^3J(HH) = 7 Hz, H^m]; 7.71 [d, 2H, ^3J(HH) = 7 Hz, H^6]; 8.99 [s, 2H, ^3J(PtH) = 34 Hz, N=CH].

7b: NMR in dmso-d_6: δ(^{1}H) = 0.37 [s, 6H, ^2J(PtH) = 64 Hz, MePt]; 0.86 [s, 3H, ^3J(PtH) = 20 Hz, MeS]; 0.88 [s, 6H, ^2J(PtH) = 70 Hz, MePt]; 1.42 [s, 3H, ^3J(PtH) = 19 Hz, MeS]; 7.09 [t, 2H, ^3J(HH) = 7 Hz, H^3]; 7.17 [d, 2H, ^3J(HH) = 7 Hz, H^5]; 7.21 [t, 2H, ^3J(HH) = 7 Hz, H^4]; 7.41 [t, 2H, ^3J(HH) = 7 Hz, H^p]; 7.49 [d, 4H, ^3J(HH) = 7 Hz, H^o]; 7.53 [t, 4H, ^3J(HH) = 7 Hz, H^m]; 7.65 [d, 2H, ^3J(HH) = 7 Hz, H^6]; 8.85 [s, 2H, ^3J(PtH) = 34 Hz, N=CH].

7c: NMR in acetone-d_6: δ(^{1}H) = 0.49 [s, 6H, ^2J(PtH) = 68 Hz, MePt]; 1.29 [s, 3H, ^3J(PtH) = 21 Hz, MeS]; 1.73 [s, 6H, ^2J(PtH) = 74 Hz, MePt]; 1.94 [s, 3H, ^3J(PtH) = 20 Hz, MeS]; 8.61 [s, 2H, ^3J(PtH) = 38 Hz, N=CH].

7d: NMR in acetone-d_6: δ(^{1}H) = 0.42 [s, 6H, ^2J(PtH) = 68 Hz, MePt]; 1.47 [s, 6H, ^3J(PtH) = 20 Hz, MeS]; 1.68 [s, 6H, ^2J(PtH) = 74 Hz, MePt]; 8.64 [s, 2H, ^3J(PtH) = 39 Hz, N=CH].

Selected data from the DFT calculations

DFT calculated structures

Complex **6a**

	Atom	Cartesian (a.u./angstrom) X	Y	Z
1	C	-1.008660000000	9.980520000000	5.342200000000
2	C	-1.286820000000	9.996880000000	6.723770000000
3	C	-1.116190000000	11.086100000000	3.147450000000
4	N	-0.601538000000	9.999040000000	2.624190000000
5	C	-1.906980000000	11.111500000000	7.324270000000
6	C	-2.267140000000	12.239900000000	6.557830000000
7	C	-2.006690000000	12.248800000000	5.181690000000

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8	S	-2.482790000000	7.217490000000	4.000070000000
9	C	-0.265319000000	9.965450000000	1.168810000000
10	N	1.585590000000	9.989170000000	-0.512187000000
11	C	1.272030000000	10.059200000000	0.941051000000
12	C	-3.755870000000	8.472640000000	3.253720000000
13	C	1.764770000000	9.303550000000	4.460290000000
14	Pt	-0.191976000000	8.457920000000	4.197640000000
15	C	0.227006000000	7.252660000000	5.891560000000
16	C	2.845750000000	9.254850000000	-0.814916000000
17	C	1.512410000000	11.302900000000	-1.205010000000
18	C	-1.384090000000	11.130600000000	4.575000000000
19	C	-0.942438000000	3.947020000000	1.106260000000
20	C	-0.642048000000	3.947050000000	-0.271246000000
21	C	-0.883190000000	2.806880000000	3.288240000000
22	N	-1.371460000000	3.900920000000	3.819340000000
23	C	-0.019529100000	2.836900000000	-0.876303000000
24	C	0.314597000000	1.693280000000	-0.120808000000
25	C	0.029223200000	1.667260000000	1.250400000000
26	S	0.543860000000	6.700300000000	2.467320000000
27	C	-1.773290000000	4.002340000000	5.256420000000
28	N	-2.011150000000	2.967110000000	7.522590000000
29	C	-1.694250000000	2.699120000000	6.089010000000
30	C	1.810080000000	5.436660000000	3.211980000000
31	C	-2.177330000000	6.669610000000	0.567929000000
32	Pt	-1.754540000000	5.465020000000	2.260660000000
33	C	-3.713920000000	4.616010000000	2.061350000000
34	C	-1.514730000000	1.882040000000	8.416440000000
35	C	-3.452240000000	3.264370000000	7.768430000000
36	C	-0.588413000000	2.784500000000	1.862840000000
37	H	-1.028710000000	9.141760000000	7.343140000000
38	H	-1.349730000000	11.955800000000	2.520620000000
39	H	-2.111860000000	11.099400000000	8.395300000000
40	H	-2.744640000000	13.096200000000	7.032190000000
41	H	-2.284400000000	13.112100000000	4.574920000000
42	H	-0.607491000000	9.014130000000	0.755684000000
43	H	-0.781940000000	10.789700000000	0.650900000000
44	H	1.666380000000	10.983200000000	1.412460000000
45	H	1.730720000000	9.198220000000	1.436260000000
46	H	-3.985840000000	9.185720000000	4.054000000000
47	H	-4.651970000000	7.911850000000	2.964320000000
48	H	-3.327540000000	8.993130000000	2.392450000000
49	H	2.050600000000	9.244500000000	5.518370000000
50	H	1.737630000000	10.354800000000	4.140740000000
51	H	2.466240000000	8.728230000000	3.840040000000
52	H	-0.720252000000	6.877170000000	6.300020000000
53	H	0.742374000000	7.863020000000	6.645960000000
54	H	0.875667000000	6.416570000000	5.601710000000
55	H	2.936010000000	9.140330000000	-1.905150000000
56	H	2.792680000000	8.253480000000	-0.367188000000
57	H	3.755470000000	9.774430000000	-0.438306000000
58	H	1.617590000000	11.145100000000	-2.288280000000
59	H	2.304150000000	12.012200000000	-0.869705000000
60	H	0.531017000000	11.763900000000	-1.027250000000
61	H	-0.879685000000	4.813860000000	-0.882599000000

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62	H	-0.697679000000	1.905620000000	3.878010000000
63	H	0.207658000000	2.863390000000	-1.942620000000
64	H	0.792243000000	0.839465000000	-0.599640000000
65	H	0.284851000000	0.791305000000	1.848450000000
66	H	-1.139180000000	4.759480000000	5.729340000000
67	H	-2.794520000000	4.399010000000	5.245210000000
68	H	-2.364850000000	1.923580000000	5.654680000000
69	H	-0.664935000000	2.314710000000	6.064200000000
70	H	2.712900000000	5.989660000000	3.495520000000
71	H	2.029310000000	4.718460000000	2.413420000000
72	H	1.382010000000	4.923180000000	4.077460000000
73	H	-2.736840000000	6.069980000000	-0.163788000000
74	H	-1.227190000000	7.001890000000	0.128886000000
75	H	-2.781830000000	7.535570000000	0.865091000000
76	H	-4.364240000000	5.116880000000	2.792820000000
77	H	-3.649800000000	3.538600000000	2.273270000000
78	H	-4.086630000000	4.773890000000	1.041240000000
79	H	-2.013230000000	0.903527000000	8.232530000000
80	H	-1.693030000000	2.174400000000	9.460790000000
81	H	-0.431470000000	1.762590000000	8.274290000000
82	H	-3.760050000000	4.147190000000	7.195090000000
83	H	-3.585920000000	3.495570000000	8.834570000000
84	H	-4.116770000000	2.410910000000	7.501950000000

#===END

Complex **6b**

Atom	Cartesian (a.u./angstrom)		
	X	Y	Z
1 C	-1.006170000000	9.882630000000	5.406170000000
2 C	-1.288640000000	9.834910000000	6.785750000000
3 C	-1.130710000000	11.079200000000	3.262060000000
4 N	-0.613781000000	10.016400000000	2.691980000000
5 C	-1.892650000000	10.927700000000	7.440480000000
6 C	-2.257220000000	12.089100000000	6.726180000000
7 C	-1.984710000000	12.165000000000	5.354120000000
8 S	-2.447270000000	7.193460000000	3.930450000000
9 C	-0.283259000000	10.052700000000	1.235550000000
10 N	1.550890000000	10.418700000000	-0.433798000000
11 C	1.217950000000	10.401300000000	1.014950000000
12 C	-3.743940000000	8.383070000000	3.110980000000
13 C	1.738820000000	9.405390000000	4.476490000000
14 Pt	-0.156538000000	8.425480000000	4.200270000000
15 C	0.314935000000	7.170270000000	5.836000000000
16 C	2.960050000000	10.027300000000	-0.717448000000

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17	C	1.170230000000	11.683100000000	-1.119690000000
18	C	-1.377330000000	11.068600000000	4.693330000000
19	C	-3.521150000000	4.602410000000	1.933130000000
20	C	-4.542520000000	4.950860000000	1.026150000000
21	C	-2.750990000000	3.224110000000	3.820680000000
22	N	-1.626750000000	3.894680000000	3.787090000000
23	C	-5.788140000000	4.290320000000	1.045090000000
24	C	-6.045700000000	3.257710000000	1.969220000000
25	C	-5.052710000000	2.899640000000	2.890570000000
26	S	0.603876000000	6.739590000000	2.412360000000
27	C	-0.494717000000	3.613120000000	4.720760000000
28	N	0.552434000000	2.259710000000	6.538820000000
29	C	-0.700651000000	2.474580000000	5.752300000000
30	C	2.095190000000	5.663050000000	3.031640000000
31	C	-1.904150000000	6.695040000000	0.464868000000
32	Pt	-1.643020000000	5.443510000000	2.161800000000
33	C	-0.783582000000	4.026170000000	0.793727000000
34	C	0.650932000000	0.873007000000	7.080410000000
35	C	0.758639000000	3.280190000000	7.608870000000
36	C	-3.800810000000	3.559870000000	2.872040000000
37	H	-1.045660000000	8.947190000000	7.363870000000
38	H	-1.371470000000	11.973400000000	2.673050000000
39	H	-2.106590000000	10.862100000000	8.507870000000
40	H	-2.729910000000	12.924800000000	7.240350000000
41	H	-2.262500000000	13.055100000000	4.787460000000
42	H	-0.467019000000	9.064490000000	0.812279000000
43	H	-0.928317000000	10.789800000000	0.731775000000
44	H	1.453170000000	11.366700000000	1.513250000000
45	H	1.812120000000	9.617050000000	1.494160000000
46	H	-4.371150000000	8.761220000000	3.927650000000
47	H	-4.345450000000	7.794540000000	2.408840000000
48	H	-3.238480000000	9.211460000000	2.604270000000
49	H	2.076730000000	9.268320000000	5.512610000000
50	H	1.607730000000	10.475900000000	4.266490000000
51	H	2.460620000000	8.958830000000	3.778020000000
52	H	-0.600696000000	6.654040000000	6.158150000000
53	H	0.708229000000	7.784190000000	6.658000000000
54	H	1.083790000000	6.448370000000	5.532980000000
55	H	3.095330000000	9.953760000000	-1.806250000000
56	H	3.152490000000	9.038500000000	-0.279924000000
57	H	3.703110000000	10.753000000000	-0.316946000000
58	H	1.351350000000	11.574000000000	-2.198660000000
59	H	1.744240000000	12.563700000000	-0.748764000000
60	H	0.098372100000	11.877900000000	-0.979275000000
61	H	-4.384150000000	5.735700000000	0.292268000000
62	H	-2.934920000000	2.431710000000	4.550200000000
63	H	-6.560690000000	4.583280000000	0.333480000000
64	H	-7.011350000000	2.754440000000	1.977400000000
65	H	-5.239140000000	2.109210000000	3.619120000000
66	H	0.376323000000	3.359190000000	4.105270000000
67	H	-0.285849000000	4.558040000000	5.229480000000
68	H	-1.566130000000	2.694560000000	6.413880000000
69	H	-0.907205000000	1.538440000000	5.215040000000
70	H	2.929100000000	6.349310000000	3.218910000000

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71 H	2.347530000000	4.973770000000	2.217590000000
72 H	1.850310000000	5.109920000000	3.941060000000
73 H	-2.425250000000	6.126410000000	-0.316449000000
74 H	-0.917166000000	6.996770000000	0.091264600000
75 H	-2.489910000000	7.579590000000	0.747664000000
76 H	-1.548820000000	3.301920000000	0.481784000000
77 H	0.029350800000	3.515070000000	1.331050000000
78 H	-0.388180000000	4.569650000000	-0.073878400000
79 H	-0.148051000000	0.636096000000	7.818290000000
80 H	1.626670000000	0.755098000000	7.572590000000
81 H	0.596260000000	0.154585000000	6.250640000000
82 H	0.765549000000	4.287570000000	7.175940000000
83 H	1.738240000000	3.108140000000	8.077140000000
84 H	-0.027348300000	3.236610000000	8.396720000000

#===END

Complex **6c**

Atom	Cartesian (a.u./angstrom)		
	X	Y	Z
1 C	-0.766877000000	9.859230000000	5.305250000000
2 C	-0.961525000000	9.843590000000	6.700160000000
3 C	-0.944681000000	11.071000000000	3.159140000000
4 N	-0.519362000000	9.984680000000	2.560610000000
5 C	-1.470680000000	10.971000000000	7.378430000000
6 C	-1.774380000000	12.159700000000	6.683610000000
7 C	-1.626230000000	12.194700000000	5.289600000000
8 S	-2.513360000000	7.415400000000	3.544140000000
9 C	-0.279242000000	9.975990000000	1.088210000000
10 N	1.489780000000	10.147700000000	-0.681597000000
11 C	1.212850000000	10.287100000000	0.772035000000
12 C	-3.326890000000	7.012850000000	5.255600000000
13 C	1.875840000000	9.106560000000	4.282840000000
14 Pt	-0.121406000000	8.364570000000	4.008320000000
15 C	0.319345000000	7.025310000000	5.596630000000
16 C	2.899410000000	9.762930000000	-0.973045000000
17 C	1.041820000000	11.311300000000	-1.493470000000
18 C	-1.117440000000	11.065000000000	4.606010000000
19 C	-0.961531000000	3.842510000000	1.051060000000
20 C	-0.329893000000	2.624340000000	1.368910000000
21 C	-1.700140000000	5.465710000000	-0.647952000000
22 N	-2.139720000000	6.218250000000	0.331184000000
23 C	0.202234000000	1.796950000000	0.358237000000
24 C	0.111153000000	2.165290000000	-0.999782000000
25 C	-0.518066000000	3.368730000000	-1.345430000000

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26	S	0.592906000000	6.547170000000	2.325990000000
27	C	-2.898900000000	7.468370000000	0.034808200000
28	N	-5.173820000000	8.496530000000	-0.124304000000
29	C	-4.435040000000	7.232810000000	0.143069000000
30	C	1.956860000000	5.404430000000	3.088330000000
31	C	-1.401130000000	4.169610000000	4.084240000000
32	Pt	-1.731320000000	5.293470000000	2.318840000000
33	C	-3.632700000000	4.298580000000	2.245990000000
34	C	-6.399260000000	8.663140000000	0.705692000000
35	C	-5.425000000000	8.750360000000	-1.567960000000
36	C	-1.048600000000	4.204060000000	-0.333341000000
37	H	-0.726593000000	8.956020000000	7.280570000000
38	H	-1.204960000000	11.968300000000	2.582900000000
39	H	-1.603640000000	10.930100000000	8.460170000000
40	H	-2.156780000000	13.028200000000	7.218310000000
41	H	-1.876690000000	13.099800000000	4.733650000000
42	H	-0.490743000000	8.973660000000	0.710365000000
43	H	-0.946258000000	10.702000000000	0.598832000000
44	H	1.472760000000	11.297000000000	1.158600000000
45	H	1.821210000000	9.550140000000	1.306150000000
46	H	-2.630840000000	6.471860000000	5.902290000000
47	H	-4.224930000000	6.413820000000	5.067200000000
48	H	-3.590670000000	7.978220000000	5.702110000000
49	H	2.186690000000	8.948850000000	5.323980000000
50	H	1.880360000000	10.181500000000	4.051930000000
51	H	2.534210000000	8.560130000000	3.593720000000
52	H	-0.494408000000	6.301040000000	5.708180000000
53	H	0.449183000000	7.591640000000	6.526330000000
54	H	1.255010000000	6.495480000000	5.378500000000
55	H	2.997510000000	9.563540000000	-2.049990000000
56	H	3.137530000000	8.838530000000	-0.429758000000
57	H	3.633370000000	10.550500000000	-0.690450000000
58	H	1.197060000000	11.084400000000	-2.558240000000
59	H	1.592100000000	12.248400000000	-1.245650000000
60	H	-0.032281300000	11.483800000000	-1.341180000000
61	H	-0.238186000000	2.308540000000	2.405200000000
62	H	-1.818780000000	5.774020000000	-1.694340000000
63	H	0.682441000000	0.856647000000	0.631447000000
64	H	0.521548000000	1.518020000000	-1.773570000000
65	H	-0.592443000000	3.668980000000	-2.391730000000
66	H	-2.635060000000	8.220700000000	0.781178000000
67	H	-2.633830000000	7.837050000000	-0.968380000000
68	H	-4.739290000000	6.413700000000	-0.541826000000
69	H	-4.648310000000	6.915440000000	1.168610000000
70	H	2.719340000000	6.039950000000	3.552940000000
71	H	2.381270000000	4.847020000000	2.244980000000
72	H	1.528230000000	4.715410000000	3.821770000000
73	H	-0.378599000000	4.329920000000	4.445560000000
74	H	-1.558830000000	3.103910000000	3.869910000000
75	H	-2.119560000000	4.486340000000	4.852310000000
76	H	-4.372340000000	4.942240000000	2.742900000000
77	H	-3.560530000000	3.330850000000	2.758470000000
78	H	-3.899220000000	4.144450000000	1.191000000000
79	H	-7.191330000000	7.917270000000	0.471097000000

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80 H	-6.807840000000	9.670140000000	0.536033000000
81 H	-6.127670000000	8.578190000000	1.766430000000
82 H	-4.477820000000	8.710450000000	-2.123660000000
83 H	-5.843000000000	9.760490000000	-1.688310000000
84 H	-6.132150000000	8.016450000000	-2.018990000000

#===END

Complex **6d**

Atom	Cartesian (a.u./angstrom) X	Y	Z
1 C	-0.936952000000	9.776760000000	5.428550000000
2 C	-1.176080000000	9.599590000000	6.806350000000
3 C	-1.094570000000	11.188300000000	3.420590000000
4 N	-0.580600000000	10.193200000000	2.741300000000
5 C	-1.775110000000	10.617400000000	7.576320000000
6 C	-2.148000000000	11.844600000000	6.989900000000
7 C	-1.919090000000	12.049700000000	5.623720000000
8 S	-2.507420000000	7.504900000000	3.396810000000
9 C	-0.298903000000	10.352200000000	1.286200000000
10 N	1.551800000000	10.627200000000	-0.397821000000
11 C	1.214000000000	10.622800000000	1.052670000000
12 C	-3.398340000000	6.939230000000	5.019200000000
13 C	1.819370000000	9.187500000000	4.420970000000
14 Pt	-0.161775000000	8.433140000000	4.053810000000
15 C	0.309829000000	6.981630000000	5.523340000000
16 C	2.983080000000	10.294500000000	-0.651051000000
17 C	1.141860000000	11.875300000000	-1.100670000000
18 C	-1.322430000000	11.027800000000	4.846120000000
19 C	-3.525380000000	4.540380000000	2.049850000000
20 C	-4.116250000000	3.613140000000	2.930760000000
21 C	-3.690360000000	5.958590000000	0.046013900000
22 N	-2.442580000000	6.305630000000	0.249732000000
23 C	-5.453450000000	3.200320000000	2.758370000000
24 C	-6.235110000000	3.703080000000	1.697960000000
25 C	-5.669100000000	4.617570000000	0.800359000000
26 S	0.496978000000	6.854580000000	2.095000000000
27 C	-1.756330000000	7.192390000000	-0.745989000000
28 N	-0.774495000000	7.268610000000	-3.068790000000
29 C	-1.301580000000	6.380440000000	-1.993240000000
30 C	2.056470000000	5.795360000000	2.545650000000
31 C	-1.109950000000	4.271570000000	3.846980000000
32 Pt	-1.644750000000	5.391660000000	2.129770000000
33 C	-0.793392000000	3.767950000000	1.010240000000
34 C	-0.784835000000	6.594170000000	-4.399570000000
35 C	0.566417000000	7.850260000000	-2.759190000000
36 C	-4.325530000000	5.031940000000	0.967481000000
37 H	-0.905084000000	8.667780000000	7.295130000000
38 H	-1.367050000000	12.128800000000	2.925630000000

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39	H	-1.951290000000	10.451200000000	8.639840000000
40	H	-2.613220000000	12.624400000000	7.591920000000
41	H	-2.209160000000	12.990500000000	5.153760000000
42	H	-0.557873000000	9.416930000000	0.787780000000
43	H	-0.918892000000	11.164200000000	0.874837000000
44	H	1.501420000000	11.572200000000	1.554860000000
45	H	1.769540000000	9.806930000000	1.525060000000
46	H	-2.740270000000	6.319530000000	5.635260000000
47	H	-4.287260000000	6.376030000000	4.714070000000
48	H	-3.676930000000	7.852310000000	5.557380000000
49	H	2.165410000000	8.870720000000	5.413420000000
50	H	1.788710000000	10.285500000000	4.370630000000
51	H	2.481840000000	8.786310000000	3.640890000000
52	H	-0.563039000000	6.349650000000	5.719330000000
53	H	0.619442000000	7.493850000000	6.443530000000
54	H	1.143180000000	6.364400000000	5.163470000000
55	H	3.142580000000	10.215800000000	-1.735610000000
56	H	3.211970000000	9.321550000000	-0.196664000000
57	H	3.685320000000	11.056800000000	-0.245608000000
58	H	1.359460000000	11.769800000000	-2.173060000000
59	H	1.672590000000	12.776700000000	-0.717174000000
60	H	0.060237900000	12.029500000000	-0.992005000000
61	H	-3.545430000000	3.203930000000	3.759980000000
62	H	-4.256420000000	6.350130000000	-0.808639000000
63	H	-5.887370000000	2.482150000000	3.455090000000
64	H	-7.268660000000	3.381540000000	1.576140000000
65	H	-6.260080000000	5.013980000000	-0.026596700000
66	H	-2.430930000000	7.997380000000	-1.074820000000
67	H	-0.889904000000	7.620900000000	-0.241013000000
68	H	-0.565714000000	5.611760000000	-1.681340000000
69	H	-2.178100000000	5.858510000000	-2.402190000000
70	H	2.845420000000	6.481780000000	2.871520000000
71	H	2.357660000000	5.271740000000	1.631620000000
72	H	1.821390000000	5.078390000000	3.337020000000
73	H	-0.058623200000	4.452280000000	4.097830000000
74	H	-1.255670000000	3.203780000000	3.629120000000
75	H	-1.745510000000	4.569770000000	4.690180000000
76	H	-1.528920000000	2.956490000000	0.923079000000
77	H	0.105511000000	3.415740000000	1.534590000000
78	H	-0.530489000000	4.153150000000	0.016155700000
79	H	-0.100349000000	5.717560000000	-4.449330000000
80	H	-0.479554000000	7.320530000000	-5.166130000000
81	H	-1.806320000000	6.259620000000	-4.630240000000
82	H	0.525954000000	8.473820000000	-1.857870000000
83	H	0.862643000000	8.498810000000	-3.596200000000
84	H	1.346300000000	7.066470000000	-2.623710000000

#===END

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