Supporting Information

MW-Promoted Cu(I)-Catalyzed P–C Coupling Reactions without the Addition of Conventional Ligands; An Experimental and A Theoretical Study

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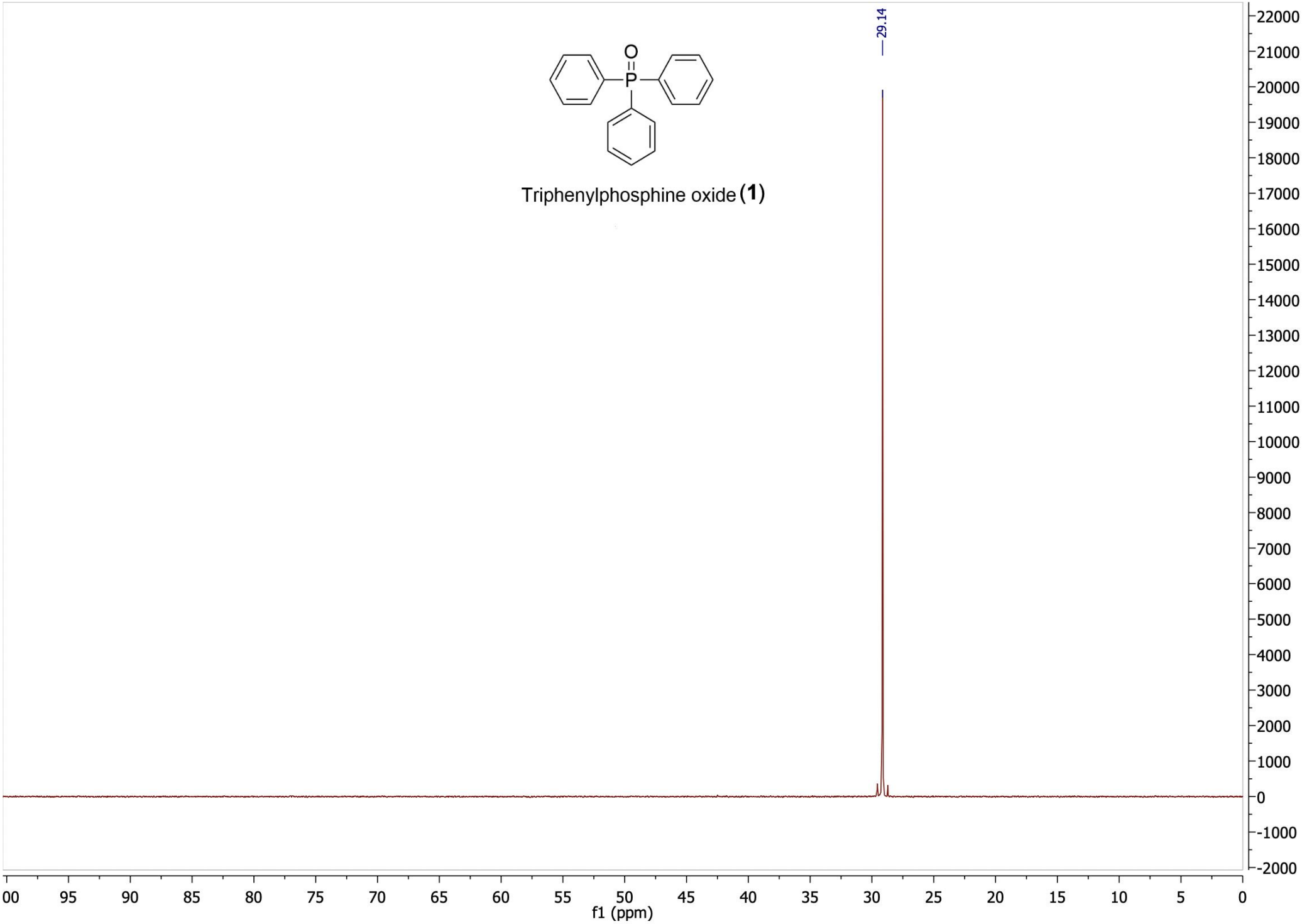
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12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
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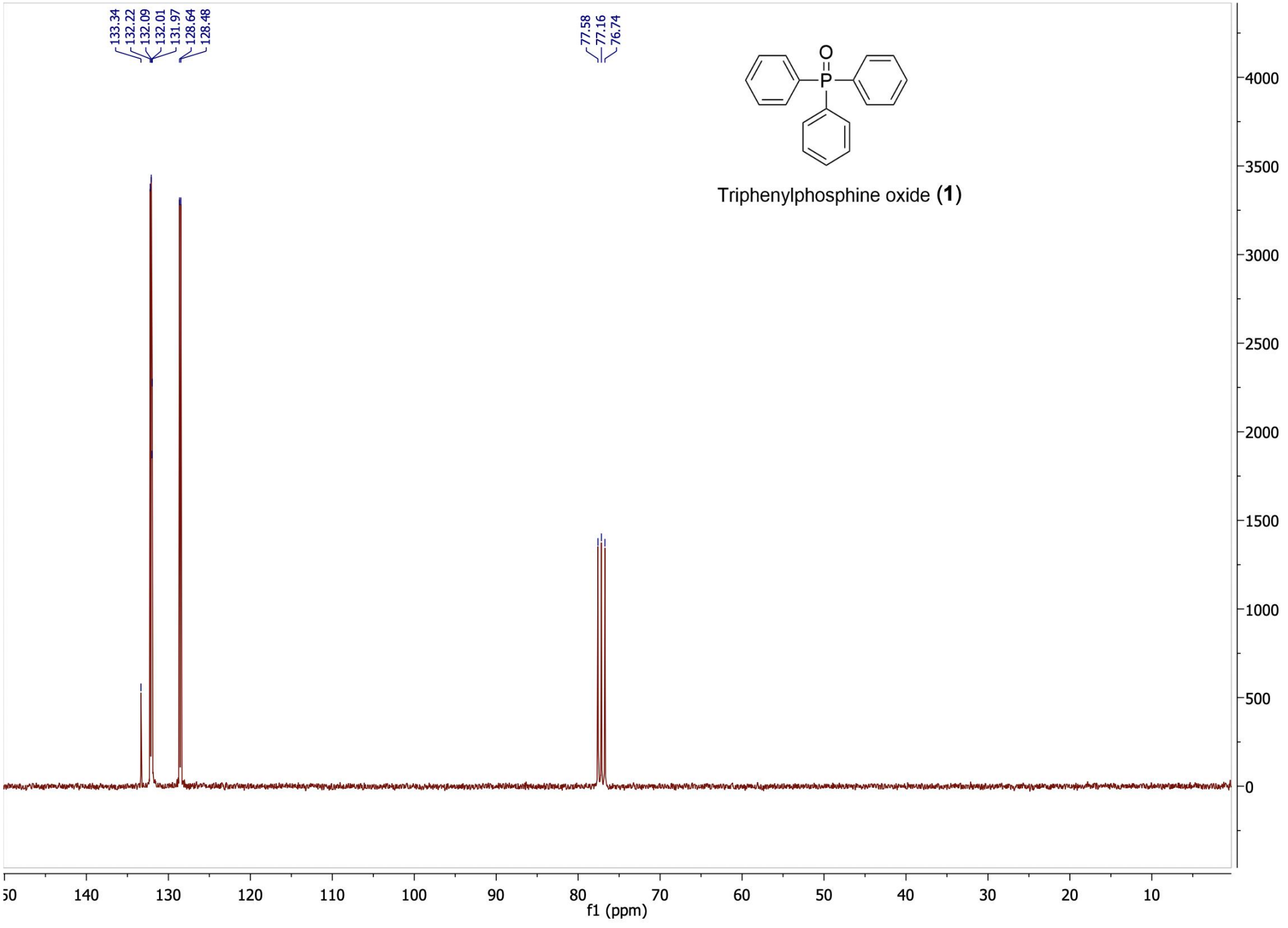
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4000
3500
3000
2500
2000
1500
1000
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120
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100
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70
60
50
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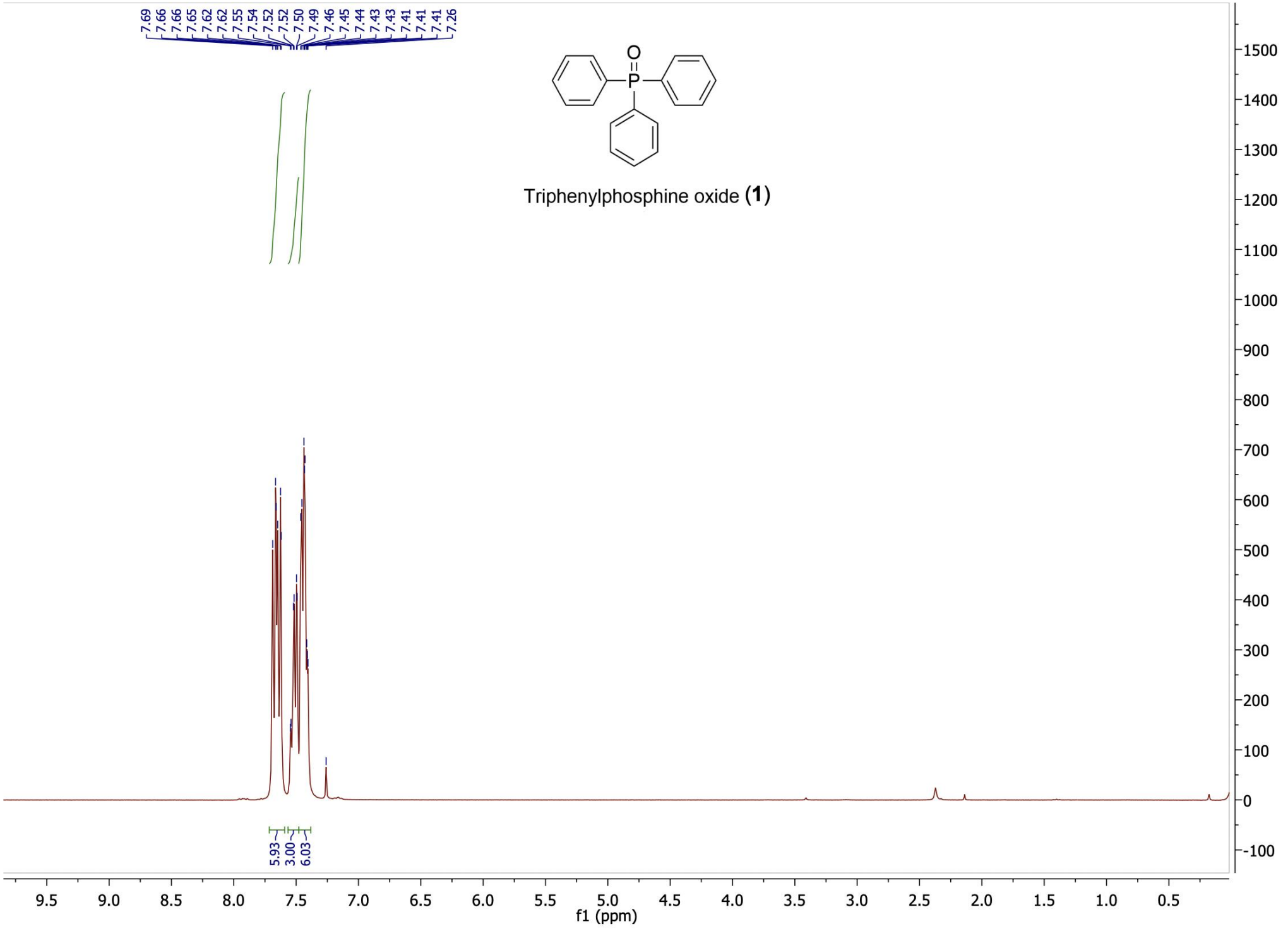
30
20
10
f1 (ppm)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7.46
7.45
7.44
7.43
7.43
7.41
7.41
7.41
7.26
O
P
Triphenylphosphine oxide (1)
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3.00
6.03
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1400
1300
1200
1100
1000
900
800
700
600
500
400
300
200
100
0
-100
9.5
9.0
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8.0
7.5
7.0
6.5
6.0
5.5
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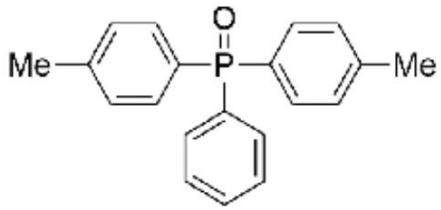
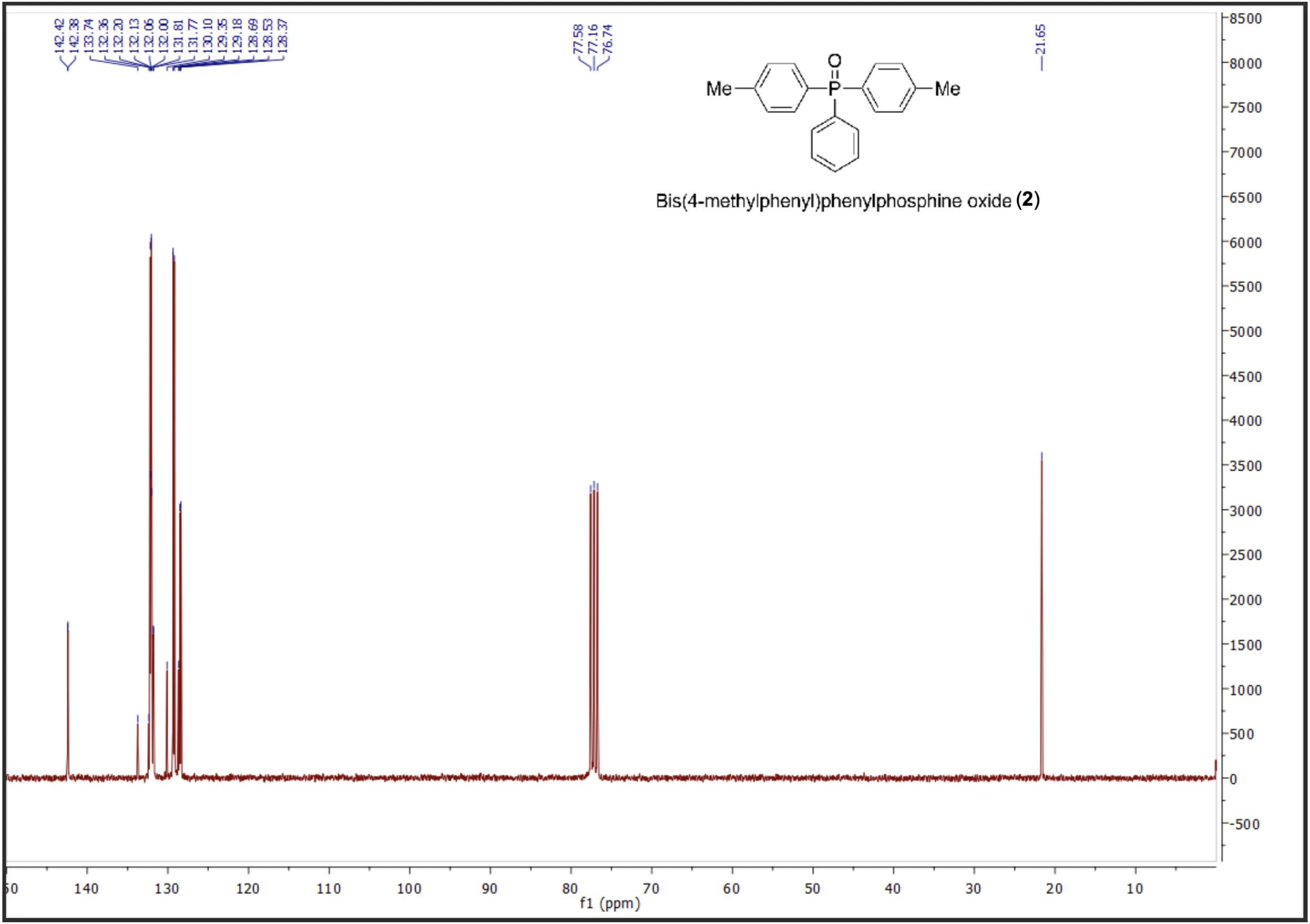
0.5
f1 (ppm)



Bis(4-methylphenyl)phenylphosphine oxide (**2**)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128.69
128.53
128.37
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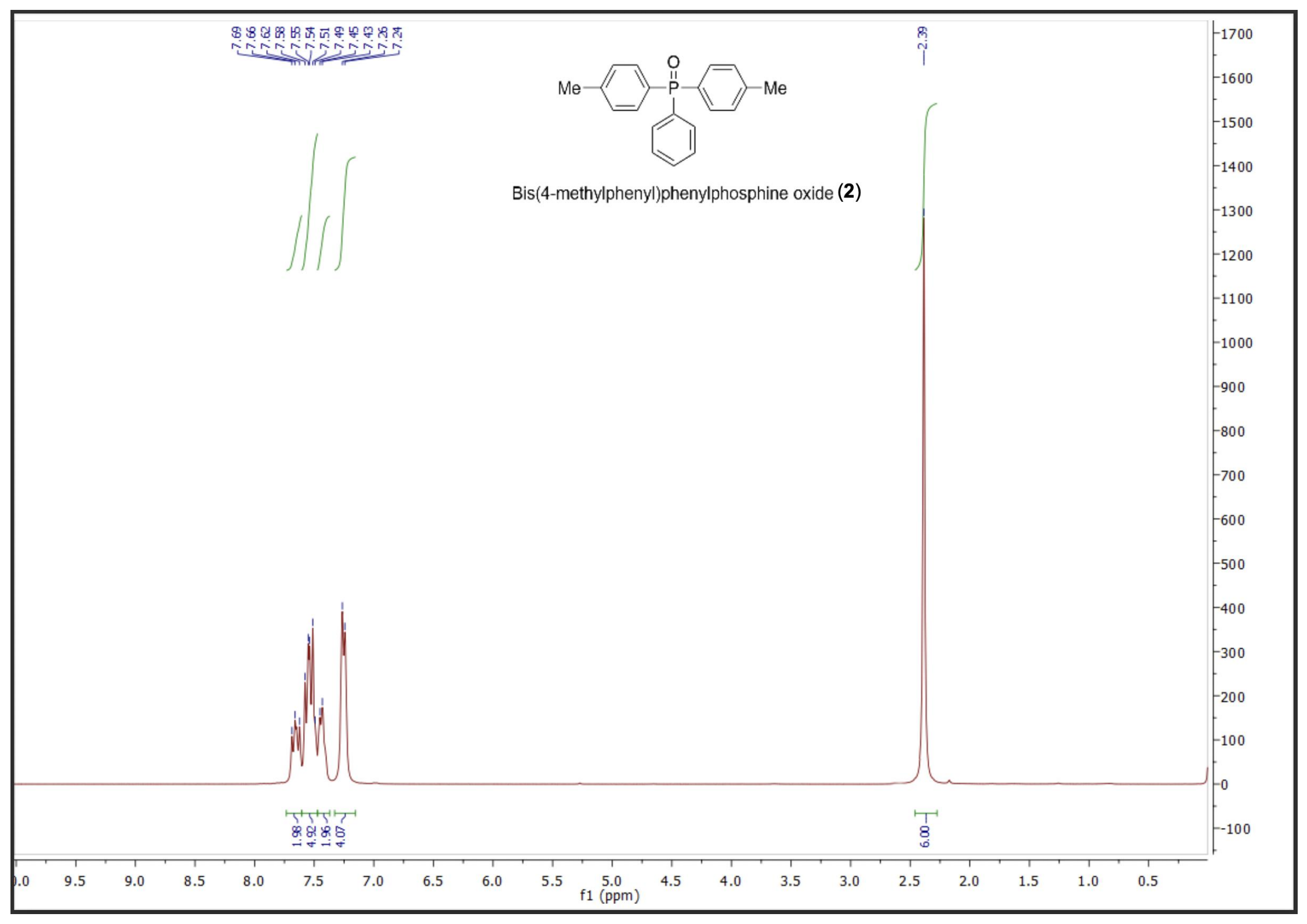
77.16
76.74
21.65
Me
P
O
Me
Bis(4-methylphenyl)phenylphosphine oxide (2)
f1 (ppm)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7.49
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7.26
7.24
2.39
Me
O
P
Me
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1.96
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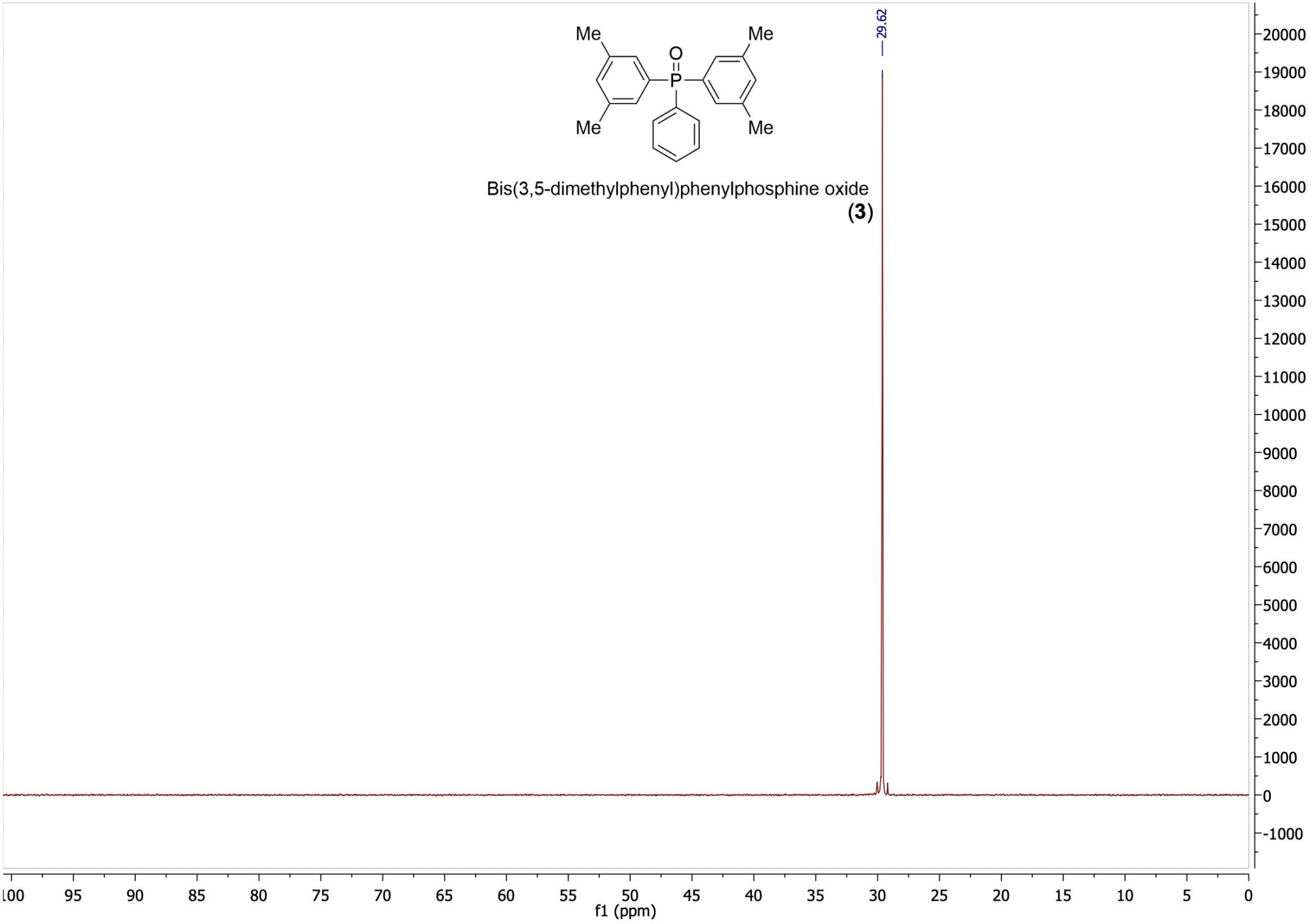
6.00
f1 (ppm)


Me
Me
O
P
Me
Me
29.62
Bis(3,5-dimethylphenyl)phenylphosphine oxide
(3)
20000
19000
18000
17000
16000
15000
14000
13000
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
100
95
90
85
80
75
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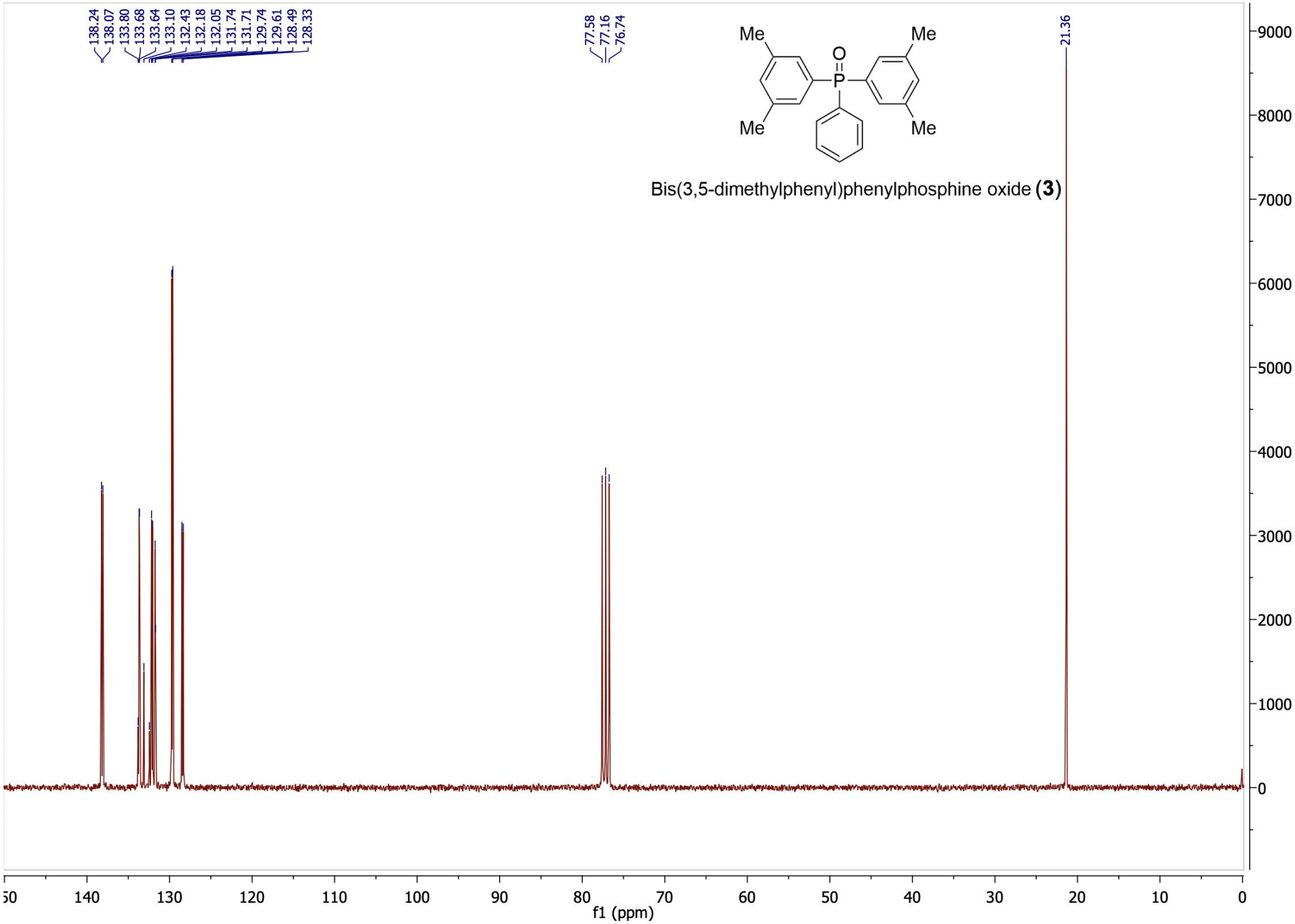
65
60
55
50
45
40
35
30
25
20
15
10
5
0
f1 (ppm)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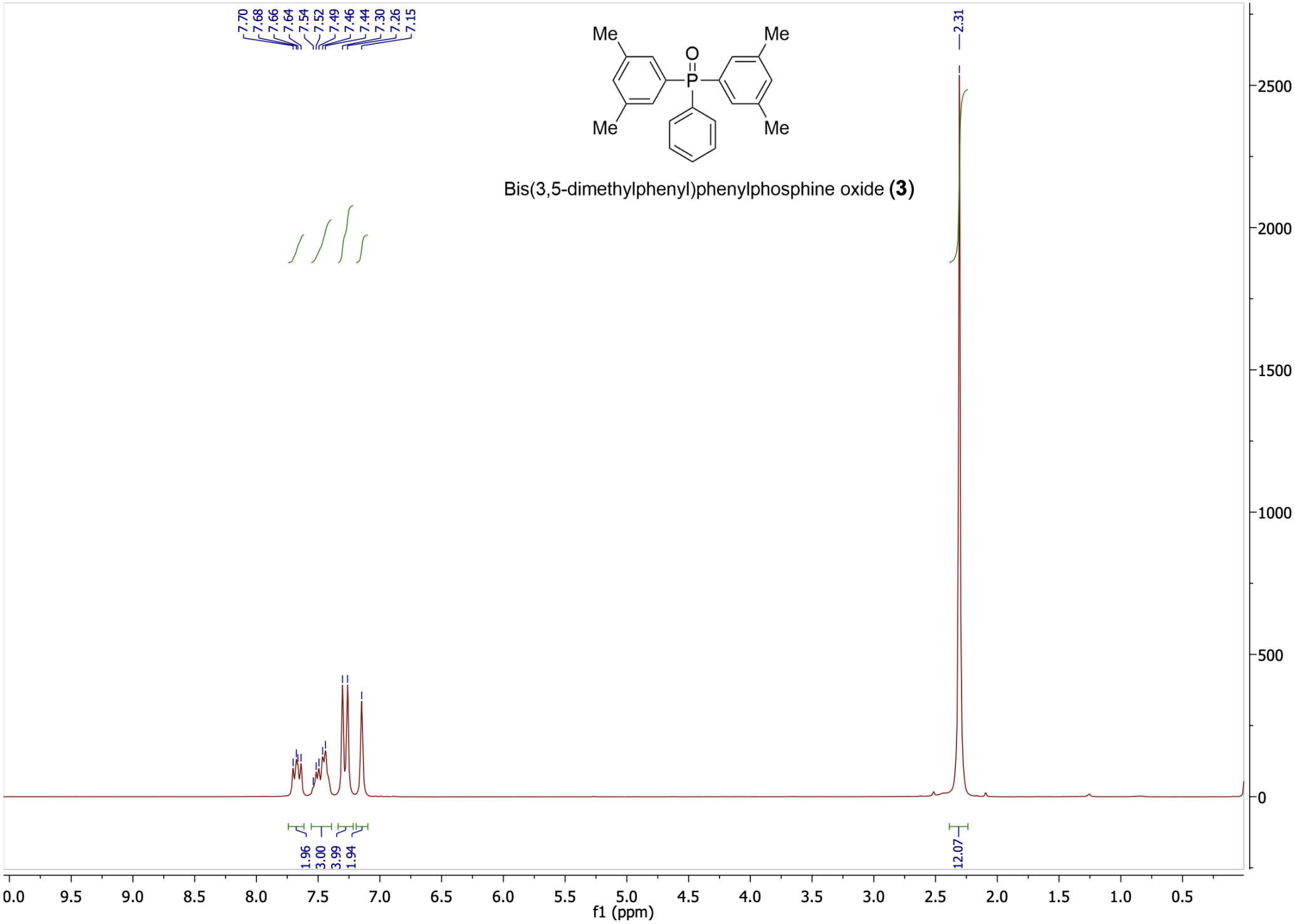
129.61
128.49
128.33
77.58
77.16
76.74
21.36
Me
Me
Me
Me
O
P
Bis(3,5-dimethylphenyl)phenylphosphine oxide (3)
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
50
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.66
7.64
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7.52
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7.46
7.44
7.30
7.26
7.15
2.31
Me
Me
Me
Me
O
P
Bis(3,5-dimethylphenyl)phenylphosphine oxide (3)
1.96
3.00
3.99
1.94
12.07
2500
2000
1500
1000
500
0
0.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
f1 (ppm)

2. Tables containing the computed row data

Table S1. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at M06-2X/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of EtOH for **small molecules and ions**.

Name	Number	E	ZPE	U	H	G	S
CuBr		-4211.98477644	-4211.984018	-4211.981277	-4211.980333	-4212.008417	59.108
Cu^+		-1639.92259300	-1639.922600	-1639.921200	-1639.920200	-1639.938400	38.337
Br^-		-2571.92996300	-2571.929963	-2571.928547	-2571.927603	-2571.946139	39.012
I^-		-11.54638300	-11.546383	-11.544966	-11.544022	-11.563231	40.428
HBr		-2572.37172100	-2572.365531	-2572.363171	-2572.362226	-2572.384741	47.387
HI		-11.95576600	-11.950644	-11.948284	-11.947340	-11.970781	49.338
NEt_3		-292.27215906	-292.064204	-292.054881	-292.053937	-292.098218	93.198
$NEt_3 + H^+$		-292.72766900	-292.503977	-292.494605	-292.493661	-292.538322	93.997
PPh_3		-1035.98423600	-1035.708238	-1035.693338	-1035.692394	-1035.752522	126.549
PhBr		-2803.32880000	-2803.237306	-2803.231664	-2803.230719	-2803.268117	78.710
PhI		-242.91063496	-242.819728	-242.813876	-242.812932	-242.851454	81.077
Ph_2POH conf 1		-880.23745910	-880.038493	-880.026309	-880.025365	-880.078844	112.556
Ph_2POH conf 2		-880.23687896	-880.037855	-880.025579	-880.024635	-880.078754	113.903
Ph_2PHO		-880.23902538	-880.040644	-880.028806	-880.027862	-880.081110	112.070
$Ph_3P(O)$	**1**	-1111.21498115	-1110.933946	-1110.917256	-1110.916312	-1110.981071	136.297

Table S2. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at M06-2X/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of EtOH for **$Cu^{+}(PPh_3)_x$ and $Cu^{+}(PPh_2POH)_x$ complexes**.

Name	Number	E	ZPE	U	H	G	S
$Cu^{+}(PPh_3)$		-2676.01298379	-2675.735701	-2675.717986	-2675.717042	-2675.784234	141.418
$Cu^{+}(PPh_3)_2$		-3712.07463274	-3711.518202	-3711.483257	-3711.482313	-3711.589331	225.240
$Cu^{+}(PPh_3)_3$		-4748.12807878	-4747.292128	-4747.240634	-4747.239690	-4747.380160	295.644
$Cu^{+}(PPh_3)_4$		-5784.14508000	-5783.031610	-5782.964331	-5782.963387	-5783.138696	368.970
$Cu^{+}(PPh_2OH)$		-2520.26221079	-2520.061161	-2520.047309	-2520.046365	-2520.103783	120.847
$Cu^{+}(PPh_2OH)_2$	**4**	-3400.57394647	-3400.171807	-3400.144031	-3400.143087	-3400.232307	187.778
$Cu^{+}(PPh_2OH)_3$		-4280.87179492	-4280.268732	-4280.227569	-4280.226625	-4280.345662	250.536
$Cu^{+}(PPh_2OH)_4$		-5161.16367655	-5160.359666	-5160.305164	-5160.304219	-5160.451514	310.007

Table S3. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at M06-2X/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of EtOH for **Cu^{+} complexes containing $PPh_2(OH)$ and NEt_3 ligands**.

Name	Number	E	ZPE	U	H	G	S
$Cu^{+}(PPh_2OH)_2$	**4**	-3400.57293955	-3400.170449	-3400.142742	-3400.141798	-3400.231288	188.348
$Cu^{3+}(PPh_2OH)_2$		-3400.05578331	-3399.650011	-3399.623729	-3399.622785	-3399.704858	172.738
$Cu^{+}(PPh_2OH)(NEt_3)$	**8**	-2812.61911095	-2812.206408	-2812.182193	-2812.181249	-2812.262155	170.283
$Cu^{3+}(PPh_2OH)(NEt_3)$		-2812.08247295	-2811.667631	-2811.644557	-2811.643613	-2811.718920	158.498
$Cu^{+}(NEt_3)_2$	**9**	-2224.66403274	-2224.241580	-2224.220911	-2224.219967	-2224.289680	146.724
$Cu^{3+}(NEt_3)_2$		-2224.06797610	-2223.640117	-2223.621753	-2223.620809	-2223.683741	132.452

Table S4. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at M06-2X/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of EtOH for **Cu^+ complexes containing $(PAr_2OH)_x$ and $(NR_3)_x$ ligands.**

Name	Number	E	ZPE	U	H	G	S
$Cu^+[4\text{-}MeC_6H_4)_2POH]$		-2598.86207188	-2598.606205	-2598.588511	-2598.587567	-2598.655294	142.544
$Cu^+[4\text{-}MeC_6H_4)_2POH]_2$		-3557.77564417	-3557.262862	-3557.229204	-3557.228260	-3557.329015	212.057
$Cu^+[4\text{-}MeC_6H_4)_2POH]_3$		-4516.66890000					
$Cu^+[4\text{-}MeC_6H_4)_2POH]_4$		-5475.56441442					
$Cu^+(NEt_3)$		-1932.31332203	-1932.102462	-1932.091931	-1932.090987	-1932.138350	99.683
$Cu^+(NEt_3)_2$	**9**	-2224.67366643	-2224.251859	-2224.231527	-2224.230582	-2224.299832	145.749
$Cu^+(NEt_3)_3$		-2516.96619796	-2516.331918	-2516.301340	-2516.300396	-2516.390347	189.318
$Cu^+(NEt_3)_4$		-2809.24493133	-2808.398718	-2808.358880	-2808.357936	-2808.467144	229.849
$Cu^+(N^iPr_2Et)$		-2010.89927645	-2010.631644	-2010.618618	-2010.617674	-2010.670833	111.883
$Cu^+(N^iPr_2Et)_2$		-2381.85210500	-2381.317442	-2381.292062	-2381.291117	-2381.369381	164.719
$Cu^+(N^iPr_2Et)_3$		-2752.72230999	-2751.918955	-2751.880710	-2751.879766	-2751.985251	222.012
$Cu^+(NMe_3)$		-1814.41165700	-1814.287364	-1814.280400	-1814.279456	-1814.318454	82.080
$Cu^+(NMe_3)_2$		-1988.88710979	-1988.637443	-1988.625103	-1988.624159	-1988.675854	108.801
$Cu^+(NMe_3)_3$		-2163.30568513	-2162.931256	-2162.911887	-2162.910942	-2162.977160	139.366
$Cu^+(NMe_3)_4$		-2337.71788961	-2337.219046	-2337.193427	-2337.192483	-2337.270420	164.032
$Cu^+[(3,5\text{-diMe } C_6H_3)_2POH]$		-2677.46045276	-2677.149360	-2677.127869	-2677.126925	-2677.204444	163.152
$Cu^+[(3,5\text{-diMe } C_6H_3)_2POH]_2$		-3714.97490000					
$Cu^+[(3,5\text{-diMe } C_6H_3)_2POH]_3$		-4752.46490000					
$Cu^+[(3,5\text{-diMe } C_6H_3)_2POH]_4$		-5789.96566380	-5788.717569	-5788.636036	-5788.635092	-5788.836210	423.288

Table S5. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at M06-2X/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of EtOH for the mechanism of **Cu^+ complexes containing $PPh_2(OH)$ ligands.**

Name	Number	E	ZPE	U	H	G	S
$Cu^+(PPh_2OH)(PPh_2O^-)$	**4'**	-3400.13180900	-3399.742303	-3399.715224	-3399.714280	-3399.803827	188.468
$Cu^+(PPh_2OH)(PPh_2O^-)$---PhBr	**5**	-6203.49281987	-6203.011881	-6202.976747	-6202.975802	-6203.085393	230.652
TS[$Cu^+(PPh_2OH)(PPh_2O^-)$···Ph···Br]	**TS5,6**	-6203.47201000	-6202.991604	-6202.957151	-6202.956206	-6203.062849	224.449
$Cu^{3+}(PPh_2OH)(PPh_2O^-)(Ph)(Br)$	**6**	-6203.49220276	-6203.008851	-6202.974930	-6202.973986	-6203.077145	217.117
TS[$Cu^+(PPh_2OH)(PPh_2O^-)(Ph)(Br)$]	**TS6,7**	-6203.45135600	-6202.969553	-6202.936989	-6202.936045	-6203.036418	211.254
$Cu^+(PPh_2OH)(Br)(Ph)(PPh_2O)$	**7**	-6203.57382635	-6203.090434	-6203.055951	-6203.055007	-6203.162049	225.289

Table S6. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at M06-2X/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of EtOH for the mechanism of **Cu^+ complexes containing $PPh_2(O^-)$ and NEt_3 ligands.**

Name	Number	E	ZPE	U	H	G	S
$Cu^+(PPh_2O^-)(NEt_3)$	**8'**	-2812.17637910	-2811.776603	-2811.752922	-2811.751978	-2811.831208	166.754
$Cu^+(PPh_2O^-)(NEt_3)$---PhBr	**10**	-5615.52399407	-5615.031699	-5615.000528	-5614.999584	-5615.096606	204.199
TS[$Cu^+(PPh_2O^-)(NEt_3)$···Ph···Br]	**TS10,11**	-5615.51392030	-5615.022717	-5614.992198	-5614.991254	-5615.086287	200.015
$Cu^{3+}(PPh_2O^-)(NEt_3)(Ph)(Br)$	**11**	-5615.52500963	-5615.031804	-5615.001197	-5615.000253	-5615.095369	200.188
TS[$Cu^+(PPh_2O^-)(NEt_3)(Ph)(Br)$]	**TS11,12**	-5615.47529200					
$Cu^+(NEt_3)(Br)(Ph)(PPh_2O)$	**12**	-5615.60632996	-5615.112761	-5615.081499	-5615.080555	-5615.179600	208.459

Table S7. Computed energies (*E*), zero point energies, internal energies (*U*), enthalpies (*H*) and Gibbs free energies (*G*) given in Hartree as well as entropies (*S*) given in J mol^{-1} K^{-1} at M06-2X/6-31G(d,p) basis set with the consideration of PCM solvent method using the parameter set of EtOH for the mechanism of **Cu^{+} complexes containing NEt_3 ligands.**

Name	Number	E	ZPE	U	H	G	S
$Cu^{+}(NEt_3)_2$---PhBr	**13**	-5028.01684904	-5027.501507	-5027.473258	-5027.472314	-5027.559928	184.399
TS[$Cu^{+}(NEt_3)_2$···Ph···Br]	**TS13,14**	-5027.97390900					
$Cu^{3+}(NEt_3)_2$(Ph)(Br)	**14**	-5027.99244260	-5027.474995	-5027.447847	-5027.446903	-5027.530631	176.221

3. Tables containing XYZ geometries of computed species

CuBr

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000000	0.000000	-1.181702
2	35	0	0.000000	0.000000	0.979124

Cu^{+}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.000000	0.000000	0.000000

Br^{-}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.000000	0.000000	0.000000

HBr

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	35	0	0.000000	0.000000	0.039244
2	1	0	0.000000	0.000000	-1.373537

HI

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	53	0	0.000000	0.000000	0.029964
2	1	0	0.000000	0.000000	-1.588113

NEt_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-0.000085	-0.000083	-0.174561
2	6	0	0.447559	1.315349	0.285372
3	1	0	1.472927	1.457577	-0.064151
4	1	0	0.480263	1.353752	1.392782
5	6	0	-1.362818	-0.270346	0.286098
6	1	0	-1.998874	0.546885	-0.062231
7	1	0	-1.411612	-0.262298	1.393544
8	6	0	0.915416	-1.045421	0.285181
9	1	0	0.526067	-2.004488	-0.064626
10	1	0	0.932168	-1.093194	1.392579
11	6	0	2.337542	-0.894626	-0.246148
12	1	0	2.885963	-0.083123	0.236862
13	1	0	2.896267	-1.816996	-0.069491
14	1	0	2.317276	-0.705526	-1.323271
15	6	0	-0.393813	2.471569	-0.246361
16	1	0	-1.370856	2.541160	0.236517
17	1	0	0.125769	3.416600	-0.069981
18	1	0	-0.547308	2.358909	-1.323453
19	6	0	-1.943876	-1.576484	-0.246578
20	1	0	-1.515001	-2.458027	0.234603
21	1	0	-3.021924	-1.599347	-0.069230
22	1	0	-1.770590	-1.651545	-1.323903

$NEt_3 + H^+$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.000113	-0.000780	-0.196197
2	6	0	-0.055579	1.441463	0.245237
3	1	0	0.803761	1.930898	-0.210635
4	1	0	0.082718	1.431013	1.329207
5	6	0	-1.220300	-0.768718	0.249459
6	1	0	-2.075350	-0.266865	-0.200759
7	1	0	-1.276482	-0.646881	1.334084
8	6	0	1.277116	-0.671570	0.249028
9	1	0	1.271223	-1.662758	-0.201438
10	1	0	1.200251	-0.780623	1.333803
11	6	0	2.529834	0.083102	-0.160575
12	1	0	2.674976	0.999849	0.411338
13	1	0	3.386432	-0.565463	0.029859
14	1	0	2.525550	0.320747	-1.228251
15	6	0	-1.337835	2.147055	-0.159570
16	1	0	-2.201510	1.813826	0.416242
17	1	0	-1.204799	3.213622	0.028393
18	1	0	-1.544606	2.021728	-1.226057
19	6	0	-1.193686	-2.230329	-0.161381
20	1	0	-0.468916	-2.813945	0.406486
21	1	0	-2.182522	-2.649818	0.030370
22	1	0	-0.988056	-2.341359	-1.229700
23	1	0	-0.000760	-0.004525	-1.222756

Ph_3P

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.002528	-0.007112	-1.275968
2	6	0	1.325228	-0.983774	-0.449886
3	6	0	1.133806	-1.753439	0.702442
4	6	0	2.603946	-0.920002	-1.017216
5	6	0	2.202239	-2.439539	1.277311
6	1	0	0.147918	-1.815884	1.153704
7	6	0	3.673289	-1.595593	-0.436117
8	6	0	3.472847	-2.358888	0.712462
9	1	0	2.042328	-3.035071	2.170770
10	1	0	4.660201	-1.532654	-0.883422

11	6	0	0.182036	1.631820	-0.449980
12	6	0	-0.540957	2.702043	-0.992410
13	6	0	0.986000	1.858907	0.671657
14	6	0	-0.476214	3.967617	-0.416539
15	6	0	1.060123	3.129525	1.240883
16	1	0	1.555718	1.041624	1.104470
17	6	0	0.327957	4.183843	0.701472
18	1	0	4.304234	-2.891972	1.162730
19	1	0	0.386164	5.171632	1.147345
20	1	0	1.688582	3.292977	2.110855
21	1	0	-1.045488	4.786480	-0.845142
22	1	0	2.761401	-0.334756	-1.920031
23	1	0	-1.159121	2.541786	-1.872713
24	6	0	-1.512303	-0.663474	-0.445893
25	6	0	-2.097677	-1.809001	-0.999721
26	6	0	-2.089496	-0.093019	0.693239
27	6	0	-3.226129	-2.381584	-0.420154
28	1	0	-1.665991	-2.254465	-1.892911
29	6	0	-3.226477	-0.659733	1.266765
30	1	0	-1.649078	0.796174	1.134915
31	6	0	-3.794131	-1.805263	0.714148
32	1	0	-3.667302	-3.271276	-0.858340
33	1	0	-3.666948	-0.206269	2.149239
34	1	0	-4.679218	-2.244324	1.163266

PhBr

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.866508	0.000006	0.000001
2	6	0	2.169223	1.205851	-0.000003
3	6	0	0.776385	1.214397	0.000001
4	6	0	0.100128	-0.000027	-0.000000
5	6	0	0.776393	-1.214405	-0.000004
6	6	0	2.169267	-1.205824	0.000002
7	1	0	3.951156	0.000044	0.000007
8	1	0	2.706804	2.148334	-0.000004
9	1	0	0.223087	2.146620	0.000007
10	1	0	0.223169	-2.146671	0.000001
11	1	0	2.706822	-2.148322	0.000001
12	35	0	-1.798813	0.000000	0.000000

PhI

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.578709	-0.000019	-0.000000
2	6	0	-1.256161	1.214262	0.000004
3	6	0	-2.650283	1.205073	-0.000005
4	6	0	-3.347704	0.000007	0.000002
5	6	0	-2.650319	-1.205056	0.000004
6	6	0	-1.256173	-1.214264	-0.000005
7	1	0	-0.713953	2.153170	-0.000000
8	1	0	-3.187334	2.147997	-0.000003
9	1	0	-4.432408	0.000035	-0.000001
10	1	0	-3.187350	-2.147992	0.000007
11	1	0	-0.714015	-2.153202	-0.000010
12	53	0	1.559833	-0.000000	0.000000

$Ph_2P(OH)$ conf. 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.017413	1.470066	-0.595511
2	8	0	0.093970	2.451659	0.742950
3	1	0	0.119436	1.956220	1.575689
4	6	0	-1.408923	0.344707	-0.159734
5	6	0	-2.569723	0.399751	-0.935711
6	6	0	-1.361211	-0.530242	0.933811
7	6	0	-3.665877	-0.405955	-0.628971
8	1	0	-2.613854	1.074066	-1.787070
9	6	0	-2.456879	-1.326167	1.248361
10	1	0	-0.454770	-0.600730	1.531447
11	6	0	-3.609697	-1.265518	0.464038
12	1	0	-4.560371	-0.361987	-1.241807
13	1	0	-2.412564	-1.999565	2.098338
14	1	0	-4.462159	-1.892271	0.705975
15	6	0	1.391580	0.323344	-0.296024
16	6	0	1.416736	-0.931734	-0.916652
17	6	0	2.486955	0.722103	0.474906
18	6	0	2.510377	-1.775568	-0.758232
19	1	0	0.568460	-1.256178	-1.515041
20	6	0	3.581007	-0.127281	0.637658
21	1	0	2.483021	1.698636	0.950765

22	6	0	3.595084	-1.375261	0.022463
23	1	0	2.515662	-2.748898	-1.238709
24	1	0	4.423006	0.189075	1.245387
25	1	0	4.446993	-2.035700	0.148609

$Ph_2P(OH)$ conf. 2

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.012390	1.376948	-0.836426
2	8	0	0.170150	2.485445	0.400080
3	1	0	-0.013508	3.373272	0.070304
4	6	0	-1.401938	0.374714	-0.225132
5	6	0	-2.299808	-0.163519	-1.148543
6	6	0	-1.591980	0.136381	1.141028
7	6	0	-3.369363	-0.948150	-0.715590
8	1	0	-2.165391	0.033837	-2.209431
9	6	0	-2.665813	-0.632378	1.573854
10	1	0	-0.893980	0.562117	1.857260
11	6	0	-3.552797	-1.179708	0.643903
12	1	0	-4.062283	-1.366933	-1.438371
13	1	0	-2.812743	-0.812694	2.634185
14	1	0	-4.388901	-1.783375	0.982600
15	6	0	1.380193	0.256737	-0.334267
16	6	0	1.420504	-1.045061	-0.847086
17	6	0	2.415191	0.698111	0.492053
18	6	0	2.475465	-1.894244	-0.531048
19	1	0	0.614891	-1.400773	-1.486241
20	6	0	3.470384	-0.156260	0.810865
21	1	0	2.382620	1.705660	0.893300
22	6	0	3.503940	-1.450576	0.300249
23	1	0	2.494586	-2.903755	-0.929539
24	1	0	4.266968	0.191790	1.461271
25	1	0	4.326816	-2.113209	0.548683

Ph_2PHO

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.006992	1.410988	-0.349110
2	8	0	-0.142700	2.621819	0.526079
3	1	0	0.118020	1.695952	-1.725355
4	6	0	1.435938	0.357429	-0.072362
5	6	0	2.487904	0.333671	-0.990199
6	6	0	1.502080	-0.424830	1.086567
7	6	0	3.601128	-0.469753	-0.751980
8	1	0	2.439794	0.938534	-1.891943
9	6	0	2.616334	-1.220167	1.324737
10	1	0	0.676799	-0.416850	1.794280
11	6	0	3.664503	-1.242998	0.404270
12	1	0	4.416186	-0.491912	-1.467721
13	1	0	2.666574	-1.827448	2.222301
14	1	0	4.531680	-1.868779	0.589366
15	6	0	-1.424301	0.290786	-0.226464
16	6	0	-1.433785	-0.935611	-0.897446
17	6	0	-2.514079	0.672656	0.556338
18	6	0	-2.536680	-1.774922	-0.788320
19	1	0	-0.577270	-1.236667	-1.496115
20	6	0	-3.614693	-0.174985	0.669753
21	1	0	-2.485710	1.627180	1.073644
22	6	0	-3.625495	-1.393931	-0.002914
23	1	0	-2.547367	-2.726773	-1.308907
24	1	0	-4.461900	0.116190	1.281913
25	1	0	-4.483450	-2.052871	0.084672

$Ph_3P(O)$ (**1**)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.001378	0.011621	0.944573
2	6	0	1.358502	0.994252	0.248411
3	6	0	1.262306	1.678512	-0.966612
4	6	0	2.554129	1.027077	0.973534
5	6	0	2.361264	2.378868	-1.458149
6	1	0	0.330553	1.672880	-1.525726
7	6	0	3.648635	1.730384	0.480579
8	6	0	3.552836	2.403070	-0.736397

9	1	0	2.284773	2.910239	-2.401099
10	1	0	4.574331	1.756020	1.045989
11	6	0	0.181021	-1.652442	0.238566
12	6	0	-0.320374	-2.720972	0.987492
13	6	0	0.769500	-1.889966	-1.007181
14	6	0	-0.247239	-4.017244	0.486154
15	6	0	0.836309	-3.187714	-1.507610
16	1	0	1.182846	-1.065595	-1.582720
17	6	0	0.326669	-4.249284	-0.762499
18	1	0	4.406798	2.952046	-1.120304
19	1	0	0.383592	-5.260167	-1.153293
20	1	0	1.292790	-3.370032	-2.474941
21	1	0	-0.634100	-4.846217	1.069738
22	1	0	2.614790	0.510207	1.927044
23	1	0	-0.753784	-2.529014	1.964755
24	6	0	-1.533664	0.684715	0.237873
25	6	0	-2.238078	1.618529	1.003433
26	6	0	-2.015285	0.308785	-1.019499
27	6	0	-3.411187	2.180936	0.507833
28	1	0	-1.869514	1.886617	1.989369
29	6	0	-3.186224	0.877127	-1.513673
30	1	0	-1.485257	-0.435690	-1.607663
31	6	0	-3.882484	1.812528	-0.750717
32	1	0	-3.959774	2.902089	1.104790
33	1	0	-3.559892	0.582084	-2.488617
34	1	0	-4.798784	2.248975	-1.135072
35	8	0	-0.011064	0.006035	2.446241

$Cu^{+}(PPh_3)$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.218677	0.017470	-0.704370
2	6	0	1.266653	-1.352963	-0.148438
3	6	0	2.166873	-1.904654	-1.065837
4	6	0	1.219252	-1.839401	1.162942
5	6	0	3.019989	-2.931188	-0.671527
6	1	0	2.195864	-1.533121	-2.086347
7	6	0	2.069587	-2.870274	1.549837
8	1	0	0.512846	-1.419172	1.873864
9	6	0	2.970182	-3.413526	0.634383
10	6	0	0.990827	1.581645	-0.224122
11	6	0	0.646459	2.726115	-0.950618
12	6	0	1.879959	1.674796	0.851053
13	6	0	1.172058	3.962715	-0.588778

14	1	0	-0.028096	2.648790	-1.799723
15	6	0	2.411133	2.912095	1.200889
16	1	0	2.155858	0.785191	1.409953
17	6	0	2.054891	4.054362	0.484844
18	1	0	3.630773	-4.218332	0.939553
19	1	0	2.471409	5.017252	0.761911
20	1	0	3.103097	2.985485	2.033107
21	1	0	0.901497	4.850172	-1.150682
22	1	0	3.717790	-3.357000	-1.384469
23	1	0	2.029695	-3.249421	2.565457
24	6	0	-1.280996	-0.112213	0.380947
25	6	0	-1.711053	0.916899	1.225251
26	6	0	-2.109336	-1.250225	0.204511
27	6	0	-2.927131	0.808928	1.894693
28	1	0	-1.091392	1.798102	1.362146
29	6	0	-3.318779	-1.348272	0.894342
30	1	0	-1.736026	-2.138604	-0.314345
31	6	0	-3.734955	-0.315219	1.727525
32	1	0	-3.242488	1.608350	2.557044
33	1	0	-3.927864	-2.239035	0.783288
34	1	0	-4.678810	-0.390298	2.255978
35	29	0	-1.724413	-0.317522	-1.745261

$Cu^{+}(PPh_3)_2$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.081856	-0.059829	0.481552
2	6	0	2.053039	1.126261	-0.904051
3	6	0	2.317141	2.480756	-0.667360
4	6	0	1.587381	0.720046	-2.157361
5	6	0	2.137812	3.412947	-1.684886
6	1	0	2.666737	2.807249	0.308724
7	6	0	1.396950	1.660216	-3.167919
8	1	0	1.365833	-0.327626	-2.343796
9	6	0	1.672384	3.005097	-2.934754
10	6	0	3.556580	0.347300	1.460147
11	6	0	3.521896	0.093175	2.834738
12	6	0	4.723153	0.859824	0.879641
13	6	0	4.642746	0.343273	3.621566
14	1	0	2.615863	-0.297614	3.290647
15	6	0	5.840038	1.111829	1.669864
16	1	0	4.753215	1.077242	-0.184577
17	6	0	5.800409	0.852952	3.039033
18	1	0	1.525137	3.735656	-3.723177
19	1	0	6.672137	1.055294	3.652604
20	1	0	6.740738	1.512988	1.217502
21	1	0	4.609315	0.146250	4.687684
22	1	0	2.356331	4.459747	-1.499287
23	1	0	1.035373	1.337329	-4.139087
24	15	0	-2.081784	0.059858	0.481517
25	6	0	-2.053158	-1.126339	-0.903985
26	6	0	-1.587708	-0.720213	-2.157399
27	6	0	-2.317159	-2.480828	-0.667132
28	6	0	-1.397391	-1.660464	-3.167906
29	1	0	-1.366235	0.327454	-2.343954
30	6	0	-2.137948	-3.413098	-1.684604
31	6	0	-1.672727	-3.005336	-2.934579
32	1	0	-1.035972	-1.337651	-4.139156
33	1	0	-2.356387	-4.459894	-1.498881
34	6	0	-3.556400	-0.347167	1.460342
35	6	0	-3.521584	-0.092888	2.834900
36	6	0	-4.723024	-0.859782	0.880015
37	6	0	-4.642350	-0.342926	3.621870
38	6	0	-5.839824	-1.111722	1.670378
39	1	0	-4.753190	-1.077312	-0.184176
40	6	0	-5.800061	-0.852695	3.039515
41	1	0	-1.525565	-3.735957	-3.722960
42	1	0	-6.671721	-1.054990	3.653198
43	1	0	-6.740565	-1.512943	1.218152

44	1	0	-4.608809	-0.145786	4.687963
45	1	0	-2.666584	-2.807248	0.309038
46	1	0	-2.615523	0.297975	3.290689
47	6	0	2.366914	-1.677036	-0.303048
48	6	0	3.609115	-2.062296	-0.816510
49	6	0	1.271800	-2.538070	-0.413563
50	6	0	3.744156	-3.296935	-1.442455
51	1	0	4.468678	-1.404369	-0.725560
52	6	0	1.407605	-3.769888	-1.047911
53	1	0	0.311275	-2.234294	-0.005503
54	6	0	2.645163	-4.148499	-1.560029
55	1	0	4.708554	-3.598117	-1.837769
56	1	0	0.549388	-4.427933	-1.132980
57	1	0	2.758114	-5.110906	-2.048295
58	6	0	-2.366908	1.677005	-0.303164
59	6	0	-3.609101	2.062100	-0.816773
60	6	0	-1.271886	2.538165	-0.413572
61	6	0	-3.744227	3.296711	-1.442750
62	1	0	-4.468588	1.404060	-0.725917
63	6	0	-1.407777	3.769962	-1.047949
64	1	0	-0.311364	2.234505	-0.005421
65	6	0	-2.645324	4.148412	-1.560207
66	1	0	-4.708615	3.597766	-1.838183
67	1	0	-0.549632	4.428110	-1.132941
68	1	0	-2.758339	5.110797	-2.048501
69	29	0	0.000034	0.000024	1.298104

$Cu^{+}(PPh_3)_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.062347	1.093271	-0.373453
2	15	0	-2.044028	1.162832	-0.240752
3	6	0	3.383040	-0.168273	-0.385584
4	6	0	4.364895	-0.292850	0.599844
5	6	0	3.333299	-1.098641	-1.429878
6	6	0	5.270786	-1.351899	0.546308
7	1	0	4.411274	0.419436	1.418558
8	6	0	4.226588	-2.162871	-1.474660
9	1	0	2.577389	-1.002979	-2.206082
10	6	0	5.195665	-2.292271	-0.479550
11	1	0	6.029574	-1.448393	1.316267
12	1	0	4.149751	-2.896375	-2.272035
13	6	0	2.575646	2.312985	-1.624349
14	6	0	1.589198	3.026762	-2.313237

15	6	0	3.926205	2.580083	-1.874898
16	6	0	1.950226	4.002944	-3.238882
17	1	0	0.537203	2.827306	-2.120390
18	6	0	4.283123	3.551056	-2.804532
19	1	0	4.695255	2.024413	-1.344851
20	6	0	3.295845	4.263304	-3.485140
21	6	0	-2.488322	0.648082	1.464560
22	6	0	-1.848310	1.275587	2.541415
23	6	0	-3.314302	-0.455362	1.709692
24	6	0	-2.056248	0.827419	3.842072
25	1	0	-1.184189	2.118623	2.370501
26	6	0	-3.530181	-0.891068	3.016172
27	1	0	-3.790552	-0.984141	0.889021
28	6	0	-2.905002	-0.251899	4.084489
29	6	0	-2.045172	2.993800	-0.189947
30	6	0	-0.872928	3.638627	0.220649
31	6	0	-3.152572	3.764796	-0.556751
32	6	0	-0.810156	5.027064	0.285240
33	1	0	0.003273	3.057081	0.493630
34	6	0	-3.085027	5.154707	-0.502689
35	1	0	-4.066639	3.285921	-0.893615
36	6	0	-1.918015	5.787955	-0.079856
37	1	0	-3.071992	-0.597132	5.099724
38	1	0	5.890446	-3.125423	-0.503222
39	1	0	3.577553	5.020302	-4.209897
40	1	0	-1.871400	6.871284	-0.040987
41	1	0	5.331311	3.753139	-2.998478
42	1	0	1.180538	4.554440	-3.768382
43	1	0	-3.948483	5.744136	-0.793026
44	1	0	0.107490	5.506988	0.611677
45	1	0	-1.553725	1.324931	4.665570
46	1	0	-4.180511	-1.742331	3.191529
47	15	0	-0.028822	-2.163457	-0.154529
48	6	0	-1.708763	-2.870002	-0.006297
49	6	0	-2.152488	-3.667977	1.050568
50	6	0	-2.589290	-2.557112	-1.047209
51	6	0	-3.476158	-4.101904	1.084464
52	1	0	-1.475731	-3.936510	1.856179
53	6	0	-3.909619	-2.994345	-1.016540
54	6	0	-4.357889	-3.757292	0.060686
55	1	0	-3.819322	-4.709725	1.915518
56	1	0	-4.585004	-2.721775	-1.822134
57	6	0	0.839600	-3.373366	-1.207165
58	6	0	0.914667	-3.104507	-2.577176
59	6	0	1.374543	-4.564247	-0.707731
60	6	0	1.543437	-4.002297	-3.435877
61	6	0	2.015168	-5.454161	-1.564712
62	1	0	1.301013	-4.791444	0.352097
63	6	0	2.103975	-5.172206	-2.927058
64	1	0	-5.390324	-4.088989	0.100309

65	1	0	2.604355	-5.867551	-3.593151
66	1	0	2.439536	-6.371289	-1.169782
67	1	0	1.601345	-3.785901	-4.497441
68	1	0	-2.247199	-1.949608	-1.881055
69	1	0	0.488769	-2.184182	-2.972835
70	6	0	-3.455698	0.729865	-1.306553
71	6	0	-4.784325	0.738822	-0.866904
72	6	0	-3.177950	0.409056	-2.639959
73	6	0	-5.812969	0.401075	-1.742134
74	1	0	-5.016163	1.001025	0.161562
75	6	0	-4.207559	0.076620	-3.515793
76	1	0	-2.148313	0.404935	-2.993419
77	6	0	-5.525747	0.065730	-3.064159
78	1	0	-6.839537	0.401931	-1.391249
79	1	0	-3.980645	-0.176089	-4.546141
80	1	0	-6.329595	-0.200519	-3.742635
81	6	0	2.219503	1.945382	1.231523
82	6	0	2.515821	3.305897	1.343913
83	6	0	1.904254	1.206809	2.379173
84	6	0	2.481718	3.922260	2.594167
85	1	0	2.758068	3.887851	0.458885
86	6	0	1.882871	1.823604	3.624940
87	1	0	1.680912	0.145363	2.298488
88	6	0	2.162908	3.185796	3.732606
89	1	0	2.704629	4.981134	2.676058
90	1	0	1.636890	1.239496	4.506669
91	1	0	2.133131	3.672052	4.702175
92	6	0	0.723212	-2.252532	1.505236
93	6	0	2.090745	-2.504313	1.664384
94	6	0	-0.031619	-1.843195	2.614040
95	6	0	2.680805	-2.391153	2.921915
96	1	0	2.704874	-2.777510	0.809762
97	6	0	0.561569	-1.740647	3.869023
98	1	0	-1.083754	-1.598879	2.497819
99	6	0	1.918815	-2.018710	4.027122
100	1	0	3.743157	-2.586190	3.029258
101	1	0	-0.040121	-1.428993	4.717498
102	1	0	2.382308	-1.932242	5.004550
103	29	0	-0.019317	0.113337	-0.605013

$Cu^{+}(PPh_3)_4$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.974106	-1.620080	0.189087
2	15	0	0.138528	1.697738	1.851556
3	6	0	1.481678	-3.321957	-0.309812
4	6	0	0.637550	-4.070231	0.515345
5	6	0	1.814700	-3.831660	-1.589702
6	6	0	0.187829	-5.318123	0.116938
7	1	0	0.350103	-3.686460	1.499556
8	6	0	1.335605	-5.083411	-1.988382
9	1	0	2.443705	-3.256188	-2.258381
10	6	0	0.526690	-5.830621	-1.122915
11	1	0	-0.441463	-5.901469	0.781376
12	1	0	1.623081	-5.469931	-2.962039
13	6	0	3.532480	-1.304753	-0.741664
14	6	0	3.825031	0.001313	-1.152227
15	6	0	4.489699	-2.310602	-0.963667
16	6	0	5.008930	0.288851	-1.831861
17	1	0	3.121763	0.804494	-0.945526
18	6	0	5.666273	-2.020843	-1.642638
19	1	0	4.301050	-3.321538	-0.611562
20	6	0	5.920454	-0.721993	-2.085224
21	6	0	-1.007466	1.290091	3.236882
22	6	0	-0.531448	0.593092	4.371372
23	6	0	-2.381175	1.484790	3.129061
24	6	0	-1.409853	0.139903	5.354028
25	1	0	0.529129	0.429769	4.498515
26	6	0	-3.251870	1.007981	4.086805
27	1	0	-2.806463	1.994254	2.276016
28	6	0	-2.780349	0.342013	5.211374
29	6	0	1.706986	2.057636	2.715093
30	6	0	2.874015	1.536081	2.158161
31	6	0	1.774086	2.797079	3.903576
32	6	0	4.109381	1.760564	2.769030
33	1	0	2.812991	0.931092	1.245275
34	6	0	3.001850	3.012160	4.513987
35	1	0	0.868436	3.210898	4.339543
36	6	0	4.170560	2.501947	3.942302
37	1	0	-3.470279	-0.017082	5.969698
38	1	0	0.159467	-6.808221	-1.417179
39	1	0	6.845848	-0.503405	-2.608851
40	1	0	5.126229	2.682342	4.426353
41	1	0	6.387477	-2.813583	-1.819530
42	1	0	5.212297	1.306637	-2.152027
43	1	0	3.046544	3.581924	5.435599

44	1	0	5.017313	1.359290	2.333436
45	1	0	-1.019016	-0.365946	6.233352
46	1	0	-4.322616	1.155149	3.947980
47	15	0	-2.083302	-1.194794	-0.000235
48	6	0	-3.556480	-0.133709	0.267522
49	6	0	-4.569944	-0.535741	1.140592
50	6	0	-3.743988	1.017231	-0.508379
51	6	0	-5.720517	0.233345	1.298534
52	1	0	-4.445945	-1.440843	1.724478
53	6	0	-4.928176	1.748652	-0.400711
54	6	0	-5.908531	1.371065	0.518436
55	1	0	-6.485274	-0.081803	1.999424
56	1	0	-5.075005	2.605399	-1.052833
57	6	0	-2.546713	-2.107691	-1.519541
58	6	0	-1.574432	-2.915594	-2.095227
59	6	0	-3.806225	-2.016409	-2.131428
60	6	0	-1.838035	-3.642868	-3.241671
61	6	0	-4.078625	-2.751539	-3.282608
62	1	0	-4.577932	-1.388367	-1.701202
63	6	0	-3.095743	-3.572472	-3.840129
64	1	0	-6.822446	1.944597	0.606988
65	1	0	-3.300327	-4.139161	-4.741966
66	1	0	-5.060111	-2.669761	-3.738905
67	1	0	-1.051441	-4.250139	-3.672826
68	1	0	-2.993102	1.350282	-1.221841
69	1	0	-0.585725	-2.968061	-1.639745
70	15	0	0.284959	1.308563	-2.035245
71	6	0	-1.313720	1.627983	-2.889120
72	6	0	-1.968878	0.565737	-3.525962
73	6	0	-1.968760	2.855624	-2.800242
74	6	0	-3.240749	0.725578	-4.070527
75	1	0	-1.494423	-0.411384	-3.581396
76	6	0	-3.241196	3.019312	-3.349534
77	6	0	-3.879844	1.960251	-3.984846
78	1	0	-3.728299	-0.119717	-4.554684
79	1	0	-3.735852	3.988828	-3.298082
80	6	0	1.080087	2.962218	-2.019851
81	6	0	0.879146	3.859490	-3.073940
82	6	0	1.911360	3.346205	-0.960182
83	6	0	1.515771	5.092468	-3.083471
84	6	0	2.518572	4.599484	-0.955986
85	1	0	2.076872	2.670096	-0.117667
86	6	0	2.335784	5.462227	-2.024699
87	1	0	-4.864105	2.104883	-4.416890
88	1	0	2.812349	6.438747	-2.025754
89	1	0	3.134868	4.886779	-0.109779
90	1	0	1.359066	5.778363	-3.910932
91	1	0	-1.508532	3.685050	-2.281854
92	1	0	0.205227	3.601182	-3.884848
93	6	0	-0.473181	3.349635	1.288743

94	6	0	0.150567	4.559243	1.574234
95	6	0	-1.673382	3.350273	0.580063
96	6	0	-0.418033	5.756074	1.145218
97	1	0	1.099875	4.563903	2.112626
98	6	0	-2.268828	4.544206	0.196131
99	1	0	-2.188120	2.431407	0.336345
100	6	0	-1.637978	5.757152	0.470744
101	1	0	0.085156	6.692130	1.354287
102	1	0	-3.221010	4.512540	-0.317641
103	1	0	-2.086845	6.692433	0.162425
104	6	0	2.542588	-1.914269	1.910859
105	6	0	3.893185	-2.057798	2.240446
106	6	0	1.579117	-1.960917	2.921020
107	6	0	4.281906	-2.224175	3.554390
108	1	0	4.657495	-1.984763	1.471648
109	6	0	1.973747	-2.136369	4.252357
110	1	0	0.520562	-1.850243	2.684041
111	6	0	3.333719	-2.260829	4.567556
112	1	0	5.335743	-2.301486	3.793974
113	1	0	1.219655	-2.171700	5.030811
114	1	0	3.651045	-2.384812	5.596627
115	6	0	-2.231108	-2.484365	1.310616
116	6	0	-2.709583	-3.776276	1.059582
117	6	0	-1.942313	-2.111517	2.630335
118	6	0	-2.854467	-4.687266	2.107217
119	1	0	-2.966716	-4.081117	0.051715
120	6	0	-2.052823	-3.028705	3.663878
121	1	0	-1.622935	-1.089952	2.847453
122	6	0	-2.509845	-4.318055	3.408747
123	1	0	-3.227154	-5.684935	1.898960
124	1	0	-1.792150	-2.738590	4.676312
125	1	0	-2.607008	-5.031961	4.219226
126	6	0	1.263677	0.387470	-3.333553
127	6	0	2.361072	0.933646	-4.013184
128	6	0	0.985922	-0.973723	-3.537973
129	6	0	3.151230	0.148471	-4.852148
130	1	0	2.650385	1.967621	-3.836640
131	6	0	1.742610	-1.746118	-4.406911
132	1	0	0.192660	-1.475972	-3.014940
133	6	0	2.844315	-1.189058	-5.057937
134	1	0	4.016085	0.597944	-5.331229
135	1	0	1.488997	-2.795147	-4.566264
136	1	0	3.459127	-1.802239	-5.707291
137	29	0	0.041787	0.001561	0.048582

$Cu^{+}(PPh_2OH)$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.018834	0.684498	0.478455
2	6	0	-1.514336	-0.244916	0.075769
3	6	0	-1.521980	-1.169369	-0.973498
4	6	0	-2.691398	0.031447	0.778149
5	6	0	-2.703138	-1.824952	-1.305782
6	1	0	-0.608104	-1.386090	-1.519559
7	6	0	-3.867498	-0.632907	0.443921
8	1	0	-2.681912	0.754257	1.588691
9	6	0	-3.873451	-1.559354	-0.596668
10	6	0	1.354631	-0.459291	0.233886
11	6	0	2.495711	0.061156	-0.381343
12	6	0	1.334855	-1.793904	0.656188
13	6	0	3.618284	-0.736693	-0.572656
14	1	0	2.483334	1.097179	-0.710122
15	6	0	2.459567	-2.588904	0.470128
16	1	0	0.441688	-2.212991	1.111524
17	6	0	3.597879	-2.060438	-0.141194
18	1	0	-4.791115	-2.077003	-0.855509
19	1	0	4.471011	-2.688231	-0.285900
20	1	0	2.450008	-3.623348	0.796152
21	1	0	4.500597	-0.329268	-1.053743
22	1	0	-2.708784	-2.548407	-2.114154
23	1	0	-4.778660	-0.426557	0.995252
24	29	0	0.375827	2.509942	-0.568702
25	8	0	-0.154005	1.004015	2.076187
26	1	0	-0.297251	0.221307	2.631994

$Cu^{+}(PPh_2OH)_2$ (**4**)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.859027	-0.999970	1.111854
2	6	0	2.863713	0.145986	0.137321
3	6	0	4.040785	0.682035	0.664290
4	6	0	2.387911	0.580788	-1.104688
5	6	0	4.748776	1.636922	-0.061358
6	1	0	4.404822	0.340994	1.627789
7	6	0	3.094176	1.542773	-1.818960

8	1	0	1.467955	0.167076	-1.512978
9	6	0	4.275709	2.069564	-1.298165
10	1	0	4.827717	2.817417	-1.857879
11	1	0	5.670207	2.044208	0.341156
12	1	0	2.723376	1.880527	-2.781014
13	15	0	-1.808780	0.962702	1.112933
14	6	0	-2.844665	-0.170776	0.150338
15	6	0	-2.511225	-0.485337	-1.171857
16	6	0	-3.888621	-0.847392	0.789027
17	6	0	-3.234458	-1.458509	-1.854664
18	1	0	-1.691382	0.028803	-1.667802
19	6	0	-4.612027	-1.815340	0.098101
20	6	0	-4.284696	-2.121817	-1.221256
21	1	0	-2.977638	-1.699799	-2.880833
22	1	0	-5.428463	-2.332160	0.591129
23	1	0	-4.846857	-2.879697	-1.756778
24	1	0	-4.135685	-0.612145	1.820168
25	6	0	1.356921	-2.267073	-0.075015
26	6	0	2.280189	-2.914269	-0.904950
27	6	0	0.002922	-2.601848	-0.139868
28	6	0	1.840698	-3.891134	-1.789357
29	1	0	3.331890	-2.643857	-0.862139
30	6	0	-0.438290	-3.571430	-1.036978
31	1	0	-0.704052	-2.085698	0.505071
32	6	0	0.483267	-4.216389	-1.856037
33	1	0	2.551361	-4.396756	-2.434408
34	1	0	-1.494481	-3.813869	-1.093377
35	1	0	0.145733	-4.975020	-2.554696
36	6	0	-1.372710	2.284205	-0.039789
37	6	0	-2.303494	2.869557	-0.907720
38	6	0	-0.050896	2.737325	-0.029236
39	6	0	-1.908273	3.904768	-1.745968
40	1	0	-3.326510	2.503664	-0.940064
41	6	0	0.346861	3.765555	-0.878715
42	1	0	0.669897	2.262206	0.631916
43	6	0	-0.585182	4.351603	-1.730300
44	1	0	-2.626993	4.359258	-2.419308
45	1	0	1.379283	4.098716	-0.876483
46	1	0	-0.281207	5.155918	-2.392136
47	29	0	0.027406	-0.009993	1.885940
48	8	0	-2.809836	1.573360	2.253406
49	1	0	-3.603610	2.007052	1.902414
50	8	0	3.012512	-1.657970	2.070015
51	1	0	2.650408	-1.959744	2.913669

$Cu^{+}(PPh_2OH)_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.628532	2.176606	-0.341080
2	15	0	-1.549768	-1.497083	-0.273469
3	6	0	-1.915172	2.985136	-1.330721
4	6	0	-3.059537	2.246832	-1.659398
5	6	0	-1.759658	4.285045	-1.815532
6	6	0	-4.054529	2.824467	-2.442272
7	1	0	-3.173882	1.226392	-1.296066
8	6	0	-2.754111	4.852394	-2.608392
9	1	0	-0.859983	4.848484	-1.588852
10	6	0	-3.901696	4.126110	-2.917444
11	6	0	-1.088806	-2.126811	1.368067
12	6	0	-1.363467	-1.323282	2.480841
13	6	0	-0.343798	-3.301312	1.523031
14	6	0	-0.918284	-1.707498	3.742749
15	1	0	-1.926774	-0.400343	2.361364
16	6	0	0.095412	-3.681361	2.788483
17	1	0	-0.107936	-3.916162	0.659515
18	6	0	-0.192451	-2.886637	3.898491
19	1	0	0.152124	-3.186884	4.882909
20	1	0	-4.673938	4.571140	-3.536258
21	1	0	-2.630174	5.861136	-2.988074
22	1	0	-4.944238	2.255215	-2.690046
23	1	0	-1.138157	-1.080011	4.601048
24	1	0	0.661868	-4.599059	2.908489
25	15	0	2.150710	-0.567255	-0.522065
26	6	0	3.525048	-0.101557	-1.605400
27	6	0	3.228439	0.369292	-2.887261
28	6	0	4.861127	-0.239505	-1.207924
29	6	0	4.256479	0.707647	-3.763970
30	6	0	5.885646	0.091128	-2.086892
31	1	0	5.099076	-0.590400	-0.206487
32	6	0	5.582085	0.566056	-3.363359
33	1	0	6.384145	0.828748	-4.045408
34	1	0	6.919951	-0.014661	-1.777253
35	1	0	4.022890	1.078824	-4.756074
36	1	0	2.191972	0.474216	-3.198387
37	6	0	-1.903285	-2.972621	-1.261960
38	6	0	-2.622226	-4.060649	-0.750353
39	6	0	-1.470522	-2.991341	-2.591243
40	6	0	-2.906730	-5.150370	-1.564851
41	1	0	-2.944431	-4.063725	0.288089
42	6	0	-1.750849	-4.087485	-3.403680
43	1	0	-0.909486	-2.148719	-2.989120

44	6	0	-2.470337	-5.162770	-2.890254
45	1	0	-3.462741	-5.992890	-1.167355
46	1	0	-1.409118	-4.100878	-4.433010
47	1	0	-2.690803	-6.017215	-3.521831
48	6	0	-1.232012	2.173036	1.378465
49	6	0	-2.586871	2.200805	1.720001
50	6	0	-0.263799	2.014128	2.378644
51	6	0	-2.965741	2.080046	3.055218
52	1	0	-3.345443	2.319715	0.952836
53	6	0	-0.648211	1.899760	3.710474
54	1	0	0.791086	1.982478	2.115478
55	6	0	-1.999840	1.929570	4.049949
56	1	0	-4.017820	2.106910	3.319353
57	1	0	0.110438	1.775955	4.477132
58	1	0	-2.302335	1.836008	5.088063
59	6	0	2.619600	0.070251	1.116024
60	6	0	3.253831	1.309594	1.261663
61	6	0	2.177379	-0.623660	2.247621
62	6	0	3.468768	1.833059	2.533924
63	1	0	3.577484	1.863798	0.385120
64	6	0	2.393741	-0.094159	3.517134
65	1	0	1.666254	-1.576690	2.135306
66	6	0	3.040371	1.131957	3.661608
67	1	0	3.967947	2.789911	2.645748
68	1	0	2.049944	-0.639684	4.390808
69	1	0	3.207304	1.545141	4.651281
70	29	0	0.000282	0.062275	-0.836280
71	8	0	-2.994100	-0.757063	0.013440
72	1	0	-3.640403	-1.312293	0.476902
73	8	0	2.230349	-2.198285	-0.324069
74	1	0	3.070594	-2.506806	0.050248
75	8	0	0.632702	3.225871	-0.292659
76	1	0	0.462719	4.016378	0.243297

$Cu^{+}(PPh_2OH)_3$ -H^{+}

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.591035	-1.790703	-0.472979
2	15	0	0.603366	2.050751	-0.294972
3	6	0	3.128673	-1.690746	-1.481076
4	6	0	3.710568	-0.465371	-1.827680
5	6	0	3.685921	-2.871972	-1.974322
6	6	0	4.851019	-0.427926	-2.627046
7	1	0	3.273502	0.463329	-1.460814
8	6	0	4.820975	-2.835415	-2.782466
9	1	0	3.207653	-3.814096	-1.720565
10	6	0	5.407531	-1.613833	-3.106409
11	6	0	0.000138	2.359904	1.395528
12	6	0	0.705971	1.765998	2.448551
13	6	0	-1.199502	3.031626	1.654428
14	6	0	0.225730	1.862392	3.751616
15	1	0	1.629906	1.229554	2.245356
16	6	0	-1.672714	3.128857	2.960669
17	1	0	-1.763928	3.470973	0.837539
18	6	0	-0.961581	2.545157	4.009472
19	1	0	-1.336575	2.619917	5.025436
20	1	0	6.290831	-1.584176	-3.736972
21	1	0	5.246743	-3.759273	-3.163087
22	1	0	5.301904	0.526112	-2.883994
23	1	0	0.778159	1.392282	4.559446
24	1	0	-2.599069	3.657836	3.160299
25	15	0	-2.077944	-0.495144	-0.416902
26	6	0	-3.141647	-1.522840	-1.470749
27	6	0	-2.684121	-1.873996	-2.742771
28	6	0	-4.411825	-1.938810	-1.052455
29	6	0	-3.486567	-2.636323	-3.589913
30	6	0	-5.215425	-2.690284	-1.901249
31	1	0	-4.765422	-1.689199	-0.054637
32	6	0	-4.750883	-3.039534	-3.169920
33	1	0	-5.376212	-3.633334	-3.828809
34	1	0	-6.198441	-3.012115	-1.573784
35	1	0	-3.124130	-2.915043	-4.573634
36	1	0	-1.694321	-1.559394	-3.065138
37	6	0	-0.008248	3.474642	-1.245252
38	6	0	0.168135	4.795226	-0.812869
39	6	0	-0.661056	3.227464	-2.455495
40	6	0	-0.296780	5.851888	-1.586806
41	1	0	0.653160	4.998050	0.139492
42	6	0	-1.134987	4.286753	-3.226891
43	1	0	-0.803545	2.203095	-2.792530

44	6	0	-0.949061	5.596206	-2.793871
45	1	0	-0.158145	6.873468	-1.248532
46	1	0	-1.645030	4.089050	-4.163672
47	1	0	-1.314953	6.422506	-3.394858
48	6	0	2.225138	-1.396668	1.224815
49	6	0	3.394117	-0.685794	1.516328
50	6	0	1.384384	-1.766274	2.283292
51	6	0	3.718343	-0.360238	2.833508
52	1	0	4.061923	-0.386502	0.713891
53	6	0	1.703208	-1.438309	3.598117
54	1	0	0.472672	-2.320346	2.067363
55	6	0	2.873430	-0.733340	3.878017
56	1	0	4.634563	0.183412	3.044895
57	1	0	1.034493	-1.731525	4.402985
58	1	0	3.126848	-0.478132	4.902806
59	6	0	-2.156073	-1.313816	1.206359
60	6	0	-2.150543	-2.708696	1.313673
61	6	0	-2.047540	-0.527193	2.357799
62	6	0	-2.068832	-3.308192	2.567230
63	1	0	-2.199890	-3.323670	0.419663
64	6	0	-1.964834	-1.132181	3.608962
65	1	0	-2.024397	0.556683	2.276019
66	6	0	-1.977029	-2.521237	3.715512
67	1	0	-2.068720	-4.390219	2.647483
68	1	0	-1.880322	-0.513783	4.497801
69	1	0	-1.907470	-2.992373	4.690986
70	29	0	0.111234	-0.102310	-0.812137
71	8	0	2.229233	2.271794	-0.131115
72	1	0	2.472676	3.083432	0.339252
73	8	0	-2.919447	0.901292	-0.154639
74	1	0	-3.767561	0.764930	0.295489
75	8	0	1.075997	-3.235684	-0.481774

$Cu^{+}(PPh_2OH)_3$ –H^{+} O ligation

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.087395	0.738887	-2.867149
2	15	0	-2.547047	0.559529	-1.000732
3	6	0	3.148609	-0.299496	-1.737892
4	6	0	4.361393	0.167613	-1.212000
5	6	0	2.781737	-1.623693	-1.480687
6	6	0	5.173370	-0.659238	-0.442020
7	1	0	4.667757	1.195461	-1.390935
8	6	0	3.593426	-2.457644	-0.708164

9	1	0	1.841852	-1.997182	-1.880868
10	6	0	4.790454	-1.977561	-0.185012
11	6	0	-2.790593	1.559839	0.504023
12	6	0	-2.210455	2.833246	0.519590
13	6	0	-3.411245	1.071083	1.657661
14	6	0	-2.251919	3.610111	1.674407
15	1	0	-1.725554	3.213582	-0.376469
16	6	0	-3.452761	1.851827	2.810862
17	1	0	-3.853473	0.079726	1.654864
18	6	0	-2.870294	3.118603	2.822349
19	1	0	-2.901498	3.722776	3.723420
20	1	0	5.420296	-2.622232	0.420346
21	1	0	3.280237	-3.478389	-0.503477
22	1	0	6.104456	-0.274761	-0.035458
23	1	0	-1.802299	4.598527	1.676919
24	1	0	-3.940058	1.470099	3.702367
25	15	0	0.009221	-1.176385	0.813088
26	6	0	0.814150	-2.784596	1.085401
27	6	0	0.533983	-3.791091	0.153756
28	6	0	1.657015	-3.061221	2.165082
29	6	0	1.088475	-5.058847	0.299779
30	6	0	2.222853	-4.326294	2.303037
31	1	0	1.884810	-2.284656	2.889594
32	6	0	1.938720	-5.324067	1.372933
33	1	0	2.382863	-6.308307	1.481901
34	1	0	2.885306	-4.533640	3.137178
35	1	0	0.871245	-5.833846	-0.427860
36	1	0	-0.102422	-3.574577	-0.702283
37	6	0	-3.941735	-0.604844	-0.985897
38	6	0	-5.265025	-0.193375	-0.786279
39	6	0	-3.667087	-1.954986	-1.217231
40	6	0	-6.298400	-1.122336	-0.824713
41	1	0	-5.487093	0.852374	-0.585639
42	6	0	-4.701406	-2.887503	-1.246179
43	1	0	-2.638609	-2.274476	-1.370837
44	6	0	-6.015164	-2.469525	-1.053783
45	1	0	-7.323082	-0.800013	-0.671533
46	1	0	-4.482218	-3.935171	-1.422819
47	1	0	-6.822976	-3.193849	-1.080370
48	6	0	2.065641	2.244559	-1.774010
49	6	0	3.047290	3.225913	-1.947811
50	6	0	1.116648	2.428366	-0.767247
51	6	0	3.107802	4.335040	-1.105201
52	1	0	3.773494	3.120486	-2.751722
53	6	0	1.167476	3.533162	0.076644
54	1	0	0.326437	1.691058	-0.635946
55	6	0	2.171147	4.487141	-0.085656
56	1	0	3.881017	5.083687	-1.249596
57	1	0	0.433974	3.636908	0.870695
58	1	0	2.215340	5.349229	0.572692

59	6	0	0.925411	0.022648	1.823135
60	6	0	2.315133	0.136935	1.695073
61	6	0	0.215017	0.964708	2.572892
62	6	0	2.987243	1.168701	2.342021
63	1	0	2.870500	-0.575455	1.088851
64	6	0	0.896626	1.990647	3.224244
65	1	0	-0.868310	0.901851	2.640484
66	6	0	2.280899	2.093710	3.110327
67	1	0	4.064609	1.252356	2.236087
68	1	0	0.338701	2.717357	3.807476
69	1	0	2.808338	2.900298	3.609735
70	29	0	-0.416860	-0.254304	-1.188428
71	8	0	-2.880036	1.656251	-2.186094
72	1	0	-3.710355	2.138216	-2.053759
73	8	0	-1.431641	-1.325069	1.613163
74	1	0	-1.328320	-1.574223	2.544635
75	8	0	0.640909	0.093307	-2.746064

$Cu^{+}(PPh_2OH)_4$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.109254	-1.717030	-1.271546
2	15	0	-0.212721	-0.200313	2.146173
3	6	0	-0.068512	-3.185575	-1.520264
4	6	0	0.582704	-3.717666	-0.398887
5	6	0	0.171920	-3.725401	-2.784548
6	6	0	1.435601	-4.806611	-0.541353
7	1	0	0.434495	-3.271184	0.584533
8	6	0	1.038708	-4.807463	-2.923363
9	1	0	-0.301881	-3.295881	-3.662044
10	6	0	1.665122	-5.350460	-1.804405
11	6	0	-1.814509	0.395897	2.783641
12	6	0	-2.934333	-0.406689	2.527779
13	6	0	-1.978302	1.642605	3.394468
14	6	0	-4.203560	0.031292	2.893355
15	1	0	-2.814325	-1.372943	2.041636
16	6	0	-3.253017	2.079445	3.748604
17	1	0	-1.118014	2.272402	3.597694
18	6	0	-4.364820	1.276169	3.500061
19	1	0	-5.355549	1.620493	3.779206
20	1	0	2.345083	-6.188864	-1.917003
21	1	0	1.226158	-5.223664	-3.907878
22	1	0	1.942589	-5.210642	0.328814
23	1	0	-5.064872	-0.597332	2.690255

24	1	0	-3.376686	3.047153	4.223683
25	15	0	-0.943400	1.997736	-0.782404
26	6	0	-0.187195	2.766740	-2.243793
27	6	0	0.059338	1.948695	-3.354150
28	6	0	0.265732	4.087305	-2.235913
29	6	0	0.734097	2.462724	-4.457621
30	6	0	0.950745	4.592842	-3.338129
31	1	0	0.109556	4.714008	-1.363137
32	6	0	1.184670	3.782590	-4.447744
33	1	0	1.723380	4.177384	-5.303083
34	1	0	1.307765	5.617585	-3.327231
35	1	0	0.923708	1.828716	-5.317601
36	1	0	-0.261864	0.907401	-3.349073
37	15	0	2.214241	-0.169793	-0.852632
38	6	0	3.239776	1.292369	-0.481838
39	6	0	3.179196	2.379815	-1.362753
40	6	0	3.969027	1.401966	0.705464
41	6	0	3.860957	3.556256	-1.064517
42	1	0	2.602642	2.306728	-2.282328
43	6	0	4.646156	2.582224	0.998528
44	6	0	4.594701	3.658988	0.115833
45	1	0	3.811341	4.392611	-1.754996
46	1	0	5.211509	2.659194	1.921889
47	6	0	3.179856	-1.588229	-0.240461
48	6	0	3.951101	-2.379414	-1.093354
49	6	0	3.074598	-1.930799	1.112574
50	6	0	4.634037	-3.484167	-0.590719
51	6	0	3.770590	-3.025039	1.615832
52	1	0	2.439322	-1.348084	1.776228
53	6	0	4.553088	-3.802164	0.763002
54	1	0	5.124842	4.576895	0.348243
55	1	0	5.087953	-4.663131	1.151122
56	1	0	3.691330	-3.277095	2.668560
57	1	0	5.226970	-4.100543	-1.258768
58	1	0	4.012664	0.571295	1.405754
59	1	0	4.002978	-2.152332	-2.153724
60	6	0	1.054602	0.658386	3.129689
61	6	0	1.795537	-0.007405	4.109626
62	6	0	1.347454	1.993566	2.822028
63	6	0	2.810247	0.662094	4.789909
64	1	0	1.594571	-1.052006	4.329934
65	6	0	2.348516	2.662663	3.520141
66	1	0	0.797717	2.508133	2.034689
67	6	0	3.082009	1.997646	4.500930
68	1	0	3.386736	0.139941	5.546415
69	1	0	2.572155	3.696967	3.279612
70	1	0	3.872541	2.517139	5.032693
71	6	0	-2.668657	-2.330403	-0.556428
72	6	0	-2.733323	-3.462855	0.261170
73	6	0	-3.802251	-1.525201	-0.719189

74	6	0	-3.922263	-3.780669	0.913848
75	1	0	-1.863037	-4.098654	0.390534
76	6	0	-4.989706	-1.853440	-0.072555
77	1	0	-3.754275	-0.639348	-1.347691
78	6	0	-5.049431	-2.976916	0.750916
79	1	0	-3.967997	-4.660676	1.547017
80	1	0	-5.862571	-1.220988	-0.204772
81	1	0	-5.972869	-3.227850	1.262996
82	6	0	-2.732334	1.935653	-1.125191
83	6	0	-3.258119	1.795333	-2.413070
84	6	0	-3.587478	1.909587	-0.016692
85	6	0	-4.631147	1.636339	-2.586440
86	1	0	-2.603345	1.812163	-3.278881
87	6	0	-4.958879	1.757225	-0.197003
88	1	0	-3.178892	2.007408	0.986519
89	6	0	-5.481991	1.616951	-1.481294
90	1	0	-5.038427	1.531280	-3.586693
91	1	0	-5.612992	1.737229	0.669320
92	1	0	-6.550943	1.492994	-1.623016
93	29	0	-0.013300	-0.026098	-0.144383
94	8	0	-1.548251	-1.206232	-2.773411
95	1	0	-2.158712	-1.803749	-3.232555
96	8	0	-0.845998	3.121452	0.416610
97	1	0	-1.427587	3.886655	0.286989
98	8	0	-0.164746	-1.766604	2.652278
99	1	0	-0.485400	-1.896361	3.558722
100	8	0	2.300308	-0.277732	-2.491305
101	1	0	3.182894	-0.090469	-2.847048

$Cu^{+}(Ph_2POH)(NEt_3)$ (8)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.300499	-1.874278	-0.065028
2	6	0	4.759103	-2.245240	-0.303598
3	29	0	1.037660	-0.317203	0.277887
4	1	0	2.981823	-2.250059	0.912661
5	1	0	2.670462	-2.362184	-0.815104
6	1	0	5.434971	-1.704096	0.363870
7	1	0	4.882892	-3.312730	-0.106911
8	1	0	5.061470	-2.064639	-1.337061
9	6	0	3.578542	0.310429	1.045331
10	1	0	3.446408	-0.305778	1.940089
11	1	0	4.655249	0.431679	0.890341
12	6	0	2.905244	1.658998	1.251201

13	1	0	3.018376	2.317107	0.384669
14	1	0	1.833405	1.514557	1.432090
15	1	0	3.324917	2.170468	2.118569
16	6	0	3.214379	0.223264	-1.408289
17	1	0	2.959029	-0.520818	-2.168682
18	1	0	2.499386	1.044418	-1.527564
19	6	0	4.616190	0.777834	-1.650462
20	1	0	5.400391	0.034548	-1.504818
21	1	0	4.668863	1.125885	-2.684625
22	1	0	4.831306	1.633925	-1.006245
23	7	0	2.957174	-0.425011	-0.084731
24	15	0	-1.085843	-0.083202	0.735032
25	6	0	-1.672049	1.534925	0.181795
26	6	0	-0.700365	2.451622	-0.228649
27	6	0	-3.022904	1.902260	0.184411
28	6	0	-1.067267	3.731162	-0.632604
29	1	0	0.341965	2.142833	-0.229728
30	6	0	-3.387596	3.183235	-0.213432
31	1	0	-3.785250	1.187195	0.482799
32	6	0	-2.411398	4.094417	-0.620277
33	1	0	-0.310757	4.438247	-0.954937
34	1	0	-4.433055	3.472373	-0.212772
35	1	0	-2.703665	5.091288	-0.933320
36	6	0	-2.269832	-1.277622	0.061061
37	6	0	-2.777134	-1.125959	-1.233979
38	6	0	-2.604176	-2.404578	0.817943
39	6	0	-3.626743	-2.093650	-1.760287
40	1	0	-2.520037	-0.250509	-1.824030
41	6	0	-3.460010	-3.365576	0.286998
42	1	0	-2.202404	-2.522266	1.819933
43	6	0	-3.970165	-3.210602	-1.000028
44	1	0	-4.026969	-1.972720	-2.761220
45	1	0	-3.727692	-4.234922	0.877993
46	1	0	-4.637720	-3.960177	-1.411834
47	8	0	-1.298196	-0.167900	2.355529
48	1	0	-2.208421	-0.002280	2.647889

$Cu^{3+}(Ph_2POH)(NEt_3)$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.081339	-0.100064	-0.356193
2	6	0	4.397568	0.352752	-0.982291
3	29	0	0.837506	-0.529627	-0.121806
4	1	0	3.291156	-0.671287	0.552502
5	1	0	2.607263	-0.783971	-1.102027
6	1	0	4.914803	1.045270	-0.315435
7	1	0	5.023888	-0.531244	-1.108379
8	1	0	4.251156	0.811139	-1.959809
9	6	0	2.381053	1.594382	1.308536
10	1	0	2.576473	0.798209	2.030720
11	1	0	3.311917	2.159049	1.186031
12	6	0	1.268694	2.494917	1.806807
13	1	0	1.011525	3.285193	1.098922
14	1	0	0.372607	1.911996	2.036583
15	1	0	1.588172	2.967301	2.736961
16	6	0	1.815775	1.932382	-1.115400
17	1	0	1.865067	1.366490	-2.050509
18	1	0	0.790176	2.291822	-1.005070
19	6	0	2.754844	3.134317	-1.167173
20	1	0	3.804156	2.858198	-1.257184
21	1	0	2.484264	3.715216	-2.051103
22	1	0	2.636944	3.784739	-0.299189
23	7	0	2.075807	0.950929	-0.002228
24	15	0	-1.137989	-0.294538	0.934744
25	6	0	-2.316342	0.710636	0.160133
26	6	0	-2.333833	2.100756	0.410765
27	6	0	-3.237746	0.093405	-0.718110
28	6	0	-3.295957	2.868788	-0.217316
29	1	0	-1.609516	2.561881	1.073837
30	6	0	-4.189084	0.890673	-1.328769
31	1	0	-3.236089	-0.979506	-0.879792
32	6	0	-4.214250	2.266519	-1.083574
33	1	0	-3.331208	3.936573	-0.039137
34	1	0	-4.920207	0.440687	-1.989539
35	1	0	-4.963559	2.879347	-1.572765
36	6	0	-0.771296	-1.897595	0.329988
37	6	0	-0.579233	-2.029970	-1.081705
38	6	0	-0.473217	-2.961613	1.220072
39	6	0	-0.133531	-3.247929	-1.580187
40	1	0	-0.882248	-1.244185	-1.774961
41	6	0	-0.055380	-4.163632	0.683121
42	1	0	-0.597412	-2.832604	2.289960
43	6	0	0.119213	-4.304425	-0.703255

44	1	0	-0.002053	-3.374425	-2.648043
45	1	0	0.141087	-5.002913	1.339993
46	1	0	0.457634	-5.255018	-1.100884
47	8	0	-0.890595	-0.211825	2.472510
48	1	0	-1.521411	0.271607	3.042364

$Cu^{+}(NEt_3)_2$ (**9**)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.392767	-0.748831	-1.034869
2	6	0	-2.348945	1.277683	0.882055
3	6	0	-3.843304	1.501653	1.080775
4	29	0	-0.002695	0.193075	-0.006458
5	1	0	-1.867588	1.122832	1.852995
6	1	0	-1.902814	2.175232	0.442911
7	1	0	-4.357780	0.598037	1.417552
8	1	0	-3.977838	2.265273	1.850460
9	1	0	-4.323901	1.865775	0.170775
10	6	0	-2.282361	-1.174914	0.655843
11	1	0	-1.959020	-1.122775	1.700739
12	1	0	-3.367333	-1.323236	0.662294
13	6	0	-1.591290	-2.337308	-0.041733
14	1	0	-1.922628	-2.455465	-1.076289
15	1	0	-0.507565	-2.179537	-0.048780
16	1	0	-1.795429	-3.269834	0.487096
17	6	0	-2.422446	0.232931	-1.380138
18	1	0	-2.346950	1.290583	-1.650227
19	1	0	-1.713529	-0.304498	-2.017825
20	6	0	-3.824575	-0.294882	-1.674753
21	1	0	-4.594567	0.159598	-1.051466
22	1	0	-4.058484	-0.068756	-2.717704
23	1	0	-3.884098	-1.379203	-1.554195
24	7	0	-1.934584	0.125350	0.030212
25	7	0	1.930002	0.234237	-0.005229
26	1	0	2.274687	-0.256073	-2.004556
27	1	0	1.694216	-1.591577	-1.027945
28	6	0	3.807224	-1.303810	-0.885345
29	1	0	3.902440	-1.940667	-0.002432
30	1	0	4.021590	-1.922845	-1.759565
31	1	0	4.569153	-0.526290	-0.829230
32	6	0	2.301257	1.640049	-0.337897
33	1	0	1.844062	2.266400	0.434556
34	1	0	1.804765	1.883378	-1.282149
35	6	0	3.786749	1.962877	-0.445114

36	1	0	3.898870	3.045951	-0.535281
37	1	0	4.343606	1.644276	0.439835
38	1	0	4.238634	1.511321	-1.330280
39	6	0	2.354340	-0.137981	1.368147
40	1	0	3.443435	-0.233999	1.422964
41	1	0	2.066823	0.687714	2.025939
42	6	0	1.682212	-1.420909	1.832421
43	1	0	1.936532	-2.275286	1.198727
44	1	0	1.987876	-1.659404	2.852428
45	1	0	0.593303	-1.302550	1.824685

$Cu^{3+}(NEt_3)_2$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.937710	-0.096420	-1.258985
2	6	0	-1.765365	1.112612	1.238312
3	6	0	-3.213175	1.621749	1.312743
4	29	0	0.058923	-0.876879	0.168890
5	1	0	-1.494016	0.606993	2.168507
6	1	0	-1.102567	1.959693	1.065299
7	1	0	-3.928291	0.809053	1.450292
8	1	0	-3.255908	2.269755	2.190340
9	1	0	-3.475255	2.218942	0.440230
10	6	0	-2.289062	-1.140880	0.314094
11	1	0	-2.312546	-1.352842	1.385382
12	1	0	-3.315916	-1.031821	-0.045729
13	6	0	-1.609479	-2.284786	-0.473333
14	1	0	-1.530914	-2.101507	-1.547329
15	1	0	-0.643312	-2.669538	-0.074347
16	1	0	-2.226137	-3.175373	-0.328031
17	6	0	-1.711775	0.770377	-1.257981
18	1	0	-1.493175	1.831674	-1.137470
19	1	0	-0.952628	0.337741	-1.922037
20	6	0	-3.079262	0.570598	-1.914241
21	1	0	-3.896232	0.933829	-1.290822
22	1	0	-3.061233	1.160873	-2.831977
23	1	0	-3.258564	-0.468845	-2.192087
24	7	0	-1.578526	0.155371	0.112357
25	7	0	1.516147	0.372702	0.101396
26	1	0	1.565867	0.636846	-1.975584
27	1	0	1.443450	-1.061115	-1.488663
28	6	0	3.439951	-0.349815	-1.419575
29	1	0	3.782619	-1.211917	-0.847565
30	1	0	3.599183	-0.563576	-2.477484

31	1	0	4.023111	0.530040	-1.149688
32	6	0	1.334411	1.836970	0.219514
33	1	0	0.973904	2.046226	1.226388
34	1	0	0.603795	2.154388	-0.528041
35	6	0	2.653512	2.589556	-0.023372
36	1	0	2.434498	3.643206	0.159168
37	1	0	3.436150	2.276842	0.669372
38	1	0	2.991208	2.484924	-1.054202
39	6	0	2.234416	-0.253901	1.257166
40	1	0	3.307907	-0.103702	1.112464
41	1	0	1.921471	0.275808	2.158751
42	6	0	1.910180	-1.748814	1.356063
43	1	0	2.224901	-2.351053	0.498800
44	1	0	2.451016	-2.147097	2.218801
45	1	0	0.863137	-1.968947	1.650767

$Cu^{+}[(4\text{-}MeC_6H_4)_2POH]$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.017634	1.004203	0.487085
2	6	0	-1.481965	-0.005228	0.189548
3	6	0	-1.482515	-1.022799	-0.768255
4	6	0	-2.663093	0.300976	0.874229
5	6	0	-2.650410	-1.733869	-1.021669
6	1	0	-0.572616	-1.267515	-1.309369
7	6	0	-3.821374	-0.420515	0.615702
8	1	0	-2.671225	1.097986	1.612397
9	6	0	-3.832927	-1.449008	-0.332644
10	6	0	1.393236	-0.092958	0.278237
11	6	0	2.486269	0.413231	-0.426904
12	6	0	1.457925	-1.386095	0.813794
13	6	0	3.633465	-0.352280	-0.597177
14	1	0	2.419835	1.415556	-0.843021
15	6	0	2.608567	-2.142092	0.646755
16	1	0	0.608596	-1.803065	1.349505
17	6	0	3.710577	-1.638852	-0.059784
18	1	0	2.660677	-3.142542	1.066847
19	1	0	4.476883	0.052000	-1.148822
20	1	0	-2.643347	-2.527577	-1.763331
21	1	0	-4.733566	-0.182437	1.155601
22	29	0	0.250614	2.769901	-0.691142
23	8	0	-0.132983	1.418539	2.065433
24	1	0	-0.263698	0.664166	2.661709
25	6	0	-5.086998	-2.242356	-0.585537

26	1	0	-5.216406	-3.009062	0.184973
27	1	0	-5.970402	-1.600177	-0.560115
28	1	0	-5.049573	-2.745313	-1.553779
29	6	0	4.939115	-2.486645	-0.249005
30	1	0	4.763669	-3.246894	-1.016628
31	1	0	5.793373	-1.883412	-0.560991
32	1	0	5.199151	-3.009252	0.674655

$Cu^{+}[(4\text{-}MeC_6H_4)_2POH]_2$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	0.594439	-1.981020	-1.359960
2	6	0	-0.665193	-2.245908	-0.092030
3	6	0	-1.840865	-2.927385	-0.427893
4	6	0	-0.573559	-1.599659	1.142645
5	6	0	-2.903720	-2.956815	0.464438
6	1	0	-1.916401	-3.432674	-1.386673
7	6	0	-1.652754	-1.621045	2.022124
8	1	0	0.338393	-1.074251	1.414937
9	6	0	-2.834083	-2.287519	1.693120
10	1	0	-3.813047	-3.489945	0.199160
11	1	0	-1.577016	-1.105048	2.975486
12	15	0	-0.589067	1.846796	-1.456832
13	6	0	0.660316	2.278085	-0.221555
14	6	0	0.592313	1.784375	1.085281
15	6	0	1.817128	2.940719	-0.645687
16	6	0	1.669599	1.949163	1.948471
17	1	0	-0.303974	1.274908	1.428776
18	6	0	2.884706	3.107878	0.229091
19	6	0	2.834510	2.599929	1.531413
20	1	0	1.607833	1.562837	2.962250
21	1	0	3.776936	3.629923	-0.105985
22	1	0	1.880183	3.325260	-1.660395
23	6	0	2.133570	-1.746924	-0.450228
24	6	0	2.649667	-2.715035	0.422125
25	6	0	2.820402	-0.546272	-0.628531
26	6	0	3.837225	-2.471020	1.095083
27	1	0	2.117994	-3.650812	0.572601
28	6	0	4.007723	-0.304752	0.057312
29	1	0	2.410810	0.210269	-1.293906
30	6	0	4.532355	-1.263696	0.924026
31	1	0	4.239080	-3.222950	1.768698
32	1	0	4.528643	0.637834	-0.087285
33	6	0	-2.124864	1.649050	-0.529908
34	6	0	-2.584198	2.572244	0.420497
35	6	0	-2.876559	0.499679	-0.781174

36	6	0	-3.775165	2.339190	1.092168
37	1	0	-2.002771	3.462291	0.648588
38	6	0	-4.067952	0.269976	-0.100635
39	1	0	-2.510033	-0.234048	-1.495161
40	6	0	-4.533905	1.185862	0.842936
41	1	0	-4.127857	3.057717	1.826825
42	1	0	-4.635289	-0.634475	-0.302042
43	29	0	0.004512	-0.089205	-2.373953
44	8	0	-0.688794	3.165309	-2.421258
45	1	0	-0.837417	3.996827	-1.944492
46	8	0	0.635013	-3.466109	-2.053149
47	1	0	0.929739	-3.420268	-2.972730
48	6	0	-5.812102	0.942931	1.599945
49	1	0	-5.597460	0.678053	2.640275
50	1	0	-6.434800	1.841135	1.613843
51	1	0	-6.387831	0.128945	1.154978
52	6	0	-4.015845	-2.285296	2.625159
53	1	0	-4.936685	-2.052116	2.081840
54	1	0	-4.150604	-3.267384	3.088955
55	1	0	-3.890239	-1.548406	3.421248
56	6	0	5.814750	-1.017870	1.673619
57	1	0	5.626848	-0.955049	2.750020
58	1	0	6.522079	-1.836455	1.515169
59	1	0	6.288719	-0.087423	1.354537
60	6	0	4.020316	2.709345	2.451011
61	1	0	4.597878	1.777815	2.430568
62	1	0	4.684973	3.521790	2.150654
63	1	0	3.707250	2.877032	3.484112

$Cu^{+}[(4\text{-}MeC_6H_4)_2POH]_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.707393	-0.026691	-2.208986
2	15	0	-1.579356	-0.186026	1.451630
3	6	0	-2.165923	-0.669270	-3.071092
4	6	0	-3.335491	-0.891734	-2.333591
5	6	0	-2.140587	-0.986043	-4.430411
6	6	0	-4.468111	-1.395253	-2.963333
7	1	0	-3.365522	-0.656490	-1.270308
8	6	0	-3.277437	-1.499421	-5.046629
9	1	0	-1.232632	-0.843660	-5.008419
10	6	0	-4.456304	-1.709492	-4.325907
11	6	0	-0.802627	1.239407	2.266917
12	6	0	-0.833028	2.475666	1.615761

13	6	0	-0.044886	1.098491	3.436331
14	6	0	-0.132933	3.559080	2.140348
15	1	0	-1.405087	2.593423	0.698837
16	6	0	0.643700	2.188567	3.953777
17	1	0	0.006040	0.138160	3.941337
18	6	0	0.614077	3.433844	3.313634
19	1	0	-3.249451	-1.742317	-6.105329
20	1	0	-5.375725	-1.554592	-2.387603
21	1	0	-0.164339	4.514831	1.622317
22	1	0	1.218496	2.074380	4.869062
23	15	0	2.013047	-1.076308	0.438931
24	6	0	3.129337	-2.358276	-0.180703
25	6	0	2.575486	-3.526541	-0.708515
26	6	0	4.524402	-2.242797	-0.095859
27	6	0	3.399064	-4.558443	-1.150966
28	6	0	5.338326	-3.277135	-0.533549
29	1	0	4.973809	-1.335850	0.301611
30	6	0	4.788461	-4.448957	-1.070562
31	1	0	6.418200	-3.178684	-0.464190
32	1	0	2.956902	-5.460342	-1.563816
33	1	0	1.495434	-3.632213	-0.779117
34	6	0	-2.152362	-1.243621	2.801193
35	6	0	-2.736268	-0.728192	3.967522
36	6	0	-2.050966	-2.628047	2.645833
37	6	0	-3.205363	-1.586893	4.950218
38	1	0	-2.810196	0.347264	4.111857
39	6	0	-2.519389	-3.483775	3.639205
40	1	0	-1.602380	-3.041405	1.745278
41	6	0	-3.102675	-2.977364	4.801569
42	1	0	-3.654902	-1.179707	5.851768
43	1	0	-2.431181	-4.558368	3.509198
44	6	0	-0.996567	1.761383	-2.019373
45	6	0	-2.275582	2.325070	-1.960107
46	6	0	0.118073	2.572599	-1.797491
47	6	0	-2.426746	3.679472	-1.689730
48	1	0	-3.154571	1.708490	-2.124425
49	6	0	-0.046017	3.929715	-1.534150
50	1	0	1.116660	2.148130	-1.829006
51	6	0	-1.317901	4.502021	-1.470042
52	1	0	-3.424044	4.109334	-1.647936
53	1	0	0.830168	4.548505	-1.362548
54	6	0	2.834159	0.483989	-0.002177
55	6	0	3.499592	0.639968	-1.223467
56	6	0	2.646332	1.598122	0.821340
57	6	0	3.999817	1.884815	-1.590982
58	1	0	3.627555	-0.209614	-1.888736
59	6	0	3.149366	2.837924	0.442597
60	1	0	2.103176	1.497209	1.757216
61	6	0	3.839008	3.000307	-0.763069
62	1	0	4.520992	1.994319	-2.538032

63	1	0	2.991545	3.697616	1.090168
64	29	0	-0.152374	-0.863485	-0.183596
65	8	0	-2.921464	0.479727	0.760745
66	1	0	-3.462023	0.999470	1.375816
67	8	0	2.118694	-1.097262	2.082012
68	1	0	3.017543	-0.953970	2.415917
69	8	0	0.528218	-0.095807	-3.289194
70	1	0	0.447033	0.545363	-4.012187
71	6	0	4.407554	4.339483	-1.152542
72	1	0	5.415689	4.462067	-0.743566
73	1	0	4.476160	4.440663	-2.237896
74	1	0	3.795486	5.157871	-0.764326
75	6	0	5.688113	-5.550745	-1.563501
76	1	0	6.203395	-5.243842	-2.478956
77	1	0	6.455384	-5.788678	-0.822133
78	1	0	5.122880	-6.458534	-1.781595
79	6	0	-5.673634	-2.293808	-4.992732
80	1	0	-5.714104	-2.020697	-6.049477
81	1	0	-5.656022	-3.386965	-4.934090
82	1	0	-6.591521	-1.952107	-4.509368
83	6	0	-1.503165	5.964254	-1.160035
84	1	0	-2.061606	6.465099	-1.955960
85	1	0	-2.070311	6.096020	-0.233232
86	1	0	-0.541632	6.469206	-1.046534
87	6	0	1.392259	4.595720	3.872944
88	1	0	1.191285	4.726290	4.939639
89	1	0	2.468883	4.427687	3.764361
90	1	0	1.141312	5.525452	3.358437
91	6	0	-3.605866	-3.893020	5.885248
92	1	0	-3.029872	-3.754626	6.805119
93	1	0	-4.651574	-3.677070	6.121059
94	1	0	-3.528347	-4.940362	5.588430

$Cu^{+}[(4\text{-}MeC_6H_4)_2POH]_4$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.076139	1.842257	-1.208265
2	15	0	0.085088	0.100919	2.021669
3	6	0	0.017292	3.308578	-1.355927
4	6	0	-0.648281	3.761224	-0.208817
5	6	0	-0.205447	3.949456	-2.574420
6	6	0	-1.479113	4.871226	-0.280314
7	1	0	-0.516840	3.244093	0.741843
8	6	0	-1.063913	5.044397	-2.638997

9	1	0	0.279052	3.590126	-3.477503
10	6	0	-1.707158	5.523742	-1.496508
11	6	0	1.655505	-0.489293	2.735944
12	6	0	2.770885	0.345409	2.606121
13	6	0	1.819589	-1.767567	3.281369
14	6	0	4.025510	-0.091001	3.021544
15	1	0	2.664615	1.338802	2.175399
16	6	0	3.079616	-2.195681	3.684473
17	1	0	0.967871	-2.431269	3.392789
18	6	0	4.201972	-1.368280	3.558434
19	1	0	-1.235577	5.534321	-3.593696
20	1	0	-1.979673	5.223706	0.617970
21	1	0	4.882324	0.568711	2.906148
22	1	0	3.197078	-3.190156	4.107106
23	15	0	1.061896	-1.950347	-0.967945
24	6	0	0.484692	-2.683123	-2.526765
25	6	0	0.195512	-1.822807	-3.592929
26	6	0	0.252786	-4.052526	-2.669777
27	6	0	-0.283801	-2.337020	-4.791980
28	6	0	-0.244363	-4.554621	-3.868782
29	1	0	0.436187	-4.729636	-1.840243
30	6	0	-0.511732	-3.708303	-4.948269
31	1	0	-0.431365	-5.620335	-3.967469
32	1	0	-0.503021	-1.662454	-5.615200
33	1	0	0.341878	-0.748887	-3.484348
34	15	0	-2.240062	0.026758	-0.957550
35	6	0	-3.258448	-1.361013	-0.353890
36	6	0	-2.827466	-2.648245	-0.707857
37	6	0	-4.388197	-1.224528	0.453137
38	6	0	-3.514758	-3.768274	-0.262415
39	1	0	-1.955195	-2.768857	-1.348404
40	6	0	-5.065492	-2.355087	0.904802
41	6	0	-4.639193	-3.638900	0.562570
42	1	0	-3.172096	-4.758981	-0.550208
43	1	0	-5.945497	-2.234301	1.531916
44	6	0	-3.182010	1.510218	-0.495478
45	6	0	-3.782158	2.327287	-1.451438
46	6	0	-3.253911	1.871912	0.856094
47	6	0	-4.470051	3.473459	-1.058441
48	6	0	-3.948420	3.011234	1.238996
49	1	0	-2.775061	1.250587	1.611892
50	6	0	-4.566267	3.831365	0.286499
51	1	0	-4.006406	3.277254	2.291481
52	1	0	-4.939472	4.099718	-1.812947
53	1	0	-4.747877	-0.239825	0.734479
54	1	0	-3.704906	2.079201	-2.505725
55	6	0	-1.221027	-0.845922	2.854903
56	6	0	-2.078306	-0.276963	3.796604
57	6	0	-1.427586	-2.173158	2.450577
58	6	0	-3.125152	-1.027477	4.330410

59	1	0	-1.945353	0.757099	4.103374
60	6	0	-2.454686	-2.918250	3.010560
61	1	0	-0.783200	-2.622129	1.695530
62	6	0	-3.327109	-2.354055	3.948834
63	1	0	-3.795387	-0.573155	5.054967
64	1	0	-2.602024	-3.948306	2.695504
65	6	0	2.576863	2.419921	-0.349316
66	6	0	2.589108	3.491662	0.550037
67	6	0	3.735138	1.652192	-0.508586
68	6	0	3.737882	3.775029	1.280928
69	1	0	1.706156	4.107917	0.685763
70	6	0	4.882420	1.952253	0.219095
71	1	0	3.741905	0.813667	-1.200629
72	6	0	4.900346	3.010275	1.130829
73	1	0	3.734939	4.607642	1.979622
74	1	0	5.772592	1.341507	0.086086
75	6	0	2.866179	-1.800001	-1.167681
76	6	0	3.465744	-1.561091	-2.409091
77	6	0	3.655953	-1.792279	-0.013364
78	6	0	4.833016	-1.322662	-2.486500
79	1	0	2.867187	-1.558906	-3.315255
80	6	0	5.024715	-1.557161	-0.104073
81	1	0	3.204638	-1.962580	0.961426
82	6	0	5.633830	-1.313862	-1.336956
83	1	0	5.290768	-1.139547	-3.455173
84	1	0	5.623221	-1.544784	0.804039
85	29	0	0.011918	0.005646	-0.290482
86	8	0	1.613681	1.522846	-2.731566
87	1	0	2.217555	2.197582	-3.079139
88	8	0	0.919787	-3.146495	0.157326
89	1	0	1.568493	-3.860063	0.054300
90	8	0	-0.044474	1.638496	2.599051
91	1	0	0.207844	1.726792	3.531521
92	8	0	-2.388815	-0.065913	-2.595491
93	1	0	-3.296110	-0.243058	-2.887923
94	6	0	-4.472171	-3.163179	4.495469
95	1	0	-4.130549	-4.140440	4.848015
96	1	0	-4.966675	-2.650433	5.322795
97	1	0	-5.218076	-3.342352	3.713076
98	6	0	5.561216	-1.856154	3.986917
99	1	0	5.566912	-2.113340	5.050161
100	1	0	5.842883	-2.757306	3.433816
101	1	0	6.326295	-1.096161	3.815431
102	6	0	-5.270273	5.094253	0.707391
103	1	0	-5.936829	5.458488	-0.077628
104	1	0	-5.856652	4.937140	1.616298
105	1	0	-4.543197	5.886477	0.920479
106	6	0	-5.344382	-4.859568	1.091619
107	1	0	-6.334994	-4.609708	1.478411
108	1	0	-5.456943	-5.620671	0.315311

109	1	0	-4.771572	-5.311473	1.909757
110	6	0	-2.666429	6.681256	-1.573776
111	1	0	-2.440405	7.330999	-2.422127
112	1	0	-3.692654	6.316396	-1.697897
113	1	0	-2.640248	7.280039	-0.659803
114	6	0	6.136515	3.333785	1.928592
115	1	0	6.584577	4.271732	1.586164
116	1	0	5.898146	3.455053	2.988959
117	1	0	6.887450	2.546767	1.831207
118	6	0	7.112486	-1.045640	-1.439372
119	1	0	7.621061	-1.861048	-1.962569
120	1	0	7.304713	-0.127822	-2.002488
121	1	0	7.565551	-0.943759	-0.450827
122	6	0	-1.024107	-4.255351	-6.254649
123	1	0	-0.205787	-4.362894	-6.973849
124	1	0	-1.481458	-5.237751	-6.120856
125	1	0	-1.763957	-3.584997	-6.698638

$Cu^{+}(NEt_3)$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.753180	-0.496468	0.509583
2	6	0	-2.434596	-0.103862	-0.790127
3	29	0	0.687206	-0.034995	-1.066108
4	1	0	-1.709700	-1.586174	0.582481
5	1	0	-2.309026	-0.134181	1.383887
6	1	0	-1.920303	-0.569404	-1.637390
7	1	0	-3.472628	-0.442370	-0.795556
8	1	0	-2.434113	0.979283	-0.940840
9	6	0	-0.330574	1.436367	1.015977
10	1	0	-1.222289	1.929876	0.622945
11	1	0	-0.376650	1.490047	2.110295
12	6	0	0.912707	2.121695	0.469162
13	1	0	1.833459	1.682220	0.863895
14	1	0	0.918976	2.036087	-0.628731
15	1	0	0.923599	3.184660	0.714298
16	6	0	0.493818	-0.846293	1.425139
17	1	0	1.325663	-0.244771	1.800083
18	1	0	-0.071475	-1.199018	2.295358
19	6	0	1.038705	-2.005596	0.599551
20	1	0	1.690056	-1.617399	-0.201083
21	1	0	1.644989	-2.678188	1.207890
22	1	0	0.239203	-2.592464	0.138976
23	7	0	-0.364288	0.020227	0.574987

$Cu^{+}(NEt_3)_2$ (**9**)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.479969	0.431927	1.125342
2	6	0	-2.491723	-0.576377	-1.042801
3	6	0	-4.013392	-0.642168	-1.086232
4	29	0	0.003982	0.034339	-0.041661
5	1	0	-2.103968	-0.184176	-1.987356
6	1	0	-2.084075	-1.584441	-0.931494
7	1	0	-4.465976	0.345554	-1.200216
8	1	0	-4.310217	-1.243963	-1.947844
9	1	0	-4.430209	-1.115764	-0.193993
10	6	0	-2.229110	1.706543	-0.196348

11	1	0	-2.005447	1.910096	-1.247915
12	1	0	-3.301802	1.876873	-0.046390
13	6	0	-1.422124	2.647481	0.687139
14	1	0	-1.726303	2.605963	1.734479
15	1	0	-0.355763	2.401559	0.627796
16	1	0	-1.552895	3.675219	0.343406
17	6	0	-2.363058	-0.153947	1.387302
18	1	0	-1.867972	0.494109	2.113439
19	1	0	-3.442593	0.015927	1.483088
20	6	0	-2.010635	-1.601996	1.692171
21	1	0	-0.944916	-1.778000	1.504738
22	1	0	-2.207662	-1.815379	2.744030
23	1	0	-2.588016	-2.309780	1.092987
24	7	0	-1.908463	0.272836	0.037183
25	7	0	1.908641	-0.269966	-0.062373
26	1	0	2.007223	-0.014083	2.005682
27	1	0	2.150487	1.473600	1.086807
28	6	0	3.996381	0.368960	1.259180
29	1	0	4.504098	0.886522	0.441575
30	1	0	4.285158	0.860841	2.190450
31	1	0	4.360604	-0.660413	1.299877
32	6	0	2.122151	-1.739643	0.043408
33	1	0	1.938503	-2.016566	1.086162
34	1	0	3.167805	-1.979742	-0.181977
35	6	0	1.191545	-2.535452	-0.860469
36	1	0	1.357712	-3.604108	-0.712249
37	1	0	0.146418	-2.318727	-0.616796
38	1	0	1.348538	-2.318045	-1.919009
39	6	0	2.477050	0.245233	-1.337328
40	1	0	3.546722	0.006332	-1.380744
41	1	0	1.992326	-0.297187	-2.151929
42	6	0	2.248269	1.736975	-1.522847
43	1	0	2.840231	2.339274	-0.829995
44	1	0	2.523523	2.027166	-2.538307
45	1	0	1.189811	1.980200	-1.374897

$Cu^{+}(NEt_3)_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.533298	1.861282	-1.117077
2	6	0	-1.583929	-2.052109	1.197666
3	6	0	-2.255274	-3.402476	1.441185
4	29	0	0.117745	-0.039725	-0.072367
5	1	0	-0.666560	-1.994622	1.796254

6	1	0	-2.236189	-1.250906	1.553313
7	1	0	-1.581177	-4.238784	1.244649
8	1	0	-2.557687	-3.460347	2.489349
9	1	0	-3.151940	-3.533061	0.829316
10	6	0	-0.270048	-2.787839	-0.692482
11	1	0	0.500555	-2.914879	0.071300
12	1	0	-0.790427	-3.750632	-0.782796
13	6	0	0.353765	-2.415464	-2.026572
14	1	0	-0.349187	-2.507512	-2.856388
15	1	0	0.693350	-1.377692	-1.971222
16	1	0	1.213431	-3.054536	-2.243888
17	6	0	-2.383078	-1.771479	-1.127123
18	1	0	-2.066765	-1.313647	-2.069111
19	1	0	-2.610491	-2.822747	-1.356830
20	6	0	-3.673649	-1.108947	-0.662908
21	1	0	-3.605501	-0.022966	-0.591119
22	1	0	-4.440651	-1.328504	-1.409691
23	1	0	-4.031418	-1.497055	0.293367
24	7	0	-1.205121	-1.742329	-0.206213
25	7	0	-0.919176	1.783780	0.236926
26	1	0	-1.924310	0.866329	-1.348122
27	1	0	-0.730878	2.050445	-1.834399
28	6	0	-2.642343	2.893511	-1.306678
29	1	0	-2.333758	3.892218	-0.984758
30	1	0	-2.897665	2.948480	-2.367350
31	1	0	-3.550758	2.627498	-0.760918
32	6	0	-1.983868	1.558855	1.247759
33	1	0	-2.585785	0.715091	0.906406
34	1	0	-2.643386	2.436812	1.278752
35	6	0	-1.484422	1.274829	2.656629
36	1	0	-0.871272	2.086574	3.055113
37	1	0	-2.349006	1.160808	3.315365
38	1	0	-0.907852	0.347255	2.708723
39	6	0	-0.218090	3.049806	0.595048
40	1	0	-0.953913	3.767539	0.987096
41	1	0	0.462178	2.822158	1.418613
42	6	0	0.556695	3.716778	-0.531773
43	1	0	-0.101154	4.176333	-1.272861
44	1	0	1.182770	4.505020	-0.107770
45	1	0	1.207721	3.015643	-1.055060
46	7	0	2.236542	-0.240186	-0.086986
47	6	0	2.669559	-1.509993	0.566102
48	1	0	2.413313	-2.314599	-0.127425
49	1	0	2.061499	-1.656317	1.464902
50	6	0	2.878921	-0.155830	-1.424787
51	1	0	3.951586	0.046028	-1.311761
52	1	0	2.788193	-1.139099	-1.891606
53	6	0	2.668692	0.926525	0.724846
54	1	0	2.318231	1.826757	0.215093
55	1	0	3.764877	0.983870	0.751388

56	6	0	4.148485	-1.624013	0.928828
57	1	0	4.450795	-0.896291	1.685608
58	1	0	4.326164	-2.619891	1.341109
59	1	0	4.796786	-1.507289	0.057332
60	6	0	2.093737	0.881849	2.128593
61	1	0	1.023487	0.672023	2.049979
62	1	0	2.554046	0.110841	2.750540
63	1	0	2.224571	1.842680	2.630971
64	6	0	2.249527	0.894538	-2.325794
65	1	0	1.157077	0.853955	-2.242017
66	1	0	2.580790	1.904552	-2.078102
67	1	0	2.517693	0.706711	-3.367552

$Cu^{+}(NEt_3)_4$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.748575	0.211359	0.619100
2	1	0	-3.743899	1.018134	-0.123243
3	1	0	-4.481267	0.486181	1.388595
4	6	0	-2.140376	1.525522	1.812168
5	1	0	-2.224430	2.226671	0.984353
6	1	0	-1.100588	1.554315	2.147336
7	6	0	3.247704	-1.120170	1.778052
8	1	0	2.208635	-1.185362	2.122301
9	1	0	3.454513	-2.061846	1.254595
10	6	0	4.605744	-0.083947	0.062695
11	1	0	4.764934	-1.122001	-0.251477
12	1	0	5.451190	0.183255	0.720811
13	6	0	0.353529	-1.943678	-2.462312
14	1	0	-0.378275	-1.448495	-3.107387
15	1	0	0.444940	-2.973655	-2.827565
16	6	0	0.995450	2.119095	-1.145084
17	1	0	1.100629	2.654200	-0.201963
18	1	0	1.528905	1.175317	-0.995168
19	6	0	-1.270275	3.051442	-1.161550
20	1	0	-1.273118	3.595828	-2.117474
21	1	0	-2.306074	2.743102	-0.991652
22	6	0	-1.424978	-2.825540	-1.111575
23	1	0	-1.900782	-2.758750	-0.130246
24	1	0	-2.114134	-2.373788	-1.831641
25	6	0	-0.715557	1.265816	-2.658984
26	1	0	-0.678333	2.064996	-3.411355
27	1	0	0.085797	0.568715	-2.907014
28	6	0	3.063586	1.270328	1.353271

29	1	0	3.842214	1.566437	2.078750
30	1	0	3.111254	2.001726	0.541626
31	6	0	0.838320	-2.548960	-0.193690
32	1	0	1.598086	-1.773826	-0.057753
33	1	0	1.318179	-3.393505	-0.711030
34	6	0	-2.368880	-0.854442	2.307370
35	1	0	-3.310776	-0.816887	2.874703
36	1	0	-2.332769	-1.834466	1.824220
37	6	0	-2.056756	0.555860	-2.736379
38	1	0	-2.896119	1.206917	-2.481230
39	1	0	-2.230332	0.169949	-3.743412
40	1	0	-2.057577	-0.302619	-2.053671
41	6	0	-0.830196	4.020188	-0.068825
42	1	0	0.055678	4.587020	-0.364179
43	1	0	-1.636275	4.736252	0.109214
44	1	0	-0.609050	3.518972	0.876314
45	6	0	1.642158	2.925245	-2.266962
46	1	0	1.100505	3.854730	-2.469032
47	1	0	2.661148	3.191966	-1.973830
48	1	0	1.705040	2.356547	-3.198794
49	6	0	-4.215165	-1.075842	-0.036355
50	1	0	-3.600046	-1.346860	-0.893589
51	1	0	-4.233021	-1.916346	0.661658
52	1	0	-5.235363	-0.928318	-0.397991
53	6	0	-1.193126	-0.715249	3.267265
54	1	0	-1.086472	-1.637286	3.843606
55	1	0	-0.256073	-0.540305	2.731210
56	1	0	-1.326170	0.107113	3.973112
57	6	0	-3.064181	1.997104	2.936462
58	1	0	-2.668064	2.938098	3.326782
59	1	0	-4.079729	2.192876	2.587345
60	1	0	-3.119745	1.292508	3.769400
61	6	0	4.638000	0.812447	-1.170215
62	1	0	3.773659	0.616377	-1.811701
63	1	0	4.647325	1.874894	-0.913963
64	1	0	5.543993	0.610210	-1.747015
65	6	0	1.691126	1.352371	2.009856
66	1	0	1.648885	0.795172	2.950202
67	1	0	1.437901	2.393543	2.232738
68	1	0	0.925778	0.947610	1.332310
69	6	0	4.172562	-1.001731	2.992518
70	1	0	4.051139	-1.879456	3.632638
71	1	0	5.224345	-0.945614	2.699259
72	1	0	3.938750	-0.118397	3.593868
73	6	0	0.335993	-3.018613	1.159010
74	1	0	1.190435	-3.319569	1.769896
75	1	0	-0.181187	-2.215710	1.681397
76	1	0	-0.340053	-3.874045	1.089893
77	6	0	-1.248556	-4.297728	-1.488167
78	1	0	-2.198456	-4.807036	-1.308007

79	1	0	-1.002367	-4.436650	-2.541967
80	1	0	-0.485995	-4.800702	-0.889115
81	6	0	1.722792	-1.287477	-2.578010
82	1	0	1.775856	-0.359706	-2.007698
83	1	0	2.518854	-1.939634	-2.211842
84	1	0	1.929873	-1.061148	-3.627156
85	7	0	3.328321	-0.048081	0.779207
86	7	0	-0.448782	1.812908	-1.308305
87	7	0	-2.394529	0.176555	1.235321
88	7	0	-0.207319	-1.967148	-1.082654
89	29	0	-0.968200	-0.099231	-0.316618

$Cu^{+}(N^{i}Pr_2Et)$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.729755	-1.310060	-0.914642
2	6	0	1.578963	-2.404683	-0.277774
3	29	0	-0.612873	1.113975	-1.034552
4	1	0	-0.109033	-1.744464	-1.457262
5	1	0	1.314191	-0.772235	-1.663866
6	1	0	1.087714	-2.854657	0.589343
7	1	0	1.750779	-3.193070	-1.013928
8	1	0	2.554875	-2.034186	0.043872
9	6	0	-0.995811	-0.776779	0.858051
10	1	0	-0.625675	-1.011347	1.863229
11	6	0	-2.036106	0.348572	0.934382
12	1	0	-1.666201	1.262739	1.396245
13	1	0	-2.382435	0.577158	-0.087781
14	1	0	-2.913213	0.026766	1.499327
15	6	0	1.275174	0.304177	0.857413
16	1	0	1.735167	-0.507321	1.434896
17	6	0	2.313246	0.939669	-0.065053
18	1	0	1.792961	1.615056	-0.756824
19	1	0	3.021270	1.530932	0.517795
20	1	0	2.883188	0.216390	-0.649499
21	7	0	0.171802	-0.290685	0.027505
22	6	0	0.790379	1.360203	1.844976
23	1	0	0.346636	2.213047	1.318124
24	1	0	0.073769	0.977929	2.573169
25	1	0	1.654697	1.729529	2.400582
26	6	0	-1.697203	-2.015944	0.305920
27	1	0	-1.046350	-2.886838	0.228125
28	1	0	-2.510402	-2.270231	0.989167
29	1	0	-2.141625	-1.816603	-0.674878

$Cu^{+}(N^{i}Pr_2Et)_2$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.483952	0.325027	1.130948
2	6	0	2.572936	1.284286	0.283516
3	6	0	4.087282	1.253731	0.469856
4	29	0	-0.004761	0.118730	-0.028606

5	1	0	2.139385	1.858990	1.108705
6	1	0	4.586850	0.765727	-0.371802
7	1	0	4.456568	2.281018	0.518823
8	1	0	4.383479	0.746647	1.392119
9	6	0	2.556159	-1.158542	-0.390999
10	1	0	3.597495	-1.251543	-0.055831
11	6	0	1.870455	-2.503017	-0.156241
12	1	0	1.913367	-2.835729	0.881947
13	1	0	0.820954	-2.463396	-0.465760
14	1	0	2.365095	-3.263312	-0.764016
15	6	0	2.030812	-0.459682	1.894411
16	1	0	2.817379	-1.211212	2.011131
17	1	0	2.357130	0.417815	2.455434
18	6	0	0.723248	-0.943695	2.498737
19	1	0	0.326012	-1.831551	2.000296
20	1	0	0.873250	-1.193982	3.551523
21	1	0	-0.025103	-0.148954	2.452826
22	7	0	1.915507	-0.075352	0.440996
23	7	0	-1.973146	0.171939	-0.278147
24	1	0	-2.045018	-0.503487	1.694582
25	6	0	-4.002253	0.225057	1.269149
26	1	0	-4.397375	-0.704677	0.854057
27	1	0	-4.258034	0.248963	2.331340
28	1	0	-4.518354	1.060765	0.790144
29	6	0	-2.489159	1.290214	-1.144145
30	1	0	-3.212769	1.876380	-0.576283
31	1	0	-3.043572	0.858864	-1.980684
32	6	0	-1.398044	2.205470	-1.664680
33	1	0	-1.839246	3.016923	-2.248906
34	1	0	-0.836378	2.654795	-0.839428
35	1	0	-0.704506	1.664522	-2.317089
36	6	0	-2.381016	-1.141469	-0.893897
37	1	0	-3.447046	-1.069984	-1.146362
38	6	0	-2.192745	-2.335546	0.036794
39	1	0	-2.868222	-2.327926	0.893629
40	1	0	-2.385309	-3.249493	-0.529693
41	1	0	-1.165026	-2.392120	0.410033
42	6	0	2.184020	2.030182	-0.992053
43	1	0	1.164164	1.772817	-1.277462
44	1	0	2.218267	3.105104	-0.798593
45	1	0	2.840797	1.826095	-1.837087
46	6	0	2.548254	-0.843686	-1.884646
47	1	0	1.563055	-0.488383	-2.207669
48	1	0	3.291727	-0.097969	-2.162866
49	1	0	2.774945	-1.754979	-2.442176
50	6	0	-1.587295	-1.361037	-2.178678
51	1	0	-1.633821	-0.507977	-2.859773
52	1	0	-0.534463	-1.547864	-1.942551
53	1	0	-1.970729	-2.234700	-2.710045
54	6	0	-1.965835	1.623177	1.744873

55	1	0	-2.198602	1.640013	2.812048
56	1	0	-0.879645	1.714216	1.635413
57	1	0	-2.422369	2.507494	1.291978

$Cu^{+}(N^{i}Pr_2Et)_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.981379	-1.313628	-0.997336
2	6	0	2.373072	-1.862538	1.369622
3	6	0	3.046738	-3.229636	1.460813
4	29	0	1.456226	0.462905	0.113968
5	1	0	2.698466	-1.282329	2.240755
6	1	0	4.130284	-3.169001	1.336130
7	1	0	2.849259	-3.646327	2.451694
8	1	0	2.645204	-3.930198	0.724328
9	6	0	4.092602	-0.352708	0.557499
10	1	0	3.932221	0.183290	1.497110
11	1	0	4.844702	-1.121630	0.768434
12	6	0	4.633694	0.615056	-0.486381
13	1	0	4.980330	0.110414	-1.390262
14	1	0	3.890396	1.365012	-0.781664
15	1	0	5.484746	1.147587	-0.056095
16	6	0	2.874852	-1.628239	-1.163549
17	1	0	3.012070	-0.767723	-1.827968
18	6	0	1.579961	-2.304301	-1.599406
19	1	0	0.710282	-1.656562	-1.458253
20	1	0	1.652248	-2.531973	-2.666060
21	1	0	1.402427	-3.246521	-1.074421
22	7	0	2.789983	-0.996719	0.205564
23	7	0	-3.044242	-0.887700	-0.084733
24	1	0	-1.832843	-0.543337	-1.759505
25	6	0	-2.153645	-2.669107	-1.688825
26	1	0	-3.093314	-2.711820	-2.249162
27	1	0	-1.335378	-2.840221	-2.395252
28	1	0	-2.149441	-3.491802	-0.967651
29	6	0	-3.106505	-1.780252	1.102208
30	1	0	-2.144695	-2.310312	1.114511
31	6	0	-3.158602	-0.992103	2.414522
32	1	0	-4.056021	-0.374822	2.492059
33	1	0	-3.146874	-1.680745	3.265346
34	1	0	-2.287664	-0.336171	2.499879
35	6	0	-4.332247	-0.606839	-0.747194
36	1	0	-4.835401	-1.544616	-1.040279
37	6	0	-4.135976	0.219436	-2.020134

38	1	0	-3.639164	-0.336206	-2.818545
39	1	0	-5.111015	0.534983	-2.398923
40	1	0	-3.549652	1.121172	-1.804400
41	7	0	0.205658	2.016595	0.101150
42	6	0	1.051112	3.188459	0.514364
43	1	0	1.570020	3.500725	-0.399268
44	6	0	-0.338378	2.100553	-1.297739
45	1	0	-1.160331	1.375018	-1.310740
46	6	0	-0.851653	1.632699	1.084633
47	1	0	-1.112928	0.589458	0.875899
48	6	0	0.316481	4.397588	1.096123
49	1	0	-0.114484	4.160412	2.073578
50	1	0	1.045853	5.197658	1.246812
51	1	0	-0.468936	4.782620	0.447599
52	6	0	0.717170	1.628829	-2.295752
53	1	0	1.033611	0.604806	-2.065930
54	1	0	0.315229	1.633687	-3.311396
55	1	0	1.603512	2.273301	-2.281995
56	6	0	-4.186962	-2.871045	1.066268
57	1	0	-4.025063	-3.562080	1.898214
58	1	0	-5.195445	-2.462457	1.172367
59	1	0	-4.152465	-3.447223	0.138134
60	6	0	-5.276374	0.161448	0.179955
61	1	0	-5.572276	-0.412156	1.058831
62	1	0	-4.796892	1.085159	0.518925
63	1	0	-6.189488	0.421866	-0.362215
64	6	0	-2.174795	2.392819	1.082097
65	1	0	-2.801155	1.965677	1.870681
66	1	0	-2.076339	3.461406	1.271217
67	1	0	-2.709364	2.240605	0.141073
68	6	0	-0.895462	3.456044	-1.733146
69	1	0	-1.682751	3.823457	-1.074500
70	1	0	-0.107796	4.212708	-1.798176
71	1	0	-1.323895	3.343837	-2.732697
72	6	0	2.115698	2.736742	1.514109
73	1	0	2.748521	3.579679	1.799813
74	1	0	1.669187	2.332025	2.428427
75	1	0	2.761439	1.970495	1.077276
76	6	0	4.060998	-2.566204	-1.418679
77	1	0	4.146996	-2.700672	-2.500342
78	1	0	5.012956	-2.163494	-1.067105
79	1	0	3.918679	-3.552269	-0.976312
80	6	0	0.856563	-1.990146	1.500741
81	1	0	0.383700	-1.001003	1.482099
82	1	0	0.411235	-2.606673	0.717465
83	1	0	0.615107	-2.448451	2.463304
84	1	0	-1.055476	-1.327498	-0.410154
85	1	0	-0.394251	1.662199	2.079489

$Cu^{+}(NMe_3)$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.058890	-1.031152	-0.967048
2	29	0	1.242996	0.002206	0.027558
3	1	0	-0.650691	-1.991630	-0.649457
4	1	0	-2.154936	-1.109148	-1.016759
5	6	0	-1.106353	1.331341	-0.442829
6	1	0	-0.639083	1.581269	-1.397316
7	1	0	-2.196982	1.339770	-0.564650
8	6	0	-1.215806	-0.307885	1.324653
9	1	0	-0.963860	0.492728	2.019870
10	1	0	-2.311332	-0.382173	1.255621
11	7	0	-0.645557	0.000946	0.004222
12	1	0	-0.830689	2.074421	0.304567
13	1	0	-0.681125	-0.775144	-1.962200
14	1	0	-0.812987	-1.254497	1.692946

$Cu^{+}(NMe_3)_2$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.355155	0.932560	1.053038
2	6	0	-2.432525	-0.982561	-0.967674
3	29	0	0.000355	0.013587	-0.051209
4	1	0	-2.126265	-0.703718	-1.977126
5	1	0	-2.037650	-1.972807	-0.734697
6	6	0	-2.432075	1.342268	-0.322380
7	1	0	-2.119327	1.625624	-1.328639
8	1	0	-3.528297	1.338919	-0.271323
9	6	0	-2.320893	-0.378806	1.365242
10	1	0	-1.922798	0.341758	2.081558
11	1	0	-3.415793	-0.392221	1.437955
12	7	0	-1.903484	0.001100	-0.000791
13	7	0	1.903586	0.000331	-0.000864
14	1	0	1.927213	0.634518	2.011709
15	1	0	2.024403	1.943809	0.811368
16	6	0	2.356193	-1.368003	0.324119
17	1	0	1.938236	-1.670667	1.285714
18	1	0	3.451679	-1.401779	0.380296
19	6	0	2.472955	0.413466	-1.299444

20	1	0	3.569367	0.401292	-1.251659
21	1	0	2.139062	-0.272626	-2.079389
22	1	0	-1.933476	-1.371320	1.602257
23	1	0	-3.528496	-1.009777	-0.917448
24	1	0	-2.041197	2.069423	0.391291
25	1	0	3.450002	0.918811	1.127051
26	1	0	2.134890	1.422268	-1.541637
27	1	0	2.014589	-2.059095	-0.448046

$Cu^{+}(NMe_3)_3$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.628527	-2.257777	1.392470
2	6	0	-2.087200	1.272515	-1.400702
3	29	0	0.015173	0.035656	-0.044608
4	1	0	-1.279683	1.646209	-2.035007
5	1	0	-2.357612	0.267811	-1.733582
6	6	0	-1.325579	2.602750	0.441315
7	1	0	-0.604924	3.054564	-0.240708
8	1	0	-2.233399	3.222673	0.453103
9	6	0	-2.720424	0.721159	0.852032
10	1	0	-2.376004	0.663030	1.887223
11	1	0	-3.597185	1.382878	0.806236
12	7	0	-1.636020	1.233082	0.000422
13	7	0	-0.273291	-1.998109	-0.012294
14	1	0	-1.523832	-1.694178	1.661186
15	1	0	0.191418	-1.944269	2.043601
16	6	0	-1.382376	-2.412398	-0.886149
17	1	0	-2.293388	-1.874412	-0.618707
18	1	0	-1.575056	-3.490721	-0.790777
19	6	0	0.904386	-2.807887	-0.360621
20	1	0	0.683306	-3.880286	-0.259663
21	1	0	1.198775	-2.602033	-1.392104
22	7	0	1.917996	0.766944	-0.012188
23	6	0	2.011507	2.225574	-0.180466
24	1	0	1.452324	2.724508	0.611787
25	1	0	1.594526	2.510442	-1.149785
26	6	0	2.419378	0.414415	1.325991
27	1	0	3.449071	0.771293	1.470791
28	1	0	1.778020	0.868491	2.085924
29	6	0	2.760644	0.135532	-1.040695
30	1	0	2.780392	-0.944549	-0.897304
31	1	0	3.790376	0.516909	-0.988578
32	1	0	3.059644	2.554495	-0.132949

33	1	0	-0.900193	2.576783	1.448009
34	1	0	-2.960872	1.929643	-1.515259
35	1	0	-3.024317	-0.274010	0.523043
36	1	0	-0.821823	-3.326581	1.560545
37	1	0	1.735800	-2.564675	0.304941
38	1	0	2.351215	0.351725	-2.030186
39	1	0	2.404900	-0.670190	1.456648
40	1	0	-1.133142	-2.186308	-1.925426

$Cu^{+}(NMe_3)_4$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.629672	1.916459	1.644389
2	1	0	-1.657344	2.585372	0.783187
3	1	0	-1.815640	2.513267	2.549987
4	6	0	0.711476	2.287142	1.812953
5	1	0	0.741252	2.874061	0.892687
6	1	0	1.689322	1.828285	1.966212
7	6	0	2.632046	-0.861988	1.171609
8	1	0	2.583323	-0.006325	1.846898
9	1	0	2.057286	-1.682861	1.604980
10	6	0	2.296643	-1.632664	-1.052332
11	1	0	1.812856	-2.525747	-0.653417
12	1	0	3.369793	-1.846080	-1.169409
13	6	0	-1.268509	-2.498029	-1.093121
14	1	0	-1.821423	-1.881847	-1.803951
15	1	0	-1.804080	-3.452098	-0.976806
16	6	0	-0.066162	0.407079	-2.975120
17	1	0	1.023539	0.460696	-2.968792
18	1	0	-0.363992	-0.642757	-3.009638
19	6	0	-0.136313	2.442141	-1.749327
20	1	0	-0.395482	2.958288	-2.685933
21	1	0	-0.601895	2.981717	-0.923444
22	6	0	-2.513179	-1.508108	0.673204
23	1	0	-2.472422	-1.077708	1.674917
24	1	0	-3.000789	-0.794464	0.005924
25	6	0	-2.074184	1.073068	-1.892422
26	1	0	-2.384843	1.660296	-2.769629
27	1	0	-2.454371	0.057460	-2.009877
28	6	0	2.862260	0.641578	-0.654773
29	1	0	3.937319	0.407495	-0.669437
30	1	0	2.551781	0.879360	-1.673184
31	6	0	-0.527420	-2.723715	1.154532
32	1	0	0.447660	-3.041791	0.782850

33	1	0	-1.148932	-3.620025	1.299388
34	6	0	-0.286799	0.458889	2.958371
35	1	0	-0.389881	1.109709	3.839649
36	1	0	-1.108113	-0.259436	2.968129
37	7	0	2.082791	-0.496244	-0.143230
38	7	0	-0.608620	1.049229	-1.768275
39	7	0	-0.322462	1.245738	1.715696
40	7	0	-1.152536	-1.799469	0.196143
41	29	0	0.000005	-0.000543	0.000792
42	1	0	-3.120081	-2.424969	0.718088
43	1	0	-0.276379	-2.698682	-1.502796
44	1	0	-0.389577	-2.230474	2.118995
45	1	0	3.683965	-1.172525	1.085500
46	1	0	0.655974	-0.087151	3.031693
47	1	0	2.702234	1.520048	-0.026442
48	1	0	1.871824	-1.414278	-2.034465
49	1	0	-0.429147	0.909054	-3.884609
50	1	0	-2.521742	1.512424	-0.998394
51	1	0	0.947594	2.471125	-1.618973
52	1	0	0.511777	2.962673	2.658285
53	1	0	-2.426827	1.177746	1.538755

$Cu^{+}[(3,5\text{-}diMeC_6H_3)_2POH]$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.015162	-1.071495	-0.494367
2	6	0	-1.497286	-0.115314	-0.109967
3	6	0	-1.483279	0.811704	0.938856
4	6	0	-2.672609	-0.374151	-0.811085
5	6	0	-2.646045	1.495887	1.280867
6	1	0	-0.561104	1.013479	1.478816
7	6	0	-3.849792	0.309557	-0.486832
8	1	0	-2.675970	-1.101104	-1.619747
9	6	0	-3.815328	1.232449	0.555846
10	6	0	1.371317	0.070852	-0.351219
11	6	0	2.547085	-0.453963	0.181147
12	6	0	1.323832	1.399650	-0.787692
13	6	0	3.697090	0.331127	0.288777
14	1	0	2.551941	-1.489433	0.516512
15	6	0	2.458158	2.201782	-0.697586
16	1	0	0.399151	1.812808	-1.184300
17	6	0	3.628896	1.648549	-0.160513
18	1	0	-4.725083	1.769453	0.816095
19	1	0	4.516631	2.274153	-0.090216

20	29	0	0.398262	-2.821212	0.667084
21	8	0	-0.181109	-1.478761	-2.069994
22	1	0	-0.311915	-0.720616	-2.661891
23	6	0	-5.118900	0.038587	-1.252332
24	1	0	-4.968053	0.192843	-2.324329
25	1	0	-5.442450	-0.997289	-1.114173
26	1	0	-5.926995	0.694032	-0.922856
27	6	0	-2.659828	2.504706	2.399432
28	1	0	-2.996549	3.480439	2.038338
29	1	0	-3.348360	2.195534	3.191203
30	1	0	-1.667651	2.625750	2.838036
31	6	0	2.442565	3.634919	-1.161033
32	1	0	2.690661	4.311271	-0.338222
33	1	0	3.183250	3.794538	-1.949602
34	1	0	1.462174	3.915131	-1.550369
35	6	0	4.957640	-0.226461	0.895001
36	1	0	4.907363	-0.189882	1.987797
37	1	0	5.106052	-1.269647	0.606012
38	1	0	5.832503	0.346917	0.582897

$Cu^{+}[(3,5\text{-}diMeC_6H_3)_2POH]_4$

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.388300	1.600538	-1.143112
2	15	0	-0.156759	0.214577	2.145365
3	6	0	0.446016	3.139484	-1.362496
4	6	0	-0.062199	3.756886	-0.211921
5	6	0	0.166486	3.666178	-2.619698
6	6	0	-0.775701	4.948534	-0.307883
7	1	0	0.098658	3.307012	0.768958
8	6	0	-0.594354	4.834813	-2.741272
9	1	0	0.523952	3.164593	-3.515749
10	6	0	-1.035556	5.468455	-1.581166
11	6	0	1.338857	-0.432972	2.957715
12	6	0	2.493574	0.338355	2.807667
13	6	0	1.397863	-1.665500	3.613044
14	6	0	3.710506	-0.093417	3.340020
15	1	0	2.447951	1.290824	2.278522
16	6	0	2.606868	-2.122403	4.138449
17	1	0	0.502136	-2.271142	3.721766
18	6	0	3.745409	-1.320418	4.002429
19	1	0	4.687788	-1.668633	4.421872
20	1	0	-1.612646	6.387948	-1.666466
21	15	0	0.918991	-2.097669	-0.582239

22	6	0	0.243299	-2.843422	-2.096382
23	6	0	0.053478	-1.995530	-3.191206
24	6	0	-0.162446	-4.176104	-2.163032
25	6	0	-0.544825	-2.470148	-4.358649
26	6	0	-0.742051	-4.678701	-3.330270
27	1	0	-0.045660	-4.830523	-1.302609
28	6	0	-0.933733	-3.811234	-4.409389
29	1	0	-1.405661	-4.191413	-5.314037
30	1	0	0.347232	-0.948126	-3.132659
31	15	0	-2.062088	0.279144	-1.135835
32	6	0	-3.292759	-1.026183	-0.782734
33	6	0	-3.206561	-2.208861	-1.524928
34	6	0	-4.242404	-0.912926	0.236210
35	6	0	-4.074808	-3.272629	-1.266804
36	1	0	-2.467952	-2.306768	-2.318988
37	6	0	-5.124705	-1.959852	0.501263
38	6	0	-5.026272	-3.129337	-0.256700
39	6	0	-2.900670	1.828282	-0.680055
40	6	0	-3.380955	2.712857	-1.641215
41	6	0	-2.992272	2.157911	0.676506
42	6	0	-3.993582	3.910435	-1.257716
43	6	0	-3.619901	3.332121	1.082664
44	1	0	-2.574079	1.496203	1.432825
45	6	0	-4.121118	4.192879	0.101304
46	1	0	-5.710520	-3.951188	-0.052343
47	1	0	-4.600229	5.121176	0.407027
48	1	0	-4.310247	-0.004490	0.828956
49	1	0	-3.259414	2.492313	-2.699104
50	6	0	-1.568851	-0.637907	2.907162
51	6	0	-2.440372	0.022869	3.776073
52	6	0	-1.838960	-1.949726	2.509719
53	6	0	-3.572398	-0.625991	4.270178
54	1	0	-2.251911	1.055858	4.057871
55	6	0	-2.956428	-2.623512	3.006775
56	1	0	-1.181053	-2.456129	1.804037
57	6	0	-3.805242	-1.949381	3.885321
58	1	0	-4.687621	-2.460996	4.266391
59	6	0	3.022717	2.145751	-0.527450
60	6	0	3.198476	3.323047	0.206501
61	6	0	4.122061	1.322552	-0.793340
62	6	0	4.462324	3.690265	0.668860
63	1	0	2.355425	3.978277	0.404308
64	6	0	5.402219	1.692068	-0.368882
65	1	0	3.991108	0.401419	-1.359383
66	6	0	5.551475	2.872774	0.358593
67	1	0	6.544722	3.165216	0.694634
68	6	0	2.726030	-2.190819	-0.796777
69	6	0	3.322538	-2.131971	-2.058427
70	6	0	3.515897	-2.275666	0.353727
71	6	0	4.711116	-2.180724	-2.183273

72	1	0	2.707877	-2.062632	-2.952134
73	6	0	4.906899	-2.356350	0.246797
74	1	0	3.046798	-2.307972	1.337354
75	6	0	5.481184	-2.312746	-1.024765
76	1	0	6.563543	-2.382814	-1.117284
77	29	0	0.048744	0.009270	-0.132256
78	8	0	1.738174	1.073060	-2.665472
79	1	0	2.358905	1.647379	-3.140499
80	8	0	0.646588	-3.199229	0.612690
81	1	0	1.201631	-3.991392	0.543885
82	8	0	-0.246935	1.764044	2.704906
83	1	0	-0.054453	1.841007	3.652427
84	8	0	-2.007378	0.305336	-2.781416
85	1	0	-2.882115	0.225112	-3.192470
86	6	0	2.698975	-3.454154	4.838151
87	1	0	3.155710	-3.347256	5.825874
88	1	0	1.713042	-3.905835	4.963230
89	1	0	3.320865	-4.149837	4.265564
90	6	0	4.949523	0.744232	3.167273
91	1	0	5.277104	0.724900	2.122086
92	1	0	4.756208	1.791934	3.416357
93	1	0	5.768079	0.382463	3.793899
94	6	0	4.657938	4.946053	1.478470
95	1	0	5.493128	5.536698	1.092770
96	1	0	3.761384	5.569111	1.467741
97	1	0	4.886082	4.701606	2.520957
98	6	0	6.598380	0.824545	-0.664427
99	1	0	6.722363	0.056512	0.108155
100	1	0	6.484842	0.304871	-1.619011
101	1	0	7.514792	1.418328	-0.694573
102	6	0	5.769596	-2.492867	1.474686
103	1	0	5.912818	-1.523239	1.963855
104	1	0	5.306937	-3.157743	2.209095
105	1	0	6.755605	-2.887957	1.219349
106	6	0	5.367604	-2.078106	-3.535671
107	1	0	6.303818	-2.640007	-3.565369
108	1	0	4.711535	-2.453069	-4.324312
109	1	0	5.601705	-1.033663	-3.770417
110	6	0	-1.141599	-6.127901	-3.436273
111	1	0	-2.124260	-6.234609	-3.903988
112	1	0	-0.424049	-6.680315	-4.051154
113	1	0	-1.174857	-6.603437	-2.453201
114	6	0	-0.807483	-1.545394	-5.518315
115	1	0	-0.414831	-1.958184	-6.451587
116	1	0	-1.883570	-1.396544	-5.653725
117	1	0	-0.352136	-0.567517	-5.349924
118	6	0	-3.960063	-4.556333	-2.046689
119	1	0	-3.647489	-4.362858	-3.076613
120	1	0	-3.204972	-5.212121	-1.598260
121	1	0	-4.907973	-5.099097	-2.061998

122	6	0	-6.190407	-1.823641	1.558010
123	1	0	-7.170608	-1.656383	1.099897
124	1	0	-6.263771	-2.732815	2.162431
125	1	0	-5.977789	-0.985436	2.225586
126	6	0	-4.535686	0.081442	5.188260
127	1	0	-5.527425	0.154449	4.730721
128	1	0	-4.651720	-0.462879	6.129759
129	1	0	-4.193920	1.092882	5.418270
130	6	0	-3.232487	-4.047004	2.597811
131	1	0	-2.790639	-4.749338	3.312477
132	1	0	-4.307061	-4.245338	2.559481
133	1	0	-2.810212	-4.256568	1.611490
134	6	0	-1.224122	5.676974	0.931386
135	1	0	-0.511988	6.468430	1.188997
136	1	0	-2.202062	6.143085	0.786747
137	1	0	-1.289567	4.994279	1.782554
138	6	0	-0.936811	5.376845	-4.105611
139	1	0	-1.378004	6.373782	-4.036693
140	1	0	-0.049844	5.436835	-4.742355
141	1	0	-1.656090	4.723429	-4.611077
142	6	0	-4.478628	4.877593	-2.305723
143	1	0	-5.213745	4.409551	-2.966912
144	1	0	-4.938390	5.758149	-1.852018
145	1	0	-3.643145	5.212691	-2.929679
146	6	0	-3.740743	3.654059	2.549764
147	1	0	-4.585502	3.121650	3.000202
148	1	0	-2.835893	3.348375	3.084062
149	1	0	-3.893438	4.723973	2.711335

$Cu^{+}(PPh_2OH)(PPh_2O^{-})$ (4')

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.824021	-1.463296	-1.021492
2	6	0	3.930131	-0.193239	-0.249119
3	6	0	4.019907	1.092229	-0.785033
4	6	0	4.728483	-0.529285	0.850404
5	6	0	4.885969	2.032723	-0.224693
6	1	0	3.405593	1.341881	-1.646205
7	6	0	5.588378	0.407419	1.413434
8	1	0	4.667708	-1.530506	1.274450
9	6	0	5.669785	1.692771	0.874402
10	1	0	6.345304	2.422850	1.309234
11	1	0	4.950673	3.030637	-0.648621
12	1	0	6.197079	0.138826	2.271601

13	15	0	-1.751517	0.533589	-1.095686
14	6	0	-2.130892	1.924583	0.010819
15	6	0	-2.517289	1.735662	1.341270
16	6	0	-1.951919	3.222133	-0.482336
17	6	0	-2.723556	2.836802	2.168391
18	1	0	-2.665868	0.730477	1.726502
19	6	0	-2.168509	4.319140	0.345050
20	6	0	-2.551457	4.126991	1.671341
21	1	0	-3.027018	2.686566	3.199309
22	1	0	-2.036945	5.323140	-0.044614
23	1	0	-2.718323	4.982812	2.317318
24	1	0	-1.653073	3.368925	-1.516703
25	6	0	1.615286	-1.559388	0.405011
26	6	0	1.083379	-0.391238	0.980096
27	6	0	1.187797	-2.796495	0.889662
28	6	0	0.159472	-0.466611	2.020026
29	1	0	1.481725	0.583363	0.690859
30	6	0	0.254711	-2.875572	1.926499
31	1	0	1.595430	-3.706654	0.456548
32	6	0	-0.263639	-1.711902	2.487853
33	1	0	-0.215797	0.444963	2.475595
34	1	0	-0.067258	-3.845226	2.294001
35	1	0	-0.986639	-1.772115	3.295293
36	6	0	-2.801828	-0.813411	-0.492987
37	6	0	-4.177971	-0.677517	-0.272334
38	6	0	-2.179622	-2.040503	-0.261195
39	6	0	-4.919739	-1.769939	0.160583
40	1	0	-4.666941	0.281989	-0.423341
41	6	0	-2.920400	-3.131191	0.186308
42	1	0	-1.106410	-2.125895	-0.414164
43	6	0	-4.290318	-2.996027	0.388741
44	1	0	-5.986861	-1.667849	0.327735
45	1	0	-2.426475	-4.079041	0.373831
46	1	0	-4.873717	-3.845276	0.729677
47	29	0	0.318452	-0.077625	-1.351228
48	8	0	-2.392443	1.030249	-2.526458
49	1	0	-3.305406	1.349182	-2.460197
50	8	0	1.969140	-0.598392	-2.068290

$Cu^{+}(PPh_2OH)(PPh_2O^{-})$---PhBr (**5**)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.289007	0.914825	-0.638234
2	6	0	3.070591	0.651909	0.978408
3	6	0	4.336744	0.072032	1.076644
4	6	0	2.322436	0.893512	2.135989
5	6	0	4.858265	-0.249846	2.328904
6	1	0	4.912031	-0.117028	0.175409
7	6	0	2.845035	0.567267	3.382929
8	1	0	1.328362	1.328519	2.055529
9	6	0	4.114010	-0.004413	3.480815
10	1	0	4.521206	-0.257694	4.454418
11	1	0	5.846613	-0.691824	2.404592
12	1	0	2.263478	0.759426	4.278677
13	15	0	-1.674365	0.137340	0.400842
14	6	0	-2.750553	1.601074	0.017668
15	6	0	-3.157012	2.476197	1.028011
16	6	0	-3.097598	1.885023	-1.305542
17	6	0	-3.909928	3.608733	0.725487
18	1	0	-2.872578	2.278037	2.060100
19	6	0	-3.847787	3.019294	-1.613048
20	6	0	-4.255402	3.883873	-0.597510
21	1	0	-4.219770	4.282681	1.518702
22	1	0	-4.112413	3.232528	-2.644927
23	1	0	-4.834417	4.770549	-0.836537
24	1	0	-2.756234	1.206901	-2.083722
25	6	0	1.626958	2.597240	-0.495877
26	6	0	2.369183	3.668171	0.016405
27	6	0	0.301797	2.792213	-0.890633
28	6	0	1.781443	4.922828	0.125420
29	1	0	3.395544	3.512484	0.338922
30	6	0	-0.295245	4.044741	-0.755832
31	1	0	-0.266283	1.950542	-1.279886
32	6	0	0.449044	5.107667	-0.253734
33	1	0	2.353474	5.756953	0.518986
34	1	0	-1.337966	4.174817	-1.033058
35	1	0	-0.008228	6.086393	-0.146703
36	6	0	-3.024907	-1.049018	0.850881
37	6	0	-3.516071	-1.944536	-0.102516
38	6	0	-3.512663	-1.111655	2.158352
39	6	0	-4.482203	-2.886068	0.245102
40	1	0	-3.114520	-1.891163	-1.111532
41	6	0	-4.485799	-2.045755	2.507336
42	1	0	-3.119352	-0.432816	2.913166
43	6	0	-4.969513	-2.938056	1.551096

44	1	0	-4.858558	-3.580893	-0.500376
45	1	0	-4.859631	-2.086700	3.526133
46	1	0	-5.719860	-3.673883	1.823866
47	29	0	0.680364	-0.542018	-1.044704
48	8	0	-1.246425	-0.358535	-1.057365
49	8	0	3.626117	1.031742	-1.597729
50	1	0	3.470641	0.597742	-2.446686
51	6	0	0.894163	-2.791935	-0.663921
52	6	0	1.970677	-2.447679	0.152780
53	6	0	1.799498	-2.508654	1.538205
54	6	0	0.585118	-2.921266	2.074708
55	6	0	-0.468185	-3.289980	1.233891
56	6	0	-0.320153	-3.237972	-0.146823
57	1	0	2.926885	-2.162155	-0.274014
58	1	0	2.624267	-2.219217	2.183221
59	1	0	0.453476	-2.955344	3.150781
60	1	0	-1.422393	-3.598971	1.649538
61	1	0	-1.144964	-3.479724	-0.806445
62	35	0	1.119195	-2.640841	-2.556905

TS[Cu^{+}(PPh_2OH)(PPh_2O^{-})···Ph···Br] (**TS5,6**)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-1.379019	-1.447706	0.062034
2	6	0	-0.214132	-2.200104	1.214652
3	6	0	-0.063799	-1.621098	2.479963
4	6	0	0.457568	-3.383345	0.895794
5	6	0	0.743480	-2.237878	3.429303
6	1	0	-0.561891	-0.685667	2.726340
7	6	0	1.274001	-3.987032	1.847673
8	1	0	0.344829	-3.830330	-0.087099
9	6	0	1.411164	-3.419333	3.112305
10	1	0	2.048729	-3.893697	3.851503
11	1	0	0.860959	-1.789025	4.409755
12	1	0	1.804199	-4.900077	1.599189
13	15	0	1.716694	0.868191	0.824384
14	6	0	2.973825	-0.427572	0.410113
15	6	0	3.499347	-1.225229	1.425563
16	6	0	3.367936	-0.666337	-0.913570
17	6	0	4.397210	-2.253247	1.130323
18	1	0	3.196237	-1.049015	2.454577
19	6	0	4.254803	-1.694100	-1.213597
20	6	0	4.770576	-2.490803	-0.188070
21	1	0	4.795132	-2.871563	1.929582

22	1	0	4.552500	-1.873960	-2.242546
23	1	0	5.464480	-3.292603	-0.421155
24	1	0	2.967707	-0.037162	-1.706655
25	6	0	-1.011832	-1.931443	-1.627188
26	6	0	-2.077685	-2.249641	-2.475743
27	6	0	0.303553	-1.916882	-2.105507
28	6	0	-1.820246	-2.567473	-3.805986
29	1	0	-3.092553	-2.262482	-2.091472
30	6	0	0.547494	-2.243593	-3.434325
31	1	0	1.117424	-1.650309	-1.439706
32	6	0	-0.511192	-2.565890	-4.283144
33	1	0	-2.641979	-2.820141	-4.467304
34	1	0	1.566919	-2.244006	-3.806582
35	1	0	-0.314462	-2.817087	-5.320369
36	6	0	2.507801	2.271898	-0.075929
37	6	0	1.952688	2.804164	-1.240650
38	6	0	3.665322	2.850534	0.454992
39	6	0	2.551966	3.895870	-1.868948
40	1	0	1.052549	2.351851	-1.646779
41	6	0	4.267043	3.935762	-0.173658
42	1	0	4.101543	2.445282	1.366602
43	6	0	3.707804	4.463259	-1.337865
44	1	0	2.114951	4.305148	-2.775072
45	1	0	5.168043	4.374267	0.244493
46	1	0	4.171557	5.314490	-1.826474
47	29	0	-1.258082	0.757568	0.207390
48	8	0	0.534195	0.446313	-0.208559
49	8	0	-2.791428	-2.184908	0.365565
50	1	0	-3.478010	-1.556744	0.647179
51	6	0	-3.145838	0.666678	0.329709
52	6	0	-3.869913	0.694727	-0.861482
53	6	0	-5.265358	0.686267	-0.819514
54	6	0	-5.930512	0.636845	0.402793
55	6	0	-5.200875	0.601514	1.589258
56	6	0	-3.804857	0.618470	1.557537
57	1	0	-3.363392	0.721267	-1.823822
58	1	0	-5.828682	0.712473	-1.746790
59	1	0	-7.014748	0.622656	0.431734
60	1	0	-5.713335	0.565727	2.545343
61	1	0	-3.242685	0.603264	2.487115
62	35	0	-1.229227	3.026271	0.657513

$Cu^{3+}(PPh_2OH)(PPh_2O^-)(Ph)(Br)$ (**6**)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	1.340868	1.371273	-0.306058
2	6	0	1.941391	1.747771	1.350824
3	6	0	3.168435	2.399088	1.499832
4	6	0	1.216219	1.325628	2.471670
5	6	0	3.665557	2.639107	2.777326
6	1	0	3.727280	2.713373	0.624314
7	6	0	1.723296	1.571806	3.743552
8	1	0	0.261091	0.819203	2.344947
9	6	0	2.945449	2.225281	3.895769
10	1	0	3.339027	2.409990	4.889960
11	1	0	4.617528	3.144800	2.898129
12	1	0	1.163835	1.251772	4.615969
13	15	0	-1.726501	-0.263633	0.631635
14	6	0	-3.161366	0.542964	-0.202697
15	6	0	-3.892714	1.526973	0.461748
16	6	0	-3.524364	0.181661	-1.504275
17	6	0	-4.983977	2.137253	-0.158541
18	1	0	-3.596724	1.834583	1.462889
19	6	0	-4.605476	0.794508	-2.128169
20	6	0	-5.338168	1.774026	-1.454255
21	1	0	-5.545384	2.905686	0.364646
22	1	0	-4.881819	0.511379	-3.139705
23	1	0	-6.181401	2.253499	-1.942010
24	1	0	-2.938043	-0.575660	-2.018597
25	6	0	-0.130868	2.349726	-0.644142
26	6	0	-0.622925	3.287590	0.267699
27	6	0	-0.730674	2.191688	-1.897168
28	6	0	-1.713292	4.075447	-0.087356
29	1	0	-0.157837	3.405258	1.241224
30	6	0	-1.815278	2.987657	-2.244168
31	1	0	-0.364550	1.438643	-2.589824
32	6	0	-2.305751	3.927228	-1.339713
33	1	0	-2.102728	4.802441	0.617432
34	1	0	-2.289909	2.860751	-3.210970
35	1	0	-3.163337	4.535821	-1.607175
36	6	0	-2.596059	-1.812695	1.150083
37	6	0	-2.147293	-3.066326	0.730760
38	6	0	-3.677046	-1.738016	2.036912
39	6	0	-2.776758	-4.225930	1.185085
40	1	0	-1.301211	-3.127965	0.052630
41	6	0	-4.305552	-2.893939	2.487184
42	1	0	-4.038547	-0.766065	2.368514
43	6	0	-3.855115	-4.144408	2.061400

44	1	0	-2.421450	-5.196164	0.850107
45	1	0	-5.147615	-2.822525	3.169156
46	1	0	-4.343238	-5.048002	2.413334
47	29	0	1.022090	-0.831469	-0.628122
48	8	0	-0.839566	-0.756027	-0.623407
49	8	0	2.378046	2.046345	-1.352509
50	1	0	3.129653	1.461977	-1.556179
51	6	0	2.924787	-0.726488	-0.690762
52	6	0	3.550986	-0.688105	-1.938618
53	6	0	4.943914	-0.721361	-2.009529
54	6	0	5.703418	-0.811924	-0.843979
55	6	0	5.069903	-0.867796	0.393664
56	6	0	3.676772	-0.821815	0.475336
57	1	0	2.964684	-0.645610	-2.853407
58	1	0	5.430769	-0.688637	-2.978959
59	1	0	6.786198	-0.839966	-0.902826
60	1	0	5.654850	-0.938856	1.305089
61	1	0	3.194042	-0.850124	1.449347
62	35	0	1.198748	-3.104963	-1.080047

TS[Cu^{+}(PPh_2OH)(PPh_2O^{-})(Ph)(Br) (**TS6,7**)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	2.168349	-0.079250	-0.782318
2	6	0	3.404562	-0.111113	0.537546
3	6	0	4.743843	-0.383015	0.247006
4	6	0	2.996813	0.122942	1.857551
5	6	0	5.678769	-0.407770	1.277896
6	1	0	5.042967	-0.579232	-0.777845
7	6	0	3.941795	0.104508	2.879297
8	1	0	1.949899	0.324622	2.077858
9	6	0	5.279409	-0.160737	2.589849
10	1	0	6.011773	-0.179973	3.390455
11	1	0	6.719495	-0.620218	1.056625
12	1	0	3.632897	0.292080	3.902254
13	15	0	-1.812678	0.183682	1.218993
14	6	0	-2.041520	2.022436	1.492228
15	6	0	-3.016320	2.477369	2.380775
16	6	0	-1.248196	2.958567	0.817113
17	6	0	-3.209578	3.844547	2.585882
18	1	0	-3.628290	1.758267	2.922131
19	6	0	-1.429830	4.321015	1.027840
20	6	0	-2.415114	4.767045	1.911298
21	1	0	-3.972756	4.188060	3.277753

22	1	0	-0.807187	5.036646	0.497307
23	1	0	-2.559519	5.830759	2.073805
24	1	0	-0.482771	2.609829	0.126912
25	6	0	1.921328	1.652751	-1.236352
26	6	0	1.298085	1.915659	-2.462752
27	6	0	2.217666	2.700757	-0.362396
28	6	0	0.968739	3.221081	-2.808462
29	1	0	1.073887	1.095204	-3.141084
30	6	0	1.888659	4.007510	-0.716482
31	1	0	2.701543	2.502936	0.589075
32	6	0	1.259890	4.266888	-1.931942
33	1	0	0.483796	3.422151	-3.757818
34	1	0	2.120174	4.822583	-0.038626
35	1	0	0.998430	5.285564	-2.199615
36	6	0	-2.554514	0.215508	-0.479360
37	6	0	-1.784526	0.411668	-1.625997
38	6	0	-3.922938	-0.033569	-0.618401
39	6	0	-2.358103	0.331721	-2.894235
40	1	0	-0.730202	0.661594	-1.529913
41	6	0	-4.504461	-0.094836	-1.881608
42	1	0	-4.532037	-0.201632	0.268241
43	6	0	-3.720428	0.075188	-3.023087
44	1	0	-1.742856	0.478873	-3.777285
45	1	0	-5.567512	-0.292146	-1.978698
46	1	0	-4.171774	0.008115	-4.007638
47	29	0	0.198936	-1.180551	-0.092938
48	8	0	-0.192371	0.245491	0.940347
49	8	0	2.895510	-0.722131	-2.088207
50	1	0	2.465813	-1.574509	-2.297196
51	6	0	-1.215119	-1.990052	0.946856
52	6	0	-2.255412	-2.698013	0.341642
53	6	0	-2.911509	-3.691736	1.063015
54	6	0	-2.475654	-4.044220	2.339151
55	6	0	-1.357261	-3.416288	2.886310
56	6	0	-0.705311	-2.410324	2.180138
57	1	0	-2.584266	-2.445960	-0.661215
58	1	0	-3.751131	-4.210174	0.610192
59	1	0	-2.986791	-4.825326	2.892037
60	1	0	-0.990749	-3.708254	3.865464
61	1	0	0.138930	-1.891357	2.627669
62	35	0	0.502752	-2.890252	-1.617281

$Cu^{+}(PPh_2OH)(Br)(Ph)(PPh_2O)$ (7)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-2.409973	0.158347	-0.067351
2	6	0	-3.062881	1.846502	0.012284
3	6	0	-4.408005	2.119206	-0.251787
4	6	0	-2.179321	2.892987	0.305717
5	6	0	-4.868548	3.432536	-0.213799
6	1	0	-5.081476	1.303836	-0.494817
7	6	0	-2.651483	4.202565	0.352622
8	1	0	-1.130677	2.673328	0.499358
9	6	0	-3.993339	4.473166	0.091990
10	1	0	-4.356448	5.495539	0.121476
11	1	0	-5.912419	3.643902	-0.422888
12	1	0	-1.968671	5.013594	0.584926
13	15	0	1.759771	0.581600	0.356764
14	6	0	3.266344	1.582828	0.429333
15	6	0	4.311112	1.438098	-0.488780
16	6	0	3.366300	2.518229	1.463526
17	6	0	5.459067	2.213921	-0.358887
18	1	0	4.228709	0.731174	-1.310002
19	6	0	4.514220	3.295757	1.585096
20	6	0	5.560323	3.140020	0.677541
21	1	0	6.269176	2.101663	-1.071537
22	1	0	4.591819	4.024734	2.384853
23	1	0	6.454741	3.747172	0.773053
24	1	0	2.539204	2.638069	2.156957
25	6	0	-2.341931	-0.441580	1.648804
26	6	0	-1.900682	0.353376	2.708742
27	6	0	-2.567129	-1.808319	1.850490
28	6	0	-1.694472	-0.215547	3.963095
29	1	0	-1.701544	1.408522	2.549851
30	6	0	-2.362124	-2.371804	3.106988
31	1	0	-2.890081	-2.427881	1.018440
32	6	0	-1.920115	-1.576366	4.162940
33	1	0	-1.352980	0.404401	4.785765
34	1	0	-2.541773	-3.431474	3.259690
35	1	0	-1.753274	-2.016448	5.140931
36	6	0	2.116072	-1.015797	1.124724
37	6	0	1.026247	-1.729391	1.634196
38	6	0	3.399849	-1.565851	1.175368
39	6	0	1.218636	-2.998816	2.170740
40	1	0	0.036108	-1.281751	1.628405
41	6	0	3.586346	-2.836236	1.714378
42	1	0	4.253539	-1.006432	0.801819
43	6	0	2.496836	-3.552676	2.206442

44	1	0	0.367754	-3.546557	2.563355
45	1	0	4.582552	-3.263942	1.755158
46	1	0	2.646370	-4.542348	2.625837
47	29	0	-0.592481	-0.482744	-1.295351
48	8	0	0.559347	1.267740	0.951775
49	8	0	-3.696360	-0.671931	-0.676056
50	1	0	-3.353270	-1.383877	-1.247225
51	6	0	1.493199	0.208388	-1.407299
52	6	0	0.642936	1.076602	-2.127441
53	6	0	0.449989	0.863312	-3.500373
54	6	0	1.128125	-0.162023	-4.153461
55	6	0	1.994268	-1.000830	-3.448248
56	6	0	2.159942	-0.832536	-2.079737
57	1	0	0.204779	1.943197	-1.638175
58	1	0	-0.213821	1.518464	-4.054186
59	1	0	0.978661	-0.311418	-5.217400
60	1	0	2.512126	-1.804233	-3.959786
61	1	0	2.789732	-1.517034	-1.517861
62	35	0	-1.245899	-2.665104	-1.909400

$Cu^{+}(Ph_2PO^{-})(NEt_3)$ (8')

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.095682	-1.825013	-0.468254
2	6	0	4.399230	-2.221371	0.217249
3	29	0	0.848225	-0.417848	-1.116352
4	1	0	2.389758	-2.660790	-0.426776
5	1	0	3.289294	-1.626994	-1.526574
6	1	0	4.285177	-2.329629	1.298908
7	1	0	4.717382	-3.188558	-0.180022
8	1	0	5.199442	-1.506591	0.015833
9	6	0	1.864043	-0.892748	1.442453
10	1	0	1.365080	-1.868234	1.425124
11	1	0	2.704990	-0.974386	2.140914
12	6	0	0.884439	0.170430	1.917347
13	1	0	1.319081	1.174025	1.904025
14	1	0	-0.010517	0.188299	1.289695
15	1	0	0.576914	-0.051712	2.941861
16	6	0	3.144991	0.626485	-0.035419
17	1	0	3.669054	0.587181	-0.995633
18	1	0	2.424831	1.447386	-0.106105
19	6	0	4.122542	0.946051	1.093590
20	1	0	4.857514	0.159326	1.265051
21	1	0	4.663020	1.857399	0.825775

22	1	0	3.603805	1.138931	2.035912
23	7	0	2.363994	-0.642508	0.068094
24	15	0	-1.953701	0.360825	-1.720039
25	6	0	-1.370456	1.688904	-0.547836
26	6	0	-0.156889	2.333240	-0.814775
27	6	0	-2.108029	2.094453	0.569416
28	6	0	0.317361	3.343957	0.021083
29	1	0	0.421696	2.034613	-1.685907
30	6	0	-1.630982	3.093373	1.414166
31	1	0	-3.051632	1.605664	0.799795
32	6	0	-0.414649	3.720223	1.144796
33	1	0	1.259931	3.835446	-0.204617
34	1	0	-2.206949	3.380099	2.288876
35	1	0	-0.044045	4.499057	1.803647
36	6	0	-2.502307	-0.847784	-0.415718
37	6	0	-3.844378	-0.871170	-0.025348
38	6	0	-1.616619	-1.745301	0.184187
39	6	0	-4.282541	-1.747698	0.966665
40	1	0	-4.554756	-0.198996	-0.503141
41	6	0	-2.048779	-2.631059	1.165660
42	1	0	-0.573627	-1.739777	-0.126663
43	6	0	-3.385129	-2.630047	1.563871
44	1	0	-5.326498	-1.749761	1.265099
45	1	0	-1.345311	-3.322459	1.620749
46	1	0	-3.726878	-3.319874	2.329001
47	8	0	-0.569112	-0.224555	-2.269436

$Cu^{+}(Ph_2PO^{-})(NEt_3)$----PhBr (**10**)

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.155456	0.514914	-1.829596
2	6	0	-4.165230	1.492024	-2.427115
3	29	0	-0.713269	-0.319621	-0.497058
4	1	0	-2.844589	-0.204071	-2.594695
5	1	0	-3.639673	-0.054971	-1.033121
6	1	0	-3.710447	2.166028	-3.157603
7	1	0	-4.939971	0.919549	-2.943797
8	1	0	-4.659772	2.089228	-1.658064
9	6	0	-1.100737	1.730440	-2.325347
10	1	0	-1.121194	1.062201	-3.192478
11	1	0	-1.569509	2.672721	-2.634089
12	6	0	0.338076	1.966118	-1.897818
13	1	0	0.400057	2.554037	-0.976485
14	1	0	0.846313	1.014686	-1.718695
15	1	0	0.874251	2.510653	-2.679126
16	6	0	-2.130533	1.947763	-0.076394
17	1	0	-2.918031	1.462809	0.510940
18	1	0	-1.223137	1.917967	0.535036
19	6	0	-2.454646	3.419487	-0.324606
20	1	0	-3.315544	3.573576	-0.976326
21	1	0	-2.672009	3.888010	0.639029
22	1	0	-1.598902	3.946568	-0.756380
23	7	0	-1.905857	1.075355	-1.265842
24	6	0	-2.452334	-1.625302	0.954738
25	6	0	-3.762420	-1.227243	1.198702
26	6	0	-1.408106	-1.301820	1.818603
27	6	0	-4.023487	-0.436896	2.315900
28	1	0	-4.562051	-1.528858	0.531041
29	6	0	-1.693396	-0.515364	2.935435
30	1	0	-0.410656	-1.694027	1.654327
31	6	0	-2.990180	-0.070363	3.177277
32	1	0	-5.040715	-0.115873	2.513949
33	1	0	-0.890084	-0.269369	3.622924
34	1	0	-3.202196	0.540939	4.047801
35	35	0	-2.067772	-2.691622	-0.571836
36	15	0	2.003650	-0.680361	0.953100
37	6	0	2.128537	1.183980	0.897352
38	6	0	1.203952	1.893874	1.672894
39	6	0	3.019265	1.914165	0.101557
40	6	0	1.144200	3.286764	1.639361
41	1	0	0.513251	1.344109	2.311920
42	6	0	2.976140	3.306812	0.073336
43	1	0	3.750338	1.389235	-0.507791

44	6	0	2.035001	3.996667	0.836635
45	1	0	0.412259	3.815449	2.243426
46	1	0	3.674237	3.856999	-0.550861
47	1	0	2.000553	5.081433	0.810445
48	6	0	3.648062	-1.060837	0.201163
49	6	0	4.809791	-0.979562	0.976085
50	6	0	3.751377	-1.445827	-1.136711
51	6	0	6.053576	-1.265545	0.420853
52	1	0	4.739718	-0.686855	2.022425
53	6	0	4.995196	-1.740054	-1.694204
54	1	0	2.840946	-1.505477	-1.726674
55	6	0	6.148227	-1.648754	-0.917309
56	1	0	6.949889	-1.196882	1.030171
57	1	0	5.066171	-2.039020	-2.736121
58	1	0	7.117144	-1.878260	-1.350116
59	8	0	0.998394	-1.061435	-0.229053
