Electronic Supplementary Material (ESI) for Dalton Transactions.

Electronic Supplementary Maetrial:

Versatile Coordination Chemistry of a Bis(methyliminophosphoranyl)pyridine Ligand on Copper Centers

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I. VT-^{31}P NMR Eyring plot for **2** and **4**

1. Compound **2**

Compound **2** was diluted in THF-d^8, 7 spectrums of 300 scans were recorded between -30°C and -85°C. Half widths of peaks were determined using the MestReNova software, exchange rates at each temperature were determined using the formula of Takeda and Stejskal:[1]

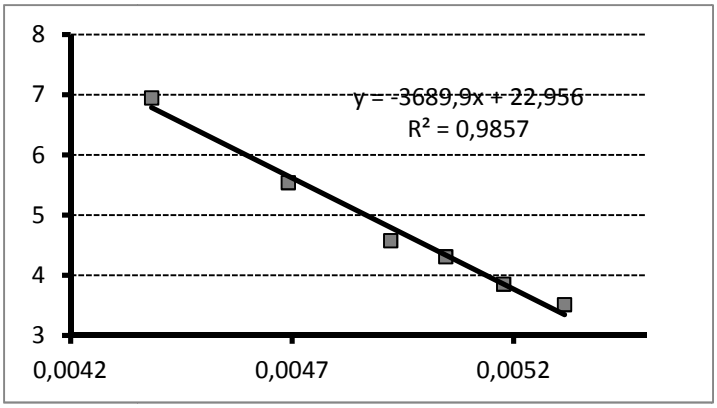
$$k = \frac{\pi\delta\nu^2(W^* - W_0)\sqrt{1 + 2\left(\frac{W^*}{\delta\nu}\right)^2 - \left(\frac{W^*}{\delta\nu}\right)^4}}{2\left(W^{*2} - {W_0}^2\right)}$$

With :

- $\delta\nu$: the peak separation after coalescence (in Hz)
- W^* the half width of the peak
- W_0 the half width of a reference peak

$\delta\nu$ = 1807 Hz for **2**.

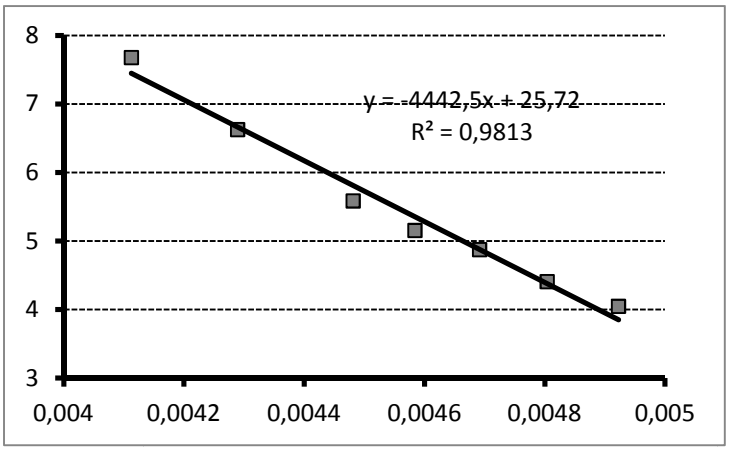
Activation parameters were determined by ploting $\ln\left(\frac{k}{T}\right) = a\left(\frac{1}{T}\right) + b$:



2. Compound **4**

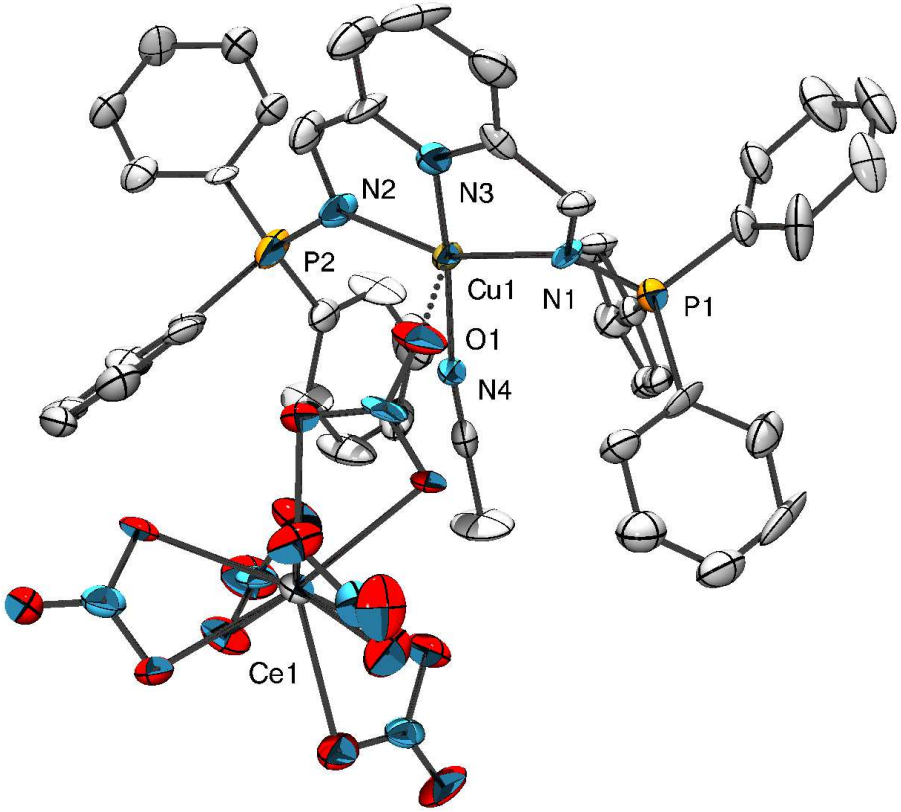
Compound **4** was diluted in THF-d^8, 8 spectrums of 100 scans were recorded between -20°C and -70°C. Half widths of peaks were determined using the MestReNova software, and the same methodology as previously was used.

$\delta\nu$ = 2521 Hz for **4**.



II. X-Ray Data

Structure of [**L**CuBr(MeCN)][Ce(NO_3)$_5$] (**6**)



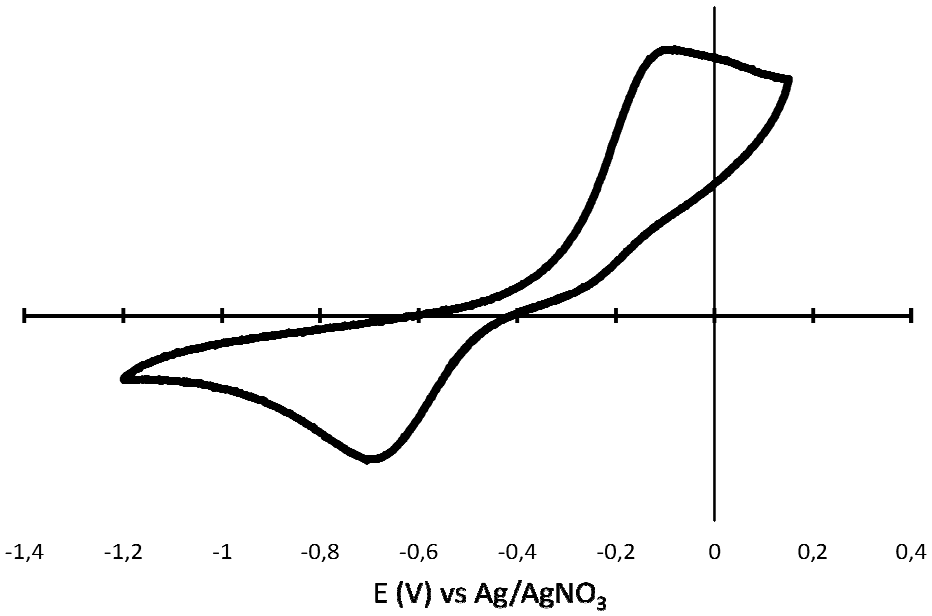
ORTEP of the solid-state structure of **6** with 50% probability thermal ellipsoids. Hydrogens were omitted for clarity. Selected bond lenghs [Å] and angles (deg): N1-Cu1 1.97(1), N2-Cu1 1.99(1), N3-Cu1 1.92(1), N4-Cu1 1.93(1), O1-Cu1 2.79(1), P1-N1 1.59(1), P2-N2 1.63(1); N1-Cu1-N3 82.8(5), N2-Cu1-N3 81.1(6), N3-Cu1-N4 160.3(8), N1-Cu1-O1 81.1(5), N2-Cu1-O1 109.8(5), N3-Cu1-O1 76.9(5).

Table S1: Crystal data and refinement details for complexes **2**, **3, 4, 5, 6**

Compound	**2**	**3**	**4**	**5**	**6**
Formula	$C_{43}H_{37}BrCuN_3P_2$, C_6H_6	$C_{86}H_{74}Cu_2N_6P_4$, $2(F_6P)$	$C_{49}H_{52}CuN_3P_3,F_6P$	$C_{44}H_{37}Br_2Cl_2CuN_3P_2$	$C_{45}H_{40}CeCuN_9O_{15}P_2$
M_r	879.25	1732.41	984.36	965.98	1212.46
Space group	P-1	P-1	P-1	$P2_{1/c}$	Cc
λ (Å)	0.71069	0.71069	0.71069	0.71069	0.71069
a(Å)	10.315(1)	12.216(1)	10.981(1)	11.030(1)	21.754(1)
b(Å)	13.914(1)	13.441(1)	14.582(1)	26.032(1)	21.836(1)
c(Å)	15.143(1)	27.368(1)	16.352(1)	18.0004(10)	10.390(1)
α(°)	100.336(1)	97.350(1)	70.160(1)	90.00	90
β(°)	91.375(1)	95.160(1)	71.273(1)	121.879(3)	93.913(1)
γ(°)	95.391(1)	116.043(1)	77.074(1)	90.00	90
V($Å^3$)	2126.8(3)	3950.1(5)	2313.1(3)	4388.9(5)	4924.0(6)
Z	2	2	2	4	4
d(g cm^{-3})	1.373	1.457	1.413	1.462	1.636
μ(cm^{-1})	1.566	0.739	0.673	2.547	1.487
F(000)	904	1776	1020	1948	2440
θmax	30.03	27.48	30.00	27.48	27.48
Rflns measd.	17505	62056	27032	30986	16546
Unique data	8870	18067	13347	10014	8888
Rint	0.0403	0.0389	0.0493	0.0506	0.0648
GoF	1.1068	1.024	1.107	1.038	1.161
R_1[a)]	0.0491	0.0362	0.0664	0.0517	0.0696
wR_2[b)]	0.1146	0.0948	0.1369	0.1093	0.1503
CCDC Number	996862	996863	996864	996894	996866

III. Cyclic voltammogram of **L**CuBr (**2**)

The electrochemical experiments were performed using a VERSATAT potentiostat/galvanostat with a three-electrode cell using a Au disk as working electrode, a Pt gauze as the counter electrode, and a $Ag/AgNO_3$ reference electrode. Measurements were made in THF with a concentration of 3.0 $mmol.L^{-1}$ for **2**. Tetrabutylammonium tetrafluoroborate salt served as electrolyte (concentration 0.12 $mol.L^{-1}$). Potentials were recorded at 50 $mV\ s^{-1}$.



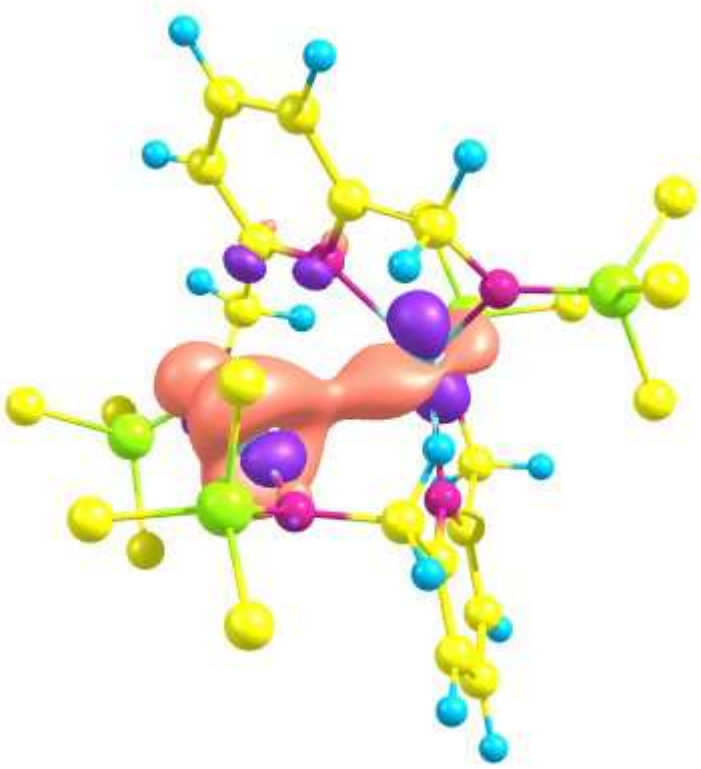
	vs $Ag/AgNO_3$	Vs Fc^+/Fc
E^a, V	-0.13	-0.36
E^c, V	-0.67	-0.90

IV. Computational details

General considerations

All calculations were performed using the Gaussian 09 series of programs (revision B.01).[2] The ω-B97XD functional was used in combination with the 6-31G* basis set for carbons and hydrogens; the 6-311+G** basis set for bromine, phosphorus, nitrogen and oxygen; and the Def2-TZVP basis set for copper.[3] The stationary points and transition states were characterised by full vibration frequencies calculations, with no imaginary frequency for minima (stationary point), and one imaginary frequency for transition states. Solvent effects were introduced through PCM single-point calculations,[4] using standard Gaussian parameters, solvent was THF. The PCM Gibbs energies were calculated using the correction proposed by Maseras and coworkers.[5]

1. Figure S1: HOMO-6 orbital of the computed dimer V



2. Energies and three lower frequencies for the hemilability process (in hartrees)

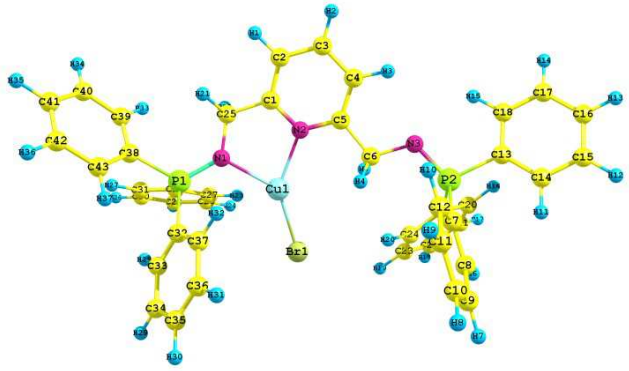
	ZPE	E	H	G	E PCM	G PCM	Freq1 (cm^{-1})	Freq2 (cm^{-1})	Freq3 (cm^{-1})
LCuBr_tri (I)	-6721,414481	-6721,369022	-6721,368078	-6721,503285	-6722,138756	-6722,273019	10,06	10,79	12,22
LCuBr_linear (II)	-6721,398799	-6721,353499	-6721,352554	-6721,487803	-6722,120256	-6722,254560	10,27	14,30	15,33
LCuBr_twisted (III)	-6721,408602	-6721,363170	-6721,362226	-6721,496403	-6722,133927	-6722,267160	7,37	14,25	17,02
LCuBr_TS (IV)	-6721,407121	-6721,362717	-6721,361773	-6721,490913	-6722,130241	-6722,258437	-15,59	10,36	20,64

3. Energies and three lower frequencies for the dimerisation process (in hartrees)

	ZPE	E	H	G	E PCM	G PCM	Freq1 (cm^{-1})	Freq2 (cm^{-1})	Freq3 (cm^{-1})
LCuDimer (V)	-8294,111587	-8294,026170	-8294,025226	-8294,238637	-8295,643519	-8295,855986	12,30	17,32	18,78
LOMePhCN (VI)	-4814,726582	-4814,669020	-4814,668076	-4814,822985	-4815,672919	-4815,826884	14,45	15,92	19,76
OMePhCN	-667,652415	-667,638661	-667,637717	-667,692737	-667,867089	-667,921165	60,36	75,56	96,81
LCuMeCN (VII)	-4279,729691	-4279,682507	-4279,681562	-4279,815163	-4280,521766	-4280,654422	10,22	13,34	24,40
MeCN	-132,675831	-132,672227	-132,671283	-132,698814	-132,729392	-132,755979	381,13	381,35	943,55
LCu (VIII)	-4147,030016	-4146,987721	-4146,986777	-4147,108927	-4147,772981	-4147,894187	14,03	19,33	22,34
LCuPEt3 (IX)	-4725,841629	-4725,787579	-4725,786634	-4725,935044	-4726,774082	-4726,921547	64,68	80,59	83,35
PEt3	-578,764199	-578,753729	-578,752785	-578,800104	-578,944914	-578,991289	39,75	92,82	100,18

4. Optimised geometries

LCuBr_tri (I)



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78	6	0	-5.974629	2.302464	-0.304421
79	1	0	-5.588748	2.349328	-1.320064
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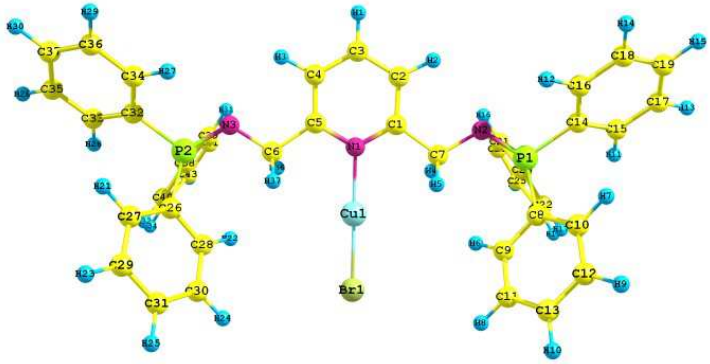
LCuBr_linear (II)



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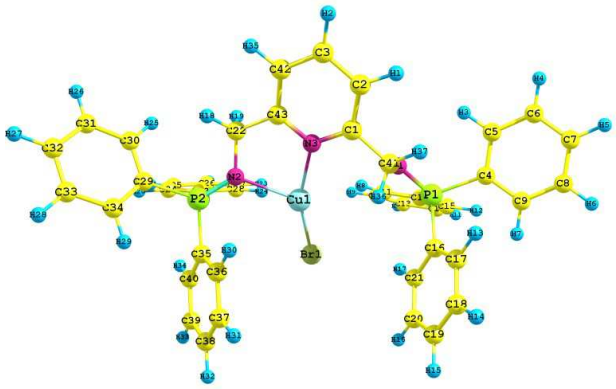
72	1	0	-9.256176	-3.898771	-1.803831
73	6	0	-5.253411	-0.177793	1.677615
74	6	0	-4.694130	-1.034554	2.630943
75	6	0	-5.999811	0.928475	2.094598
76	6	0	-4.888939	-0.792974	3.986973
77	1	0	-4.102354	-1.883638	2.297209
78	6	0	-6.196279	1.165491	3.452165
79	1	0	-6.416056	1.612231	1.359624
80	6	0	-5.642597	0.304677	4.396952
81	1	0	-4.450401	-1.458709	4.724150
82	1	0	-6.774439	2.027021	3.772300
83	1	0	-5.793274	0.493954	5.455665
84	1	0	-2.319836	-0.128218	0.788873
85	1	0	-2.299073	0.174777	-0.946956
86	29	0	-0.000007	1.127967	-0.097631
87	35	0	-0.000069	3.366972	0.056738

PCM: SCF Done: E(RwB97XD) = -6722.12025558 A.U. after 18 cycles
Convg = 0.3650D-08 -V/T = 2.0026

LCuBr_twisted (III)

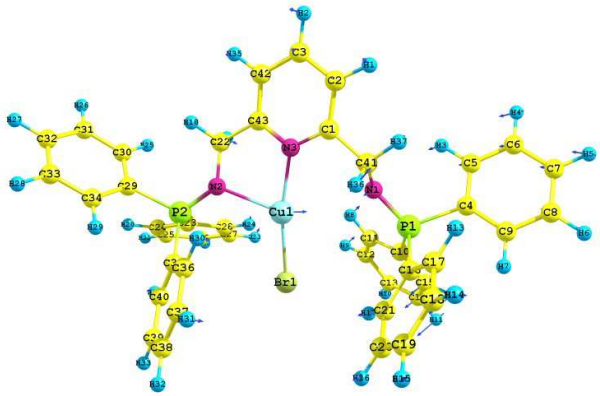


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.461464	0.292143	-0.300215
2	15	0	-3.883781	0.198000	0.130669
3	15	0	3.747527	0.139792	0.009892
4	7	0	-2.711031	1.236258	0.245896
5	7	0	2.475370	1.072668	-0.145766
6	7	0	0.069556	2.306715	-0.223056
7	6	0	-1.119536	2.882720	-0.470939
8	6	0	-1.307374	4.250974	-0.311090
9	1	0	-2.281718	4.682963	-0.513570
10	6	0	-0.243873	5.040285	0.111690
11	1	0	-0.368253	6.111097	0.243189
12	6	0	-5.557084	0.951770	0.105081
13	6	0	-5.689802	2.211971	0.695296
14	1	0	-4.807620	2.689014	1.115936
15	6	0	-6.931765	2.838596	0.741751
16	1	0	-7.028394	3.817492	1.202149
17	6	0	-8.049862	2.209952	0.198683
18	1	0	-9.019268	2.698541	0.234677
19	6	0	-7.924672	0.955277	-0.393910
20	1	0	-8.794604	0.466438	-0.822648
21	6	0	-6.682731	0.328782	-0.443915
22	1	0	-6.586294	-0.642942	-0.921094
23	6	0	-3.833499	-0.870051	1.588360
24	6	0	-2.606324	-1.049472	2.230855
25	1	0	-1.732744	-0.525380	1.858209
26	6	0	-2.518890	-1.912727	3.319086
27	1	0	-1.560803	-2.061095	3.807688
28	6	0	-3.648133	-2.592241	3.767474
29	1	0	-3.575225	-3.268393	4.614697
30	6	0	-4.874013	-2.409917	3.129872
31	1	0	-5.756916	-2.934611	3.482512
32	6	0	-4.968081	-1.550055	2.040716
33	1	0	-5.926867	-1.405064	1.550468
34	6	0	-3.872393	-0.875930	-1.341780
35	6	0	-4.257037	-0.345032	-2.580365
36	1	0	-4.662239	0.662800	-2.639098
37	6	0	-4.140012	-1.106012	-3.737931
38	1	0	-4.442929	-0.687834	-4.693345
39	6	0	-3.632109	-2.402328	-3.667220
40	1	0	-3.536481	-2.996302	-4.571669
41	6	0	-3.239582	-2.931683	-2.442000
42	1	0	-2.822805	-3.932102	-2.384349
43	6	0	-3.354450	-2.171389	-1.281159
44	1	0	-3.016196	-2.580659	-0.335246
45	6	0	2.415821	2.368136	0.478300
46	1	0	3.223636	3.038984	0.141869
47	1	0	2.499809	2.313789	1.580815
48	6	0	3.960636	-0.621871	1.651845
49	6	0	5.215192	-0.897330	2.207630
50	1	0	6.121231	-0.633110	1.669305
51	6	0	5.307663	-1.509186	3.454229
52	1	0	6.283313	-1.717416	3.882923

53	6	0	4.149773	-1.849286	4.150289
54	1	0	4.223950	-2.326217	5.123247
55	6	0	2.899473	-1.583720	3.597704
56	1	0	1.995084	-1.858262	4.131661
57	6	0	2.800540	-0.972434	2.351843
58	1	0	1.824605	-0.793378	1.908456
59	6	0	5.323417	1.004930	-0.310151
60	6	0	5.799964	1.942507	0.615920
61	1	0	5.283789	2.081674	1.562914
62	6	0	6.944678	2.683186	0.341568
63	1	0	7.307729	3.404855	1.067084
64	6	0	7.623993	2.495755	-0.860537
65	1	0	8.519965	3.071374	-1.073288
66	6	0	7.156090	1.568003	-1.786603
67	1	0	7.683876	1.418357	-2.723527
68	6	0	6.008889	0.826971	-1.515403
69	1	0	5.648877	0.104152	-2.241422
70	6	0	3.616566	-1.190790	-1.196977
71	6	0	2.965143	-0.940512	-2.407493
72	1	0	2.510025	0.030074	-2.577891
73	6	0	2.872588	-1.945571	-3.362473
74	1	0	2.351768	-1.755780	-4.295520
75	6	0	3.428049	-3.198273	-3.112858
76	1	0	3.346581	-3.984877	-3.857087
77	6	0	4.075271	-3.449062	-1.905967
78	1	0	4.496363	-4.429371	-1.705954
79	6	0	4.170031	-2.447318	-0.945434
80	1	0	4.654277	-2.652927	0.004856
81	6	0	-2.256730	1.985242	-0.897959
82	6	0	0.978715	4.436203	0.357054
83	1	0	1.839716	5.013792	0.679791
84	6	0	1.098597	3.059000	0.179262
85	1	0	-1.888167	1.333015	-1.710274
86	1	0	-3.037395	2.631742	-1.340127
87	35	0	0.063874	-1.986896	-0.230060

PCM: SCF Done: E(RwB97XD) = -6722.13392695 A.U. after 19 cycles
Convg = 0.3049D-08 -V/T = 2.0026

LCuBr_TS (TS IV)

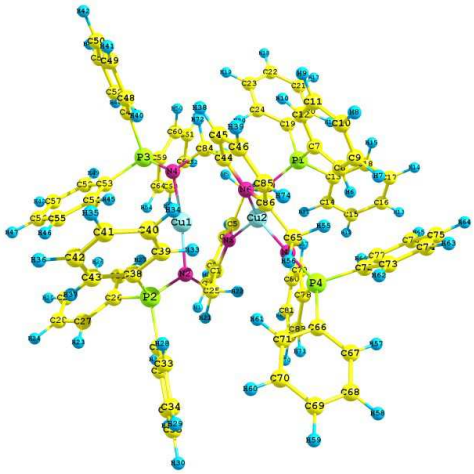


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-0.029620	0.390264	0.056301
2	15	0	3.640847	0.116866	-0.069958
3	15	0	-3.596884	0.111732	0.011408
4	7	0	2.461435	1.150490	-0.238192
5	7	0	-2.353067	1.080435	0.073487
6	7	0	0.004089	2.444664	0.044005
7	6	0	1.145471	3.102683	0.297826
8	6	0	1.217924	4.489255	0.236034
9	1	0	2.158809	4.988515	0.443677
10	6	0	0.078116	5.210467	-0.101796
11	1	0	0.107551	6.294619	-0.160791
12	6	0	5.296331	0.850889	-0.362790
13	6	0	5.346605	1.984944	-1.179087
14	1	0	4.418507	2.395784	-1.569786
15	6	0	6.569218	2.572182	-1.491198
16	1	0	6.599995	3.454379	-2.123914
17	6	0	7.750491	2.027013	-0.994613
18	1	0	8.704901	2.485340	-1.236796
19	6	0	7.708496	0.893575	-0.185553
20	1	0	8.628349	0.466503	0.202896
21	6	0	6.486453	0.307619	0.130588
22	1	0	6.460181	-0.568378	0.773134
23	6	0	3.459441	-1.163354	-1.327249
24	6	0	2.485029	-1.017264	-2.313907
25	1	0	1.823176	-0.158491	-2.278686
26	6	0	2.359748	-1.984293	-3.306131
27	1	0	1.592177	-1.877586	-4.066417
28	6	0	3.199710	-3.094014	-3.312630
29	1	0	3.092878	-3.851798	-4.083400
30	6	0	4.175661	-3.239326	-2.328259
31	1	0	4.830349	-4.105538	-2.330425
32	6	0	4.308952	-2.272677	-1.338161
33	1	0	5.067258	-2.390490	-0.567978
34	6	0	3.776199	-0.680779	1.561666
35	6	0	4.387547	0.005680	2.619374
36	1	0	4.889171	0.953404	2.438437
37	6	0	4.369693	-0.525890	3.904871
38	1	0	4.850026	0.009410	4.718627
39	6	0	3.736231	-1.743597	4.143928
40	1	0	3.723116	-2.160500	5.146930
41	6	0	3.112600	-2.421775	3.100173
42	1	0	2.601847	-3.361771	3.283930
43	6	0	3.124331	-1.892210	1.813300
44	1	0	2.597883	-2.405531	1.014690
45	6	0	-2.351314	2.343897	-0.605286
46	1	0	-3.212683	2.981171	-0.340096
47	1	0	-2.379415	2.238841	-1.708446
48	6	0	-3.858260	-0.738444	-1.581913
49	6	0	-5.116481	-1.163943	-2.023651
50	1	0	-6.001473	-0.966377	-1.424492
51	6	0	-5.240947	-1.836036	-3.235738
52	1	0	-6.219338	-2.164832	-3.573657

53	6	0	-4.111711	-2.084521	-4.013702
54	1	0	-4.211200	-2.608601	-4.959887
55	6	0	-2.858449	-1.662464	-3.578585
56	1	0	-1.974522	-1.864240	-4.175703
57	6	0	-2.728708	-0.991941	-2.366079
58	1	0	-1.748671	-0.689848	-2.008493
59	6	0	-5.197018	0.938074	0.334967
60	6	0	-5.738853	1.791952	-0.634974
61	1	0	-5.260802	1.879218	-1.607994
62	6	0	-6.897352	2.514754	-0.370038
63	1	0	-7.309716	3.172434	-1.129457
64	6	0	-7.527475	2.391018	0.866499
65	1	0	-8.435430	2.950494	1.071810
66	6	0	-6.995084	1.546461	1.836605
67	1	0	-7.485825	1.444951	2.799880
68	6	0	-5.832099	0.826636	1.575299
69	1	0	-5.421058	0.169193	2.335849
70	6	0	-3.398064	-1.144681	1.288586
71	6	0	-2.649564	-0.830685	2.424995
72	1	0	-2.160631	0.136137	2.487849
73	6	0	-2.506478	-1.771920	3.438030
74	1	0	-1.911599	-1.533147	4.314196
75	6	0	-3.105216	-3.023668	3.317880
76	1	0	-2.983788	-3.761209	4.105988
77	6	0	-3.848377	-3.338284	2.182906
78	1	0	-4.303206	-4.318821	2.081524
79	6	0	-3.995386	-2.399989	1.166559
80	1	0	-4.553033	-2.657185	0.270463
81	6	0	2.348131	2.264566	0.668102
82	6	0	-1.094933	4.520796	-0.364573
83	1	0	-2.009243	5.042992	-0.629172
84	6	0	-1.096473	3.128613	-0.281573
85	1	0	2.209611	1.942074	1.718548
86	1	0	3.231887	2.927261	0.666143
87	35	0	-0.067387	-1.945716	0.072207

PCM: SCF Done: E(RwB97XD) = -6722.13024142 A.U. after 19 cycles
Convg = 0.4260D-08 -V/T = 2.0026

LCu_dimer (V)



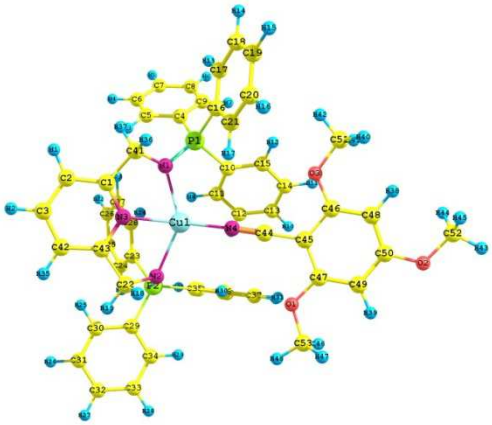
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	1.725926	-0.038550	0.159002
2	29	0	-1.153067	-0.018863	0.069583
3	15	0	-3.223608	-2.522643	-0.272283
4	15	0	3.097948	2.618928	-0.156179
5	15	0	2.938731	-2.838351	0.195263
6	15	0	-2.922066	2.781338	0.253355
7	7	0	-1.934407	-1.753716	-0.797743
8	7	0	1.750636	1.795475	-0.435094
9	7	0	-0.214510	0.078148	-1.861511
10	7	0	1.924086	-1.802847	0.896941
11	7	0	-1.898605	1.735284	0.905539
12	7	0	-0.510221	-0.319789	2.062122
13	6	0	0.392437	1.158083	-2.380168
14	6	0	0.672866	1.255973	-3.736999
15	1	0	1.160369	2.142823	-4.128192
16	6	0	0.300148	0.210842	-4.577586
17	1	0	0.491939	0.267826	-5.644797
18	6	0	-0.334753	-0.895502	-4.032388
19	1	0	-0.649324	-1.726219	-4.656459
20	6	0	-0.572402	-0.931150	-2.659191
21	6	0	-1.221026	-2.133147	-2.002968
22	1	0	-1.840757	-2.644045	-2.754346
23	1	0	-0.406538	-2.837173	-1.766219
24	6	0	-3.436015	-2.156050	1.486750
25	6	0	-4.118498	-0.999795	1.879835
26	1	0	-4.565686	-0.343118	1.140488
27	6	0	-4.238477	-0.687907	3.229735
28	1	0	-4.791270	0.198980	3.523519
29	6	0	-3.661454	-1.512965	4.192165
30	1	0	-3.760068	-1.270562	5.245773
31	6	0	-2.974022	-2.660556	3.804780
32	1	0	-2.533565	-3.311736	4.552896
33	6	0	-2.867461	-2.986761	2.456697
34	1	0	-2.351152	-3.896963	2.167172
35	6	0	-4.790352	-2.039565	-1.066703
36	6	0	-4.735605	-1.460153	-2.336395
37	1	0	-3.773225	-1.306045	-2.815496
38	6	0	-5.903300	-1.070037	-2.985267
39	1	0	-5.850846	-0.612012	-3.967937
40	6	0	-7.137131	-1.271735	-2.371336
41	1	0	-8.050084	-0.974777	-2.878115
42	6	0	-7.201629	-1.860175	-1.108730
43	1	0	-8.163039	-2.019966	-0.630886
44	6	0	-6.033456	-2.238659	-0.454559
45	1	0	-6.090900	-2.682415	0.535790
46	6	0	-3.097520	-4.326023	-0.468666
47	6	0	-4.179191	-5.124292	-0.854272
48	1	0	-5.141300	-4.674035	-1.076425
49	6	0	-4.026442	-6.504027	-0.962188

50	1	0	-4.869843	-7.116477	-1.264178
51	6	0	-2.798239	-7.096807	-0.682684
52	1	0	-2.684683	-8.173258	-0.762511
53	6	0	-1.714072	-6.306866	-0.305346
54	1	0	-0.755656	-6.768906	-0.086164
55	6	0	-1.859460	-4.928029	-0.207669
56	1	0	-1.008318	-4.313323	0.071439
57	6	0	0.747775	2.249780	-1.400202
58	1	0	1.064799	3.137367	-1.958947
59	1	0	-0.163172	2.516773	-0.855383
60	6	0	4.449595	2.204393	-1.297417
61	6	0	5.618077	2.972051	-1.375424
62	1	0	5.733278	3.864180	-0.764971
63	6	0	6.626421	2.616248	-2.264567
64	1	0	7.530998	3.213087	-2.322597
65	6	0	6.464797	1.508756	-3.095270
66	1	0	7.248207	1.240196	-3.797023
67	6	0	5.294391	0.757071	-3.038528
68	1	0	5.164618	-0.098299	-3.693955
69	6	0	4.290566	1.099900	-2.138861
70	1	0	3.372106	0.521187	-2.091115
71	6	0	2.930648	4.419969	-0.287353
72	6	0	2.801573	5.209598	0.860613
73	1	0	2.815393	4.751410	1.845085
74	6	0	2.685711	6.592249	0.744286
75	1	0	2.616162	7.203356	1.639144
76	6	0	2.673210	7.190274	-0.513076
77	1	0	2.582760	8.268273	-0.600734
78	6	0	2.794576	6.408361	-1.660354
79	1	0	2.799205	6.875371	-2.639771
80	6	0	2.936143	5.029986	-1.549289
81	1	0	3.076852	4.432389	-2.446390
82	6	0	3.598159	2.256025	1.545747
83	6	0	2.615201	1.882048	2.470024
84	1	0	1.580241	1.791189	2.152366
85	6	0	2.966977	1.617423	3.789876
86	1	0	2.199640	1.319798	4.496874
87	6	0	4.294304	1.734444	4.196483
88	1	0	4.567332	1.528386	5.226603
89	6	0	5.271069	2.129252	3.284592
90	1	0	6.303611	2.233286	3.602443
91	6	0	4.924974	2.391571	1.962737
92	1	0	5.694799	2.689315	1.258316
93	6	0	0.187337	-1.365706	2.534889
94	6	0	0.456574	-1.514419	3.887408
95	1	0	1.010169	-2.378839	4.239192
96	6	0	-0.002183	-0.543056	4.774258
97	1	0	0.191090	-0.632848	5.838919
98	6	0	3.395222	-4.187501	1.317851
99	6	0	3.408772	-3.909436	2.690021
100	1	0	3.079371	-2.935775	3.044036
101	6	0	3.859338	-4.867099	3.591441
102	1	0	3.866106	-4.649936	4.654856
103	6	0	4.313475	-6.100471	3.128483
104	1	0	4.667992	-6.846323	3.832643
105	6	0	4.326419	-6.372547	1.762681
106	1	0	4.696247	-7.326238	1.400222
107	6	0	3.873156	-5.418743	0.856369
108	1	0	3.902402	-5.636963	-0.207191
109	6	0	4.490168	-1.999447	-0.182168
110	6	0	4.924231	-0.966459	0.654502
111	1	0	4.276005	-0.592900	1.442425
112	6	0	6.194259	-0.426545	0.479492
113	1	0	6.530758	0.367923	1.135679
114	6	0	7.033994	-0.912169	-0.518112
115	1	0	8.023133	-0.485457	-0.649237
116	6	0	6.609089	-1.951171	-1.342532
117	1	0	7.266293	-2.339995	-2.113636
118	6	0	5.343931	-2.501521	-1.171474
119	1	0	5.030077	-3.324800	-1.806685
120	6	0	2.298189	-3.579077	-1.335681
121	6	0	1.547373	-4.760122	-1.302661
122	1	0	1.426708	-5.304520	-0.369947
123	6	0	0.957980	-5.250452	-2.464561
124	1	0	0.377802	-6.166577	-2.430415
125	6	0	1.113282	-4.566284	-3.667288
126	1	0	0.667579	-4.959947	-4.575356

127	6	0	1.841266	-3.378630	-3.703648
128	1	0	1.958213	-2.838685	-4.637515
129	6	0	2.417986	-2.877928	-2.542057
130	1	0	2.968569	-1.941584	-2.577290
131	6	0	-1.832815	1.719283	2.354873
132	1	0	-2.822070	1.568624	2.819609
133	1	0	-1.449829	2.669191	2.764817
134	6	0	-2.558623	4.494709	0.725528
135	6	0	-3.543925	5.487384	0.757810
136	1	0	-4.580011	5.238008	0.547110
137	6	0	-3.199504	6.801312	1.059843
138	1	0	-3.966289	7.568631	1.084328
139	6	0	-1.872671	7.127761	1.331168
140	1	0	-1.607051	8.153326	1.568058
141	6	0	-0.888167	6.143008	1.297468
142	1	0	0.145866	6.397255	1.501317
143	6	0	-1.225527	4.828817	0.992816
144	1	0	-0.456852	4.059252	0.957692
145	6	0	-4.659565	2.497466	0.723503
146	6	0	-5.061921	2.835845	2.024467
147	1	0	-4.394466	3.394715	2.675301
148	6	0	-6.329381	2.490468	2.482711
149	1	0	-6.633465	2.765526	3.487903
150	6	0	-7.208160	1.802565	1.648573
151	1	0	-8.197873	1.536137	2.005906
152	6	0	-6.823435	1.477493	0.350513
153	1	0	-7.508053	0.955529	-0.309395
154	6	0	-5.556186	1.820951	-0.112473
155	1	0	-5.279667	1.561199	-1.128889
156	6	0	-2.803336	2.710366	-1.548730
157	6	0	-2.996317	1.495487	-2.214289
158	1	0	-3.169892	0.586263	-1.647510
159	6	0	-2.940368	1.443689	-3.601468
160	1	0	-3.094308	0.499039	-4.113662
161	6	0	-2.668225	2.595729	-4.335341
162	1	0	-2.618202	2.550338	-5.418912
163	6	0	-2.461494	3.804761	-3.678324
164	1	0	-2.251489	4.706236	-4.244874
165	6	0	-2.537491	3.867134	-2.289421
166	1	0	-2.385510	4.817723	-1.789053
167	6	0	0.698233	-2.342140	1.505303
168	1	0	0.878664	-3.309336	1.993546
169	1	0	-0.090050	-2.478031	0.751884
170	6	0	-0.718837	0.533050	4.276650
171	1	0	-1.105138	1.303800	4.937041
172	6	0	-0.968346	0.604916	2.903860

PCM: SCF Done: E(RwB97XD) = -8295.64351887 A.U. after 23 cycles
Convg = 0.3570D-08 -V/T = 2.0035

LCu_OMePhCN (VI)

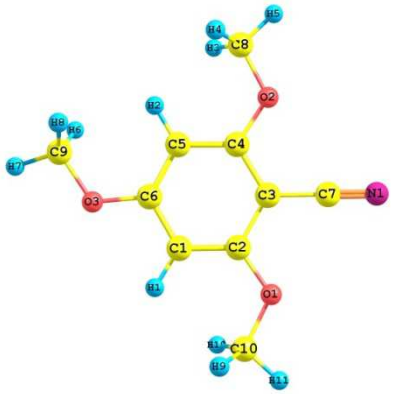


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.415646	0.169565	-1.294495
2	15	0	-0.957242	2.849924	0.191024
3	15	0	3.062927	-1.470751	0.095801
4	7	0	0.210659	2.354698	-0.765800
5	7	0	2.179666	-1.220186	-1.200027
6	7	0	1.815725	1.134843	-2.492560
7	6	0	1.797213	2.462231	-2.570761
8	6	0	2.870752	3.162841	-3.112466
9	1	0	2.845855	4.246194	-3.173585
10	6	0	3.981086	2.442999	-3.544504
11	1	0	4.837607	2.961739	-3.964035
12	6	0	-0.511273	4.232536	1.288476
13	6	0	0.700303	4.896693	1.085466
14	1	0	1.353524	4.589745	0.274298
15	6	0	1.082992	5.931762	1.934457
16	1	0	2.026233	6.444188	1.772328
17	6	0	0.259414	6.302385	2.993616
18	1	0	0.558884	7.106515	3.658551
19	6	0	-0.945147	5.634451	3.210170
20	1	0	-1.581022	5.914885	4.043984
21	6	0	-1.328769	4.599987	2.363659
22	1	0	-2.259677	4.068676	2.547463
23	6	0	-1.382456	1.482856	1.290703
24	6	0	-0.343182	0.841308	1.975929
25	1	0	0.679374	1.193118	1.874086
26	6	0	-0.618512	-0.257487	2.777713
27	1	0	0.190408	-0.760779	3.296554
28	6	0	-1.927362	-0.722138	2.901562
29	1	0	-2.133936	-1.592482	3.516946
30	6	0	-2.963472	-0.075170	2.237273
31	1	0	-3.983094	-0.437074	2.332487
32	6	0	-2.693529	1.031724	1.435314
33	1	0	-3.501737	1.522214	0.904101
34	6	0	-2.463465	3.338770	-0.703867
35	6	0	-3.115166	4.561421	-0.523559
36	1	0	-2.754534	5.271845	0.213911
37	6	0	-4.229148	4.878726	-1.297716
38	1	0	-4.730300	5.830866	-1.155019
39	6	0	-4.689985	3.983068	-2.258791
40	1	0	-5.553553	4.237514	-2.866064
41	6	0	-4.036539	2.765895	-2.450711
42	1	0	-4.387990	2.067615	-3.204158
43	6	0	-2.926034	2.443137	-1.678963
44	1	0	-2.417939	1.494016	-1.828023
45	6	0	2.778998	-1.042896	-2.517905
46	1	0	2.113748	-1.511450	-3.255870
47	1	0	3.760473	-1.524929	-2.629945
48	6	0	3.770176	-0.006987	0.930685
49	6	0	4.877242	-0.100632	1.783962
50	1	0	5.388573	-1.050780	1.914299
51	6	0	5.340224	1.024050	2.459917

52	1	0	6.199585	0.942100	3.118170
53	6	0	4.703129	2.251287	2.290221
54	1	0	5.064258	3.127532	2.819933
55	6	0	3.608242	2.352381	1.436469
56	1	0	3.105288	3.304950	1.302687
57	6	0	3.143623	1.231153	0.754674
58	1	0	2.288330	1.333629	0.091877
59	6	0	4.484564	-2.562881	-0.202402
60	6	0	5.662407	-2.038901	-0.751045
61	1	0	5.767112	-0.966157	-0.894516
62	6	0	6.708670	-2.885796	-1.101844
63	1	0	7.619355	-2.473153	-1.524462
64	6	0	6.587262	-4.259780	-0.906467
65	1	0	7.405472	-4.920127	-1.176703
66	6	0	5.418180	-4.787538	-0.364132
67	1	0	5.324063	-5.857666	-0.209212
68	6	0	4.366842	-3.944210	-0.017632
69	1	0	3.456542	-4.360536	0.404645
70	6	0	2.005780	-2.287535	1.321503
71	6	0	0.794862	-2.848582	0.909259
72	1	0	0.478764	-2.737700	-0.122817
73	6	0	0.000116	-3.528148	1.828791
74	1	0	-0.950956	-3.937845	1.506557
75	6	0	0.416957	-3.669006	3.149215
76	1	0	-0.200611	-4.209730	3.860478
77	6	0	1.626821	-3.112464	3.562371
78	1	0	1.953751	-3.217845	4.592093
79	6	0	2.415883	-2.414934	2.653322
80	1	0	3.349151	-1.971196	2.986915
81	6	0	0.564528	3.103254	-1.968114
82	6	0	4.005550	1.057662	-3.397165
83	1	0	4.876699	0.476795	-3.683541
84	6	0	2.891629	0.432405	-2.848625
85	1	0	-0.245657	3.072072	-2.717429
86	1	0	0.774154	4.168000	-1.789560
87	6	0	-2.176281	-1.450541	-0.989826
88	7	0	-1.235446	-0.819863	-1.212620
89	6	0	-3.310420	-2.249301	-0.706855
90	6	0	-4.576561	-1.661756	-0.535570
91	6	0	-3.166879	-3.650508	-0.586966
92	6	0	-5.682410	-2.447441	-0.215094
93	6	0	-4.261076	-4.438724	-0.275575
94	6	0	-5.510094	-3.830346	-0.086549
95	1	0	-6.655564	-1.997784	-0.082919
96	1	0	-4.196373	-5.513636	-0.172883
97	8	0	-1.922318	-4.114678	-0.790390
98	8	0	-6.504485	-4.676423	0.218778
99	8	0	-4.622052	-0.330123	-0.707252
100	6	0	-5.847957	0.348973	-0.499604
101	1	0	-6.611091	0.011315	-1.209748
102	1	0	-6.207186	0.209387	0.526777
103	1	0	-5.631832	1.402951	-0.674964
104	6	0	-7.810414	-4.165976	0.420662
105	1	0	-8.429971	-5.028857	0.662372
106	1	0	-7.833536	-3.455944	1.255470
107	1	0	-8.192633	-3.686119	-0.487616
108	6	0	-1.701809	-5.515354	-0.755447
109	1	0	-1.942529	-5.929607	0.230250
110	1	0	-2.291559	-6.022819	-1.526188
111	1	0	-0.639357	-5.648814	-0.955424

PCM : SCF Done: E(RwB97XD) = -4815.67291924 A.U. after 21 cycles
Convg = 0.6147D-08 -V/T = 2.0038

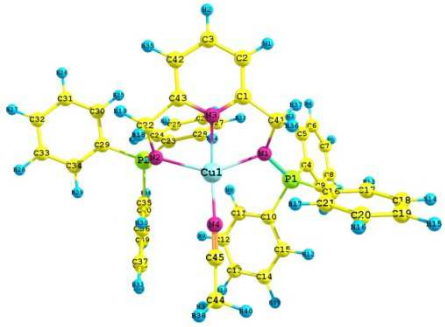
OMePhCN



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.246292	0.249388	0.014877
2	6	0	-0.145806	-0.048093	1.367430
3	6	0	1.117728	-0.110607	1.991874
4	6	0	2.273171	0.130898	1.232078
5	6	0	2.182859	0.431053	-0.129641
6	6	0	0.919348	0.486104	-0.720611
7	1	0	-1.195480	0.306916	-0.500663
8	1	0	3.075108	0.615991	-0.709674
9	6	0	1.221055	-0.416095	3.381823
10	7	0	1.306383	-0.663417	4.507198
11	8	0	-1.195531	-0.292300	2.169151
12	8	0	3.434151	0.051287	1.904894
13	8	0	0.717911	0.766965	-2.025568
14	6	0	4.643599	0.281694	1.214191
15	1	0	4.788805	-0.449651	0.409631
16	1	0	4.679853	1.297453	0.801692
17	1	0	5.433258	0.164426	1.955917
18	6	0	1.838570	1.019770	-2.845875
19	1	0	2.506444	0.150579	-2.890477
20	1	0	1.440442	1.218798	-3.841225
21	1	0	2.399550	1.896286	-2.498600
22	6	0	-2.494273	-0.247446	1.614705
23	1	0	-2.720877	0.748308	1.215432
24	1	0	-2.613744	-0.997014	0.823392
25	1	0	-3.173661	-0.473659	2.436077

PCM : SCF Done: E(RwB97XD) = -667.867088698 A.U. after 14 cycles
Convg = 0.4097D-08 -V/T = 2.0059

LCu_MeCN (VII)

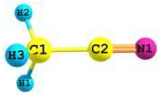


Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.027484	0.234263	-1.534795
2	15	0	2.918932	-0.257842	0.159660
3	15	0	-2.984356	0.099400	0.009621
4	7	0	1.721090	-0.942424	-0.629539
5	7	0	-2.191067	0.055961	-1.366485
6	7	0	-0.309626	-1.718825	-2.158627
7	6	0	0.631734	-2.636274	-1.955638
8	6	0	0.351086	-3.992795	-2.088388
9	1	0	1.126202	-4.733997	-1.921925
10	6	0	-0.949117	-4.372012	-2.409824
11	1	0	-1.199356	-5.423273	-2.514093
12	6	0	3.484428	-1.152150	1.640308
13	6	0	3.076464	-2.473516	1.837160
14	1	0	2.430925	-2.954187	1.108408
15	6	0	3.474289	-3.167267	2.976711
16	1	0	3.155603	-4.194523	3.124144
17	6	0	4.276172	-2.541639	3.927311
18	1	0	4.584036	-3.081026	4.817594
19	6	0	4.676741	-1.219252	3.743135
20	1	0	5.291247	-0.726968	4.490158
21	6	0	4.280754	-0.524385	2.605400
22	1	0	4.579765	0.513001	2.475745
23	6	0	2.341360	1.344288	0.771194
24	6	0	1.098811	1.405279	1.412231
25	1	0	0.511074	0.503203	1.555025
26	6	0	0.608645	2.623884	1.863769
27	1	0	-0.359712	2.667232	2.349669
28	6	0	1.359851	3.785790	1.693700
29	1	0	0.974455	4.734617	2.055765
30	6	0	2.606430	3.725828	1.076744
31	1	0	3.201885	4.626653	0.959705
32	6	0	3.097944	2.506904	0.611535
33	1	0	4.066106	2.468112	0.120875
34	6	0	4.379699	0.049178	-0.874018
35	6	0	5.684519	-0.287373	-0.506242
36	1	0	5.881015	-0.745141	0.458425
37	6	0	6.738856	-0.042521	-1.383580
38	1	0	7.751726	-0.305340	-1.095334
39	6	0	6.494766	0.531821	-2.627466
40	1	0	7.318448	0.718047	-3.309646
41	6	0	5.192462	0.858962	-3.004451
42	1	0	5.001579	1.296007	-3.979558
43	6	0	4.137303	0.615887	-2.134185
44	1	0	3.117207	0.854704	-2.428365
45	6	0	-2.527067	-0.886342	-2.427825
46	1	0	-2.413885	-0.368609	-3.390119
47	1	0	-3.563742	-1.248583	-2.388571
48	6	0	-2.456147	-1.053216	1.323149
49	6	0	-3.293444	-1.382724	2.397346
50	1	0	-4.310365	-1.000840	2.436461
51	6	0	-2.835569	-2.214389	3.414443
52	1	0	-3.492505	-2.467221	4.240793
53	6	0	-1.539944	-2.724776	3.367503
54	1	0	-1.183874	-3.373246	4.162134
55	6	0	-0.706872	-2.408271	2.298323

56	1	0	0.304073	-2.801144	2.258381
57	6	0	-1.161450	-1.580198	1.275643
58	1	0	-0.495648	-1.349028	0.448212
59	6	0	-4.767171	-0.191196	-0.172532
60	6	0	-5.250585	-1.503947	-0.255788
61	1	0	-4.576042	-2.343661	-0.106146
62	6	0	-6.596634	-1.738368	-0.514729
63	1	0	-6.966490	-2.757025	-0.576201
64	6	0	-7.468992	-0.666198	-0.689624
65	1	0	-8.520818	-0.849894	-0.885080
66	6	0	-6.994546	0.640720	-0.610687
67	1	0	-7.675405	1.475418	-0.743749
68	6	0	-5.647074	0.880030	-0.358849
69	1	0	-5.282451	1.901664	-0.299153
70	6	0	-2.773828	1.771858	0.681600
71	6	0	-2.415982	2.798746	-0.196334
72	1	0	-2.218342	2.554174	-1.235101
73	6	0	-2.319492	4.107448	0.268630
74	1	0	-2.053262	4.905331	-0.418813
75	6	0	-2.588776	4.398524	1.603966
76	1	0	-2.524306	5.421500	1.962569
77	6	0	-2.949006	3.376660	2.481030
78	1	0	-3.159517	3.599449	3.522227
79	6	0	-3.036882	2.064679	2.023348
80	1	0	-3.307916	1.274504	2.717009
81	6	0	1.968642	-2.076167	-1.517146
82	6	0	-1.935356	-3.398749	-2.554581
83	1	0	-2.967079	-3.667959	-2.757309
84	6	0	-1.573580	-2.064654	-2.406942
85	1	0	2.529676	-1.769292	-2.416751
86	1	0	2.551827	-2.887598	-1.058621
87	6	0	1.089010	4.615039	-1.923460
88	1	0	0.712440	5.080310	-2.837965
89	1	0	0.617964	5.078659	-1.053049
90	1	0	2.169862	4.761527	-1.858411
91	6	0	0.785962	3.190320	-1.927431
92	7	0	0.534957	2.067665	-1.923385

PCM : SCF Done: E(RwB97XD) = -4280.52176634 A.U. after 20 cycles
Convg = 0.7201D-08 -V/T = 2.0035

MeCN



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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2	1	0	0.000000	1.027294	-1.552294
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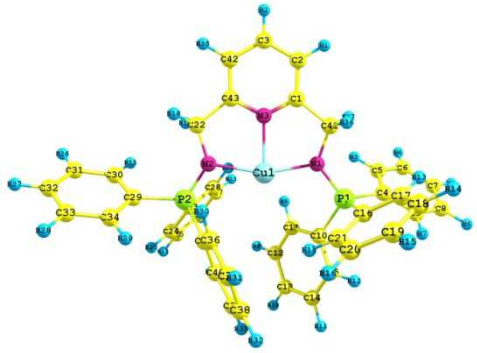
4	1	0	0.889662	-0.513647	-1.552294
5	6	0	0.000000	0.000000	0.282002
6	7	0	0.000000	0.000000	1.434324

PCM : SCF Done: E(RwB97XD) = -132.729391706 A.U. after 11 cycles
Convg = 0.1848D-08 -V/T = 2.0053

LCu (VIII)



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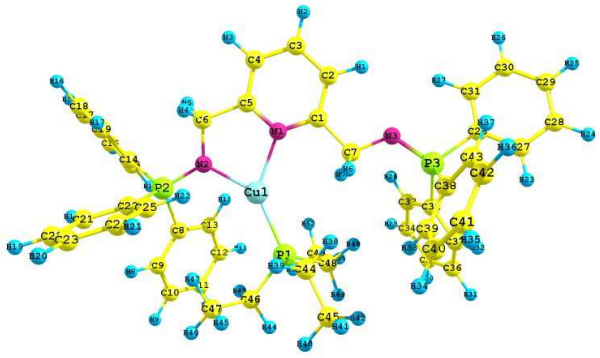
3	15	0	2.871306	-0.102222	-0.085764
4	7	0	-1.884294	1.189551	0.193495
5	7	0	1.998627	1.168571	-0.493012
6	7	0	0.052171	2.889531	-0.284666
7	6	0	-1.120778	3.495046	-0.227627
8	6	0	-1.170447	4.885549	-0.228798
9	1	0	-2.113863	5.420028	-0.180190
10	6	0	0.043177	5.575399	-0.294506
11	1	0	0.039476	6.661232	-0.300351
12	6	0	-4.442476	0.124968	0.901112
13	6	0	-4.483164	0.987388	2.002422
14	1	0	-3.592799	1.543097	2.284942
15	6	0	-5.654956	1.120380	2.740210
16	1	0	-5.684793	1.795467	3.589542
17	6	0	-6.785425	0.386236	2.389868
18	1	0	-7.700274	0.491941	2.964424
19	6	0	-6.744575	-0.487501	1.305396
20	1	0	-7.623918	-1.064424	1.037265
21	6	0	-5.576427	-0.621860	0.562691
22	1	0	-5.552512	-1.304901	-0.281791
23	6	0	-2.028798	-1.481704	0.830983
24	6	0	-1.063644	-1.250112	1.816457
25	1	0	-0.789503	-0.230496	2.069006
26	6	0	-0.461243	-2.320757	2.469168
27	1	0	0.296781	-2.130478	3.223426
28	6	0	-0.833072	-3.625846	2.154571
29	1	0	-0.369073	-4.462090	2.668964
30	6	0	-1.805674	-3.860271	1.185135
31	1	0	-2.100754	-4.876590	0.943752
32	6	0	-2.405186	-2.792317	0.524209
33	1	0	-3.159363	-2.985639	-0.233738
34	6	0	-3.210448	-0.508379	-1.677488
35	6	0	-4.290349	0.073067	-2.352134
36	1	0	-5.015298	0.674839	-1.811090
37	6	0	-4.447238	-0.125118	-3.721197
38	1	0	-5.290385	0.323021	-4.236953
39	6	0	-3.525851	-0.896975	-4.423449
40	1	0	-3.653575	-1.055233	-5.489697
41	6	0	-2.438786	-1.463154	-3.759877
42	1	0	-1.716849	-2.061200	-4.307161
43	6	0	-2.273213	-1.263670	-2.394627
44	1	0	-1.413709	-1.696923	-1.888952
45	6	0	2.425150	2.556603	-0.318267
46	1	0	3.126620	2.851840	-1.110369
47	1	0	2.946255	2.725594	0.638626
48	6	0	2.894984	-0.440772	1.702583
49	6	0	3.718211	-1.431206	2.250984
50	1	0	4.383449	-2.005272	1.610483
51	6	0	3.691190	-1.678879	3.619282
52	1	0	4.326193	-2.451305	4.041229
53	6	0	2.862288	-0.923294	4.448707
54	1	0	2.852046	-1.110257	5.518084

55	6	0	2.058391	0.078485	3.910466
56	1	0	1.424118	0.676393	4.557396
57	6	0	2.070454	0.316560	2.538199
58	1	0	1.438544	1.092298	2.112184
59	6	0	4.622686	-0.011448	-0.549208
60	6	0	5.473433	0.784210	0.230564
61	1	0	5.100687	1.262403	1.133177
62	6	0	6.803577	0.952215	-0.134553
63	1	0	7.457161	1.568321	0.474567
64	6	0	7.296213	0.322957	-1.276198
65	1	0	8.336878	0.450204	-1.557295
66	6	0	6.458616	-0.474140	-2.051423
67	1	0	6.844891	-0.970486	-2.935835
68	6	0	5.123536	-0.641155	-1.693324
69	1	0	4.480458	-1.271235	-2.300133
70	6	0	2.090984	-1.497775	-0.932978
71	6	0	1.775907	-1.336025	-2.290102
72	1	0	2.000493	-0.397019	-2.787265
73	6	0	1.153838	-2.365255	-2.985990
74	1	0	0.927183	-2.239707	-4.040210
75	6	0	0.817283	-3.548683	-2.328739
76	1	0	0.323918	-4.349939	-2.870634
77	6	0	1.109207	-3.702420	-0.976795
78	1	0	0.832519	-4.614471	-0.458586
79	6	0	1.754454	-2.684080	-0.279044
80	1	0	1.966578	-2.811042	0.776867
81	6	0	-2.310852	2.534950	-0.207910
82	6	0	1.260474	4.893635	-0.346322
83	1	0	2.200927	5.433819	-0.391023
84	6	0	1.220703	3.501256	-0.333387
85	1	0	-2.748798	2.543645	-1.220746
86	1	0	-3.080128	2.932643	0.467800

PCM : SCF Done: E(RwB97XD) = -4147.77298114 A.U. after 18 cycles
Convg = 0.6891D-08 -V/T = 2.0035

LCuPEt3 (IX)



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
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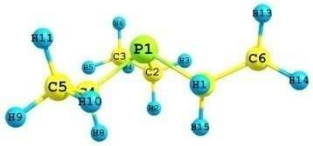
3	15	0	-4.216430	0.494931	-0.075196
4	15	0	4.581113	0.542216	-0.063167
5	7	0	-0.227043	1.948039	0.331026
6	7	0	-2.766548	1.150462	0.050305
7	7	0	3.381490	1.556882	-0.138771
8	6	0	1.079425	2.259313	0.273962
9	6	0	1.519161	3.568551	0.406538
10	1	0	2.583765	3.759499	0.349849
11	6	0	0.577459	4.574442	0.597571
12	1	0	0.892411	5.608389	0.701369
13	6	0	-0.770816	4.246774	0.644658
14	1	0	-1.532291	5.008477	0.779771
15	6	0	-1.137743	2.911449	0.505423
16	6	0	-2.593050	2.491879	0.575323
17	1	0	-2.903622	2.572036	1.632059
18	1	0	-3.190291	3.229627	0.020071
19	6	0	2.035483	1.107150	0.056466
20	1	0	1.913446	0.433807	0.929106
21	1	0	1.642689	0.539947	-0.808678
22	6	0	-4.095668	-0.840710	-1.289081
23	6	0	-4.863816	-2.003216	-1.190276
24	1	0	-5.521594	-2.157485	-0.340414
25	6	0	-4.772294	-2.982981	-2.175623
26	1	0	-5.364542	-3.888460	-2.091000
27	6	0	-3.922018	-2.802842	-3.264095
28	1	0	-3.856665	-3.566815	-4.032466
29	6	0	-3.155974	-1.642367	-3.367191
30	1	0	-2.492811	-1.498900	-4.214489
31	6	0	-3.238253	-0.663886	-2.382316
32	1	0	-2.637165	0.237816	-2.452118
33	6	0	-5.490582	1.653430	-0.644153
34	6	0	-5.867941	1.707198	-1.990005
35	1	0	-5.458865	0.997622	-2.703089
36	6	0	-6.782783	2.664509	-2.418823
37	1	0	-7.078124	2.697814	-3.462577
38	6	0	-7.318466	3.574101	-1.511065
39	1	0	-8.032841	4.318607	-1.848054
40	6	0	-6.944595	3.527484	-0.169316
41	1	0	-7.363848	4.234722	0.539176
42	6	0	-6.035242	2.570170	0.265308
43	1	0	-5.758158	2.529119	1.315900
44	6	0	-4.854619	-0.187064	1.483921
45	6	0	-6.207906	-0.497572	1.663362
46	1	0	-6.924783	-0.302192	0.869733
47	6	0	-6.642935	-1.041982	2.867235
48	1	0	-7.692631	-1.281019	3.004198
49	6	0	-5.733727	-1.266374	3.899994
50	1	0	-6.077589	-1.685962	4.840232
51	6	0	-4.389839	-0.943661	3.732229
52	1	0	-3.684240	-1.106654	4.540794
53	6	0	-3.949266	-0.405563	2.526593
54	1	0	-2.901139	-0.151524	2.388741

55	6	0	6.115728	1.474615	-0.244686
56	6	0	7.353998	0.829810	-0.165932
57	1	0	7.408010	-0.239716	0.021087
58	6	0	8.526711	1.559501	-0.321193
59	1	0	9.487823	1.059496	-0.256393
60	6	0	8.465460	2.931733	-0.559648
61	1	0	9.382913	3.499143	-0.682441
62	6	0	7.232943	3.573539	-0.642620
63	1	0	7.186894	4.641819	-0.830022
64	6	0	6.055361	2.848059	-0.485236
65	1	0	5.083596	3.326886	-0.548749
66	6	0	4.578939	-0.721683	-1.385041
67	6	0	3.896306	-0.384839	-2.558949
68	1	0	3.389155	0.574917	-2.621741
69	6	0	3.880096	-1.264242	-3.637806
70	1	0	3.357821	-0.991681	-4.550053
71	6	0	4.536734	-2.489303	-3.548084
72	1	0	4.523887	-3.176614	-4.388604
73	6	0	5.220977	-2.830274	-2.382873
74	1	0	5.739794	-3.781426	-2.314420
75	6	0	5.247623	-1.948413	-1.306756
76	1	0	5.785276	-2.223294	-0.403444
77	6	0	4.708333	-0.388866	1.500900
78	6	0	4.054394	-1.612483	1.685611
79	1	0	3.559813	-2.099526	0.848904
80	6	0	4.054011	-2.230408	2.933386
81	1	0	3.561547	-3.189499	3.059941
82	6	0	4.694065	-1.625165	4.011150
83	1	0	4.698328	-2.109871	4.982513
84	6	0	5.332420	-0.398515	3.841105
85	1	0	5.831099	0.076481	4.680088
86	6	0	5.337170	0.218321	2.594818
87	1	0	5.836808	1.174901	2.468968
88	6	0	0.452234	-2.515124	1.726622
89	1	0	1.237096	-1.779272	1.937136
90	1	0	-0.313209	-2.364718	2.497487
91	6	0	1.013729	-3.935005	1.802087
92	1	0	0.253380	-4.688479	1.572076
93	1	0	1.381316	-4.141884	2.811958
94	1	0	1.848437	-4.077631	1.107577
95	6	0	-1.560857	-3.341347	-0.204514
96	1	0	-2.070225	-3.065782	-1.133702
97	1	0	-1.038498	-4.287158	-0.393720
98	6	0	-2.586799	-3.511784	0.915989
99	1	0	-2.126835	-3.895927	1.832849
100	1	0	-3.362528	-4.221079	0.612160
101	1	0	-3.079107	-2.564327	1.156147
102	6	0	0.971673	-2.360351	-1.140228
103	1	0	1.874036	-1.802255	-0.864597
104	1	0	1.228632	-3.425759	-1.116234
105	6	0	0.521352	-1.953319	-2.544351
106	1	0	-0.390010	-2.481750	-2.844058
107	1	0	1.303393	-2.184820	-3.271937
108	1	0	0.319824	-0.876855	-2.595563

PCM : SCF Done: E(RwB97XD) = -4726.77408248 A.U. after 21 cycles
Convg = 0.3541D-08 -V/T = 2.0035

PEt3



Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	15	0	-0.001662	-0.002050	-0.531358
2	6	0	-0.897285	1.370345	0.348607
3	1	0	-1.965554	1.247984	0.133309
4	6	0	1.633782	0.089598	0.349859
5	1	0	1.476061	0.030984	1.435988
6	1	0	2.055434	1.080401	0.141888
7	6	0	2.624784	-0.984402	-0.104571
8	1	0	3.587680	-0.865105	0.403304
9	1	0	2.259839	-1.993172	0.118242
10	1	0	2.802120	-0.924499	-1.183809
11	6	0	-0.741258	-1.462930	0.350696
12	1	0	-0.097276	-2.325455	0.140525
13	1	0	-0.709988	-1.297634	1.436814
14	6	0	-2.169523	-1.779583	-0.100248
15	1	0	-2.548031	-2.673678	0.406330
16	1	0	-2.856988	-0.957551	0.127141
17	1	0	-2.210597	-1.959936	-1.179956
18	6	0	-0.451999	2.765060	-0.097902
19	1	0	0.602045	2.948793	0.137255
20	1	0	-0.579997	2.892328	-1.178286
21	1	0	-1.039544	3.540235	0.405409
22	1	0	-0.775126	1.258617	1.435119

PCM : SCF Done: E(RwB97XD) = -578.944913714 A.U. after 13 cycles
Convg = 0.4111D-08 -V/T = 2.0028

1. References

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