Supporting Information

Unusual Homo-Coupling in the Reaction of Diorganocuprates with an Allylic Halide

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1. Experimental Procedures

General Remarks: All experiments were performed by standard Schlenk techniques under an argon atmosphere. Unless otherwise noted, all materials were obtained from commercial suppliers and used without further purification. THF was distilled from sodium benzophenone ketyl radical prior to use.

General Procedure for the reaction of allylic halides with diorganocuprates.

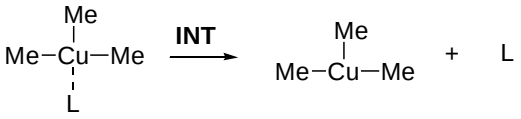
The reaction of *n*-Hex_2CuLi with C_3F_5I serves as an example: To a Schlenk tube were added CuBr•SMe_2 (74.0 mg, 0.360 mmol) and tridecane (43.3 mg) as internal standard. After addition of THF (5 ml) the tube was cooled to –20° C and *n*-hexyllithium (0.30 ml, 0.70 mmol in hexane) was added. The reaction mixture was stirred for one hour at –20° C and subsequently cooled to –60° C. The allylic substrate, C_3F_5I (75.0 mg, 0.291 mmol) dissolved in THF (0.5 ml) was added. The reaction was monitored by GC and after 20 minutes no further progress of the reaction was detected. Analytical samples were prepared by quenching aliquots of the reaction mixture with 2 M $HCl_{(aq)}$. The product mixture was extracted with pentane, dried with Na_2SO_4 and filtered through a plug of celite prior to injection on the GC. A parallel control experiment, employing the same reaction conditions, but without addition of allylic substrate, was always performed. The amount of homo-coupling product (*n*-dodecane) obtained under these conditions was subtracted from the yield obtained in the reaction with the

allylic substrate. This gave a corrected yield of 70% of *n*-dodecane, followed by 13% of *n*-hexyl iodide, according to GC.

Interaction energies between Me_3Cu^{III} and L in Me_3Cu^{III}•L complexes (L = C_2F_4, C_2H_4, Me_2O)

After geometry optimization of a series of Me_3Cu•L complexes, single-point energy calculation of the Me_3Cu and L fragments in each complex was performed to obtain the interaction energy (Table S1).

Table S1. Energies of Me_3Cu^{III}•L complexes and their Me_3Cu^{III} and L fragments, and corresponding interaction energies



L	Me_3Cu^{III}•L (hartree)	Me_3Cu^{III} (hartree)	L (hartree)	**INT** (kcal/mol)
C_2F_4	-792.522829179	-317.014676620	-475.499369172	5.5
C_2H_4	-395.614233386	-317.010585861	-78.5869993716	10.4
Me_2O	-472.059776746	-317.011745390	-155.024151649	15.0

Energies and Cartesian coordinates of stationary points

5a

SCF Done: E(RB+HF-LYP) = -1045.60917874 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	0.926174	-1.974771	-1.650854
2	6	0	1.289710	-1.013799	-0.809978
3	6	0	0.990603	0.325262	-1.132775
4	6	0	1.038792	1.346236	-0.116550
5	9	0	0.484964	2.523490	-0.444225
6	9	0	2.209790	1.542557	0.524320
7	9	0	2.433123	-1.316952	-0.182454
8	9	0	0.104940	0.514029	-2.118029
9	6	0	-0.237983	-1.992721	1.565918
10	29	0	0.078852	-0.221143	0.800953
11	6	0	-0.337895	0.856581	2.374498
12	1	0	-1.201710	-1.959704	2.080630
13	1	0	-0.241642	-2.785005	0.811165

14	1	0	0.561055	-2.171874	2.291826
15	1	0	-0.891296	0.220974	3.067169
16	1	0	-0.933118	1.724141	2.077898
17	1	0	0.607764	1.179016	2.818214
18	8	0	-2.190139	-0.039185	-0.539669
19	6	0	-3.139054	-1.058947	-0.276688
20	6	0	-2.793237	1.237380	-0.677586
21	1	0	-3.308069	1.537032	0.247764
22	1	0	-3.519869	1.241435	-1.503915
23	1	0	-1.996057	1.949170	-0.895532
24	1	0	-3.872364	-1.132760	-1.093806
25	1	0	-3.676567	-0.872465	0.665497
26	1	0	-2.590263	-1.998466	-0.197047

6a

SCF Done: E(RB+HF-LYP) = -1045.62324654 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	0.259893	-0.471330	1.980674
2	6	0	0.609737	0.268983	0.837861
3	6	0	1.532840	-0.572655	0.022902
4	6	0	2.754441	-0.295908	-0.433472
5	9	0	3.404753	-1.085670	-1.279517
6	9	0	3.455743	0.783604	-0.135344
7	9	0	1.335116	1.343195	1.315187
8	9	0	0.972083	-1.736556	-0.412470
9	6	0	-0.406201	2.522990	-0.520478
10	29	0	-1.122966	0.781398	-0.081785
11	6	0	-2.800851	1.460208	-0.845788
12	1	0	0.616266	2.326641	-0.843680
13	1	0	-0.980900	3.043799	-1.282077
14	1	0	-0.416920	3.054808	0.432309
15	1	0	-3.548311	0.714250	-0.553720
16	1	0	-2.736047	1.530727	-1.936498
17	1	0	-3.068679	2.437758	-0.437901
18	8	0	-2.018088	-1.157641	0.037894
19	6	0	-1.922539	-2.074211	1.138222
20	6	0	-2.090584	-1.834122	-1.223090
21	1	0	-0.977854	-2.624149	1.098283
22	1	0	-2.771809	-2.767038	1.095475
23	1	0	-1.964245	-1.486074	2.052511
24	1	0	-2.937796	-2.530889	-1.218969
25	1	0	-1.160573	-2.376310	-1.422208
26	1	0	-2.251769	-1.073831	-1.988622

TS_{6a-7a}

SCF Done: E(RB+HF-LYP) = -1045.59728018 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	-0.025713	-1.871725	1.302524
2	6	0	0.653077	-0.730785	1.008513
3	6	0	1.070921	-0.820706	-0.432544
4	6	0	2.169108	-0.276787	-0.980399
5	9	0	2.448299	-0.375626	-2.260617
6	9	0	3.070281	0.409558	-0.314338
7	9	0	1.759441	-0.653587	1.796097
8	9	0	0.225728	-1.483053	-1.244461
9	6	0	-0.603629	0.418447	2.232162
10	29	0	-0.089371	1.061550	0.382092
11	6	0	-0.371229	2.752145	-0.526808
12	1	0	-1.649263	0.267544	1.962133
13	1	0	-0.262570	-0.324429	2.946230
14	1	0	-0.379272	1.422657	2.600210

15	1	0	-1.219494	3.304719	-0.099120
16	1	0	-0.580208	2.610685	-1.596588
17	1	0	0.508731	3.405340	-0.448829
18	8	0	-2.625042	-0.347308	-0.288766
19	6	0	-2.908759	-1.709547	-0.549593
20	6	0	-3.407349	0.530839	-1.078681
21	1	0	-2.726071	-1.961740	-1.605365
22	1	0	-3.954936	-1.953909	-0.306881
23	1	0	-2.241742	-2.301811	0.078609
24	1	0	-4.480660	0.413433	-0.861006
25	1	0	-3.245392	0.352149	-2.152807
26	1	0	-3.092182	1.547123	-0.835877

TS_{6a-8a}

SCF Done: E(RB+HF-LYP) = -1045.61214021 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	-0.485901	0.393426	2.006720
2	6	0	-0.664919	-0.325301	0.800731
3	6	0	-1.594297	0.472077	-0.051810
4	6	0	-2.855747	0.234839	-0.407065
5	9	0	-3.511219	0.970376	-1.300543
6	9	0	-3.601876	-0.759119	0.042952
7	9	0	-1.341545	-1.488327	1.176957
8	9	0	-1.002279	1.560960	-0.628985
9	6	0	1.042976	-2.439400	-1.071270
10	29	0	1.107143	-0.774316	0.016948
11	6	0	2.870028	-1.562258	-0.383450
12	1	0	0.193809	-2.005978	-1.611947
13	1	0	1.725891	-2.892782	-1.785034
14	1	0	0.709774	-3.163278	-0.327298
15	1	0	3.173079	-0.856151	0.410919
16	1	0	3.313710	-1.268634	-1.334899
17	1	0	3.174659	-2.566313	-0.097418
18	8	0	2.133962	1.378363	0.073280
19	6	0	1.730218	2.304783	1.085735
20	6	0	2.208314	1.994233	-1.209361
21	1	0	0.731510	2.699478	0.870643
22	1	0	2.455493	3.127726	1.148364
23	1	0	1.702089	1.758689	2.027983
24	1	0	2.930175	2.822786	-1.197182
25	1	0	1.226023	2.369059	-1.521197
26	1	0	2.550877	1.233970	-1.915643

7a

SCF Done: E(RB+HF-LYP) = -1045.68921310 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	-1.045926	-2.226186	-0.276969
2	6	0	-1.726538	-1.027209	-0.407646
3	6	0	-1.049966	-0.026412	0.486576
4	6	0	-0.970724	1.364102	0.302680
5	9	0	-0.979609	2.174091	1.362983
6	9	0	-1.516885	1.969100	-0.764116
7	9	0	-2.985933	-1.274861	0.100555
8	9	0	-0.996548	-0.448510	1.792913
9	6	0	-1.846816	-0.696365	-1.879398
10	29	0	0.827165	0.679833	-0.081319
11	6	0	2.033446	2.131157	-0.579928
12	1	0	-0.867772	-0.479296	-2.314840
13	1	0	-2.272671	-1.571462	-2.377247
14	1	0	-2.504228	0.160223	-2.030503
15	1	0	2.346634	2.025668	-1.629318

16	1	0	2.939059	2.102693	0.043078
17	1	0	1.586542	3.125387	-0.471408
18	8	0	2.006991	-1.100497	-0.062968
19	6	0	1.873993	-2.059712	0.993583
20	6	0	3.341162	-1.032651	-0.572497
21	1	0	2.513049	-1.782994	1.842391
22	1	0	2.160344	-3.053884	0.628415
23	1	0	0.829196	-2.066698	1.295315
24	1	0	3.631842	-2.010009	-0.978325
25	1	0	4.044033	-0.738988	0.217799
26	1	0	3.347008	-0.281998	-1.361873

8a

SCF Done: E(RB+HF-LYP) = -1045.69503206 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	9	0	-3.415049	-0.992885	1.677598
2	6	0	-2.753019	-0.974706	0.526279
3	6	0	-1.621059	-0.297224	0.347738
4	6	0	-0.700654	-0.269601	-0.828915
5	9	0	-0.852325	0.976519	-1.457833
6	9	0	-1.150155	-1.201255	-1.753431
7	9	0	-3.341992	-1.726824	-0.386242
8	9	0	-1.167973	0.429595	1.407666
9	6	0	0.541770	3.907844	-0.330754
10	29	0	1.131473	-0.526515	-0.357608
11	6	0	-0.807995	3.861969	0.389090
12	1	0	0.744573	4.900360	-0.750859
13	1	0	1.365667	3.668275	0.354677
14	1	0	0.563482	3.181630	-1.149953
15	1	0	-1.625128	4.122219	-0.293403
16	1	0	-0.840331	4.565686	1.229617
17	1	0	-1.010744	2.859092	0.776084
18	8	0	3.034750	-0.765633	0.127318
19	6	0	3.489676	-2.086733	0.459866
20	6	0	3.656686	0.261124	0.917785
21	1	0	4.743158	0.215147	0.780824
22	1	0	3.406435	0.135118	1.977819
23	1	0	3.276866	1.216998	0.556257
24	1	0	3.225313	-2.336474	1.494358
25	1	0	4.576448	-2.140531	0.327995
26	1	0	2.998555	-2.775900	-0.227673

5b

SCF Done: E(RB+HF-LYP) = -549.472972359 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.994950	1.876480	-1.012696
2	29	0	-0.932681	0.265322	0.088506
3	6	0	-1.420900	-1.087547	-1.493876
4	6	0	-0.777696	1.215455	1.784053
5	1	0	0.166747	1.767738	1.747917
6	1	0	-0.789203	0.551315	2.651485
7	1	0	-1.608404	1.925435	1.842272
8	6	0	-0.779041	-1.775900	-0.453066
9	1	0	-0.953526	-1.015482	-2.470057
10	1	0	-2.496372	-0.918125	-1.467898
11	1	0	-0.651160	2.728220	-0.421583
12	1	0	-2.033300	2.037241	-1.323013
13	1	0	-0.366914	1.754458	-1.900167
14	6	0	-1.231269	-1.700057	0.873411
15	1	0	0.256638	-2.071151	-0.613351
16	1	0	-0.619805	-2.088360	1.680834

17	1	0	-2.291240	-1.583605	1.094961
18	8	0	2.236770	-0.439545	-0.206375
19	6	0	2.835821	-0.400217	1.074084
20	6	0	2.816843	0.492485	-1.098413
21	1	0	3.905122	-0.661870	1.025744
22	1	0	2.316316	-1.131619	1.697634
23	1	0	2.738591	0.594637	1.535299
24	1	0	2.702556	1.524427	-0.732690
25	1	0	2.295528	0.394999	-2.053528
26	1	0	3.889163	0.289572	-1.250506

$TS_{5b\text{-}6b}$

SCF Done: E(RB+HF-LYP) = -549.455732954 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.412724	-0.841602	0.693365
2	29	0	-0.660876	-0.367475	0.009006
3	6	0	-0.718045	1.361987	1.036613
4	6	0	-0.726898	-1.832855	-1.298585
5	1	0	-0.519289	-2.775862	-0.778716
6	1	0	0.053756	-1.663515	-2.053405
7	1	0	-1.696885	-1.905410	-1.800430
8	6	0	0.065389	2.095866	0.042969
9	1	0	-0.253091	1.272248	2.021120
10	1	0	-1.758234	1.680371	1.117351
11	1	0	-2.558989	-1.911095	0.544939
12	1	0	-3.125366	-0.262410	0.102001
13	1	0	-2.466277	-0.568364	1.747938
14	6	0	-0.398547	2.609485	-1.120176
15	1	0	1.141264	2.157368	0.217642
16	1	0	0.261643	3.091902	-1.834960
17	1	0	-1.458061	2.590186	-1.367460
18	8	0	1.611231	-0.574428	0.141860
19	6	0	2.236214	-0.495504	1.417176
20	6	0	2.505562	-0.289280	-0.927510
21	1	0	3.076539	-1.200808	1.474942
22	1	0	1.485027	-0.763659	2.161494
23	1	0	2.604961	0.520891	1.616763
24	1	0	2.914049	0.727110	-0.838765
25	1	0	1.936397	-0.372937	-1.853430
26	1	0	3.332401	-1.012399	-0.936181

6b

SCF Done: E(RB+HF-LYP) = -549.457380324 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.388165	1.916231	0.146967
2	29	0	-0.074992	0.664608	0.037680
3	6	0	1.128581	-0.765439	0.840813
4	6	0	-1.214773	2.134335	-0.620483
5	1	0	-1.140108	3.032264	0.001154
6	1	0	-2.248288	1.764799	-0.619259
7	1	0	-0.926047	2.390532	-1.646683
8	6	0	2.060068	-1.342649	-0.141436
9	1	0	0.406508	-1.506360	1.211942
10	1	0	1.651131	-0.318367	1.693111
11	1	0	1.199136	2.796670	-0.465008
12	1	0	2.260675	1.356170	-0.195362
13	1	0	1.468403	2.183086	1.203968
14	6	0	3.382531	-1.109614	-0.232509
15	1	0	1.616302	-1.993442	-0.901003
16	1	0	3.985462	-1.535264	-1.030045
17	1	0	3.905341	-0.501131	0.502946

18	8	0	-1.718295	-0.708597	-0.200648
19	6	0	-1.506328	-1.928605	-0.912546
20	6	0	-2.523034	-0.879641	0.967108
21	1	0	-0.960770	-2.656765	-0.299860
22	1	0	-0.922588	-1.682536	-1.800693
23	1	0	-2.473118	-2.351193	-1.213455
24	1	0	-3.482887	-1.335680	0.694175
25	1	0	-2.696222	0.114847	1.381862
26	1	0	-2.013048	-1.510186	1.707188

TS_{6b-7b}

SCF Done: E(RB+HF-LYP) = -549.444109655 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.398183	-0.456291	0.879702
2	29	0	0.795249	-0.986429	-0.141632
3	6	0	1.493814	0.742676	-0.857186
4	6	0	-0.311088	-2.590617	-0.033059
5	1	0	0.292863	-3.503971	-0.131663
6	1	0	-1.065437	-2.623764	-0.833760
7	1	0	-0.850852	-2.662947	0.921776
8	6	0	0.851887	1.927840	-0.265269
9	1	0	0.947577	0.341281	-1.732465
10	1	0	2.544584	0.872227	-1.113135
11	1	0	2.050932	-1.083368	1.709465
12	1	0	2.602688	0.555639	1.220584
13	1	0	3.254998	-0.905399	0.374145
14	6	0	1.523986	3.013130	0.148708
15	1	0	-0.232173	1.890269	-0.163902
16	1	0	1.011797	3.867681	0.581896
17	1	0	2.605381	3.091586	0.051427
18	8	0	-2.366125	0.919524	0.051392
19	6	0	-2.667287	0.411066	1.337663
20	6	0	-3.135798	0.302677	-0.963111
21	1	0	-3.725179	0.578949	1.596256
22	1	0	-2.037570	0.947845	2.052037
23	1	0	-2.450413	-0.664917	1.405477
24	1	0	-2.944863	-0.779662	-1.011447
25	1	0	-2.845931	0.760694	-1.912439
26	1	0	-4.213795	0.465222	-0.802748

TS_{6b-8b}

SCF Done: E(RB+HF-LYP) = -549.443788477 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.492924	1.821204	0.616170
2	29	0	-0.232679	0.622146	-0.335797
3	6	0	-1.036085	-1.065011	-1.019080
4	6	0	0.534149	2.384543	0.096303
5	1	0	0.116148	3.363114	-0.129590
6	1	0	1.237304	2.102632	-0.710655
7	1	0	1.044992	2.377969	1.059571
8	6	0	-1.750246	-1.725737	0.094686
9	1	0	-0.251531	-1.712729	-1.433317
10	1	0	-1.724437	-0.794777	-1.831957
11	1	0	-1.299936	2.455546	1.478405
12	1	0	-2.013495	0.904804	0.928757
13	1	0	-2.057962	2.354331	-0.148316
14	6	0	-3.054388	-1.622784	0.414651
15	1	0	-1.124544	-2.324441	0.765161
16	1	0	-3.470164	-2.114920	1.289761
17	1	0	-3.752726	-1.068773	-0.211553
18	8	0	2.124004	-0.307329	0.245266

19	6	0	2.051385	-1.100188	1.421140
20	6	0	2.772232	-0.987857	-0.819215
21	1	0	1.468074	-2.015654	1.248482
22	1	0	1.557370	-0.498333	2.187426
23	1	0	3.057324	-1.375696	1.771170
24	1	0	3.807926	-1.240841	-0.547953
25	1	0	2.780632	-0.312533	-1.677819
26	1	0	2.235947	-1.908319	-1.089535

TS_{5b-7b}

SCF Done: E(RB+HF-LYP) = -549.449501298 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.077866	1.451984	-0.814840
2	6	0	1.760562	0.318221	-1.413156
3	6	0	1.345999	1.924830	0.454418
4	29	0	0.728998	-0.199537	0.413676
5	6	0	1.214477	-1.704129	-1.043945
6	6	0	0.238935	-1.126107	2.046736
7	1	0	1.533991	0.152870	-2.460910
8	1	0	0.719910	2.690824	0.900832
9	1	0	2.816302	0.197066	-1.177604
10	1	0	2.297965	1.737639	0.946962
11	1	0	1.129404	-1.585383	2.500171
12	1	0	1.453572	-2.358304	-0.203517
13	1	0	-0.225393	-0.484037	2.805556
14	1	0	1.932957	-1.887124	-1.840732
15	1	0	-0.464482	-1.939049	1.810770
16	1	0	0.202509	-1.890511	-1.409643
17	1	0	0.151260	1.767206	-1.291469
18	8	0	-2.125417	0.386594	-0.644359
19	6	0	-2.755882	-0.855938	-0.890084
20	6	0	-2.649120	1.028428	0.505039
21	1	0	-3.838557	-0.731141	-1.051966
22	1	0	-2.601704	-1.556300	-0.055425
23	1	0	-2.309332	-1.273577	-1.796180
24	1	0	-2.492153	0.421203	1.407951
25	1	0	-3.725450	1.233634	0.390329
26	1	0	-2.115439	1.975064	0.618132

7b

SCF Done: E(RB+HF-LYP) = -549.530317523 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.826386	-1.076308	0.853647
2	6	0	-1.827837	-1.911082	0.093577
3	6	0	-1.143626	-0.188109	1.838517
4	29	0	-0.814699	1.016034	0.111794
5	6	0	-1.527255	-2.038410	-1.406782
6	6	0	-0.651041	2.519708	-1.069601
7	1	0	-1.816060	-2.916174	0.543340
8	1	0	-0.378189	0.233575	2.487200
9	1	0	-2.839029	-1.514918	0.249361
10	1	0	-2.177484	-0.005479	2.128786
11	1	0	-1.635768	2.899944	-1.374336
12	1	0	-1.579240	-1.064361	-1.905332
13	1	0	-0.109621	3.347456	-0.590112
14	1	0	-2.247880	-2.707274	-1.889209
15	1	0	-0.102416	2.255587	-1.985355
16	1	0	-0.524200	-2.448583	-1.573204
17	1	0	0.227242	-1.307401	0.681337
18	8	0	2.493608	-0.861902	0.117505
19	6	0	2.636952	-0.507301	-1.246599

20	6	0	3.152227	0.049429	0.976161
21	1	0	3.697551	-0.485682	-1.543558
22	1	0	2.187622	0.474690	-1.457540
23	1	0	2.119406	-1.269562	-1.834627
24	1	0	2.741175	1.066672	0.880535
25	1	0	4.233228	0.088047	0.767143
26	1	0	3.002872	-0.303870	1.999974

8b

SCF Done: E(RB+HF-LYP) = -549.530513505 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.825633	1.604232	-0.199168
2	29	0	0.985392	-0.746429	-0.063983
3	6	0	0.039964	-2.408906	0.030954
4	6	0	-2.753808	2.682396	-0.020526
5	1	0	-3.184407	3.690559	-0.047374
6	1	0	-1.999340	2.625268	-0.814844
7	1	0	-2.237919	2.571346	0.941542
8	6	0	-1.347741	-2.229357	0.535401
9	1	0	0.621260	-3.057395	0.701082
10	1	0	0.046548	-2.857907	-0.971444
11	1	0	-4.580596	1.661585	0.593708
12	1	0	-3.387462	0.600314	-0.173094
13	1	0	-4.344459	1.717639	-1.158130
14	6	0	-2.482266	-2.288869	-0.180048
15	1	0	-1.436528	-2.028413	1.606581
16	1	0	-3.456745	-2.144014	0.279016
17	1	0	-2.472090	-2.493372	-1.249682
18	8	0	1.966333	1.013912	-0.197348
19	6	0	1.456177	2.141628	0.526139
20	6	0	3.397127	1.000422	-0.272091
21	1	0	1.786492	2.111443	1.572076
22	1	0	0.368237	2.088544	0.477627
23	1	0	1.804109	3.068321	0.053537
24	1	0	3.748102	1.919575	-0.757002
25	1	0	3.677646	0.134745	-0.872891
26	1	0	3.837186	0.917633	0.729605

$Me_3Cu^{III}•C_2F_4$

SCF Done: E(RB+HF-LYP) = -792.522829179 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	-1.220262	0.001856	-0.150723
2	6	0	-1.165251	-1.946810	-0.221450
3	6	0	-1.169005	1.951418	-0.190369
4	6	0	-3.107658	-0.003097	0.273383
5	1	0	-1.994422	-2.370337	-0.798219
6	1	0	-1.172248	-2.385489	0.783544
7	1	0	-0.221694	-2.217074	-0.720799
8	1	0	-1.999620	2.382853	-0.759152
9	1	0	-0.226608	2.231443	-0.686471
10	1	0	-1.175590	2.373695	0.821660
11	1	0	-3.312232	-0.915964	0.828065
12	1	0	-3.583154	0.002972	-0.708138
13	1	0	-3.314610	0.901537	0.840506
14	6	0	1.860397	0.011707	-0.542886
15	6	0	1.645803	-0.014337	0.772102
16	9	0	1.996293	1.132594	-1.230095
17	9	0	1.995319	-1.081353	-1.273902
18	9	0	1.561169	-1.135274	1.464940
19	9	0	1.558561	1.078394	1.508532

$Me_3Cu^{III}•C_2H_4$

SCF Done: E(RB+HF-LYP) = -395.614233386 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.244103	0.004061	-0.004984
2	6	0	0.306699	-1.980944	-0.000430
3	6	0	0.328876	1.986425	0.025082
4	6	0	2.187688	-0.018473	-0.010813
5	1	0	0.494603	-2.314645	1.029183
6	1	0	1.103009	-2.374987	-0.639624
7	1	0	-0.651148	-2.402612	-0.334674
8	1	0	0.977040	2.361371	-0.775165
9	1	0	0.744948	2.314685	0.985747
10	1	0	-0.668115	2.432193	-0.093348
11	1	0	2.450560	-0.174656	-1.059840
12	1	0	2.525337	-0.853653	0.602510
13	1	0	2.568766	0.934173	0.353807
14	6	0	-2.077680	-0.036528	0.671730
15	6	0	-2.103907	0.041382	-0.672587
16	1	0	-2.092583	0.856044	1.290850
17	1	0	-2.098679	-0.993719	1.184376
18	1	0	-2.143705	-0.850347	-1.291022
19	1	0	-2.139078	0.997199	-1.186158

$Me_3Cu^{III}•OMe_2$

SCF Done: E(RB+HF-LYP) = -472.059776746 A.U.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	29	0	0.606862	0.004156	-0.012088
2	6	0	0.338686	1.940597	0.312882
3	6	0	0.938943	-1.921393	-0.276079
4	6	0	2.514282	0.282728	0.024099
5	1	0	0.237072	2.457888	-0.651966
6	1	0	1.160722	2.407031	0.864285
7	1	0	-0.587539	2.091064	0.887617
8	1	0	1.674672	-2.321647	0.429942
9	1	0	1.305518	-2.091776	-1.296073
10	1	0	-0.016263	-2.448693	-0.151016
11	1	0	2.765306	0.376520	1.083186
12	1	0	2.718970	1.214307	-0.504372
13	1	0	3.031597	-0.561078	-0.429997
14	6	0	-2.266332	0.523321	-1.003254
15	8	0	-1.500768	-0.343210	-0.163288
16	6	0	-2.135198	-0.602599	1.089922
17	1	0	-2.395910	1.509066	-0.542025
18	1	0	-3.246511	0.070458	-1.198303
19	1	0	-1.716654	0.625718	-1.939876
20	1	0	-3.131019	-1.031194	0.920829
21	1	0	-2.224407	0.317235	1.682023
22	1	0	-1.510713	-1.325673	1.617191