Supporting Information

Cross C-S coupling reaction catalyzed by copper (I) *N*-heterocyclic carbene complexes

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DOSY Experiment

In a glove box, IMes-Cu-SPh (8 mg, 16.8 μmol) was transferred to an NMR tube, and d_8-toluene (0.5 mL) was added. A DOSY spectrum was acquired on a Bruker AVIII-500 and probe temperature of 25 ℃. Hydrodynamic Radii was calculated from the diffusion constants (D) using the Stokes-Einstein equation.

Table S1. Measured Hydrodynamic Radii.

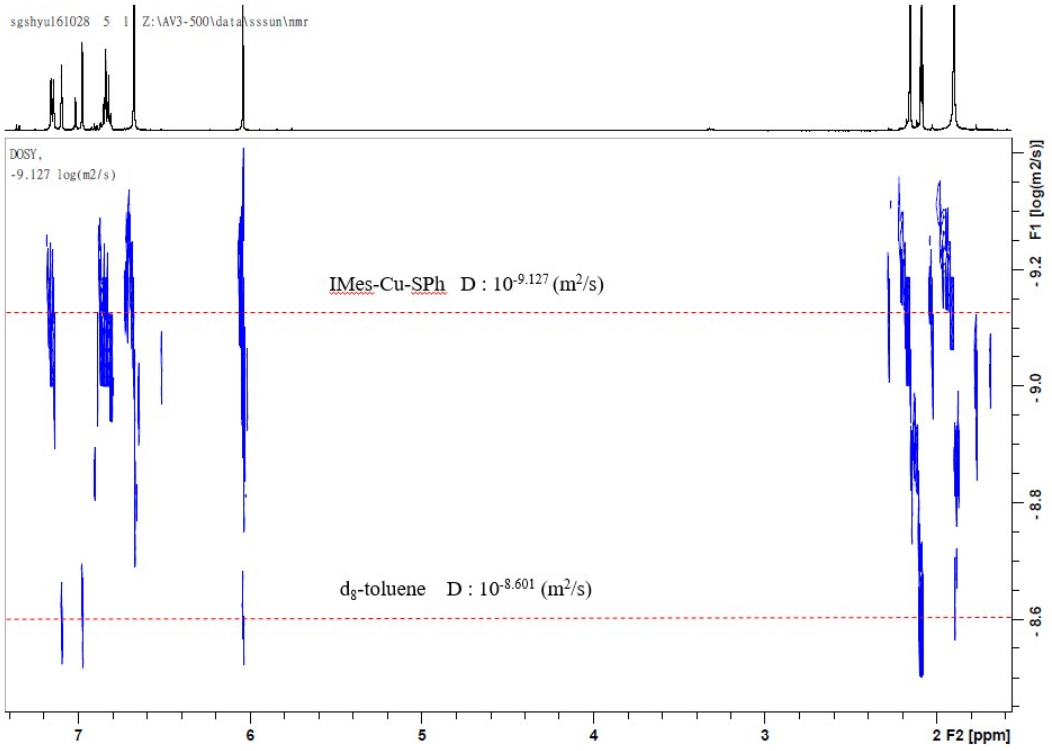
Compound	D (10^{-10} m^2/s)	Hydrodynamic Radii (Å)
d^8-toluene	25.06 (1)	1.50
IMes-Cu-SPh	7.46 (4)	5.04

Calculation of Molar Volumes. In order to obtain molar volume, Monte-Carlo integration over the electron density grid was carried out by the single point calculation with "Volume" keyword (0.001 $e^-/Bohr^3$ cutoff density, 1000 test points/$Bohr^3$). The B3LYP functional with the basis set of SDD for heavy atoms (Cu and I) and 6-311+G(d,p) for others was employed. All volume calculations were run in triplicate due to the random error associated with Monte-Carlo methods.

Table S2. DFT Calculated Radii.

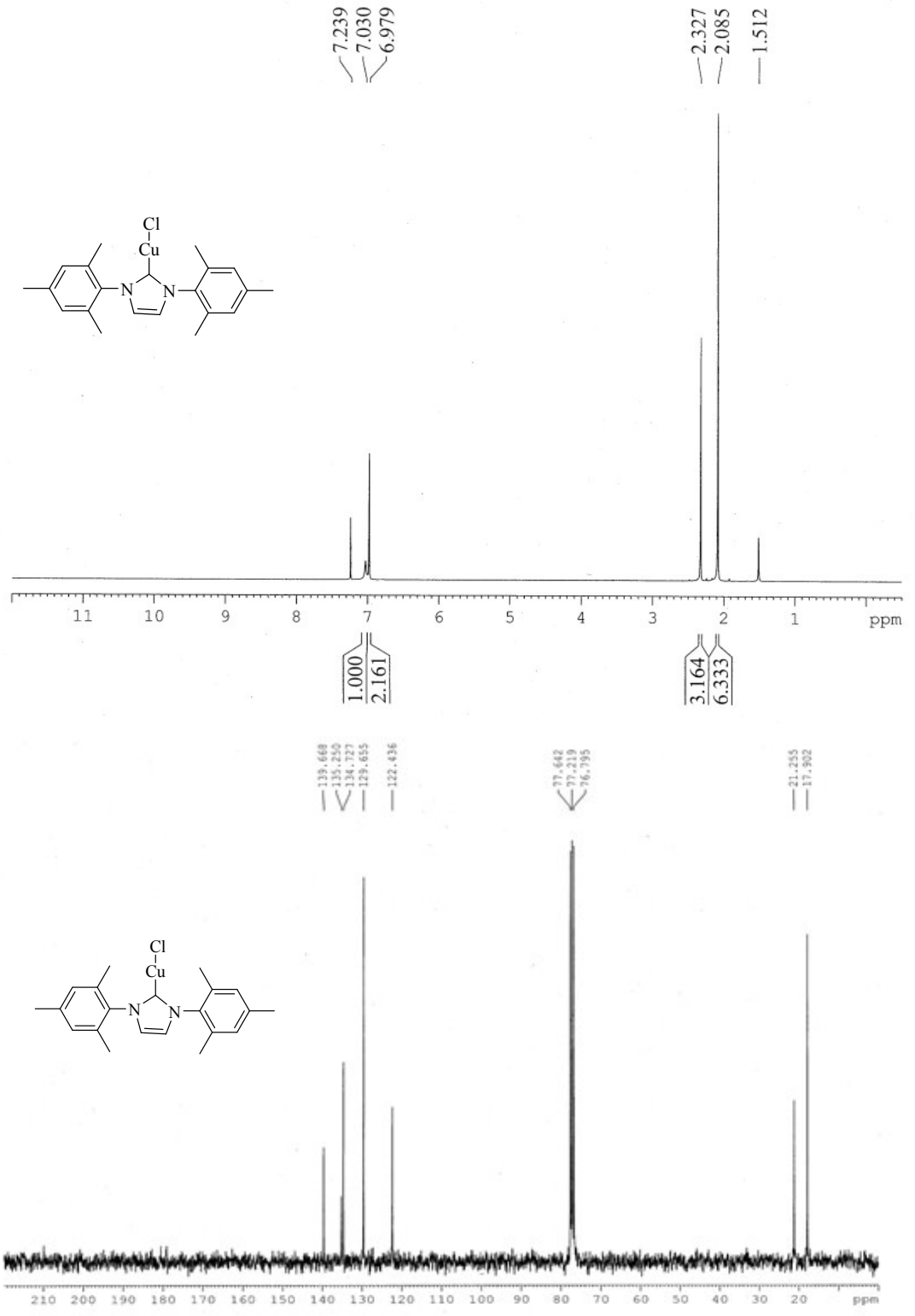
Species	Volume (cm^3/mol)			Average (cm^3/mol)	Radii (Å)
	1st Run	2nd Run	3rd Run		
IMes-Cu-SPh	369.9	352.9	357.2	360.0 (72)	5.23
$(IMes\text{-}Cu\text{-}SPh)_2$	698.6	704.7	707.3	703.5 (36)	6.53

Proton 2D DOSY-NMR Spectrum (IMes-Cu-SPh)

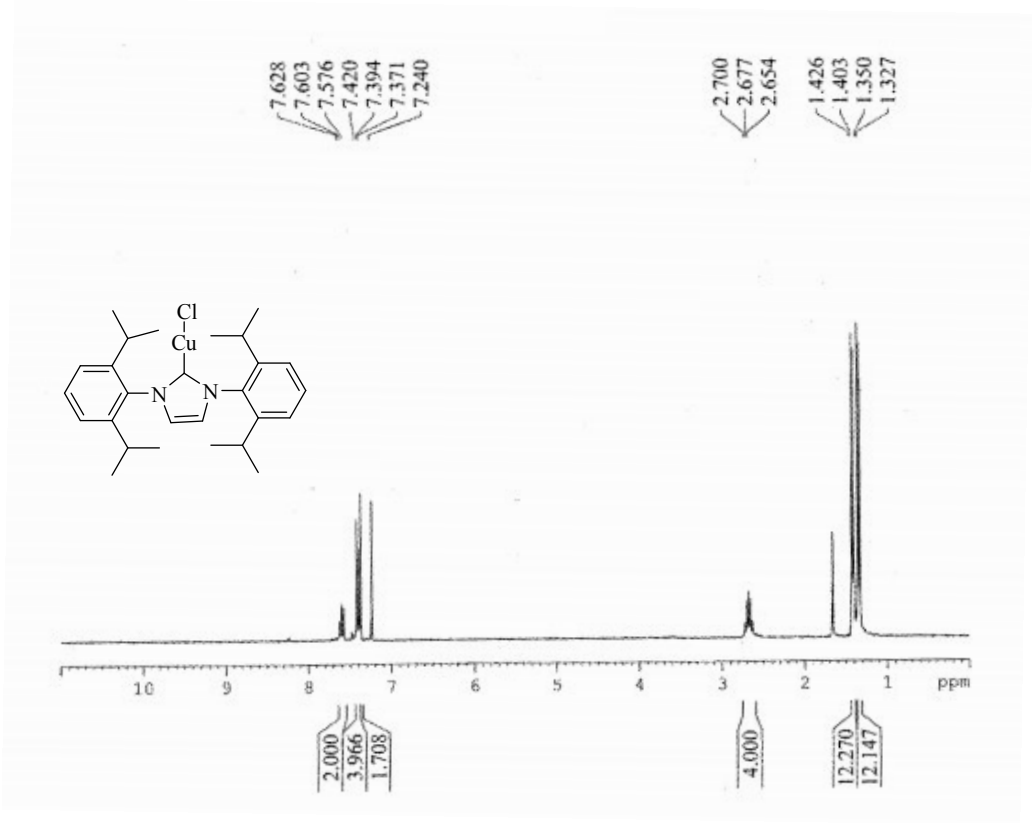


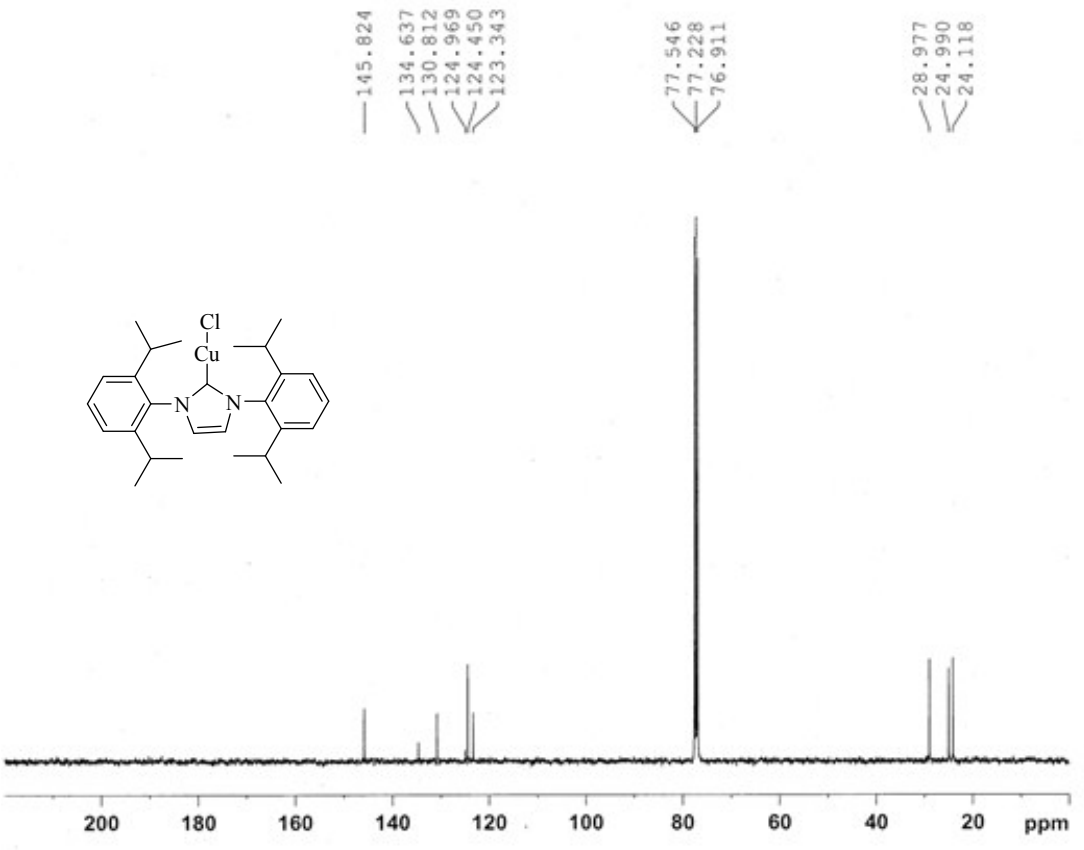
NMR Spectra

^{1}H and $^{13}C\{^{1}H\}$ NMR ($CDCl_3$); IMes-Cu-Cl

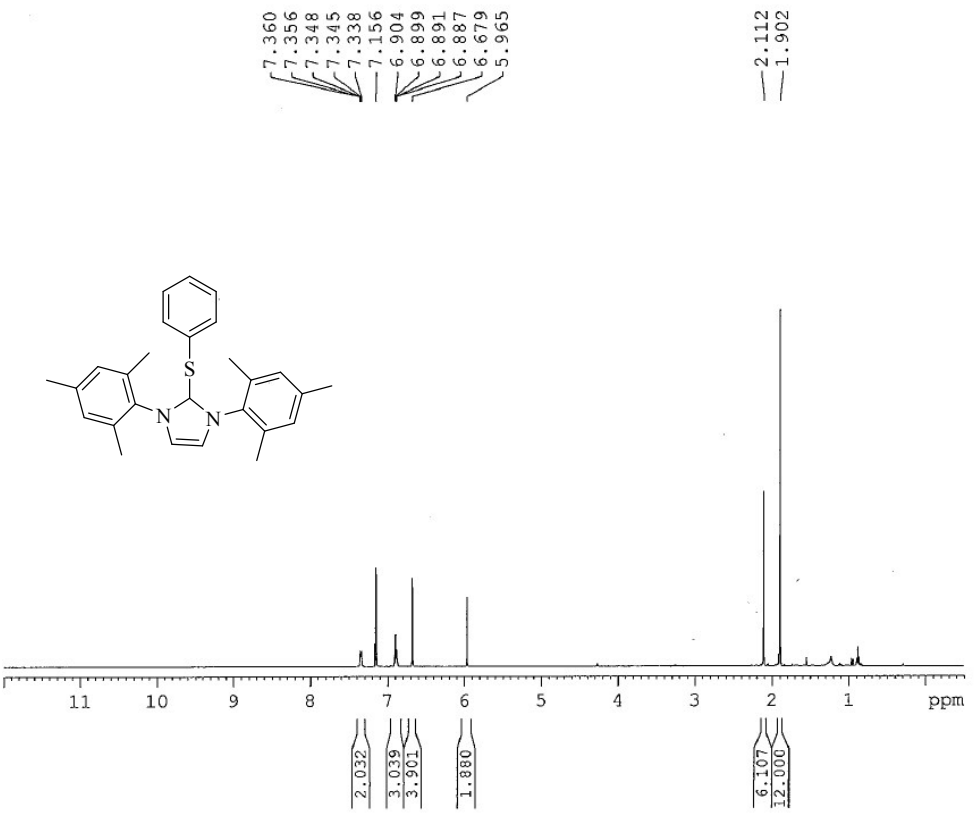


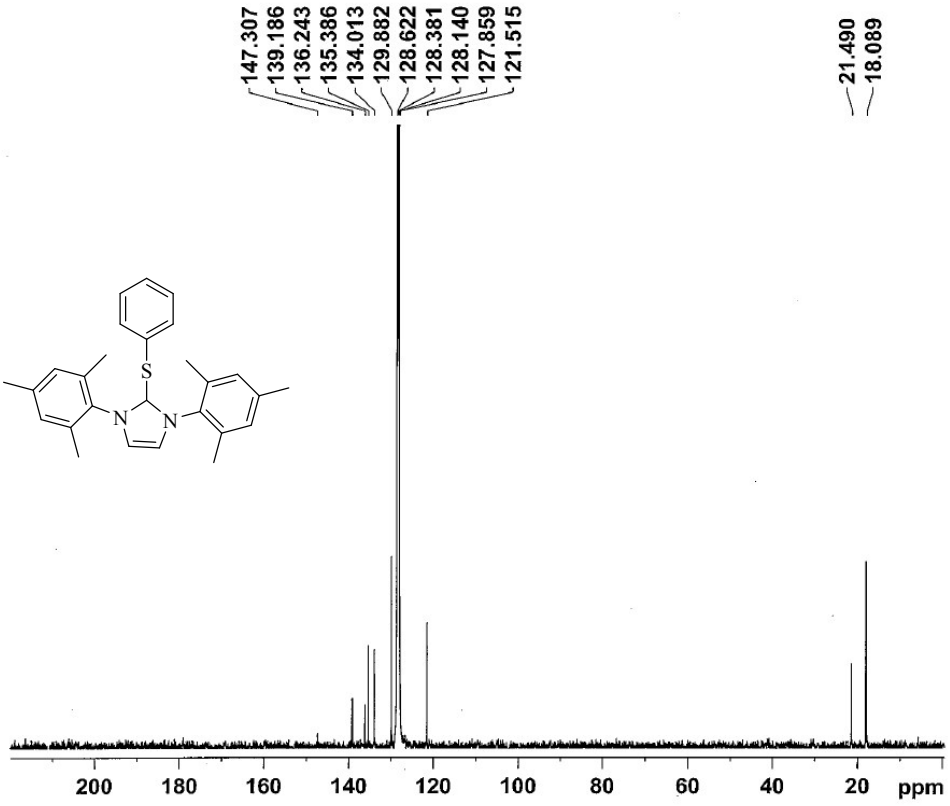
^{1}H and $^{13}C\{^{1}H\}$ NMR ($CDCl_3$); IPr-Cu-Cl





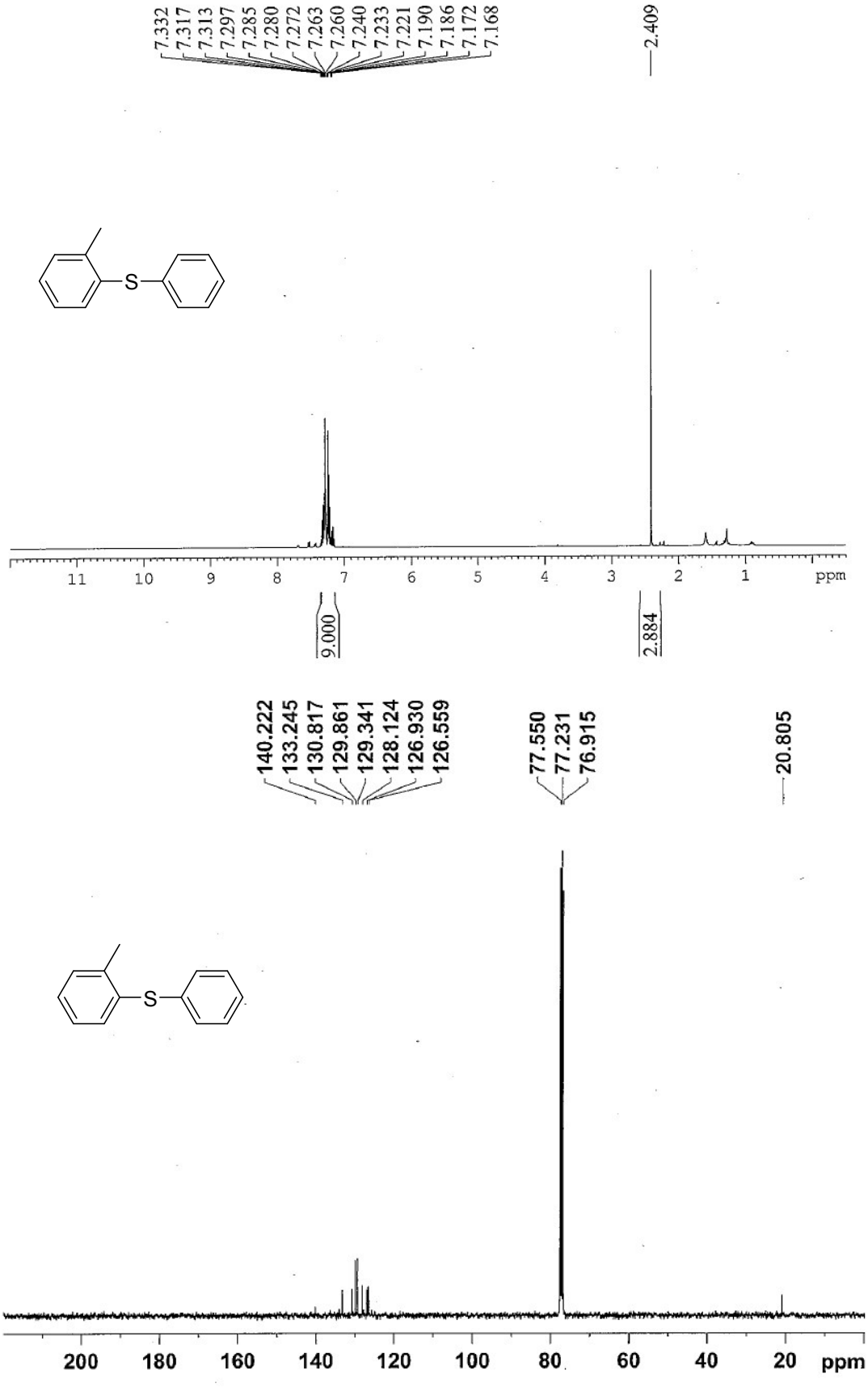
^{1}H and $^{13}C\{^{1}H\}$ NMR (C_6D_6); IMes-Cu-SPh



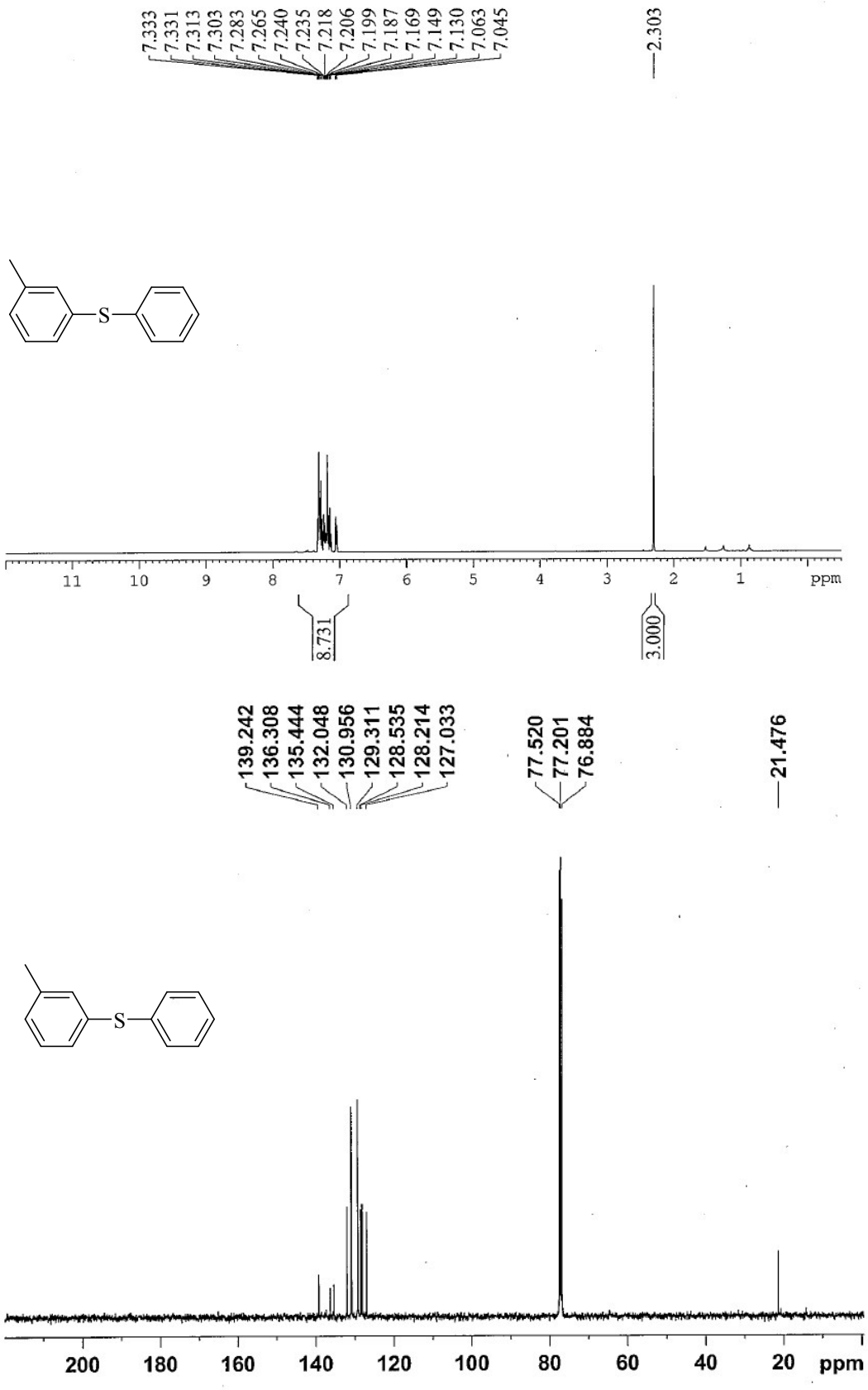


^{1}H and $^{13}C\{^{1}H\}$ NMR ($CDCl_3$); Table 2, entry 1

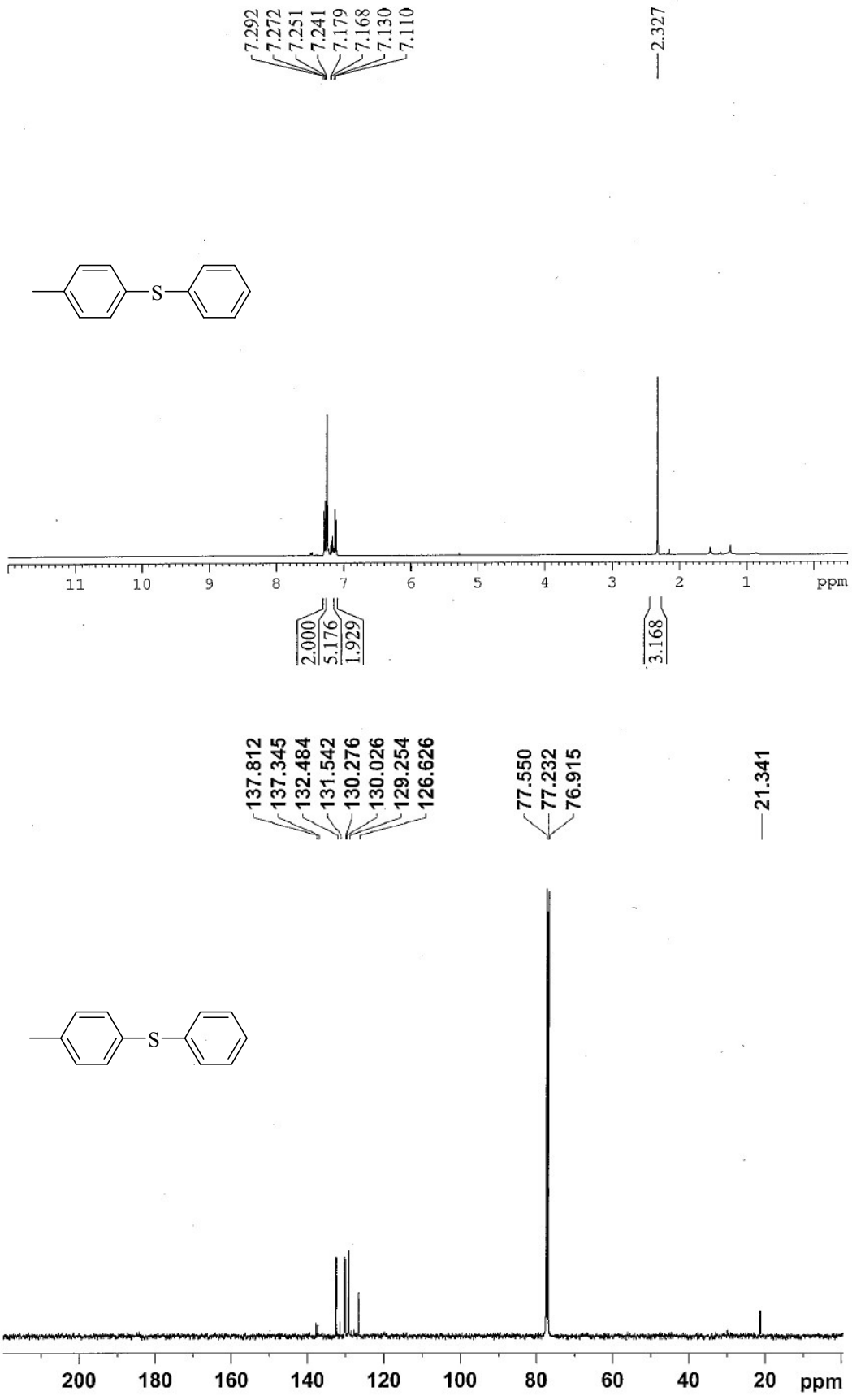
^{1}H and $^{13}C\{^{1}H\}$ NMR ($CDCl_3$); Table 2, entry 2



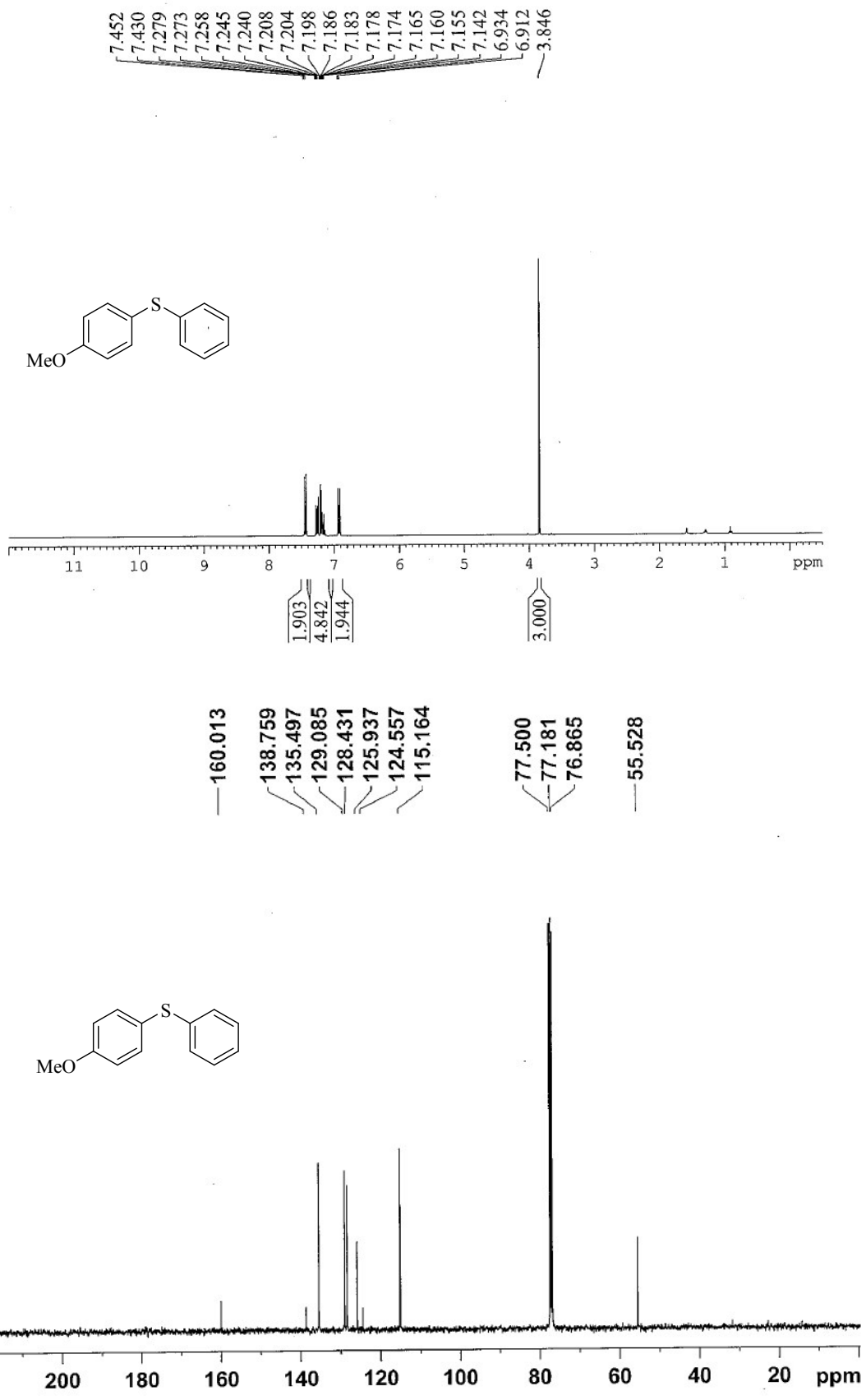
^{1}H and $^{13}C\{^{1}H\}$ NMR ($CDCl_3$); Table 1, entry 3



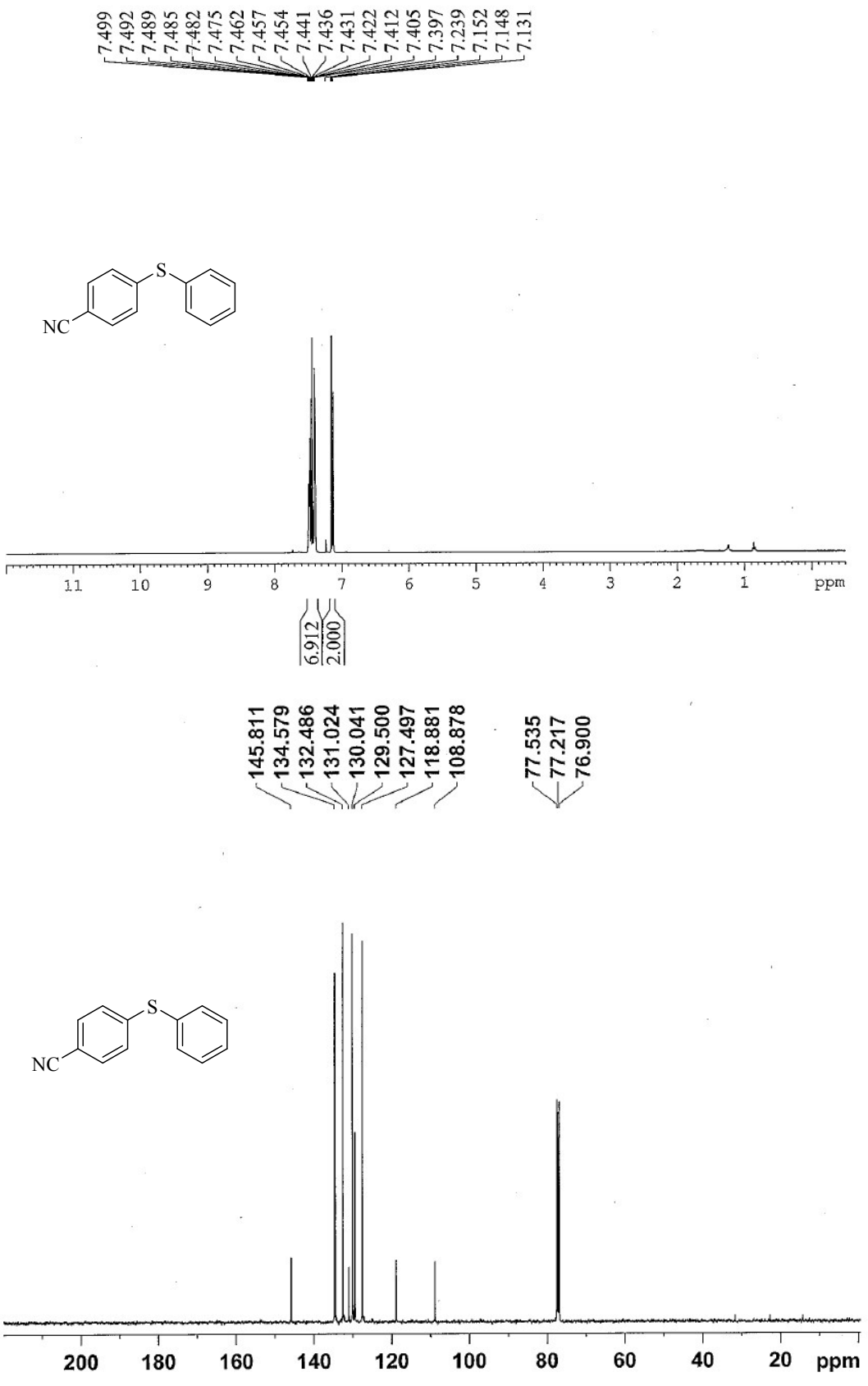
^{1}H and $^{13}C\{^{1}H\}$ NMR ($CDCl_3$); Table 2, entry 4



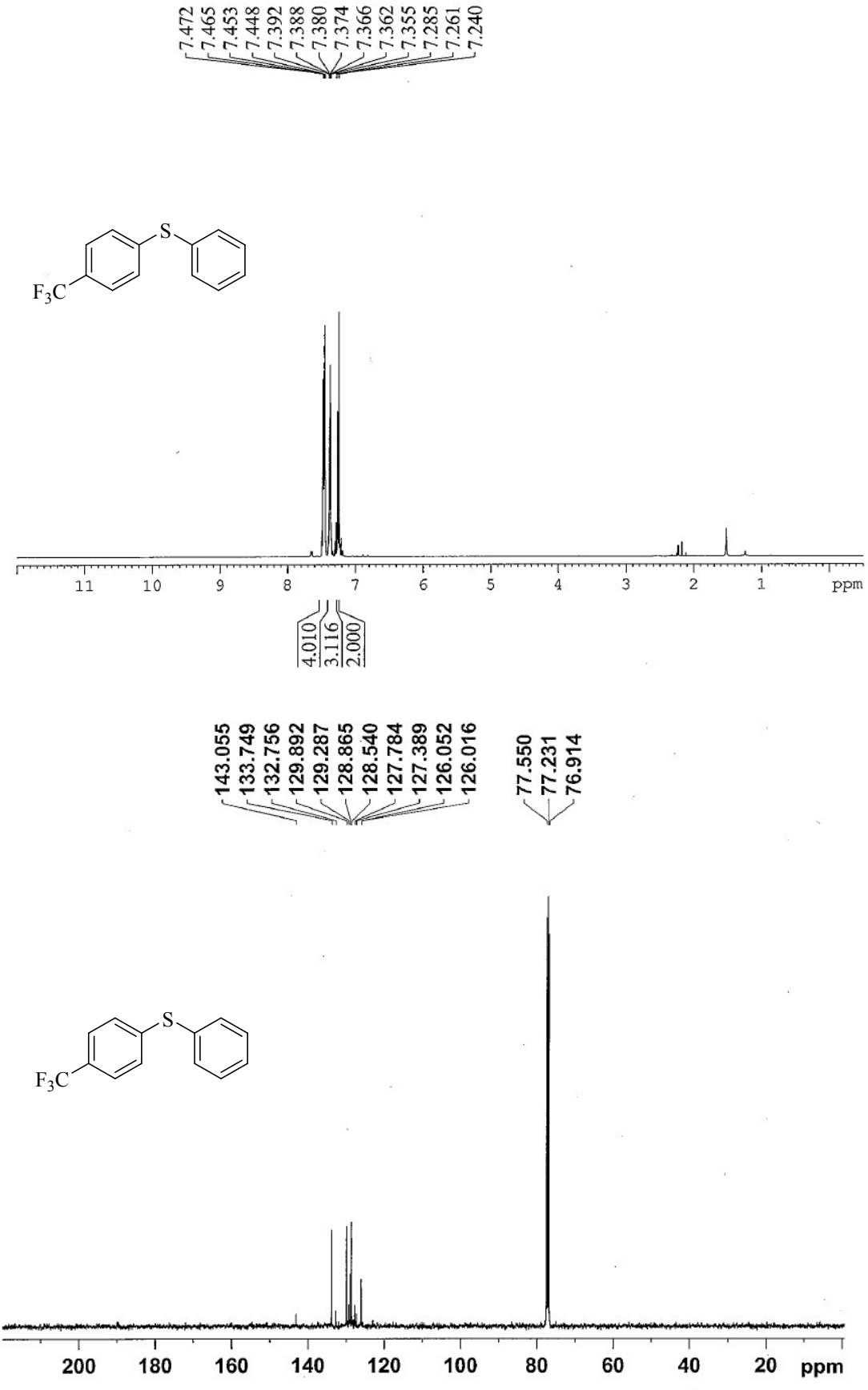
^{1}H and $^{13}C\{^{1}H\}$ NMR ($CDCl_3$); Table 2, entry 5



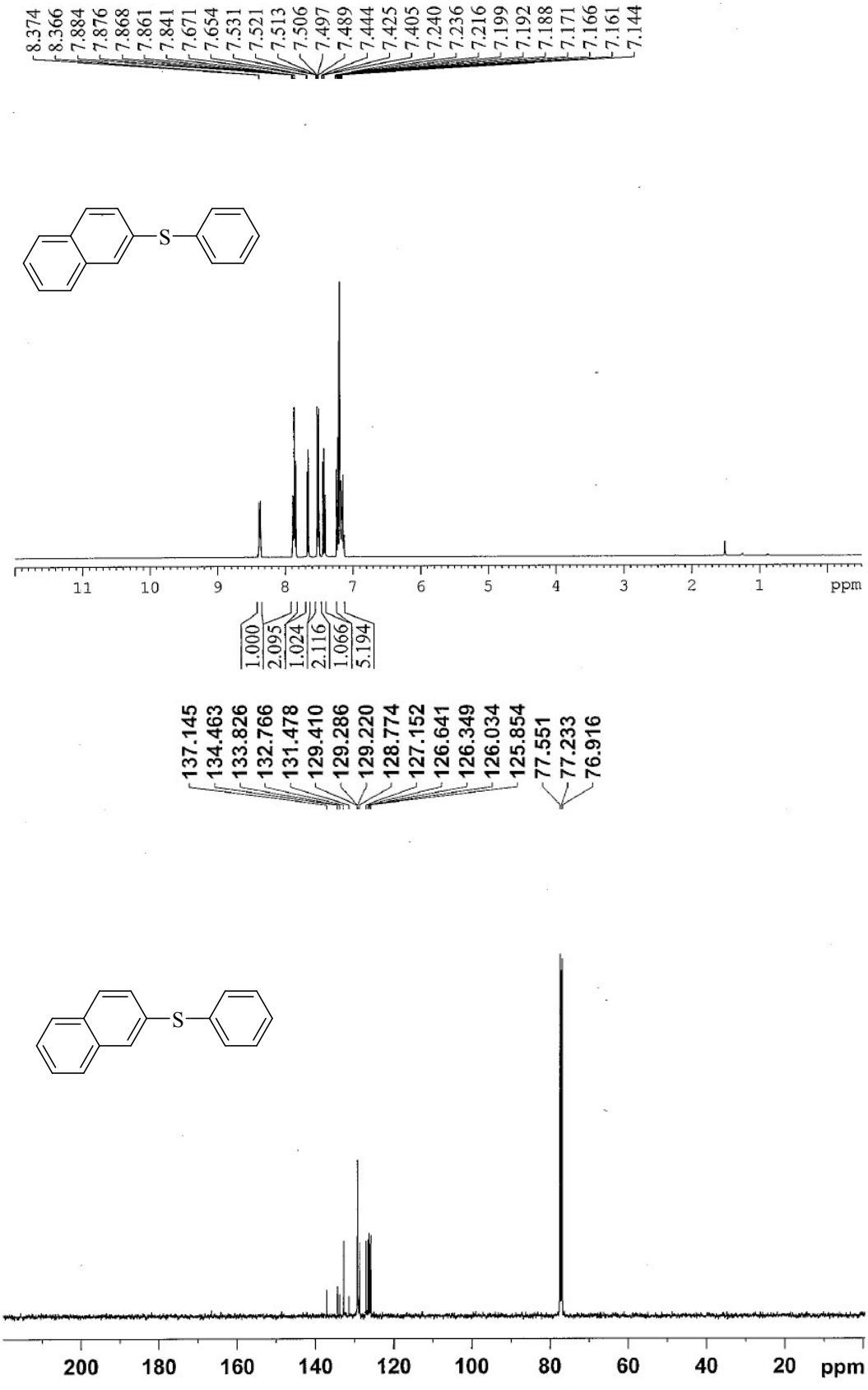
^{1}H and $^{13}C\{^{1}H\}$ NMR ($CDCl_3$); Table 2, entry 6



^{1}H and $^{13}C\{^{1}H\}$ NMR ($CDCl_3$); Table 2, entry 7

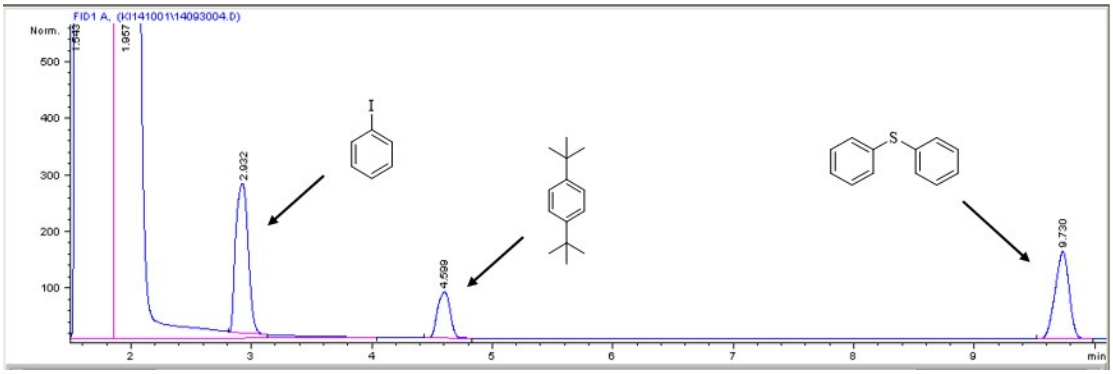


^{1}H and $^{13}C\{^{1}H\}$ NMR ($CDCl_3$); Table 2, entry 8



GC Data

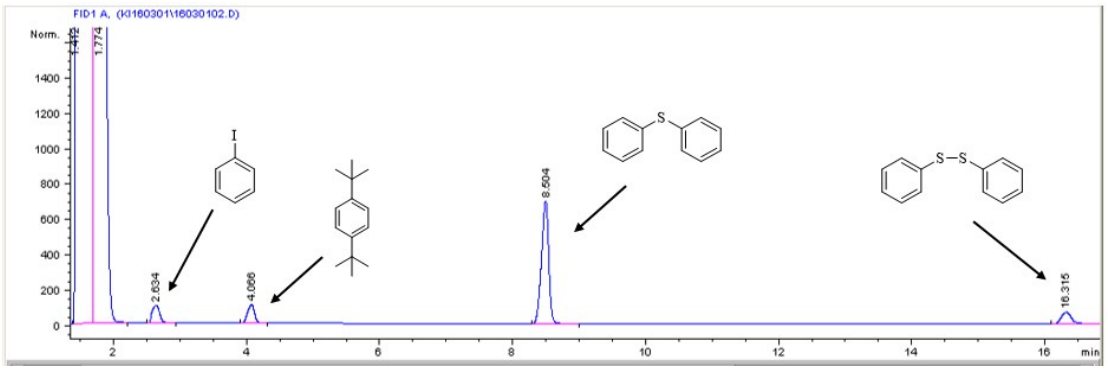
Table 1, entry 1; HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.543	1697268	276613.9	0.0736	95.835	6.59E-2
2	1.957	70043.6	7723.9	0.1511	3.955	0.886
3	2.932	1886.2	264.1	0.1183	0.107	1.084
4	4.599	583.9	81.3	0.1177	0.033	1.173
5	9.73	1247.3	155.1	0.1198	0.070	1.159

The yield (24%) of diphenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (iodobenzene/internal standard = 10 and product response factor = 1.11).

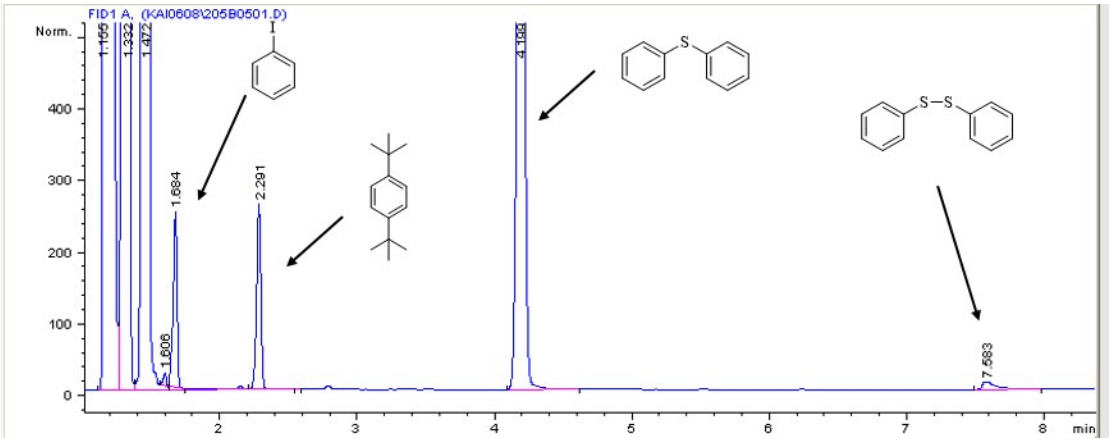
Table 1, entry 2 (no radical scavenger); HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.412	2372735.3	393356.5	0.0754	96.035	8.52E-2
2	1.774	90564.4	9593.3	0.1573	3.666	0.861
3	2.634	726.3	97.6	0.1118	0.029	1.143
4	4.066	732.1	104.9	0.1054	0.030	1.256
5	8.504	5249.3	692.8	0.1134	0.212	1.227
6	16.315	694.4	66.5	0.1479	0.028	0.887

The yield (81%) of product diphenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (iodobenzene/internal standard = 10 and product response factor = 1.13).

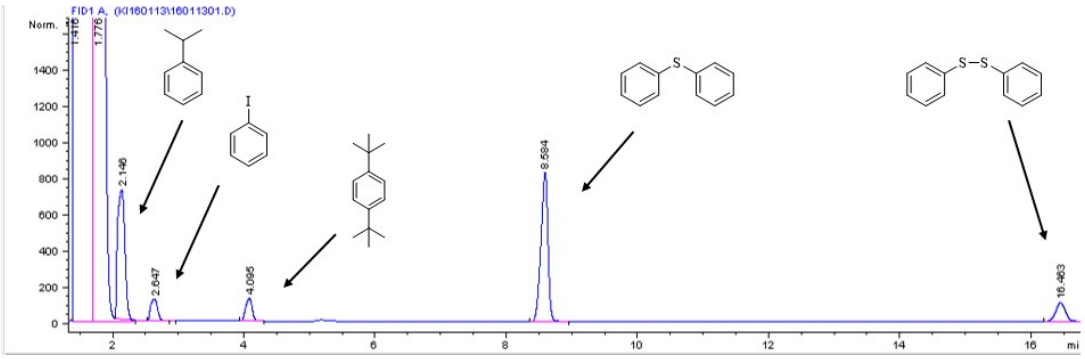
Table 1, entry 2 (TEMPO as radical scavenger); HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.155	459801.4	147643.3	0.0393	87.308	0.169
2	1.332	32422.3	13173.4	0.0357	6.156	2.031
3	1.472	28770.2	13720	0.0305	5.463	1.55
4	1.606	29	17.6	0.0252	0.006	1.195
5	1.684	498.2	245.3	0.0307	0.095	1.399
6	2.291	576.3	258.4	0.035	0.109	1.113
7	4.199	4470.8	1363.2	0.0513	0.849	1.071
8	7.583	75.6	11	0.0953	0.014	0.309

The yield (86%) of product diphenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (iodobenzene/internal standard = 10 and product response factor = 1.11).

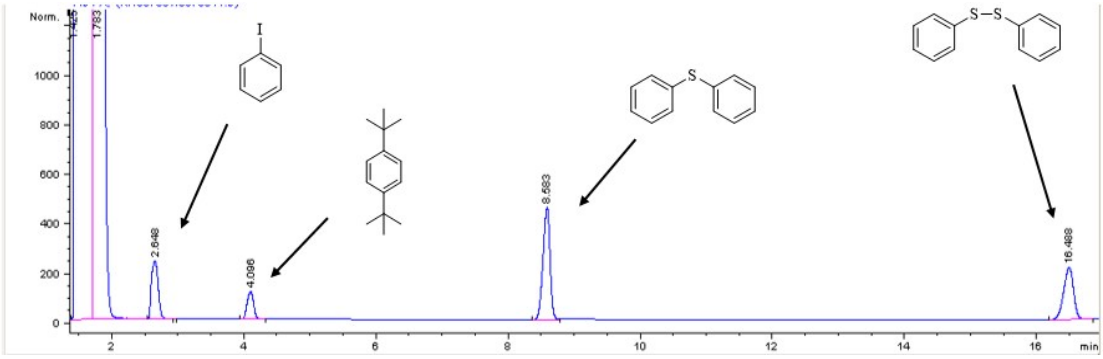
Table 1, entry 2 (cumene as radical scavenger); HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.416	2422032	394776.7	0.0816	95.079	8.08E-2
2	1.776	110928.7	11699.9	0.158	4.355	0.776
3	2.146	5526.9	713.5	0.1134	0.217	1.159
4	2.647	864.8	118.7	0.107	0.034	1.159
5	4.095	876.7	128.5	0.0996	0.034	1.31
6	8.584	6110.6	822.4	0.1087	0.240	1.294
7	16.463	1043.7	102.5	0.1518	0.041	1.004

The yield (78%) of product diphenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (iodobenzene/internal standard = 10 and product response factor = 1.11).

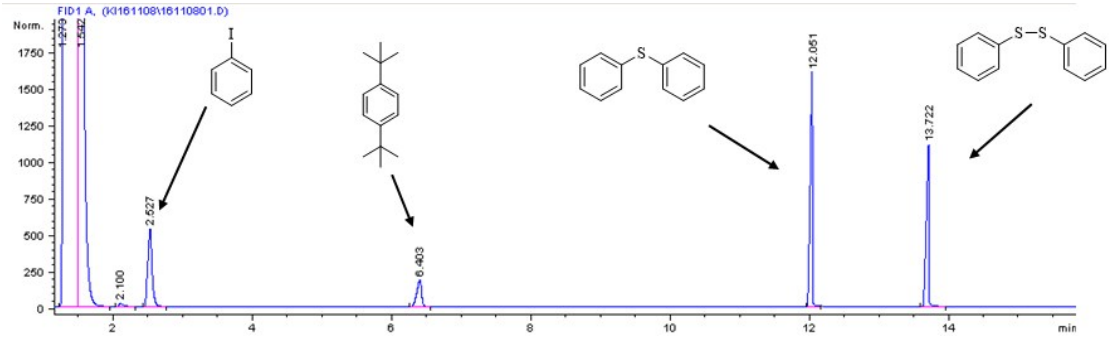
Table 1, entry 3 (in toluene); HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.425	2221728.5	364058.1	0.0752	95.758	7.97E-2
2	1.783	90494.4	9972	0.1512	3.900	0.755
3	2.648	1659.2	234.8	0.1174	0.072	1.015
4	4.096	759.1	113.1	0.1123	0.033	1.139
5	8.583	3335.4	451.6	0.1142	0.144	1.275
6	16.488	2173.8	211.4	0.1499	0.094	1.242

The yield (48%) of product diphenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (iodobenzene/internal standard = 10 and product response factor = 1.11).

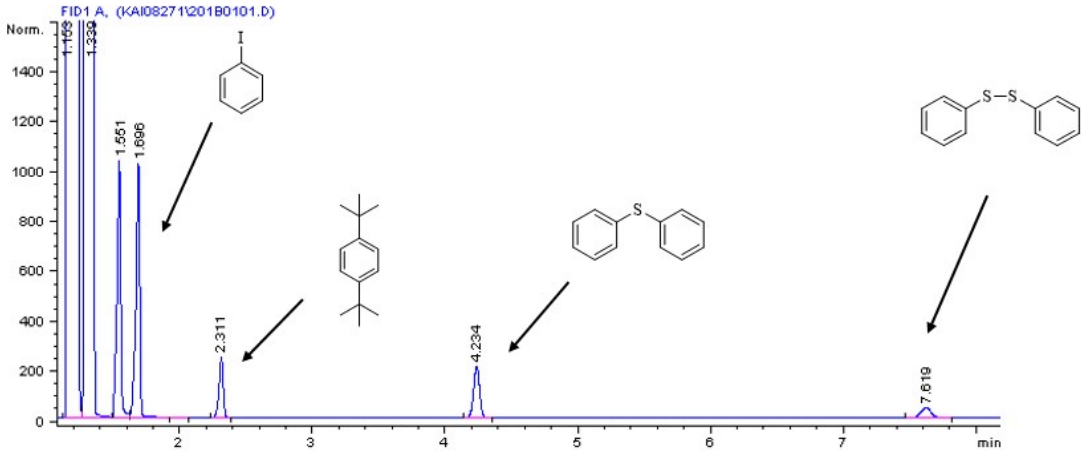
Table 1, entry 3 (in DMF); DB-5MS capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.273	2026076	474510	0.0513	97.949	0.118
2	1.542	32886.2	7441.8	0.0737	1.590	1.363
3	2.1	79.7	17.2	0.065	0.004	0.454
4	2.527	2274.7	529.2	0.0601	0.110	1.042
5	6.403	889.4	185.6	0.0652	0.043	1.796
6	12.051	3502.4	1597.8	0.0278	0.169	5.333
7	13.722	2790	1109.5	0.0318	0.135	5.065

The yield (39%) of product diphenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (iodobenzene/internal standard = 10 and product response factor = 0.99).

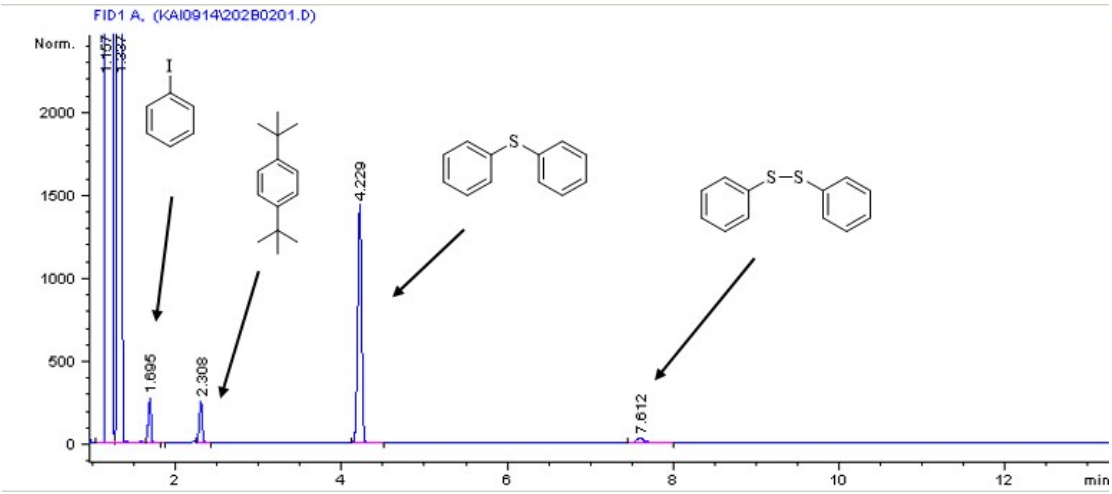
Table 1, entry 4; HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.153	458844.8	140546	0.0568	86.648	9.59E-2
2	1.339	65236.2	27302.1	0.0334	12.319	2.214
3	1.551	1994.1	1026	0.0284	0.377	1.389
4	1.696	2051.3	1018.6	0.0292	0.387	1.648
5	2.311	535.6	241.2	0.0337	0.101	1.234
6	4.234	656.7	207.2	0.0495	0.124	1.053
7	7.619	233.2	40	0.0885	0.044	1.035

The yield (14%) of product diphenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (iodobenzene/internal standard = 10 and product response factor = 1.11).

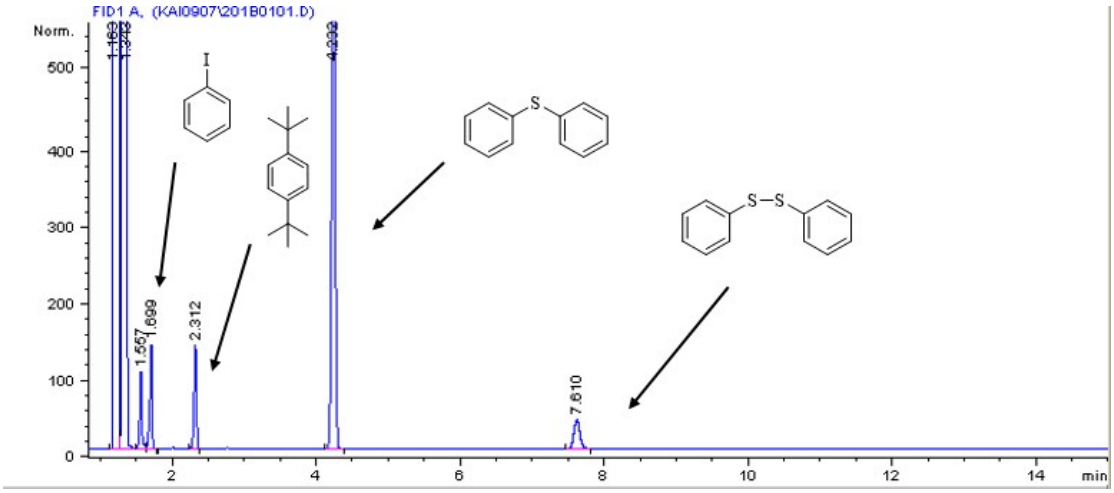
Table 1, entry 5; HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.157	465226.2	149290.4	0.0554	85.362	0.144
2	1.337	73614.5	28811.2	0.0388	13.507	1.867
3	1.695	604.2	268.1	0.0343	0.111	1.607
4	2.308	598.7	245.8	0.0374	0.110	1.212
5	4.229	4775.8	1430.9	0.0529	0.876	1.089
6	7.612	186.4	28.1	0.1015	0.034	0.75

The yield (89%) of product diphenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (iodobenzene/internal standard = 10 and product response factor = 1.11).

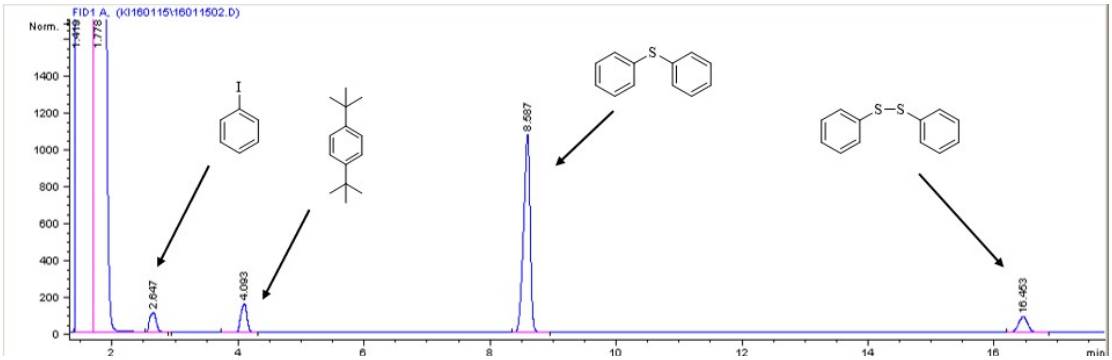
Table 1, entry 6; HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.163	458232.8	132966.3	0.0577	91.809	0.236
2	1.343	37581.5	14781	0.0379	7.530	2.127
3	1.557	200.8	101.3	0.0299	0.040	1.116
4	1.699	289.8	136.3	0.0323	0.058	1.642
5	2.312	302.7	134	0.0344	0.061	1.209
6	4.232	2290.7	711.6	0.0506	0.459	1.062
7	7.61	219.7	37.5	0.0869	0.044	0.922

The yield (84%) of product diphenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (iodobenzene/internal standard = 10 and product response factor = 1.11).

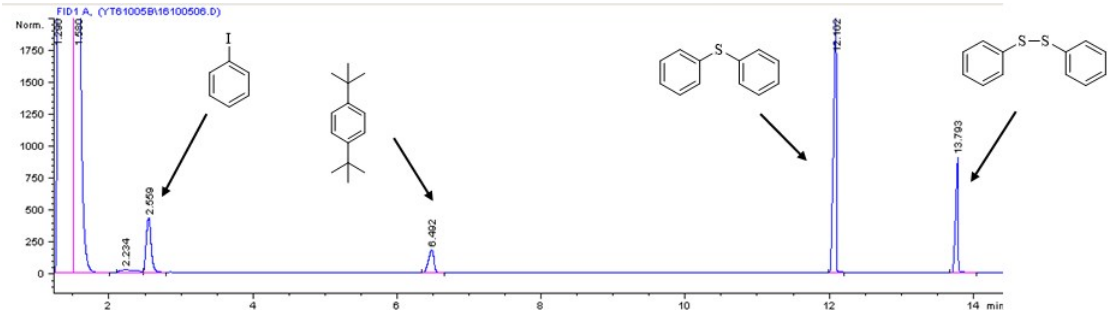
Table 1, entry7; HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.419	2332839.2	388146.7	0.0741	94.130	8.66E-2
2	1.778	135112.1	15031.6	0.1498	5.452	0.789
3	2.647	735.7	103.2	0.1022	0.030	1.23
4	4.093	1037.1	154.8	0.1102	0.042	1.358
5	8.587	7739.6	1073.2	0.1061	0.312	1.491
6	16.453	865.4	85.3	0.1293	0.035	0.935

The yield (83%) of product diphenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (iodobenzene/internal standard = 10 and product response factor = 1.11).

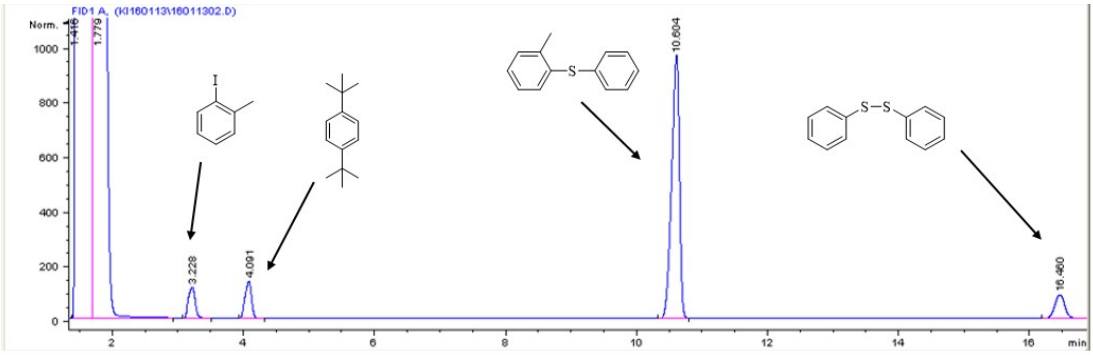
Table 2, entry 1 (in DMF); DB-5MS capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.29	1753662.6	451652.5	0.0473	97.149	5.53E-2
2	1.58	40626.7	7670.8	0.0883	2.251	2.014
3	2.234	358.1	22.1	0.1906	0.020	0.48
4	2.559	2086.3	428.6	0.075	0.116	0.872
5	6.492	959.9	181.8	0.0786	0.053	1.639
6	12.102	5286.4	2080.2	0.0331	0.293	5.832
7	13.793	2137.8	900.4	0.0317	0.118	3.984

The yield (55%) of product diphenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (iodobenzene/internal standard = 10 and product response factor = 0.99).

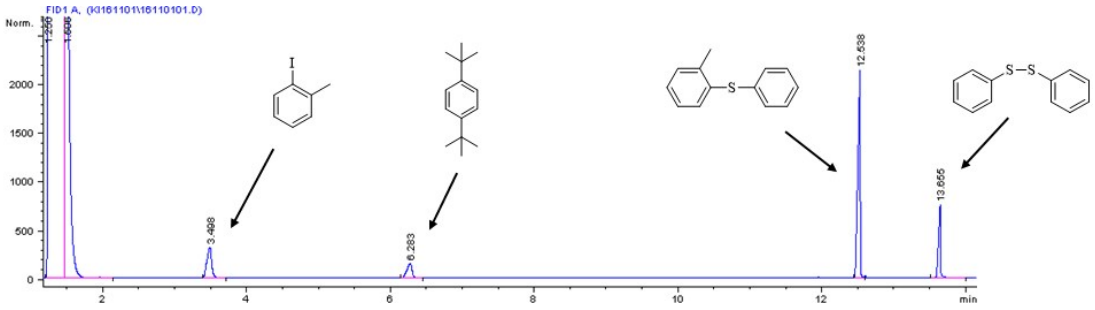
Table 2, entry2 (in toluene); HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.416	2430979.7	406745	0.0747	94.839	7.41E-2
2	1.779	121713.3	12858.7	0.1578	4.748	0.839
3	3.228	798.2	111.7	0.1024	0.031	1.205
4	4.091	915.4	134.4	0.0984	0.036	1.295
5	10.604	7953.2	962.3	0.1214	0.310	1.604
6	16.46	907.4	86.7	0.1341	0.035	1.174

The yield (94%) of product 2-methylphenyl phenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (2-iodotoluene/internal standard = 10 and product response factor = 1.08).

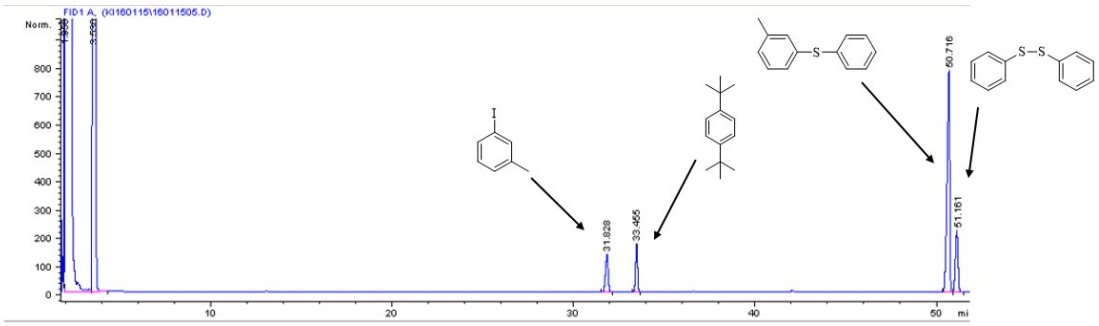
Table 2, entry 2 (in DMF); DB-5MS capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.25	2190516	520263.6	0.0504	98.501	0.152
2	1.506	24655.6	6298.6	0.0652	1.109	0.829
3	3.498	1458.6	321.3	0.0607	0.066	1.444
4	6.283	769.6	155.5	0.0678	0.035	1.605
5	12.538	4872.5	2138.9	0.0288	0.219	5.406
6	13.655	1569.7	757.7	0.0277	0.071	2.905

The yield (61%) of product 2-methylphenyl phenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (2-iodotoluene/internal standard = 10 and product response factor = 0.96).

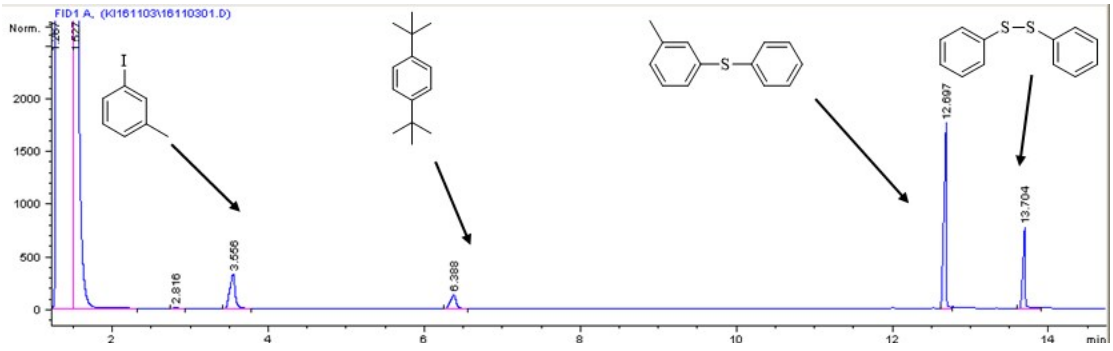
Table 2, entry3 (in toluene); HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.956	2168154.8	223299	0.1618	92.533	5.81E-2
2	3.536	162230.6	22187.4	0.1183	6.924	0.421
3	31.828	1376.1	131.8	0.1288	0.059	1.562
4	33.455	1253	168.2	0.1029	0.053	1.119
5	50.716	8038.7	780.2	0.1372	0.343	2.278
6	51.161	2067	215.4	0.1259	0.088	1.417

The yield (69%) of product 3-methylphenyl phenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (3-iodotoluene/internal standard = 10 and product response factor = 1.08).

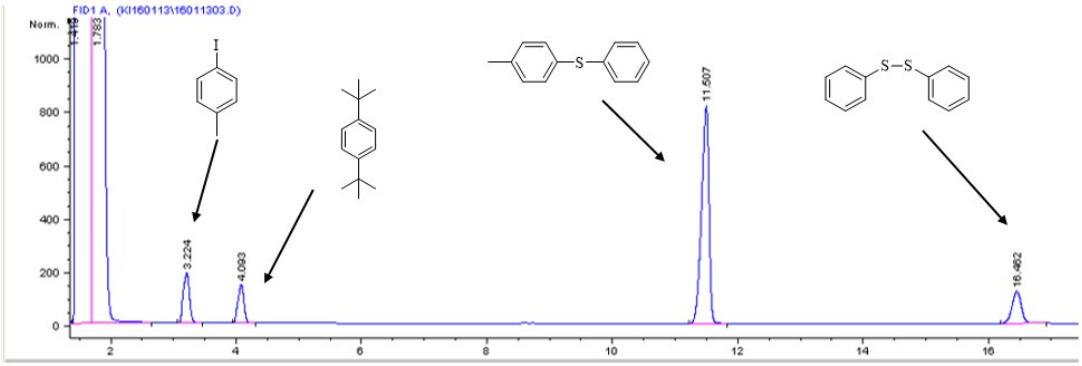
Table 2, entry3 (in DMF); DB-5MS capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.267	2244226.7	531933.4	0.054	98.725	0.105
2	1.527	21243.5	6082.6	0.0582	0.935	0.472
3	2.816	11.2	2.6	0.0586	0.000	0.869
4	3.556	1520	325.9	0.0639	0.067	1.435
5	6.388	635.8	125.5	0.0708	0.028	1.499
6	12.697	3958.4	1751.9	0.0289	0.174	4.968
7	13.704	1617.5	765.6	0.0281	0.071	2.961

The yield (60%) of product 3-methylphenyl phenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (3-iodotoluene/internal standard = 10 and product response factor = 0.96).

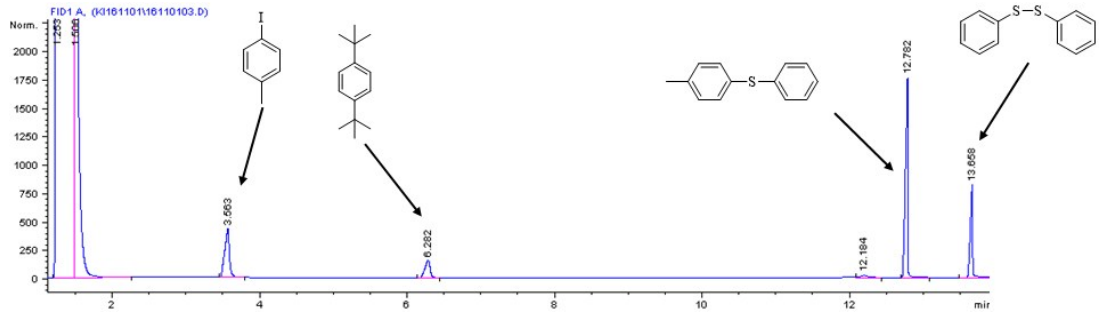
Table 2, entry 4 (in toluene); HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.419	2393249.7	392754.9	0.0781	94.688	8.34E-2
2	1.783	124116.3	13290.1	0.1557	4.911	0.902
3	3.224	1278.1	186.6	0.0979	0.051	1.262
4	4.093	958.8	143.6	0.0969	0.038	1.274
5	11.507	6695.1	816.6	0.1187	0.265	1.646
6	16.462	1217	118.9	0.1484	0.048	1.076

The yield (75%) of product 4-methylphenyl phenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (4-iodotoluene/internal standard = 10 and product response factor = 1.08).

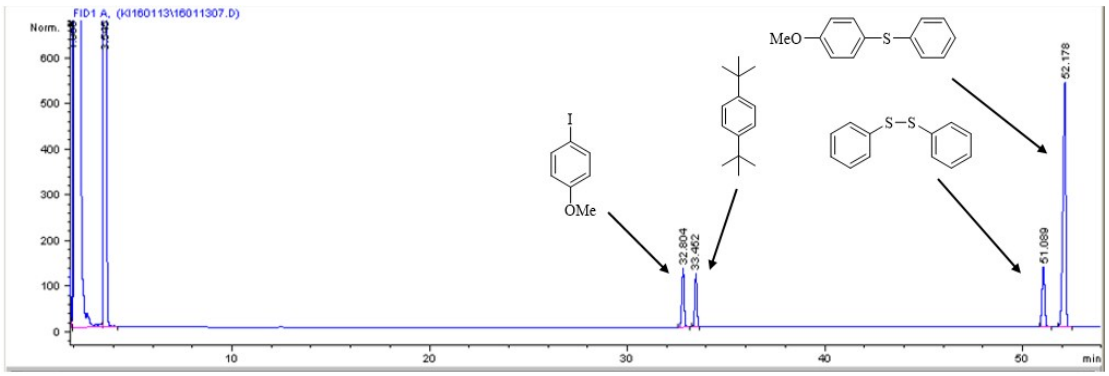
Table 2, entry 4 (in DMF); DB-5MS capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.253	2248564.5	552399.6	0.0485	98.590	0.214
2	1.506	23689.3	6347.2	0.0622	1.039	0.626
3	3.563	1892.5	427.6	0.0611	0.083	1.765
4	6.282	751.3	154.8	0.0691	0.033	1.659
5	12.184	131.3	20	0.0805	0.006	0.838
6	12.782	3903.3	1761.2	0.0289	0.171	4.745
7	13.658	1784.4	817.5	0.03	0.078	2.637

The yield (50%) of product 4-methylphenyl phenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (4-iodotoluene/internal standard = 10 and product response factor = 0.96).

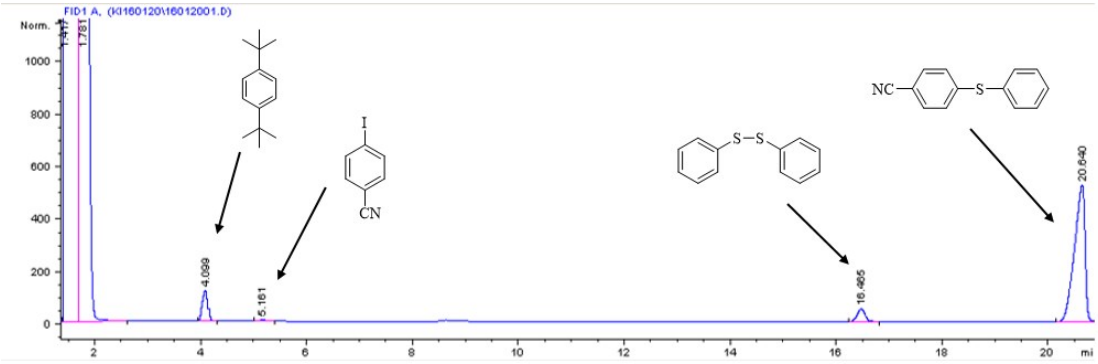
Table 2, entry 5; HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.908	2841.1	2722.6	0.0162	0.123	0.789
2	1.956	2198618	225293.9	0.1626	95.057	6.18E-2
3	3.545	102880.4	13949.5	0.12	4.448	0.471
4	32.804	1061	128.9	0.119	0.046	1.153
5	33.452	863.6	116.2	0.1097	0.037	1.04
6	51.089	1185.1	131.6	0.1311	0.051	1.03
7	52.178	5496.7	535.7	0.1367	0.238	2.079

The yield (93%) of product 4-methoxyphenyl phenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (4-iodoanisole/internal standard = 10 and product response factor = 1.47).

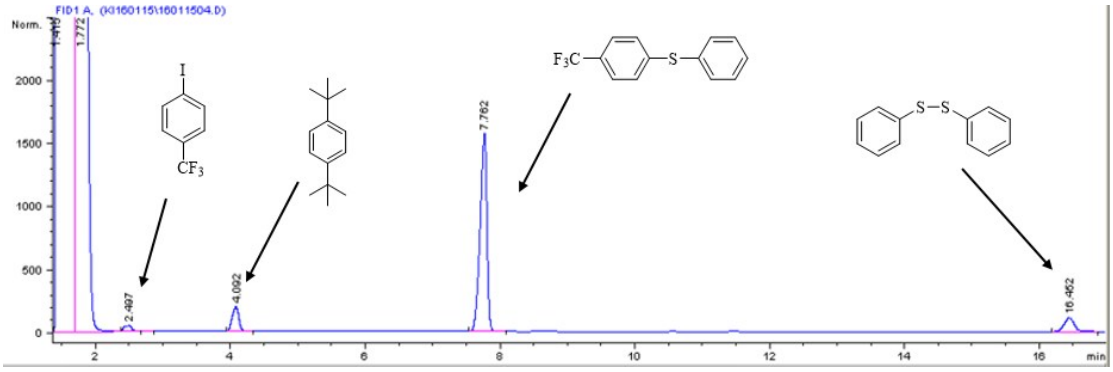
Table 2, entry 6; HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.417	2446139.7	400769.1	0.0792	95.810	6.8E-2
2	1.781	98500.6	10207.3	0.1608	3.858	0.846
3	4.099	774.3	116.8	0.0994	0.030	1.309
4	5.161	39.3	7	0.085	0.002	0.797
5	16.465	480.9	47.8	0.1564	0.019	0.956
6	20.64	7169.2	520.2	0.1948	0.281	2.529

The yield (99%) of product 4-cyanophenyl phenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (4-iodobenzonitrile/internal standard = 10 and product response factor = 1.09).

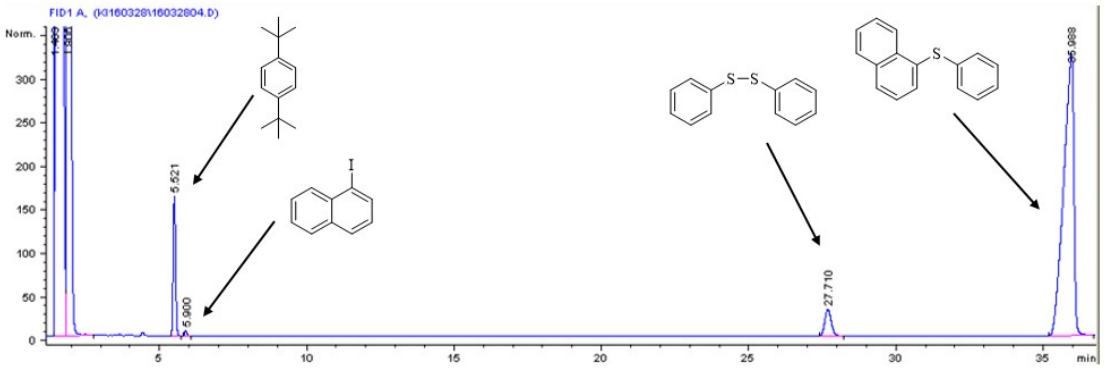
Table 2, entry 7; HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.415	2407560.8	394477.3	0.0762	92.910	8.25E-2
2	1.772	170082.3	18546.6	0.1528	6.564	0.758
3	2.497	299.2	42.3	0.1026	0.012	1.342
4	4.092	1279.2	191.2	0.1021	0.049	1.271
5	7.762	10980.1	1566.8	0.0988	0.424	1.608
6	16.452	1069	106.1	0.1455	0.041	1.005

The yield (99%) of product 4-trifluoromethylphenyl phenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (4-iodobenzotrifluoride/internal standard = 10 and product response factor = 1.18).

Table 2, entry 8; HP-1 capillary column was used



#	Time	Area	Height	Width	Area%	Symmetry
1	1.463	1545133.1	273512.9	0.0689	95.679	8.85E-2
2	1.906	60552.1	10043.4	0.0973	3.750	0.655
3	5.521	875.6	160.1	0.0888	0.054	0.956
4	5.9	30.2	5.7	0.0821	0.002	0.932
5	27.71	464.2	30.7	0.2302	0.029	0.862
6	35.988	7856.3	324.4	0.3276	0.486	3.211

The yield (91%) of product 1-naphtylphenyl sulfide was calculated with the internal standard 1,4-di-*tert*-butylbenzene (1-iodonaphthalene/internal standard = 5 and product response factor = 0.505).

The Basis Set Effect on Molecular Geometry

Basis set effect for Cu atom:

The selected bond distances of experimental and computational results were listed in Table S3.
All bond distances obtained by SDD basis set for Cu were more close to experimental results, so that the basis set SDD was used for Cu atom in all calculations.

Table S3. The geometric parameters of experimental and computational results.

DFT method		B3LYP		
Basis set for Cu		LanL2DZ(f)	SDD	SDD
Basis set for others		6-31G(d)	6-31G(d)	6-31+G(d)
	Exp.			
IMes-Cu-Cl[a]				
C-Cu	1.897 (7)	1.922	1.892	1.890
Cu-Cl	2.095 (2)	2.151	2.126	2.126
C-Cu-Cl	180.0 (2)	180.00	180.00	180.00
IMes-Cu-SPh[b]				
Cu-C	1.807 (6)	1.940	1.909	1.909
Cu-S	2.047 (2)	2.201	2.170	2.170
C-Cu-S	174.06 (8)	177.46	177.66	174.77
IPr-Cu-SPh[b]				
Cu-C	1.895 (1)	1.939	1.909	1.908
Cu-S	2.139 (1)	2.199	2.170	2.170
C-Cu-S	178.3 (1)	177.35	176.72	174.73

[a] X-ray data obtained from *Dalton Trans.*,**2010**, *39*, 4489.
[b] X-ray data obtained from *Inorg. Chem.*, **2007**, *46*, 2365.

Basis set effect for S atoms:

Based on the large size and high electronegativity of S atom, the smallest basis set for S is 6-31+G(d). However, regardless of 6-31+G(d) or 6-311+G(d,p) for S, the Cu-S bond distance of computational data is longer than that of experimental one. Maybe B3LYP is not good enough to reproduce the experimental Cu-S distances. Based on the basis set balance and computational cost, 6-31+G(d) is selected for main group atoms (H, C N, O, S, Cl, Li and Na) to perform structure optimization.

Table S4. Experimental and computational results of Cu-S distances.

		B3LYP		
Symmetry		C2v	C2v	C2v
Basis Set		BS1	BS2	BS3
Basis set for Cu		SDD	SDD	SDD
Basis set for S		6-31+G(d)	6-311+G(d,p)	6-311+G(d,p)
Basis set for others		6-31+G(d)	6-31G(d)	6-311G(d,p)
	Exp.			
Cu-SPh	-	2.135	2.139	2.140
$Cu(SPh)_2^-$	-	2.196	2.199	2.200
IMes-Cu-SPh	2.047 (2)	2.170	2.174	2.174
IPr-Cu-SPh	2.139 (1)	2.170	2.174	2.174
Phen-Cu-SPh[a]	-	2.166	2.171	2.171
$Cu_4(SPh)_6^{2-}$	2.290[b,c] 2.281[b,d]	2.346[b]	2.349[b]	2.353[b]

[a] The calculated Cu-S distance 2.21 Å was reported in *Organometallics*, **2013**, *32*, 4944. The basis set of LANL2DZ for Cu, 6-311+G(d) for S, 6-31(d) for others was used. The DFT method is also B3LYP.
[b] Average Cu-S distance.
[c] *Inorg. Chim. Acta*, **1976**, *19*, L41.
[d] *Inorg. Chim. Acta*, **1987**, *136*,139.

The Equilibriums of Copper Species in Toluene or in DMF

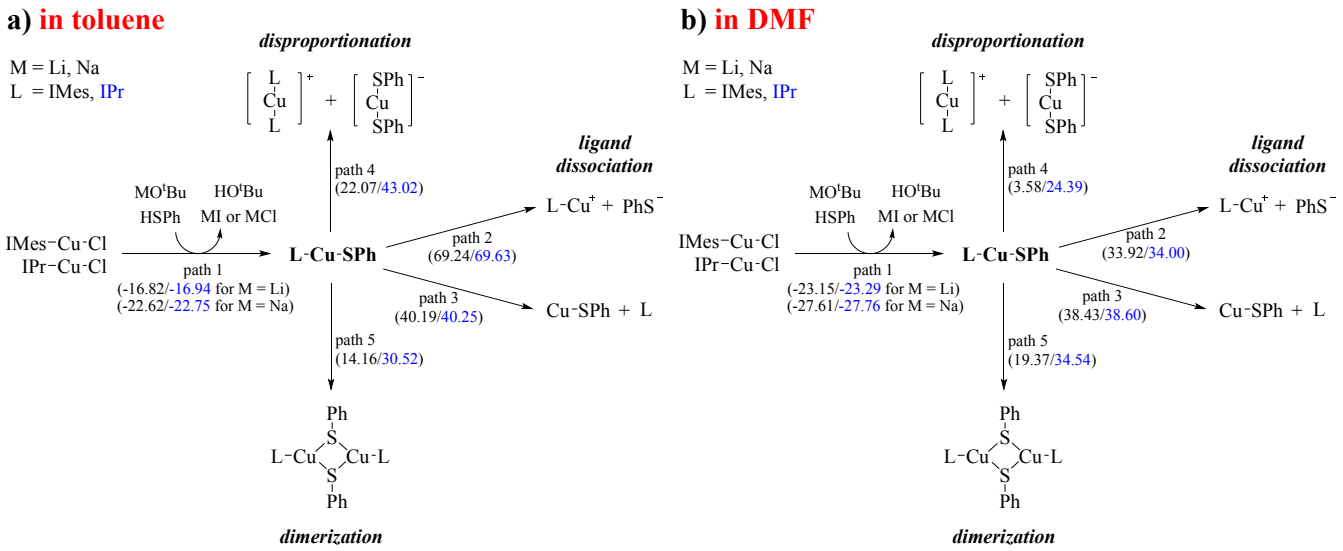


Fig. S1. The possible copper species in toluene solvent. The ΔG values (kcal/mol; black for L = IMes and blue for L = IPr) are shown in parentheses. (a) in toluene, (b) in DMF.

Even if in DMF, the disproportionation with positive ΔG_{path4} values (3.58 kcal/mol for L = IMes and 24.39 kcal/mol for L = IPr) is also unfavorable to form $Cu(SPh_2)^-$ and L_2-Cu^+ species. This result is different from the result reported by Organometallics, 2013, 32, 4944 (1,10-phenanthroline is used as ligand). The stronger binding capacity and higher steric hindrance of carbene ligands are main reasons to prevent disproportionation.

Free Energy Profile (kcal/mol) for (a) Oxidative Addition/Reductive Elimination Paths and (b) σ-Bond Metathesis Paths When Base is NaO^{t}Bu

In Toluene

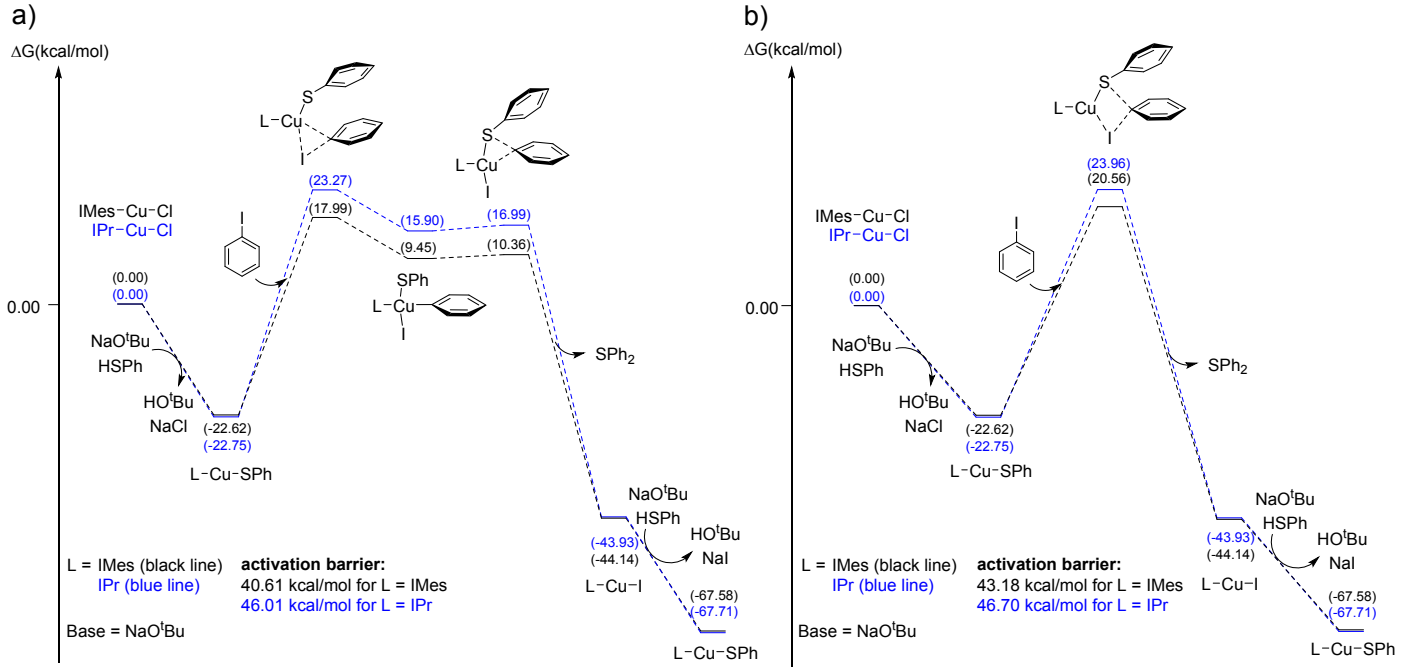


Fig. S2. Free energy profile (kcal/mol) for (a) oxidative addition/reductive elimination paths and (b) σ-bond metathesis paths in toluene.

In DMF

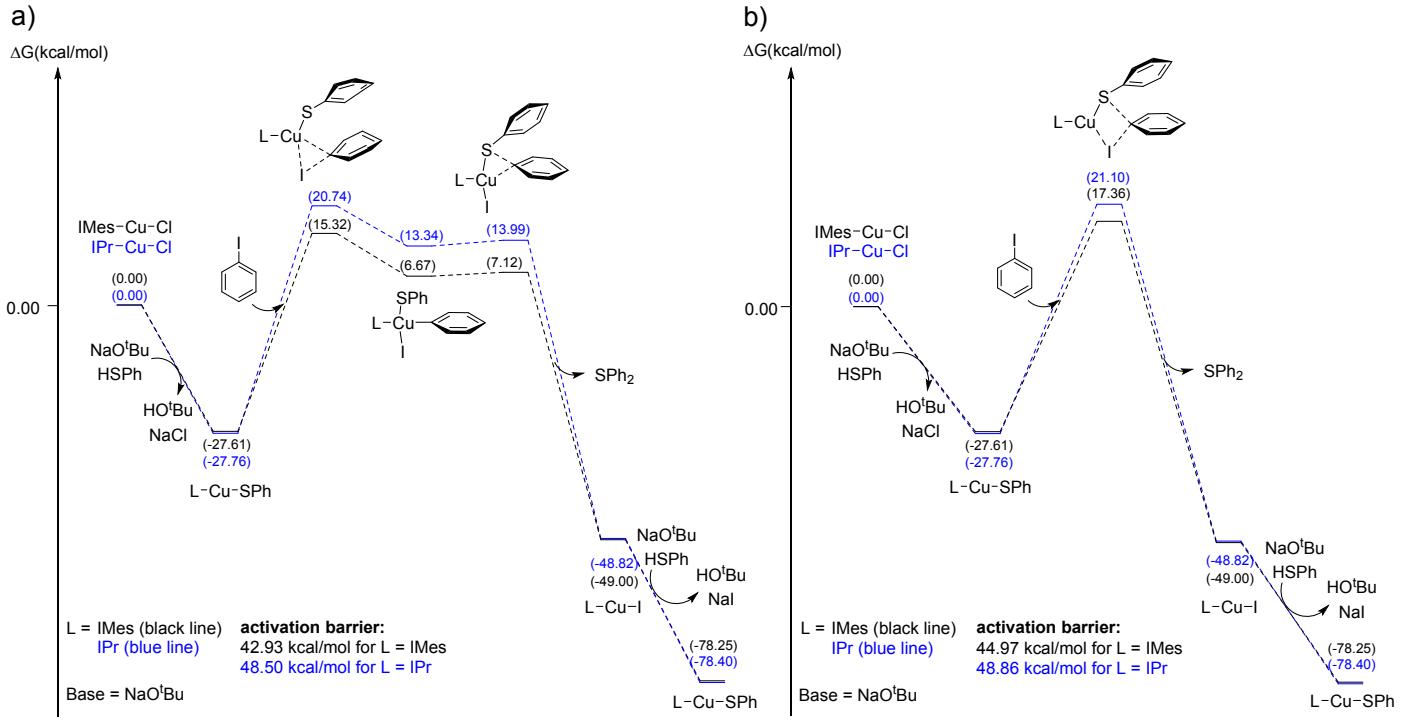


Fig. S3. Free energy profile (kcal/mol) for (a) oxidative addition/reductive elimination paths and (b) σ-bond metathesis paths in DMF.

The Results Obtained by B3LYP/BS-1

Based on the former discussions, the geometry optimization and free energy correction (at 298.15 K and 1 atm) was calculated by basis sets of SDD for heavy atoms (Cu and I) and 6-31+G(d) for main group atoms (H, C N, O, S, Cl, Li and Na). This basis set is noted as BS-1. Single-point solvent effect (toluene solvent, $\varepsilon = 2.37$; DMF, $\varepsilon = 37.22$) was calculated by self-consistent reaction filed with CPCM solvation model, and these calculations were carried out on the optimized gas-phase geometries. Using smaller basis set also can produce consistent results.

Using smaller basis set also can produce consistent results, especially on activation energy results. Based on the sense of computational chemistry, we prefer to obtain ΔG by using larger basis set. However, these two basis sets provide the consistent results and no effect on the conclusions.

The equilibriums of copper species in toluene or in DMF:

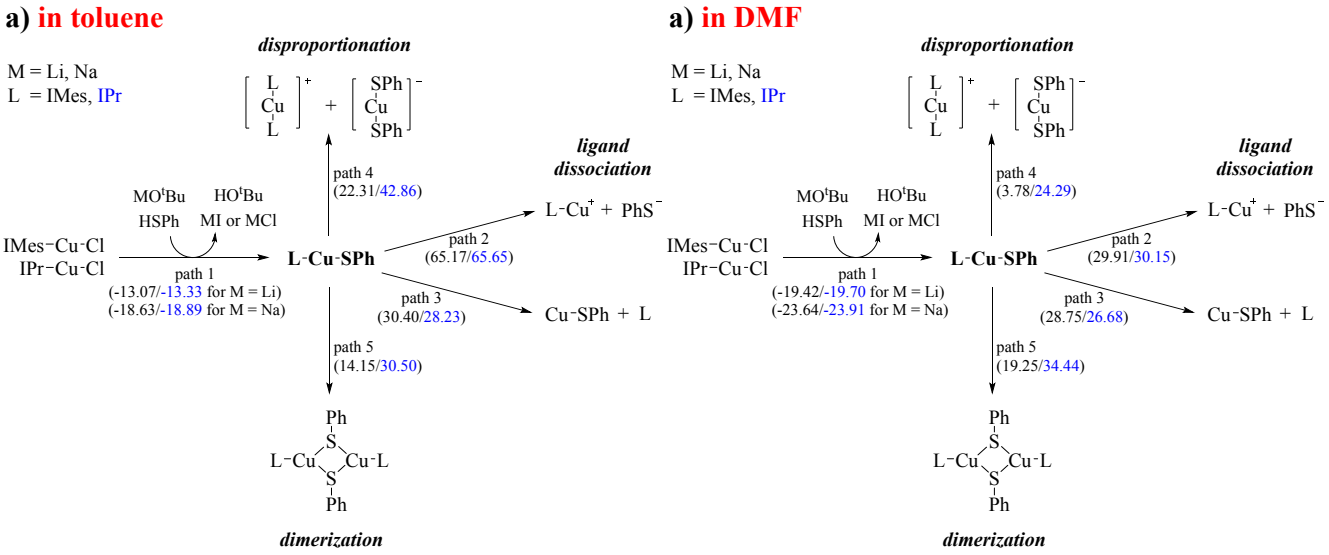


Fig. S4. The possible copper species in toluene solvent. The ΔG values (kcal/mol; black for L = IMes and blue for L = IPr) are shown in parentheses. (a) in toluene, (b) in DMF.

Oxidative addition/reductive elimination vs. σ-bond metathesis in toluene:

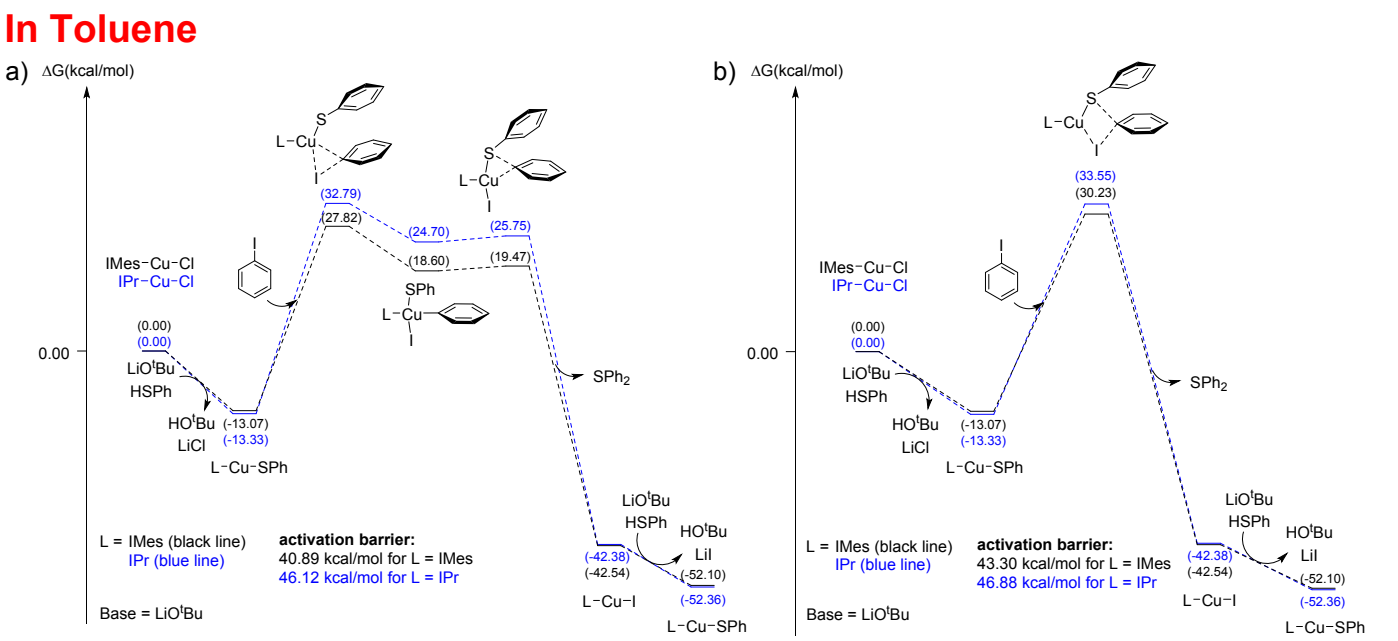


Fig. S5. Free energy profile (kcal/mol) for (a) oxidative addition/ reductive elimination paths and (b) σ-bond metathesis paths in toluene. The used base is LiO^{t}Bu.

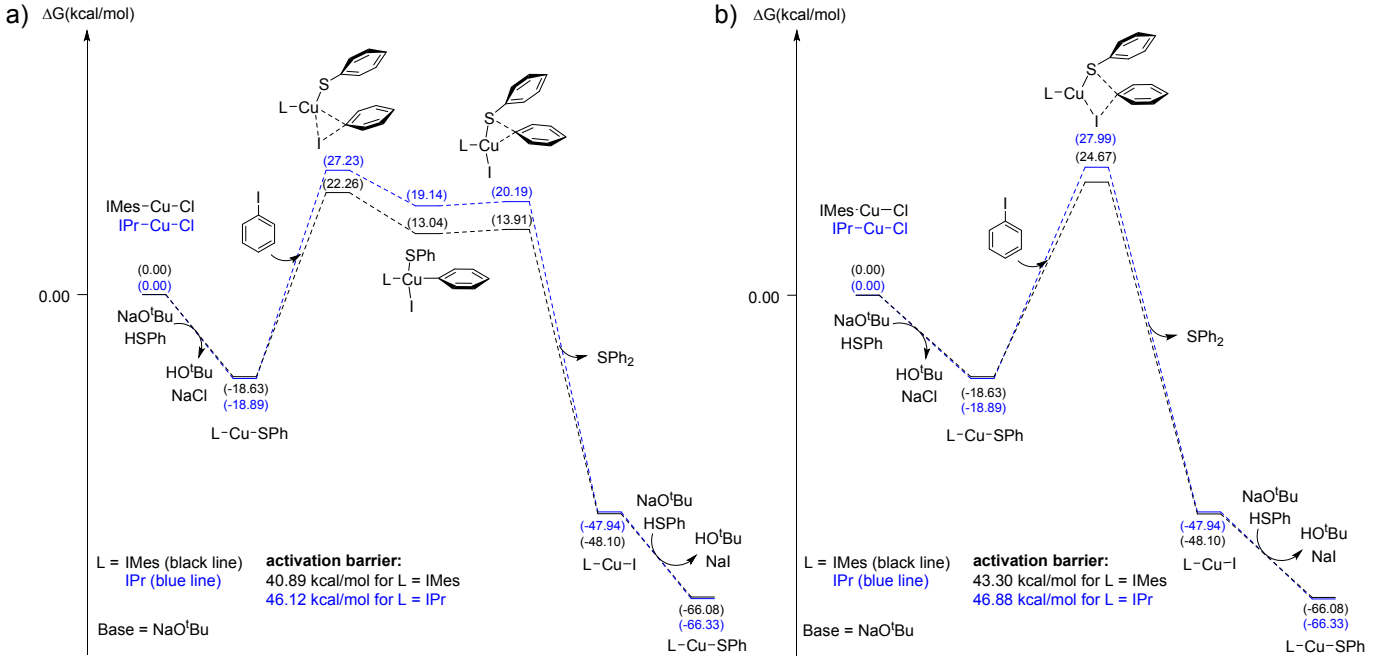


Fig. S6. Free energy profile (kcal/mol) for (a) oxidative addition/ reductive elimination paths and (b) σ-bond metathesis paths in toluene. The used base is NaO^{t}Bu.

Oxidative addition/reductive elimination vs. σ-bond metathesis in DMF:

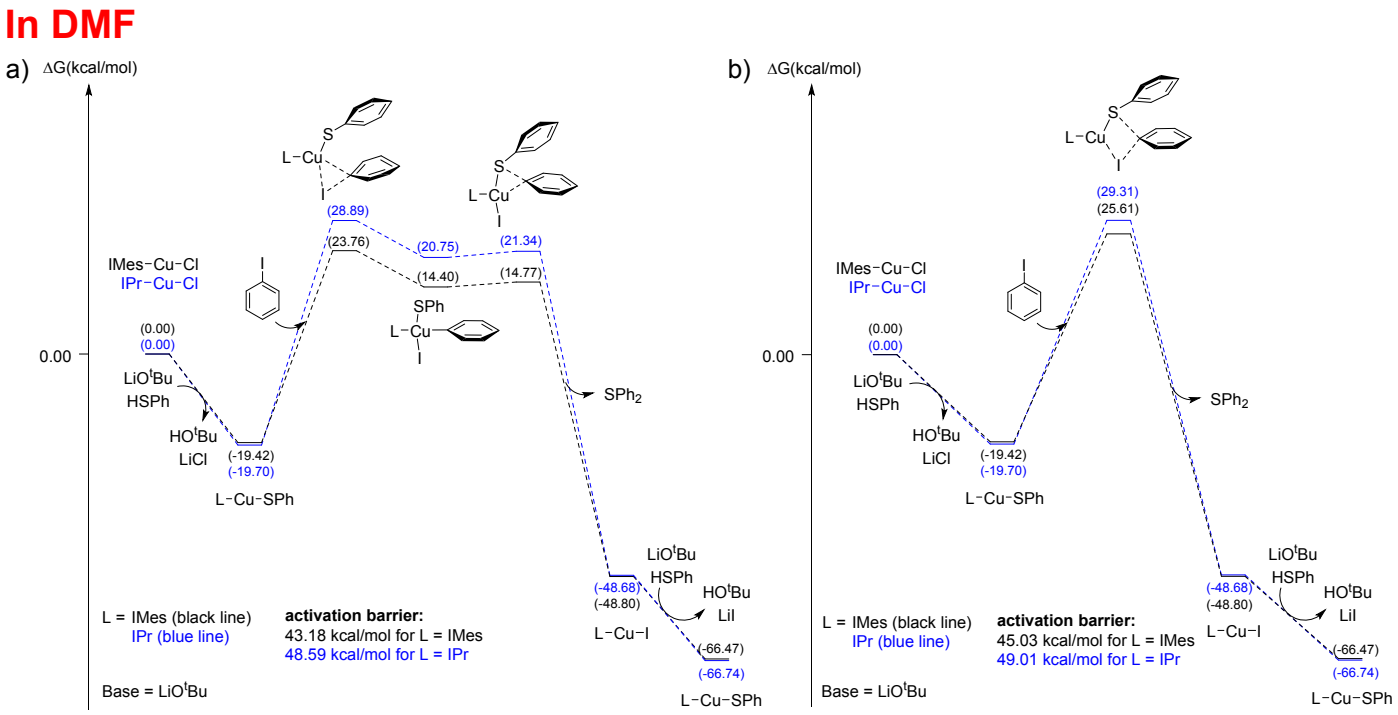


Fig. S7. Free energy profile (kcal/mol) for (a) oxidative addition/ reductive elimination paths and (b) σ-bond metathesis paths in DMF. The used base is LiO^{t}Bu.

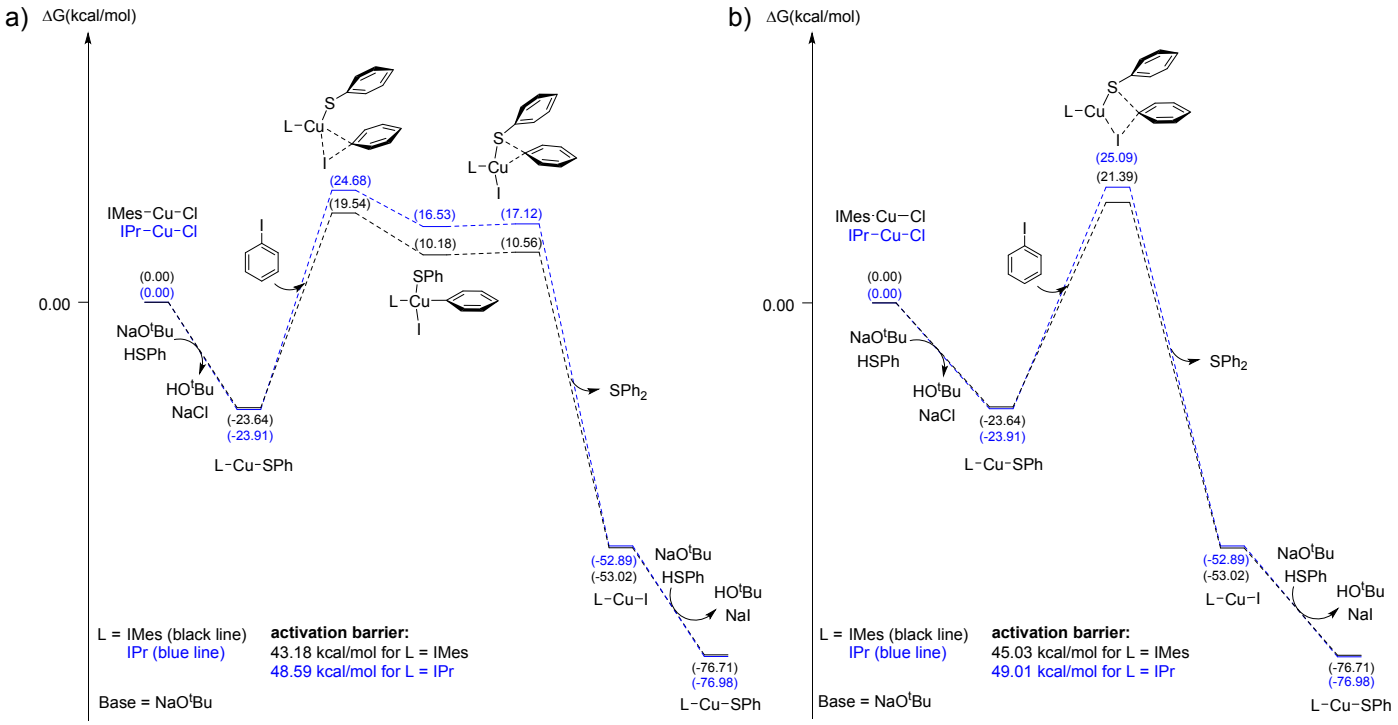


Fig. S8. Free energy profile (kcal/mol) for (a) oxidative addition/ reductive elimination paths and (b) σ-bond metathesis paths in DMF. The used base is NaO^{t}Bu.

Molecular Geometry, Free Energy Correction and PCM Energy

LiO^{t}Bu

O	0.00000000	0.00000000	1.27671900
C	0.00000000	0.00000000	-0.11302400
C	0.00000000	1.45544400	-0.63339000
C	1.26045200	-0.72772200	-0.63339000
C	-1.26045200	-0.72772200	-0.63339000
H	0.00000000	1.50485100	-1.73088800
H	0.88774400	1.98430000	-0.26422700
H	-0.88774400	1.98430000	-0.26422700
H	1.30323900	-0.75242500	-1.73088800
H	1.27458200	-1.76095900	-0.26422700
H	2.16232600	-0.22334100	-0.26422700
H	-1.30323900	-0.75242500	-1.73088800
H	-2.16232600	-0.22334100	-0.26422700
H	-1.27458200	-1.76095900	-0.26422700
Li	0.00000000	0.00000000	2.88114700

Thermal correction to Gibbs Free Energy= 0.095932
PCM energy (toluene) = -240.735427260
PCM energy (DMF) = -240.753442092

NaO^{t}Bu

O	0.00000100	0.00003300	-0.75901700
C	0.00000000	0.00001400	0.62505300
C	-1.25996200	0.72743600	1.15677700
C	0.00000000	-1.45485300	1.15680200
C	1.25996200	0.72743600	1.15677800
H	-1.30358200	0.75238000	2.25525800
H	-2.16235600	0.22340400	0.78696400
H	-1.27448800	1.76107200	0.78730300
H	-0.00000100	-1.50500900	2.25528200
H	0.88780800	-1.98429900	0.78720300
H	-0.88780800	-1.98429800	0.78720300
H	1.30358100	0.75238000	2.25525900
H	1.27448900	1.76107200	0.78730400
H	2.16235600	0.22340400	0.78696600
Na	-0.00000100	-0.00017000	-2.72288600

Thermal correction to Gibbs Free Energy= 0.091091
PCM energy (toluene) = -395.490623789
PCM energy (DMF) = -395.510419091

HO^{t}Bu

O	-0.48717000	1.37230200	0.00000000
C	0.00131300	0.01260300	0.00000000
C	1.52588100	0.14688400	0.00000000
C	-0.48717000	-0.70829800	1.26559000
C	-0.48717000	-0.70829800	-1.26559000
H	2.00275300	-0.83983200	0.00000000
H	1.85965200	0.69592600	0.88719300
H	1.85965200	0.69592600	-0.88719300
H	-0.09474900	-1.73129600	1.31650700
H	-1.58370200	-0.77246500	1.28176400
H	-0.16346600	-0.16671200	2.16113400
H	-0.09474900	-1.73129600	-1.31650700
H	-0.16346600	-0.16671200	-2.16113400
H	-1.58370200	-0.77246500	-1.28176400
H	-1.45798300	1.35315700	0.00000000

Thermal correction to Gibbs Free Energy= 0.106761
PCM energy (toluene) = -233.755357364
PCM energy (DMF) = -233.757758660

LiCl

Li	0.00000000	0.00000000	-1.74644300
Cl	0.00000000	0.00000000	0.30819600

Thermal correction to Gibbs Free Energy= -0.019319
PCM energy (toluene) = -467.870003679
PCM energy (DMF) = -467.898475865

LiI

Li	0.00000000	0.00000000	-2.30639100
I	0.00000000	0.00000000	0.13055000

Thermal correction to Gibbs Free Energy= -0.021763
PCM energy (toluene) = -19.0589803868
PCM energy (DMF) = -19.0889807628

NaCl

Na	0.00000000	0.00000000	-1.45122500
Cl	0.00000000	0.00000000	0.93902800

Thermal correction to Gibbs Free Energy= -0.021635
PCM energy (toluene) = -622.636973294
PCM energy (DMF) = -622.665093915

NaI

Na	0.00000000	0.00000000	-2.27258400
I	0.00000000	0.00000000	0.47166800

Thermal correction to Gibbs Free Energy= -0.023921
PCM energy (toluene) = -173.831126285
PCM energy (DMF) = -173.858996453

CuSPh

Cu	1.31281000	-1.94612600	0.00000000
S	-0.73964000	-1.35985900	0.00000000
C	-0.63547400	0.43623100	0.00000000
C	-0.64045700	1.14957200	1.21074700
C	-0.64045700	2.54682700	1.20857400
C	-0.63829800	3.25104000	0.00000000
C	-0.64045700	2.54682700	-1.20857400
C	-0.64045700	1.14957200	-1.21074700
H	-0.64746800	0.60321100	2.14954700
H	-0.64481700	3.08528000	2.15333700
H	-0.63908200	4.33802200	0.00000000
H	-0.64481700	3.08528000	-2.15333700
H	-0.64746800	0.60321100	-2.14954700

Thermal correction to Gibbs Free Energy= 0.057192
PCM energy (toluene) = -827.301515038
PCM energy (DMF) = -827.308847576

Cu(SPh)$_2^-$

Cu	0.00000000	0.00000000	-1.15383300
S	-1.06143200	1.92081200	-1.22612300
C	-0.31046600	3.04014200	-0.07095800
C	-0.84832900	4.34046100	0.06211300
C	-0.30206200	5.26699400	0.95172000
C	0.80322400	4.93134900	1.74370000
C	1.34779100	3.64702600	1.62360500
C	0.80383100	2.71779500	0.73418800
H	-1.70699900	4.61499300	-0.54624300
H	-0.74436500	6.25969600	1.02657800
H	1.22928400	5.65287500	2.43760900
H	2.20701800	3.36130100	2.22861300
H	1.24061400	1.72573400	0.65482200
S	1.06143200	-1.92081200	-1.22612300
C	0.31046600	-3.04014200	-0.07095800
C	0.84832900	-4.34046000	0.06211300
C	0.30206200	-5.26699400	0.95172000
C	-0.80322400	-4.93134900	1.74370000
C	-1.34779100	-3.64702600	1.62360400
C	-0.80383100	-2.71779500	0.73418800
H	1.70699900	-4.61499300	-0.54624300
H	0.74436500	-6.25969500	1.02657800
H	-1.22928400	-5.65287500	2.43760900
H	-2.20701800	-3.36130100	2.22861300
H	-1.24061500	-1.72573400	0.65482200

Thermal correction to Gibbs Free Energy= 0.135047
PCM energy (toluene) = -1457.41472830
PCM energy (DMF) = -1457.44456656

HSPh

S	-0.08370400	2.29490800	0.00000000
C	0.00000000	0.50912100	0.00000000
C	1.21205100	-0.19568800	0.00000000
C	1.20909200	-1.59267500	0.00000000
C	0.00465800	-2.30081600	0.00000000
C	-1.20304800	-1.59663100	0.00000000
C	-1.21023000	-0.20082300	0.00000000
H	2.15834400	0.33952000	0.00000000
H	2.15644800	-2.12610700	0.00000000
H	0.00680700	-3.38727600	0.00000000

H	-2.14811600	-2.13389200	0.00000000
H	-2.15569700	0.33589400	0.00000000
H	1.24634000	2.51839500	0.00000000

Thermal correction to Gibbs Free Energy= 0.068298
PCM energy (toluene) = -630.528019251
PCM energy (DMF) = -630.530213567

SPh^-

S	0.00000000	0.00000000	2.34805700
C	0.00000000	0.00000000	0.59786900
C	0.00000000	1.20327700	-0.16366400
C	0.00000000	1.20243500	-1.55854300
C	0.00000000	0.00000000	-2.28188400
C	0.00000000	-1.20243500	-1.55854300
C	0.00000000	-1.20327700	-0.16366400
H	0.00000000	2.14682600	0.37775100
H	0.00000000	2.15448400	-2.09160600
H	0.00000000	0.00000000	-3.37062500
H	0.00000000	-2.15448400	-2.09160600
H	0.00000000	-2.14682600	0.37775100

Thermal correction to Gibbs Free Energy= 0.060345
PCM energy (toluene) = -630.030325629
PCM energy (DMF) = -630.067809142

IMes

N	0.00000000	1.06605400	-0.58248500
C	0.00000000	0.00000000	0.28288100
N	0.00000000	-1.06605400	-0.58248500
C	0.00000000	-0.67828300	-1.92531200
C	0.00000000	0.67828300	-1.92531200
H	0.00000000	-1.39027400	-2.73770800
H	0.00000000	1.39027400	-2.73770800
C	0.00000000	2.44022800	-0.15367400
C	-1.22666700	3.09495700	0.04580700
C	-1.20100400	4.43763000	0.44204200
C	0.00000000	5.12637100	0.64651300
C	1.20100400	4.43763000	0.44204200
C	1.22666700	3.09495700	0.04580700
C	-2.53953000	2.37204900	-0.14229400
H	-2.61912800	1.52174500	0.54496500
H	-2.64394900	1.97181000	-1.15797100
H	-3.38219200	3.04534100	0.04429000
H	-2.14576700	4.95567000	0.59765600
C	0.00000000	6.56636500	1.10819500
H	-0.88660000	7.10223500	0.75129900
H	0.88660000	7.10223500	0.75129900
H	0.00000000	6.62918100	2.20499700
H	2.14576700	4.95567000	0.59765600
C	2.53953000	2.37204900	-0.14229400
H	2.61912800	1.52174500	0.54496500
H	3.38219200	3.04534100	0.04429000
H	2.64394900	1.97181000	-1.15797100
C	0.00000000	-2.44022800	-0.15367400
C	1.22666700	-3.09495700	0.04580700
C	1.20100400	-4.43763000	0.44204200
C	0.00000000	-5.12637100	0.64651300
C	-1.20100400	-4.43763000	0.44204200
C	-1.22666700	-3.09495700	0.04580700
C	2.53953000	-2.37204900	-0.14229400
H	2.61912800	-1.52174500	0.54496500
H	2.64394900	-1.97181000	-1.15797100
H	3.38219200	-3.04534100	0.04429000
H	2.14576700	-4.95567000	0.59765600
C	0.00000000	-6.56636500	1.10819500
H	-0.88660000	-7.10223500	0.75129900
H	0.00000000	-6.62918100	2.20499700
H	0.88660000	-7.10223500	0.75129900
H	-2.14576700	-4.95567000	0.59765600
C	-2.53953000	-2.37204900	-0.14229400
H	-2.61912800	-1.52174500	0.54496500
H	-3.38219200	-3.04534100	0.04429000
H	-2.64394900	-1.97181000	-1.15797100

Thermal correction to Gibbs Free Energy= 0.339465
PCM energy (toluene) = -924.410770459
PCM energy (DMF) = -924.416351313

IPr

N	0.00000000	1.06627100	-0.50918900
C	0.00000000	0.00000000	0.35825500
N	0.00000000	-1.06627100	-0.50918900
C	0.00000000	-0.67857000	-1.85044900
C	0.00000000	0.67857000	-1.85044900
H	0.00000000	-1.39052500	-2.66261700
H	0.00000000	1.39052500	-2.66261700
C	0.00000000	2.44450100	-0.08550200
C	-1.23472700	3.09658500	0.11167900
C	-1.20650600	4.43818200	0.51625800
C	0.00000000	5.10573100	0.71632200
C	1.20650600	4.43818200	0.51625800
C	1.23472700	3.09658500	0.11167900
C	-2.57250100	2.38583300	-0.06905100
H	-2.37165500	1.38914200	-0.47213700
C	-3.28096000	2.19221700	1.28714600
H	-2.64737600	1.63069300	1.98167600
H	-4.21858700	1.63827300	1.15256300
H	-3.52474000	3.15619400	1.75102600
C	-3.48716700	3.11111700	-1.07559700
H	-2.99347900	3.23771900	-2.04638300
H	-3.78039100	4.10553300	-0.71781600
H	-4.40648900	2.53403700	-1.23474400
H	-2.14173500	4.96639700	0.68220000
H	0.00000000	6.14629700	1.03196200
H	2.14173500	4.96639700	0.68220000
C	2.57250100	2.38583300	-0.06905100
H	2.37165500	1.38914200	-0.47213700
C	3.28096000	2.19221700	1.28714600
H	2.64737600	1.63069300	1.98167600
H	3.52474000	3.15619400	1.75102600
H	4.21858700	1.63827300	1.15256300
C	3.48716700	3.11111700	-1.07559700
H	2.99347900	3.23771900	-2.04638300
H	4.40648900	2.53403700	-1.23474400
H	3.78039100	4.10553300	-0.71781600
C	0.00000000	-2.44450100	-0.08550200
C	1.23472700	-3.09658500	0.11167900
C	1.20650600	-4.43818200	0.51625800
C	0.00000000	-5.10573100	0.71632200
C	-1.20650600	-4.43818200	0.51625800
C	-1.23472700	-3.09658500	0.11167900
C	2.57250100	-2.38583300	-0.06905100
H	2.37165500	-1.38914200	-0.47213700
C	3.28096000	-2.19221700	1.28714600
H	2.64737600	-1.63069300	1.98167600
H	4.21858700	-1.63827300	1.15256300
H	3.52474000	-3.15619400	1.75102600
C	3.48716700	-3.11111700	-1.07559700
H	2.99347900	-3.23771900	-2.04638300
H	3.78039100	-4.10553300	-1.71781600
H	4.40648900	-2.53403700	-1.23474400
H	2.14173500	-4.96639700	0.68220000
H	0.00000000	-6.14629700	1.03196200
H	-2.14173500	-4.96639700	0.68220000
C	-2.57250100	-2.38583300	-0.06905100
H	-2.37165500	-1.38914200	-0.47213700
C	-3.28096000	-2.19221700	1.28714600
H	-2.64737600	-1.63069300	1.98167600
H	-3.52474000	-3.15619400	1.75102600
H	-4.21858700	-1.63827300	1.15256300
C	-3.48716700	-3.11111700	-1.07559700
H	-2.99347900	-3.23771900	-2.04638300
H	-4.40648900	-2.53403700	-1.23474400
H	-3.78039100	-4.10553300	-1.71781600

Thermal correction to Gibbs Free Energy= 0.505897
PCM energy (toluene) = -1160.33831538
PCM energy (DMF) = -1160.34376366

IMes-Cu^+

N	0.79004400	0.74320000	-0.91207000
C	0.00000000	0.00000000	-0.09699600
N	-0.79004400	-0.74320000	-0.91207000
C	-0.49576400	-0.46640700	-2.24031700
C	0.49576400	0.46640700	-2.24031700
H	-1.01499200	-0.95484900	-3.05096900
H	1.01499200	0.95484900	-3.05096900
C	1.79329100	1.68694100	-0.46032700
C	1.41643300	3.02663800	-0.25727000
C	2.40652400	3.91556400	0.17706300
C	3.72911800	3.50799500	0.39568500
C	4.05609700	2.16364800	0.17332700
C	3.10849000	1.22979600	-0.26101900
C	0.00483100	3.50864400	-0.50458400
H	-0.72901100	2.96367700	0.10154100
H	-0.28999600	3.38341000	-1.55369700
H	-0.08632100	4.57056700	-0.26126000
H	2.13657100	4.95589500	0.34331200
C	4.78305200	4.49884500	0.82965100
H	4.34895600	5.31903400	1.41035800
H	5.27993900	4.94274000	-0.04312300
H	5.55791800	4.02089800	1.43772600
H	5.07870900	1.83133700	0.33671700
C	3.50416300	-0.20769200	-0.51238400
H	2.91556000	-0.90895800	0.09147100
H	4.55855600	-0.36372100	-0.26925100

H	3.36162500	-0.49134000	-1.56238000
C	-1.79329100	-1.68694100	-0.46032700
C	-1.41643300	-3.02663800	-0.25727000
C	-2.40652400	-3.91556400	0.17706300
C	-3.72911800	-3.50799500	0.39568500
C	-4.05609700	-2.16364800	0.17332700
C	-3.10849000	-1.22979600	-0.26101900
C	-0.00483100	-3.50864400	-0.50458400
H	0.72901100	-2.96367700	0.10154100
H	0.28999600	-3.38341000	-1.55369700
H	0.08632100	-4.57056700	-0.26126000
H	-2.13657100	-4.95589500	0.34331200
C	-4.78305200	-4.49884500	0.82965100
H	-5.27993900	-4.94274000	-0.04312300
H	-5.55791800	-4.02089800	1.43772600
H	-4.34895600	-5.31903400	1.41035800
H	-5.07870900	-1.83133700	0.33671700
C	-3.50416300	0.20769200	-0.51238400
H	-2.91556000	0.90895800	0.09147100
H	-4.55855600	0.36372100	-0.26925100
H	-3.36162500	0.49134000	-1.56238100
Cu	0.00000000	0.00000000	1.78348200

Thermal correction to Gibbs Free Energy= 0.338920
PCM energy (toluene) = -1121.63827303
PCM energy (DMF) = -1121.66718489

IMes-Cu^{+}-IMes

N	0.00000000	1.07761300	2.75815400
C	0.00000000	0.00000000	1.92251400
N	0.00000000	-1.07761300	2.75815400
C	0.00000000	-0.67921400	4.09010300
C	0.00000000	0.67921400	4.09010300
H	0.00000000	-1.39284200	4.90002100
H	0.00000000	1.39284200	4.90002100
C	0.00000000	2.45887500	2.32981200
C	1.23142500	3.11084900	2.14429400
C	1.20234400	4.45474500	1.75266100
C	0.00000000	5.14572200	1.55563800
C	-1.20234400	4.45474500	1.75266100
C	-1.23142500	3.11084900	2.14429400
C	2.54804500	2.39900900	2.35495800
H	2.67387300	1.56559900	1.65329000
H	2.63035700	1.98319400	3.36623900
H	3.38474400	3.08835500	2.20996600
H	2.14576000	4.97652800	1.60625200
C	0.00000000	6.60871100	1.17725800
H	0.88696000	6.87297800	0.59182900
H	0.00000000	7.24287900	2.07374900
H	-0.88696000	6.87297800	0.59182900
H	-2.14576000	4.97652800	1.60625200
C	-2.54804500	2.39900900	2.35495800
H	-2.67387300	1.56559900	1.65329000
H	-3.38474400	3.08835500	2.20996600
H	-2.63035700	1.98319400	3.36623900
C	0.00000000	-2.45887500	2.32981200
C	-1.23142500	-3.11084900	2.14429400
C	-1.20234400	-4.45474500	1.75266100
C	0.00000000	-5.14572200	1.55563800
C	1.20234400	-4.45474500	1.75266100
C	1.23142500	-3.11084900	2.14429400
C	-2.54804500	-2.39900900	2.35495800
H	-2.67387300	-1.56559900	1.65329000
H	-2.63035700	-1.98319400	3.36623900
H	-3.38474400	-3.08835500	2.20996600
H	-2.14576000	-4.97652800	1.60625200
C	0.00000000	-6.60871100	1.17725800
H	0.88696000	-6.87297800	0.59182900
H	-0.88696000	-6.87297800	0.59182900
H	0.00000000	-7.24287900	2.07374900
H	2.14576000	-4.97652800	1.60625200
C	2.54804500	-2.39900900	2.35495800
H	2.67387300	-1.56559900	1.65329000
H	3.38474400	-3.08835500	2.20996600
H	2.63035700	-1.98319400	3.36623900
Cu	0.00000000	0.00000000	0.00000000
N	-1.07761300	0.00000000	-2.75815400
C	0.00000000	0.00000000	-1.92251400
N	1.07761300	0.00000000	-2.75815400
C	0.67921400	0.00000000	-4.09010300
C	-0.67921400	0.00000000	-4.09010300
H	1.39284200	0.00000000	-4.90002100
H	-1.39284200	0.00000000	-4.90002100
C	-2.45887500	0.00000000	-2.32981200
C	-3.11084900	-1.23142500	-2.14429400
C	-4.45474500	-1.20234400	-1.75266100
C	-5.14572200	0.00000000	-1.55563800
C	-4.45474500	1.20234400	-1.75266100
C	-3.11084900	1.23142500	-2.14429400
C	-2.39900900	-2.54804500	-2.35495800
H	-1.56559900	-2.67387300	-1.65329000
H	-1.98319400	-2.63035700	-3.36623900
H	-3.08835500	-3.38474400	-2.20996600
H	-4.97652800	-2.14576000	-1.60625200
C	-6.60871100	0.00000000	-1.17725800
H	-7.24287900	0.00000000	-2.07374900
H	-6.87297800	0.88696000	-0.59182900
H	-6.87297800	-0.88696000	-0.59182900
H	-4.97652800	2.14576000	-1.60625200
C	-2.39900900	2.54804500	-2.35495800
H	-1.56559900	2.67387300	-1.65329000
H	-3.08835500	3.38474400	-2.20996600
H	-1.98319400	2.63035700	-3.36623900
C	2.45887500	0.00000000	-2.32981200
C	3.11084900	1.23142500	-2.14429400
C	4.45474500	1.20234400	-1.75266100
C	5.14572200	0.00000000	-1.55563800
C	4.45474500	-1.20234400	-1.75266100
C	3.11084900	-1.23142500	-2.14429400
C	2.39900900	2.54804500	-2.35495800
H	1.56559900	2.67387300	-1.65329000
H	1.98319400	2.63035700	-3.36623900
H	3.08835500	3.38474400	-2.20996600
H	4.97652800	2.14576000	-1.60625200
C	6.60871100	0.00000000	-1.17725800
H	6.87297800	-0.88696000	-0.59182900
H	6.87297800	0.88696000	-0.59182900
H	7.24287900	0.00000000	-2.07374900
H	4.97652800	-2.14576000	-1.60625200
C	2.39900900	-2.54804500	-2.35495800
H	1.56559900	-2.67387300	-1.65329000
H	3.08835500	-3.38474400	-2.20996600
H	1.98319400	-2.63035700	-3.36623900

Thermal correction to Gibbs Free Energy= 0.704325
PCM energy (toluene) = -2046.14881300
PCM energy (DMF) = -2046.16865742

IMes-Cu-Cl

N	0.00000000	1.07746100	-1.22776400
C	0.00000000	0.00000000	-0.38742400
N	0.00000000	-1.07746100	-1.22776400
C	0.00000000	-0.67899800	-2.56108200
C	0.00000000	0.67899800	-2.56108200
H	0.00000000	-1.39295200	-3.37059700
H	0.00000000	1.39295200	-3.37059700
C	0.00000000	2.45588300	-0.79591900
C	-1.23014100	3.10560200	-0.59985800
C	-1.20206600	4.44680700	-0.20074300
C	0.00000000	5.13338600	0.00746300
C	1.20206600	4.44680700	-0.20074300
C	1.23014100	3.10560200	-0.59985800
C	-2.54483300	2.38497900	-0.78669900
H	-2.65789300	1.57630600	-0.05446100
H	-2.62976200	1.93371800	-1.78253900
H	-3.38382400	3.07509000	-0.65676200
H	-2.14590400	4.96436500	-0.04178300
C	0.00000000	6.56953200	0.47872600
H	-0.88704400	7.10766300	0.12703300
H	0.88704400	7.10766300	0.12703300
H	0.00000000	6.61968300	1.57589700
H	2.14590400	4.96436500	-0.04178300
C	2.54483300	2.38497900	-0.78669900
H	2.65789300	1.57630600	-0.05446100
H	3.38382400	3.07509000	-0.65676200
H	2.62976200	1.93371800	-1.78253900
C	0.00000000	-2.45588300	-0.79591900
C	1.23014100	-3.10560200	-0.59985800
C	1.20206600	-4.44680700	-0.20074300
C	0.00000000	-5.13338600	0.00746300
C	-1.20206600	-4.44680700	-0.20074300
C	-1.23014100	-3.10560200	-0.59985800
C	2.54483300	-2.38497900	-0.78669900
H	2.65789300	-1.57630600	-0.05446100
H	2.62976200	-1.93371800	-1.78253900
H	3.38382400	-3.07509000	-0.65676200
H	2.14590400	-4.96436500	-0.04178300
C	0.00000000	-6.56953200	0.47872600
H	-0.88704400	-7.10766300	0.12703300
H	0.00000000	-6.61968300	1.57589700
H	0.88704400	-7.10766300	0.12703300
H	-2.14590400	-4.96436500	-0.04178300
C	-2.54483300	-2.38497900	-0.78669900
H	-2.65789300	-1.57630600	-0.05446100
H	-3.38382400	-3.07509000	-0.65676200
H	-2.62976200	-1.93371800	-1.78253900
Cu	0.00000000	0.00000000	1.50287200
Cl	0.00000000	0.00000000	3.62931400

Thermal correction to Gibbs Free Energy= 0.338089
PCM energy (toluene) = -1582.12965948

PCM energy (DMF) = -1582.14034486

IMes-Cu-I

N	0.00000000	1.07733200	-1.83577600
C	0.00000000	0.00000000	-0.99631100
N	0.00000000	-1.07733200	-1.83577600
C	0.00000000	-0.67907500	-3.16911500
C	0.00000000	0.67907500	-3.16911500
H	0.00000000	-1.39303700	-3.97864500
H	0.00000000	1.39303700	-3.97864500
C	0.00000000	2.45567800	-1.40298900
C	-1.23026000	3.10502700	-1.20630500
C	-1.20207900	4.44585700	-0.80600000
C	0.00000000	5.13216700	-0.59695100
C	1.20207900	4.44585700	-0.80600000
C	1.23026000	3.10502700	-1.20630500
C	-2.54516500	2.38482800	-1.39365700
H	-2.66040400	1.57818500	-0.65949100
H	-2.62887800	1.93117200	-2.38848100
H	-3.38381300	3.07588700	-1.26677300
H	-2.14587700	4.96324500	-0.64639200
C	0.00000000	6.56761500	-0.12370100
H	-0.88705900	7.10622700	-0.47457600
H	0.88705900	7.10622700	-0.47457600
H	0.00000000	6.61600500	0.97353200
H	2.14587700	4.96324500	-0.64639200
C	2.54516500	2.38482800	-1.39365700
H	2.66040400	1.57818500	-0.65949100
H	3.38381300	3.07588700	-1.26677300
H	2.62887800	1.93117200	-2.38848100
C	0.00000000	-2.45567800	-1.40298900
C	1.23026000	-3.10502700	-1.20630500
C	1.20207900	-4.44585700	-0.80600000
C	0.00000000	-5.13216700	-0.59695100
C	-1.20207900	-4.44585700	-0.80600000
C	-1.23026000	-3.10502700	-1.20630500
C	2.54516500	-2.38482800	-1.39365700
H	2.66040400	-1.57818500	-0.65949100
H	2.62887800	-1.93117200	-2.38848100
H	3.38381300	-3.07588700	-1.26677300
H	2.14587700	-4.96324500	-0.64639200
C	0.00000000	-6.56761500	-0.12370100
H	-0.88705900	-7.10622700	-0.47457600
H	0.00000000	-6.61600500	0.97353200
H	0.88705900	-7.10622700	-0.47457600
H	-2.14587700	-4.96324500	-0.64639200
C	-2.54516500	-2.38482800	-1.39365700
H	-2.66040400	-1.57818500	-0.65949100
H	-3.38381300	-3.07588700	-1.26677300
H	-2.62887800	-1.93117200	-2.38848100
Cu	0.00000000	0.00000000	0.90884300
I	0.00000000	0.00000000	3.36474600

Thermal correction to Gibbs Free Energy= 0.335481
PCM energy (toluene) = -1133.32218200
PCM energy (DMF) = -1133.33130983

IPr-Cu^{+}

N	0.00000000	1.08406600	-0.74802600
C	0.00000000	0.00000000	0.06824000
N	0.00000000	-1.08406600	-0.74802600
C	0.00000000	-0.68094700	-2.07511600
C	0.00000000	0.68094700	-2.07511600
H	0.00000000	-1.39355700	-2.88571000
H	0.00000000	1.39355700	-2.88571000
C	0.00000000	2.46461600	-0.29722900
C	-1.24217100	3.10375400	-0.09668100
C	-1.20864200	4.43506600	0.34051100
C	0.00000000	5.09383600	0.55878100
C	1.20864200	4.43506600	0.34051100
C	1.24217100	3.10375400	-0.09668100
C	-2.58466200	2.41904400	-0.34150700
H	-2.39381400	1.39474100	-0.67915300
C	-3.41824000	2.32394700	0.95286600
H	-2.87487100	1.79092800	1.74345400
H	-4.35434500	1.78613200	0.76394300
H	-3.67771800	3.31553400	1.34022100
C	-3.38267500	3.12301200	-1.45906300
H	-2.80922300	3.17489800	-2.39156000
H	-3.65282200	4.14681900	-1.17693000
H	-4.31191100	2.57803300	-1.66123800
H	-2.14154600	4.96540700	0.50756200
H	0.00000000	6.12705300	0.89494800
H	2.14154600	4.96540700	0.50756200
C	2.58466200	2.41904400	-0.34150700
H	2.39381400	1.39474100	-0.67915300
C	3.41824000	2.32394700	0.95286600
H	2.87487100	1.79092800	1.74345400
H	3.67771800	3.31553400	1.34022100
H	4.35434500	1.78613200	0.76394300
C	3.38267500	3.12301200	-1.45906300
H	2.80922300	3.17489800	-2.39156000
H	3.65282200	4.14681900	-1.17693000
H	4.31191100	2.57803300	-1.66123800
H	2.14154600	4.96540700	0.50756200
H	0.00000000	6.12705300	0.89494800
H	-2.14154600	4.96540700	0.50756200
C	-2.58466200	2.41904400	-0.34150700
H	-2.39381400	1.39474100	-0.67915300
C	-3.41824000	2.32394700	0.95286600
H	-2.87487100	1.79092800	1.74345400
H	-3.67771800	3.31553400	1.34022100
H	-4.35434500	1.78613200	0.76394300
C	-3.38267500	3.12301200	-1.45906300
H	-2.80922300	3.17489800	-2.39156000
H	-4.31191100	2.57803300	-1.66123800
H	-3.65282200	4.14681900	-1.17693000
Cu	0.00000000	0.00000000	1.94879300

Thermal correction to Gibbs Free Energy= 0.505459
PCM energy (toluene) = -1357.56539592
PCM energy (DMF) = -1357.59484415

IPr-Cu^{+}-IPr

N	-1.07456600	0.00000000	2.82750400
C	0.00000000	0.00000000	1.97534800
N	1.07456600	0.00000000	2.82750400
C	0.67745000	0.00000000	4.15628000
C	-0.67745000	0.00000000	4.15628000
H	1.39150700	0.00000000	4.96466200
H	-1.39150700	0.00000000	4.96466200
C	-2.47114800	0.00000000	2.45106300
C	-3.13075200	1.24149600	2.32965400
C	-4.48000300	1.20987700	1.95086700
C	-5.14125500	0.00000000	1.74147600
C	-4.48000300	-1.20987700	1.95086700
C	-3.13075200	-1.24149600	2.32965400
C	-2.46825900	2.55958500	2.73320800
H	-1.39458300	2.38032000	2.84839600
C	-2.62233500	3.68811500	1.70013100
H	-2.16093100	3.42623400	0.74419700
H	-2.13192200	4.59595300	2.07086200
H	-3.67359600	3.93770500	1.51569800
C	-3.01096500	3.01382400	4.10781300
H	-2.88263200	2.23994200	4.87318300
H	-2.48586400	3.91525300	4.44531600
H	-4.08044400	3.24854200	4.05069800
H	-5.02774500	2.14139100	1.84098500
H	-6.18792600	0.00000000	1.44848500
H	-5.02774500	-2.14139100	1.84098500
C	-2.46825900	-2.55958500	2.73320800
H	-1.39458300	-2.38032000	2.84839600
C	-2.62233500	-3.68811500	1.70013100
H	-2.16093100	-3.42623400	0.74419700
H	-3.67359600	-3.93770500	1.51569800
H	-2.13192200	-4.59595300	2.07086200
C	-3.01096500	-3.01382400	4.10781300
H	-2.88263200	-2.23994200	4.87318300
H	-2.48586400	-3.91525300	4.44531600
H	-4.08044400	-3.24854200	4.05069800
C	2.47114800	0.00000000	2.45106300
C	3.13075200	-1.24149600	2.32965400
C	4.48000300	-1.20987700	1.95086700
C	5.14125500	0.00000000	1.74147600
C	4.48000300	1.20987700	1.95086700
C	3.13075200	1.24149600	2.32965400
C	2.46825900	-2.55958500	2.73320800
H	1.39458300	-2.38032000	2.84839600
C	2.62233500	-3.68811500	1.70013100
H	2.16093100	-3.42623400	0.74419700
H	2.13192200	-4.59595300	2.07086200

H	3.67359600	-3.93770500	1.51569800
C	3.01096500	-3.01382400	4.10781300
H	2.88263200	-2.23994200	4.87318300
H	4.08044400	-3.24854200	4.05069800
H	2.48586400	-3.91525300	4.44531600
H	5.02774500	-2.14139100	1.84098500
H	6.18792600	0.00000000	1.44848500
H	5.02774500	2.14139100	1.84098500
C	2.46825900	2.55958500	2.73320800
H	1.39458300	2.38032000	2.84839600
C	2.62233500	3.68811500	1.70013100
H	2.16093100	3.42623400	0.74419700
H	3.67359600	3.93770500	1.51569800
H	2.13192200	4.59595300	2.07086200
C	3.01096500	3.01382400	4.10781300
H	2.88263200	2.23994200	4.87318300
H	2.48586400	3.91525300	4.44531600
H	4.08044400	3.24854200	4.05069800
Cu	0.00000000	0.00000000	0.00000000
N	0.00000000	-1.07456600	-2.82750400
C	0.00000000	0.00000000	-1.97534800
N	0.00000000	1.07456600	-2.82750400
C	0.00000000	0.67745000	-4.15628000
C	0.00000000	-0.67745000	-4.15628000
H	0.00000000	1.39150700	-4.96466200
H	0.00000000	-1.39150700	-4.96466200
C	0.00000000	-2.47114800	-2.45106300
C	1.24149600	-3.13075200	-2.32965400
C	1.20987700	-4.48000300	-1.95086700
C	0.00000000	-5.14125500	-1.74147600
C	-1.20987700	-4.48000300	-1.95086700
C	-1.24149600	-3.13075200	-2.32965400
C	2.55958500	-2.46825900	-2.73320800
H	2.38032000	-1.39458300	-2.84839600
C	3.68811500	-2.62233500	-1.70013100
H	3.42623400	-2.16093100	-0.74419700
H	4.59595300	-2.13192200	-2.07086200
H	3.93770500	-3.67359600	-1.51569800
C	3.01382400	-3.01096500	-4.10781300
H	2.23994200	-2.88263200	-4.87318300
H	3.24854200	-4.08044400	-4.05069800
H	3.91525300	-2.48586400	-4.44531600
H	2.14139100	-5.02774500	-1.84098500
H	0.00000000	-6.18792600	-1.44848500
H	-2.14139100	-5.02774500	-1.84098500
C	-2.55958500	-2.46825900	-2.73320800
H	-2.38032000	-1.39458300	-2.84839600
C	-3.68811500	-2.62233500	-1.70013100
H	-3.42623400	-2.16093100	-0.74419700
H	-3.93770500	-3.67359600	-1.51569800
H	-4.59595300	-2.13192200	-2.07086200
C	-3.01382400	-3.01096500	-4.10781300
H	-2.23994200	-2.88263200	-4.87318300
H	-3.91525300	-2.48586400	-4.44531600
H	-3.24854200	-4.08044400	-4.05069800
C	0.00000000	2.47114800	-2.45106300
C	-1.24149600	3.13075200	-2.32965400
C	-1.20987700	4.48000300	-1.95086700
C	0.00000000	5.14125500	-1.74147600
C	1.20987700	4.48000300	-1.95086700
C	1.24149600	3.13075200	-2.32965400
C	-2.55958500	2.46825900	-2.73320800
H	-2.38032000	1.39458300	-2.84839600
C	-3.68811500	2.62233500	-1.70013100
H	-3.42623400	2.16093100	-0.74419700
H	-4.59595300	2.13192200	-2.07086200
H	-3.93770500	3.67359600	-1.51569800
C	-3.01382400	3.01096500	-4.10781300
H	-2.23994200	2.88263200	-4.87318300
H	-3.24854200	4.08044400	-4.05069800
H	-3.91525300	2.48586400	-4.44531600
H	-2.14139100	5.02774500	-1.84098500
H	0.00000000	6.18792600	-1.44848500
H	2.14139100	5.02774500	-1.84098500
C	2.55958500	2.46825900	-2.73320800
H	2.38032000	1.39458300	-2.84839600
C	3.68811500	2.62233500	-1.70013100
H	3.42623400	2.16093100	-0.74419700
H	3.93770500	3.67359600	-1.51569800
H	4.59595300	2.13192200	-2.07086200
C	3.01382400	3.01096500	-4.10781300
H	2.23994200	2.88263200	-4.87318300
H	3.91525300	2.48586400	-4.44531600
H	3.24854200	4.08044400	-4.05069800

Thermal correction to Gibbs Free Energy= 1.046337
PCM energy (toluene) = -2517.97985885
PCM energy (DMF) = -2518.00000191

IPr-Cu-Cl

N	0.00000000	1.07744000	-1.02095300
C	0.00000000	0.00000000	-0.17944900
N	0.00000000	-1.07744000	-1.02095300
C	0.00000000	-0.67926700	-2.35278600
C	0.00000000	0.67926700	-2.35278600
H	0.00000000	-1.39282000	-3.16234100
H	0.00000000	1.39282000	-3.16234100
C	0.00000000	2.46046400	-0.59475100
C	-1.23804700	3.10830200	-0.40448300
C	-1.20739000	4.45421800	-0.01537400
C	0.00000000	5.12275100	0.17598200
C	1.20739000	4.45421800	-0.01537400
C	1.23804700	3.10830200	-0.40448300
C	-2.57886700	2.40291800	-0.58684200
H	-2.38219700	1.37310400	-0.90070900
C	-3.35943700	2.33155300	0.74186100
H	-2.77264000	1.83656000	1.52300300
H	-4.29083500	1.76869500	0.60372100
H	-3.62553100	3.33189000	1.10410700
C	-3.42566300	3.06265300	-1.69432500
H	-2.88739700	3.09155800	-2.64933500
H	-3.69829800	4.09238900	-1.43393900
H	-4.35589000	2.50130500	-1.84492700
H	-2.14194300	4.98384200	0.14727900
H	0.00000000	6.16577200	0.48218600
H	2.14194300	4.98384200	0.14727900
C	2.57886700	2.40291800	-0.58684200
H	2.38219700	1.37310400	-0.90070900
C	3.35943700	2.33155300	0.74186100
H	2.77264000	1.83656000	1.52300300
H	3.62553100	3.33189000	1.10410700
H	4.29083500	1.76869500	0.60372100
C	3.42566300	3.06265300	-1.69432500
H	2.88739700	3.09155800	-2.64933500
H	4.35589000	2.50130500	-1.84492700
H	3.69829800	4.09238900	-1.43393900
C	0.00000000	-2.46046400	-0.59475100
C	1.23804700	-3.10830200	-0.40448300
C	1.20739000	-4.45421800	-0.01537400
C	0.00000000	-5.12275100	0.17598200
C	-1.20739000	-4.45421800	-0.01537400
C	-1.23804700	-3.10830200	-0.40448300
C	2.57886700	-2.40291800	-0.58684200
H	2.38219700	-1.37310400	-0.90070900
C	3.35943700	-2.33155300	0.74186100
H	2.77264000	-1.83656000	1.52300300
H	4.29083500	-1.76869500	0.60372100
H	3.62553100	-3.33189000	1.10410700
C	3.42566300	-3.06265300	-1.69432500
H	2.88739700	-3.09155800	-2.64933500
H	3.69829800	-4.09238900	-1.43393900
H	4.35589000	-2.50130500	-1.84492700
H	2.14194300	-4.98384200	0.14727900
H	0.00000000	-6.16577200	0.48218600
H	-2.14194300	-4.98384200	0.14727900
C	-2.57886700	-2.40291800	-0.58684200
H	-2.38219700	-1.37310400	-0.90070900
C	-3.35943700	-2.33155300	0.74186100
H	-2.77264000	-1.83656000	1.52300300
H	-3.62553100	-3.33189000	1.10410700
H	-4.29083500	-1.76869500	0.60372100
C	-3.42566300	-3.06265300	-1.69432500
H	-2.88739700	-3.09155800	-2.64933500
H	-4.35589000	-2.50130500	-1.84492700
H	-3.69829800	-4.09238900	-1.43393900
Cu	0.00000000	0.00000000	1.71010300
Cl	0.00000000	0.00000000	3.83642000

Thermal correction to Gibbs Free Energy= 0.504570
PCM energy (toluene) = -1818.05714993
PCM energy (DMF) = -1818.06784999

IPr-Cu-I

N	0.00000000	1.07728400	-1.55044800
C	0.00000000	0.00000000	-0.70950800
N	0.00000000	-1.07728400	-1.55044800
C	0.00000000	-0.67931800	-2.88225900
C	0.00000000	0.67931800	-2.88225900
H	0.00000000	-1.39287300	-3.69183400
H	0.00000000	1.39287300	-3.69183400
C	0.00000000	2.46058000	-1.12438300
C	-1.23816300	3.10842400	-0.93471300
C	-1.20739400	4.45430400	-0.54550300
C	0.00000000	5.12269400	-0.35379900
C	1.20739400	4.45430400	-0.54550300
C	1.23816300	3.10842400	-0.93471300
C	-2.57924700	2.40436300	-1.12060100
H	-2.38280700	1.37179500	-1.42551600
C	-3.37018500	2.34453600	0.20242800
H	-2.79014900	1.85577400	0.99249400

H	-4.30075200	1.78104700	0.06153500
H	-3.63883800	3.34778800	0.55446900
C	-3.41614500	3.05826200	-2.23914200
H	-2.87129800	3.07774600	-3.19065100
H	-3.68639000	4.09104400	-1.98851500
H	-4.34741800	2.49919400	-2.39171600
H	-2.14191700	4.98404000	-0.38315100
H	0.00000000	6.16560500	-0.04728900
H	2.14191700	4.98404000	-0.38315100
C	2.57924700	2.40436300	-1.12060100
H	2.38280700	1.37179500	-1.42551600
C	3.37018500	2.34453600	0.20242800
H	2.79014900	1.85577400	0.99249400
H	3.63883800	3.34778800	0.55446900
H	4.30075200	1.78104700	0.06153500
C	3.41614500	3.05826200	-2.23914200
H	2.87129800	3.07774600	-3.19065100
H	4.34741800	2.49919400	-2.39171600
H	3.68639000	4.09104400	-1.98851500
C	0.00000000	-2.46058000	-1.12438300
C	1.23816300	-3.10842400	-0.93471300
C	1.20739400	-4.45430400	-0.54550300
C	0.00000000	-5.12269400	-0.35379900
C	-1.20739400	-4.45430400	-0.54550300
C	-1.23816300	-3.10842400	-0.93471300
C	2.57924700	-2.40436300	-1.12060100
H	2.38280700	-1.37179500	-1.42551600
C	3.37018500	-2.34453600	0.20242800
H	2.79014900	-1.85577400	0.99249400
H	4.30075200	-1.78104700	0.06153500
H	3.63883800	-3.34778800	0.55446900
C	3.41614500	-3.05826200	-2.23914200
H	2.87129800	-3.07774600	-3.19065100
H	3.68639000	-4.09104400	-1.98851500
H	4.34741800	-2.49919400	-2.39171600
H	2.14191700	-4.98404000	-0.38315100
H	0.00000000	-6.16560500	-0.04728900
H	-2.14191700	-4.98404000	-0.38315100
C	-2.57924700	-2.40436300	-1.12060100
H	-2.38280700	-1.37179500	-1.42551600
C	-3.37018500	-2.34453600	0.20242800
H	-2.79014900	-1.85577400	0.99249400
H	-3.63883800	-3.34778800	0.55446900
H	-4.30075200	-1.78104700	0.06153500
C	-3.41614500	-3.05826200	-2.23914200
H	-2.87129800	-3.07774600	-3.19065100
H	-4.34741800	-2.49919400	-2.39171600
H	-3.68639000	-4.09104400	-1.98851500
Cu	0.00000000	0.00000000	1.19561200
I	0.00000000	0.00000000	3.65054800

Thermal correction to Gibbs Free Energy= 0.502160
PCM energy (toluene) = -1369.24952503
PCM energy (DMF) = -1369.25873494

IMes-Cu-SPh

N	-2.10361700	-1.43450200	0.06035000
C	-0.80632500	-1.00758800	0.01371000
N	-0.07580000	-2.16169900	0.04937400
C	-0.90032500	-3.28132000	0.11672000
C	-2.17833800	-2.82281700	0.12350900
H	-0.50107200	-4.28352200	0.15261300
H	-3.12317300	-3.34293000	0.16676700
C	-3.25410900	-0.56128300	0.04624100
C	-3.76882800	-0.09670900	1.26840000
C	-4.89477300	0.73356900	1.22740200
C	-5.49853600	1.10522600	0.02018800
C	-4.95313900	0.61764600	-1.17334600
C	-3.82849100	-0.21549800	-1.18852000
C	-3.12318700	-0.45492500	2.58650400
H	-2.11326500	-0.03300900	2.65716700
H	-3.03089800	-1.53959800	2.71871200
H	-3.71019700	-0.06204200	3.42201800
H	-5.30472600	1.10427200	2.16468600
C	-6.68923700	2.03615700	0.00461100
H	-7.30223800	1.91913800	0.90500400
H	-7.32717400	1.85761500	-0.86782400
H	-6.36411400	3.08446300	-0.03606200
H	-5.40887500	0.89722700	-2.12102400
C	-3.24738500	-0.70162100	-2.49574700
H	-2.23772500	-0.30237200	-2.65076400
H	-3.86862900	-0.37915200	-3.33662900
H	-3.17177300	-1.79506700	-2.53160600
C	1.36673200	-2.22219400	0.01803900
C	2.01601300	-2.30190800	-1.22724000
C	3.41202000	-2.38267600	-1.22956600
C	4.15753500	-2.38147600	-0.04295900
C	3.47059200	-2.29806900	1.17261800
C	2.07301500	-2.21547800	1.23130600
C	1.24249900	-2.27839500	-2.52483500
H	0.72742200	-1.31950400	-2.65905000
H	0.47820500	-3.06388800	-2.56223900
H	1.91467800	-2.42062200	-3.37622600
H	3.93053300	-2.44011900	-2.18466400
C	5.66692500	-2.45284700	-0.08458300
H	6.01029000	-3.29043500	-0.70384900
H	6.08981000	-2.57782800	0.91745100
H	6.09272500	-1.53697700	-0.51434300
H	4.03342900	-2.28981400	2.10354900
C	1.36371500	-2.10292200	2.56066100
H	0.83277100	-1.14715800	2.64563300
H	2.08002100	-2.16364300	3.38534000
H	0.62128200	-2.89818900	2.69894200
Cu	-0.18447700	0.79433500	-0.07980600
S	0.33316600	2.89849600	-0.20251100
C	2.10133600	3.07419600	-0.06534900
C	2.99752300	1.99962000	0.09814200
C	4.37334100	2.21879300	0.20316400
C	4.89718400	3.51433900	0.14668300
C	4.01766600	4.59039800	-0.01735300
C	2.64243600	4.37515800	-0.12161100
H	2.61209500	0.98436900	0.14375100
H	5.03881000	1.36711400	0.33138500
H	5.96812300	3.68238500	0.22903300
H	4.40337400	5.60682700	-0.06422500
H	1.97022800	5.21995000	-0.24781700

Thermal correction to Gibbs Free Energy= 0.417988
PCM energy (toluene) = -1751.79766135
PCM energy (DMF) = -1751.80776551

$(IMes\text{-}Cu\text{-}SPh)_2$

N	4.40407100	0.90349900	0.03358800
C	3.43725600	-0.06801700	0.00915100
N	4.15724100	-1.23240000	-0.04044400
C	5.53025600	-0.98868500	-0.04741700
C	5.68488000	0.35776600	-0.00063300
H	6.25274700	-1.78985400	-0.08513600
H	6.57018100	0.97533300	0.01148300
Cu	1.54221400	0.32344700	0.03350700
S	0.04946100	0.97951400	1.75710800
C	-0.04936500	-0.23983300	3.05834300
C	-0.00029300	-1.62563300	2.81173800
C	-0.07697900	-2.54464000	3.86133300
C	-0.20571900	-2.10799700	5.18430500
C	-0.25645500	-0.73359700	5.44237600
C	-0.17891000	0.18783200	4.39487700
H	0.09774400	-1.97974300	1.78934800
H	-0.03582800	-3.60956500	3.64043200
H	-0.26430100	-2.82516900	5.99943200
H	-0.35496600	-0.37434600	6.46475900
H	-0.21569600	1.25374800	4.60485100
N	-4.24742200	1.44962100	-0.03449900
C	-3.41281100	0.36236500	-0.01008600
N	-4.27604400	-0.70071200	0.02789200
C	-5.60671100	-0.28332000	0.02789700
C	-5.58765700	1.07202200	-0.01163700
H	-6.42587200	-0.98576700	0.05633900
H	-6.38668000	1.79773700	-0.02536500
Cu	-1.48373700	0.51361200	-0.02110600
S	0.07991400	1.00010400	-1.73935000
C	0.01916200	-0.20631600	-3.05464500
C	0.17762100	0.22005100	-4.38851800
C	0.13419300	-0.69127300	-5.44676600
C	-0.06966300	-2.05396900	-5.20246300
C	-0.22855400	-2.48925000	-3.88232900
C	-0.18476700	-1.58038200	-2.82204500
H	0.33354600	1.27725100	-4.58767400
H	0.25871500	-0.33312800	-6.46670000
H	-0.10484700	-2.76312200	-6.02590400
H	-0.38760900	-3.54518500	-3.67195000
H	-0.30822800	-1.93350700	-1.80208600
C	-3.80569200	2.82270700	-0.08010700
C	-3.61074400	3.43274400	-1.33205700
C	-3.60610600	3.51277200	1.12678200
C	-3.21991300	4.77584300	-1.34901100
C	-3.21464900	4.85571800	1.05366900
C	-3.01631700	5.50363100	-0.16999600
H	-3.06305000	5.26192400	-2.31022400
H	-3.05447800	5.40380400	1.98006000
C	-3.88669300	-2.08780100	0.06567400
C	-3.76169000	-2.79027800	-1.14401800
C	-3.68279400	-2.70212500	1.31394500
C	-3.41625800	-4.14673600	-1.07812700
C	-3.33885800	-4.05873300	1.32388600
C	-3.20422400	-4.79814500	0.14188100
H	-3.31242300	-4.70455800	-2.00679600
H	-3.17259300	-4.54753400	2.28204300
C	3.59057500	-2.55680200	-0.08154000

C	3.37856500	-3.24137900	1.12709600
C	3.30989000	-3.13672800	-1.33051400
C	2.85897600	-4.54013700	1.05851600
C	2.79169900	-4.43747300	-1.34325600
C	2.55610400	-5.15303600	-0.16315900
H	2.69095400	-5.08499100	1.98560900
H	2.56922100	-4.90070200	-2.30259300
C	4.14175500	2.32149500	0.08873900
C	4.02424400	3.03793100	-1.11366500
C	4.03389400	2.94450600	1.34467900
C	3.80783800	4.41930000	-1.03170000
C	3.81754300	4.32649200	1.37052800
C	3.70082400	5.08053400	0.19636600
H	3.71321700	4.98838500	-1.95445500
H	3.73011800	4.82340200	2.33499600
C	-3.81868700	-1.92884000	2.60396400
H	-3.05568900	-1.14610500	2.67774400
H	-4.79720900	-1.43968900	2.68188600
H	-3.69938500	-2.59176500	3.46579100
C	-3.97980200	-2.11271600	-2.47634200
H	-4.96928900	-1.64363800	-2.53678700
H	-3.23554600	-1.32697500	-2.64732600
H	-3.89645900	-2.83441000	-3.29440600
C	-2.86554800	-6.27142200	0.18934600
H	-3.74426500	-6.87094700	0.46338800
H	-2.51188100	-6.63271300	-0.78231800
H	-2.08792700	-6.48035900	0.93347700
C	-3.76571500	2.83026000	2.46447900
H	-4.72060000	2.29828600	2.54669400
H	-2.96573000	2.09523800	2.61719400
H	-3.71259700	3.56064600	3.27803200
C	-3.77419000	2.66231000	-2.62048500
H	-2.96878300	1.92553500	-2.72983200
H	-4.72502700	2.11836900	-2.65988100
H	-3.73258900	3.33747200	-3.48101300
C	-2.56536200	6.94592700	-0.22343000
H	-1.49108400	7.01349500	-0.44188900
H	-3.09128900	7.50240200	-1.00819100
H	-2.74042400	7.45624700	0.72981600
C	3.55259900	-2.38830400	-2.61958400
H	2.90181800	-1.51018400	-2.69517300
H	4.58820400	-2.03514700	-2.69466900
H	3.34763000	-3.02886300	-3.48221600
C	3.69404200	-2.60400000	2.45974000
H	4.73922300	-2.27650300	2.51670400
H	3.06658500	-1.72309400	2.63522900
H	3.51475100	-3.30912400	3.27681200
C	1.96800000	-6.54558300	-0.20730700
H	2.28772000	-7.08793200	-1.10428500
H	2.26338400	-7.13390600	0.66856300
H	0.87011700	-6.50903700	-0.22246100
C	4.08670200	2.34753200	-2.45532400
H	4.96574100	1.69909300	-2.54692400
H	3.19871400	1.72085700	-2.60471600
H	4.12097700	3.08281800	-3.26546200
C	4.10667100	2.15263900	2.62845800
H	3.21614200	1.52172900	2.73950700
H	4.98219600	1.49380600	2.65942600
H	4.15471100	2.82298700	3.49239800
C	3.43579300	6.56789700	0.25879700
H	4.00644600	7.04416400	1.06463900
H	3.69993900	7.06215500	-0.68237700
H	2.37311200	6.76932200	0.45018500

Thermal correction to Gibbs Free Energy= 0.858038
PCM energy (toluene) = -3503.59482097
PCM energy (DMF) = -3503.60672611

IPr-Cu-SPh

N	2.09000600	0.85383700	0.05002500
C	0.74184900	0.62763400	0.02458700
N	0.19625200	1.88011300	0.07315900
C	1.18087900	2.86046900	0.12727200
C	2.37505900	2.21308500	0.11268800
H	0.93926900	3.91134900	0.17060000
H	3.38811700	2.58395200	0.14034900
C	3.10000900	-0.18191300	0.01564500
C	3.55833300	-0.71938500	1.23639900
C	4.55053500	-1.70703300	1.17272800
C	5.06166300	-2.13894700	-0.04941900
C	4.58641500	-1.59102700	-1.23912000
C	3.59495100	-0.60064100	-1.23691700
C	3.01198600	-0.28101700	2.59223900
H	2.25749600	0.49307900	2.42142900
C	2.30996900	-1.44647800	3.31910400
H	1.50475200	-1.87005700	2.70925900
H	1.87592400	-1.09604400	4.26366100
H	3.01393400	-2.25342000	3.55571700
C	4.11256600	0.34256600	3.47495800
H	4.59670100	1.19057100	2.97582300
H	4.89218700	-0.38760800	3.72311600
H	3.68313100	0.70270700	4.41782100
H	4.92284000	-2.14907000	2.09269500
H	5.82804700	-2.90945800	-0.07505300
H	4.98630400	-1.94319200	-2.18591000
C	3.08660900	-0.03493100	-2.56000400
H	2.33074200	0.72469800	-2.33774200
C	2.40002900	-1.12422500	-3.40963200
H	1.57742000	-1.59766300	-2.86298900
H	3.10730800	-1.91015200	-3.70091900
H	1.99262600	-0.68576800	-4.32897300
C	4.21204000	0.66068000	-3.35286800
H	4.68687800	1.45543200	-2.76507200
H	3.80838000	1.10962500	-4.26861600
H	4.99464700	-0.04836300	-3.64838500
C	-1.22271700	2.16171100	0.06948000
C	-1.87047800	2.35042400	-1.16925400
C	-3.24160700	2.63941200	-1.14120600
C	-3.93403700	2.73659800	0.06413900
C	-3.26662600	2.54379000	1.27208600
C	-1.89622300	2.25209200	1.30557000
C	-1.14603500	2.24314400	-2.50825500
H	-0.09344000	2.01973100	-2.30890100
C	-1.70337500	1.08405000	-3.35976100
H	-1.64076600	0.12989100	-2.82589500
H	-1.13269300	0.99202600	-4.29203100
H	-2.75353600	1.25124700	-3.62745500
C	-1.19000400	3.57450900	-3.28605900
H	-0.76892800	4.39868300	-2.69783400
H	-2.21646000	3.84882300	-3.55742100
H	-0.61267100	3.48966800	-4.21478100
H	-3.77574800	2.78339600	-2.07622800
H	-4.99822800	2.95846800	0.06189300
H	-3.82017400	2.61358700	2.20426500
C	-1.19977600	2.03669200	2.64638000
H	-0.14238300	1.83242300	2.45194400
C	-1.77045800	0.81007500	3.38727000
H	-1.69144700	-0.09672700	2.77835200
H	-2.82712200	0.95159200	3.64390200
H	-1.22013400	0.64350700	4.32144900
C	-1.26472300	3.29926200	3.53021400
H	-0.83553700	4.17024500	3.02050100
H	-0.70540000	3.13947500	4.46007400
H	-2.29736800	3.54776700	3.80295800
Cu	-0.14761400	-1.05882100	-0.05683000
S	-0.97841100	-3.06172700	-0.14826300
C	-2.75802800	-2.95693300	-0.12527400
C	-3.48319900	-1.74983500	-0.09096400
C	-4.88035600	-1.74874500	-0.07618100
C	-5.59539600	-2.95040800	-0.09592600
C	-4.88673200	-4.15669600	-0.13071000
C	-3.49095100	-4.16128400	-0.14507700
H	-2.94751000	-0.80426200	-0.07618700
H	-5.41035500	-0.79862600	-0.04944600
H	-6.68246800	-2.94750000	-0.08457300
H	-5.42321200	-5.10325000	-0.14658800
H	-2.95257400	-5.10515500	-0.17158000

Thermal correction to Gibbs Free Energy= 0.583996
PCM energy (toluene) = -1987.72487536
PCM energy (DMF) = -1987.73502547

$(IPr\text{-}Cu\text{-}SPh)_2$

N	4.53582500	0.41308900	-0.79662700
C	3.55089300	-0.05915100	0.03801400
N	4.25746100	-0.54869400	1.11092700
C	5.63031400	-0.38176600	0.94185600
C	5.80452800	0.21658100	-0.26067400
H	6.34154700	-0.70995900	1.68346100
H	6.69863100	0.52268100	-0.78064800
Cu	1.65284500	-0.04469300	-0.35874600
S	0.03556100	1.57414200	-1.04187900
C	0.06951200	3.21923300	-0.35209600
C	0.22655700	3.46241200	1.02513300
C	0.27873800	4.76679400	1.52268000
C	0.16939200	5.86310500	0.65989900
C	0.00314800	5.63460000	-0.71022900
C	-0.04491300	4.33057700	-1.21051700
H	0.30368600	2.61844400	1.70320100
H	0.40110900	4.92648600	2.59230600
H	0.21110500	6.87755900	1.04890000
H	-0.08473300	6.47489400	-1.39602500
H	-0.16249700	4.16011700	-2.27733500
N	-4.53582400	-0.41311100	-0.79661700
C	-3.55089100	0.05914100	0.03801700
N	-4.25745900	0.54868700	1.11092900
C	-5.63031100	0.38175000	0.94186400
C	-5.80452600	-0.21660700	-0.26066100
H	-6.34154400	0.70994300	1.68346900

H	-6.69862900	-0.52271600	-0.78062900
Cu	-1.65284700	0.04470700	-0.35875600
S	-0.03555500	-1.57413000	-1.04191900
C	-0.06951600	-3.21920400	-0.35209900
C	0.04490000	-4.33056800	-1.21049700
C	-0.00316700	-5.63458000	-0.71018100
C	-0.16940700	-5.86305600	0.65995200
C	-0.27874300	-4.76672700	1.52271000
C	-0.22655700	-3.46235500	1.02513600
H	0.16248100	-4.16013100	-2.27731900
H	0.08470700	-6.47488900	-1.39596000
H	-0.21112400	-6.87750100	1.04897400
H	-0.40111100	-4.92639500	2.59234000
H	-0.30367900	-2.61837200	1.70318700
C	-4.31773700	-1.06791100	-2.06791100
C	-4.42739600	-2.47391300	-2.12377400
C	-4.05518900	-0.27891200	-3.20822900
C	-4.24111100	-3.08784100	-3.36942000
C	-3.87317400	-0.94855800	-4.42576300
C	-3.96024200	-2.33655200	-4.50819100
H	-4.31092700	-4.16907300	-3.44727000
H	-3.66244700	-0.37471600	-5.32320100
C	-3.70157400	1.25283500	2.24437000
C	-3.13679800	0.51186300	3.30591500
C	-3.80427400	2.65977500	2.26975400
C	-2.65015200	1.23080300	4.40546600
C	-3.30544100	3.32548800	3.39857500
C	-2.73132000	2.62236900	4.45349400
H	-2.20469400	0.69759100	5.23927000
H	-3.36204600	4.40918200	3.44635900
C	3.70157600	-1.25282800	2.24437700
C	3.13680600	-0.51184200	3.30591600
C	3.80427200	-2.65976800	2.26977600
C	2.65016200	-1.23076900	4.40547600
C	3.30544200	-3.32546700	3.39860600
C	2.73132700	-2.62233500	4.45352000
H	2.20470900	-0.69754600	5.23927600
H	3.36204500	-4.40916000	3.44640300
C	4.31773600	1.06788300	-2.06792400
C	4.05519000	0.27887600	-3.20823800
C	4.42739300	2.47388500	-2.12379400
C	3.87317600	0.94851500	-4.42577600
C	4.24110700	3.08780500	-3.36944400
C	3.96024100	2.33650900	-4.50821100
H	3.66245000	0.37466800	-5.32321100
H	4.31092100	4.16903700	-3.44730000
C	-4.46412500	3.46280800	1.15037600
H	-4.64774100	2.78713800	0.30988300
C	-3.11260800	-1.01539000	3.30118500
H	-3.05594600	-1.34520800	2.25919500
C	-4.04040600	1.24765800	-3.16894100
H	-3.93758000	1.55955800	-2.12592700
C	-4.77972600	-3.32423000	-0.90487700
H	-4.70295700	-2.69088600	-0.01564600
C	4.46411700	-3.46281500	1.15040400
H	4.64773800	-2.78715400	0.30990600
C	3.11262300	1.01541100	3.30117000
H	3.05596200	1.34521900	2.25917800
C	4.04040800	-1.24769300	-3.16893900
H	3.93757200	-1.55958600	-2.12592400
C	4.77972000	3.32420900	-0.90490200
H	4.70294300	2.69087200	-0.01566700
H	3.81080300	2.83371300	-5.46360100
H	2.34626100	-3.15794800	5.31802000
H	-3.81080300	-2.83376200	-5.46357800
H	-2.34625200	3.15799400	5.31798700
C	3.56677100	-4.59836800	0.62545100
H	3.38887700	-5.36505700	1.38862300
H	2.59530200	-4.22348400	0.29377000
H	4.05294100	-5.09056000	-0.22604500
C	5.83003400	-4.02109800	1.60614700
H	6.50448300	-3.22685600	1.94706400
H	5.70884900	-4.73116700	2.43359800
H	6.32003400	-4.54980900	0.77917300
C	1.89442700	1.61170400	4.02715800
H	0.95479800	1.18516000	3.65998600
H	1.94122900	1.45225300	5.11157400
H	1.86205800	2.69441000	3.86104200
C	4.41750700	1.58147000	3.90504200
H	4.52378600	1.27793900	4.95441000
H	5.30205500	1.23161600	3.36190900
H	4.41109400	2.67799500	3.86756000
C	5.38031200	-1.80872100	-3.69466100
H	5.53374400	-1.53876100	-4.74719000
H	6.23299300	-1.42261800	-3.12316300
H	5.39063300	-2.90355800	-3.62202800
C	2.85323900	-1.86151300	-3.93334500
H	1.89834800	-1.48473900	-3.55445900
H	2.90880900	-1.66009800	-5.01031200
H	2.85757800	-2.95084400	-3.80491400
C	6.23613700	3.83124300	-0.99259100
H	6.95182600	3.00736600	-1.09734200
H	6.36841100	4.49601300	-1.85526000
H	6.49901300	4.39594500	-0.08931200
C	3.81299200	4.50460900	-0.70021900
H	2.77522800	4.16829300	-0.63460600
H	4.06017000	5.03106400	0.22980500
H	3.88195900	5.23448600	-1.51592900
C	-5.83004700	4.02108300	1.60611500
H	-6.50448800	3.22683900	1.94703900
H	-5.70886700	4.73116000	2.43355900
H	-6.32005200	4.54978300	0.77913600
C	-3.56678900	4.59836400	0.62541300
H	-4.05296500	5.09054500	-0.22608700
H	-3.38890200	5.36506100	1.38857800
H	-2.59531800	4.22348600	0.29373400
C	-4.41748900	-1.58145000	3.90506100
H	-4.52377100	-1.27790800	4.95442600
H	-5.30203900	-1.23160500	3.36192400
H	-4.41107100	-2.67797500	3.86759100
C	-1.89440900	-1.61167100	4.02717800
H	-0.95478200	-1.18512500	3.66000400
H	-1.94121300	-1.45221300	5.11159300
H	-1.86203400	-2.69437900	3.86107000
C	-5.38030600	1.80868300	-3.69467900
H	-5.53372800	1.53871700	-4.74720800
H	-6.23299100	1.42258400	-3.12318600
H	-5.39062700	2.90352000	-3.62205200
C	-2.85323100	1.86147200	-3.93334100
H	-1.89834200	1.48470200	-3.55444300
H	-2.90878900	1.66004700	-5.01030600
H	-2.85757200	2.95080400	-3.80492000
C	-6.23614000	-3.83127200	-0.99256900
H	-6.95183300	-3.00740000	-1.09733100
H	-6.36840600	-4.49605000	-1.85523300
H	-6.49901800	-4.39596800	-0.08928700
C	-3.81299200	-4.50462300	-0.70018000
H	-3.88195000	-5.23450500	-1.51588600
H	-2.77523100	-4.16830000	-0.63456300
H	-4.06017300	-5.03107300	0.22984600

Thermal correction to Gibbs Free Energy= 1.202594
PCM energy (toluene) = -3975.43572416
PCM energy (DMF) = -3975.44960318

SPh_2

S	0.00000000	0.00000000	1.62174200
C	0.00000000	1.41041100	0.51076700
C	-0.88103100	1.50394700	-0.57715600
C	-0.88846000	2.65175900	-1.37091500
C	-0.03939400	3.72418000	-1.07499700
C	0.82734600	3.63689400	0.01662600
C	0.85630500	2.48087000	0.80298300
H	-1.55462700	0.68194600	-0.80129900
H	-1.56982000	2.71321000	-2.21597600
H	-0.05470800	4.61909600	-1.69147400
H	1.49427200	4.46235500	0.25266200
H	1.54716800	2.40486300	1.63830400
C	0.00000000	-1.41041100	0.51076700
C	0.88103100	-1.50394700	-0.57715600
C	0.88846000	-2.65175900	-1.37091500
C	0.03939400	-3.72418000	-1.07499700
C	-0.82734600	-3.63689400	0.01662600
C	-0.85630500	-2.48087000	0.80298300
H	1.55462700	-0.68194600	-0.80129900
H	1.56982000	-2.71321000	-2.21597600
H	0.05470800	-4.61909600	-1.69147400
H	-1.49427200	-4.46235500	0.25266200
H	-1.54716800	-2.40486300	1.63830400

Thermal correction to Gibbs Free Energy= 0.143432
PCM energy (toluene) = -861.632140581
PCM energy (DMF) = -861.634442028

Iodobenzene

C	0.00000000	0.00000000	-0.58090600
C	0.00000000	1.21662000	-1.26484500
C	0.00000000	1.20860600	-2.66428800
C	0.00000000	0.00000000	-3.36585200
C	0.00000000	-1.20860600	-2.66428800
C	0.00000000	-1.21662000	-1.26484500
I	0.00000000	0.00000000	1.56855400
H	0.00000000	2.15720800	-0.72389000
H	0.00000000	2.15365200	-3.20149100
H	0.00000000	0.00000000	-4.45246000
H	0.00000000	-2.15365200	-3.20149100
H	0.00000000	-2.15720800	-0.72389000

Thermal correction to Gibbs Free Energy= 0.059017
PCM energy (toluene) = -243.120462749

PCM energy (DMF) = -243.121998052

OA: oxidative addition
RE: reductive elimination
σBM: σ-bond metathesis
TS: transition state
IM: intermediate

OA-TS: IMes-Cu-SPh/iodobenzene

N	1.27198300	-2.37337000	-0.95138700
C	0.15367300	-1.68469100	-0.56695300
N	-0.86861200	-2.54919800	-0.84966600
C	-0.39589800	-3.73970700	-1.39503400
C	0.95360100	-3.63020100	-1.45993100
H	-1.06322300	-4.53827500	-1.68148500
H	1.71151300	-4.31192500	-1.81473200
C	2.63426100	-1.91603500	-0.81011200
C	3.24252300	-1.22272000	-1.87204600
C	4.57709500	-0.83176900	-1.71033500
C	5.30131800	-1.11465700	-0.54579300
C	4.65820400	-1.81223700	0.48300200
C	3.32475500	-2.22781000	0.37374300
C	2.49481800	-0.88573400	-3.13958700
H	1.78246900	-0.06817900	-2.97206500
H	1.92537000	-1.74076900	-3.52053600
H	3.19161200	-0.56669000	-3.92109400
H	5.06151800	-0.28961500	-2.52026300
C	6.74828900	-0.69412300	-0.41876400
H	6.88098400	0.36366600	-0.67589200
H	7.38943700	-1.27352100	-1.09605400
H	7.12151800	-0.84386100	0.59973400
H	5.20555300	-2.04432900	1.39447700
C	2.66094900	-2.98095100	1.50421100
H	1.79872100	-2.43322500	1.90269200
H	3.36652200	-3.14233800	2.32490900
H	2.29323000	-3.96189400	1.17943600
C	-2.27391800	-2.32741100	-0.58713100
C	-2.79188200	-2.72217400	0.65947100
C	-4.15646500	-2.52090800	0.89381700
C	-4.99857000	-1.96032400	-0.07439500
C	-4.44922900	-1.62338000	-1.31591700
C	-3.08943300	-1.80218300	-1.60404400
C	-1.92079400	-3.36725900	1.71198000
H	-1.10257900	-2.70620600	2.01616700
H	-1.47117700	-4.30006500	1.34862300
H	-2.50940100	-3.60532700	2.60333600
H	-4.57058300	-2.81462700	1.85639700
C	-6.46130200	-1.71648500	0.21945700
H	-7.06312900	-1.73581500	-0.69569200
H	-6.60829000	-0.73339000	0.68701300
H	-6.86368400	-2.46792800	0.90811300
H	-5.09357200	-1.21074100	-2.08966000
C	-2.54296300	-1.43817600	-2.96254000
H	-1.90444800	-0.54799700	-2.89921900
H	-3.36060200	-1.22065100	-3.65708800
H	-1.94129600	-2.24801500	-3.39228100
Cu	0.06813900	0.25921500	0.05732000
S	-0.33862000	1.39834200	-1.90149600
C	-1.08824800	2.97859700	-1.60731200
C	-2.28872200	3.10468700	-0.87741200
C	-2.89515200	4.35074000	-0.70172100
C	-2.32417900	5.50199300	-1.25629700
C	-1.13529800	5.39049000	-1.98619000
C	-0.52159200	4.14708700	-2.15510800
H	-2.74459900	2.21342100	-0.45477500
H	-3.82074800	4.42092700	-0.13413400
H	-2.79992400	6.47056700	-1.12390200
H	-0.68025000	6.27684300	-2.42350800
H	0.40593800	4.06775700	-2.71539700
C	0.92158800	1.71997200	1.24060400
C	0.59363000	3.07897500	1.19704400
C	1.62651300	4.01552700	1.15833600
C	2.96629600	3.60685000	1.21045100
C	3.27311600	2.24913600	1.31397400
C	2.24942900	1.29404300	1.37048000
I	-0.67359300	0.36338800	2.60927700
H	-0.44034900	3.40171200	1.15534900
H	1.37792800	5.07127900	1.08520400
H	3.76218800	4.34672900	1.19062800
H	4.30730400	1.91941300	1.37651900
H	2.49628400	0.24579900	1.49686000

Thermal correction to Gibbs Free Energy= 0.500673

PCM energy (toluene) = -1994.87707465
PCM energy (DMF) = -1994.88501063

OA-TS: IPr-Cu-SPh/iodobenzene

N	2.21270000	0.45408600	1.06825400
C	1.00912000	0.80795300	0.51723700
N	0.94226800	2.16019500	0.73661700
C	2.07324400	2.62318800	1.40338200
C	2.87218600	1.55048600	1.61518100
H	2.19789200	3.66299700	1.65941700
H	3.83455900	1.46027100	2.09407000
C	2.79811500	-0.86928700	1.06098700
C	2.49718300	-1.75530300	2.11790700
C	3.12506300	-3.00875200	2.10318400
C	4.01388600	-3.36167300	1.08970800
C	4.29793400	-2.46290400	0.06335900
C	3.70036500	-1.19523000	0.02445300
C	1.57698300	-1.37241800	3.27463100
H	0.95675300	-0.53170300	2.95037300
C	0.61433900	-2.50294000	3.68131400
H	0.02968200	-2.85405800	2.82632300
H	-0.09253600	-2.12916600	4.43039900
H	1.14471200	-3.35505800	4.12444800
C	2.40678900	-0.90390300	4.49079000
H	3.05666800	-0.05734400	4.24024000
H	3.04284300	-1.71510500	4.86715200
H	1.74204700	-0.59007500	5.30482700
H	2.91513600	-3.71856500	2.89720700
H	4.48976500	-4.33928900	1.10161400
H	4.99702500	-2.74858800	-0.71737100
C	4.07479000	-0.21444000	-1.08538300
H	3.37247900	0.62389100	-1.04856300
C	3.96375400	-0.83304900	-2.49233500
H	2.95896000	-1.22307900	-2.68262300
H	4.68288200	-1.64761000	-2.63959600
H	4.17512600	-0.07007700	-3.25125400
C	5.49226500	0.35407600	-0.85612300
H	5.58038600	0.84220300	0.12127800
H	5.73601600	1.09470600	-1.62768200
H	6.24723900	-0.44053700	-0.90130200
C	-0.12513800	3.06031000	0.33537600
C	-0.08400900	3.61918800	-0.96249500
C	-1.10100100	4.51837800	-1.31026500
C	-2.10286400	4.86072100	-0.40482200
C	-2.10079300	4.31753700	0.87672900
C	-1.11232100	3.40983200	1.28336700
C	1.05138400	3.33401100	-1.94519200
H	1.44056600	2.33403500	-1.72842800
C	0.60390300	3.33521700	-3.41858400
H	-0.27551200	2.70314200	-3.57516600
H	1.41381700	2.95104500	-4.04971500
H	0.36917700	4.34571500	-3.77474700
C	2.20441700	4.34671500	-1.75727000
H	2.61005700	4.32550600	-0.74072400
H	1.85811800	5.36779600	-1.96069200
H	3.02472100	4.12357600	-2.45116600
H	-1.10947300	4.95913900	-2.30179400
H	-2.88443300	5.55736700	-0.69819100
H	-2.88274800	4.59951200	1.57436100
C	-1.10260600	2.89843300	2.72297700
H	-0.52808800	1.96739600	2.74584800
C	-2.50745900	2.57161700	3.26183600
H	-3.03968200	1.89189100	2.59201200
H	-3.11029100	3.47622700	3.41032800
H	-2.41851600	2.07725800	4.23636900
C	-0.41232000	3.91768600	3.65857400
H	0.61620900	4.13611800	3.35178200
H	-0.38134200	3.52919500	4.68414200
H	-0.96408700	4.86603300	3.67404500
Cu	-0.41047000	-0.47250500	-0.21269400
S	-1.93348500	-0.59350300	1.49806400
C	-3.55020800	-0.98099300	0.88109700
C	-4.15709800	-0.22337300	-0.14296700
C	-5.45160400	-0.51270600	-0.58089400
C	-6.17945200	-1.55874200	-0.00216100
C	-5.59223800	-2.31480500	1.01878100
C	-4.29368800	-2.03489100	1.45072900
H	-3.60442100	0.59948500	-0.58826900
H	-5.89512300	0.08646700	-1.37341600
H	-7.18897000	-1.77953600	-0.33990800
H	-6.14588700	-3.13093000	1.47858400
H	-3.83938700	-2.63235100	2.23640800
C	-0.77858700	-2.25678400	-1.21163400
C	-2.03910600	-2.85238000	-1.33011000
C	-2.16336800	-4.21481700	-1.06050700
C	-1.04032800	-4.98418900	-0.72562900
C	0.21883500	-4.38451800	-0.67196400
C	0.36710100	-3.01958400	-0.95333500

I	-0.39685500	-0.44215200	-2.86959800
H	-2.91141000	-2.26284500	-1.58804500
H	-3.14709700	-4.67454400	-1.11291200
H	-1.14767600	-6.04765000	-0.52879600
H	1.10162400	-4.97291900	-0.43421400
H	1.35534900	-2.57319500	-0.95254500

Thermal correction to Gibbs Free Energy= 0.668619
PCM energy (toluene) = -2230.79761463
PCM energy (DMF) = -2230.80534192

OA-IM: IMes-Cu-SPh/iodobenzene

N	1.74197300	-1.83404400	-1.09211500
C	0.53053400	-1.48761200	-0.55878300
N	-0.23937700	-2.60593700	-0.73150000
C	0.48279600	-3.62308000	-1.34974900
C	1.72625100	-3.13741900	-1.57877900
H	0.03994000	-4.58428700	-1.56066100
H	2.59552300	-3.58277100	-2.03751800
C	2.92534800	-1.00248300	-1.15990300
C	3.05495800	-0.07863200	-2.21206800
C	4.21571400	0.70605100	-2.24910400
C	5.23224100	0.57599200	-1.29744200
C	5.08792600	-0.40010600	-0.30421300
C	3.95099600	-1.21079200	-0.21812000
C	2.01485400	0.05936100	-3.29860700
H	1.11664200	0.57654000	-2.94374400
H	1.69482400	-0.91831300	-3.67799300
H	2.42035100	0.63004300	-4.14021900
H	4.32846100	1.42910600	-3.05457200
C	6.45430900	1.46459400	-1.33670200
H	6.34266800	2.31379800	-0.64905900
H	6.62136500	1.87349500	-2.33905600
H	7.35662000	0.92024600	-1.03579600
H	5.88178700	-0.53857000	0.42688600
C	3.86808000	-2.29417200	0.83094900
H	2.92577200	-2.25000700	1.38404400
H	4.68391000	-2.18897600	1.55241300
H	3.94925000	-3.29292600	0.38143200
C	-1.63172600	-2.77865200	-0.36926700
C	-1.95362400	-3.18097400	0.93922700
C	-3.30847900	-3.34983300	1.25360100
C	-4.32118000	-3.15938700	0.30759600
C	-3.94979400	-2.82633100	-1.00020900
C	-2.61218000	-2.64150000	-1.36959500
C	-0.89329300	-3.47536500	1.97218700
H	-0.34491100	-2.57544300	2.26863100
H	-0.15399300	-4.19239100	1.59372400
H	-1.34675800	-3.90441400	2.87111400
H	-3.57272600	-3.65279300	2.26476800
C	-5.77657700	-3.31113300	0.68696800
H	-6.38342900	-3.62969200	-0.16777200
H	-6.19034800	-2.35846600	1.04475800
H	-5.90756600	-4.04448600	1.49037300
H	-4.71984000	-2.71177800	-1.76052400
C	-2.25874100	-2.35056500	-2.80899100
H	-1.64447200	-1.45031000	-2.89881600
H	-3.16647000	-2.19733000	-3.40067300
H	-1.70383400	-3.18208200	-3.26277200
Cu	0.05036800	0.31985700	0.27079000
S	-1.18077600	0.87333700	-1.54009400
C	-2.29883500	2.24768600	-1.38504400
C	-3.60792900	2.03408800	-0.91618500
C	-4.53282500	3.07975600	-0.89971000
C	-4.16335300	4.35235200	-1.34807900
C	-2.86334000	4.57235800	-1.81541800
C	-1.93630900	3.52877500	-1.83545700
H	-3.89198100	1.04331800	-0.57303800
H	-5.54235100	2.90111200	-0.53678800
H	-4.88344800	5.16674800	-1.33391900
H	-2.56912200	5.55970800	-2.16310400
H	-0.92627600	3.69924800	-2.19462800
C	-0.20302900	2.15161400	0.89765300
C	-1.27889300	2.53072900	1.69853700
C	-1.36796300	3.85154700	2.15519300
C	-0.38802100	4.78706800	1.81072600
C	0.68529800	4.39642800	1.00552500
C	0.78104800	3.07627100	0.54463200
I	1.16118000	-0.10063500	2.59736500
H	-2.04161300	1.81232100	1.98509000
H	-2.20535400	4.14242100	2.78570100
H	-0.45994300	5.81139600	2.16801400
H	1.45603500	5.11432400	0.73224200
H	1.62675200	2.78565700	-0.07321200

Thermal correction to Gibbs Free Energy= 0.502000
PCM energy (toluene) = -1994.89200440
PCM energy (DMF) = -1994.90012182

OA-IM: IPr-Cu-SPh/iodobenzene

N	2.06904000	0.32002300	1.16851000
C	0.96301300	0.70188300	0.45561000
N	0.99809900	2.07076000	0.49143600
C	2.10714400	2.52293900	1.20052300
C	2.77253600	1.42685200	1.63268300
H	2.31069700	3.57385400	1.32677700
H	3.66708600	1.32593100	2.22527000
C	2.48177000	-1.03761600	1.48514500
C	1.87710500	-1.68521400	2.58730000
C	2.30591700	-2.98600800	2.88626700
C	3.30833600	-3.60523400	2.14414700
C	3.91949200	-2.92493200	1.09453500
C	3.53125500	-1.62480000	0.74138500
C	0.86952100	-0.99283300	3.50334000
H	0.38141100	-0.19524400	2.93739600
C	-0.24669200	-1.92522000	4.00611400
H	-0.74296900	-2.43674500	3.17628400
H	-1.00595300	-1.33656400	4.53318300
H	0.13046800	-2.67787300	4.70927100
C	1.59865600	-0.34268200	4.70145100
H	2.35508100	0.38025600	4.37608800
H	2.10177800	-1.10349600	5.31128900
H	0.88126200	0.18496700	5.34222900
H	1.85561000	-3.51745500	3.71845400
H	3.62221400	-4.61623800	2.39211000
H	4.71159200	-3.41278800	0.53590100
C	4.29001700	-0.88766200	-0.36131400
H	3.64331800	-0.09116800	-0.74233600
C	4.65289100	-1.78845400	-1.55750500
H	3.78179800	-2.33383700	-1.92916100
H	5.43810400	-2.51042500	-1.30129200
H	5.03673500	-1.17010200	-2.37735400
C	5.57966200	-0.24385100	0.19893800
H	5.37865900	0.45613100	1.01637900
H	6.10154600	0.30717600	-0.59321300
H	6.26238800	-1.01324500	0.58066900
C	0.02274000	3.00113800	-0.05673100
C	0.15162000	3.41101100	-1.40228300
C	-0.79435200	4.32361700	-1.89139000
C	-1.80153900	4.82987700	-1.07432900
C	-1.87055100	4.44960100	0.26361000
C	-0.95949400	3.53521500	0.80969200
C	1.31806400	2.97875500	-2.28739600
H	1.67996800	2.01118200	-1.92958600
C	0.93081300	2.78864000	-3.76456700
H	0.06947000	2.12265800	-3.87212100
H	1.76780700	2.33395200	-4.30583500
H	0.70190400	3.74201700	-4.25683300
C	2.47881800	3.99358900	-2.17376000
H	2.83016000	4.10200600	-1.14153500
H	2.16814800	4.98455900	-2.52840400
H	3.32878800	3.66588700	-2.78506600
H	-0.73476100	4.64900800	-2.92478400
H	-2.52495600	5.53489000	-1.47679900
H	-2.64531100	4.87105600	0.89636100
C	-1.01381300	3.22691400	2.30566000
H	-0.48175300	2.28637200	2.47801200
C	-2.44545800	3.04300500	2.84337300
H	-3.00340400	2.31095200	2.25428400
H	-3.00422600	3.98677100	2.85009400
H	-2.40560300	2.68500200	3.87912400
C	-0.30221300	4.33688900	3.11384200
H	0.74010500	4.47259600	2.80720500
H	-0.30912600	4.09180300	4.18323100
H	-0.81433300	5.29846800	2.98487000
Cu	-0.37980600	-0.54762500	-0.43678700
S	-1.91082700	-0.14276300	1.16164700
C	-3.59419700	-0.56980500	0.77487900
C	-4.39793600	0.32495100	0.04477100
C	-5.75043100	0.05056900	-0.16668300
C	-6.31917400	-1.12002300	0.34645700
C	-5.52655500	-2.01469600	1.07309300
C	-4.17371100	-1.74362300	1.28658700
H	-3.95445700	1.23485700	-0.34987000
H	-6.36049700	0.75143400	-0.73177700
H	-7.37227100	-1.33354300	0.18115000
H	-5.96126900	-2.92825400	1.47154600
H	-3.55651600	-2.44091600	1.84451800
C	-1.54497500	-1.97527800	-1.07959300
C	-2.53070000	-1.78199700	-2.04565400
C	-3.28331300	-2.87481200	-2.49295900
C	-3.05171700	-4.15297100	-1.97602200
C	-2.06210600	-4.33546000	-1.00652300
C	-1.30567700	-3.24569400	-0.55318900
I	1.01405100	-0.94502300	-2.59465500
H	-2.71359900	-0.79775500	-2.46698400
H	-4.04689100	-2.72125500	-3.25237100
H	-3.63717000	-4.99932400	-2.32674300
H	-1.87076500	-5.32509000	-0.59656500

H	-0.53594700	-3.40588900	0.19744600

Thermal correction to Gibbs Free Energy= 0.671223
PCM energy (toluene) = -2230.81195233
PCM energy (DMF) = -2230.81974692

RE-TS: IMes-Cu-SPh/iodobenzene

N	1.32900400	-2.27913600	-0.89040900
C	0.20345600	-1.59635700	-0.52018100
N	-0.80465200	-2.49809700	-0.72060200
C	-0.31338600	-3.71059700	-1.19962000
C	1.03045800	-3.57407500	-1.30671500
H	-0.96699500	-4.54217800	-1.41448400
H	1.79690800	-4.26060200	-1.63266600
C	2.67217400	-1.74714900	-0.89076200
C	3.15189000	-1.12735500	-2.05741600
C	4.46471600	-0.63686000	-2.04353600
C	5.28987800	-0.76183500	-0.92053400
C	4.77676300	-1.40521900	0.21304200
C	3.47329100	-1.91297000	0.25463500
C	2.29858600	-0.99457200	-3.29789300
H	1.40334300	-0.39064700	-3.11427100
H	1.95828500	-1.97196700	-3.66138000
H	2.86479600	-0.51599600	-4.10258500
H	4.84867500	-0.14787300	-2.93643100
C	6.70846700	-0.23860000	-0.93111900
H	6.91484000	0.34131400	-1.83660100
H	7.43403200	-1.06141700	-0.88916100
H	6.90209500	0.40622700	-0.06539700
H	5.40656400	-1.51672900	1.09354200
C	2.95919900	-2.61063100	1.49066700
H	2.15483000	-2.03808500	1.96773600
H	3.76358600	-2.73468400	2.22208800
H	2.55720600	-3.60417000	1.25821800
C	-2.21829900	-2.28116500	-0.49903500
C	-2.79387800	-2.72636000	0.70570100
C	-4.16679400	-2.52224000	0.88370900
C	-4.96279000	-1.91647700	-0.09627100
C	-4.35830900	-1.53800900	-1.29953400
C	-2.98827800	-1.72019200	-1.53238600
C	-1.98111700	-3.42554200	1.76837200
H	-1.18086400	-2.78006900	2.14531000
H	-1.51853800	-4.34385300	1.38473600
H	-2.61709100	-3.70048200	2.61539200
H	-4.62430500	-2.84978600	1.81512100
C	-6.43686100	-1.68189100	0.14413600
H	-6.96990900	-1.48647000	-0.79242600
H	-6.59537900	-0.81662200	0.80171200
H	-6.90657700	-2.54575600	0.62885700
H	-4.96616700	-1.09767000	-2.08735500
C	-2.38605500	-1.34899700	-2.86650400
H	-1.66941900	-0.52613100	-2.76703500
H	-3.16811700	-1.03361000	-3.56419100
H	-1.85391100	-2.19569300	-3.31783800
Cu	0.20882400	0.34372900	0.16723400
S	-0.23112800	1.53038600	-1.71091700
C	-1.50914300	2.72839100	-1.40696500
C	-2.69345700	2.38983400	-0.72804700
C	-3.70684200	3.33751700	-0.56944100
C	-3.56092400	4.62397800	-1.09980900
C	-2.38758400	4.96343700	-1.78151600
C	-1.36125800	4.02734900	-1.92473600
H	-2.81715300	1.38757500	-0.32853600
H	-4.61427300	3.06687500	-0.03525600
H	-4.35460100	5.35703800	-0.98029400
H	-2.26388400	5.96309700	-2.19082000
H	-0.43907500	4.29613300	-2.43165000
C	0.97380100	2.15831700	0.43239800
C	0.36084700	3.19389500	1.13417000
C	1.15264200	4.22012700	1.65835200
C	2.53920300	4.21851100	1.46621900
C	3.13404600	3.18731500	0.73613100
C	2.34894000	2.16158000	0.19114900
I	-0.09309700	-0.07302900	2.75108300
H	-0.71000700	3.19333800	1.30849200
H	0.68021600	5.01513400	2.23074100
H	3.14798700	5.02085500	1.87517700
H	4.20817700	3.18279400	0.56457600
H	2.82026800	1.38802300	-0.40875200

Thermal correction to Gibbs Free Energy= 0.501471
PCM energy (toluene) = -1994.89002473
PCM energy (DMF) = -1994.89888036

RE-TS: IPr-Cu-SPh/iodobenzene

N	-1.85257700	-1.33816600	0.85087000
C	-0.57981000	-1.09497200	0.40816600
N	0.04407400	-2.30878500	0.52388600
C	-0.82506900	-3.27632500	1.02272700
C	-2.01629900	-2.66733700	1.22969700
H	-0.51127900	-4.29526300	1.18222500
H	-2.95314300	-3.04373100	1.60886500
C	-2.90175000	-0.35181500	1.01975200
C	-2.99335000	0.31942700	2.26007300
C	-4.04159000	1.23609900	2.42275500
C	-4.96081900	1.46780000	1.40203400
C	-4.85487500	0.77916800	0.19560200
C	-3.82933600	-0.15080300	-0.02630900
C	-2.04837200	0.03710700	3.42694500
H	-1.17572300	-0.49590700	3.03732300
C	-1.52780200	1.31776000	4.10744500
H	-1.04662300	1.99042400	3.39086000
H	-0.78459800	1.05536100	4.86980800
H	-2.33069800	1.86825600	4.61212900
C	-2.73029700	-0.88230900	4.46435300
H	-3.06154100	-1.82562600	4.01558200
H	-3.60929400	-0.39341600	4.90240900
H	-2.03518900	-1.12053300	5.27888400
H	-4.14176800	1.77197600	3.36193300
H	-5.76517200	2.18456800	1.54853100
H	-5.58029600	0.96830500	-0.58897100
C	-3.77846200	-0.93982000	-1.33237300
H	-2.74873600	-1.27865400	-1.48121400
C	-4.15098500	-0.09694400	-2.56546700
H	-3.55479200	0.81829200	-2.62017300
H	-5.21490400	0.17126000	-2.57445100
H	-3.95128100	-0.67412800	-3.47508800
C	-4.68850900	-2.18620700	-1.24921500
H	-4.40857300	-2.84735900	-0.42152000
H	-4.62180900	-2.76514100	-2.17849200
H	-5.73704500	-1.89530700	-1.10647400
C	1.43986300	-2.61045800	0.25201000
C	1.79111100	-3.14607300	-1.00737200
C	3.14078400	-3.46525100	-1.21640400
C	4.09320700	-3.27782100	-0.21842300
C	3.71203100	-2.78065300	1.02558700
C	2.37865700	-2.44472800	1.29684800
C	0.76323900	-3.44922000	-2.09591900
H	-0.09313700	-2.78480600	-1.94610600
C	1.28874200	-3.18758700	-3.51929900
H	1.71472800	-2.18488400	-3.61102800
H	0.46035000	-3.26116200	-4.23290600
H	2.04438300	-3.92446900	-3.81943600
C	0.27093200	-4.91101100	-1.98866200
H	-0.17992400	-5.12867700	-1.01470300
H	1.10122400	-5.61295800	-2.13769000
H	-0.48369700	-5.11226000	-2.75907500
H	3.44938200	-3.86664400	-2.17607200
H	5.13436400	-3.52834700	-0.40708200
H	4.46224000	-2.65397700	1.79943900
C	1.98150400	-1.99916500	2.70355500
H	1.06380200	-1.40889500	2.62289900
C	3.03343700	-1.10500300	3.38532300
H	3.32805500	-0.26854200	2.74578500
H	3.93441900	-1.66776000	3.65867000
H	2.61851500	-0.69154700	4.31214700
C	1.68719200	-3.22522300	3.59833100
H	0.89067900	-3.85449000	3.18801300
H	1.37673000	-2.90004100	4.59928500
H	2.58394300	-3.84771300	3.70873400
Cu	0.07074300	0.72657500	-0.28614800
S	1.27850900	1.52346400	1.44380400
C	2.82500700	2.18091200	0.86319800
C	3.63849700	1.46600900	-0.03461300
C	4.88133400	1.97630400	-0.41548700
C	5.33592000	3.19214900	0.10667400
C	4.53415800	3.90352300	1.00561300
C	3.28113100	3.40920600	1.37395500
H	3.29539800	0.51439100	-0.42978900
H	5.49715400	1.41832000	-1.11647400
H	6.30679000	3.58326600	-0.18662500
H	4.87785700	4.85210000	1.41088800
H	2.64627100	3.97187300	2.05222100
C	0.01370700	2.70329600	-0.43321700
C	0.83409800	3.48166800	-1.24641000
C	0.40236300	4.75642800	-1.62480400
C	-0.82904500	5.25246300	-1.18039000
C	-1.62758700	4.46968000	-0.34423300
C	-1.19748900	3.19627800	0.05601300
I	-0.19576200	0.35295200	-2.87167100
H	1.77934400	3.09812600	-1.61577200
H	1.02876800	5.35534400	-2.28190700
H	-1.15715800	6.24520600	-1.47776000
H	-2.57984700	4.84773400	0.02105500
H	-1.81374200	2.61421600	0.73541700

Thermal correction to Gibbs Free Energy= 0.671188
PCM energy (toluene) = -2230.81018289
PCM energy (DMF) = -2230.81866615

σBM-TS: IMes-Cu-SPh/iodobenzene

N	-2.90931300	1.45305400	0.12017200
C	-1.54706800	1.43914400	0.01720700
N	-1.22654400	2.72627100	-0.31063100
C	-2.36424100	3.52272200	-0.40991800
C	-3.42448700	2.71994800	-0.13808400
H	-2.30781800	4.57047000	-0.66310700
H	-4.48395600	2.92337500	-0.10369800
C	-3.72070200	0.30713500	0.46009500
C	-4.28170900	-0.45893400	-0.57607000
C	-5.07933600	-1.55184600	-0.21774300
C	-5.31728200	-1.89027800	1.11969600
C	-4.74262800	-1.09591600	2.11876800
C	-3.93854500	0.00918300	1.81585200
C	-4.02189400	-0.13893700	-2.02933500
H	-2.96118200	-0.26839500	-2.27606800
H	-4.29243500	0.89393900	-2.27942100
H	-4.59885200	-0.80470700	-2.67807400
H	-5.51814300	-2.15822700	-1.00748300
C	-6.14931900	-3.10127900	1.47486900
H	-6.93223500	-3.28294100	0.73029300
H	-6.62900100	-2.98622100	2.45297400
H	-5.52528900	-4.00404600	1.51966500
H	-4.91971700	-1.34222500	3.16376900
C	-3.31710500	0.83350500	2.91913600
H	-2.22607000	0.72197500	2.92764500
H	-3.69475000	0.51603100	3.89579200
H	-3.53230500	1.90254000	2.80390600
C	0.11708800	3.21407600	-0.51399100
C	0.81316300	3.75149000	0.58316400
C	2.10667000	4.23755100	0.36046400
C	2.70541800	4.19755600	-0.90521100
C	1.97214300	3.66197200	-1.97017000
C	0.67415600	3.16222700	-1.80295000
C	0.19904700	3.79842100	1.96318900
H	-0.01861500	2.79060700	2.33609200
H	-0.74534600	4.35603000	1.97233300
H	0.88007900	4.27944200	2.67161600
H	2.65851600	4.65886100	1.19858000
C	4.11679900	4.69003800	-1.10981700
H	4.35200900	5.52499200	-0.42944300
H	4.27356000	5.04790800	-2.13621400
H	4.84758600	3.90120700	-0.92033100
H	2.41912900	3.62865900	-2.96166400
C	-0.08066600	2.57636300	-2.97259500
H	-0.18986400	1.49001700	-2.86713800
H	0.45276300	2.76826100	-3.90848500
H	-1.08808300	2.99886400	-3.06363000
Cu	-0.37647800	-0.05934000	0.28125500
S	0.86928000	-1.67624400	1.17308000
C	2.14200300	-1.05487300	2.24153900
C	2.60404500	0.27377200	2.18279400
C	3.63548200	0.70497700	3.01993300
C	4.23449600	-0.18137800	3.92100600
C	3.79025900	-1.50716400	3.97805500
C	2.75507000	-1.94125100	3.14882500
H	2.14899500	0.96592300	1.47974500
H	3.97645100	1.73638300	2.96212200
H	5.03914700	0.15584900	4.56948700
H	4.25019700	-2.20639300	4.67250000
H	2.41033900	-2.97031100	3.19880900
C	2.13223700	-2.44721000	-0.80821400
C	3.20862200	-1.59478100	-1.03689900
C	4.48390700	-2.15833900	-1.16941100
C	4.67096500	-3.54146800	-1.08446700
C	3.56438100	-4.36826000	-0.86204100
C	2.27882600	-3.83010500	-0.72679100
I	0.06448700	-1.77534200	-2.18493200
H	3.06989500	-0.52172700	-1.11053100
H	5.33186700	-1.49924400	-1.34408100
H	5.66384500	-3.96942000	-1.19206200
H	3.68985200	-5.44699500	-0.79413900
H	1.42325500	-4.47423900	-0.55613400

Thermal correction to Gibbs Free Energy= 0.496844

PCM energy (toluene) = -1994.86914840

PCM energy (DMF) = -1994.87793612

σBM-TS: IPr-Cu-SPh/iodobenzene

N	2.83143400	-0.18727500	-0.43063500
C	1.68783100	0.45368700	-0.03351900
N	2.13673000	1.66032000	0.43226900
C	3.52009900	1.76579800	0.32488900
C	3.95669000	0.60345700	-0.22162100
H	4.05243800	2.64941600	0.64100600
H	4.94812800	0.26635800	-0.48076000
C	2.88529800	-1.50877300	-1.01890800
C	3.19644400	-2.60652100	-0.18750500
C	3.27046600	-3.86953300	-0.78963200
C	3.04360900	-4.03292500	-2.15482100
C	2.74517800	-2.92983200	-2.95124300
C	2.66328400	-1.64094800	-2.40616100
C	3.48876400	-2.45311000	1.30339600
H	3.13608900	-1.46480200	1.61591100
C	2.74883400	-3.49070800	2.16885800
H	1.67195600	-3.48006900	1.97458600
H	2.90496600	-3.26642900	3.23101600
H	3.11958600	-4.50787600	1.99395800
C	5.00854400	-2.51500800	1.57281800
H	5.55583700	-1.75105500	1.00849400
H	5.41616100	-3.49334900	1.28957200
H	5.21395000	-2.36003100	2.63925500
H	3.50253200	-4.73836000	-0.18103300
H	3.10011900	-5.02359400	-2.59902200
H	2.57512900	-3.07052800	-4.01481500
C	2.39165400	-0.44918000	-3.32097700
H	2.22795300	0.43143100	-2.69313700
C	1.12087100	-0.63518300	-4.17243400
H	0.24150800	-0.81496200	-3.54557200
H	1.21968200	-1.47222500	-4.87416500
H	0.93398800	0.26879700	-4.76499000
C	3.61643700	-0.15772100	-4.21481400
H	4.51833700	0.02233600	-3.61749100
H	3.43470700	0.73055800	-4.83244500
H	3.82478800	-0.99790600	-4.88859000
C	1.29603800	2.72953400	0.92401200
C	0.88651200	3.73017700	0.01709600
C	0.10213700	4.77620400	0.52228600
C	-0.25585800	4.82329100	1.86797200
C	0.16776300	3.82276200	2.74122900
C	0.95555400	2.75333600	2.29345500
C	1.29110000	3.72706500	-1.45527000
H	1.78403300	2.77408200	-1.66939700
C	0.07849600	3.82907200	-2.40067000
H	-0.64712200	3.03233000	-2.21129100
H	0.41136400	3.74875900	-3.44273200
H	-0.44068000	4.78915300	-2.29520800
C	2.30998700	4.84931100	-1.74837400
H	3.20065700	4.76329200	-1.11460800
H	1.87081600	5.83909000	-1.57317700
H	2.63324000	4.80632700	-2.79573200
H	-0.23443800	5.56233500	-0.14764600
H	-0.86563800	5.64352700	2.23885600
H	-0.11642800	3.87469600	3.78799400
C	1.45761000	1.70423200	3.28241100
H	1.82693200	0.84909800	2.70827000
C	0.34882700	1.17481600	4.21085200
H	-0.49327600	0.77192200	3.63966100
H	-0.02875800	1.95311600	4.88498800
H	0.74431200	0.36569000	4.83615300
C	2.64031800	2.25947600	4.10616700
H	3.46307800	2.59115200	3.46173600
H	3.02921300	1.48842400	4.78259500
H	2.32699700	3.11618900	4.71579000
Cu	-0.12273600	-0.19893000	-0.16769200
S	-2.02702300	-0.52440800	-1.34823200
C	-3.04283100	0.92560400	-1.41160800
C	-2.90209800	1.99155500	-0.50167600
C	-3.75972900	3.09268200	-0.55805800
C	-4.77980900	3.14855600	-1.51323300
C	-4.93456900	2.08951300	-2.41517200
C	-4.07763800	0.98911600	-2.36621400
H	-2.11415800	1.95544500	0.24536400
H	-3.63013000	3.90674000	0.15145300
H	-5.44773300	4.00531700	-1.55344000
H	-5.72623000	2.11961600	-3.16025300
H	-4.20142700	0.16840500	-3.06716800
C	-3.34658800	-1.93910500	0.25474900
C	-4.34185000	-1.16789600	0.84203900
C	-5.66117900	-1.63838200	0.78684800
C	-5.96313800	-2.85633500	0.17096900
C	-4.93118500	-3.61111300	-0.39858500
C	-3.60555600	-3.16299500	-0.35573200
I	-1.20524300	-2.01618800	1.70409900
H	-4.11372700	-0.22297000	1.32334300
H	-6.44965200	-1.04025700	1.23882300
H	-6.98812700	-3.21547100	0.13792000
H	-5.14827500	-4.56120600	-0.88245400
H	-2.80818700	-3.75023400	-0.79843300

Thermal correction to Gibbs Free Energy= 0.664407

PCM energy (toluene) = -2230.79230552

PCM energy (DMF) = -2230.80056161