Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting information

for

Reaching strong absorption up to 700 nm with new benzo[g]quinoxaline-based heteroleptic copper(I) complexes for light-harvesting applications

Cecilia Bruschi,[a] Xin Gui, [b] Olaf Fuhr, [c,d] Wim Klopper[b,c] and Claudia Bizzarri*[a]

Table of contents

1. Experimental procedures

Photoluminescence measurements in solution

UV/Vis absorption spectra were recorded for all the compounds in a solution of CH_2Cl_2 (concentrations ~10^{-5}M). The instrument used was a Lambda 750 double-beam UV/Vis-NIR spectrometer. Emission and excitation spectra at 298 K were recorded with a Fluoromax 4 from Horiba Jobin. The copper complex solutions were air-free by letting Ar bubbling inside for 10 minutes at least. Lifetime experiments were performed by time-correlated singlephoton counting method (TCSPC) with a DeltaTime kit for DeltaDiode source on FluoroMax systems, including DeltaHub and DeltaDiode controller. NanoLED 370 was used as the excitation source (l=366 nm).

Electrochemistry

Cyclic voltammetry experiments were performed with a Gamry Interface 1010B in a three electrodes electrochemical cell. The electrochemical cell was equipped with a GC-disc working electrode, $Ag/AgNO_3$ reference electrode and a Pt wire as the auxiliary electrode. All the experiments were performed in acetonitrile (0.1 M $TBAPF_6$) solution, under Ar atmosphere, unless otherwise specified. Ferrocene (Fc) was added after each experiment as an internal standard, according to IUPAC recommendation. The redox properties are reported versus Fc/Fc+ couple.

2. Experimental procedures ^{1}H, ^{13}C NMR of 1-10

2-(bromomethyl)-3-methylbenzo[g]quinoxaline (7)

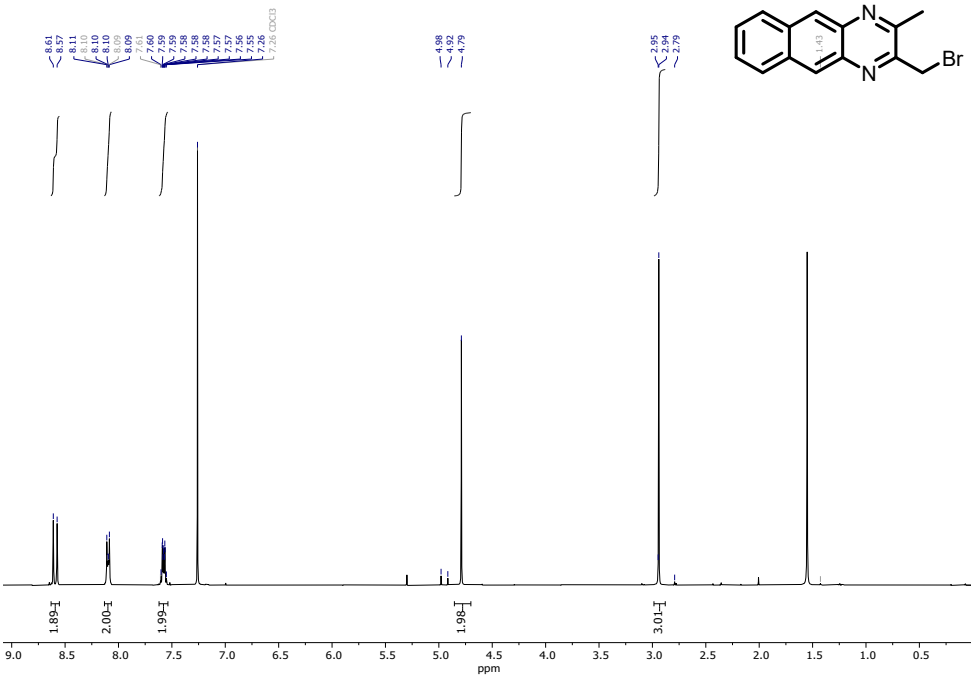


Figure S2.1 ^{1}H NMR of **7** in $CDCl_3$. (Solvent residuals: 1.55 ppm (water)).

2,3-bis(bromomethyl)benzo[g]quinoxaline (8)

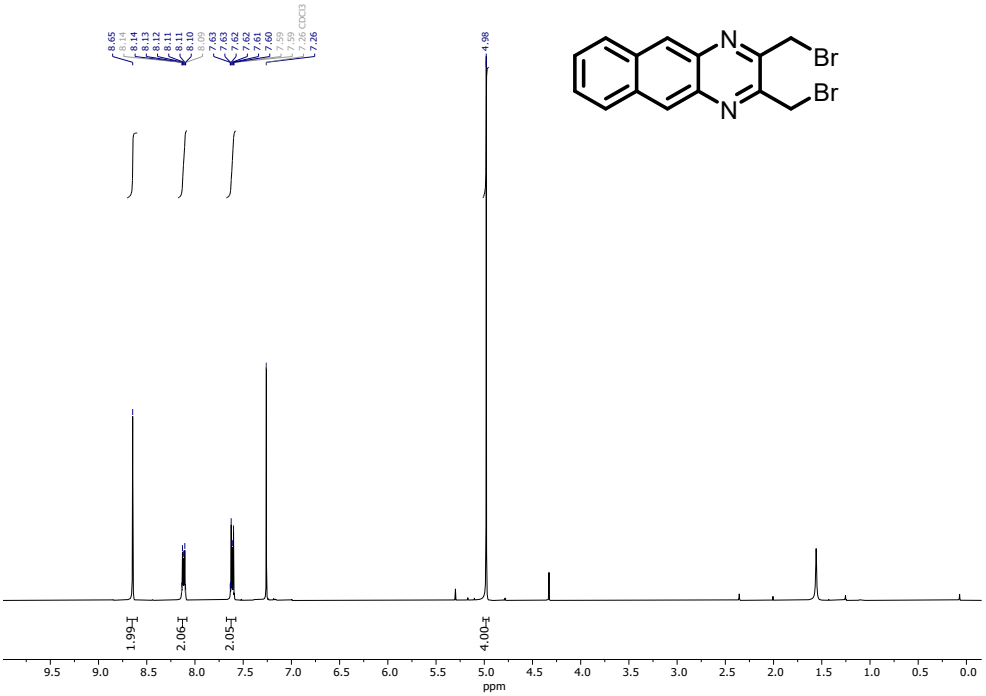


Figure S2.2 ^{1}H NMR of **8** in $CDCl_3$. (Solvent residuals: 1.55 ppm (water)).

2-methyl-3-((4'-phenyl-1'*H*-1',2',3'-triazol-1'-yl)methyl)benzo[g]quinoxaline (4)

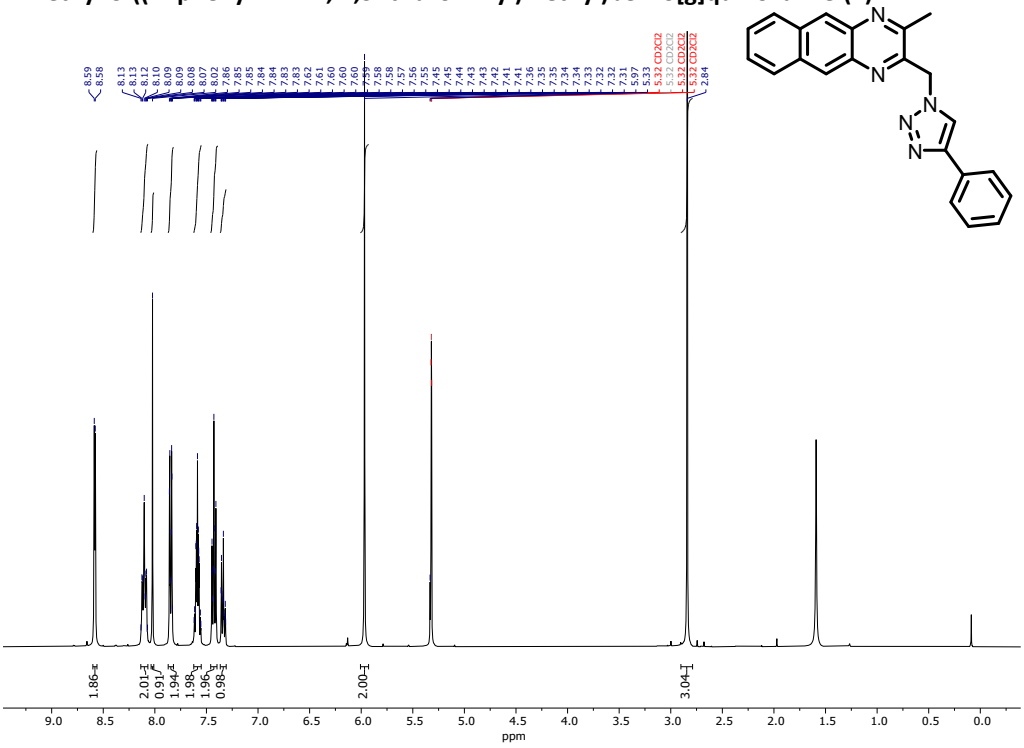


Figure S2.3 ^{1}H NMR of **4** in $CDCl_3$. (Solvent residuals: 1.55 ppm (water)).

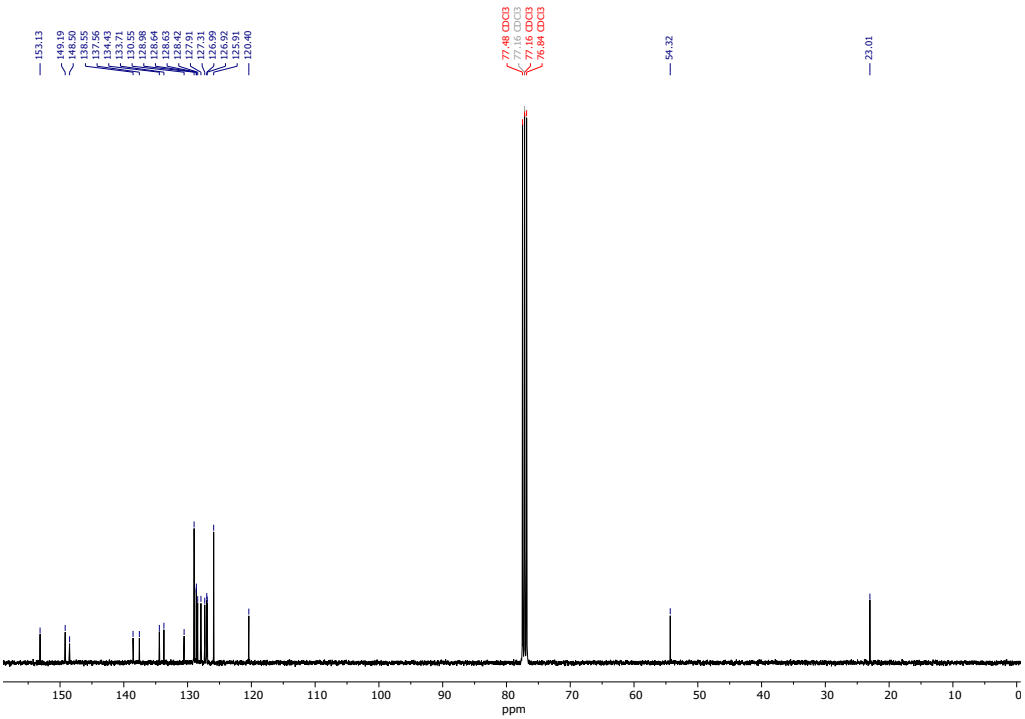
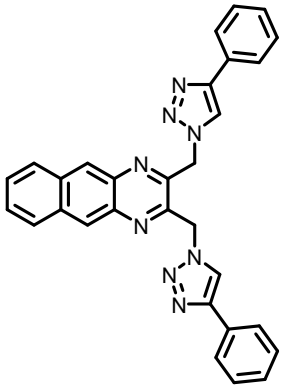


Figure S2.4 ^{13}C NMR of **4** in $CDCl_3$.

2,3-bis((4'-phenyl-1'*H*-1',2',3'-triazol-1'-yl)methyl)benzo[g]quinoxaline (5)



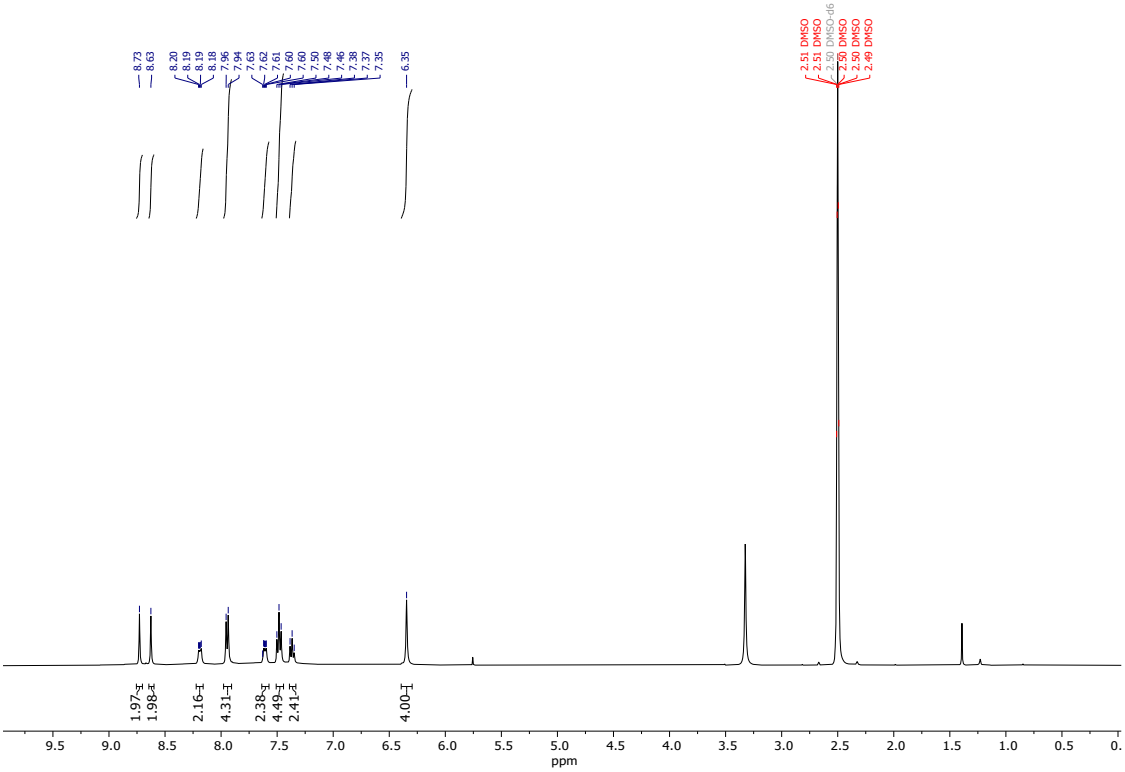


Figure S2.5 ^{1}H NMR of **5** in C_2D_6OS.

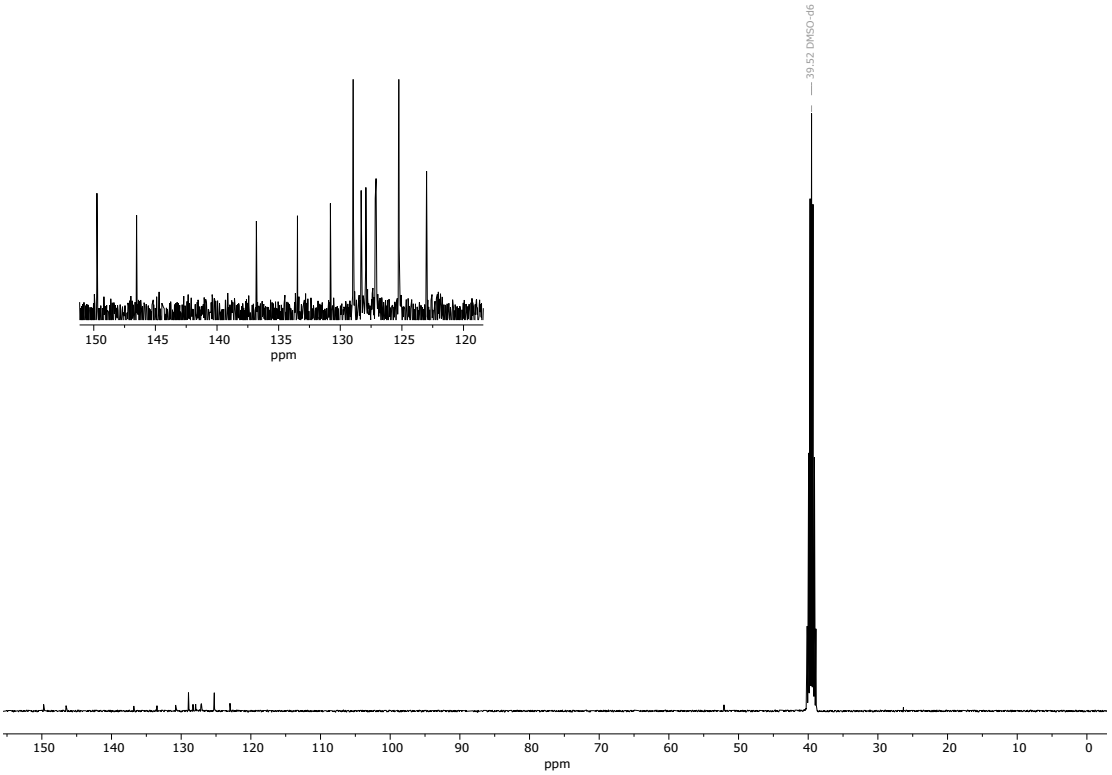
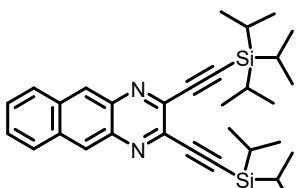


Figure S2.6 ^{13}C NMR of **5** in C_2D_6OS.

2,3-bis((triisopropylsilyl)ethynyl)benzo[g]quinoxaline (10)



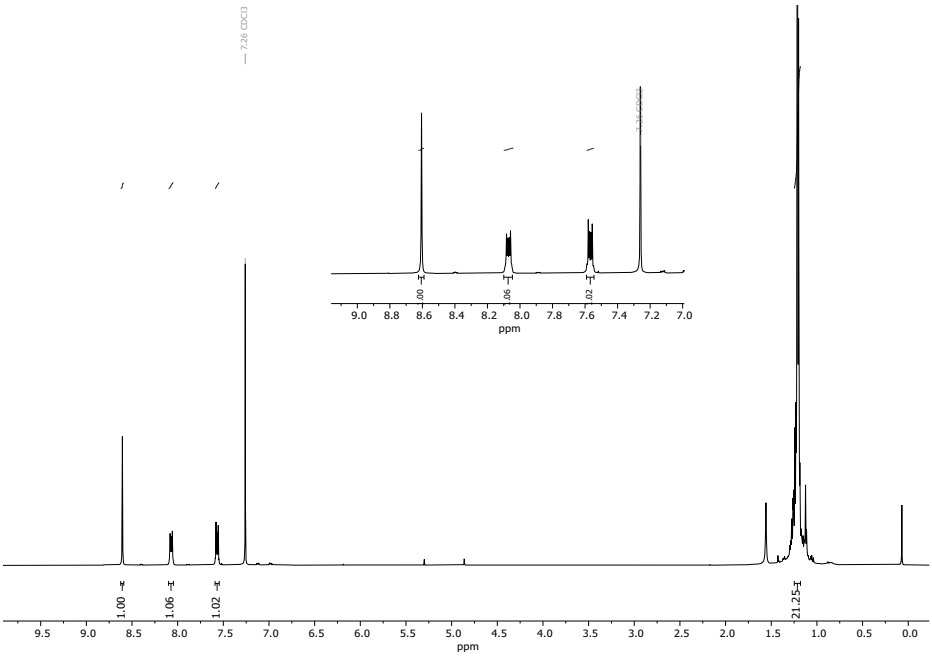


Figure S2.7 ^{1}H NMR of **10** in $CDCl_3$ (Residual solvent peaks:1.56 ppm (water))

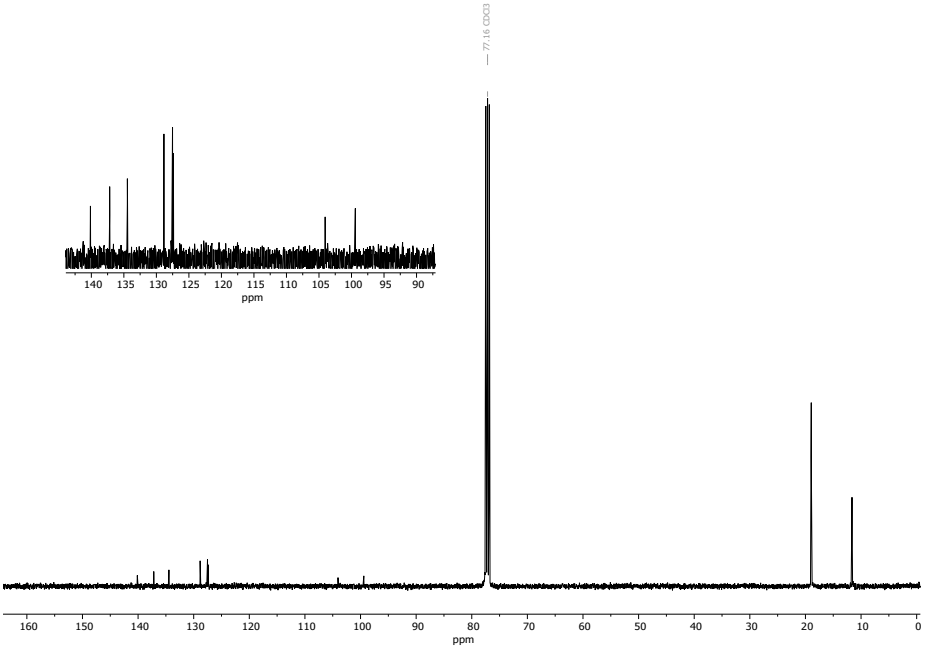


Figure S2.8 ^{13}C NMR of **10** in $CDCl_3$.

2,3-bis(1'-benzyl-1'*H*-1',2',3'-triazol-4'-yl)benzo[g]quinoxaline (6)

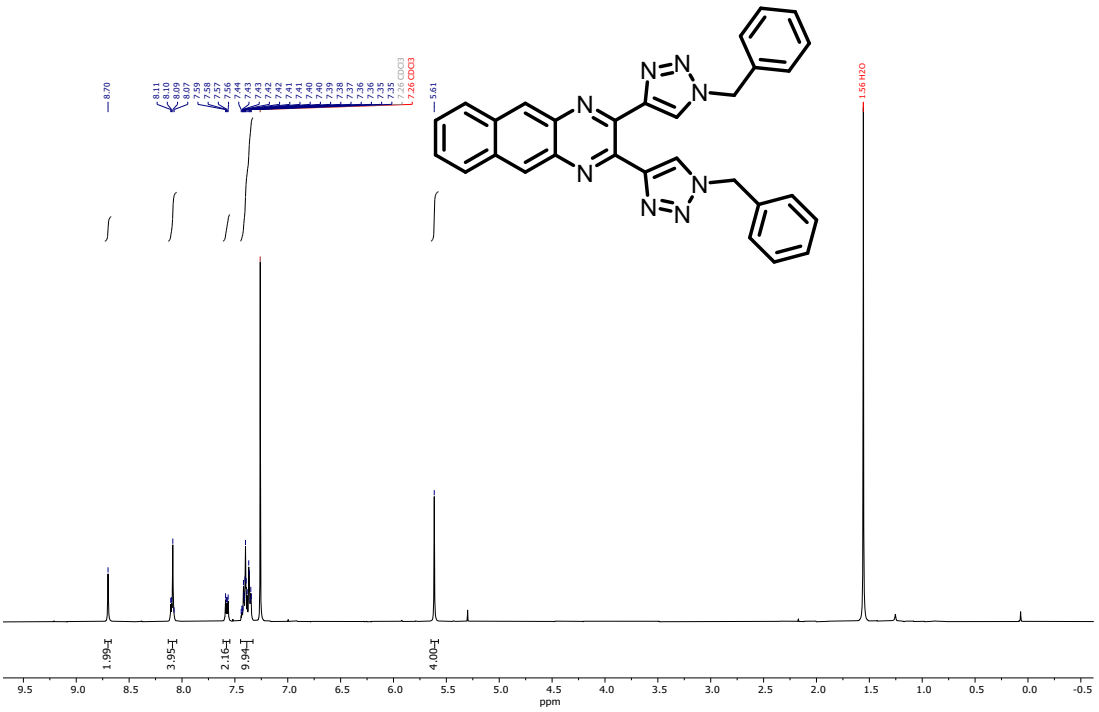


Figure S2.9 ^{1}H NMR of **6** in $CDCl_3$ (Residual solvent peaks:1.56 ppm (water))

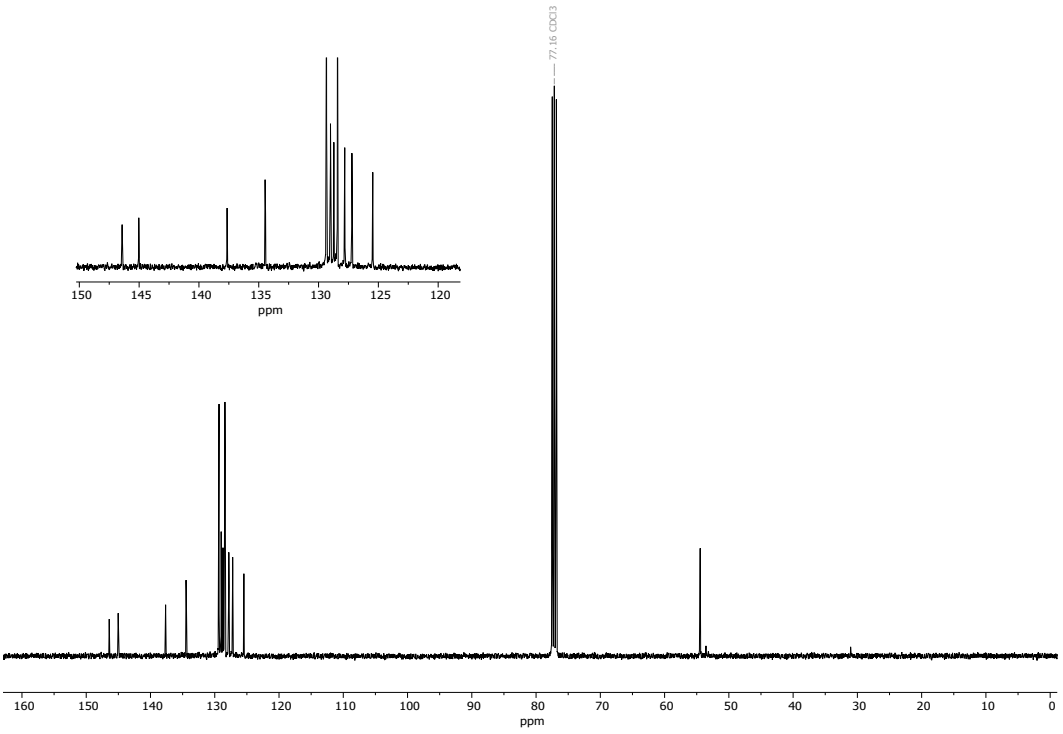
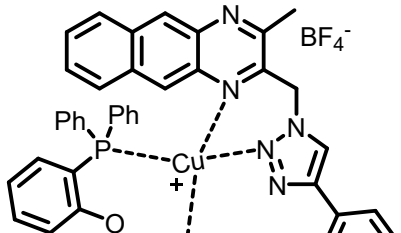


Figure S2.10 ^{13}C NMR of **6** in $CDCl_3$.

Copper complex 1



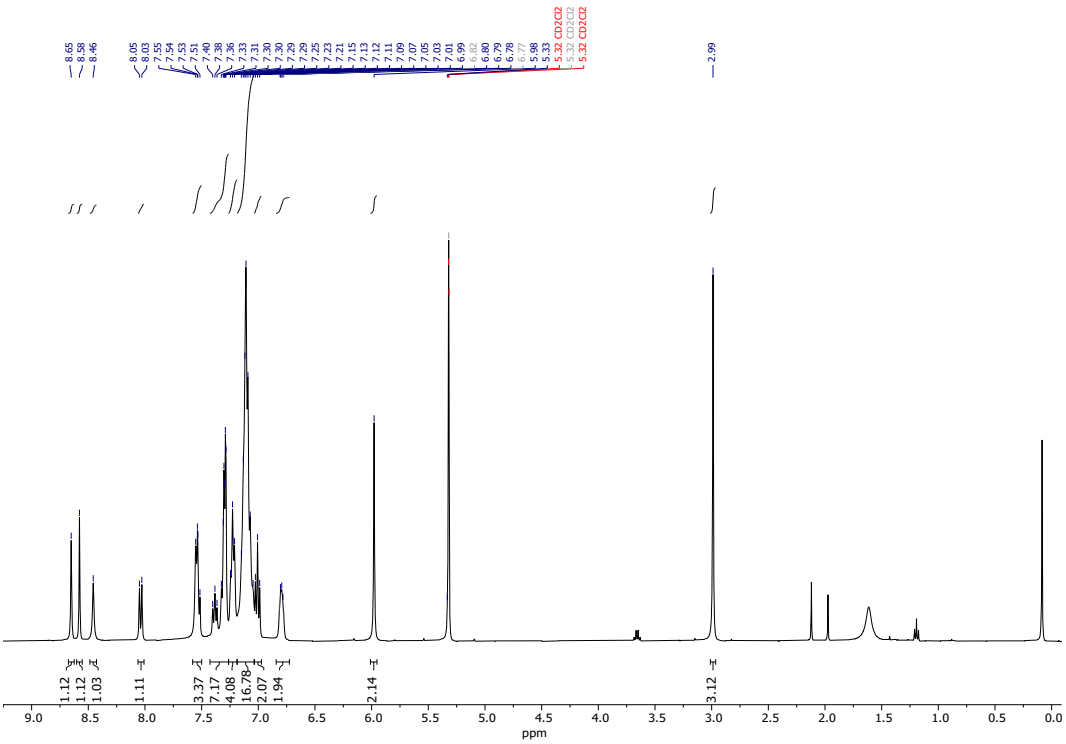


Figure S2.11 ^{1}H NMR of **1** in CD_2Cl_2 (Residual solvent peaks: 1.56 ppm (water)).

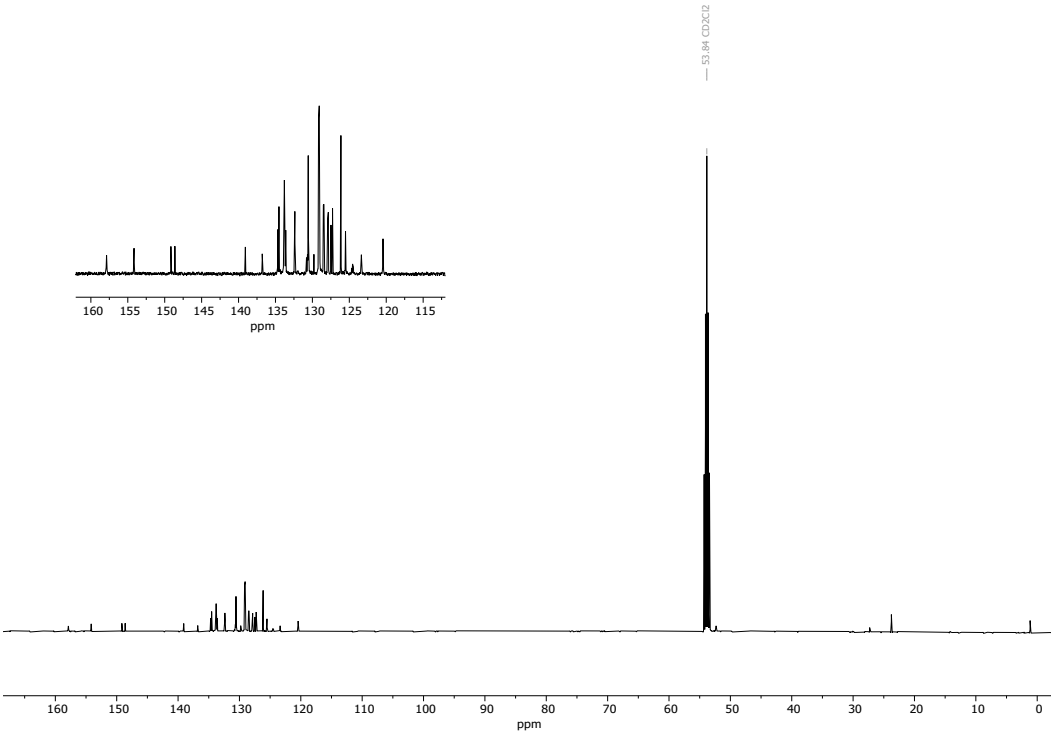
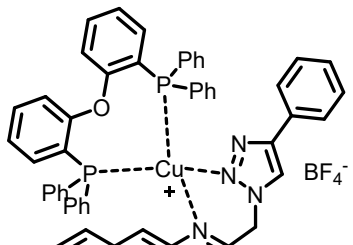


Figure S2.12 ^{13}C NMR of **1** in CD_2Cl_2.

Copper complex 2



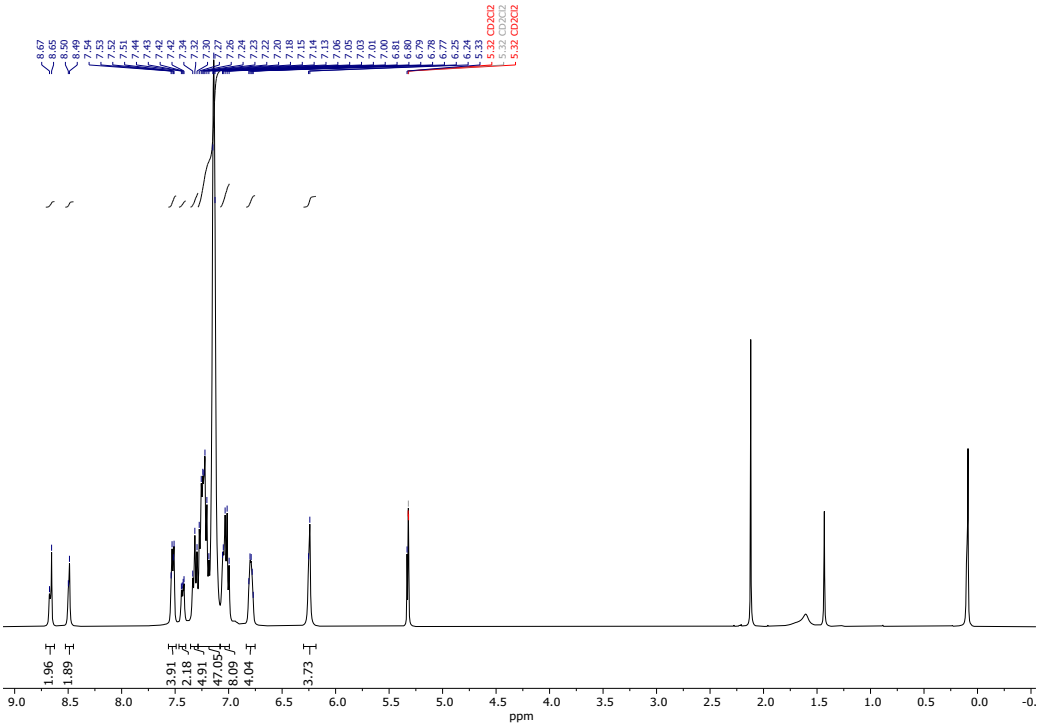


Figure S2.13 ^{1}H NMR of **2** in CD_2Cl_2 (Residual solvent peaks: 1.56 ppm (water)).

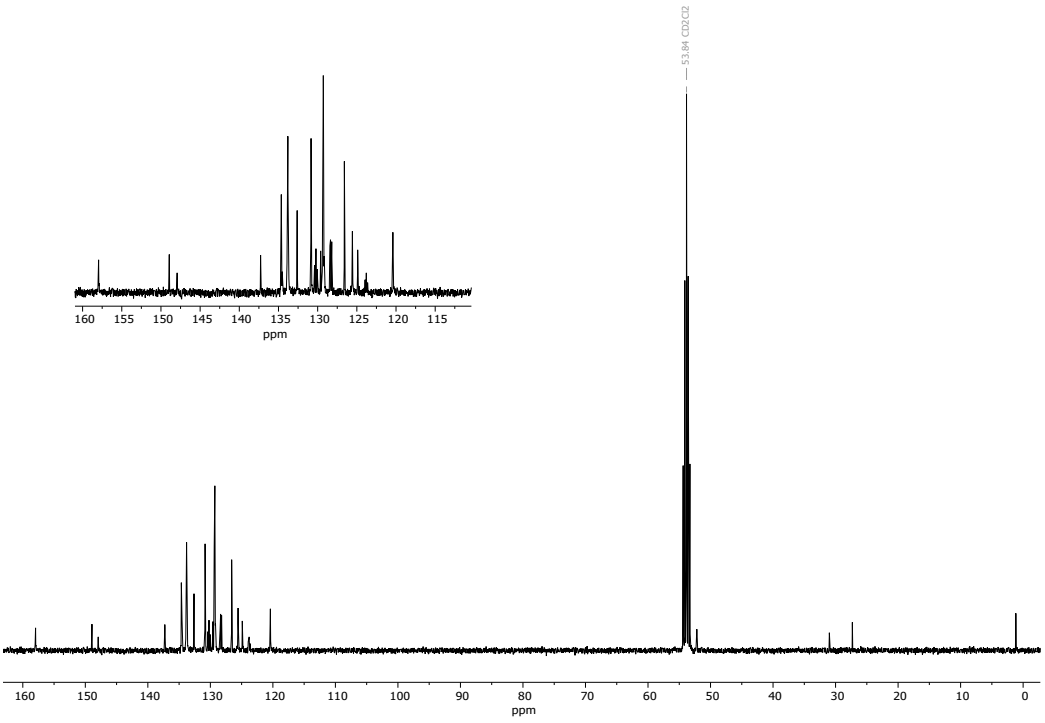


Figure S2.14 ^{13}C NMR of **2** in CD_2Cl_2.

Copper complex 3

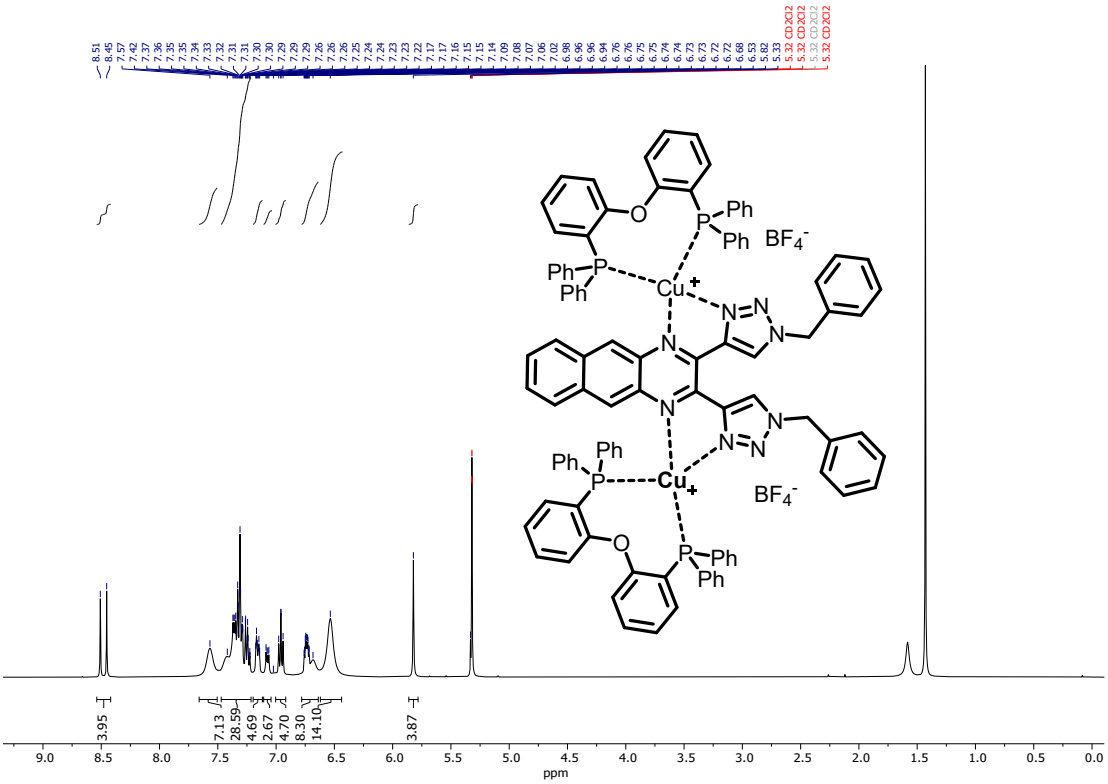


Figure S2.15 ^{1}H NMR of **3** in CD_2Cl_2 (Residual solvent peaks: 1.56 ppm (water), 1.43 ppm (cyclohexane))).

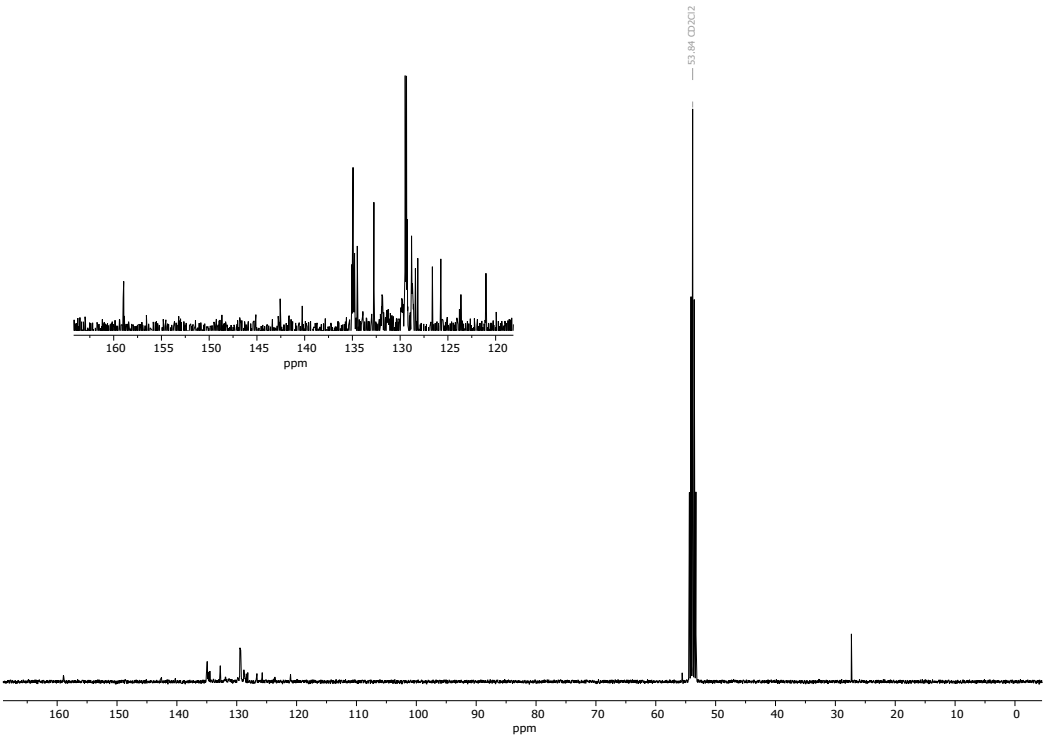


Figure S2.16 ^{13}C NMR of **1** in CD_2Cl_2.

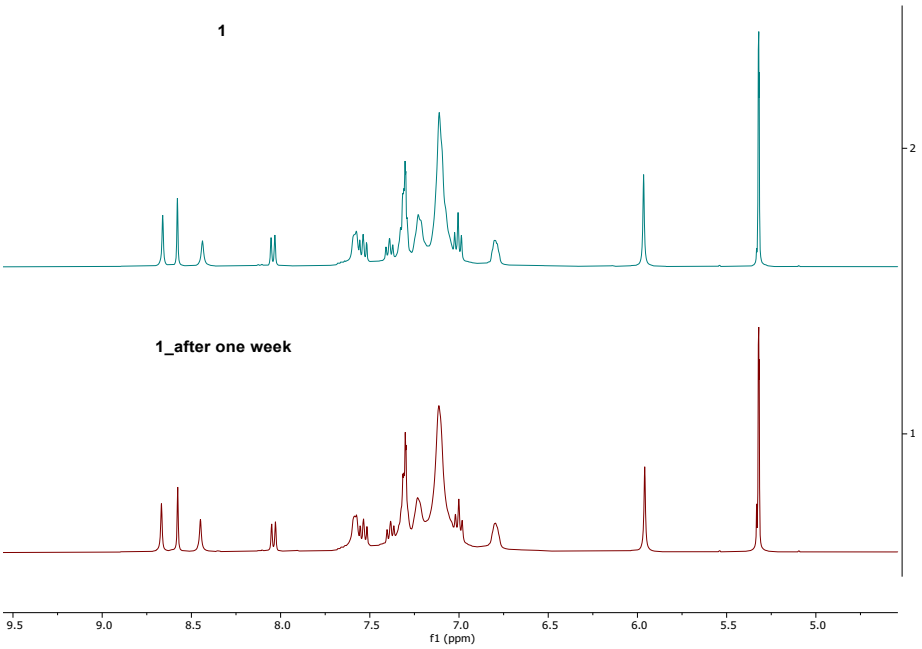


Figure S2.17 ^{1}H NMR of **1** in CD_2Cl_2: freshly prepared solution (top) and after a week (bottom).

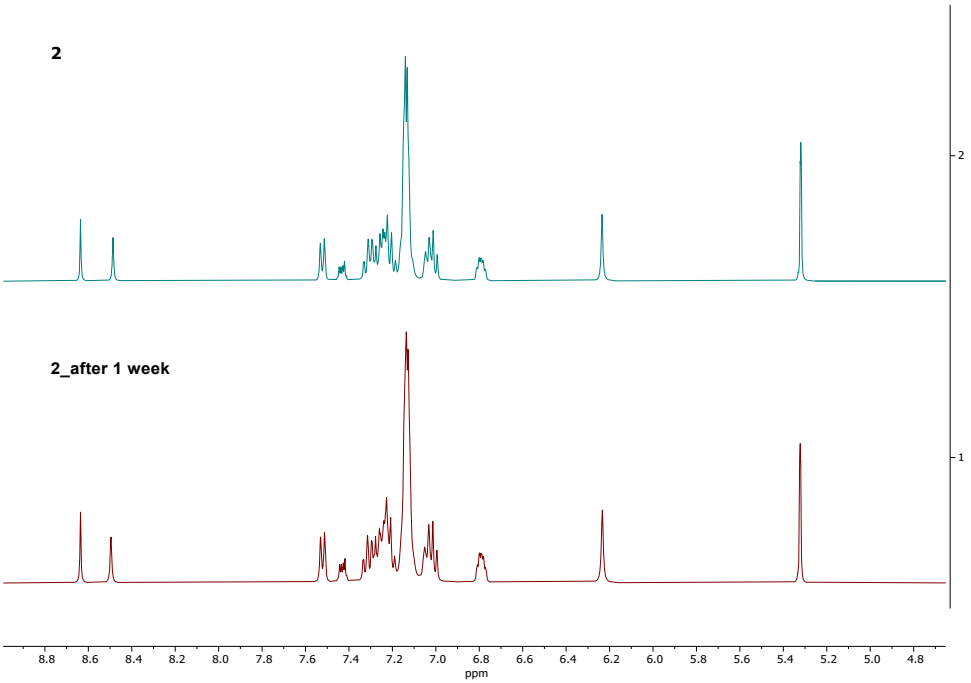


Figure S2.18 ^{1}H NMR of **2** in CD_2Cl_2: freshly prepared solution (top) and after a week (bottom).

3. Reaction monitoring

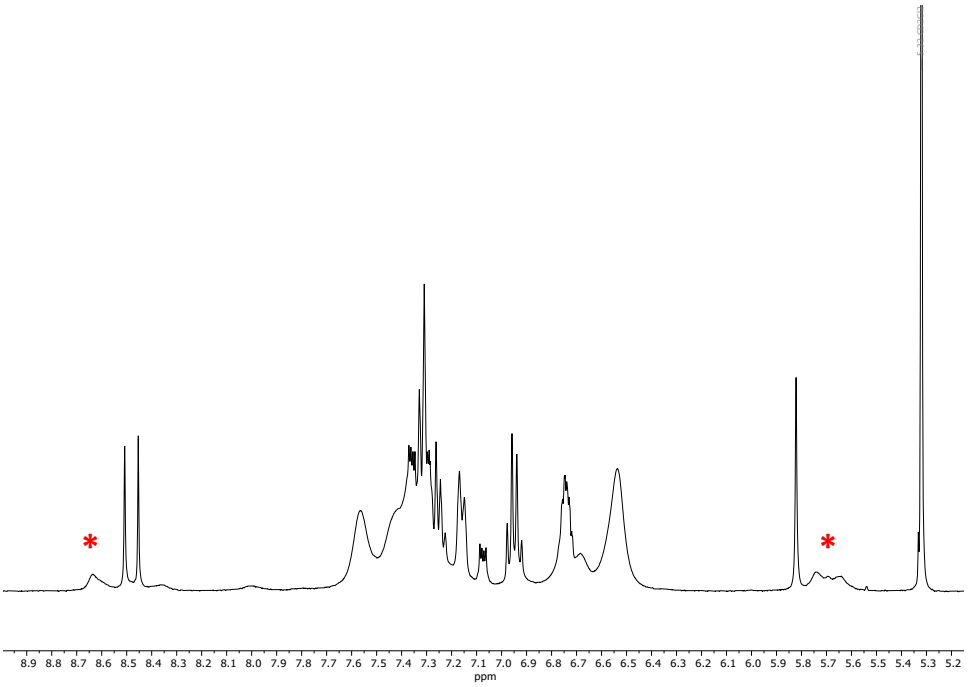


Figure S3.1 ^{1}H NMR of the product of the reaction of the ligand **6** and of the Cu(I) precursor and DPEPhos in a ratio 1:2. The asterisks indicate the peak of the unknown species (most probably the mononuclear species).

Figure S3.2 ^{1}H NMR of the product of the reaction mixture (S4.1) after reaction with an excess of $[Cu(DPEPhos)_2]^+$.

4. Cyclic voltammetry of 4-6

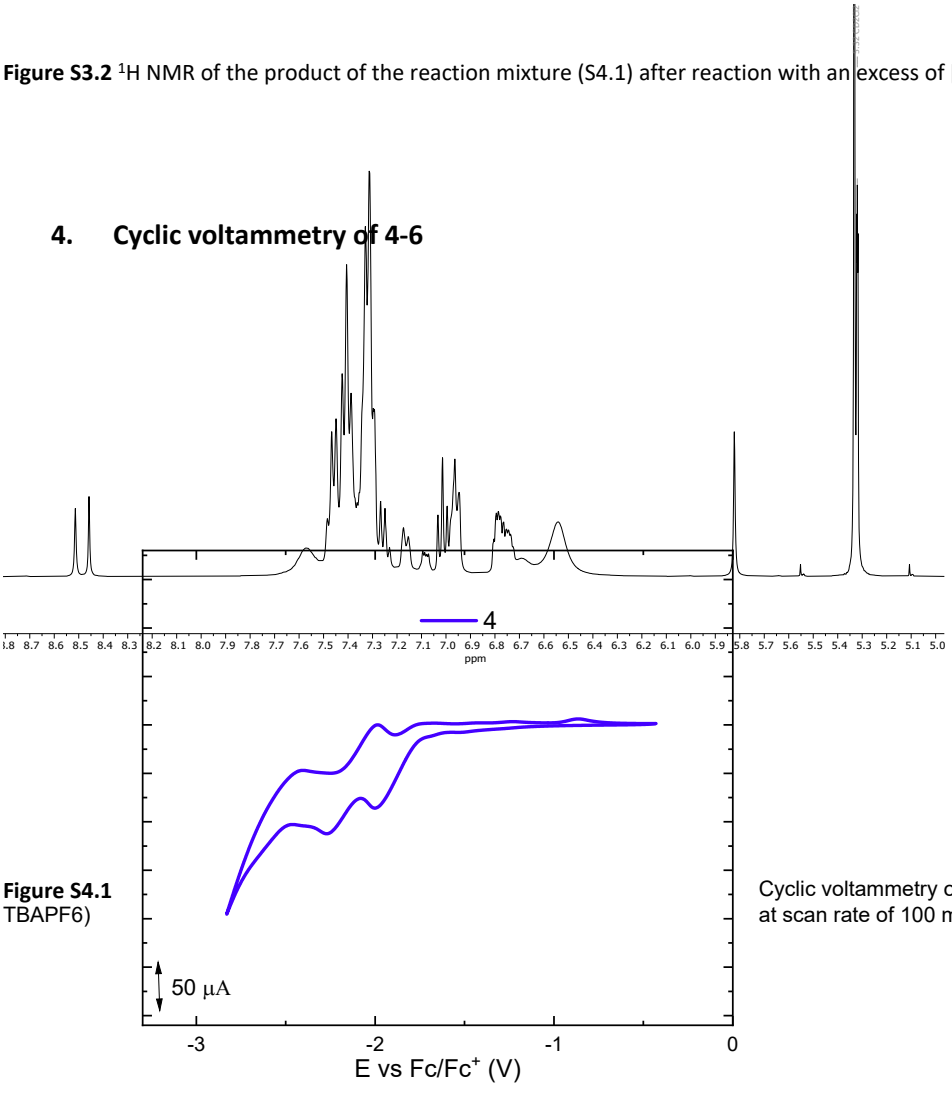


Figure S4.1 Cyclic voltammetry of compound **4** in DCM (0.1 M TBAPF6) at scan rate of 100 mV/s.

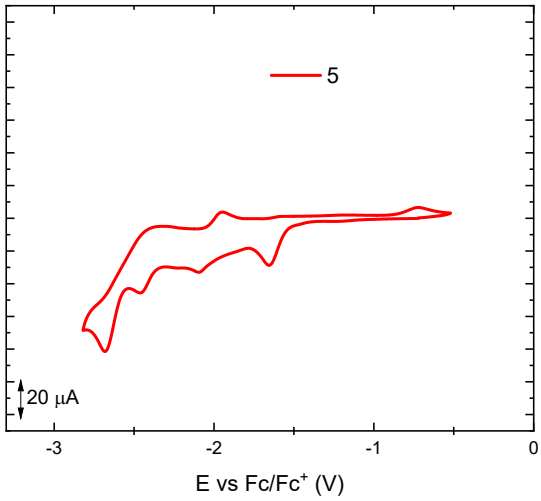


Figure S4.2 Cyclic voltammetry of compound **5** in DMF (0.1 M TBAPF6) at scan rate of 100 mV/s.

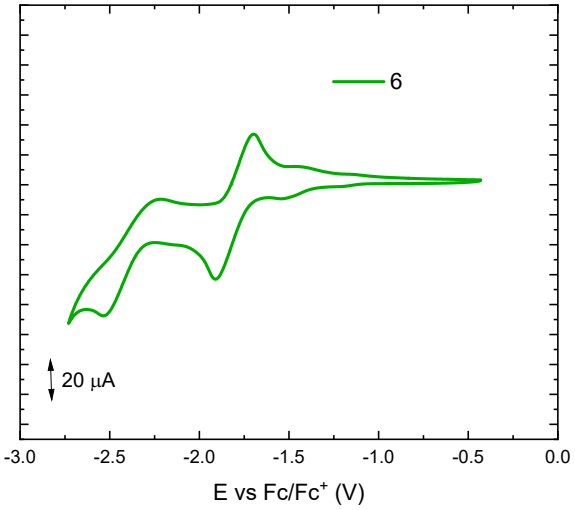


Figure S4.3 Cyclic voltammetry of compound **6** in DCM (0.1 M TBAPF6) at scan rate of 100 mV/s.

5. Quantum chemical calculations

5.1 DFT optimized geometries

1 S_0 state:

C	0.2444166	1.5264529	-5.2557089
C	0.9919206	1.5538621	-4.1207589
C	-0.9836749	0.8205170	-5.2930841
C	-1.4399806	0.1655279	-4.1935648

1 T_1 state:

C	-0.1924717	1.2468231	-5.7884846
C	0.6805386	0.4988873	-4.9950924
C	-1.4043050	1.6629981	-5.2789783
C	-1.7703319	1.3220758	-3.9740784

C	1.2918275	0.9019505	-1.7719835
C	0.5529020	0.8828247	-2.9490705
C	-0.6953517	0.1762568	-2.9860457
C	-1.1603590	-0.4579802	-1.8392480
C	-0.4336826	-0.4071313	-0.6619054
C	0.8200786	0.2740645	-0.6280851
H	0.5883519	2.0442079	-6.1464491
H	1.9374359	2.0887869	-4.0884278
H	-1.5604103	0.8074074	-6.2135376
H	-2.3792673	-0.3765543	-4.2167550
H	2.2436051	1.4222519	-1.7186480
H	-2.1211044	-0.9635522	-1.8468268
N	-0.9399885	-0.9397513	0.4938290
N	1.5430254	0.3462896	0.5181718
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H	1.3341111	0.4545629	3.6464426
H	2.1350386	-1.0882641	3.2439435
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H	-0.0630879	-1.4147791	3.6535502
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N	-2.7456474	-2.6281023	2.2766332
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C	-2.3513788	-6.0676294	3.0283870
C	-1.2430896	-6.9021197	3.2132741
C	-1.4101903	-8.2795613	3.3251224
C	-2.6872819	-8.8372627	3.2523708
C	-3.7962836	-8.0091945	3.0715294
C	-3.6317323	-6.6318399	2.9600056
H	-0.2363393	-6.4754605	3.2462893
H	-0.5373506	-8.9234381	3.4657459
H	-2.8184718	-9.9195001	3.3411102
H	-4.7997061	-8.4416612	3.0199549
H	-4.4948022	-5.9780131	2.8126103
Cu	-2.9735973	-1.4946920	0.4641195
P	-4.1988540	0.4152905	0.4104054
P	-3.7408027	-3.2383581	-0.8126357
C	-2.7292773	-4.7355277	-0.6796564
C	-3.2500317	-6.0035024	-0.4064132
C	-2.3947022	-7.0966492	-0.2678447
C	-1.0180438	-6.9315286	-0.4031126
C	-0.4908758	-5.6670406	-0.6754107
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H	-2.8080644	-8.0810615	-0.0322694
H	-0.3509554	-7.7903053	-0.2866269
H	0.5895882	-5.5326799	-0.7812063
H	-0.9263725	-3.5778873	-1.0027942

C	1.2177164	-0.5638769	-2.8437705
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H	1.6423504	0.1836711	-5.3920476
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N	-0.7643539	-0.8138523	0.2421903
N	1.7612254	-1.5316867	-0.7481750
C	0.1871293	-1.3925819	1.0321887
C	1.4187132	-1.7679359	0.5378929
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H	2.0449949	-3.3908431	1.8243997
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H	0.6962274	-1.8363112	3.0744460
H	-0.5591972	-0.5892508	2.8584224
N	-1.2103143	-2.5346340	2.7156380
C	-1.1200960	-3.7823259	3.1995881
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N	-2.4689073	-2.2473668	2.4103256
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C	-2.1268353	-6.5300226	4.1640450
C	-2.6245806	-7.7978550	4.4524444
C	-3.9439760	-8.1211684	4.1333752
C	-4.7636380	-7.1662150	3.5296541
C	-4.2689000	-5.8978390	3.2412673
H	-1.0912941	-6.2876740	4.4196508
H	-1.9786614	-8.5388686	4.9319710
H	-4.3342484	-9.1176632	4.3587043
H	-5.7990690	-7.4130754	3.2778879
H	-4.9044781	-5.1521591	2.7570455
Cu	-2.7898694	-1.1103297	0.6295901
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C	-0.3037639	-6.2627526	0.2025051
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C	-0.8319642	-4.1016505	-0.7382524
H	-3.6512531	-5.6711898	0.3637297
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C	-3.8860574	-2.9888404	-2.6128533
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C	-4.6583808	-1.5374553	-4.4141365
C	-4.2896956	-2.5033586	-5.3502949
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H	-5.0923652	-0.5820823	-4.7198930
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H	-3.4003438	-4.4480618	-5.6618947
H	-3.0467868	-4.8742842	-3.2414536
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C	-7.3431389	-3.5040811	1.0930225
C	-6.0177305	-3.2134512	0.7781531
H	-5.7922891	-4.8763528	-2.1921101
H	-8.1391638	-5.4180555	-1.6130178
H	-9.1477581	-4.5228114	0.4822936
H	-7.7843088	-3.1016763	2.0090338
H	-5.4204125	-2.5880299	1.4457543
C	-4.5631932	1.1949750	2.0043206
C	-4.6140759	0.3790940	3.1428204
C	-4.9237921	0.9262667	4.3871506
C	-5.1716287	2.2943786	4.5033173
C	-5.1155653	3.1132216	3.3740945
C	-4.8163097	2.5672262	2.1274683
H	-4.4110280	-0.6930976	3.0476262
H	-4.9686468	0.2829657	5.2707465
H	-5.4088805	2.7264252	5.4798832
H	-5.3092369	4.1859218	3.4651145
H	-4.7745999	3.2105155	1.2439001
C	-5.8310339	0.1049485	-0.3171341
C	-5.8848087	-0.6190816	-1.5194904
C	-7.0855326	-1.1060541	-2.0237430
C	-8.2638011	-0.8520975	-1.3235224
C	-8.2417001	-0.1092980	-0.1439554
C	-7.0297401	0.3621230	0.3565072
O	-4.6823846	-0.7948617	-2.1426789
H	-7.0950957	-1.6895372	-2.9471619
H	-9.2098777	-1.2403532	-1.7107166
H	-9.1699531	0.0949860	0.3957185
H	-7.0089184	0.9191169	1.2966564
C	-3.3977705	1.7181051	-0.5623143
C	-3.8759175	2.1499193	-1.8026804
C	-3.1282968	3.0445105	-2.5689622
C	-1.9076648	3.5250591	-2.0990477
C	-1.4390284	3.1224323	-0.8466612
C	-2.1765175	2.2205021	-0.0869245
H	-4.8344394	1.7843931	-2.1770820
H	-3.5057034	3.3695433	-3.5426158
H	-1.3212715	4.2204270	-2.7060305
H	-0.4886482	3.5058766	-0.4649828

C	-3.2886515	-2.5944525	-2.5063510
C	-3.9022209	-1.4246074	-2.9832119
C	-3.9192633	-1.1144545	-4.3383918
C	-3.3000519	-1.9694407	-5.2485351
C	-2.6708952	-3.1286524	-4.7962791
C	-2.6722180	-3.4398454	-3.4373365
H	-4.4092834	-0.1943057	-4.6638785
H	-3.3057344	-1.7237863	-6.3140109
H	-2.1806762	-3.8006787	-5.5057690
H	-2.1822512	-4.3533299	-3.0900210
C	-4.9914946	-3.6601380	-0.5062137
C	-5.5053382	-4.5647932	-1.4454954
C	-6.7668270	-5.1235690	-1.2620541
C	-7.5263640	-4.7805875	-0.1413400
C	-7.0216195	-3.8785716	0.7938923
C	-5.7573183	-3.3196904	0.6130943
H	-4.9172235	-4.8307922	-2.3287556
H	-7.1615539	-5.8301970	-1.9978907
H	-8.5193638	-5.2175008	-0.0001855
H	-7.6167813	-3.6006393	1.6682764
H	-5.3573766	-2.6184253	1.3480411
C	-4.9986395	1.0765844	2.2010691
C	-5.0054615	0.1603869	3.2616050
C	-5.5290599	0.5266995	4.5000728
C	-6.0340085	1.8133506	4.6903975
C	-6.0196531	2.7327419	3.6402574
C	-5.5071057	2.3668112	2.3973054
H	-4.5928640	-0.8433924	3.1170188
H	-5.5338151	-0.1935650	5.3231521
H	-6.4370340	2.1041678	5.6649190
H	-6.4112969	3.7429218	3.7906364
H	-5.4988018	3.0888907	1.5758389
C	-5.8339053	-0.0451521	-0.2881312
C	-5.6542477	-0.6291818	-1.5519883
C	-6.6975323	-1.2680833	-2.2133399
C	-7.9540675	-1.3107569	-1.6118958
C	-8.1665091	-0.7072966	-0.3731537
C	-7.1097362	-0.0806680	0.2841007
O	-4.4006452	-0.5100457	-2.0874758
H	-6.5220543	-1.7369715	-3.1844408
H	-8.7751720	-1.8205321	-2.1232207
H	-9.1562009	-0.7348133	0.0899440
H	-7.2687554	0.3680111	1.2680042
C	-3.8393474	2.0388038	-0.2450025
C	-4.5853029	2.6301735	-1.2698379
C	-4.0966887	3.7573565	-1.9312568
C	-2.8644024	4.3031920	-1.5714684
C	-2.1194947	3.7228748	-0.5428621
C	-2.6017601	2.5934758	0.1126450
H	-5.5530199	2.2071345	-1.5534923
H	-4.6873254	4.2165042	-2.7296362
H	-2.4832120	5.1864756	-2.0918893
H	-1.1537657	4.1485811	-0.2563839

H	-1.7986353	1.8985761	0.8891088
H	2.7983894	0.4494987	2.6210916

2 S_0 state:

C	0.4901366	0.5122458	-5.5220470
C	0.9787567	1.0062801	-4.3534925
C	-0.4901366	-0.5122458	-5.5220470
C	-0.9787567	-1.0062801	-4.3534925
C	1.0194547	0.9616328	-1.9034045
C	0.5101767	0.5048955	-3.1123362
C	-0.5101767	-0.5048955	-3.1123362
C	-1.0194547	-0.9616328	-1.9034045
C	-0.5309355	-0.4786610	-0.7024035
C	0.5309355	0.4786610	-0.7024035
H	0.8518744	0.9004453	-6.4694451
H	1.7303748	1.7891888	-4.3480928
H	-0.8518744	-0.9004453	-6.4694451
H	-1.7303748	-1.7891888	-4.3480928
H	1.8099235	1.7051751	-1.8870159
H	-1.8099235	-1.7051751	-1.8870159
N	-1.0461408	-0.9279600	0.4772507
N	1.0461408	0.9279600	0.4772507
C	-0.5207939	-0.4860864	1.5884273
C	0.5207939	0.4860864	1.5884273
C	1.0664180	1.0254754	2.8920531
H	0.3048451	0.9909353	3.6801907
H	1.9286475	0.4185937	3.2172864
N	1.5079835	2.3902007	2.7982260
C	0.8609658	3.5278614	3.1077337
C	1.7453877	4.5363614	2.7803341
N	2.8667542	3.9496234	2.2989527
N	2.7121264	2.6659811	2.2994241
H	-0.1231634	3.5319020	3.5497368
C	1.6001136	5.9839277	2.8646007
C	0.3299992	6.5730920	2.9089825
C	0.1993264	7.9576221	2.9595772
C	1.3372219	8.7659383	2.9674145
C	2.6041043	8.1831421	2.9234624
C	2.7380024	6.7990649	2.8695790
H	-0.5664910	5.9456241	2.8835955
H	-0.7954499	8.4104498	2.9917224
H	1.2351112	9.8538035	3.0121667
H	3.4970099	8.8143602	2.9336353
H	3.7267479	6.3367978	2.8296442
Cu	3.0693663	1.6348462	0.4423485
P	4.1798658	-0.3589237	0.5275808
P	3.9902545	3.3018366	-0.8302086
C	3.2397621	4.9460775	-0.7205040
C	3.9767745	6.1322281	-0.6505250
C	3.3174945	7.3584823	-0.5637293
C	1.9248633	7.4096911	-0.5422408
C	1.1850820	6.2279907	-0.6034885
C	1.8409420	5.0029752	-0.6882602

H	-2.0063038	2.1229118	0.9021594
H	3.2899499	-2.7498340	0.7140199

2 T_1 state:

C	0.4669531	0.5151629	-5.5138436
C	0.9411056	1.0274317	-4.3177502
C	-0.4669535	-0.5151572	-5.5138340
C	-0.9411101	-1.0274300	-4.3177463
C	0.9784888	0.9884709	-1.8627457
C	0.4865096	0.5175768	-3.0991377
C	-0.4864981	-0.5175631	-3.0991748
C	-0.9785206	-0.9885021	-1.8627300
C	-0.5304266	-0.4821805	-0.6485092
C	0.5304385	0.4821892	-0.6485147
H	0.8277514	0.9194038	-6.4544309
H	1.6724994	1.8300314	-4.3154419
H	-0.8277520	-0.9194026	-6.4544331
H	-1.6724997	-1.8300324	-4.3154433
H	1.7411404	1.7618118	-1.8499781
H	-1.7411262	-1.7617951	-1.8499776
N	-1.0911581	-0.8927925	0.5122018
N	1.0911575	0.8927890	0.5122069
C	-0.5400062	-0.4225632	1.6663274
C	0.5400111	0.4225649	1.6663295
C	1.2267492	0.8780800	2.9279858
H	0.6017432	0.7400015	3.8153754
H	2.1630989	0.3147278	3.0729390
N	1.6019429	2.2701613	2.8760594
C	0.9043760	3.3721771	3.1935969
C	1.7318874	4.4246678	2.8504303
N	2.8716233	3.8954519	2.3485808
N	2.7792233	2.6044617	2.3521661
H	-0.0725590	3.3274324	3.6488184
C	1.5143130	5.8631396	2.9373741
C	0.2159864	6.3886610	2.9634383
C	0.0157156	7.7650843	3.0132299
C	1.1116506	8.6289989	3.0390137
C	2.4064535	8.1096932	3.0139702
C	2.6097918	6.7340830	2.9610321
H	-0.6472084	5.7167561	2.9239636
H	-1.0007528	8.1678590	3.0308645
H	0.9548758	9.7103668	3.0835863
H	3.2666872	8.7844425	3.0387496
H	3.6207993	6.3214701	2.9359166
Cu	3.0195716	1.5851441	0.4282065
P	4.2048365	-0.3895412	0.4458620
P	4.0066481	3.2644489	-0.7931936
C	3.2626335	4.9066223	-0.6351464
C	4.0069124	6.0873236	-0.5524251
C	3.3531020	7.3158356	-0.4576620
C	1.9602661	7.3736938	-0.4412288
C	1.2139961	6.1966587	-0.5131465
C	1.8645471	4.9695143	-0.6051671

H	5.0692636	6.1016227	-0.6529758
H	3.8993901	8.2822668	-0.5029166
H	1.4128507	8.3718741	-0.4594661
H	0.0925847	6.2668812	-0.5674799
H	1.2687410	4.0698799	-0.7145591
C	4.0418746	2.9854254	-2.6259666
C	4.4155782	1.7030482	-3.0565060
C	4.5205362	1.3883220	-4.4071329
C	4.2490923	2.3704029	-5.3598568
C	3.8521411	3.6449966	-4.9555201
C	3.7472906	3.9489232	-3.5976509
H	4.8055540	0.3749748	-4.7000024
H	4.3382224	2.1329251	-6.4234364
H	3.6288080	4.4123472	-5.7013268
H	3.4407554	4.9507603	-3.2852810
C	5.7462695	3.5135469	-0.4359960
C	6.6525243	4.0638472	-1.3525196
C	7.9979826	4.1892698	-1.0167121
C	8.4501403	3.7579070	0.2311746
C	7.5536836	3.2084818	1.1472689
C	6.2061684	3.0888865	0.8158396
H	6.3091494	4.3846164	-2.3402596
H	8.7004036	4.6199912	-1.7357866
H	9.5089261	3.8488439	0.4896338
H	7.9067436	2.8666339	2.1239095
H	5.5009488	2.6579288	1.5323424
C	4.6212628	-0.9926928	2.1680124
C	4.7168465	-0.0827799	3.2294689
C	5.1006156	-0.5164367	4.4989089
C	5.3863275	-1.8636229	4.7173513
C	5.2940256	-2.7766869	3.6643196
C	4.9166880	-2.3453029	2.3949447
H	4.4951166	0.9749892	3.0557940
H	5.1810939	0.2019672	5.3195595
H	5.6890541	-2.2050161	5.7113216
H	5.5278180	-3.8317737	3.8327886
H	4.8549405	-3.0634252	1.5723622
C	5.7639484	-0.2709017	-0.3517695
C	5.8009465	0.4036897	-1.5827166
C	7.0037262	0.7091229	-2.2087831
C	8.1987487	0.3239145	-1.6041178
C	8.1893014	-0.3657433	-0.3931243
C	6.9778965	-0.6546834	0.2298221
O	4.5795445	0.7247325	-2.1099918
H	7.0061663	1.2538443	-3.1552223
H	9.1471229	0.5675929	-2.0904115
H	9.1283120	-0.6698209	0.0755632
H	6.9773132	-1.1650589	1.1954531
C	3.1911737	-1.6962209	-0.2068877
C	3.2661390	-2.0026019	-1.5712450
C	2.4046344	-2.9428867	-2.1323903
C	1.4631519	-3.5969424	-1.3402387
C	1.3857497	-3.3060974	0.0220929

H	5.0993076	6.0504669	-0.5547413
H	3.9393083	8.2363526	-0.3882046
H	1.4528788	8.3378905	-0.3538708
H	0.1215761	6.2397232	-0.4805765
H	1.2894478	4.0389448	-0.6385389
C	4.0345553	3.0083278	-2.5995737
C	4.3908556	1.7399123	-3.0813528
C	4.4722490	1.4709798	-4.4435939
C	4.1951350	2.4883327	-5.3567367
C	3.8166868	3.7513070	-4.9013402
C	3.7346572	4.0084124	-3.5323606
H	4.7440055	0.4661984	-4.7759527
H	4.2668770	2.2885720	-6.4293872
H	3.5915054	4.5471618	-5.6160285
H	3.4427768	5.0017047	-3.1817210
C	5.7608067	3.4577146	-0.3926759
C	6.6795799	3.9893445	-1.3073725
C	8.0208711	4.1173032	-0.9557187
C	8.4549548	3.7092360	0.3062601
C	7.5447634	3.1798456	1.2209420
C	6.2019347	3.0556269	0.8733920
H	6.3488069	4.2959270	-2.3038441
H	8.7337620	4.5340388	-1.6726988
H	9.5101937	3.8036606	0.5776716
H	7.8832696	2.8588113	2.2097044
H	5.4847464	2.6442745	1.5890772
C	4.6682073	-1.0440971	2.0698925
C	4.8224120	-0.1435282	3.1325424
C	5.2284352	-0.5969133	4.3877997
C	5.4788133	-1.9535399	4.5904564
C	5.3293352	-2.8567954	3.5355686
C	4.9289337	-2.4065927	2.2799977
H	4.6245516	0.9208775	2.9730788
H	5.3519079	0.1132860	5.2102048
H	5.7979019	-2.3104538	5.5737899
H	5.5357377	-3.9194940	3.6913629
H	4.8227177	-3.1169493	1.4554140
C	5.7739406	-0.2970291	-0.4531412
C	5.7943535	0.3897781	-1.6766087
C	6.9873613	0.6855723	-2.3252783
C	8.1890020	0.2790706	-1.7479852
C	8.1952787	-0.4204947	-0.5423758
C	6.9936691	-0.7006856	0.1026131
O	4.5644906	0.7315994	-2.1703398
H	6.9785126	1.2389547	-3.2666075
H	9.1307735	0.5138088	-2.2512384
H	9.1396919	-0.7405619	-0.0958782
H	7.0049862	-1.2214092	1.0626223
C	3.1793633	-1.6913878	-0.2916984
C	3.2108931	-1.9732497	-1.6637480
C	2.3116861	-2.8820945	-2.2171640
C	1.3762876	-3.5278127	-1.4106294
C	1.3442471	-3.2617141	-0.0403636

C	2.2376015	-2.3573884	0.5828465
H	3.9988621	-1.5015141	-2.2037778
H	2.4776557	-3.1730833	-3.1988364
H	0.7987100	-4.3403627	-1.7876943
H	0.6585999	-3.8242188	0.6554744
H	2.1814979	-2.1489791	1.6555741
C	-1.0664180	-1.0254754	2.8920531
H	-0.3048451	-0.9909353	3.6801907
H	-1.9286475	-0.4185937	3.2172864
N	-1.5079835	-2.3902007	2.7982260
C	-0.8609658	-3.5278614	3.1077337
C	-1.7453877	-4.5363614	2.7803341
N	-2.8667542	-3.9496234	2.2989527
N	-2.7121264	-2.6659811	2.2994241
H	0.1231634	-3.5319020	3.5497368
C	-1.6001136	-5.9839277	2.8646007
C	-0.3299992	-6.5730920	2.9089825
C	-0.1993264	-7.9576221	2.9595772
C	-1.3372219	-8.7659383	2.9674145
C	-2.6041043	-8.1831421	2.9234624
C	-2.7380024	-6.7990649	2.8695790
H	0.5664910	-5.9456241	2.8835955
H	0.7954499	-8.4104498	2.9917224
H	-1.2351112	-9.8538035	3.0121667
H	-3.4970099	-8.8143602	2.9336353
H	-3.7267479	-6.3367978	2.8296442
Cu	-3.0693663	-1.6348462	0.4423485
P	-4.1798658	0.3589237	0.5275808
P	-3.9902545	-3.3018366	-0.8302086
C	-3.2397621	-4.9460775	-0.7205040
C	-3.9767745	-6.1322281	-0.6505250
C	-3.3174945	-7.3584823	-0.5637293
C	-1.9248633	-7.4096911	-0.5422408
C	-1.1850820	-6.2279907	-0.6034885
C	-1.8409420	-5.0029752	-0.6882602
H	-5.0692636	-6.1016227	-0.6529758
H	-3.8993901	-8.2822668	-0.5029166
H	-1.4128507	-8.3718741	-0.4594661
H	-0.0925847	-6.2668812	-0.5674799
H	-1.2687410	-4.0698799	-0.7145591
C	-4.0418746	-2.9854254	-2.6259666
C	-4.4155782	-1.7030482	-3.0565060
C	-4.5205362	-1.3883220	-4.4071329
C	-4.2490923	-2.3704029	-5.3598568
C	-3.8521411	-3.6449966	-4.9555201
C	-3.7472906	-3.9489232	-3.5976509
H	-4.8055540	-0.3749748	-4.7000024
H	-4.3382224	-2.1329251	-6.4234364
H	-3.6288080	-4.4123472	-5.7013268
H	-3.4407554	-4.9507603	-3.2852810
C	-5.7462695	-3.5135469	-0.4359960
C	-6.6525243	-4.0638472	-1.3525196
C	-7.9979826	-4.1892698	-1.0167121

C	2.2304419	-2.3428187	0.5125402
H	3.9382870	-1.4782605	-2.3070585
H	2.3487193	-3.0930278	-3.2893604
H	0.6822275	-4.2475648	-1.8522238
H	0.6226497	-3.7706426	0.6060523
H	2.1975222	-2.1437723	1.5871198
C	-1.2267521	-0.8780745	2.9279857
H	-0.6017396	-0.7400022	3.8153710
H	-2.1630968	-0.3147266	3.0729371
N	-1.6019317	-2.2701871	2.8760690
C	-0.9044067	-3.3721769	3.1935764
C	-1.7318846	-4.4246464	2.8504386
N	-2.8716239	-3.8954548	2.3485805
N	-2.7792232	-2.6044559	2.3521598
H	0.0725730	-3.3274320	3.6488291
C	-1.5143112	-5.8631483	2.9373770
C	-0.2159974	-6.3886927	2.9634391
C	-0.0157353	-7.7650565	3.0132346
C	-1.1116339	-8.6290069	3.0390099
C	-2.4064746	-8.1096989	3.0139737
C	-2.6097926	-6.7340779	2.9610313
H	0.6472181	-5.7167476	2.9239663
H	1.0007617	-8.1678654	3.0308674
H	-0.9548803	-9.7103647	3.0835892
H	-3.2666832	-8.7844375	3.0387497
H	-3.6207984	-6.3214699	2.9359167
Cu	-3.0195771	-1.5851457	0.4282066
P	-4.2048373	0.3895418	0.4458611
P	-4.0066489	-3.2644492	-0.7931943
C	-3.2626225	-4.9066164	-0.6351457
C	-4.0069070	-6.0873353	-0.5524247
C	-3.3530974	-7.3158226	-0.4576615
C	-1.9602775	-7.3737042	-0.4412293
C	-1.2139892	-6.1966384	-0.5131463
C	-1.8645592	-4.9695325	-0.6051668
H	-5.0993113	-6.0504662	-0.5547412
H	-3.9393097	-8.2363559	-0.3882039
H	-1.4528782	-8.3378884	-0.3538699
H	-0.1215776	-6.2397237	-0.4805759
H	-1.2894431	-4.0389364	-0.6385383
C	-4.0345538	-3.0083335	-2.5995756
C	-4.3908578	-1.7399064	-3.0813536
C	-4.4722462	-1.4709893	-4.4435967
C	-4.1951386	-2.4883246	-5.3567347
C	-3.8166839	-3.7513146	-4.9013431
C	-3.7346571	-4.0084100	-3.5323548
H	-4.7440071	-0.4661969	-4.7759527
H	-4.2668759	-2.2885736	-6.4293865
H	-3.5915043	-4.5471614	-5.6160266
H	-3.4427757	-5.0017042	-3.1817201
C	-5.7608097	-3.4577134	-0.3926773
C	-6.6795797	-3.9893394	-1.3073617
C	-8.0208694	-4.1173054	-0.9557235

C	-8.4501403	-3.7579070	0.2311746
C	-7.5536836	-3.2084818	1.1472689
C	-6.2061684	-3.0888865	0.8158396
H	-6.3091494	-4.3846164	-2.3402596
H	-8.7004036	-4.6199912	-1.7357866
H	-9.5089261	-3.8488439	0.4896338
H	-7.9067436	-2.8666339	2.1239095
H	-5.5009488	-2.6579288	1.5323424
C	-4.6212628	0.9926928	2.1680124
C	-4.7168465	0.0827799	3.2294689
C	-5.1006156	0.5164367	4.4989089
C	-5.3863275	1.8636229	4.7173513
C	-5.2940256	2.7766869	3.6643196
C	-4.9166880	2.3453029	2.3949447
H	-4.4951166	-0.9749892	3.0557940
H	-5.1810939	-0.2019672	5.3195595
H	-5.6890541	2.2050161	5.7113216
H	-5.5278180	3.8317737	3.8327886
H	-4.8549405	3.0634252	1.5723622
C	-5.7639484	0.2709017	-0.3517695
C	-5.8009465	-0.4036897	-1.5827166
C	-7.0037262	-0.7091229	-2.2087831
C	-8.1987487	-0.3239145	-1.6041178
C	-8.1893014	0.3657433	-0.3931243
C	-6.9778965	0.6546834	0.2298221
O	-4.5795445	-0.7247325	-2.1099918
H	-7.0061663	-1.2538443	-3.1552223
H	-9.1471229	-0.5675929	-2.0904115
H	-9.1283120	0.6698209	0.0755632
H	-6.9773132	1.1650589	1.1954531
C	-3.1911737	1.6962209	-0.2068877
C	-3.2661390	2.0026019	-1.5712450
C	-2.4046344	2.9428867	-2.1323903
C	-1.4631519	3.5969424	-1.3402387
C	-1.3857497	3.3060974	0.0220929
C	-2.2376015	2.3573884	0.5828465
H	-3.9988621	1.5015141	-2.2037778
H	-2.4776557	3.1730833	-3.1988364
H	-0.7987100	4.3403627	-1.7876943
H	-0.6585999	3.8242188	0.6554744
H	-2.1814979	2.1489791	1.6555741

C	-8.4549490	-3.7092341	0.3062643
C	-7.5447595	-3.1798469	1.2209388
C	-6.2019422	-3.0556289	0.8733871
H	-6.3488054	-4.2959276	-2.3038485
H	-8.7337605	-4.5340384	-1.6726976
H	-9.5101940	-3.8036621	0.5776721
H	-7.8832700	-2.8588107	2.2097068
H	-5.4847430	-2.6442712	1.5890810
C	-4.6682064	1.0440992	2.0698906
C	-4.8224179	0.1435447	3.1325538
C	-5.2284293	0.5969046	4.3877837
C	-5.4788154	1.9535380	4.5904646
C	-5.3293303	2.8567955	3.5355511
C	-4.9289377	2.4065849	2.2800190
H	-4.6245505	-0.9208863	2.9730767
H	-5.3519083	-0.1132872	5.2102065
H	-5.7979003	2.3104527	5.5737881
H	-5.5357373	3.9194934	3.6913645
H	-4.8227175	3.1169552	1.4554067
C	-5.7739407	0.2970226	-0.4531453
C	-5.7943457	-0.3897732	-1.6766024
C	-6.9873637	-0.6855792	-2.3252870
C	-8.1890040	-0.2790602	-1.7479769
C	-8.1952771	0.4204837	-0.5423834
C	-6.9936704	0.7006909	0.1026174
O	-4.5644924	-0.7315990	-2.1703410
H	-6.9785122	-1.2389520	-3.2666047
H	-9.1307741	-0.5138092	-2.2512388
H	-9.1396936	0.7405631	-0.0958761
H	-7.0049853	1.2214066	1.0626214
C	-3.1793621	1.6913869	-0.2916959
C	-3.2108867	1.9732532	-1.6637509
C	-2.3116907	2.8820921	-2.2171584
C	-1.3762876	3.5278136	-1.4106369
C	-1.3442497	3.2617127	-0.0403551
C	-2.2304382	2.3428193	0.5125329
H	-3.9382874	1.4782586	-2.3070604
H	-2.3487190	3.0930283	-3.2893626
H	-0.6822295	4.2475650	-1.8522226
H	-0.6226501	3.7706415	0.6060515
H	-2.1975217	2.1437712	1.5871221

3 S_0 state:

C	0.6854354	-0.1783649	-5.9174808
C	1.3602629	-0.3423562	-4.7473871
C	-0.6854354	0.1783649	-5.9174808
C	-1.3602629	0.3423562	-4.7473871
C	1.3721074	-0.3001606	-2.2971088
C	0.6980034	-0.1621061	-3.5073867
C	-0.6980034	0.1621061	-3.5073867
C	-1.3721074	0.3001606	-2.2971088
C	-0.6978124	0.1515696	-1.0988343
C	0.6978124	-0.1515696	-1.0988343

3 T_1 state:

C	0.6810821	-0.1271171	-5.9602923
C	1.3698575	-0.2483904	-4.7586109
C	-0.6810920	0.1271190	-5.9602754
C	-1.3698162	0.2483837	-4.7585939
C	1.3777606	-0.2289014	-2.3075731
C	0.7002876	-0.1186575	-3.5426550
C	-0.7003031	0.1186613	-3.5427148
C	-1.3777318	0.2288957	-2.3075265
C	-0.7028745	0.1323554	-1.0887710
C	0.7028507	-0.1323543	-1.0887430

H	1.1961666	-0.3198928	-6.8656873
H	2.4097506	-0.6214108	-4.7345557
H	-1.1961666	0.3198928	-6.8656873
H	-2.4097506	0.6214108	-4.7345557
H	2.4289466	-0.5364423	-2.2833729
H	-2.4289466	0.5364423	-2.2833729
N	-1.3460781	0.3399567	0.0847155
N	1.3460781	-0.3399567	0.0847155
C	-0.6838748	0.2109169	1.2107605
C	0.6838748	-0.2109169	1.2107605
Cu	3.4292924	-0.2014843	0.3229593
P	4.9127584	-1.5046849	-0.7313198
P	3.6615382	2.0518138	0.0026240
C	2.4633014	2.9321382	1.0438907
C	2.8525856	3.4696226	2.2774785
C	1.9013226	4.0135089	3.1410651
C	0.5520734	4.0272796	2.7867213
C	0.1560941	3.4928274	1.5592653
C	1.1021270	2.9431724	0.6973711
H	3.9089172	3.4750253	2.5599435
H	2.2258070	4.4518917	4.0895298
H	-0.1896209	4.4712254	3.4571521
H	-0.8984705	3.5075604	1.2662466
H	0.7796707	2.5372202	-0.2664664
C	3.3524615	2.6665376	-1.6796130
C	3.8116689	1.8997861	-2.7635348
C	3.5657186	2.2824518	-4.0778871
C	2.8585734	3.4553329	-4.3336664
C	2.4106880	4.2433241	-3.2738362
C	2.6587132	3.8514950	-1.9598014
H	3.9353048	1.6513741	-4.8888731
H	2.6642044	3.7571593	-5.3664033
H	1.8692764	5.1727554	-3.4702088
H	2.3000639	4.4739700	-1.1360199
C	5.2799652	2.7245344	0.4473458
C	5.6653747	4.0235358	0.0897150
C	6.9291825	4.4937286	0.4332471
C	7.8149102	3.6719464	1.1346240
C	7.4354838	2.3801233	1.4953148
C	6.1706041	1.9063763	1.1512256
H	4.9795998	4.6662623	-0.4699138
H	7.2290662	5.5067292	0.1502235
H	8.8095518	4.0428714	1.3983489
H	8.1302742	1.7337725	2.0384418
H	5.8727118	0.8872261	1.4180432
C	5.8316156	-2.7262139	0.2331585
C	5.9848880	-2.5075794	1.6083954
C	6.7302380	-3.3970671	2.3803083
C	7.3136822	-4.5159090	1.7854639
C	7.1527761	-4.7453342	0.4177507
C	6.4163637	-3.8534190	-0.3585727
H	5.5128642	-1.6387350	2.0790516
H	6.8518582	-3.2190792	3.4525850

H	1.2139900	-0.2312324	-6.9005985
H	2.4362207	-0.4541607	-4.7491818
H	-1.2139892	0.2312341	-6.9006058
H	-2.4362385	0.4541641	-4.7491855
H	2.4473605	-0.3994983	-2.2956405
H	-2.4473709	0.3995008	-2.2956447
N	-1.3613236	0.3086042	0.0704034
N	1.3613309	-0.3086059	0.0704140
C	-0.6612242	0.1938950	1.2371384
C	0.6612255	-0.1938936	1.2371343
Cu	3.3962778	-0.1423373	0.3215677
P	4.8767098	-1.4435991	-0.7409791
P	3.6879310	2.1050275	0.0232215
C	2.5164989	2.9948098	1.0854513
C	2.9358839	3.5562660	2.2978376
C	2.0033323	4.1021799	3.1805883
C	0.6446426	4.0938436	2.8650649
C	0.2193704	3.5369121	1.6570901
C	1.1463999	2.9857160	0.7767872
H	3.9995535	3.5761434	2.5502311
H	2.3492018	4.5564021	4.1138215
H	-0.0830499	4.5365705	3.5515484
H	-0.8435823	3.5327877	1.3962858
H	0.8009236	2.5551504	-0.1680389
C	3.3570602	2.7292435	-1.6527962
C	3.8154129	1.9788993	-2.7487659
C	3.5755123	2.3853305	-4.0575157
C	2.8692796	3.5623413	-4.2960561
C	2.4135419	4.3293029	-3.2238291
C	2.6589587	3.9159786	-1.9159496
H	3.9509087	1.7699607	-4.8780985
H	2.6819426	3.8841269	-5.3241736
H	1.8707220	5.2608942	-3.4058155
H	2.2986804	4.5240473	-1.0821102
C	5.3219079	2.7626378	0.4316984
C	5.7157802	4.0549257	0.0590275
C	6.9919713	4.5114845	0.3741449
C	7.8817281	3.6826903	1.0620148
C	7.4935101	2.3979364	1.4383974
C	6.2163304	1.9377600	1.1228961
H	5.0262953	4.7035286	-0.4891686
H	7.2980562	5.5193917	0.0799878
H	8.8860132	4.0427852	1.3034136
H	8.1910056	1.7465606	1.9720254
H	5.9104636	0.9245465	1.4028771
C	5.7723169	-2.6863395	0.2165609
C	5.9423533	-2.4687456	1.5901534
C	6.6716759	-3.3754662	2.3571130
C	7.2216934	-4.5097159	1.7595959
C	7.0433589	-4.7378369	0.3936930
C	6.3230026	-3.8292229	-0.3781978
H	5.4948202	-1.5885590	2.0633718
H	6.8062176	-3.1985264	3.4280310

H	7.8951694	-5.2169134	2.3911980
H	7.6065941	-5.6250345	-0.0473620
H	6.2933197	-4.0355241	-1.4300936
C	6.1913591	-0.4352706	-1.4418942
C	5.7756325	0.6742812	-2.1950365
C	6.6698155	1.6680072	-2.5778690
C	8.0113363	1.5483885	-2.2168865
C	8.4538405	0.4403351	-1.4965741
C	7.5461561	-0.5442429	-1.1111111
O	4.4467551	0.7058423	-2.5328929
H	6.3182299	2.5311065	-3.1480661
H	8.7165668	2.3307020	-2.5103373
H	9.5082594	0.3454328	-1.2252395
H	7.8878578	-1.3999065	-0.5231759
C	4.1982216	-2.4377085	-2.1118824
C	4.7278882	-2.4058236	-3.4056715
C	4.0913309	-3.0941112	-4.4390926
C	2.9255245	-3.8171556	-4.1872040
C	2.3970009	-3.8597431	-2.8954078
C	3.0286974	-3.1705635	-1.8646391
H	5.6407476	-1.8383512	-3.6076489
H	4.5126319	-3.0684835	-5.4483106
H	2.4279357	-4.3526674	-5.0006527
H	1.4825586	-4.4253413	-2.6941751
H	2.6033224	-3.1842101	-0.8551500
C	-1.4640447	0.5093800	2.4004592
Cu	-3.4292924	0.2014843	0.3229593
P	-4.9127584	1.5046849	-0.7313198
P	-3.6615382	-2.0518138	0.0026240
C	-2.4633014	-2.9321382	1.0438907
C	-2.8525856	-3.4696226	2.2774785
C	-1.9013226	-4.0135089	3.1410651
C	-0.5520734	-4.0272796	2.7867213
C	-0.1560941	-3.4928274	1.5592653
C	-1.1021270	-2.9431724	0.6973711
H	-3.9089172	-3.4750253	2.5599435
H	-2.2258070	-4.4518917	4.0895298
H	0.1896209	-4.4712254	3.4571521
H	0.8984705	-3.5075604	1.2662466
H	-0.7796707	-2.5372202	-0.2664664
C	-3.3524615	-2.6665376	-1.6796130
C	-3.8116689	-1.8997861	-2.7635348
C	-3.5657186	-2.2824518	-4.0778871
C	-2.8585734	-3.4553329	-4.3336664
C	-2.4106880	-4.2433241	-3.2738362
C	-2.6587132	-3.8514950	-1.9598014
H	-3.9353048	-1.6513741	-4.8888731
H	-2.6642044	-3.7571593	-5.3664033
H	-1.8692764	-5.1727554	-3.4702088
H	-2.3000639	-4.4739700	-1.1360199
C	-5.2799652	-2.7245344	0.4473458
C	-5.6653747	-4.0235358	0.0897150
C	-6.9291825	-4.4937286	0.4332471

H	7.7903323	-5.2241340	2.3619512
H	7.4708696	-5.6296832	-0.0732589
H	6.1862106	-4.0098802	-1.4483135
C	6.1701267	-0.4045556	-1.4667239
C	5.7705372	0.7167694	-2.2110356
C	6.6801462	1.6948330	-2.5967785
C	8.0221539	1.5465399	-2.2484015
C	8.4489939	0.4258840	-1.5379373
C	7.5255451	-0.5422093	-1.1485244
O	4.4393029	0.7751610	-2.5376607
H	6.3400993	2.5683262	-3.1580685
H	8.7401252	2.3166205	-2.5434902
H	9.5037263	0.3089884	-1.2763182
H	7.8549670	-1.4069525	-0.5667511
C	4.1146592	-2.3591826	-2.1076570
C	4.6159161	-2.3393031	-3.4129357
C	3.9340459	-3.0025845	-4.4339521
C	2.7497513	-3.6872643	-4.1590827
C	2.2486129	-3.7174931	-2.8562456
C	2.9254570	-3.0535154	-1.8371808
H	5.5426232	-1.8015796	-3.6328360
H	4.3348842	-2.9890685	-5.4517715
H	2.2175513	-4.2034155	-4.9631335
H	1.3197597	-4.2520228	-2.6365652
H	2.5219111	-3.0553463	-0.8188037
C	-1.4596616	0.4922977	2.4130037
Cu	-3.3962779	0.1423364	0.3215675
P	-4.8767101	1.4436001	-0.7409773
P	-3.6879280	-2.1050247	0.0232238
C	-2.5165110	-2.9948052	1.0854469
C	-2.9358637	-3.5562781	2.2978576
C	-2.0033304	-4.1021633	3.1805549
C	-0.6446550	-4.0938398	2.8650588
C	-0.2193908	-3.5369109	1.6570923
C	-1.1463805	-2.9857199	0.7767905
H	-3.9995599	-3.5761421	2.5502301
H	-2.3492068	-4.5564082	4.1138335
H	0.0830559	-4.5365752	3.5515522
H	0.8435897	-3.5327867	1.3962828
H	-0.8009255	-2.5551499	-0.1680388
C	-3.3570651	-2.7292386	-1.6528102
C	-3.8153940	-1.9789284	-2.7487659
C	-3.5755187	-2.3853194	-4.0575021
C	-2.8692791	-3.5623394	-4.2960700
C	-2.4135305	-4.3293255	-3.2238318
C	-2.6589646	-3.9159682	-1.9159391
H	-3.9509084	-1.7699611	-4.8781003
H	-2.6819431	-3.8841263	-5.3241684
H	-1.8707280	-5.2608833	-3.4058139
H	-2.2986808	-4.5240493	-1.0821096
C	-5.3219170	-2.7626621	0.4316933
C	-5.7157972	-4.0549021	0.0590436
C	-6.9919682	-4.5114554	0.3741558

C	-7.8149102	-3.6719464	1.1346240
C	-7.4354838	-2.3801233	1.4953148
C	-6.1706041	-1.9063763	1.1512256
H	-4.9795998	-4.6662623	-0.4699138
H	-7.2290662	-5.5067292	0.1502235
H	-8.8095518	-4.0428714	1.3983489
H	-8.1302742	-1.7337725	2.0384418
H	-5.8727118	-0.8872261	1.4180432
C	-5.8316156	2.7262139	0.2331585
C	-5.9848880	2.5075794	1.6083954
C	-6.7302380	3.3970671	2.3803083
C	-7.3136822	4.5159090	1.7854639
C	-7.1527761	4.7453342	0.4177507
C	-6.4163637	3.8534190	-0.3585727
H	-5.5128642	1.6387350	2.0790516
H	-6.8518582	3.2190792	3.4525850
H	-7.8951694	5.2169134	2.3911980
H	-7.6065941	5.6250345	-0.0473620
H	-6.2933197	4.0355241	-1.4300936
C	-6.1913591	0.4352706	-1.4418942
C	-5.7756325	-0.6742812	-2.1950365
C	-6.6698155	-1.6680072	-2.5778690
C	-8.0113363	-1.5483885	-2.2168865
C	-8.4538405	-0.4403351	-1.4965741
C	-7.5461561	0.5442429	-1.1111111
O	-4.4467551	-0.7058423	-2.5328929
H	-6.3182299	-2.5311065	-3.1480661
H	-8.7165668	-2.3307020	-2.5103373
H	-9.5082594	-0.3454328	-1.2252395
H	-7.8878578	1.3999065	-0.5231759
C	-4.1982216	2.4377085	-2.1118824
C	-4.7278882	2.4058236	-3.4056715
C	-4.0913309	3.0941112	-4.4390926
C	-2.9255245	3.8171556	-4.1872040
C	-2.3970009	3.8597431	-2.8954078
C	-3.0286974	3.1705635	-1.8646391
H	-5.6407476	1.8383512	-3.6076489
H	-4.5126319	3.0684835	-5.4483106
H	-2.4279357	4.3526674	-5.0006527
H	-1.4825586	4.4253413	-2.6941751
H	-2.6033224	3.1842101	-0.8551500
C	1.4640447	-0.5093800	2.4004592
N	2.8214339	-0.4546625	2.2983005
N	3.3678108	-0.7377250	3.4317940
N	2.3812552	-1.0184797	4.2743850
C	1.1804070	-0.9051825	3.6844528
H	0.2677188	-1.1186175	4.2159886
C	2.6384784	-1.1769607	5.6919930
H	2.1504672	-2.1019254	6.0373323
H	3.7278241	-1.3086400	5.7858319
C	2.1503913	0.0131035	6.4867434
C	1.8705486	-0.1469298	7.8457754
C	1.4618413	0.9396124	8.6160881

C	-7.8817127	-3.6827293	1.0619922
C	-7.4935862	-2.3979120	1.4384374
C	-6.2162665	-1.9377214	1.1228856
H	-5.0262841	-4.7035376	-0.4891773
H	-7.2980604	-5.5194041	0.0799843
H	-8.8860147	-4.0427826	1.3034160
H	-8.1909823	-1.7465799	1.9720086
H	-5.9104735	-0.9245657	1.4028733
C	-5.7723158	2.6863272	0.2165911
C	-5.9423437	2.4687445	1.5901144
C	-6.6716825	3.3754633	2.3571493
C	-7.2216894	4.5097264	1.7595515
C	-7.0433667	4.7378335	0.3937344
C	-6.3229990	3.8292257	-0.3782215
H	-5.4948183	1.5885564	2.0633756
H	-6.8062157	3.1985285	3.4280176
H	-7.7903371	5.2241376	2.3619569
H	-7.4708713	5.6296868	-0.0732634
H	-6.1862111	4.0098788	-1.4483068
C	-6.1701057	0.4045451	-1.4667370
C	-5.7705461	-0.7167715	-2.2110340
C	-6.6801184	-1.6948215	-2.5967782
C	-8.0221774	-1.5465876	-2.2484209
C	-8.4490436	-0.4258749	-1.5379230
C	-7.5255460	0.5422520	-1.1484984
O	-4.4393169	-0.7751464	-2.5376569
H	-6.3401017	-2.5683261	-3.1580675
H	-8.7401098	-2.3166023	-2.5434828
H	-9.5037008	-0.3089920	-1.2763246
H	-7.8549618	1.4069346	-0.5667636
C	-4.1146690	2.3591766	-2.1076589
C	-4.6159108	2.3393060	-3.4129364
C	-3.9340442	3.0025848	-4.4339474
C	-2.7497494	3.6872585	-4.1590582
C	-2.2486434	3.7174765	-2.8562562
C	-2.9254396	3.0535289	-1.8371931
H	-5.5426245	1.8015771	-3.6328356
H	-4.3348860	2.9890673	-5.4517744
H	-2.2175477	4.2034211	-4.9631424
H	-1.3197477	4.2520296	-2.6365621
H	-2.5219107	3.0553446	-0.8188002
C	1.4596629	-0.4922990	2.4130028
N	2.8154565	-0.4181886	2.3050345
N	3.3752680	-0.6979178	3.4339958
N	2.3990501	-0.9937679	4.2814116
C	1.1924534	-0.8970480	3.6982174
H	0.2858339	-1.1178901	4.2371304
C	2.6652562	-1.1395330	5.6982552
H	2.1929838	-2.0689163	6.0534444
H	3.7568798	-1.2536181	5.7886867
C	2.1621376	0.0495253	6.4855059
C	1.8687932	-0.1066153	7.8420478
C	1.4438571	0.9801802	8.6034939

C	1.3066369	2.1952494	8.0309815
C	1.5758528	2.3597023	6.6726193
C	2.0047754	1.2776346	5.9042555
H	1.9736642	-1.1323576	8.3106489
H	1.2567497	0.8014678	9.6813365
H	0.9860161	3.0481014	8.6358898
H	1.4711469	3.3446197	6.2082450
H	2.2456035	1.4368300	4.8476139
N	-2.8214339	0.4546625	2.2983005
N	-3.3678108	0.7377250	3.4317940
N	-2.3812552	1.0184797	4.2743850
C	-1.1804070	0.9051825	3.6844528
H	-0.2677188	1.1186175	4.2159886
C	-2.6384784	1.1769607	5.6919930
H	-2.1504672	2.1019254	6.0373323
H	-3.7278241	1.3086400	5.7858319
C	-2.1503913	-0.0131035	6.4867434
C	-1.8705486	0.1469298	7.8457754
C	-1.4618413	-0.9396124	8.6160881
C	-1.3066369	-2.1952494	8.0309815
C	-1.5758528	-2.3597023	6.6726193
C	-2.0047754	-1.2776346	5.9042555
H	-1.9736642	1.1323576	8.3106489
H	-1.2567497	-0.8014678	9.6813365
H	-0.9860161	-3.0481014	8.6358898
H	-1.4711469	-3.3446197	6.2082450
H	-2.2456035	-1.4368300	4.8476139

C	1.2860294	2.2321693	8.0114106
C	1.5681671	2.3925892	6.6549894
C	2.0127941	1.3105312	5.8958659
H	1.9731215	-1.0895795	8.3118127
H	1.2278995	0.8449712	9.6670183
H	0.9529049	3.0853948	8.6091494
H	1.4602433	3.3740340	6.1840756
H	2.2604669	1.4661741	4.8402836
N	-2.8154741	0.4181933	2.3050524
N	-3.3752678	0.6979094	3.4339625
N	-2.3990342	0.9937751	4.2814419
C	-1.1924451	0.8970497	3.6982100
H	-0.2858370	1.1178910	4.2371307
C	-2.6652967	1.1395109	5.6982345
H	-2.1929729	2.0689317	6.0534498
H	-3.7568570	1.2536188	5.7886872
C	-2.1621333	-0.0495236	6.4855093
C	-1.8687946	0.1066120	7.8420447
C	-1.4438583	-0.9801808	8.6034897
C	-1.2860297	-2.2321656	8.0114109
C	-1.5681675	-2.3925840	6.6549921
C	-2.0127953	-1.3105324	5.8958685
H	-1.9731223	1.0895804	8.3118139
H	-1.2278995	-0.8449712	9.6670186
H	-0.9529041	-3.0853972	8.6091510
H	-1.4602431	-3.3740337	6.1840757
H	-2.2604675	-1.4661738	4.8402835

4 S_0 state:

C	0.0629814	0.5448324	-5.1138637
C	0.5367251	1.1324212	-3.9827934
C	-0.6373406	-0.6842013	-5.0464722
C	-0.8457909	-1.2946031	-3.8494558
C	0.8160632	1.1144899	-1.5407032
C	0.3412845	0.5294973	-2.7121741
C	-0.3675124	-0.7159682	-2.6442881
C	-0.5695292	-1.3227269	-1.4071892
C	-0.0931182	-0.7333410	-0.2469778
C	0.6104629	0.5058817	-0.3122452
H	0.2187782	1.0169489	-6.0797248
H	1.0741223	2.0763147	-4.0291647
H	-1.0089003	-1.1368683	-5.9613810
H	-1.3838970	-2.2374407	-3.7915175
H	1.3533129	2.0582283	-1.5701831
H	-1.1070453	-2.2637767	-1.3303873
N	-0.2977965	-1.3421881	0.9554973
N	1.0822598	1.0956107	0.8239840
C	0.1532194	-0.7545840	2.0140221
C	0.8677043	0.5010983	1.9576910
C	1.3735702	1.1473326	3.2061638
H	0.5399987	1.4243958	3.8762661
H	2.0359482	0.4696403	3.7730747
C	-0.0524049	-1.4169880	3.3550003

4 T_1 state:

C	0.1020587	0.8638700	-5.3152862
C	-0.2716551	1.3226466	-4.0434516
C	0.7875587	-0.3195139	-5.4413479
C	1.1125856	-1.0657016	-4.2987674
C	-0.3290087	1.0467249	-1.6035591
C	0.0398932	0.6004249	-2.8995304
C	0.7534838	-0.6299096	-3.0306451
C	1.0745839	-1.3668421	-1.8606113
C	0.7096848	-0.9173479	-0.5628434
C	-0.0086281	0.3092318	-0.4310466
H	-0.1533037	1.4482537	-6.1939078
H	-0.8145210	2.2593250	-3.9426285
H	1.0812015	-0.6832362	-6.4213065
H	1.6556722	-2.0022763	-4.3996367
H	-0.8753195	1.9778042	-1.4804462
H	1.6206804	-2.3029266	-1.9388913
N	1.0392483	-1.6281938	0.5073176
N	-0.3815850	0.7675515	0.7570574
C	0.6633269	-1.1446061	1.7074304
C	-0.0533612	0.0357019	1.8411375
C	-0.4952232	0.5638793	3.1671024
H	-0.9821528	-0.2140215	3.7786261
H	0.3644863	0.9465002	3.7471983
C	1.0364121	-1.9931572	2.8878654

H	0.9228412	-1.7442129	3.7564316
H	-0.4776291	-0.7007972	4.0733284
N	-0.9566669	-2.5293596	3.3245330
C	-0.8126509	-3.7312893	2.7416370
C	-1.9962004	-4.3823564	2.9967557
N	-2.7807355	-3.5305622	3.7138018
N	-2.1561177	-2.4225590	3.9047833
H	0.0777564	-4.0019988	2.1986085
C	-2.4365298	-5.7210594	2.6182446
C	-1.6306565	-6.5537340	1.8295666
C	-2.0605493	-7.8291910	1.4744560
C	-3.3052956	-8.2937486	1.9005749
C	-4.1145682	-7.4702838	2.6842683
C	-3.6861673	-6.1949177	3.0413729
H	-0.6545227	-6.1995733	1.4853916
H	-1.4183652	-8.4656068	0.8581726
H	-3.6439666	-9.2958332	1.6214025
H	-5.0926100	-7.8260668	3.0222207
H	-4.3146311	-5.5449253	3.6543709
H	1.9319296	2.0561756	2.9417756

H	1.9379015	-2.5689536	2.6344483
H	1.2263852	-1.3948119	3.7876981
N	-0.0246879	-2.9139826	3.2494235
C	-0.5728133	-3.8909838	2.5060423
C	-1.5554740	-4.4231749	3.3097327
N	-1.5390281	-3.7327651	4.4821300
N	-0.6213563	-2.8280682	4.4386213
H	-0.2262822	-4.1037674	1.5068847
C	-2.4916748	-5.5148392	3.0601707
C	-2.5227318	-6.1766646	1.8250561
C	-3.4205833	-7.2163118	1.5991603
C	-4.3035333	-7.6115725	2.6045825
C	-4.2794341	-6.9572766	3.8368608
C	-3.3823240	-5.9177956	4.0649747
H	-1.8379901	-5.8733223	1.0276764
H	-3.4319604	-7.7216102	0.6287094
H	-5.0095469	-8.4282994	2.4275034
H	-4.9683078	-7.2609252	4.6309707
H	-3.3574414	-5.4013003	5.0271472
H	-1.1974738	1.3943539	3.0072515

5 S_0 state:

C	0.1499296	0.6921241	-6.0185369
C	0.2955187	1.3672619	-4.8475096
C	-0.1499296	-0.6921241	-6.0185369
C	-0.2955187	-1.3672619	-4.8475096
C	0.2935347	1.3739660	-2.3906129
C	0.1508264	0.7016401	-3.6016547
C	-0.1508264	-0.7016401	-3.6016547
C	-0.2935347	-1.3739660	-2.3906129
C	-0.1478513	-0.6981300	-1.1894863
C	0.1478513	0.6981300	-1.1894863
H	0.2631904	1.2125295	-6.9652544
H	0.5260134	2.4295608	-4.8418660
H	-0.2631904	-1.2125295	-6.9652544
H	-0.5260134	-2.4295608	-4.8418660
H	0.5240560	2.4352921	-2.3671827
H	-0.5240560	-2.4352921	-2.3671827
N	-0.2866997	-1.3689722	-0.0117945
N	0.2866997	1.3689722	-0.0117945
C	-0.1506638	-0.7047990	1.0886385
C	0.1506638	0.7047990	1.0886385
C	0.2864269	1.4429874	2.4005341
H	-0.7108915	1.5689437	2.8575746
H	0.9045006	0.8674912	3.1052520
N	0.9207117	2.7221389	2.2768299
C	0.4519892	3.8613265	1.7395414
C	1.5028573	4.7428615	1.8312419
N	2.5399307	4.0778104	2.4126018
N	2.1889983	2.8686785	2.6736856
H	-0.5451090	3.9381231	1.3380654
C	1.6021258	6.1385207	1.4166647
C	0.5340161	6.7826025	0.7771135

5 T_1 state:

C	-0.4525939	0.5166028	-6.8663924
C	-0.9132610	1.0431299	-5.6516561
C	0.4527759	-0.5171266	-6.8662205
C	0.9134517	-1.0427890	-5.6511976
C	-0.9243556	1.0545493	-3.1956689
C	-0.4703016	0.5373435	-4.4368524
C	0.4700759	-0.5366246	-4.4367455
C	0.9239270	-1.0540100	-3.1956621
C	0.4726649	-0.5361771	-1.9534017
C	-0.4730954	0.5365128	-1.9533697
H	-0.8148330	0.9297952	-7.8027031
H	-1.6295680	1.8610907	-5.6520810
H	0.8149945	-0.9309270	-7.8023042
H	1.6301462	-1.8603871	-5.6507936
H	-1.6433296	1.8688150	-3.1736551
H	1.6428202	-1.8683126	-3.1737803
N	0.9320588	-1.0426587	-0.8169092
N	-0.9324346	1.0427310	-0.8167502
C	0.4676591	-0.5086624	0.3312730
C	-0.4679282	0.5085621	0.3313502
C	-1.0082598	1.1302015	1.5896425
H	-2.0245057	1.4929308	1.3879577
H	-1.0386768	0.4204067	2.4260478
N	-0.1957157	2.2569588	2.0031048
C	-0.1851668	3.5075460	1.5107010
C	0.8589698	4.1247233	2.1616065
N	1.4155666	3.2058929	2.9966485
N	0.7827534	2.0872328	2.8914136
H	-0.8950603	3.8303894	0.7661562
C	1.3578097	5.4924473	2.0596269
C	0.8150399	6.3946907	1.1344342

C	0.6398215	8.1142136	0.3855860
C	1.8166659	8.8242965	0.6257031
C	2.8851282	8.1899072	1.2605273
C	2.7811646	6.8586811	1.6537520
H	-0.3930129	6.2360876	0.5803686
H	-0.2038964	8.6016477	-0.1121061
H	1.9004848	9.8707955	0.3181675
H	3.8116783	8.7393238	1.4526559
H	3.6135358	6.3561265	2.1515005
C	-0.2864269	-1.4429874	2.4005341
H	0.7108915	-1.5689437	2.8575746
H	-0.9045006	-0.8674912	3.1052520
N	-0.9207117	-2.7221389	2.2768299
C	-0.4519892	-3.8613265	1.7395414
C	-1.5028573	-4.7428615	1.8312419
N	-2.5399307	-4.0778104	2.4126018
N	-2.1889983	-2.8686785	2.6736856
H	0.5451090	-3.9381231	1.3380654
C	-1.6021258	-6.1385207	1.4166647
C	-0.5340161	-6.7826025	0.7771135
C	-0.6398215	-8.1142136	0.3855860
C	-1.8166659	-8.8242965	0.6257031
C	-2.8851282	-8.1899072	1.2605273
C	-2.7811646	-6.8586811	1.6537520
H	0.3930129	-6.2360876	0.5803686
H	0.2038964	-8.6016477	-0.1121061
H	-1.9004848	-9.8707955	0.3181675
H	-3.8116783	-8.7393238	1.4526559
H	-3.6135358	-6.3561265	2.1515005

C	1.2991121	7.6967681	1.0448056
C	2.3356264	8.1184876	1.8782172
C	2.8822283	7.2259669	2.8011551
C	2.3989590	5.9238734	2.8932298
H	0.0050880	6.0745518	0.4724093
H	0.8641759	8.3879324	0.3165660
H	2.7166671	9.1415826	1.8082227
H	3.6949838	7.5486269	3.4589297
H	2.8209492	5.2202470	3.6143582
C	1.0082908	-1.1301982	1.5894900
H	2.0248706	-1.4920560	1.3879627
H	1.0380006	-0.4205186	2.4260136
N	0.1963106	-2.2573401	2.0030008
C	0.1856728	-3.5081254	1.5110444
C	-0.8585955	-4.1249209	2.1621641
N	-1.4150853	-3.2057931	2.9968910
N	-0.7821660	-2.0872603	2.8912464
H	0.8957444	-3.8317166	0.7669680
C	-1.3578672	-5.4924733	2.0602255
C	-0.8151824	-6.3945467	1.1348595
C	-1.2992632	-7.6965633	1.0448231
C	-2.3358418	-8.1184317	1.8780171
C	-2.8824070	-7.2260833	2.8011619
C	-2.3991824	-5.9239683	2.8936164
H	-0.0051765	-6.0742574	0.4730214
H	-0.8642977	-8.3876233	0.3165209
H	-2.7167542	-9.1415481	1.8075123
H	-3.6951061	-7.5489410	3.4588878
H	-2.8213820	-5.2205487	3.6148602

6 S_0 state:

C	0.0045840	0.7080611	-4.4330326
C	0.0088369	1.3975522	-3.2608073
C	-0.0045840	-0.7080611	-4.4330326
C	-0.0088369	-1.3975522	-3.2608073
C	0.0160709	1.4026563	-0.8022753
C	0.0040725	0.7174133	-2.0144098
C	-0.0040725	-0.7174133	-2.0144098
C	-0.0160709	-1.4026563	-0.8022753
C	-0.0166165	-0.7137211	0.4015413
C	0.0166165	0.7137211	0.4015413
H	0.0082007	1.2413676	-5.3794471
H	0.0164135	2.4847544	-3.2551547
H	-0.0082007	-1.2413676	-5.3794471
H	-0.0164135	-2.4847544	-3.2551547
H	0.0419612	2.4885823	-0.7794215
H	-0.0419612	-2.4885823	-0.7794215
N	-0.1031151	-1.3985665	1.5738754
N	0.1031151	1.3985665	1.5738754
C	-0.0949286	-0.7188630	2.6838367
C	0.0949286	0.7188630	2.6838367
C	-0.3378111	-1.4635130	3.9158576
C	0.3378111	1.4635130	3.9158576

6 T_1 state:

C	-0.0626808	0.6844721	-4.3662786
C	-0.1249477	1.3803834	-3.1516132
C	0.0626852	-0.6844634	-4.3662757
C	0.1249485	-1.3803720	-3.1516143
C	-0.1101996	1.3981796	-0.6936323
C	-0.0629390	0.7111791	-1.9367252
C	0.0629473	-0.7111675	-1.9367262
C	0.1102002	-1.3981886	-0.6936335
C	0.0359680	-0.7144939	0.5463220
C	-0.0359624	0.7144936	0.5463116
H	-0.1130676	1.2317292	-5.3027021
H	-0.2222121	2.4634099	-3.1509681
H	0.1130691	-1.2317152	-5.3027058
H	0.2222183	-2.4634017	-3.1509738
H	-0.1772465	2.4825187	-0.6724947
H	0.1772430	-2.4825072	-0.6725025
N	-0.0024220	-1.3955702	1.6814881
N	0.0024283	1.3955654	1.6814899
C	-0.0583327	-0.6948601	2.8350702
C	0.0583382	0.6948579	2.8350700
C	-0.2905153	-1.4887723	4.0314370
C	0.2905209	1.4887719	4.0314417

C	-0.0580411	2.7365705	4.2379497
N	0.4787391	2.9497787	5.4492834
N	1.1881333	1.8885943	5.8509826
N	1.1028220	0.9898670	4.9338726
H	-0.6503769	3.4697179	3.7153959
C	0.3841416	4.1255905	6.2867470
H	-0.6645862	4.2694043	6.5932714
H	0.9687359	3.8830024	7.1878934
C	0.9096614	5.3642063	5.6073623
C	2.1698255	5.3553209	4.9982997
C	2.6621360	6.5024808	4.3826274
C	1.9020569	7.6737549	4.3707310
C	0.6465875	7.6895790	4.9743457
C	0.1523569	6.5370523	5.5863886
H	2.7656032	4.4367459	5.0034375
H	3.6473961	6.4832999	3.9076200
H	2.2897729	8.5745282	3.8858384
H	0.0428766	8.6018766	4.9646186
H	-0.8379456	6.5501547	6.0537771
C	0.0580411	-2.7365705	4.2379497
N	-0.4787391	-2.9497787	5.4492834
N	-1.1881333	-1.8885943	5.8509826
N	-1.1028220	-0.9898670	4.9338726
H	0.6503769	-3.4697179	3.7153959
C	-0.3841416	-4.1255905	6.2867470
H	0.6645862	-4.2694043	6.5932714
H	-0.9687359	-3.8830024	7.1878934
C	-0.9096614	-5.3642063	5.6073623
C	-2.1698255	-5.3553209	4.9982997
C	-2.6621360	-6.5024808	4.3826274
C	-1.9020569	-7.6737549	4.3707310
C	-0.6465875	-7.6895790	4.9743457
C	-0.1523569	-6.5370523	5.5863886
H	-2.7656032	-4.4367459	5.0034375
H	-3.6473961	-6.4832999	3.9076200
H	-2.2897729	-8.5745282	3.8858384
H	-0.0428766	-8.6018766	4.9646186
H	0.8379456	-6.5501547	6.0537771

C	-0.0983001	2.7822787	4.2799117
N	0.4178058	3.0556448	5.4887047
N	1.1109025	2.0105330	5.9580135
N	1.0361481	1.0664544	5.0878777
H	-0.6720359	3.4917909	3.7067558
C	0.3282358	4.2765653	6.2566809
H	-0.7240493	4.4606565	6.5282000
H	0.8844240	4.0723872	7.1851858
C	0.8989717	5.4665384	5.5277590
C	2.1537164	5.3854686	4.9130430
C	2.6888291	6.4903594	4.2567830
C	1.9778197	7.6910440	4.2090122
C	0.7275410	7.7783760	4.8174488
C	0.1902443	6.6682482	5.4700342
H	2.7110887	4.4437184	4.9459002
H	3.6693928	6.4144799	3.7776865
H	2.3991531	8.5583794	3.6921473
H	0.1614198	8.7137619	4.7794912
H	-0.7963319	6.7375069	5.9404487
C	0.0982865	-2.7822908	4.2799012
N	-0.4178066	-3.0556484	5.4887016
N	-1.1108925	-2.0105250	5.9580183
N	-1.0361324	-1.0664478	5.0878730
H	0.6720115	-3.4918091	3.7067486
C	-0.3282414	-4.2765623	6.2566875
H	0.7240533	-4.4606601	6.5281980
H	-0.8844244	-4.0723888	7.1851897
C	-0.8989806	-5.4665323	5.5277641
C	-2.1537161	-5.3854711	4.9130469
C	-2.6888324	-6.4903660	4.2567845
C	-1.9778221	-7.6910472	4.2090263
C	-0.7275415	-7.7783753	4.8174605
C	-0.1902451	-6.6682547	5.4700374
H	-2.7110934	-4.4437162	4.9458970
H	-3.6693959	-6.4144860	3.7776889
H	-2.3991564	-8.5583896	3.6921570
H	-0.1614192	-8.7137670	4.7795039
H	0.7963318	-6.7375028	5.9404569

5.2 Calculated electronic spectra and natural transition orbitals (NTOs)

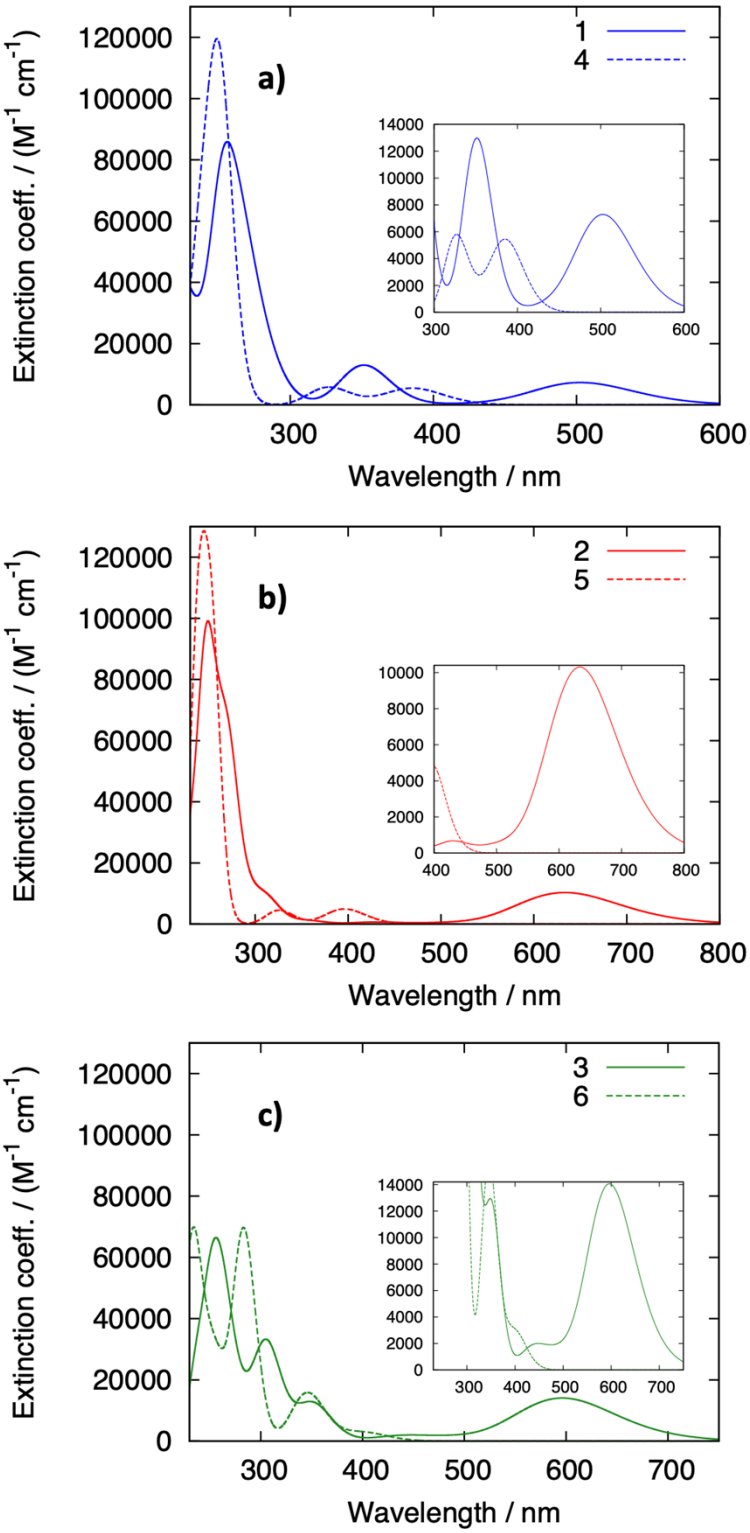


Figure S5.1. Absorption spectra (FWHM = 0.4 eV) of compounds **1-6** calculated using PBE0 ev*GW*-BSE/def2-TZVP at the optimized S_0 geometries. Inset: zoom-in in the range of MLCT.

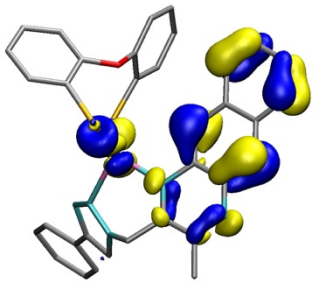
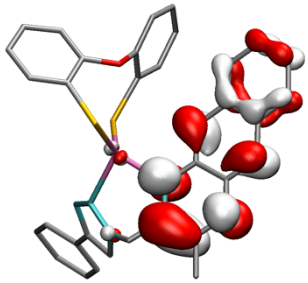
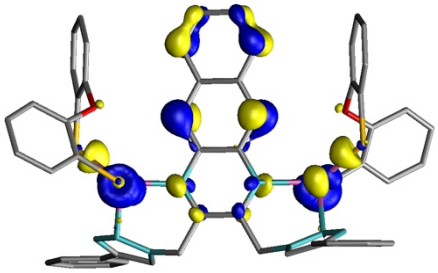
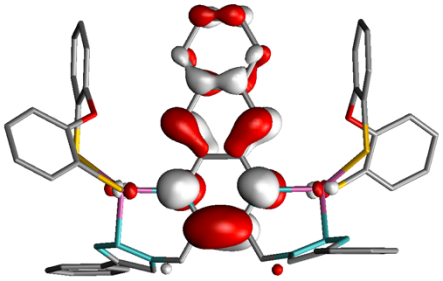
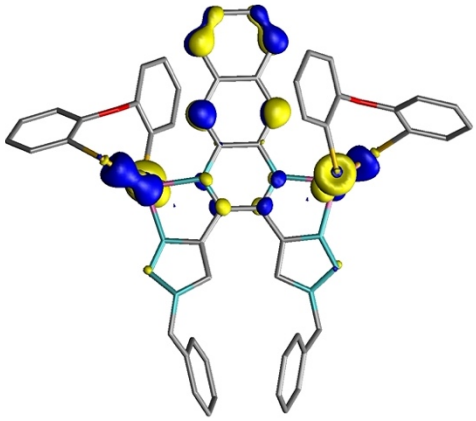
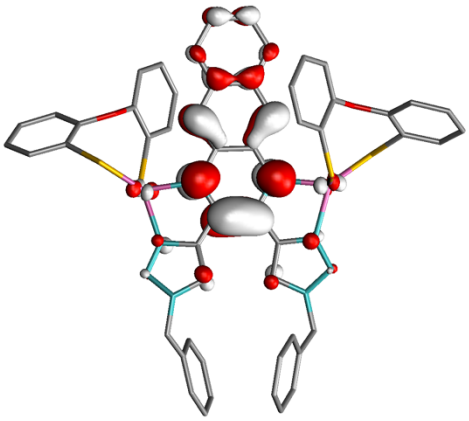
complex	λ_{abs}/nm	hole NTO	particle NTO
1	503		
2	634		
3	597		

Figure S5.2. Dominating occupied (blue/yellow) and virtual (red/white) natural transition orbitals (NTOs, iso-value: $\pm 0.04 a_0^{-3/2}$) of the MLCT excitation (S_1) in the visible region calculated using PBE0 ev*GW*-BSE/def2-TZVP at the optimized S_0 geometries. Phenyl groups of DPEPhos and all hydrogen atoms are omitted for clarity. Color code: C (silver), N (cyan), O (red), P (yellow), Cu (mauve).

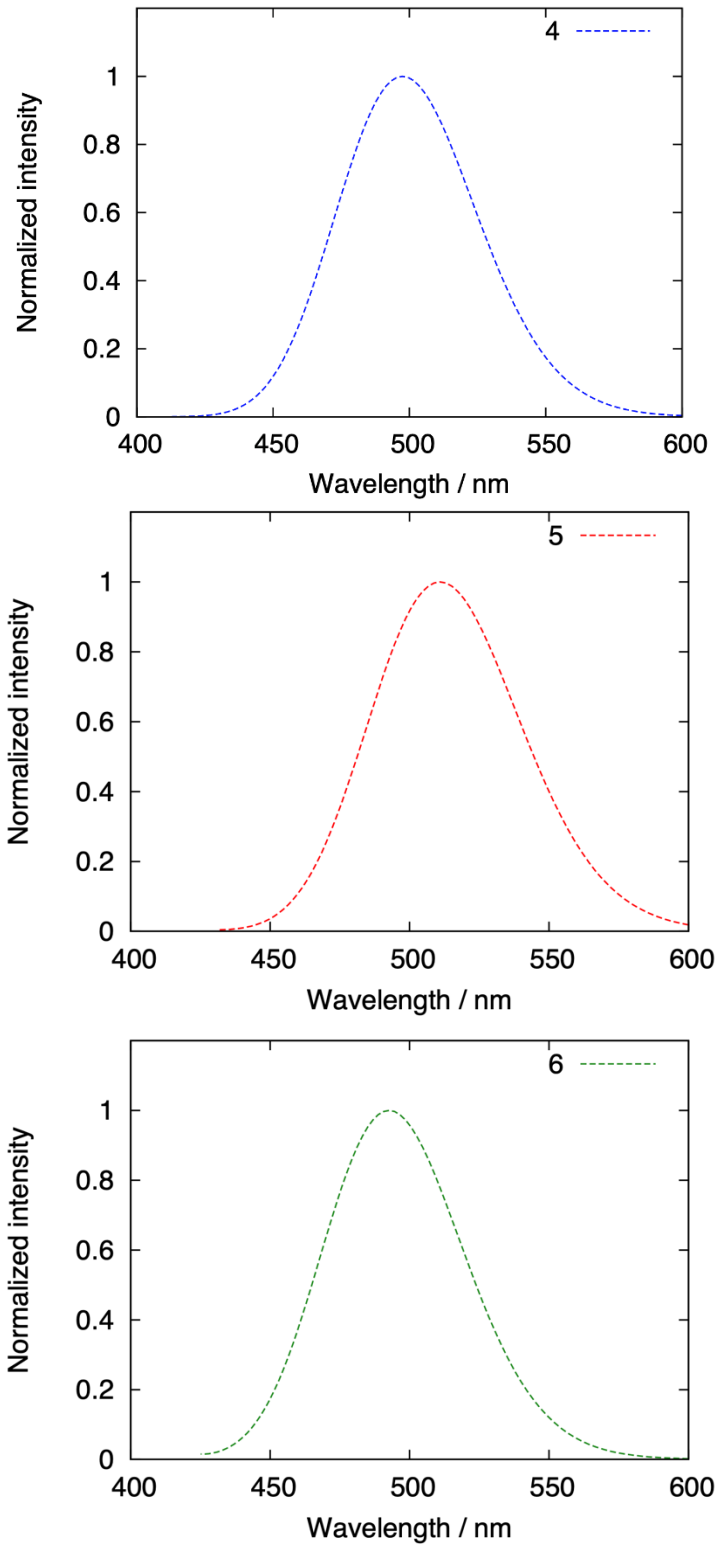


Figure S5.3. Emission spectra (FWHM = 0.3 eV) of compounds **4**-**6** calculated using PBE0 ev*GW*-BSE/x2c-TZVPall-2c at the optimized T_1 geometries.

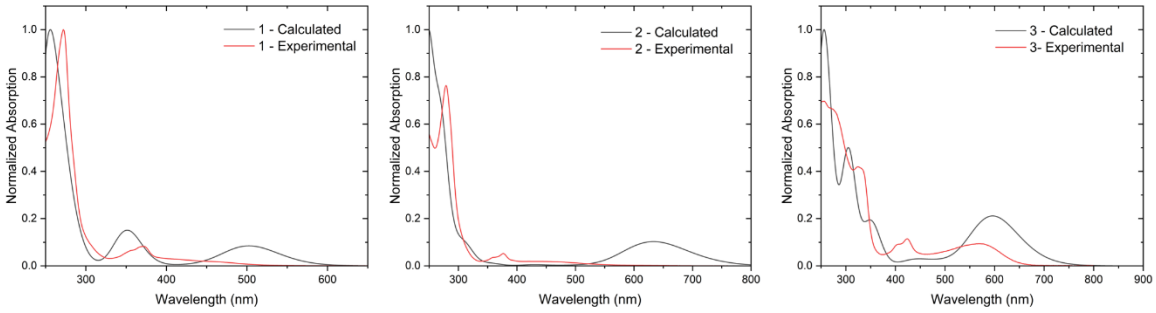


Figure S5.4. Comparison between the calculated (black curve) and experimental (red curve) absorption spectra of the complexes: **1** (left), **2** (middle), **3** (right).

6. Single crystal X-ray analysis

Single crystal X-ray diffraction data of compound **1** were collected on a STOE STADI VARI diffractometer with monochromated Ga Kα (1.34143 Å) radiation at 150 K. Using Olex2 [1], the structures were solved with the ShelXT [2] structure solution program using Intrinsic Phasing and refined with the ShelXL [3] refinement package using Least Squares minimization. Refinement was performed with anisotropic temperature factors for all non-hydrogen atoms (disordered atoms were refined isotropically); hydrogen atoms were calculated on idealized positions. Crystal data and refinement parameters of **1** are summarized in table S1.

Crystallographic data for compounds **1** reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as supplementary information no. CCDC-2074014. Copies of the data can be obtained free of charge from https://www.ccdc.cam.ac.uk/structures/.

Table S1 Crystal data and structure refinement for **1**.

Empirical formula	$C_{60}H_{49}BCl_4CuF_4N_5OP_2$
Formula weight	1210.13
Temperature/K	150
Crystal system	triclinic
Space group	*P*1
a/Å	14.6581(6)
b/Å	15.3265(7)
c/Å	16.0358(5)
α/°	62.258(3)

β/°	79.347(3)
γ/°	62.225(3)
Volume/Å^3	2818.7(2)
Z	2
ρ_{calc}g/cm^3	1.426
μ/mm^{-1}	3.899
F(000)	1240.0
Crystal size/mm^3	0.18 × 0.16 × 0.14
Radiation	GaKα (λ = 1.34143)
2Θ range for data collection/°	5.422 to 125.132
Index ranges	-19 ≤ h ≤ 12, -20 ≤ k ≤ 13, -21 ≤ l ≤ 21
Reflections collected	38702
Independent reflections	13345 [R_{int} = 0.0209, R_{sigma} = 0.0277]
Ind. Refl. with I≥2σ (I)	10663
Data/restraints/parameters	13345/0/704
Goodness-of-fit on F^2	1.048
Final R indexes [I≥2σ (I)]	R_1 = 0.0752, wR_2 = 0.2275
Final R indexes [all data]	R_1 = 0.0904, wR_2 = 0.2424
Largest diff. peak/hole / e Å^{-3}	1.29/-1.58

7. References

[1] O.V. Dolomanov, L.J. Bourhis, R.J. Gildea, J.A.K. Howard, H. Puschmann, *J. Appl. Cryst.* **2009**, *42*, 339–341.

[2] G.M. Sheldrick, *Acta Cryst. A* **2015**, *A71*, 3–8.

[3] G.M. Sheldrick, *Acta Cryst. C* **2015**, *C71*, 3–8.