

Supporting Information for

Synthesis, structure, and excited state kinetics of heteroleptic Cu(I) complexes with a new sterically demanding phenanthroline ligand

Lars Kohler,¹ Ryan G. Hadt,¹ Dugan Hayes,¹ Lin X. Chen,^{1,2} and Karen L. Mulfort^{1}*

¹Division of Chemical Sciences and Engineering, Argonne National Laboratory, 9700 South Cass Avenue, Argonne, IL 60439; ²Department of Chemistry, Northwestern University, 2145 Sheridan Road, Evanston, IL 60208

*To whom correspondence should be addressed. E-mail: mulfort@anl.gov

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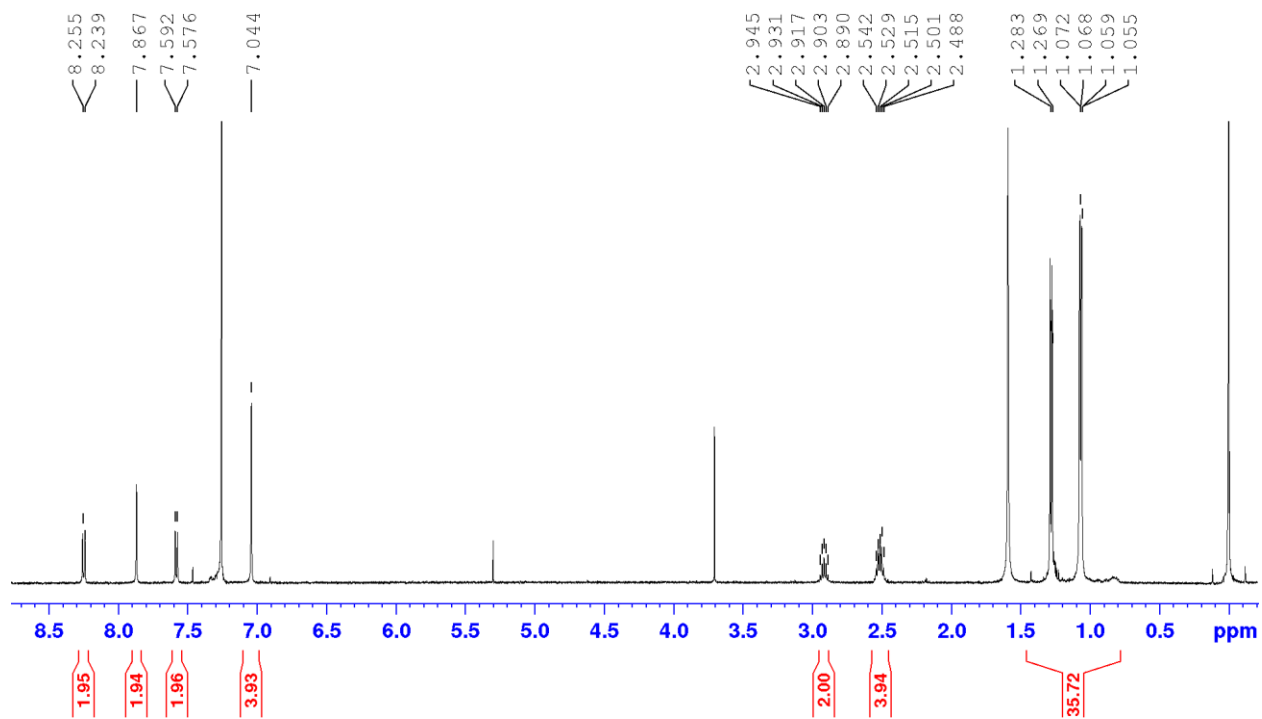


Figure S1. ^1H NMR spectrum of compound **bL2** in CDCl_3 .

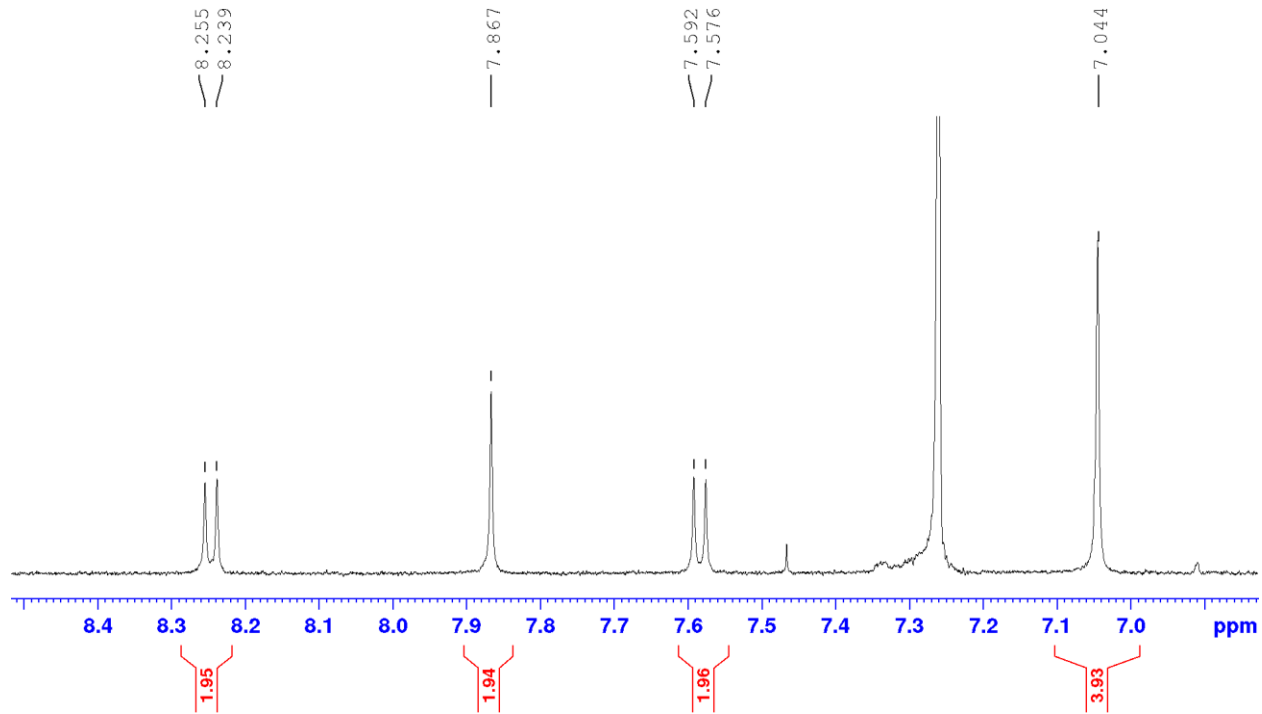


Figure S2. Aromatic region of ^1H NMR spectrum of compound **bL2** in CDCl_3 .

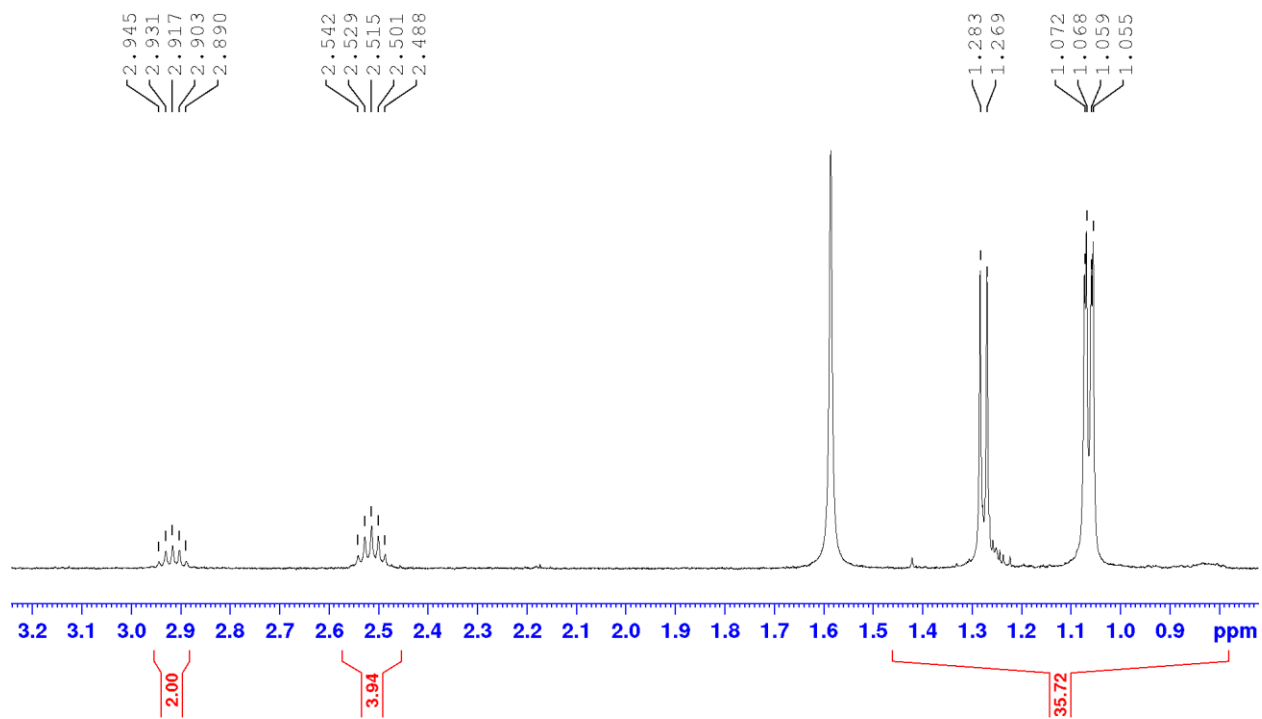


Figure S3. Aliphatic region of ^1H NMR spectrum of compound **bL2** in CDCl_3 .

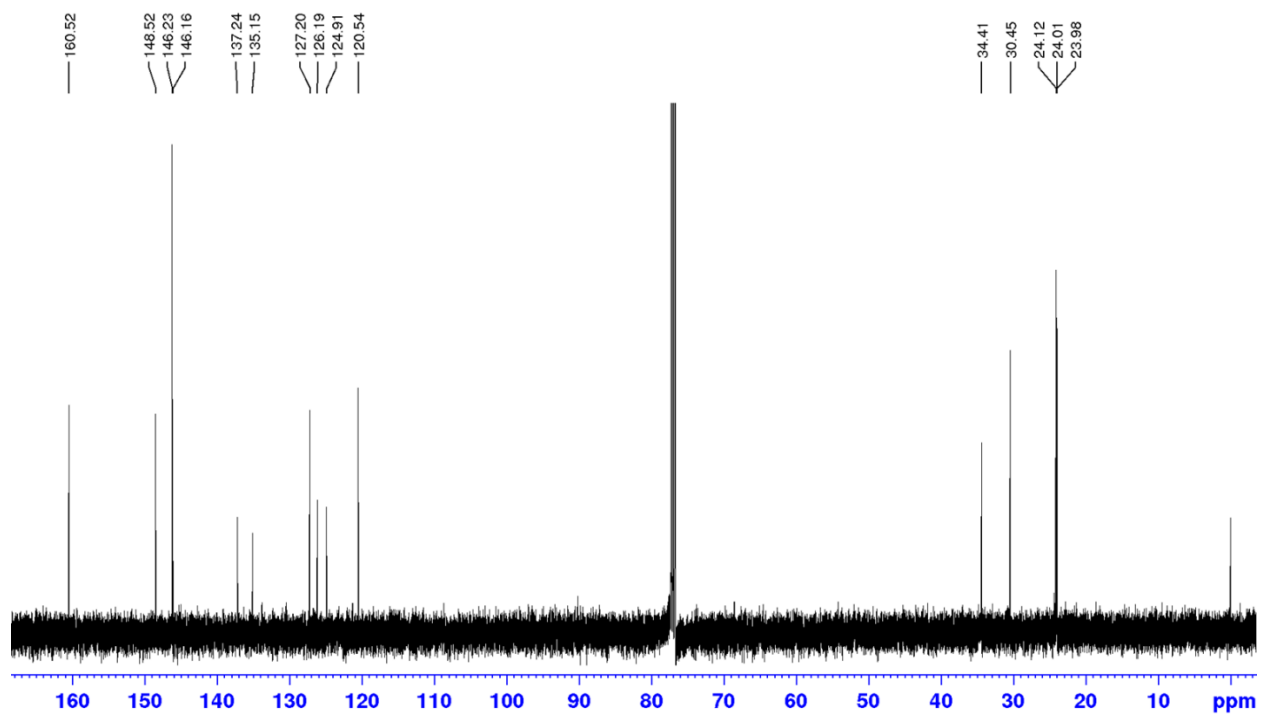


Figure S4. ^{13}C NMR spectrum of compound **bL2** in CDCl_3 .

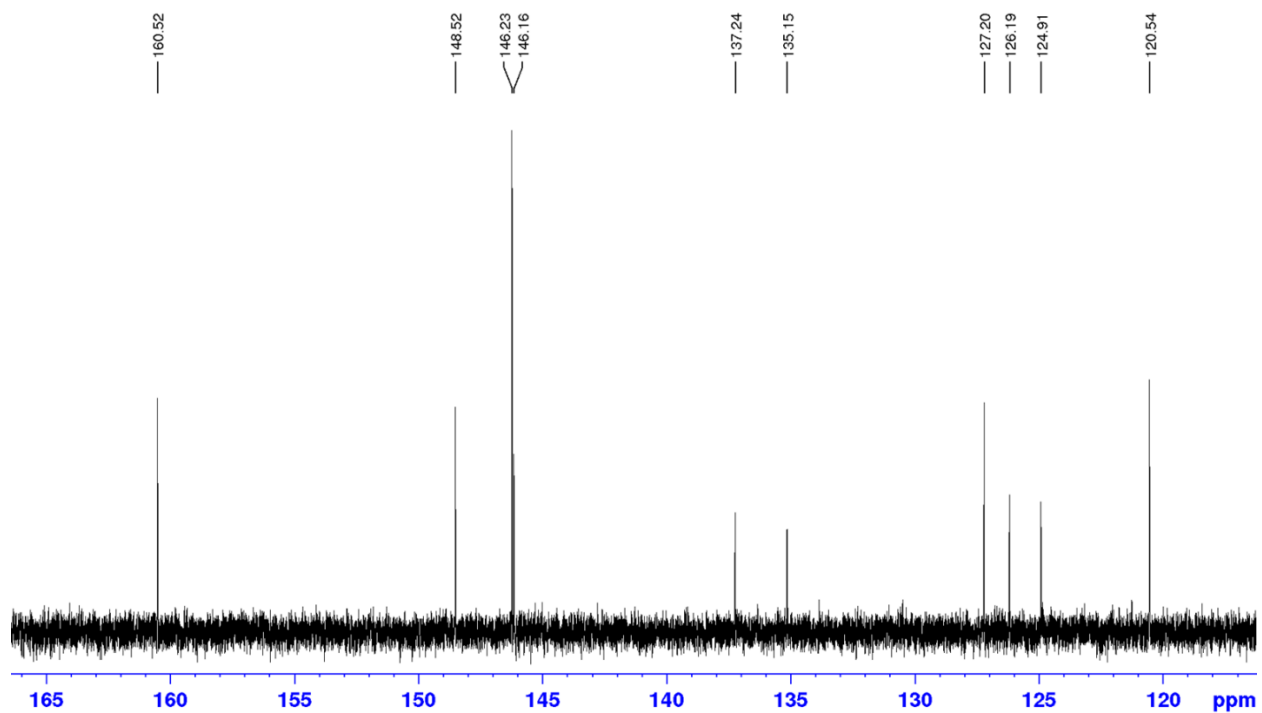


Figure S5. Aromatic region of ^{13}C NMR spectrum of compound **bL2** in CDCl_3 .

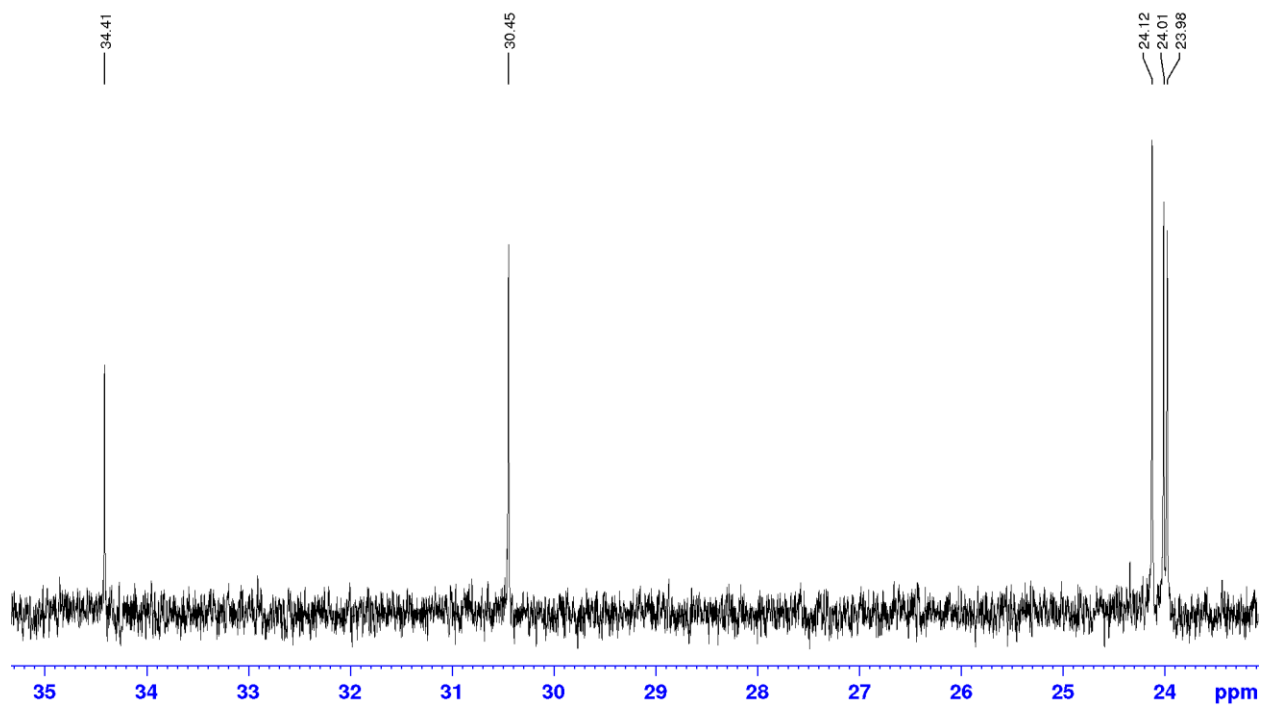


Figure S6. Aliphatic region of ^{13}C NMR spectrum of compound **bL2** in CDCl_3 .

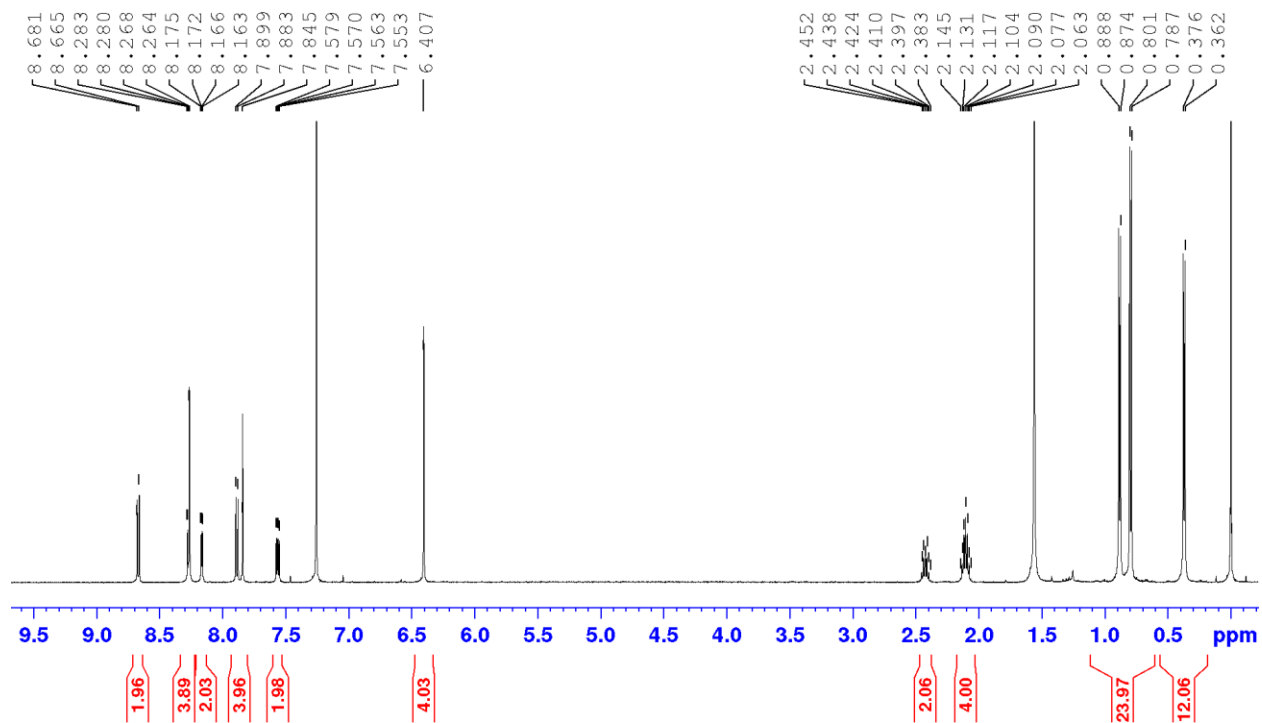


Figure S7. ^1H NMR of **3** in CDCl_3 .

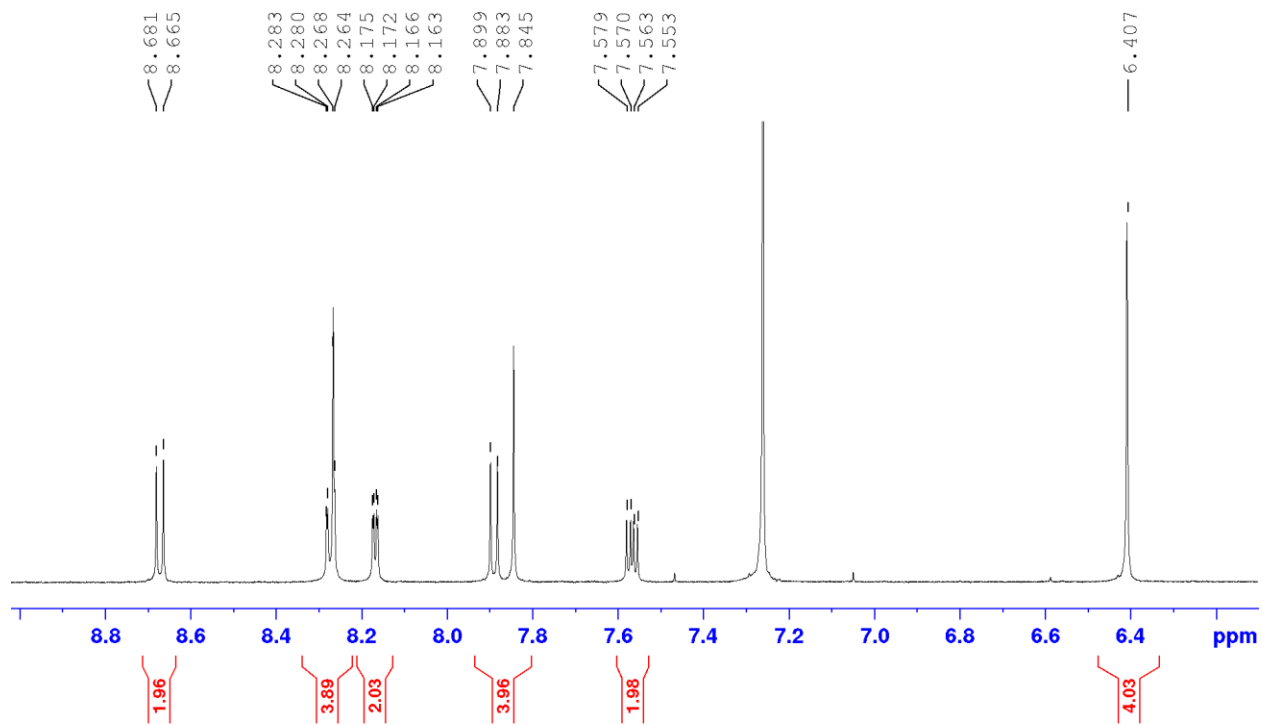


Figure S8. Aromatic region of ^1H NMR spectrum of **3** in CDCl_3 .

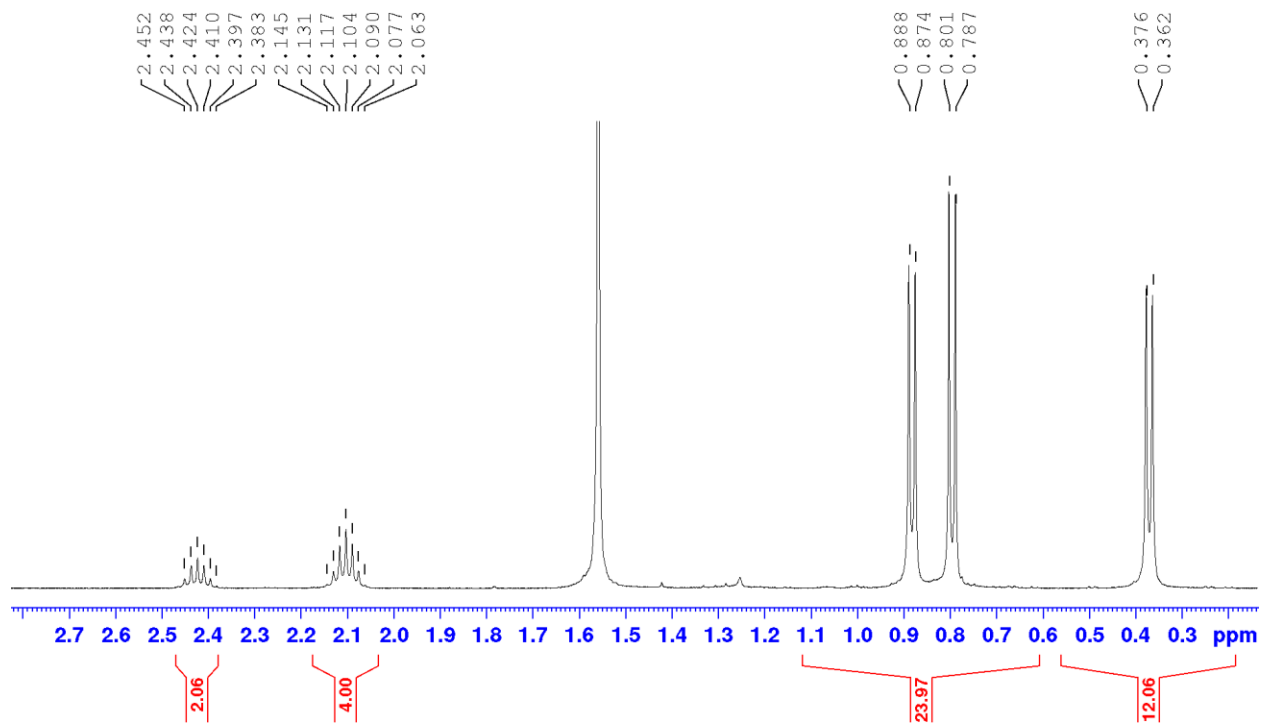


Figure S9. Aliphatic region of ^1H NMR spectrum of **3** in CDCl_3 .

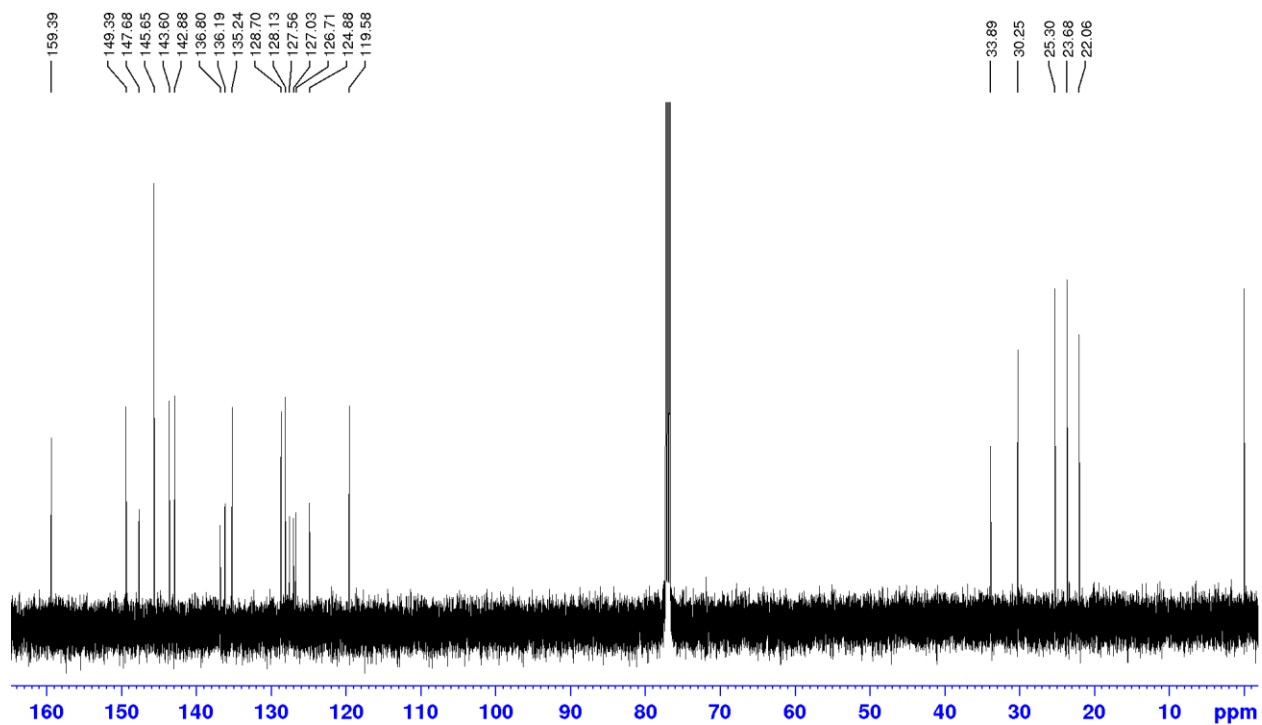


Figure S10. ^{13}C NMR spectrum of complex **3** in CDCl_3 .

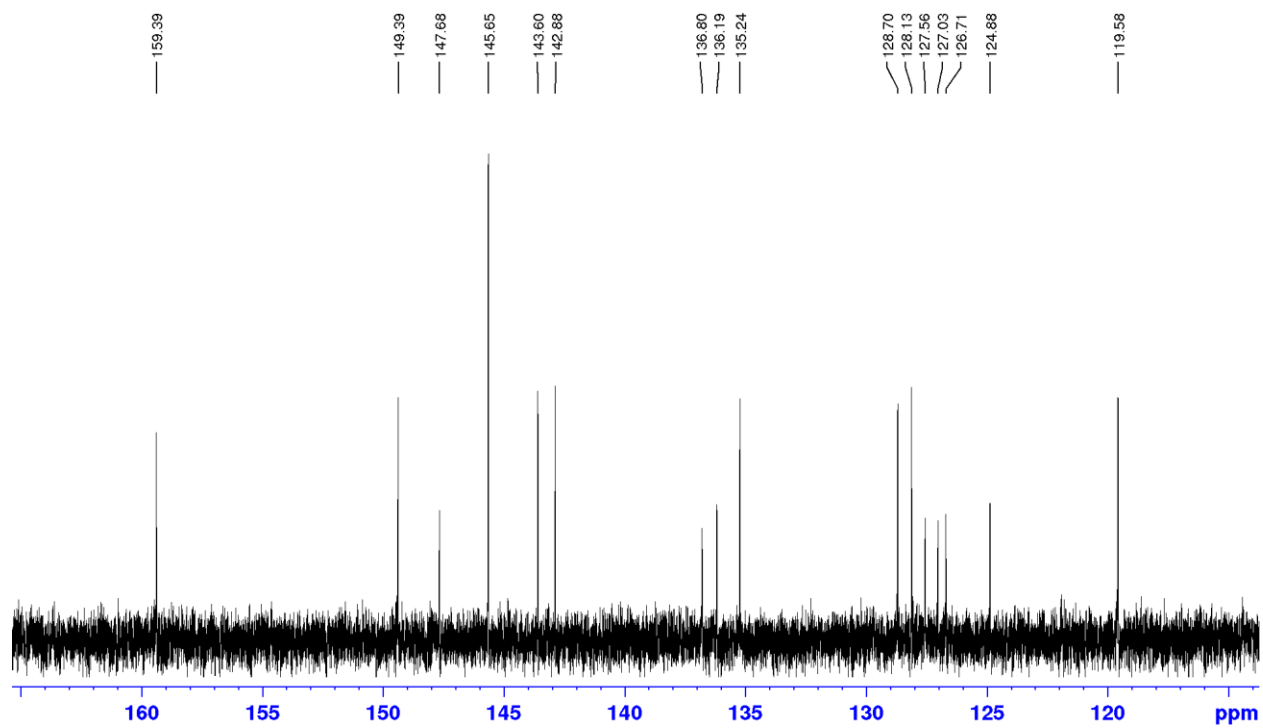


Figure S11. Aromatic region of ^{13}C NMR spectrum of **3** in CDCl_3 .

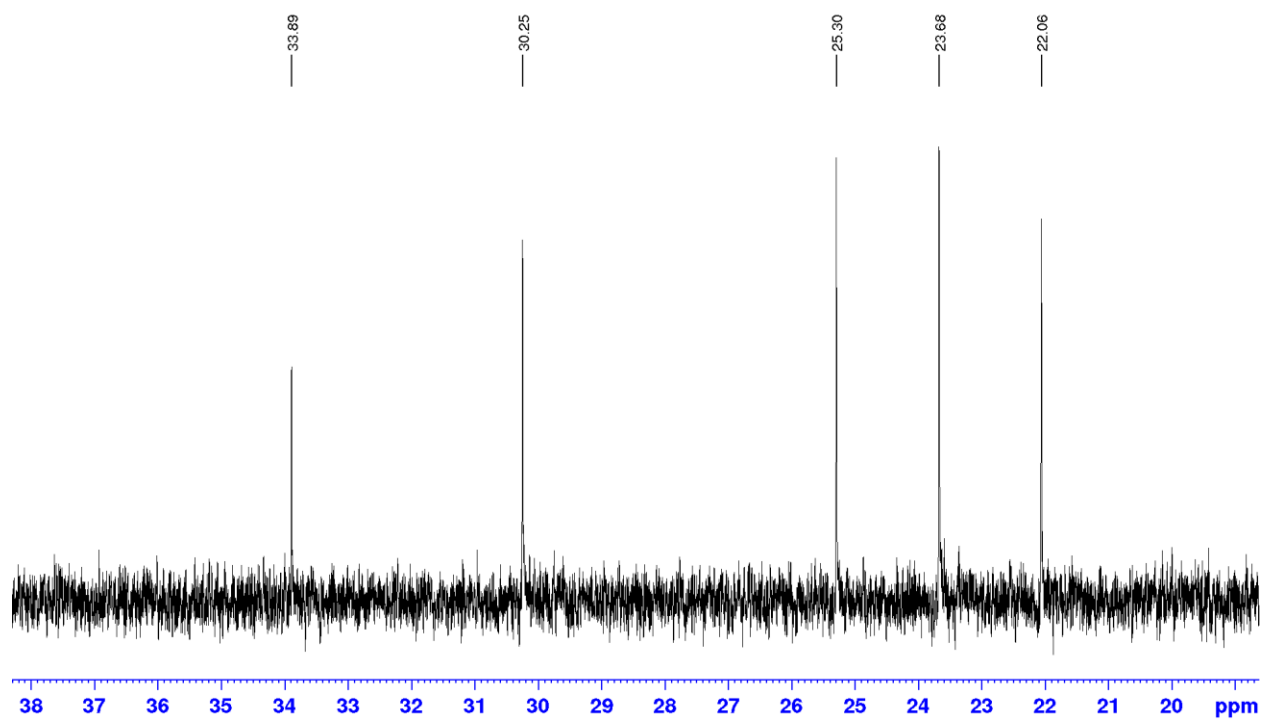


Figure S12. Aliphatic region of ^{13}C NMR spectrum of **3** in CDCl_3 .

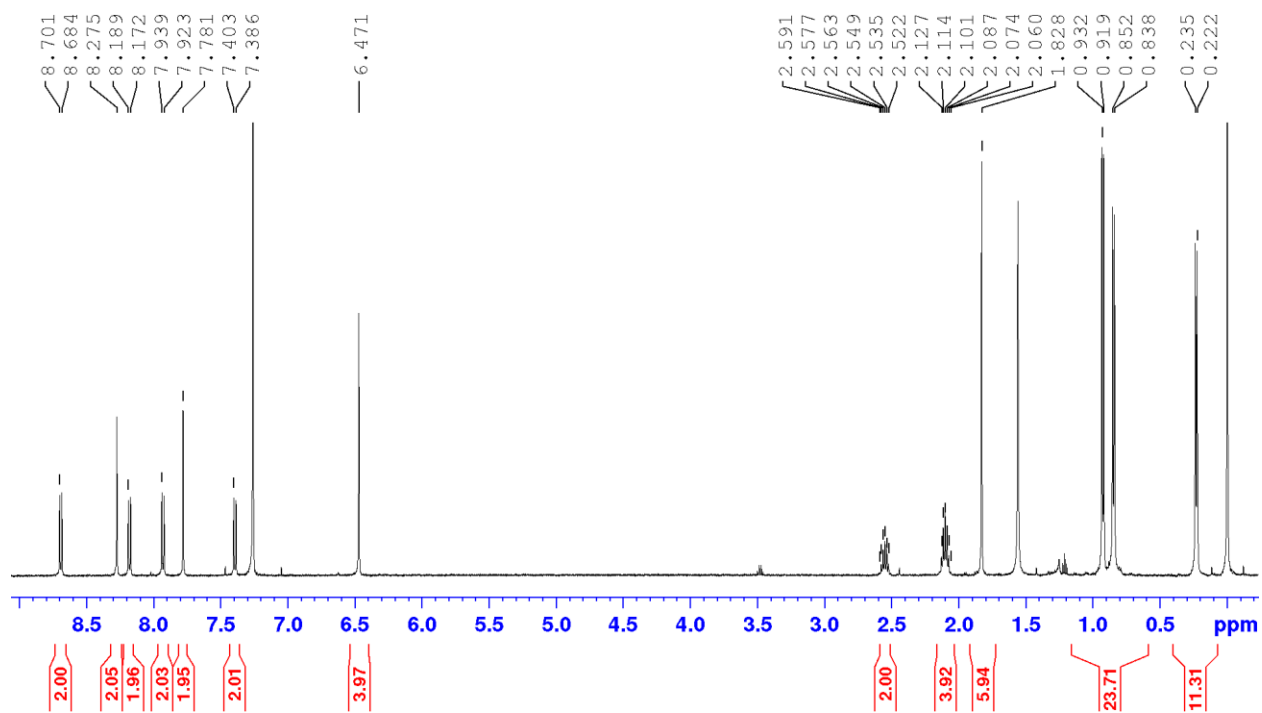


Figure S13. ^1H NMR of **4** in CDCl_3 .

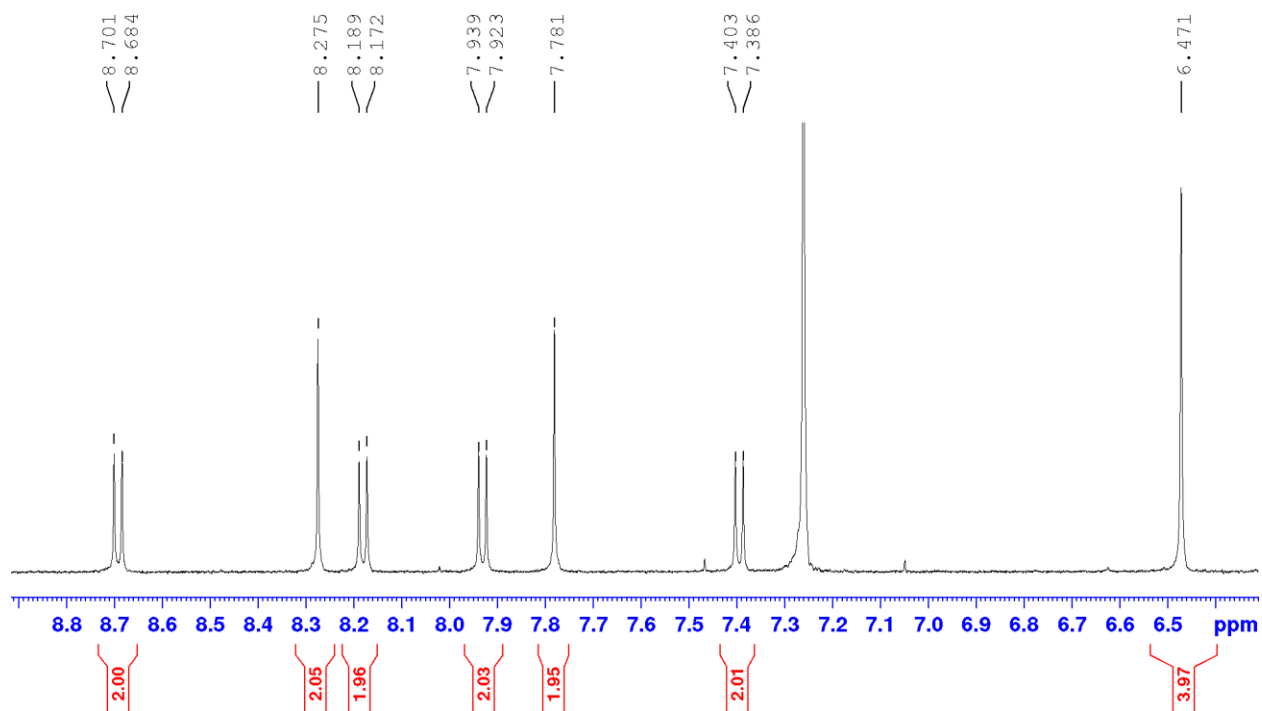


Figure S14. Aromatic region of ^1H NMR spectrum of **4** in CDCl_3 .

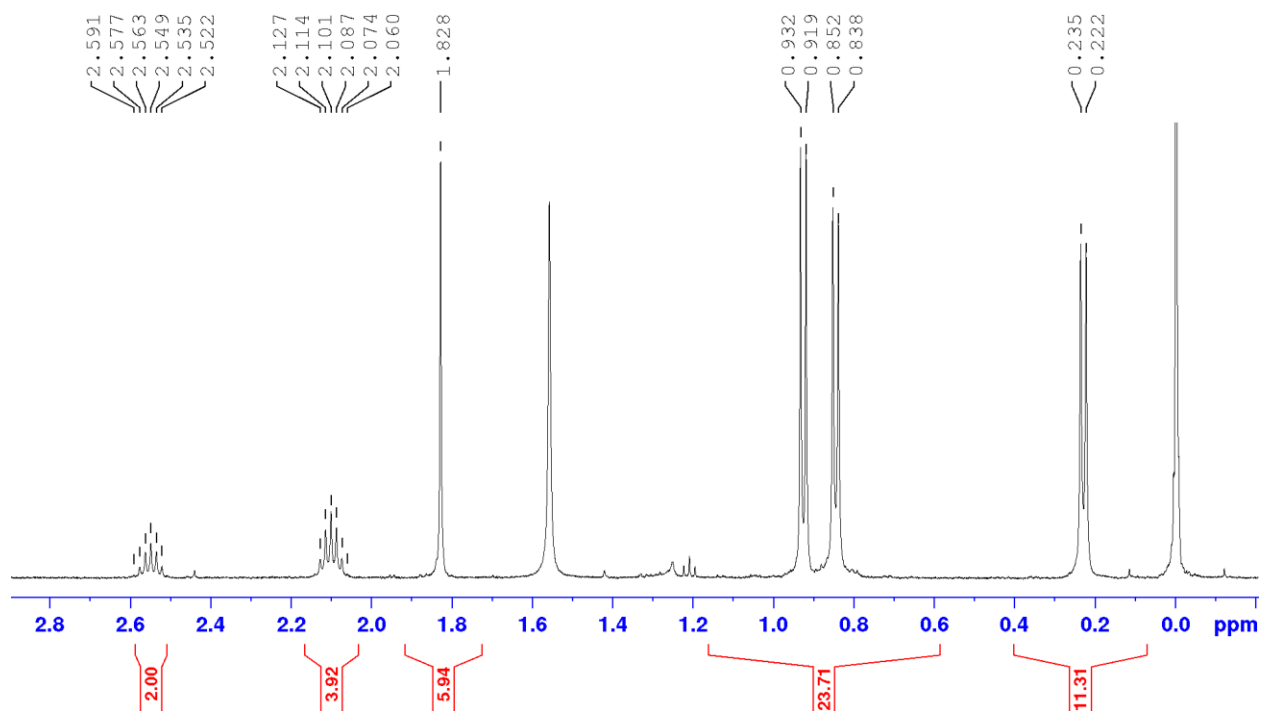


Figure S15. Aliphatic region of ^1H NMR spectrum of **4** in CDCl_3 .

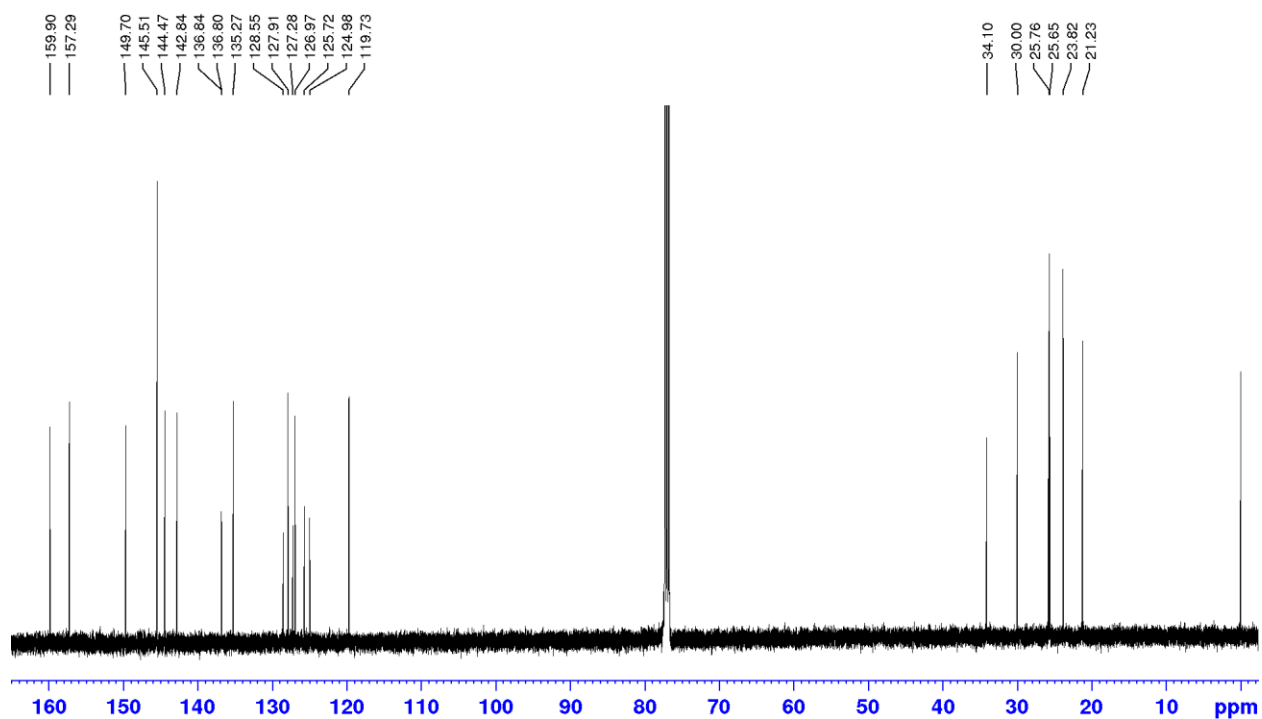


Figure S16. ^{13}C NMR spectrum of **4** in CDCl_3 .

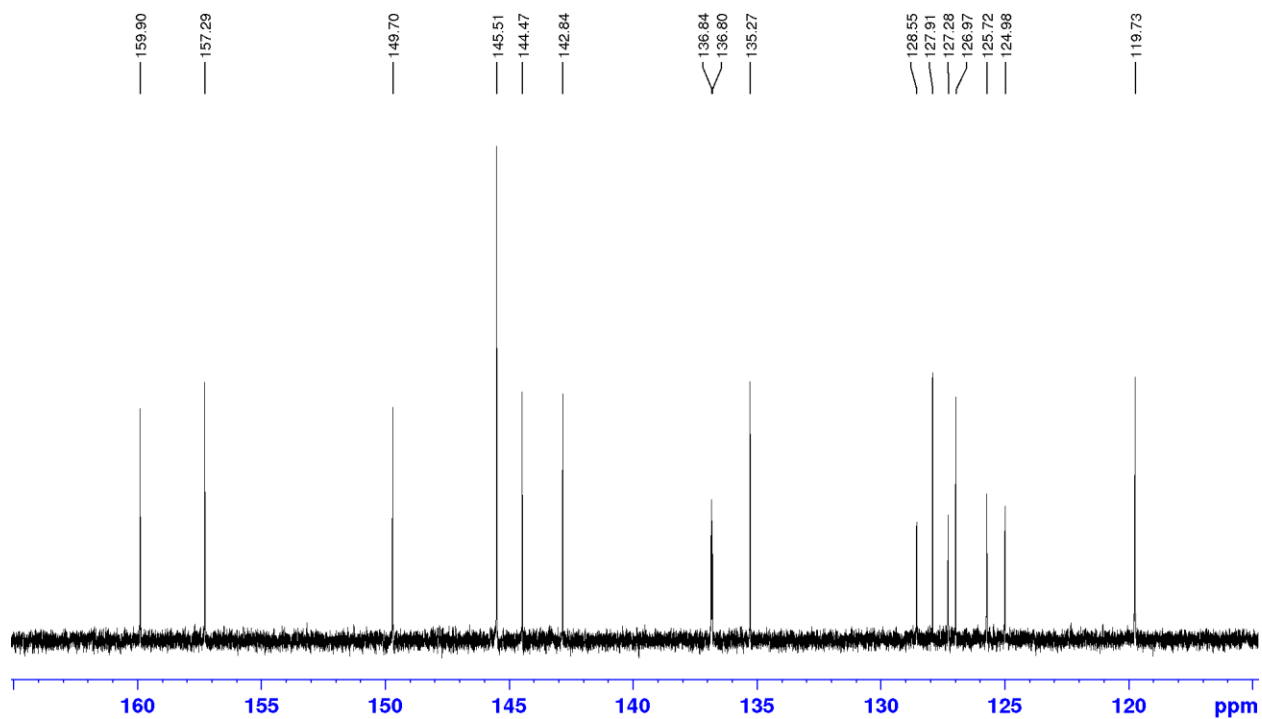


Figure S17. Aromatic region of ^{13}C NMR spectrum of **4** in CDCl_3 .

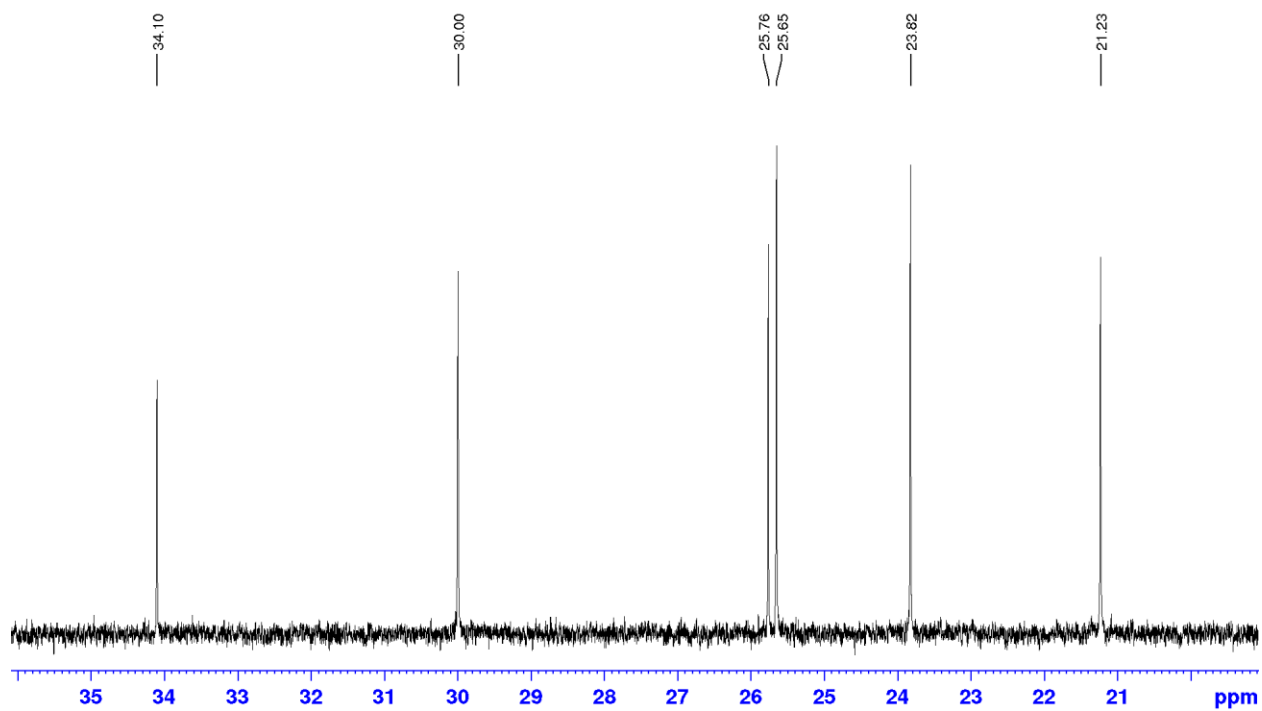


Figure S18. Aliphatic region of ^{13}C NMR spectrum of **4** in CDCl_3 .

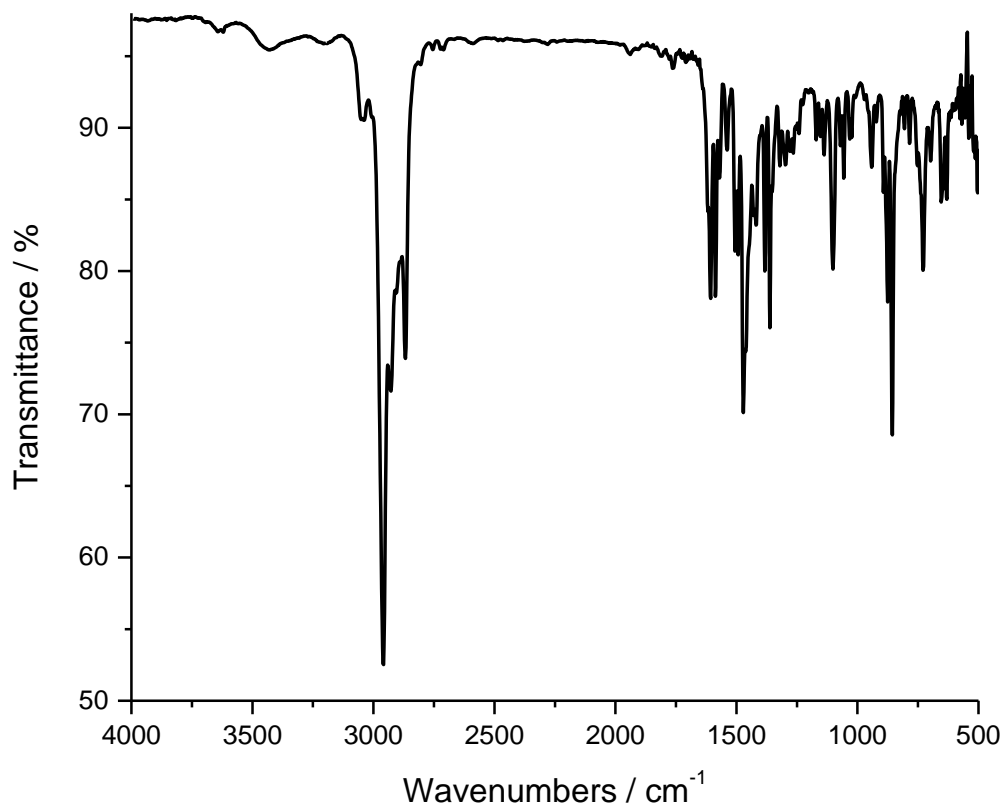


Figure S19. FTIR spectrum of **bL2**.

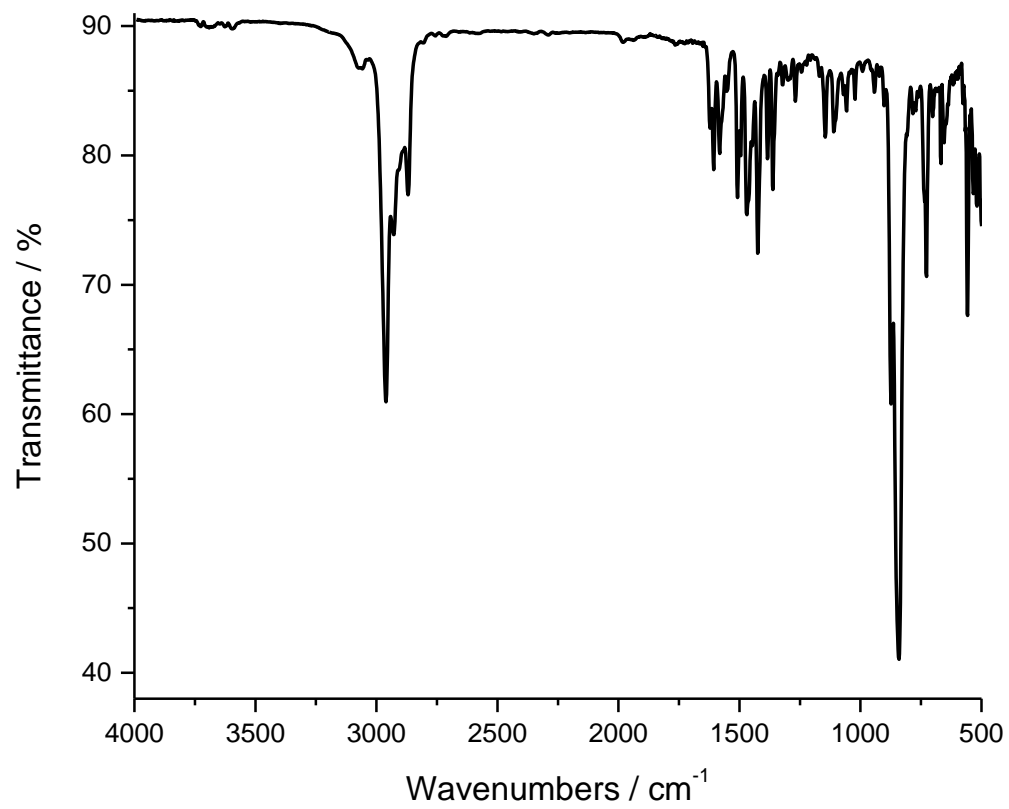


Figure S20. FTIR spectrum of **3**.

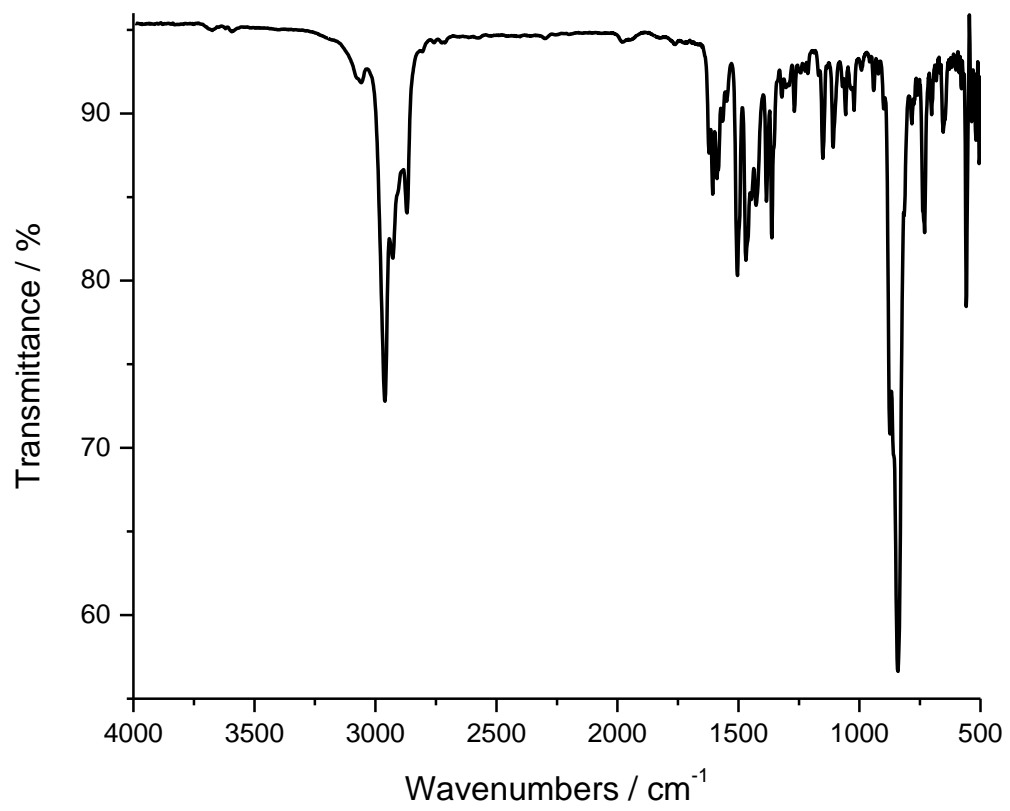


Figure S21. FTIR spectrum of **4**.

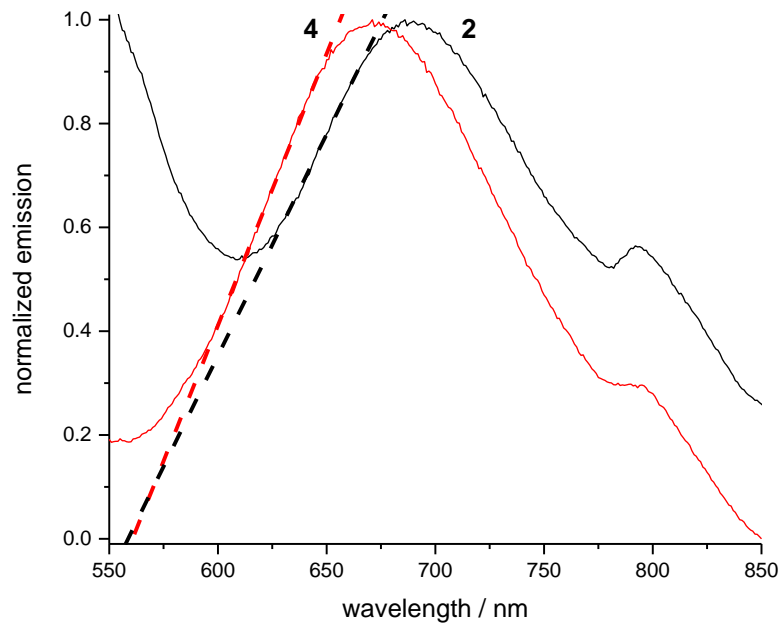


Figure S22. Emission spectra of CuHETPHEN **2** and **4** in CH₂Cl₂. Emission spectra of **2** and **4** in CH₂Cl₂ following excitation at 450 nm. No emission was detected for **1** and **3** at room temperature. Dashed lines are tangent to the high energy edge of the emission spectra and used to estimate E_{00} for **2** and **4**.

Details of fitting transient optical spectroscopy. Kinetic decay times for **1-4** were obtained by a global fit of several wavelengths to a multi-exponential decay model using Origin Pro 9.1 software. The initial decay parameters (τ_1 , τ_2) were obtained from a fit using the response from ~ 0.5 ps to ~ 100 ps, and τ_3 was calculated using the response after ~ 100 ps. The ultrafast experiment was sufficient to obtain near-complete decay of **1** and **3** in CH_3OH . The nanosecond experiment was required to obtain complete decay kinetics for all complexes in CH_2Cl_2 and **2** and **4** in CH_3OH . In kinetic plots, points represent data and lines represent fit.

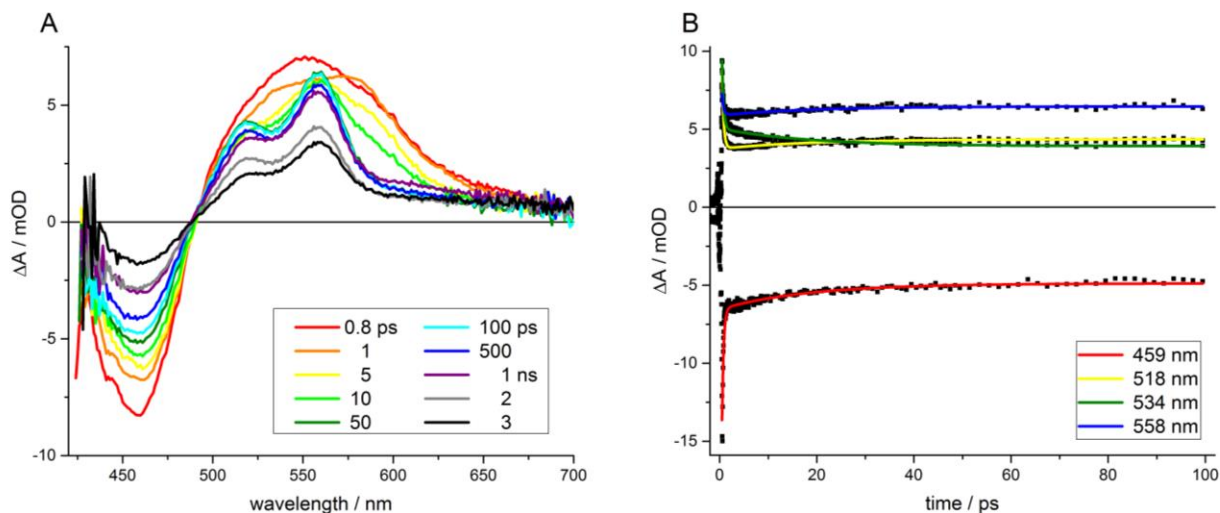


Figure S23. Ultrafast transient spectra (A) and kinetic fitting (B) for **1** in CH_2Cl_2 following 415nm excitation.

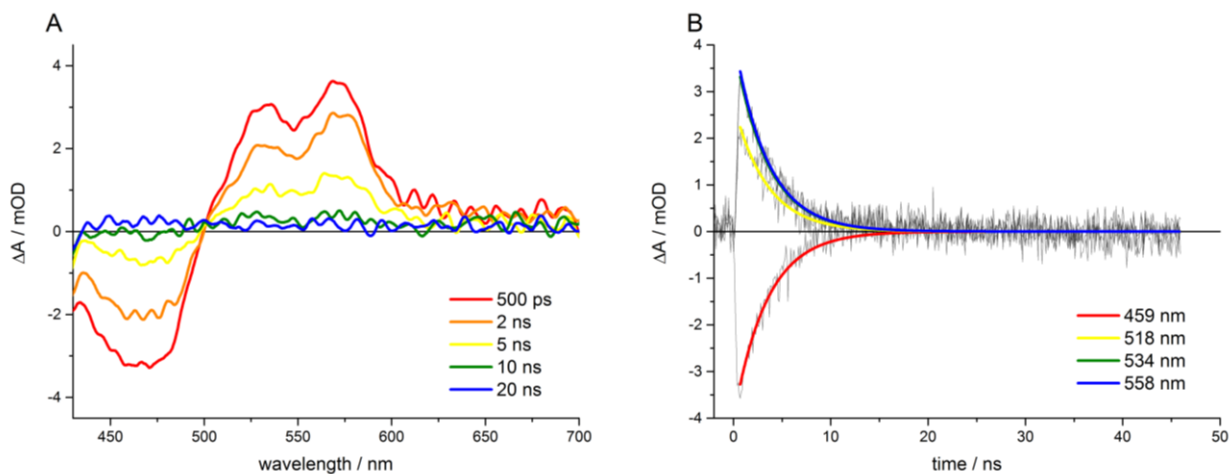


Figure S24. Nanosecond transient spectra (A) and kinetic fitting (B) for **1** in CH_2Cl_2 following 415nm excitation.

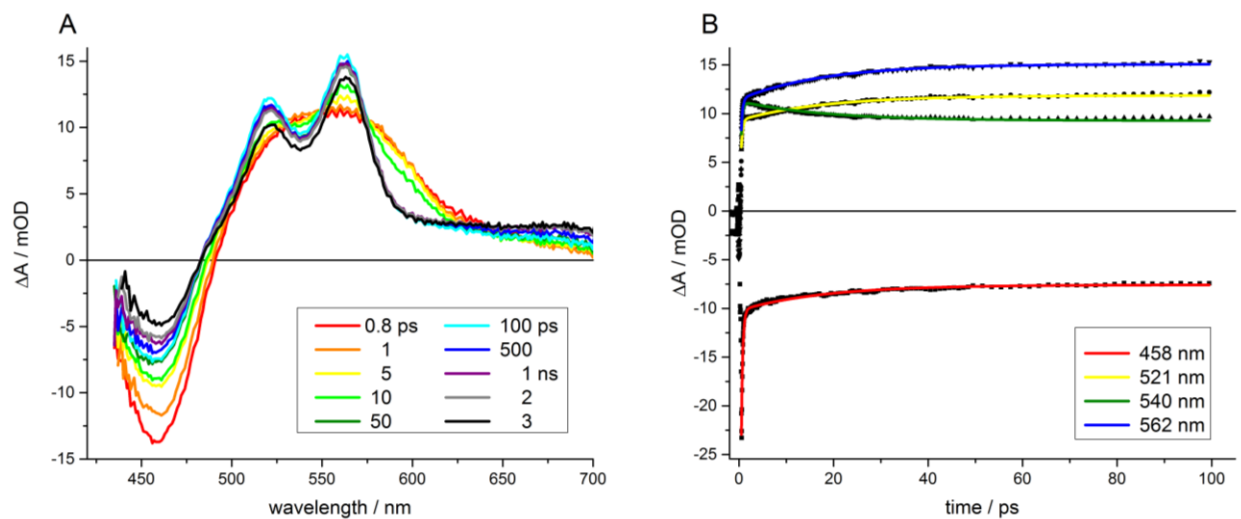


Figure S25. Ultrafast transient spectra (A) and kinetic fitting (B) for **2** in CH₂Cl₂ following 415nm excitation.

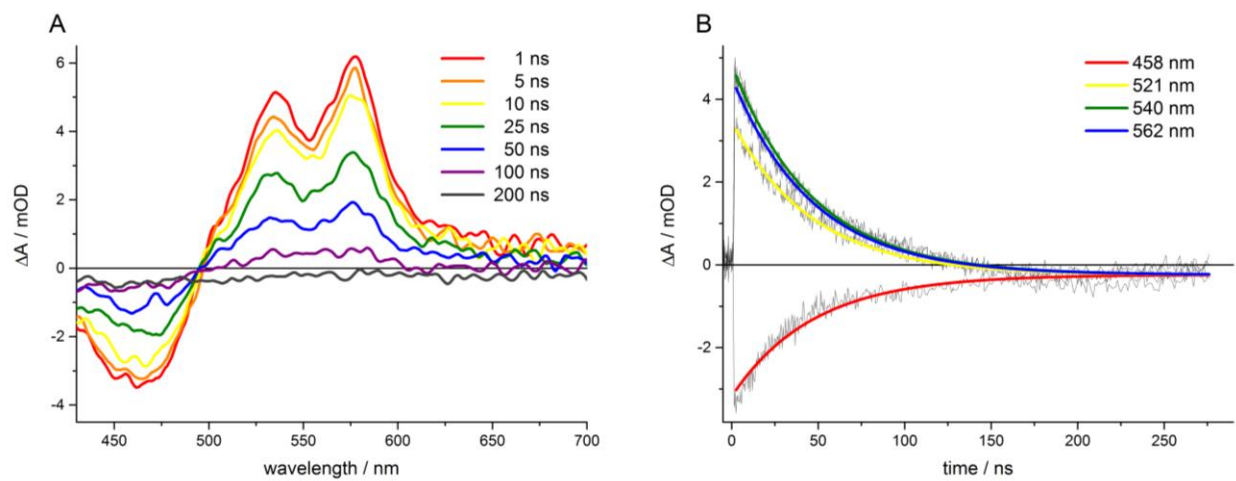


Figure S26. Nanosecond transient spectra (A) and kinetic fitting (B) for **2** in CH₂Cl₂ following 415nm excitation.

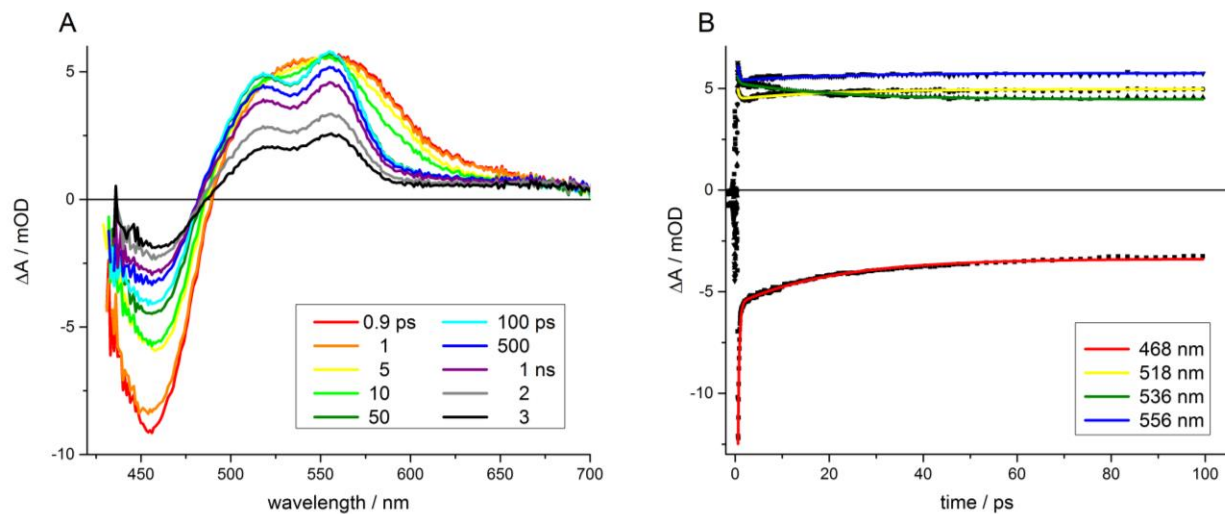


Figure S27. Ultrafast transient spectra (A) and kinetic fitting (B) for **3** in CH_2Cl_2 following 415nm excitation.

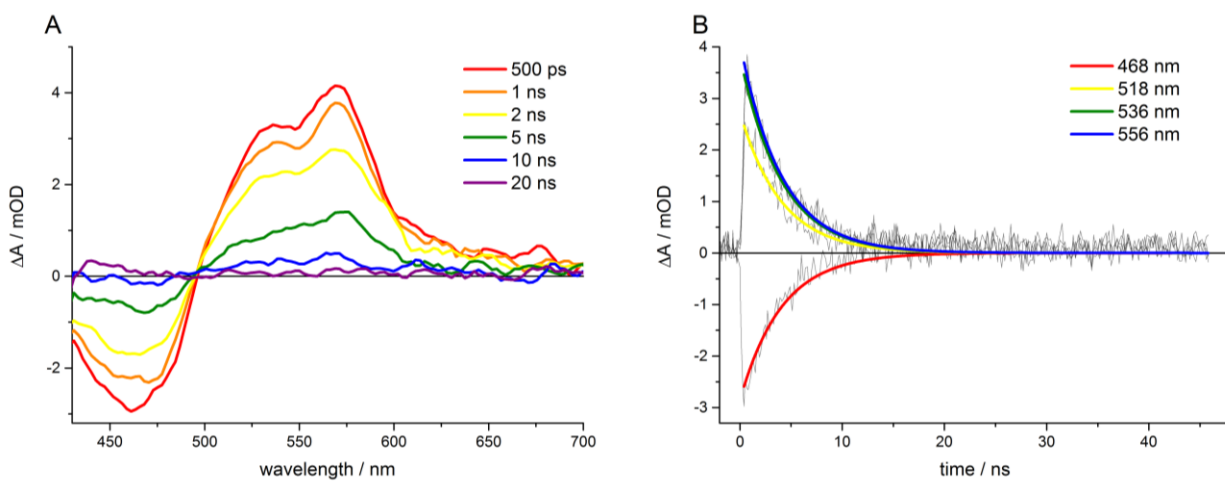


Figure S28. Nanosecond transient spectra (A) and kinetic fitting (B) for **3** in CH_2Cl_2 following 415nm excitation.

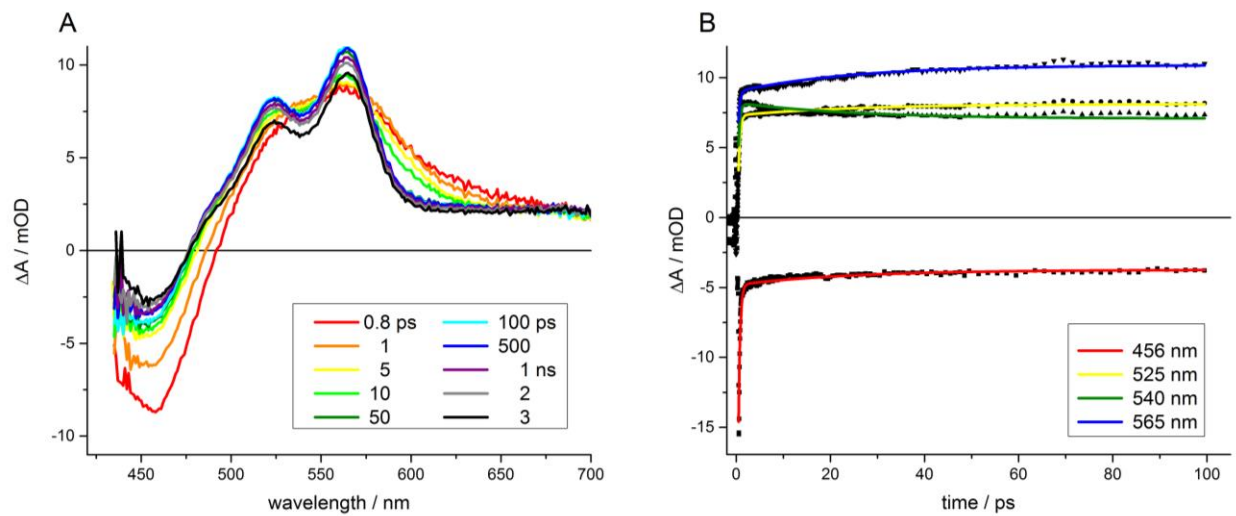


Figure S29. Ultrafast transient spectra (A) and kinetic fitting (B) for **4** in CH_2Cl_2 following 415nm excitation.

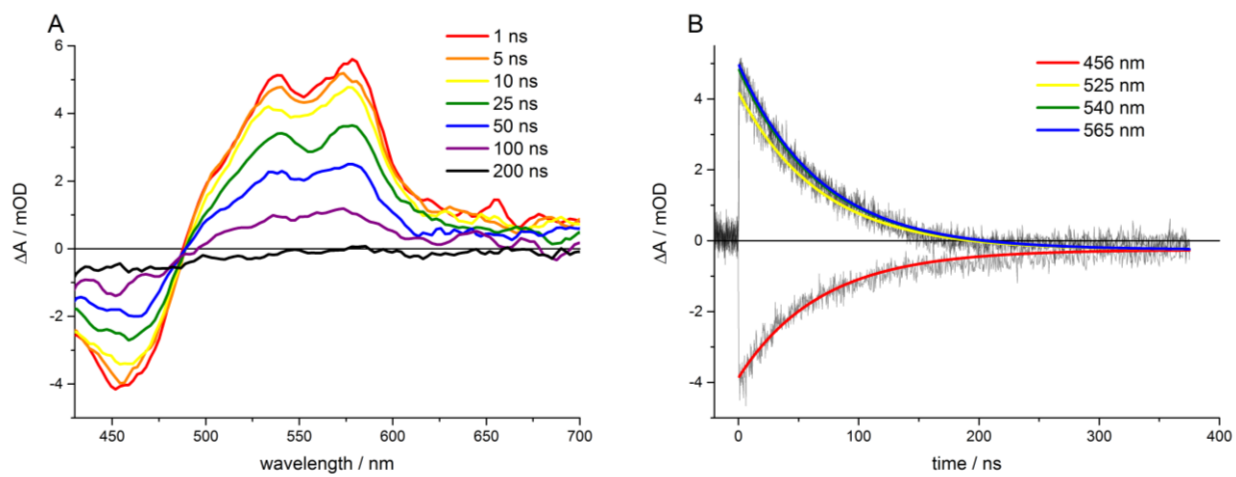


Figure S30. Nanosecond transient spectra (A) and kinetic fitting (B) for **4** in CH_2Cl_2 following 415nm excitation.

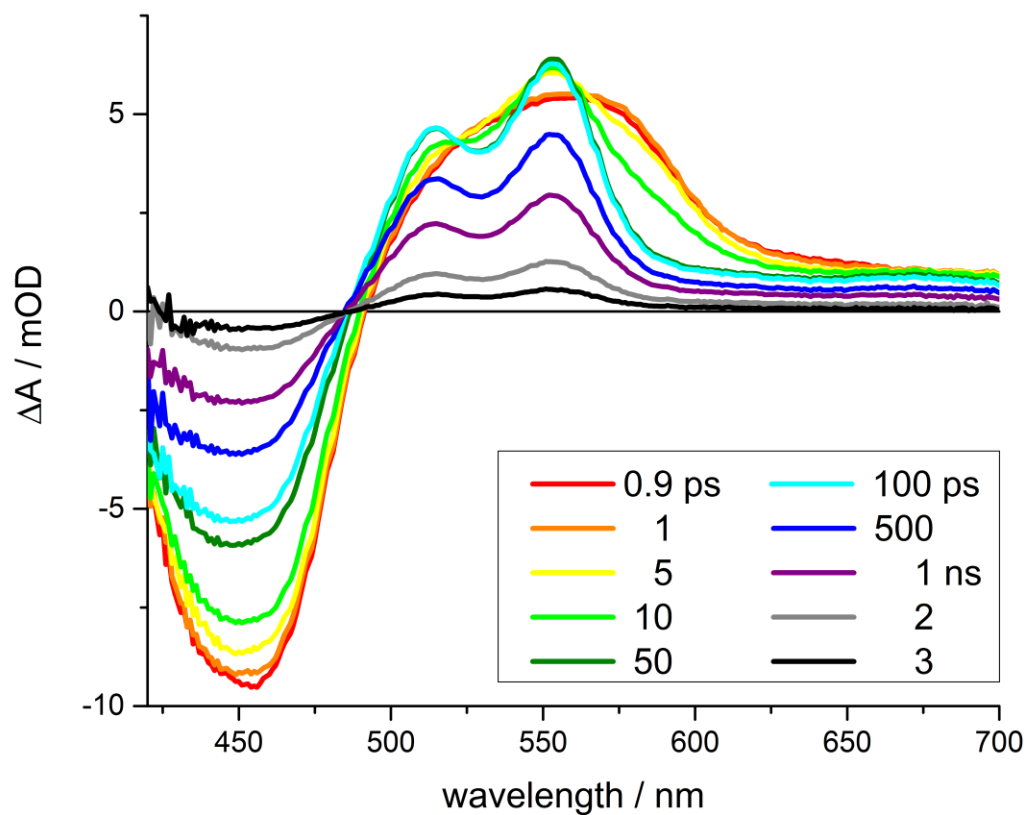


Figure S31. Ultrafast transient spectra for **1** in CH_3OH following 415 nm excitation.

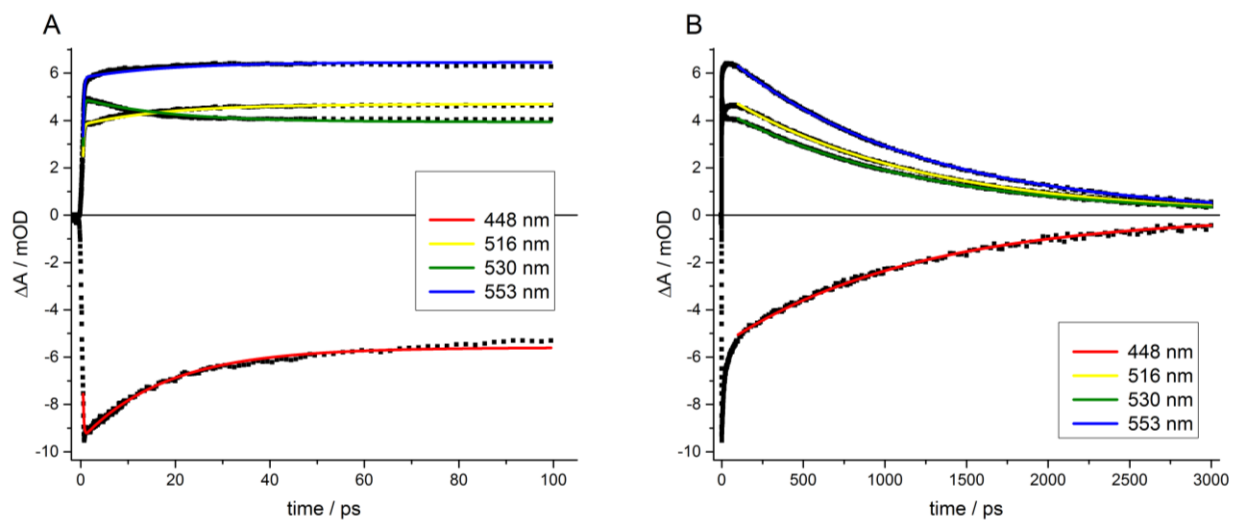


Figure S32. Kinetics for **1** following 415 nm excitation in CH_3OH . (A) Response < 100 ps for calculation of τ_1 and τ_2 (B) and up to 3 ns to model τ_3 .

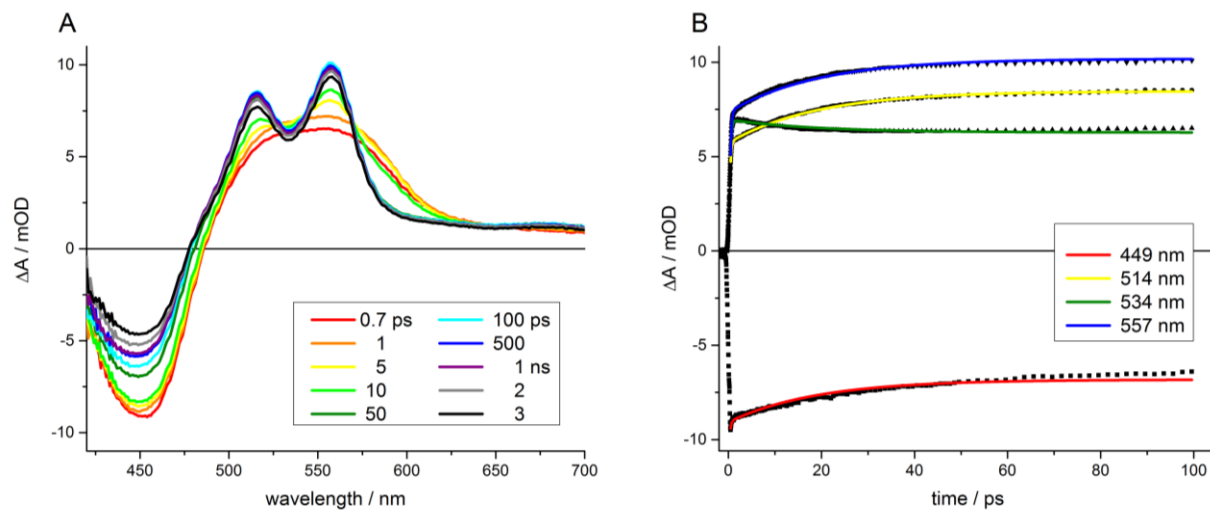


Figure S33. Ultrafast transient spectra (A) and kinetic fitting (B) for **2** in CH₃OH following 415nm excitation.

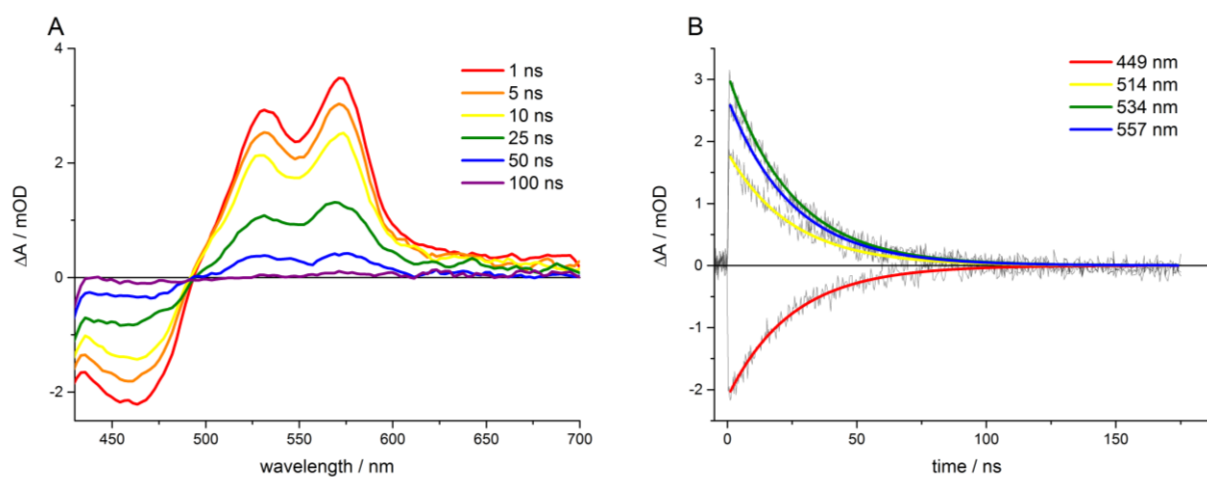


Figure S34. Nanosecond transient spectra (A) and kinetic fitting (B) for **2** in CH₃OH following 415nm excitation.

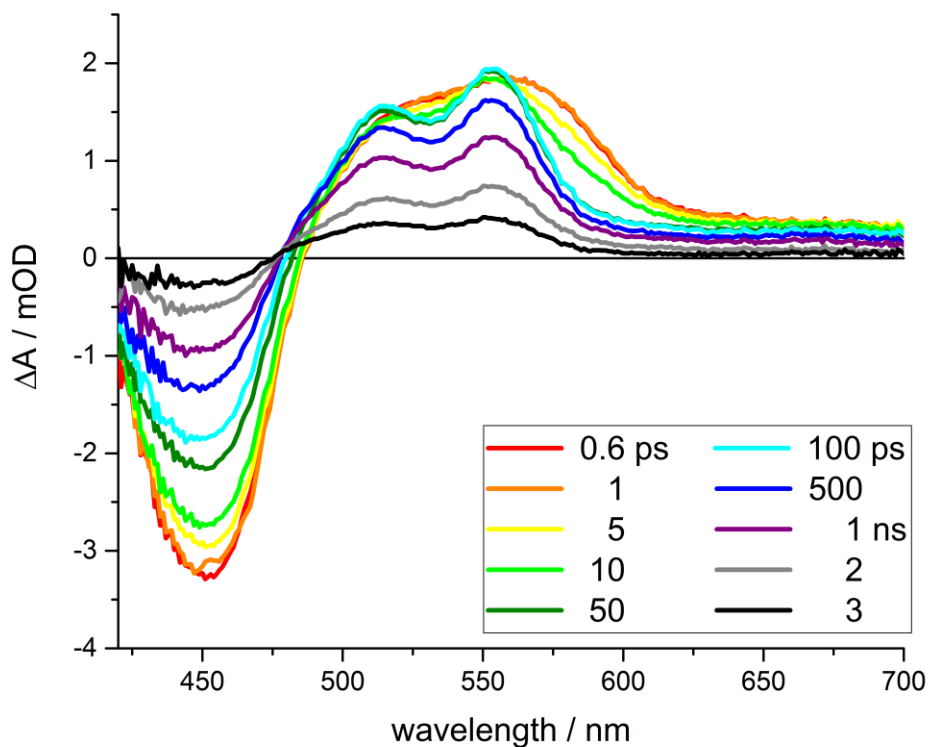


Figure S35. Ultrafast transient spectra for **3** in CH_3OH following 415nm excitation.

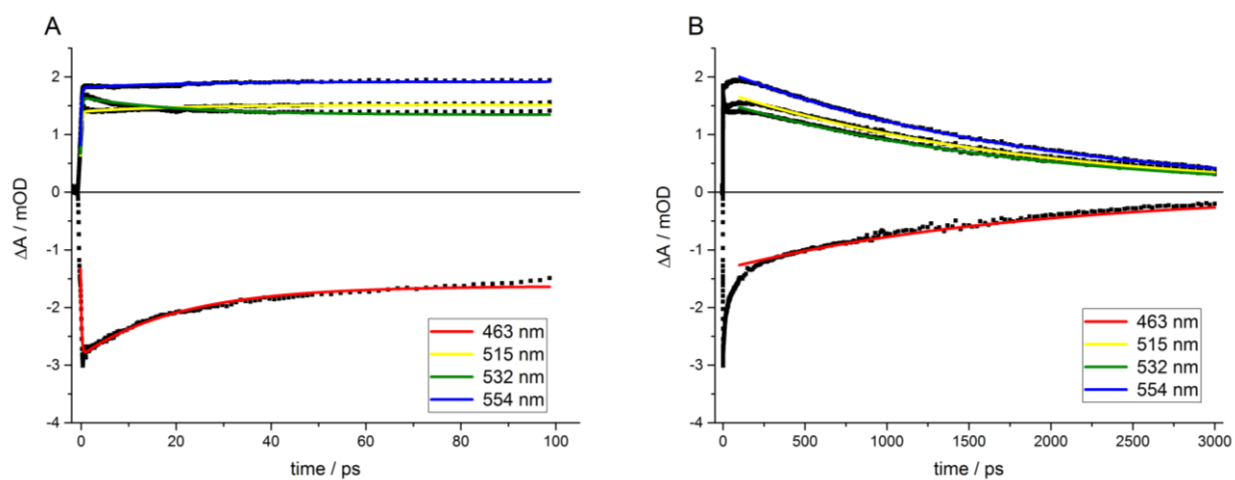


Figure S36. Kinetics for **3** following 415nm excitation in CH_3OH . (A) Response < 100 ps for calculation of τ_1 and τ_2 (B) and up to 3 ns to model τ_3 .

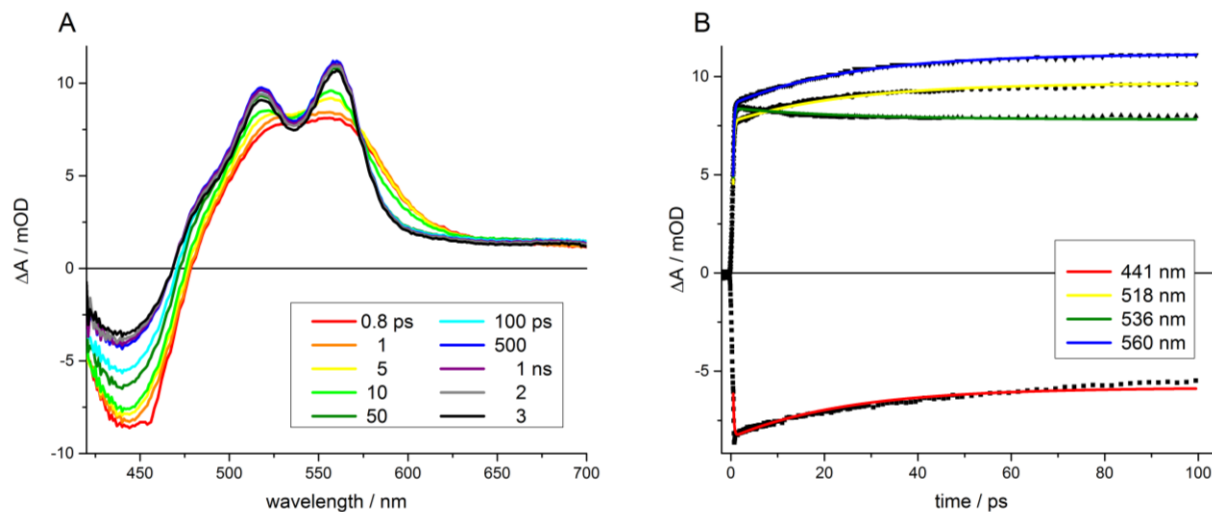


Figure S37. Ultrafast transient spectra (A) and kinetic fitting (B) for **4** in CH_3OH following 415nm excitation.

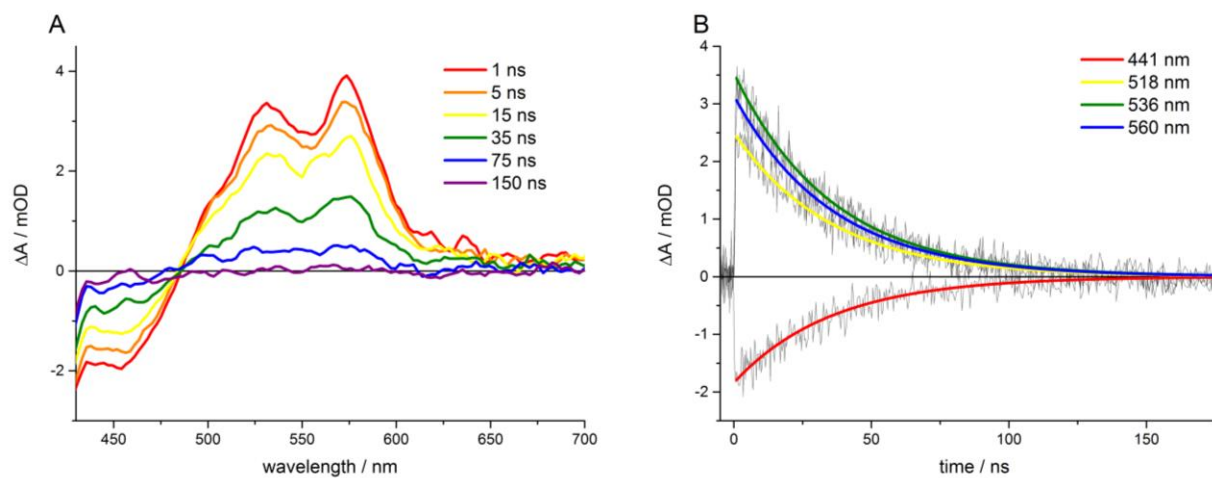


Figure S38. Nanosecond transient spectra (A) and kinetic fitting (B) for **4** in CH_3OH following 415nm excitation.

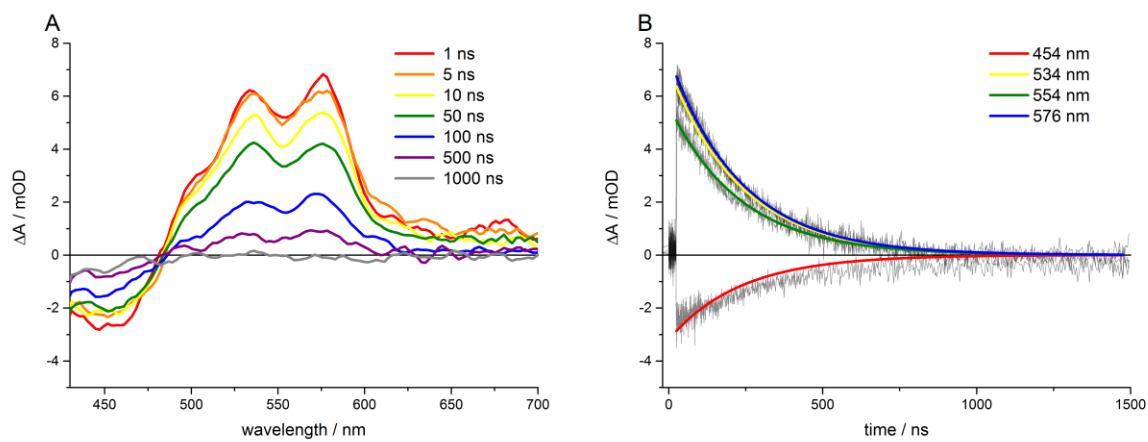


Figure S39. Nanosecond transient spectra (A) and kinetic fitting (B) for $[\text{Cu}(\text{bL1})(\text{L3})](\text{PF}_6)$ in CH_2Cl_2 following 415nm excitation. Global fit to kinetic traces shown in (B) yields $\tau_3 = 232$ ns.

Table S1. DFT calculated redox potentials and GS-³MLCT energy gaps of select CuHETPHEN complexes using three different functionals.^a

complex	E(Cu ^{2+/+})(V vs. SCE)			Energy Gap (eV)		
	BP86	TPSSh	B3LYP	BP86	TPSSh	B3LYP
Cu(bL1)(L3)	+1.26	+1.03	+1.15	2.02	2.03	2.18
3	+1.07	+0.78	+0.89	1.71	1.71	1.88
4	+1.15	+0.88	+0.99	1.87	1.87	2.03

^a Electronic energies. Note that the functionals BP86, TPSSh, and B3LYP have 0, 10, and 20% Hartree-Fock exchange, respectively.

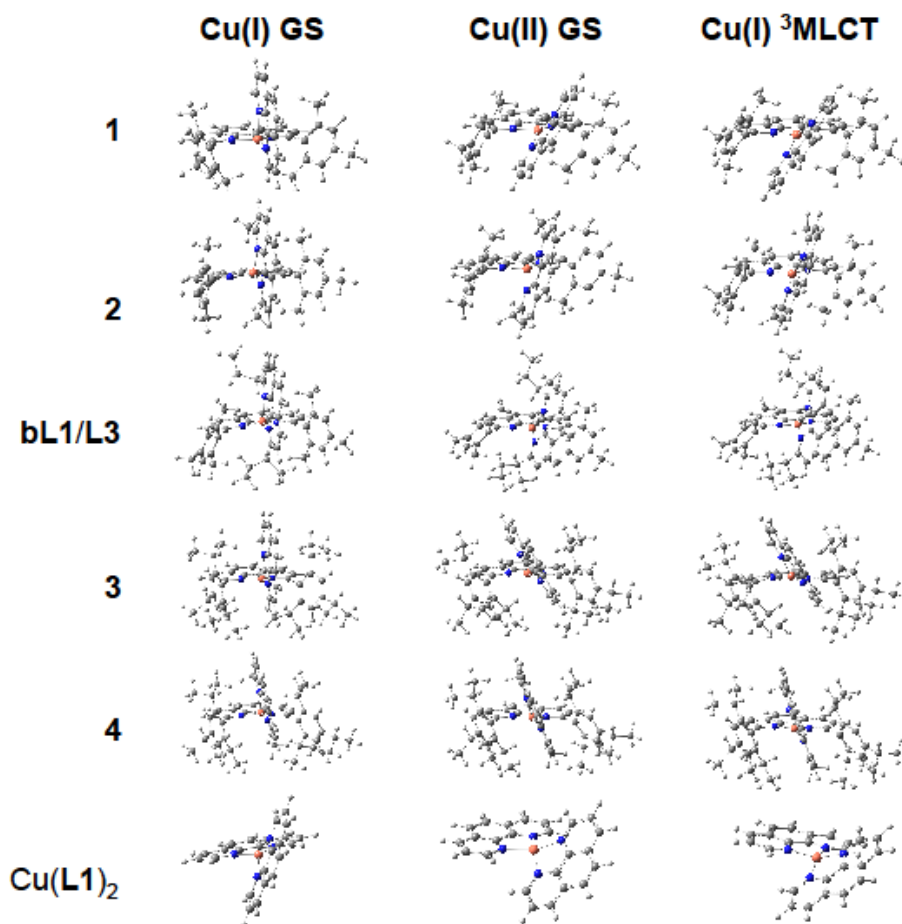


Figure S40. DFT optimized geometries of all complexes considered here. The first, second and third columns contain the Cu(I) ground state (Cu(I) GS), Cu(II) GS, and Cu(I) ³MLCT geometries, respectively.

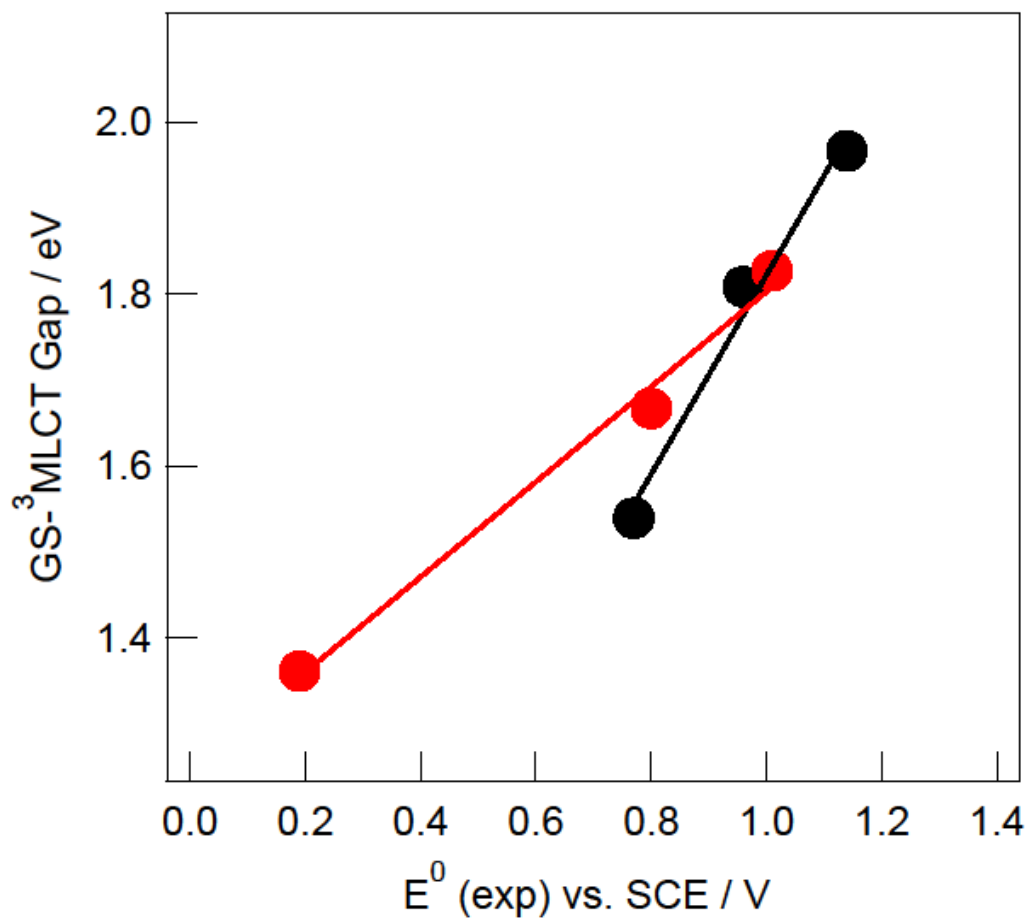


Figure S41. Correlations between the DFT calculated GS-³MLCT Gap vs. the experimental E^0 .

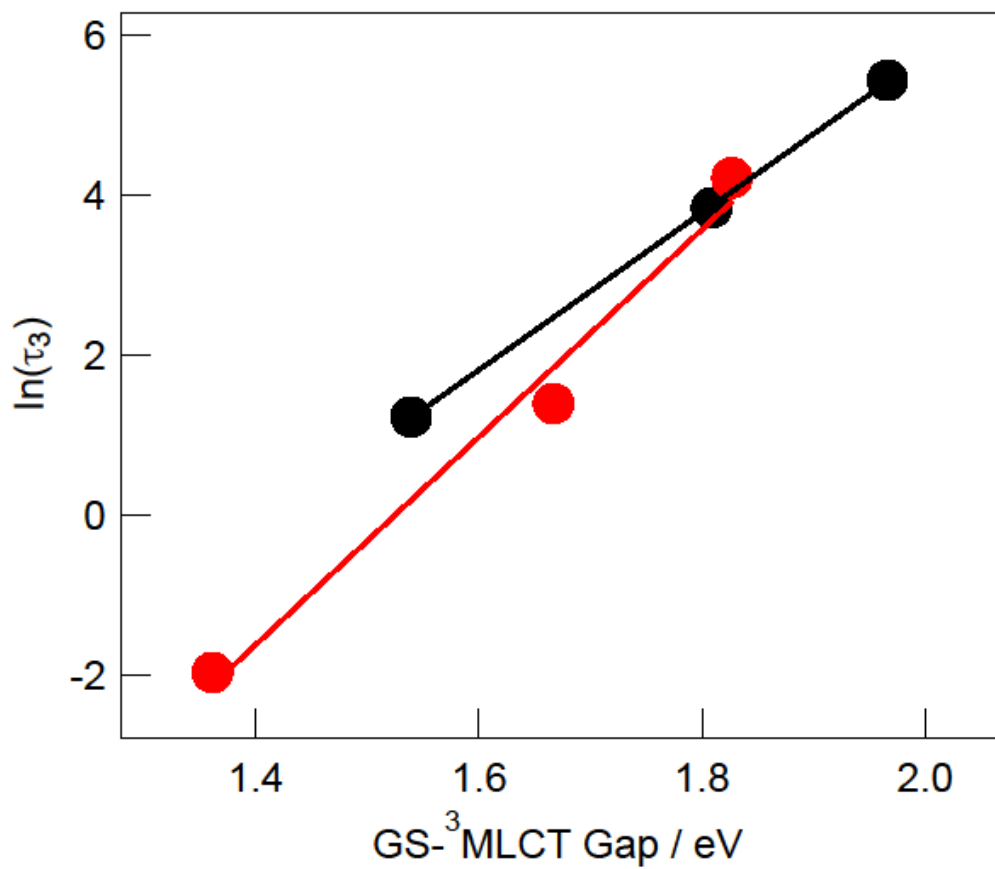


Figure S42. Correlations between the $\ln(\tau_3)$ and the DFT calculated GS-³MLCT gap.

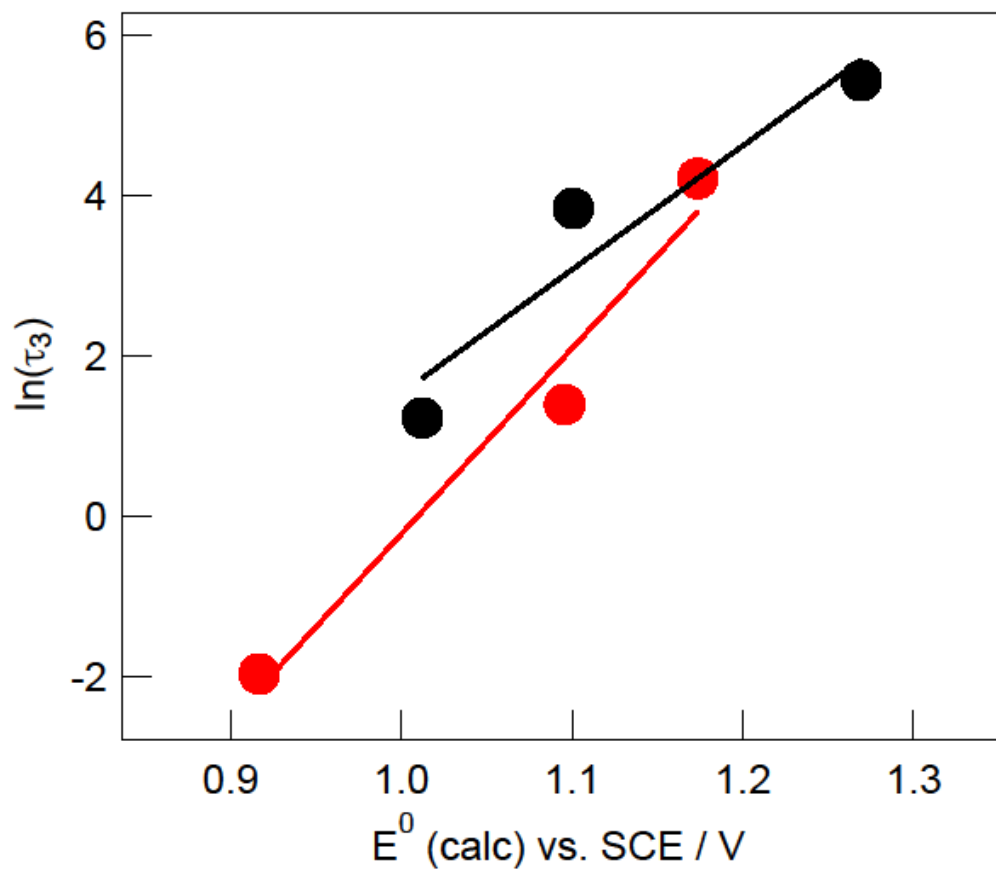


Figure S43. Correlations between the $\ln(\tau_3)$ and the DFT calculated E^0 .

Cartesian coordinates of DFT optimized structures

1 (reduced)

Cu	0.02766700	0.32895800	-0.19541600
N	-1.26574300	1.88401900	-0.23147600
N	1.40743900	1.79814500	-0.22985200
N	-0.00652300	-0.42753700	1.74075100
N	-0.05102000	-1.54851700	-0.69410200
C	-2.61736300	1.88054200	-0.25833900
C	-3.32021600	0.58919300	-0.52093600
C	-4.17157200	0.02084500	0.46370400
C	-4.34120300	0.64479500	1.83661800
H	-3.37821600	0.97168200	2.26709200
H	-4.79815300	-0.07505600	2.53618300
H	-5.00069400	1.53266400	1.81169300
C	-4.85783000	-1.16871000	0.15795500
H	-5.50114100	-1.61719900	0.92562400
C	-4.74865400	-1.79513600	-1.09617800
C	-5.53983200	-3.04505400	-1.41579900
H	-4.99996000	-3.69950100	-2.12199600
H	-6.50890400	-2.79026700	-1.88592500
H	-5.76319900	-3.62847100	-0.50614100
C	-3.89904500	-1.21014000	-2.05423000
H	-3.80094300	-1.67993300	-3.04121400
C	-3.18083700	-0.03148800	-1.79363100
C	-2.29453100	0.56764400	-2.86696200
H	-2.32460500	-0.03607100	-3.78910100
H	-1.24690400	0.62837900	-2.51499100
H	-2.59946100	1.59774200	-3.12881900
C	-3.35517200	3.08582000	-0.08897900
H	-4.44721800	3.04235500	-0.13255600
C	-2.69942900	4.29674900	0.09303200
H	-3.26406400	5.22856700	0.21037700
C	-1.27979400	4.32461400	0.10660800
C	-0.49913600	5.52094600	0.27651600
H	-1.02311300	6.47439500	0.40543700
C	0.87641700	5.47657100	0.27744700
H	1.46066400	6.39424300	0.40692100
C	1.57833600	4.23236500	0.10842000
C	2.99312400	4.11302900	0.09637900
H	3.61638200	5.00661100	0.21426000
C	3.56985400	2.86212300	-0.08397200
H	4.65708200	2.74842000	-0.12468300
C	2.75600300	1.70714500	-0.25332600
C	3.37224200	0.37082100	-0.50798700
C	4.16409100	-0.25598200	0.49017600
C	4.34922900	0.35405500	1.86719300
H	4.75893100	-0.39053600	2.57010200

H	3.39854100	0.72897200	2.28608300
H	5.05359600	1.20692000	1.85383500
C	4.77263700	-1.48934600	0.19376000
H	5.37055800	-1.98132000	0.97138700
C	4.64267800	-2.10501100	-1.06377300
C	5.35339900	-3.40462100	-1.37384100
H	5.53471700	-3.99683700	-0.46057500
H	6.33875300	-3.21447500	-1.84064000
H	4.77595500	-4.02651500	-2.07983700
C	3.85117500	-1.46254100	-2.03479100
H	3.73781900	-1.92390900	-3.02414200
C	3.21073700	-0.23783800	-1.78375600
C	2.38249100	0.42120700	-2.86831700
H	2.38628300	-0.18085800	-3.79204600
H	2.75907000	1.42940600	-3.12210100
H	1.33572200	0.55083500	-2.53224300
C	0.83067700	3.03070900	-0.06200100
C	-0.61138300	3.07694100	-0.06288000
C	0.02067600	0.16463300	2.94263800
H	0.08020300	1.25946200	2.93712600
C	-0.02310500	-0.55253900	4.15878000
H	0.00311100	-0.01079600	5.10898500
C	-0.09990500	-1.94321400	4.12429300
H	-0.13586200	-2.52828400	5.05004300
C	-0.13079600	-2.60726400	2.87076600
C	-0.20835000	-4.03621100	2.72118200
H	-0.24769500	-4.65794800	3.62239500
C	-0.23162800	-4.61442900	1.47404400
H	-0.28931100	-5.70359900	1.37043200
C	-0.17948500	-3.81651200	0.27554700
C	-0.19625400	-4.37009300	-1.03049500
H	-0.25245900	-5.45591400	-1.16329700
C	-0.13793600	-3.51132300	-2.12474000
H	-0.14591400	-3.89715300	-3.14844200
C	-0.06642500	-2.11984400	-1.91569900
H	-0.01932000	-1.43497500	-2.76716700
C	-0.10473300	-2.39724300	0.39241000
C	-0.08109400	-1.79180500	1.69945300

1 (oxidized)

Cu	0.04258400	0.39774200	0.07977700
N	-1.37769600	1.85641300	0.06846100
N	1.31141100	1.92145100	-0.07085900
N	1.03504200	-0.89751100	1.26915100
N	-0.75618700	-1.28194500	-0.66468100
C	-2.72750300	1.78520400	0.17492400
C	-3.46103300	0.48639900	0.12951000
C	-3.37799700	-0.41616700	1.22723200

C	-2.49800600	-0.12777900	2.42600300
H	-2.75362700	0.83633600	2.90294100
H	-1.42840500	-0.07205900	2.14691900
H	-2.59968900	-0.91448700	3.19074100
C	-4.17471800	-1.57341100	1.21024600
H	-4.12582000	-2.25782300	2.06624100
C	-5.06099300	-1.85911900	0.15308800
C	-5.95208700	-3.07946600	0.19122500
H	-6.22840300	-3.41764800	-0.82160600
H	-6.89454200	-2.85273500	0.72485200
H	-5.47531600	-3.91981300	0.72402400
C	-5.12153400	-0.94841700	-0.91950300
H	-5.80226300	-1.15188100	-1.75545600
C	-4.35608200	0.23231600	-0.94725800
C	-4.50209300	1.18161000	-2.12340000
H	-4.94044200	0.66377500	-2.99257100
H	-3.54161200	1.62581200	-2.44120900
H	-5.17876300	2.02440400	-1.88715500
C	-3.49622900	2.97326500	0.36199900
H	-4.57998200	2.86958100	0.46107900
C	-2.89229300	4.21711700	0.43631800
H	-3.49076600	5.12351400	0.57983900
C	-1.47949700	4.30949300	0.33319900
C	-0.75892200	5.55215900	0.38710500
H	-1.32563900	6.47894200	0.52379400
C	0.61027800	5.58375200	0.25414500
H	1.15009200	6.53607500	0.27453600
C	1.35753300	4.36945900	0.08028600
C	2.76657500	4.32144700	-0.10666200
H	3.34611700	5.25120400	-0.11058300
C	3.38851300	3.10212800	-0.32664500
H	4.45989300	3.04999200	-0.53694700
C	2.64259700	1.88634200	-0.32301800
C	3.29188500	0.59337300	-0.66108700
C	4.39999900	0.12117000	0.09866600
C	4.95909000	0.86049600	1.30142000
H	5.32051900	0.14939800	2.06395400
H	4.23129600	1.53618300	1.78130900
H	5.83280800	1.47745100	1.01764700
C	5.01249900	-1.08637500	-0.28240100
H	5.85503100	-1.45825100	0.31376600
C	4.59819200	-1.81719600	-1.41027200
C	5.31823700	-3.07602500	-1.83439000
H	5.79980200	-3.58068400	-0.98014000
H	6.11694800	-2.83696100	-2.56218500
H	4.63837300	-3.79169300	-2.32742900
C	3.51903400	-1.31030600	-2.16300300
H	3.20580600	-1.84343000	-3.06921300

C	2.85663400	-0.12089800	-1.82086500
C	1.81199500	0.42888700	-2.77934700
H	1.61168600	-0.29497100	-3.58562400
H	2.16405900	1.36261600	-3.25652600
H	0.84499000	0.67035300	-2.30174100
C	0.66711800	3.12395500	0.06741500
C	-0.76434100	3.08794100	0.16810400
C	1.85835800	-0.64747700	2.29595700
H	2.10563700	0.40168600	2.48293100
C	2.39295400	-1.67956700	3.10013900
H	3.04992000	-1.42096200	3.93507000
C	2.08590500	-3.00622000	2.80898400
H	2.50646000	-3.82120300	3.40810300
C	1.21521400	-3.30159100	1.72518300
C	0.82897500	-4.63029700	1.32458200
H	1.23295800	-5.48376800	1.87895000
C	-0.02307900	-4.83276500	0.26201200
H	-0.29385100	-5.84941000	-0.04166200
C	-0.58515500	-3.72401800	-0.46651100
C	-1.46956300	-3.85313600	-1.57155200
H	-1.76342700	-4.84862000	-1.92170400
C	-1.95140400	-2.70811000	-2.19856000
H	-2.62507200	-2.77301000	-3.05701800
C	-1.57950800	-1.43474600	-1.71118100
H	-1.96987800	-0.52186400	-2.16682500
C	-0.23839600	-2.40173400	-0.07015500
C	0.69254600	-2.19326400	0.99987600

1 (triplet)

Cu	-0.00009400	0.41042300	0.00014900
N	-1.34563300	1.88667100	0.00435500
N	1.34565500	1.88669600	-0.00439500
N	0.89894400	-1.07548500	0.96824300
N	-0.89867900	-1.07575900	-0.96811100
C	-2.70135300	1.84630900	0.16672100
C	-3.41185700	0.54477800	0.34694300
C	-3.18443800	-0.21692600	1.53023900
C	-2.23186500	0.25334500	2.61144100
H	-2.47018400	1.28021800	2.94452500
H	-1.18102700	0.26777600	2.26747400
H	-2.28170800	-0.40809400	3.49173400
C	-3.91492300	-1.39951700	1.72512100
H	-3.74487200	-1.97809300	2.64203600
C	-4.87326400	-1.85171300	0.79668300
C	-5.66473900	-3.11626200	1.05036600
H	-6.10123500	-3.51633900	0.11946600
H	-6.50113500	-2.92650900	1.74983100
H	-5.03827300	-3.90418200	1.50425300

C	-5.09515400	-1.07152200	-0.34942300
H	-5.84110200	-1.40110800	-1.08397200
C	-4.39719200	0.12814200	-0.58847100
C	-4.73483000	0.92834700	-1.83404500
H	-5.06748700	0.26180000	-2.64844100
H	-3.88641900	1.52943400	-2.20346700
H	-5.56579500	1.63501800	-1.64736900
C	-3.45434000	3.04265200	0.22791600
H	-4.53743400	2.96183700	0.35253400
C	-2.83493200	4.29277500	0.16064500
H	-3.42471800	5.21473900	0.20291200
C	-1.42692800	4.35772900	0.07264600
C	-0.68591400	5.59003600	0.04077500
H	-1.24184500	6.53320100	0.07753600
C	0.68591000	5.59005200	-0.04053300
H	1.24182300	6.53323100	-0.07720900
C	1.42693100	4.35775600	-0.07251300
C	2.83493300	4.29280500	-0.16055500
H	3.42471300	5.21477800	-0.20274000
C	3.45434400	3.04269800	-0.22795900
H	4.53743400	2.96188600	-0.35261500
C	2.70134400	1.84634300	-0.16683900
C	3.41182500	0.54482000	-0.34720700
C	4.39723600	0.12809000	0.58803500
C	4.73521600	0.92825700	1.83353500
H	5.06753000	0.26163800	2.64801400
H	3.88708500	1.52979100	2.20286900
H	5.56653900	1.63449200	1.64679500
C	5.09505900	-1.07165200	0.34883000
H	5.84112000	-1.40132800	1.08321800
C	4.87292600	-1.85178500	-0.79723300
C	5.66392100	-3.11661800	-1.05101600
H	6.10792300	-3.51184300	-0.12161400
H	6.49461100	-2.92930700	-1.75787600
H	5.03484700	-3.90738900	-1.49633800
C	3.91456100	-1.39941000	-1.72560500
H	3.74443200	-1.97783600	-2.64260500
C	3.18422700	-0.21678100	-1.53056700
C	2.23157800	0.25368500	-2.61162600
H	2.28207000	-0.40705600	-3.49240800
H	2.46923600	1.28097200	-2.94387500
H	1.18066000	0.26709100	-2.26785500
C	0.71164200	3.12088200	-0.02094900
C	-0.71163200	3.12086800	0.02100500
C	1.71308700	-1.02898800	2.04132100
H	2.02768600	-0.03315500	2.36591600
C	2.15316700	-2.18419100	2.70776900
H	2.81380100	-2.08151700	3.57287000

C	1.76130900	-3.44960000	2.24293000
H	2.11644000	-4.36185500	2.73390700
C	0.89629000	-3.53686000	1.12840400
C	0.42090100	-4.76718100	0.54538700
H	0.75326200	-5.71423800	0.98465600
C	-0.42028200	-4.76733200	-0.54453700
H	-0.75256300	-5.71450800	-0.98360800
C	-0.89580800	-3.53717200	-1.12778100
C	-1.76094800	-3.45021300	-2.24223500
H	-2.11604100	-4.36260100	-2.73299400
C	-2.15299800	-2.18493800	-2.70726700
H	-2.81374200	-2.08249600	-3.57231100
C	-1.71295900	-1.02955800	-2.04108800
H	-2.02765800	-0.03382000	-2.36587600
C	-0.45949900	-2.31213100	-0.53942200
C	0.45990500	-2.31197800	0.53976900

2 (reduced)

Cu	-0.07885300	0.35617600	0.07460700
N	-1.63903700	1.64548500	0.00886700
N	1.00958300	2.04871200	-0.14129500
N	0.30207100	-0.76966100	1.72228900
N	0.11169700	-1.38278400	-0.86781700
C	-2.97459900	1.41506800	0.01031200
C	-3.46110500	0.01474200	-0.20849900
C	-3.58851700	-0.89084300	0.87524700
C	-3.29317000	-0.45930900	2.29690600
H	-3.23006000	-1.32978400	2.97105400
H	-4.09085800	0.20215900	2.68604600
H	-2.34571300	0.09976400	2.36833500
C	-4.05708100	-2.19198400	0.61915700
H	-4.14849300	-2.89397800	1.45790700
C	-4.42677900	-2.61165300	-0.67157500
C	-4.96107500	-4.00712800	-0.91450300
H	-4.75314300	-4.34910500	-1.94304800
H	-6.05862100	-4.04100100	-0.77602200
H	-4.52317100	-4.73802300	-0.21286100
C	-4.32370100	-1.68201700	-1.72248000
H	-4.62318500	-1.98267400	-2.73477800
C	-3.86209000	-0.36950400	-1.51586400
C	-3.84018700	0.61205900	-2.67244500
H	-3.98492600	0.09097800	-3.63405800
H	-2.89531100	1.18031800	-2.72856400
H	-4.65361300	1.35709000	-2.58360600
C	-3.90728400	2.47573400	0.15975400
H	-4.97458700	2.23488700	0.17240900
C	-3.47161900	3.79029200	0.27916400
H	-4.18649500	4.61244600	0.39641100

C	-2.08086800	4.06478700	0.22817500
C	-1.52636500	5.39016000	0.30590700
H	-2.21128700	6.23753500	0.42039000
C	-0.16879500	5.59594400	0.23335900
H	0.24350300	6.60941500	0.28971400
C	0.74017200	4.49189200	0.07644000
C	2.14754800	4.63946400	-0.02147400
H	2.59600400	5.63797500	0.02909100
C	2.93771500	3.50881300	-0.19564500
H	4.02426700	3.59266700	-0.29329600
C	2.34784500	2.21858400	-0.26355800
C	3.20042000	1.01278900	-0.52005400
C	3.81836900	0.32237100	0.55193700
C	3.67889000	0.79095500	1.98659700
H	3.77705500	-0.05201400	2.69175200
H	2.71171000	1.28525300	2.17229700
H	4.47064900	1.52128800	2.24303500
C	4.62434200	-0.79530800	0.26342900
H	5.09116800	-1.33748700	1.09584500
C	4.85985800	-1.22483500	-1.05365300
C	5.76060000	-2.40720800	-1.34143000
H	5.41843500	-2.97374600	-2.22504400
H	5.80718900	-3.10054300	-0.48427000
H	6.79555000	-2.07559800	-1.55062500
C	4.26276000	-0.49869900	-2.10197100
H	4.44778500	-0.80559400	-3.13947300
C	3.44745600	0.62066700	-1.86380700
C	2.89355700	1.41592500	-3.02984300
H	3.06018700	0.88631200	-3.98295500
H	3.38882100	2.40201900	-3.11349600
H	1.81200000	1.61296600	-2.93035200
C	0.22085800	3.16476400	0.01175800
C	-1.20338100	2.94810100	0.09173800
C	0.38702000	-0.42119400	3.02306300
C	0.12588800	1.02080200	3.37479600
H	-0.06795700	1.59010200	2.45272500
H	0.98598700	1.47108400	3.90246200
H	-0.74951500	1.11750000	4.04292400
C	0.69917500	-1.37570600	4.02772700
H	0.75981400	-1.04731100	5.07038900
C	0.91571300	-2.70578100	3.69082700
H	1.15345400	-3.44862200	4.46048100
C	0.82275100	-3.10180200	2.33072500
C	1.01797900	-4.45055700	1.87131400
H	1.25447200	-5.22613600	2.60812500
C	0.90890800	-4.76714500	0.53637900
H	1.05781400	-5.79828500	0.19729600
C	0.59962700	-3.75920500	-0.44192000

C	0.47446400	-4.01352800	-1.83336000
H	0.61450200	-5.03032900	-2.21686200
C	0.17517500	-2.96329500	-2.69169300
H	0.07380500	-3.13436400	-3.76818000
C	-0.00284900	-1.64944400	-2.18469600
C	-0.33337300	-0.49004100	-3.08383700
H	-0.35759600	0.42787100	-2.47265100
H	-1.31981800	-0.62579100	-3.56168200
H	0.41271700	-0.37334200	-3.88930300
C	0.40448300	-2.41535100	-0.01268200
C	0.51359500	-2.08358900	1.38270300

2 (oxidized)

Cu	-0.00018200	0.41131400	0.00008100
N	-1.34295900	1.91559200	0.11170000
N	1.34153300	1.91645700	-0.11196300
N	0.66076600	-1.08981400	1.17122500
N	-0.66009500	-1.09055300	-1.17105500
C	-2.68391700	1.85779800	0.30732100
C	-3.34383000	0.53077900	0.45588000
C	-3.04803200	-0.28024100	1.59389700
C	-2.20102800	0.21245700	2.75327100
H	-1.78528200	-0.63571200	3.32265900
H	-2.82559300	0.79505400	3.45719200
H	-1.36814600	0.86549200	2.44965700
C	-3.70177400	-1.51759000	1.72730500
H	-3.49034700	-2.13136900	2.61166500
C	-4.64902400	-1.97231100	0.79183500
C	-5.36485400	-3.28971700	0.97691400
H	-5.52490500	-3.80660300	0.01486400
H	-6.36486700	-3.12810200	1.42256000
H	-4.81287500	-3.96578100	1.65079600
C	-4.94964800	-1.13359200	-0.30083800
H	-5.70066100	-1.45937100	-1.03140200
C	-4.33899900	0.11968200	-0.47783500
C	-4.79407300	0.98812500	-1.63704800
H	-5.09829400	0.36783800	-2.49765800
H	-4.02604800	1.70074900	-1.97968500
H	-5.68459200	1.58269400	-1.35734000
C	-3.44330400	3.05959000	0.40390200
H	-4.52099600	2.97809800	0.56944200
C	-2.82998400	4.30001700	0.31508400
H	-3.41832400	5.22111400	0.39100600
C	-1.42003400	4.37429200	0.14866000
C	-0.68599000	5.60759400	0.07673200
H	-1.23745200	6.55105900	0.14514900
C	0.68224400	5.60802900	-0.07717800
H	1.23309900	6.55184500	-0.14563900

C	1.41706900	4.37518700	-0.14901600
C	2.82707200	4.30177400	-0.31532900
H	3.41484300	5.22323500	-0.39125300
C	3.44118900	3.06172900	-0.40402000
H	4.51894600	2.98091600	-0.56946600
C	2.68254800	1.85946600	-0.30745500
C	3.34326600	0.53285100	-0.45594700
C	4.33876900	0.12244900	0.47772700
C	4.79321100	0.99107700	1.63706300
H	5.09667200	0.37091100	2.49803400
H	4.02508800	1.70393400	1.97898300
H	5.68406400	1.58537000	1.35784900
C	4.95027300	-1.13041400	0.30071800
H	5.70157300	-1.45564700	1.03123000
C	4.65009200	-1.96940400	-0.79185900
C	5.36677200	-3.28634900	-0.97693300
H	4.81516700	-3.96281400	-1.65071900
H	5.52724700	-3.80308200	-0.01487000
H	6.36663900	-3.12411700	-1.42268100
C	3.70242900	-1.51538300	-1.72725600
H	3.49130300	-2.12938500	-2.61153400
C	3.04791400	-0.27844300	-1.59389000
C	2.20051600	0.21360000	-2.75325200
H	1.78493400	-0.63488600	-3.32228900
H	2.82476600	0.79617200	-3.45747600
H	1.36747800	0.86647200	-2.44970900
C	0.71436200	3.13843100	-0.06671400
C	-0.71656200	3.13797500	0.06638200
C	1.23345000	-1.03384900	2.38920100
C	1.49516600	0.30422500	3.02362800
H	1.22476000	1.12848200	2.34732600
H	2.55613000	0.40824900	3.30689700
H	0.90416800	0.40608900	3.95217700
C	1.55906800	-2.22933000	3.09142200
H	2.02680400	-2.14664000	4.07729900
C	1.29080900	-3.47031200	2.53668800
H	1.55362000	-4.39002400	3.07084000
C	0.65596900	-3.54652800	1.26680000
C	0.31301700	-4.78037400	0.61436500
H	0.55957400	-5.72395600	1.11229800
C	-0.30833700	-4.78072300	-0.61409900
H	-0.55386900	-5.72458200	-1.11201400
C	-0.65265400	-3.54726400	-1.26654900
C	-1.28764500	-3.47177900	-2.53640300
H	-1.54950900	-4.39179100	-3.07050500
C	-1.55727900	-2.23111000	-3.09115900
H	-2.02522000	-2.14896200	-4.07698500
C	-1.23286500	-1.03525200	-2.38902200

C	-1.49589100	0.30251500	-3.02355000
H	-1.22667400	1.12707300	-2.34714700
H	-2.55684900	0.40533500	-3.30727100
H	-0.90463000	0.40503500	-3.95186400
C	-0.34196200	-2.31238200	-0.63025300
C	0.34395400	-2.31200500	0.63045900

2 (triplet)

Cu	0.01010800	0.38237400	0.03806500
N	-1.47227200	1.76395400	0.03799200
N	1.20082200	1.94091000	-0.19124400
N	0.93609200	-0.74773600	1.40586400
N	-0.52883100	-1.37006500	-0.74545900
C	-2.81743200	1.65031600	0.26037200
C	-3.49964000	0.31782800	0.21073600
C	-3.32399100	-0.62096300	1.26514700
C	-2.45794500	-0.30078400	2.46516400
H	-2.41571800	-1.15320600	3.16276700
H	-2.84970500	0.57233400	3.02005100
H	-1.42278100	-0.05556400	2.16992600
C	-4.02939300	-1.83442100	1.22255300
H	-3.89143800	-2.55169600	2.04171700
C	-4.92238000	-2.14426100	0.17874700
C	-5.68736300	-3.45013200	0.17359100
H	-6.13538800	-3.65522200	-0.81328000
H	-6.51082700	-3.43015800	0.91231800
H	-5.03742200	-4.30241400	0.44051300
C	-5.10656400	-1.18634300	-0.83249500
H	-5.81086600	-1.39800000	-1.64727400
C	-4.43046700	0.04944500	-0.82981000
C	-4.74272200	1.05576000	-1.92324600
H	-5.16289200	0.55176800	-2.81073300
H	-3.85844700	1.63293100	-2.24229400
H	-5.49836200	1.79140200	-1.58845800
C	-3.60847200	2.79120200	0.52621800
H	-4.67578200	2.64269300	0.71129700
C	-3.05497000	4.07622800	0.53529800
H	-3.68045100	4.95657500	0.71786900
C	-1.67146000	4.22519400	0.30489900
C	-0.99885800	5.49782500	0.27548900
H	-1.59470500	6.40281500	0.43732800
C	0.35189000	5.58708900	0.03528400
H	0.84610500	6.56383200	-0.00759800
C	1.14908300	4.40442700	-0.15417600
C	2.53900500	4.41409000	-0.40537000
H	3.07609800	5.36650300	-0.46991600
C	3.21166200	3.20005300	-0.59992800
H	4.27614000	3.18301000	-0.85005400

C	2.53059400	1.96594100	-0.49215700
C	3.23767400	0.67932700	-0.78004200
C	4.29945200	0.20974200	0.03691100
C	4.76771800	0.91670500	1.29553700
H	4.50356700	0.33315200	2.19723900
H	4.34083400	1.92553400	1.40780900
H	5.86754800	1.01977100	1.29625300
C	4.95413800	-0.98639600	-0.32182200
H	5.76781300	-1.34969800	0.31908800
C	4.61120300	-1.71745800	-1.46803900
C	5.33672300	-2.99250000	-1.83864800
H	4.63666300	-3.84384300	-1.92524900
H	6.10050600	-3.25688600	-1.08851000
H	5.84420600	-2.89438800	-2.81608900
C	3.58206100	-1.20900300	-2.28675300
H	3.32487000	-1.73645700	-3.21429400
C	2.89726600	-0.02577900	-1.97519600
C	1.89362000	0.53075800	-2.96725000
H	1.75019500	-0.16793800	-3.80811000
H	2.24004900	1.49358100	-3.38794400
H	0.90670900	0.72570800	-2.51256200
C	0.50200700	3.13103300	-0.08895600
C	-0.90429900	3.03649900	0.09368700
C	1.48896900	-0.37691400	2.59001700
C	1.50466600	1.08743500	2.94647200
H	2.25385700	1.64459700	2.35888700
H	1.73786700	1.22575800	4.01414700
H	0.52275900	1.54824700	2.74003600
C	2.00381600	-1.34868900	3.47530900
H	2.45220500	-1.01528100	4.41588400
C	1.94490900	-2.71174800	3.15957600
H	2.36636600	-3.46130200	3.83784400
C	1.30057100	-3.11824900	1.96887200
C	1.12297000	-4.48874800	1.56532800
H	1.53233300	-5.27841600	2.20490000
C	0.45811000	-4.80785100	0.40383500
H	0.34157800	-5.85433600	0.10125500
C	-0.11228000	-3.78555800	-0.43260000
C	-0.81674700	-4.04021000	-1.63143900
H	-0.95999300	-5.07096700	-1.97368700
C	-1.31563300	-2.96695400	-2.37012200
H	-1.84704900	-3.13527700	-3.31160900
C	-1.16294500	-1.63609600	-1.91021500
C	-1.68957900	-0.49382700	-2.73675800
H	-1.61574800	0.46086400	-2.19494300
H	-2.74384000	-0.66340100	-3.01019000
H	-1.11420200	-0.40883600	-3.67733900
C	0.03644300	-2.42064100	-0.04066800

C 0.77751500 -2.08938500 1.12815600

Cu(b11)(L3) (reduced)

Cu	-0.04241800	0.19830400	-0.04650000
N	-1.69572900	1.21192200	-0.72173000
N	0.93864000	1.44680000	-1.33858000
N	0.68224300	0.60742300	1.91204400
N	0.45235900	-1.65957200	0.43962600
C	-3.03058200	1.05311300	-0.51693000
C	-3.64198100	-0.27184600	-0.16339600
C	-3.51010400	-0.85915000	1.12170800
C	-2.63400100	-0.22749100	2.17615500
H	-2.52375200	-0.88467100	3.05456600
H	-3.04790700	0.73704700	2.52689500
H	-1.63167500	-0.02640500	1.76165500
C	-4.22168000	-2.03618500	1.41502400
H	-4.11277500	-2.47970100	2.41283600
C	-5.07602400	-2.64647500	0.48005200
C	-5.87229900	-3.88316700	0.83607500
H	-5.99310300	-4.55361500	-0.03241900
H	-6.88888800	-3.61234400	1.17984400
H	-5.39412200	-4.45465000	1.64979700
C	-5.18105500	-2.05638200	-0.79291500
H	-5.82074000	-2.52744100	-1.55012900
C	-4.48960800	-0.88048800	-1.13493200
C	-4.64283100	-0.32504300	-2.53998100
H	-5.06725600	-1.08995500	-3.21172800
H	-3.67793400	0.00183300	-2.96584300
H	-5.32155900	0.54748600	-2.57548100
C	-3.94134600	2.13135000	-0.71340000
H	-4.99513600	1.96637800	-0.47058300
C	-3.51033600	3.34899200	-1.21175400
H	-4.20905000	4.17922500	-1.36443200
C	-2.14313800	3.50221400	-1.55352100
C	-1.62201400	4.70568700	-2.14133200
H	-2.31392800	5.53300400	-2.33406900
C	-0.29070400	4.81759600	-2.45886500
H	0.10239900	5.73530000	-2.90997000
C	0.61550300	3.73216500	-2.20533900
C	1.99968300	3.79871500	-2.50748900
H	2.41595600	4.70973600	-2.95217700
C	2.80128700	2.69541300	-2.25324100
H	3.86638400	2.70235300	-2.50384500
C	2.24428900	1.51534900	-1.68786900
C	3.11473400	0.30132000	-1.56657400
C	3.99368400	0.13226700	-0.46801400
C	4.07180300	1.15499800	0.64736100
H	4.64014400	0.76062700	1.50619000

H	3.07365400	1.45553900	1.00799300
H	4.58596900	2.07594700	0.31077700
C	4.84845000	-0.98615800	-0.45135700
H	5.52272100	-1.12095300	0.40398600
C	4.88317200	-1.91581400	-1.50503000
C	5.80419100	-3.11613800	-1.45992400
H	6.21635400	-3.34806100	-2.45751500
H	5.26660500	-4.01978500	-1.11389900
H	6.64953500	-2.95301600	-0.76985400
C	4.03475800	-1.69576800	-2.60718700
H	4.07502000	-2.38478300	-3.46076900
C	3.15215900	-0.60259000	-2.66276100
C	2.30024400	-0.37369500	-3.89629200
H	2.46291000	-1.16912400	-4.64198500
H	2.54115000	0.59104200	-4.38080600
H	1.22186200	-0.34851300	-3.65632300
C	0.13187100	2.52572600	-1.61146600
C	-1.27256000	2.40356000	-1.27785000
C	0.79159700	1.75728800	2.61495500
C	0.23855200	3.01896600	1.97579200
H	0.01951200	2.72716500	0.93494300
C	1.40533100	1.77765100	3.89755700
H	1.50209700	2.72796900	4.42880400
C	1.87955100	0.60540600	4.46846000
H	2.34737300	0.61293300	5.45956800
C	1.76176300	-0.61503400	3.75618300
C	2.23110200	-1.87313400	4.26765500
H	2.68844500	-1.89711600	5.26295200
C	2.11275200	-3.02153900	3.52270500
H	2.47578200	-3.97900600	3.91237500
C	1.51876700	-2.99507700	2.21399800
C	1.40626800	-4.14434300	1.39171200
H	1.77173900	-5.11133100	1.75524200
C	0.84300700	-4.02348300	0.12960200
H	0.76771200	-4.89494800	-0.52565800
C	0.36400700	-2.76947700	-0.33271200
C	-0.28236000	-2.61324700	-1.69571500
H	-0.28916400	-1.51704700	-1.87309000
C	1.02978200	-1.76437200	1.68322500
C	1.15282800	-0.55592000	2.46527600
C	1.27085800	4.16690200	1.94405200
H	0.84829000	5.03607500	1.40958400
H	1.55548300	4.50871800	2.95435800
H	2.19362400	3.86192300	1.42077500
C	-1.12618500	3.47057400	2.58433000
H	-1.49961300	4.28827300	1.93769700
H	-1.84609300	2.63880200	2.47340400
C	-1.12348600	3.94771800	4.04487600

H	-2.13047000	4.30074100	4.32807000
H	-0.85417500	3.13817500	4.74576300
H	-0.42691600	4.78938400	4.20776800
C	0.52297600	-3.29657100	-2.81875300
H	0.52977900	-4.39584500	-2.71840800
H	0.07070100	-3.06322500	-3.79884900
H	1.57029400	-2.95229100	-2.82566800
C	-1.77456700	-3.06680200	-1.68664700
H	-2.21197600	-2.73518800	-2.64821500
H	-2.30252700	-2.50549700	-0.89710100
C	-2.04439200	-4.56794000	-1.50433800
H	-1.68750500	-4.93793400	-0.52666700
H	-3.13134000	-4.75545300	-1.54318900
H	-1.57863200	-5.18245100	-2.29518500

Cu(**bL1**)(**L3**) (oxidized)

Cu	-0.05782300	0.28115200	-0.05856400
N	-1.63131000	1.53953200	-0.57510200
N	1.03914800	1.55757400	-1.16060700
N	1.16733600	0.12604000	1.53759400
N	-0.02005100	-1.78162600	-0.00018000
C	-2.96397900	1.53172700	-0.30175400
C	-3.71928700	0.35141500	0.22510900
C	-3.47201900	-0.16710200	1.52764900
C	-2.31672100	0.32238400	2.36292700
H	-2.29697800	-0.16770800	3.34966400
H	-2.36646000	1.41499000	2.52312000
H	-1.34580700	0.11536300	1.87040800
C	-4.36997600	-1.10007100	2.08006500
H	-4.17773300	-1.47496700	3.09280400
C	-5.52809700	-1.52579600	1.39803700
C	-6.51117000	-2.47294800	2.04530900
H	-7.10505800	-3.02094300	1.29520000
H	-7.22338100	-1.91577600	2.68316900
H	-6.00409900	-3.20753500	2.69389700
C	-5.73937500	-1.01996600	0.10478900
H	-6.61370400	-1.35891000	-0.46472600
C	-4.86655900	-0.08989400	-0.49882800
C	-5.18720800	0.37171200	-1.90912900
H	-5.62248000	-0.45765500	-2.49324800
H	-4.30466300	0.74190900	-2.45535900
H	-5.94372300	1.17929600	-1.91308100
C	-3.75130300	2.70896200	-0.49740800
H	-4.80550100	2.66954200	-0.21236900
C	-3.20649300	3.86510300	-1.01981000
H	-3.81985500	4.76038100	-1.16999500
C	-1.83070400	3.88211600	-1.36255600
C	-1.19632200	5.03608400	-1.93568300

H	-1.80457200	5.92886100	-2.11462600
C	0.13822200	5.02033500	-2.26251000
H	0.61524600	5.89511100	-2.71645900
C	0.93005900	3.85018500	-2.01564400
C	2.30975400	3.76308300	-2.34569000
H	2.81194400	4.62306900	-2.80259500
C	2.99491200	2.57983200	-2.12128600
H	4.04193100	2.47037200	-2.41673700
C	2.33687000	1.46017600	-1.53613200
C	3.04645700	0.15228800	-1.44195800
C	4.22364900	0.00680600	-0.65461300
C	4.77951200	1.13156800	0.19628900
H	5.40310600	0.73343100	1.01381200
H	3.99163000	1.75840600	0.64428900
H	5.43046200	1.80079100	-0.39814200
C	4.91181100	-1.21811400	-0.69364600
H	5.81047800	-1.33565400	-0.07563700
C	4.50664600	-2.28252800	-1.52168800
C	5.30963400	-3.56020700	-1.59519100
H	4.68266200	-4.42449600	-1.87272800
H	5.81390500	-3.78295800	-0.63965600
H	6.10065500	-3.47618600	-2.36484400
C	3.36217200	-2.09617500	-2.32267900
H	3.05543700	-2.89520000	-3.00872700
C	2.62602500	-0.90069000	-2.30843600
C	1.49310600	-0.71143300	-3.29812300
H	1.38157100	-1.60620300	-3.93115900
H	1.68784300	0.14338300	-3.97212200
H	0.52308200	-0.51639000	-2.80772700
C	0.32810000	2.69858300	-1.42315300
C	-1.07884500	2.69659300	-1.10252600
C	1.62711700	1.10635400	2.34607100
C	1.01647200	2.49245600	2.23108200
H	0.30138400	2.42723500	1.38899700
C	2.63596500	0.80800300	3.30590000
H	3.03054200	1.61597100	3.92555000
C	3.11832800	-0.48399200	3.44836100
H	3.89729300	-0.70877900	4.18548400
C	2.59508000	-1.52802900	2.63989200
C	3.01846400	-2.89623300	2.73402200
H	3.77705500	-3.16404400	3.47688600
C	2.48330000	-3.85016000	1.90060300
H	2.81785800	-4.89127600	1.95861700
C	1.46842000	-3.50993200	0.94213000
C	0.90900500	-4.45105900	0.03928700
H	1.26047400	-5.48882600	0.04608300
C	-0.08033800	-4.04389200	-0.83751900
H	-0.51517500	-4.75321600	-1.54429600

C	-0.58039100	-2.70847500	-0.81254500
C	-1.79955000	-2.34600500	-1.63652800
H	-1.91735500	-1.24747400	-1.55172700
C	0.99788400	-2.16814200	0.84810800
C	1.59871400	-1.16491400	1.68699500
C	2.05650400	3.58309800	1.89351700
H	1.56696200	4.57238500	1.87308100
H	2.86809200	3.63402500	2.63884700
H	2.51771800	3.41233900	0.90579500
C	0.16096000	2.87587700	3.48744000
H	-0.43796300	3.75434400	3.17826600
H	-0.56186700	2.06385500	3.68642600
C	0.90104800	3.22067300	4.78974700
H	0.17607700	3.59329400	5.53346600
H	1.39523500	2.34414800	5.24256900
H	1.65517900	4.01439000	4.64928500
C	-1.66638400	-2.70872400	-3.13292800
H	-1.53226100	-3.79118200	-3.29582200
H	-2.58908400	-2.41390500	-3.66189200
H	-0.82112500	-2.18985000	-3.61075800
C	-3.09266800	-2.97290600	-1.01449200
H	-3.93493500	-2.51596600	-1.56499000
H	-3.18403700	-2.62298400	0.02910100
C	-3.25147600	-4.50100500	-1.05748100
H	-2.52846600	-5.02398500	-0.40753000
H	-4.25735200	-4.77121200	-0.69267200
H	-3.16111900	-4.90977600	-2.07914500

Cu(**bL1**)(**L3**) triplet

Cu	-0.05851800	0.30070400	-0.06710200
N	-1.61644800	1.50670900	-0.57784700
N	1.03529400	1.56206700	-1.14393200
N	1.18389500	0.15244100	1.50228400
N	-0.02703800	-1.75225200	0.00503600
C	-2.94870500	1.52025000	-0.25005500
C	-3.70226000	0.33031700	0.27013000
C	-3.47812200	-0.17797200	1.57958000
C	-2.34426800	0.33500900	2.43451300
H	-2.32589900	-0.16297900	3.41797300
H	-2.43242300	1.42431400	2.60230500
H	-1.36313400	0.16274500	1.95447800
C	-4.36919400	-1.12463700	2.11408700
H	-4.18891400	-1.50045900	3.12927800
C	-5.50101400	-1.57072500	1.40566800
C	-6.48096500	-2.53936300	2.03092500
H	-7.06146600	-3.08184900	1.26550800
H	-7.20601000	-2.00623100	2.67513400
H	-5.96949900	-3.28238600	2.66735800

C	-5.69659500	-1.06894400	0.10823600
H	-6.55513800	-1.42256300	-0.47716200
C	-4.82422600	-0.13115100	-0.47686500
C	-5.11110400	0.33691900	-1.89354300
H	-5.66462700	-0.43920900	-2.44990600
H	-4.19008600	0.56944000	-2.45399000
H	-5.73768900	1.24809900	-1.91236300
C	-3.72728600	2.69277000	-0.39619400
H	-4.77287700	2.65067300	-0.08080800
C	-3.19913200	3.86463600	-0.94339100
H	-3.82006700	4.75722100	-1.07435500
C	-1.84731400	3.87584400	-1.33519400
C	-1.21840700	5.02151900	-1.93739300
H	-1.82806300	5.91690600	-2.10186600
C	0.10254400	4.99839000	-2.31233100
H	0.56386200	5.86901700	-2.79129600
C	0.91072600	3.83345700	-2.07703600
C	2.27380700	3.73882700	-2.42987600
H	2.77219300	4.58766200	-2.91038100
C	2.96519100	2.54122600	-2.19604600
H	4.00337800	2.41987500	-2.51704200
C	2.32937300	1.45260100	-1.56168100
C	3.03885600	0.14059900	-1.44782200
C	4.18305000	-0.02032900	-0.62240700
C	4.73952700	1.11095700	0.21846200
H	5.34599200	0.71846600	1.05214600
H	3.94798900	1.74805600	0.64312000
H	5.39915000	1.76840900	-0.37959800
C	4.84357300	-1.26318900	-0.61557600
H	5.71644500	-1.39011600	0.03732300
C	4.43463300	-2.33494700	-1.42759000
C	5.19540400	-3.64334800	-1.43587900
H	4.53340100	-4.49790000	-1.65930800
H	5.68972500	-3.83219500	-0.46748400
H	5.98663800	-3.63626500	-2.20972200
C	3.32567700	-2.13565400	-2.27094300
H	3.00880600	-2.94470500	-2.94106800
C	2.62606300	-0.91795600	-2.30584300
C	1.51392600	-0.71946200	-3.31512600
H	1.39557100	-1.61647600	-3.94459600
H	1.72999500	0.13432700	-3.98401200
H	0.54294300	-0.50395600	-2.83433800
C	0.30546000	2.69666600	-1.44827500
C	-1.07508700	2.69012000	-1.10932900
C	1.63715800	1.13924800	2.31594500
C	1.02881400	2.52703400	2.17117400
H	0.32028200	2.45012900	1.32630300
C	2.62426200	0.84786100	3.28899500

H	3.01793100	1.66067400	3.90302400
C	3.10972500	-0.45195500	3.44794000
H	3.88345500	-0.67012500	4.19233500
C	2.59438500	-1.49660600	2.64569000
C	3.02004200	-2.86613400	2.73500900
H	3.77300600	-3.13479300	3.48399500
C	2.50637300	-3.81606200	1.88453000
H	2.85295500	-4.85412100	1.93550100
C	1.49820600	-3.48197600	0.91496000
C	0.96503100	-4.41247800	-0.00409100
H	1.32884300	-5.44590300	-0.01096600
C	-0.02943500	-3.99881800	-0.88677400
H	-0.45130300	-4.70308100	-1.60654400
C	-0.55766600	-2.68344900	-0.83122400
C	-1.79206000	-2.33115200	-1.64056300
H	-1.92327800	-1.23510100	-1.54834800
C	1.01069200	-2.14091600	0.84409400
C	1.60382600	-1.14524500	1.67824200
C	2.06918500	3.61061000	1.81429600
H	1.58229100	4.60138900	1.77985700
H	2.88607900	3.66719100	2.55436800
H	2.52003000	3.42312700	0.82530600
C	0.16337800	2.93861600	3.40782700
H	-0.43804000	3.80749000	3.07636500
H	-0.55795100	2.12899000	3.62106800
C	0.89297600	3.31563700	4.70737400
H	0.16426300	3.69877900	5.44289000
H	1.39398400	2.45039500	5.17408600
H	1.64461500	4.10932600	4.55051700
C	-1.67132400	-2.67785000	-3.14079100
H	-1.51793800	-3.75663000	-3.31463800
H	-2.60459800	-2.39407300	-3.65837200
H	-0.83948900	-2.13939900	-3.62113400
C	-3.07023200	-2.97594600	-1.01223600
H	-3.92742400	-2.53000000	-1.54783800
H	-3.15521600	-2.63397300	0.03430700
C	-3.20516100	-4.50628700	-1.06086200
H	-2.45317400	-5.01712600	-0.43470200
H	-4.19749800	-4.79744200	-0.67407900
H	-3.12875300	-4.90620600	-2.08788400

3 (reduced)

Cu	0.07730100	0.49436700	0.10560700
N	0.03415200	-1.45136400	0.09349900
N	1.41690100	1.97469600	-0.20612200
N	-1.27082300	1.96175900	-0.29532500
N	0.03405200	0.23787800	2.17198000
C	0.05040700	1.11001800	3.18848200

C	0.04354800	0.71609200	4.54501700
H	0.05714800	1.47746700	5.33060400
C	0.01612200	-0.64129800	4.85822300
H	0.00689700	-0.97845800	5.90071200
C	-0.00133700	-1.59736700	3.80952700
C	0.01377000	-1.09640400	2.47147000
C	-0.03412300	-3.02083000	4.01887100
H	-0.04580000	-3.40101500	5.04625600
C	-0.05329100	-3.88986700	2.95347900
H	-0.08129300	-4.97192500	3.12304900
C	0.00369200	-2.00698400	1.35536900
C	-0.03567200	-3.41250600	1.59428000
C	-0.05497700	-4.27099300	0.46487500
H	-0.08598300	-5.35705800	0.60386200
C	-0.03330000	-3.70642900	-0.80795500
H	-0.04848400	-4.33233200	-1.70491700
C	0.01239400	-2.30507500	-0.94915500
C	2.76841000	1.93446600	-0.22900700
C	3.53699400	3.12857300	-0.14014300
H	4.62786400	3.05207400	-0.15617100
C	2.91108300	4.36690600	-0.07216400
H	3.49820400	5.29048400	-0.01511900
C	1.49352800	4.43386200	-0.11085400
C	0.79040300	3.19426500	-0.17452800
C	0.75048600	5.66488100	-0.09163200
H	1.30220300	6.60974600	-0.03596200
C	-0.62369200	5.66117000	-0.14779300
H	-1.18266900	6.60337000	-0.13708000
C	-0.65353900	3.18830100	-0.23038600
C	-1.35971100	4.42763300	-0.22389700
C	-2.77525000	4.36039600	-0.29172400
H	-3.36629000	5.28318400	-0.29196200
C	-3.39133600	3.11899200	-0.37219400
H	-4.47964200	3.03791000	-0.44244100
C	-2.62119900	1.92122600	-0.37557800
C	3.42667100	0.60689400	-0.44977800
C	3.39574900	0.05510200	-1.76550700
C	4.00848400	-1.19020500	-1.98277600
H	3.99237800	-1.61824600	-2.99169700
C	4.67040100	-1.89068700	-0.95555400
C	4.72225000	-1.29830100	0.31661500
H	5.25814700	-1.82391100	1.11688900
C	4.12007000	-0.05590800	0.59692600
C	2.74329100	0.80772100	-2.93198700
H	2.66838200	1.87248800	-2.64181600
C	1.30418400	0.30883100	-3.19291900
H	0.69430400	0.37731600	-2.27022500
H	1.31423000	-0.74241600	-3.53633200

H	0.81474100	0.91350100	-3.97778500
C	3.58079000	0.76048500	-4.22827400
H	3.12927100	1.41770800	-4.99270200
H	3.62416400	-0.25580900	-4.65898300
H	4.61683000	1.09893200	-4.05351500
C	5.34920000	-3.23286200	-1.21957600
H	5.72397900	-3.60453800	-0.24524500
C	4.36178900	-4.28475700	-1.77147600
H	3.97717600	-3.99283900	-2.76601000
H	3.49621900	-4.41605600	-1.09820600
H	4.86293400	-5.26267600	-1.88451700
C	6.56814400	-3.07130400	-2.15713300
H	6.25933300	-2.70642700	-3.15377900
H	7.08047000	-4.03998800	-2.29763600
H	7.29814400	-2.35221000	-1.74646700
C	4.26321000	0.55194300	1.99527600
H	3.59045900	1.42885600	2.05592500
C	5.70730600	1.05520100	2.23239900
H	6.42820700	0.21870100	2.19523300
H	5.79465700	1.53317100	3.22490400
H	6.01620200	1.79140800	1.46937700
C	3.84514000	-0.42306500	3.11723500
H	3.88189800	0.08507700	4.09750300
H	4.52244900	-1.29407500	3.17444700
H	2.82092500	-0.80330500	2.96283200
C	-3.31291600	0.59450700	-0.49292000
C	-3.33638400	-0.08219700	-1.75051300
C	-4.04809700	-1.28958500	-1.84766700
H	-4.07243700	-1.80925000	-2.81124200
C	-4.74662400	-1.84414700	-0.75761900
C	-4.72564400	-1.14290100	0.45724800
H	-5.27762500	-1.55562100	1.31086700
C	-4.03185500	0.07280100	0.61731400
C	-2.70233900	0.53629000	-3.00272800
H	-1.81725200	1.11795200	-2.68412900
C	-2.21919400	-0.50056600	-4.03786500
H	-3.06297300	-1.01204600	-4.53499000
H	-1.57860500	-1.27507000	-3.58002000
H	-1.63627200	0.00128700	-4.82981500
C	-3.69353500	1.51828000	-3.67682000
H	-3.23387100	1.98478500	-4.56712400
H	-4.00251600	2.32691200	-2.99203200
H	-4.60520900	0.98533500	-4.00214000
C	-5.51748600	-3.15505200	-0.89155200
H	-5.96622700	-3.36981000	0.09859700
C	-6.67202200	-3.03766500	-1.91213500
H	-6.28927500	-2.83369800	-2.92886600
H	-7.36532600	-2.22206200	-1.64254800

H	-7.24821400	-3.97923700	-1.95464000
C	-4.58291300	-4.33398800	-1.24557700
H	-5.14775100	-5.28326300	-1.26564400
H	-3.76542800	-4.43405900	-0.50978500
H	-4.12617900	-4.19688600	-2.24302400
C	-4.10973500	0.79730500	1.96588900
H	-3.38250300	1.63088200	1.95160200
C	-5.51566300	1.40616100	2.18493400
H	-5.79088700	2.10833200	1.37842400
H	-5.55766500	1.95382400	3.14387700
H	-6.28726200	0.61573500	2.21249000
C	-3.73489900	-0.11408700	3.15508500
H	-4.46662000	-0.93057300	3.29040900
H	-3.71960500	0.47001900	4.09267700
H	-2.74126400	-0.57284600	3.01695000
H	0.06655200	2.17057000	2.91019400
H	0.04034500	-1.84638000	-1.94071400

3 (oxidized)

Cu	-0.17095700	0.51294000	0.35621600
N	0.60231400	-1.29563800	0.02652600
N	1.22501600	2.01000400	0.15488000
N	-1.46630500	1.97417200	0.06449900
N	-1.05747500	-0.42247900	1.91927900
C	-1.78206200	0.09218500	2.92110000
C	-2.23955900	-0.69813400	4.00102600
H	-2.81358200	-0.22685000	4.80353900
C	-1.97011300	-2.06435700	4.01479200
H	-2.33727300	-2.69762800	4.82971900
C	-1.20720300	-2.63795400	2.96206300
C	-0.74498600	-1.75191900	1.94738000
C	-0.86202200	-4.03299000	2.86798900
H	-1.22585600	-4.71751400	3.64128600
C	-0.09143600	-4.50439400	1.82902600
H	0.15431900	-5.56949700	1.76373400
C	0.10672300	-2.23105900	0.89829700
C	0.42705000	-3.61592900	0.81956900
C	1.25521800	-4.02524900	-0.26023100
H	1.52211900	-5.08172100	-0.37249100
C	1.72802800	-3.07174800	-1.15616300
H	2.37347500	-3.34938600	-1.99332800
C	1.39287000	-1.71097800	-0.97252200
C	2.57795700	2.00183600	0.17066700
C	3.30438100	3.22362100	0.31553700
H	4.39597900	3.16765600	0.32884100
C	2.65337000	4.44048100	0.42643300
H	3.21924300	5.37305200	0.52877600
C	1.23478000	4.47116900	0.39458700

C	0.56629400	3.21832900	0.27124500
C	0.46595600	5.68391800	0.46155200
H	0.99840100	6.63374300	0.57652600
C	-0.90610300	5.66056000	0.35596800
H	-1.48260800	6.59121900	0.37578900
C	-0.86752000	3.20018200	0.19719300
C	-1.60557600	4.41695200	0.19671500
C	-3.00895300	4.30860800	-0.01075100
H	-3.62707600	5.21305400	-0.02585900
C	-3.57309400	3.06775000	-0.25947900
H	-4.63207500	2.98045700	-0.51223500
C	-2.78332100	1.87613700	-0.23988100
C	3.37322000	0.74054500	0.02934900
C	4.05356200	0.49877600	-1.20016100
C	4.91371700	-0.61395300	-1.27962700
H	5.44212000	-0.80034000	-2.22188700
C	5.14497600	-1.46949000	-0.18604300
C	4.46013800	-1.19808700	1.01345400
H	4.64415200	-1.84786800	1.87583200
C	3.58461000	-0.10603000	1.15886600
C	3.90669400	1.41113700	-2.42525600
H	3.15297000	2.18779600	-2.19399400
C	3.40014300	0.65068400	-3.67258200
H	2.41477900	0.17885200	-3.49841100
H	4.10358100	-0.14161900	-3.98421000
H	3.28917300	1.34545900	-4.52337000
C	5.23661700	2.13559100	-2.74404300
H	5.10243800	2.82954700	-3.59221200
H	6.02746900	1.41666800	-3.02135100
H	5.60581800	2.71678300	-1.88111600
C	6.14509000	-2.61946600	-0.27079400
H	6.09673300	-3.16454600	0.69232000
C	5.80050100	-3.62224200	-1.39439500
H	5.84990000	-3.15025900	-2.39263900
H	4.78815500	-4.04586400	-1.26313800
H	6.51866500	-4.46040800	-1.39225500
C	7.58774800	-2.08365300	-0.43297900
H	7.70884700	-1.54144200	-1.38826200
H	8.30870100	-2.91951400	-0.42784900
H	7.85675500	-1.39414700	0.38558900
C	2.96100400	0.20780700	2.52454900
H	1.96939300	0.67131800	2.34114400
C	3.82498100	1.23604500	3.29826800
H	4.83161600	0.82464900	3.49001300
H	3.36299400	1.47437400	4.27276700
H	3.94840800	2.18061200	2.74170000
C	2.72827900	-1.03492200	3.40855700
H	2.14108100	-0.75553400	4.30065200

H	3.67921100	-1.45967500	3.77516400
H	2.18802800	-1.83471800	2.87197100
C	-3.35338600	0.56252400	-0.64595700
C	-2.76487100	-0.13977300	-1.75971500
C	-3.37829600	-1.32475700	-2.19086000
H	-2.95746000	-1.85307900	-3.05070100
C	-4.54187100	-1.84923600	-1.58950900
C	-5.10395200	-1.13006300	-0.52466500
H	-6.01726000	-1.51657800	-0.05778600
C	-4.55150900	0.06978600	-0.03976000
C	-1.60934600	0.44395100	-2.59911200
H	-0.81992400	0.82100800	-1.91393600
C	-0.92202200	-0.57887500	-3.52562400
H	-1.57832600	-0.88418200	-4.35960000
H	-0.61168600	-1.49240400	-2.98778500
H	-0.02555500	-0.12168800	-3.97996500
C	-2.10175700	1.64684700	-3.44099700
H	-1.27303500	2.06673500	-4.03787600
H	-2.51729000	2.45689900	-2.81768300
H	-2.89463100	1.32383400	-4.13862900
C	-5.19194000	-3.12871500	-2.10243400
H	-6.03769400	-3.35847400	-1.42552400
C	-5.77192200	-2.92646300	-3.52324500
H	-4.97428400	-2.70992900	-4.25702700
H	-6.49493900	-2.09322800	-3.55022000
H	-6.29224100	-3.84202300	-3.85428900
C	-4.22081900	-4.33045600	-2.06476400
H	-4.74278800	-5.24929600	-2.38338700
H	-3.82285400	-4.49877900	-1.04826500
H	-3.36591100	-4.18222200	-2.74975900
C	-5.28456500	0.77640000	1.10806900
H	-4.65174400	1.60836000	1.47227700
C	-6.62956500	1.37372400	0.62381900
H	-6.50954500	2.05332800	-0.23866400
H	-7.11630000	1.93677100	1.43942500
H	-7.32273000	0.57423000	0.30767700
C	-5.54175300	-0.15639800	2.31488700
H	-6.25931600	-0.95751000	2.06599700
H	-5.97551500	0.41987900	3.15109200
H	-4.61355900	-0.63724000	2.66775900
H	-2.01478500	1.15995700	2.86146900
H	1.79992200	-0.93826300	-1.62834600

3 (triplet)

Cu	-0.15253800	0.52870200	0.36719800
N	0.61117900	-1.25728300	-0.02804300
N	1.24042900	1.99283900	0.16115500
N	-1.44560400	1.99448500	0.07095700

N	-1.10936000	-0.45192300	1.81100600
C	-1.84476200	0.03812800	2.82941100
C	-2.31451800	-0.77190000	3.87604200
H	-2.90016500	-0.31827900	4.68031800
C	-2.05237300	-2.15348800	3.86214600
H	-2.43683000	-2.80422500	4.65453200
C	-1.27927200	-2.69766100	2.81225200
C	-0.79066000	-1.79361300	1.82082600
C	-0.93341400	-4.09102000	2.67453800
H	-1.31254700	-4.79870800	3.42000400
C	-0.15036700	-4.53503800	1.63318100
H	0.08785000	-5.60027900	1.53875900
C	0.07763000	-2.23651600	0.79301500
C	0.39671200	-3.62268400	0.65894500
C	1.23429900	-3.99734400	-0.41457400
H	1.49697900	-5.05012300	-0.56360900
C	1.73004700	-3.00226100	-1.27216000
H	2.38634400	-3.25186600	-2.10959100
C	1.41037800	-1.65483900	-1.03753900
C	2.60053800	1.98230800	0.24657400
C	3.33058700	3.17889300	0.45469000
H	4.41956800	3.10635700	0.51722500
C	2.69069400	4.41609900	0.54819600
H	3.26420300	5.33896600	0.68613500
C	1.28462900	4.46305100	0.44482800
C	0.59290100	3.22234200	0.27780200
C	0.52696900	5.68600700	0.48225900
H	1.06934700	6.62737900	0.62273700
C	-0.83749900	5.68496700	0.31540500
H	-1.39970800	6.62513300	0.30990900
C	-0.82647500	3.22491800	0.17033800
C	-1.55525900	4.45285300	0.13365900
C	-2.94390300	4.36848200	-0.11566200
H	-3.54712100	5.28151600	-0.16387200
C	-3.52080700	3.12064300	-0.36610600
H	-4.56964600	3.04606500	-0.66044500
C	-2.76198100	1.92606800	-0.27994700
C	3.40071600	0.72179300	0.08983200
C	4.09779200	0.50370800	-1.13393300
C	4.97613000	-0.59323800	-1.22162700
H	5.52081700	-0.75632700	-2.15950900
C	5.19581700	-1.46701100	-0.14234300
C	4.48902300	-1.22764000	1.05016600
H	4.65439100	-1.90119100	1.89839900
C	3.60034800	-0.14776300	1.20036200
C	3.95142400	1.43609100	-2.34449200
H	3.16606600	2.17951500	-2.11449400
C	3.50806100	0.68816600	-3.62282300

H	2.53747700	0.17690300	-3.48697400
H	4.24821600	-0.07154300	-3.93196300
H	3.39496600	1.39939200	-4.46044200
C	5.26231200	2.21369400	-2.61031300
H	5.13283800	2.91365200	-3.45522200
H	6.08853800	1.52622700	-2.86576900
H	5.57622000	2.79757600	-1.72759800
C	6.19133400	-2.62100500	-0.23967500
H	6.16638500	-3.15402900	0.73140100
C	5.80132600	-3.63579400	-1.33741600
H	5.82250200	-3.17267800	-2.34113900
H	4.78676900	-4.03808900	-1.16820300
H	6.50829400	-4.48447600	-1.34925700
C	7.63305000	-2.10450500	-0.45144500
H	7.73093700	-1.57467900	-1.41655400
H	8.34838700	-2.94618300	-0.45745300
H	7.93129000	-1.40549000	0.34915800
C	2.93009500	0.11972000	2.55342200
H	1.95200000	0.59788300	2.34724300
C	3.77199300	1.10713000	3.39927000
H	4.76653400	0.67716300	3.61623200
H	3.27262400	1.31391200	4.36317900
H	3.92394200	2.06951600	2.88184400
C	2.65013700	-1.15558400	3.37525500
H	2.03156300	-0.90570200	4.25516400
H	3.58253500	-1.60885200	3.75721900
H	2.11706000	-1.92064100	2.78529300
C	-3.36536300	0.61038200	-0.65545100
C	-2.80818900	-0.12543600	-1.75830600
C	-3.41577200	-1.33477000	-2.12962200
H	-3.00091900	-1.89571700	-2.97217700
C	-4.55752400	-1.84427500	-1.48041200
C	-5.10550500	-1.08451400	-0.43900700
H	-6.00732300	-1.45600100	0.06204500
C	-4.54886900	0.13706100	-0.01199500
C	-1.67206800	0.43955600	-2.63178000
H	-0.88910700	0.85578100	-1.96655400
C	-0.97738500	-0.60640500	-3.52578400
H	-1.64060800	-0.96315600	-4.33451700
H	-0.63299700	-1.48508100	-2.95285300
H	-0.09841900	-0.14845400	-4.01352800
C	-2.19494400	1.60080100	-3.51344800
H	-1.37622400	2.01993900	-4.12558500
H	-2.62459000	2.41974500	-2.91235200
H	-2.98206900	1.23654900	-4.19812900
C	-5.20006900	-3.15795600	-1.91648900
H	-6.04078700	-3.35452700	-1.22220000
C	-5.78788700	-3.05201200	-3.34292200

H	-4.99464500	-2.86763300	-4.09040600
H	-6.51929500	-2.22844400	-3.41648700
H	-6.29818000	-3.99149400	-3.62086400
C	-4.21689700	-4.34524800	-1.80894600
H	-4.72452100	-5.29018700	-2.07270600
H	-3.81471800	-4.44444600	-0.78534700
H	-3.36239600	-4.22270900	-2.49940000
C	-5.27734000	0.89677600	1.10461800
H	-4.62638600	1.72225400	1.44827800
C	-6.59642300	1.51568200	0.57764400
H	-6.44053900	2.16552400	-0.30146800
H	-7.08414200	2.11622200	1.36647000
H	-7.30288500	0.72290600	0.27198900
C	-5.58906700	0.01501100	2.33605000
H	-6.33856100	-0.76243400	2.10332600
H	-6.00876100	0.63707700	3.14724300
H	-4.68595200	-0.49004200	2.71589200
H	-2.07305300	1.10811200	2.79037800
H	1.83345600	-0.86165300	-1.65705800

4 (reduced)

Cu	0.02402400	0.44705800	0.38785700
N	0.06422300	-1.50437500	0.04807700
N	1.48839200	1.84480700	0.16248200
N	-1.18580000	1.95367000	-0.23962500
N	-0.61761400	-0.16705300	2.26614200
C	-0.67393100	2.02402200	3.33968600
H	-1.47808700	2.50866600	2.75557100
H	0.28160600	2.26920800	2.84601300
H	-0.67580100	2.46676600	4.34850400
C	-0.87640800	0.53233500	3.39081200
C	-1.31945400	-0.10996500	4.57690700
H	-1.50510000	0.49415600	5.47040800
C	-1.51047800	-1.48652500	4.60135800
H	-1.85488400	-1.98944200	5.51194900
C	-1.24520500	-2.24553500	3.43290100
C	-0.78548900	-1.52724000	2.28805800
C	-1.38998600	-3.67475200	3.35581200
H	-1.75679400	-4.21244900	4.23706400
C	-1.06551400	-4.35739700	2.20687500
H	-1.17295900	-5.44671000	2.15943300
C	-0.42840400	-2.24731100	1.09175800
C	-0.56153400	-3.66555100	1.05036500
C	-0.16679900	-4.31456900	-0.14872900
H	-0.26020200	-5.40276900	-0.23588100
C	0.34953000	-3.55710900	-1.19248900
H	0.67590100	-4.03603800	-2.12091900
C	0.46847900	-2.14875600	-1.06781100

C	1.10052400	-1.30898200	-2.14012000
H	0.86577400	-1.67734500	-3.15183900
H	2.20063400	-1.31797500	-2.02294400
H	0.76333600	-0.26398300	-2.03195800
C	2.84158600	1.77870200	0.22922200
C	3.62569600	2.94929700	0.44227300
H	4.70978400	2.83622700	0.53225100
C	3.03335200	4.20033800	0.51486800
H	3.63367900	5.10206000	0.67969600
C	1.63092200	4.30735100	0.33621300
C	0.90025500	3.09200600	0.16613500
C	0.93943200	5.56657200	0.32384900
H	1.51983800	6.48349200	0.47413600
C	-0.41731400	5.62149000	0.11626800
H	-0.94163500	6.58323600	0.09692300
C	-0.52749300	3.15012000	-0.05431400
C	-1.17832600	4.42052000	-0.09154300
C	-2.57408500	4.42547400	-0.34170400
H	-3.11859000	5.37570900	-0.37843100
C	-3.22206800	3.22080600	-0.56833900
H	-4.28906600	3.19544700	-0.80557700
C	-2.51133300	1.98716400	-0.52510300
C	3.56495200	0.48292200	-0.00582300
C	4.29154300	0.33791200	-1.22633400
C	5.02923100	-0.84374400	-1.43369500
H	5.58173800	-0.95922000	-2.37399600
C	5.09248900	-1.87025300	-0.47603400
C	4.38237100	-1.68971000	0.72450300
H	4.43487700	-2.47814300	1.48301000
C	3.62204500	-0.53656700	0.98762600
C	4.31984000	1.41414200	-2.32147100
H	3.63193100	2.22807800	-2.03027200
C	3.83397600	0.88595100	-3.69037100
H	2.80610100	0.48862100	-3.63149100
H	4.48742000	0.08284600	-4.07555500
H	3.84076200	1.70196900	-4.43515300
C	5.73279900	2.03064900	-2.45613700
H	5.73177000	2.83692500	-3.21149800
H	6.47071400	1.27258500	-2.77499100
H	6.08791400	2.45636700	-1.50099000
C	5.91467800	-3.13389400	-0.71622300
H	5.79964500	-3.77260700	0.18188200
C	5.39078000	-3.93527700	-1.92945800
H	5.49060100	-3.35644100	-2.86601300
H	4.32560200	-4.20037600	-1.80643200
H	5.96517300	-4.87069900	-2.05302500
C	7.41885800	-2.81320800	-0.87171100
H	7.60578600	-2.18815700	-1.76398300

H	8.00262800	-3.74381300	-0.98755100
H	7.80742700	-2.27074600	0.00772500
C	2.92345100	-0.35296700	2.33807800
H	1.93905100	0.10325200	2.11720200
C	3.71895300	0.60943200	3.25366500
H	4.71901900	0.19400500	3.47414400
H	3.19214200	0.75209200	4.21480000
H	3.86081400	1.60277900	2.79494700
C	2.65726200	-1.67027400	3.09133900
H	2.01822800	-1.47551000	3.97050800
H	3.59296700	-2.12261700	3.46734800
H	2.14915800	-2.41654600	2.45636900
C	-3.25788100	0.72626000	-0.85329100
C	-3.10097200	0.12672200	-2.14203700
C	-3.89288800	-0.98877000	-2.46275000
H	-3.78013900	-1.44946200	-3.44976400
C	-4.84481000	-1.52230700	-1.57285000
C	-4.99695600	-0.89567400	-0.32798100
H	-5.74587100	-1.29180300	0.36892300
C	-4.23373400	0.22549500	0.05292200
C	-2.18164600	0.73766600	-3.20794200
H	-1.28870500	1.14366800	-2.69549200
C	-1.69096900	-0.27559800	-4.26295800
H	-2.49816800	-0.56052400	-4.96161700
H	-1.30318100	-1.19915100	-3.80026800
H	-0.88610800	0.17422800	-4.87065300
C	-2.88779900	1.91538100	-3.92695000
H	-2.21711600	2.36488000	-4.68158300
H	-3.18978800	2.71112100	-3.22510000
H	-3.79579300	1.55907500	-4.44623300
C	-5.70208700	-2.72685100	-1.95292600
H	-6.35719100	-2.94482200	-1.08616300
C	-6.61491400	-2.41814800	-3.16135800
H	-6.02092200	-2.20700400	-4.06933700
H	-7.25660600	-1.54128700	-2.96634300
H	-7.26844900	-3.28083500	-3.38280800
C	-4.84242200	-3.98426300	-2.21412000
H	-5.48758300	-4.85601000	-2.42481800
H	-4.20953700	-4.22661300	-1.34229400
H	-4.17840700	-3.84260900	-3.08660600
C	-4.51485800	0.87321700	1.41303300
H	-3.71609800	1.61350300	1.61173000
C	-5.86605700	1.62792200	1.40484400
H	-5.90238400	2.40775500	0.62445900
H	-6.04558900	2.11351900	2.38118600
H	-6.70268000	0.93171100	1.21478600
C	-4.49297900	-0.14890900	2.57018800
H	-5.33646000	-0.85911300	2.50156300

H	-4.58251100	0.37024200	3.54121100
H	-3.55998600	-0.73596600	2.57450200

4 (oxidized)

Cu	-0.08644200	0.49838200	0.20199300
N	0.36954500	-1.39016000	-0.30151400
N	1.42719900	1.92993500	0.07729800
N	-1.28418400	2.03211000	-0.20508200
N	-0.96238500	-0.39451200	1.81183500
C	-1.40541600	1.65493300	3.09716000
H	-2.30678100	2.11908700	2.65594400
H	-0.52372700	2.08367400	2.59493100
H	-1.37710500	1.93683200	4.16186900
C	-1.44472400	0.15845400	2.94117200
C	-1.98328600	-0.66454600	3.97050000
H	-2.35996000	-0.18800000	4.88047000
C	-2.04011200	-2.04252200	3.81741700
H	-2.47569200	-2.67319900	4.60018000
C	-1.49934200	-2.63961200	2.64766700
C	-0.93661200	-1.75719500	1.68059800
C	-1.45094200	-4.05712900	2.41688100
H	-1.89995300	-4.72683300	3.15773900
C	-0.83802600	-4.56593800	1.29445600
H	-0.80354200	-5.64679600	1.12237300
C	-0.25082000	-2.28864800	0.53712900
C	-0.20565000	-3.69725800	0.33886700
C	0.48577700	-4.16270900	-0.81270900
H	0.54392100	-5.23758400	-1.01626400
C	1.08180700	-3.24720300	-1.66294700
H	1.61850200	-3.57924300	-2.55669600
C	1.02198800	-1.85025300	-1.38775100
C	1.70955700	-0.88258800	-2.30064400
H	1.47164200	-1.10568400	-3.35421500
H	2.80372600	-0.97120500	-2.17869200
H	1.42324400	0.15652600	-2.07788700
C	2.77421500	1.86667000	0.24290700
C	3.52815300	3.06116100	0.46613000
H	4.60215600	2.95867900	0.63931400
C	2.93060700	4.30686100	0.45168700
H	3.52087600	5.21686700	0.60574000
C	1.53318600	4.39794100	0.22750000
C	0.81773200	3.17152900	0.07708100
C	0.83959800	5.65308100	0.15985400
H	1.41645500	6.57529700	0.28516900
C	-0.51476600	5.69868700	-0.07023200
H	-1.03897700	6.65710500	-0.14423600
C	-0.60909300	3.22562100	-0.11450100
C	-1.26832100	4.48665000	-0.21389700

C	-2.66665800	4.46521400	-0.46558200
H	-3.21518900	5.40883300	-0.56057400
C	-3.31426000	3.25221900	-0.62163100
H	-4.37796800	3.21365800	-0.86760500
C	-2.60990500	2.01775800	-0.49034000
C	3.54764600	0.58614300	0.18105300
C	4.53404200	0.43332000	-0.84504300
C	5.30101500	-0.74982000	-0.86338100
H	6.04603900	-0.87391000	-1.65759800
C	5.16228600	-1.76205300	0.10282900
C	4.22342000	-1.55531800	1.12957700
H	4.14473200	-2.31281000	1.91628700
C	3.42153900	-0.40114000	1.20727400
C	4.83748400	1.49456900	-1.91525900
H	4.10683200	2.31812200	-1.81887200
C	4.71898900	0.96591500	-3.36437100
H	3.69751400	0.62195100	-3.60048700
H	5.41513600	0.13091100	-3.55735600
H	4.97052500	1.77182400	-4.07566700
C	6.25004000	2.09232200	-1.69371200
H	6.43244500	2.91440200	-2.40775500
H	7.03395500	1.33109200	-1.85323900
H	6.38450600	2.48877800	-0.67168900
C	6.01857800	-3.02345900	0.06680300
H	5.70945700	-3.65017100	0.92642400
C	5.77533600	-3.84114500	-1.22243500
H	6.08785500	-3.28040300	-2.12215300
H	4.70920900	-4.10745100	-1.33830100
H	6.35958400	-4.77735800	-1.19693700
C	7.51995500	-2.69598000	0.24239400
H	7.90207100	-2.08796600	-0.59758000
H	8.11084600	-3.62772100	0.27428000
H	7.70622500	-2.14011800	1.17736100
C	2.54035600	-0.16616700	2.43803100
H	1.58055500	0.26164100	2.07917700
C	3.19019500	0.86753200	3.39330300
H	4.16261000	0.49179100	3.75720900
H	2.54352400	1.04055100	4.27185700
H	3.36821900	1.84092600	2.90568700
C	2.20142100	-1.44365600	3.23055000
H	1.43728900	-1.21676200	3.99459500
H	3.08314000	-1.83160700	3.77038900
H	1.81744600	-2.25256500	2.58512500
C	-3.32065000	0.72496100	-0.71890100
C	-2.95126600	-0.09498700	-1.84306500
C	-3.67950000	-1.27197200	-2.07159200
H	-3.42209600	-1.89255700	-2.93465200
C	-4.76220000	-1.67046000	-1.26048100

C	-5.13325500	-0.81992400	-0.20663700
H	-5.99722800	-1.09937000	0.40760600
C	-4.45772700	0.38147400	0.07716700
C	-1.92998100	0.37354600	-2.89502400
H	-1.04117800	0.77875400	-2.37009200
C	-1.43988100	-0.74609200	-3.83522300
H	-2.24051700	-1.08267900	-4.51687200
H	-1.07106600	-1.62938800	-3.28446600
H	-0.62353200	-0.36457800	-4.47253600
C	-2.53035500	1.51594100	-3.75461300
H	-1.79902600	1.85528400	-4.50937300
H	-2.82372000	2.39120600	-3.15100900
H	-3.42971200	1.16042200	-4.28780700
C	-5.54223500	-2.94754300	-1.54726300
H	-6.28894300	-3.06243500	-0.73748300
C	-6.31576800	-2.83900600	-2.88405000
H	-5.62567200	-2.73963100	-3.74155100
H	-6.99334900	-1.96810300	-2.88932500
H	-6.92311400	-3.74657300	-3.04545700
C	-4.63653600	-4.19969100	-1.53197000
H	-5.24530300	-5.10879000	-1.67798800
H	-4.09773100	-4.29865900	-0.57284000
H	-3.88921700	-4.16843100	-2.34591900
C	-5.02373100	1.26908600	1.19430700
H	-4.30878900	2.09143500	1.39023000
C	-6.36650400	1.90677400	0.75573400
H	-6.28010800	2.47649000	-0.18623400
H	-6.74030500	2.59133900	1.53729300
H	-7.13433400	1.12995900	0.59355200
C	-5.22693600	0.51547800	2.52824300
H	-6.01212200	-0.25620300	2.44528000
H	-5.54865100	1.22107700	3.31441500
H	-4.30281700	0.01662500	2.86527600

4 (triplet)

Cu	-0.07473700	0.51477500	0.19773700
N	0.37813500	-1.35669500	-0.32066700
N	1.42063000	1.91800000	0.06476000
N	-1.27695500	2.03618600	-0.19519000
N	-0.98655000	-0.37154000	1.75463500
C	-1.39931200	1.68168600	3.04908100
H	-2.21737300	2.16030500	2.48116300
H	-0.44995400	2.08820900	2.66047200
H	-1.50219400	1.97696000	4.10536800
C	-1.43834200	0.18206500	2.90785800
C	-1.93061300	-0.63337400	3.95108100
H	-2.28874300	-0.15280200	4.86637200
C	-1.98621100	-2.02603600	3.80935600

H	-2.40120500	-2.65266900	4.60602400
C	-1.46846500	-2.62131600	2.63776400
C	-0.93040400	-1.74519200	1.64556400
C	-1.41127400	-4.03996800	2.40046700
H	-1.84129500	-4.71290200	3.15049800
C	-0.82241500	-4.54687900	1.26490000
H	-0.79099800	-5.62828600	1.09206100
C	-0.25371500	-2.26958500	0.51204400
C	-0.20637100	-3.68039400	0.29474700
C	0.46016600	-4.13523900	-0.86499700
H	0.51777000	-5.20816600	-1.07835900
C	1.04109800	-3.20223400	-1.72609600
H	1.55736100	-3.52484800	-2.63515800
C	1.00215700	-1.81823200	-1.42879300
C	1.68560100	-0.83615900	-2.33496400
H	1.45767200	-1.05629600	-3.39158700
H	2.77886700	-0.90491800	-2.20240200
H	1.38128400	0.19751300	-2.10620000
C	2.76988000	1.86031800	0.28916000
C	3.51288200	3.03481500	0.56326300
H	4.58077900	2.92531000	0.76745400
C	2.92314200	4.29925100	0.53170000
H	3.51568100	5.20325100	0.70858300
C	1.54513500	4.39718100	0.25383000
C	0.81567000	3.17832700	0.06845300
C	0.85357800	5.65424900	0.15916500
H	1.43068200	6.57466500	0.30081400
C	-0.49050800	5.70682100	-0.11809900
H	-1.00539100	6.66899500	-0.21418200
C	-0.59160200	3.23901400	-0.14190500
C	-1.25502800	4.50007000	-0.27300900
C	-2.63944200	4.48194200	-0.54781800
H	-3.18571100	5.42408500	-0.66505600
C	-3.29150000	3.25427400	-0.69535500
H	-4.35001200	3.21540000	-0.96289200
C	-2.60475100	2.02991200	-0.51466100
C	3.54518000	0.57616000	0.20889000
C	4.51043300	0.42017700	-0.83584700
C	5.27466200	-0.76237900	-0.87398900
H	6.00570400	-0.88581400	-1.68208700
C	5.14608400	-1.77689700	0.08953700
C	4.23140200	-1.56963600	1.13651400
H	4.15298000	-2.33636200	1.91483800
C	3.43725600	-0.41273600	1.23190000
C	4.80218600	1.49598900	-1.89644800
H	4.06186600	2.30799300	-1.78644800
C	4.69735100	0.98588500	-3.35225000
H	3.68173000	0.63151300	-3.59585100

H	5.40432300	0.16138600	-3.55405200
H	4.94115900	1.80458600	-4.05268900
C	6.20593900	2.10902900	-1.66446600
H	6.38784300	2.93466300	-2.37563500
H	6.99800100	1.35360700	-1.81554800
H	6.32297600	2.50631000	-0.64099000
C	5.98155700	-3.05259000	0.02380700
H	5.69663900	-3.67201500	0.89737900
C	5.66976400	-3.87045600	-1.25024500
H	5.94885600	-3.31232300	-2.16282500
H	4.59476400	-4.11539200	-1.31722600
H	6.23926100	-4.81701500	-1.25101900
C	7.49434600	-2.75587500	0.13566300
H	7.85021700	-2.15069400	-0.71804600
H	8.07180400	-3.69749200	0.14025500
H	7.72887100	-2.20395700	1.06242500
C	2.56879300	-0.18435100	2.47424500
H	1.62255200	0.28207900	2.13561500
C	3.26229900	0.79901800	3.45062000
H	4.22148900	0.37659300	3.80071700
H	2.62590700	0.97693900	4.33648900
H	3.47278800	1.77416700	2.98013200
C	2.19592300	-1.47304200	3.23311300
H	1.43623400	-1.24591100	4.00152900
H	3.06813800	-1.90049400	3.76027400
H	1.78684500	-2.24951200	2.56459700
C	-3.33203100	0.73549600	-0.72575700
C	-2.99777600	-0.08359100	-1.85532700
C	-3.71286700	-1.27563100	-2.05407700
H	-3.46423800	-1.90254000	-2.91570500
C	-4.75990400	-1.68356100	-1.20537800
C	-5.10917000	-0.83069800	-0.15023800
H	-5.94746100	-1.11610500	0.49678200
C	-4.43632100	0.38085600	0.10481500
C	-1.99629500	0.38174200	-2.92533500
H	-1.11318900	0.81110000	-2.41169300
C	-1.49261600	-0.74555400	-3.84861400
H	-2.29382400	-1.11279100	-4.51490000
H	-1.09839800	-1.60799100	-3.28332300
H	-0.68896800	-0.36020200	-4.50051800
C	-2.62004400	1.50018000	-3.79923500
H	-1.89376700	1.84875500	-4.55556200
H	-2.93288000	2.37230100	-3.20177400
H	-3.50973100	1.11723800	-4.33110200
C	-5.51636200	-2.98730400	-1.44454400
H	-6.26075700	-3.08481100	-0.62955600
C	-6.29047300	-2.95912000	-2.78254500
H	-5.60139700	-2.88087800	-3.64339200

H	-6.98534300	-2.10255100	-2.82724300
H	-6.87844200	-3.88587700	-2.90793200
C	-4.58018200	-4.21492500	-1.37182100
H	-5.16009400	-5.14878200	-1.48175000
H	-4.04096700	-4.25422300	-0.40898700
H	-3.82773500	-4.19269900	-2.18138500
C	-4.97866500	1.27400800	1.22844900
H	-4.25329000	2.08960100	1.40775600
C	-6.31941500	1.92429400	0.80353200
H	-6.22957200	2.50292800	-0.13237900
H	-6.68683200	2.60454400	1.59296300
H	-7.09146100	1.15180700	0.63608900
C	-5.17506600	0.52688000	2.56664200
H	-5.97756400	-0.22931900	2.49891000
H	-5.46906700	1.24119300	3.35679400
H	-4.25472100	0.01240900	2.88785800

Cu(L1)₂ (reduced)

Cu	0.00000000	-0.00000500	0.00002000
N	1.48550300	1.12957600	0.70687000
N	1.48548500	-1.12959500	-0.70683900
N	-1.48550600	-1.12958700	0.70686000
N	-1.48548300	1.12959700	-0.70682800
C	1.46100000	2.29860800	1.37218100
C	2.62736600	3.00479500	1.73371900
H	2.53649300	3.94676200	2.28244200
C	3.87708100	2.47970500	1.40798300
H	4.79815300	3.00076300	1.69079600
C	3.94805300	1.24909700	0.70459300
C	5.18034100	0.60187400	0.33305200
H	6.12615600	1.08567700	0.60017200
C	5.18033300	-0.60189100	-0.33312000
H	6.12614100	-1.08569300	-0.60026600
C	3.94803500	-1.24911500	-0.70462900
C	3.87704500	-2.47972200	-1.40801900
H	4.79810900	-3.00077800	-1.69085700
C	2.62732100	-3.00481200	-1.73372100
H	2.53643400	-3.94677800	-2.28244300
C	1.46096500	-2.29862600	-1.37215000
C	2.71470000	-0.62025100	-0.36431900
C	2.71470900	0.62023200	0.36431700
C	-1.46100600	-2.29862000	1.37217000
C	-2.62737400	-3.00479900	1.73371600
H	-2.53650300	-3.94676700	2.28243700
C	-3.87708700	-2.47970200	1.40798700
H	-4.79816000	-3.00075400	1.69080400
C	-3.94805500	-1.24909300	0.70459900
C	-5.18034200	-0.60186400	0.33306400

H	-6.12615900	-1.08566200	0.60018700
C	-5.18033100	0.60190200	-0.33310800
H	-6.12613800	1.08570700	-0.60025100
C	-3.94803200	1.24912100	-0.70461800
C	-3.87704000	2.47972800	-1.40800700
H	-4.79810200	3.00078700	-1.69084400
C	-2.62731500	3.00481600	-1.73371000
H	-2.53642600	3.94678200	-2.28243200
C	-1.46096000	2.29862800	-1.37213800
C	-2.71469800	0.62025300	-0.36431100
C	-2.71471000	-0.62023400	0.36431900
H	-0.46860800	-2.67976400	1.63725100
H	-0.46855300	2.67976600	-1.63719700
H	0.46855900	-2.67976400	-1.63721300
H	0.46860200	2.67974400	1.63727300

Cu(L1)₂ (oxidized)

Cu	0.00000100	0.00001600	0.00038900
N	1.49130800	1.25923600	0.43556600
N	1.49110100	-1.25942100	-0.43516400
N	-1.49128700	-1.25921600	0.43560500
N	-1.49112200	1.25944200	-0.43512100
C	1.44310800	2.49148600	0.96681000
C	2.61064800	3.21328800	1.30185400
H	2.51454400	4.21385700	1.73242100
C	3.86084000	2.64345900	1.07302800
H	4.77673200	3.19490600	1.31156900
C	3.94442300	1.33133100	0.53225100
C	5.17756500	0.63680300	0.26086300
H	6.12335700	1.14560600	0.47372500
C	5.17744600	-0.63706300	-0.26193400
H	6.12314100	-1.14589100	-0.47516300
C	3.94418100	-1.33157000	-0.53282000
C	3.86036000	-2.64373300	-1.07348000
H	4.77614700	-3.19521100	-1.31235300
C	2.61006600	-3.21356000	-1.30174600
H	2.51377000	-4.21416500	-1.73218700
C	1.44267400	-2.49171300	-0.96628400
C	2.71470800	-0.67106600	-0.25109100
C	2.71482700	0.67086400	0.25096900
C	-1.44306700	-2.49146900	0.96684200
C	-2.61059500	-3.21329200	1.30188100
H	-2.51447400	-4.21386200	1.73244200
C	-3.86079700	-2.64348300	1.07305800
H	-4.77667900	-3.19494700	1.31159600
C	-3.94440100	-1.33135300	0.53228900
C	-5.17755500	-0.63684300	0.26090600
H	-6.12333800	-1.14566300	0.47376600

C	-5.17745600	0.63702500	-0.26188400
H	-6.12316100	1.14584000	-0.47510800
C	-3.94420300	1.33155400	-0.53276800
C	-3.86040400	2.64372000	-1.07342200
H	-4.77620000	3.19518500	-1.31229000
C	-2.61012000	3.21356800	-1.30168900
H	-2.51384000	4.21417700	-1.73212400
C	-1.44271500	2.49173600	-0.96623500
C	-2.71472000	0.67106700	-0.25104500
C	-2.71481600	-0.67086500	0.25101000
H	-0.44910700	-2.91840000	1.13327700
H	-0.44869800	2.91870600	-1.13223000
H	0.44865000	-2.91866700	-1.13227600
H	0.44915500	2.91843500	1.13324600

Cu(L1)₂ (triplet)

Cu	0.00000000	0.00000000	0.00002200
N	1.47374200	-1.26280400	-0.39945200
N	1.47375300	1.26279200	0.39948100
N	-1.47374200	1.26280400	-0.39945100
N	-1.47375300	-1.26279300	0.39947700
C	1.43331500	-2.50593600	-0.92702700
C	2.59089900	-3.22882900	-1.25307800
H	2.49161600	-4.23451600	-1.67032800
C	3.85532400	-2.65743200	-1.03145300
H	4.76945800	-3.21459000	-1.26144300
C	3.93777300	-1.34524100	-0.51469500
C	5.16852700	-0.64008900	-0.25218800
H	6.11524400	-1.15139100	-0.45746300
C	5.16853300	0.64007500	0.25213600
H	6.11525500	1.15137600	0.45739000
C	3.93778500	1.34522700	0.51467000
C	3.85534800	2.65741700	1.03143200
H	4.76948800	3.21457400	1.26140400
C	2.59092900	3.22881400	1.25308700
H	2.49165600	4.23450100	1.67034200
C	1.43333700	2.50592300	0.92706000
C	2.71102100	0.66881700	0.23575300
C	2.71101500	-0.66882900	-0.23575200
C	-1.43331400	2.50593800	-0.92702100
C	-2.59089800	3.22883200	-1.25307100
H	-2.49161400	4.23452100	-1.67031800
C	-3.85532300	2.65743500	-1.03144900
H	-4.76945600	3.21459400	-1.26143900
C	-3.93777200	1.34524200	-0.51469500
C	-5.16852700	0.64009000	-0.25219200
H	-6.11524400	1.15139300	-0.45746600
C	-5.16853400	-0.64007600	0.25212800

H	-6.11525600	-1.15137700	0.45738000
C	-3.93778600	-1.34522800	0.51466200
C	-3.85535000	-2.65742000	1.03142000
H	-4.76948900	-3.21457800	1.26138900
C	-2.59093000	-3.22881800	1.25307400
H	-2.49165700	-4.23450500	1.67032600
C	-1.43333800	-2.50592600	0.92705200
C	-2.71102200	-0.66881700	0.23574800
C	-2.71101500	0.66883000	-0.23575300
H	-0.43774600	2.93142100	-1.08829400
H	-0.43777400	-2.93140800	1.08835000
H	0.43777300	2.93140600	1.08835800
H	0.43774700	-2.93141900	-1.08830100