Supporting Information

Electronic and interfacial behavior of gemini metallosurfactants with copper(II)/pseudohalide cascade cores

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Figure S1. Infrared spectra of **1** (left) and **2** (right) in bulk from KBr pellets.

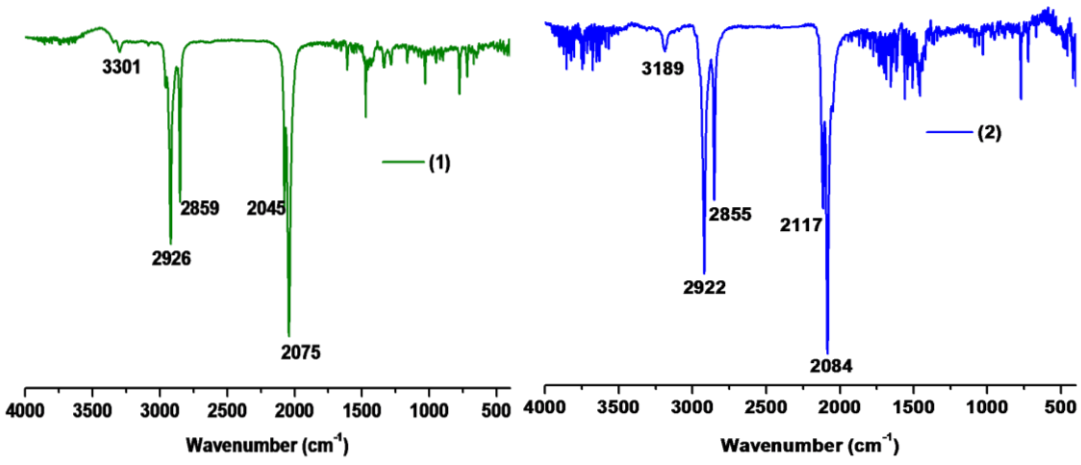
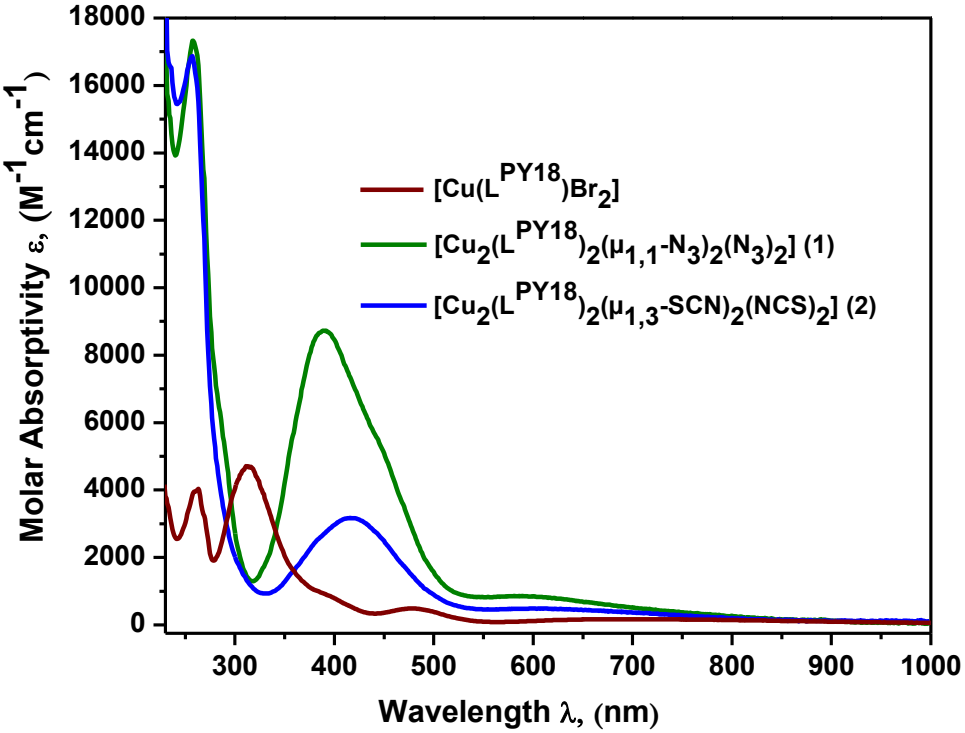


Figure S2. (a) Comparison between the electronic spectra for the precursor [Cu(L^{PY18})Br_2], **1**, **2**; (b) Spectral changes for **1**, 1.0 × 10^{-4} M, in pyridine/dichloromethane 50% v/v solution, followed for 3 hours. A similar behavior was found for **2**.



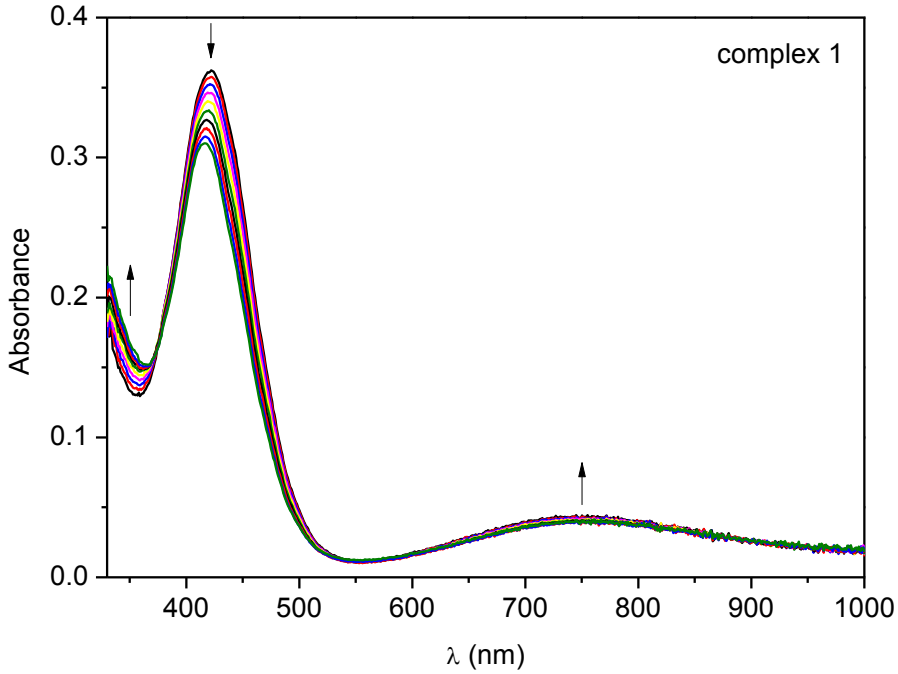


Figure S3. IRRAS spectra of the LB films of **2** with p-polarized light at an angle of incidence 30 ^{o}.

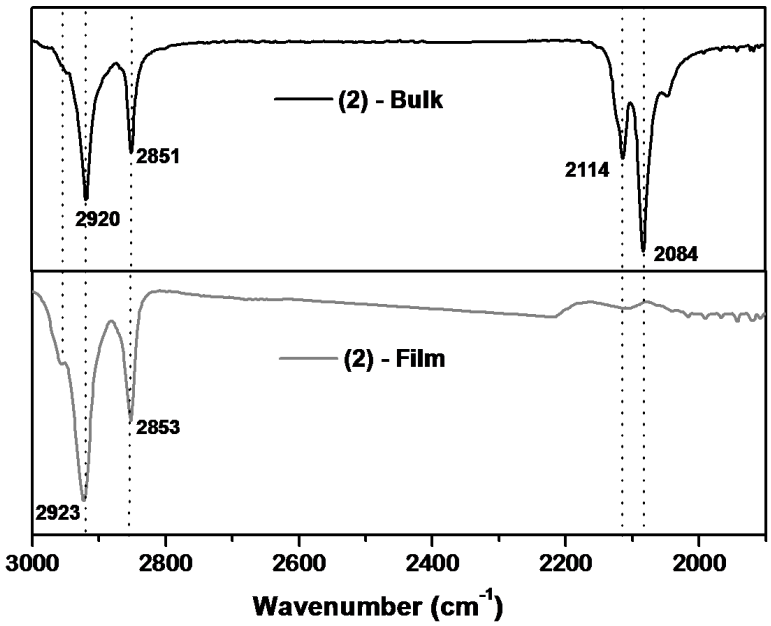


Figure S4. IR spectra of the ground LB films of **1** and **2** on gold coated glass plates.

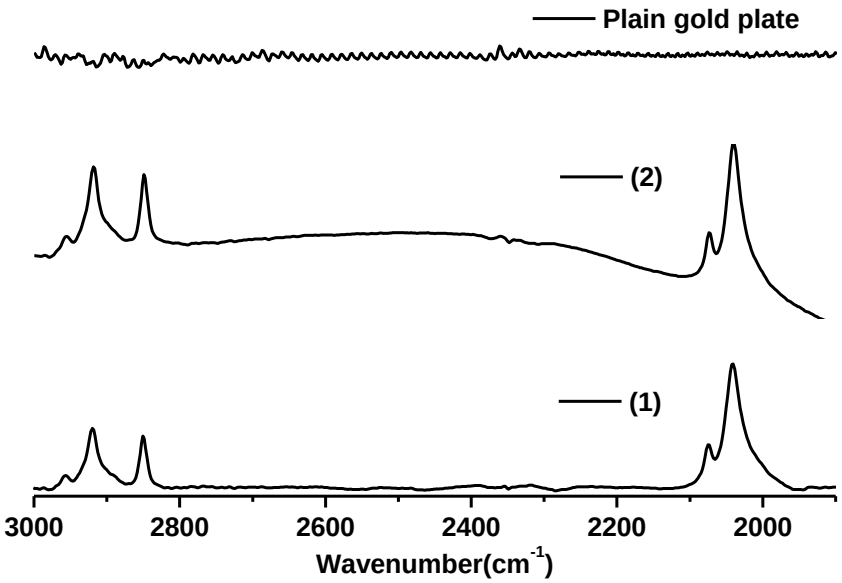


Table T1. Bond lengths and angles for **2**. CCDC 948258 contains the supplementary crystallographic data for this paper.

Bond lengths (Å)
N3—C25 1.168 (12)
C15—C16 1.5400 (10)
N3—Cu1 1.932 (9)
C16—C17 1.5400 (10)
C25—S1 1.628 (10)
C17—C18 1.5400 (10)
N4—C26 1.165 (12)
C18—C19 1.5400 (10)
N4—Cu1 1.961 (8)
C19—C20 1.5400 (10)
C26—S2 1.640 (10)
C20—C21 1.5400 (10)
Cu1—N1 2.004 (8)
C21—C22 1.5400 (10)
Cu1—N2 2.041 (9)
C22—C23 1.5400 (11)
N1—C1 1.327 (13)
C23—C24 1.5400 (11)
N1—C5 1.327 (11)
C1A—C1B 1.53 (2)
C1—C2 1.375 (13)
C1B—C1C 1.51 (4)
C2—C3 1.382 (14)
C1C—C1D 1.50 (3)
C3—C4 1.366 (15)
C1D—C1E 1.54 (3)
C4—C5 1.375 (12)
C1E—C1F 1.57 (3)
C5—C6 1.507 (14)
C1F—C1G 1.52 (3)
C6—N2 1.468 (14)
C1G—C1H 1.52 (3)
N2—C7 1.24 (6)
C1H—C1I 1.51 (3)
N2—C1A 1.509 (19)
C1I—C1J 1.54 (3)
C7—C8 1.5400 (10)
C1J—C1K 1.51 (3)
C8—C9 1.539 (10)
C1K—C1L 1.56 (3)
C9—C10 1.541 (10)
C1L—C1M 1.51 (3)
C10—C11 1.538 (10)
C1M—C1N 1.53 (3)
C11—C12 1.537 (10)
C1N—C1O 1.52 (3)
C12—C13 1.541 (10)
C1O—C1P 1.54 (3)
C13—C14 1.543 (10)
C1P—C1Q 1.54 (3)
C14—C15 1.5400 (10)
C1Q—C1R 1.59 (5)

Bond Angles (°)
C25—N3—Cu1 167.9 (8)
C12—C11—C10 110.8 (18)
N3—C25—S1 178.6 (12)
C11—C12—C13 112.9 (17)
C26—N4—Cu1 168.9 (9)
C12—C13—C14 111.0 (17)
N4—C26—S2 177.7 (10)
C15—C14—C13 111.3 (15)
N3—Cu1—N4 95.8 (3)
C16—C15—C14 111.2 (15)
N3—Cu1—N1 160.5 (4)
C15—C16—C17 110.5 (13)
N3—Cu1—N2 92.1 (3)
C16—C17—C18 111.7 (15)
N4—Cu1—N1 92.6 (3)
C19—C18—C17 113.3 (14)
N4—Cu1—N2 171.3 (3)
C18—C19—C20 111.0 (15)
N1—Cu1—N2 78.8 (3)
C21—C20—C19 109.8 (14)
C1—N1—Cu1 126.9 (6)
C20—C21—C22 114.7 (16)
C1—N1—C5 117.9 (8)
C23—C22—C21 114.0 (18)
C5—N1—Cu1 115.3 (7)
C22—C23—C24 103 (3)
N1—C1—C2 123.0 (9)
N2—C1A—C1B 114.2 (15)
C1—C2—C3 118.2 (10)
C1C—C1B—C1A 112 (2)
C4—C3—C2 119.1 (9)
C1D—C1C—C1B 110 (2)
C3—C4—C5 118.6 (9)
C1C—C1D—C1E 111 (2)
N1—C5—C4 123.0 (10)
C1D—C1E—C1F 112 (2)
N1—C5—C6 113.8 (8)
C1G—C1F—C1E 113 (2)
C4—C5—C6 123.2 (9)
C1H—C1G—C1F 113 (2)
N2—C6—C5 107.2 (9)
C1I—C1H—C1G 113 (2)
C6—N2—Cu1 106.1 (7)
C1H—C1I—C1J 114.4 (19)
C6—N2—C1A 111.0 (11)
C1K—C1J—C1I 112 (2)
C7—N2—Cu1 124 (2)
C1J—C1K—C1L 112.4 (19)
C7—N2—C6 114 (3)
C1M—C1L—C1K 113 (2)
C7—N2—C1A 10 (3)
C1L—C1M—C1N 112 (2)
C1A—N2—Cu1 118.7 (8)
C1M—C1N—C1O 112 (2)
N2—C7—C8 120 (5)
C1P—C1O—C1N 116 (2)
C9—C8—C7 126 (3)
C1Q—C1P—C1O 116 (2)
C8—C9—C10 113 (2)
C1P—C1Q—C1R 118 (4)
C11—C10—C9 111.4 (18)

Table T2. Cartesian Coordinates:

(1) Cu_2 (Azide: Side on) : E = -2999385.01724921 a.u.
(S= 2/2)

N	-2.11533700	-2.38800200	1.57516900
N	-1.10937300	-2.81785700	2.06911900
N	-0.16221200	-3.27470400	2.55995500
Cu	-2.37366200	-0.65869300	0.71951800
N	-4.04043500	-1.39017900	-0.23452100
C	-4.63040400	-0.29228800	-1.01386800
C	-3.79354700	-2.61797800	-1.02086500
H	-4.67348700	-1.62666900	0.52998900
C	-4.50012000	0.99853200	-0.25183800
H	-5.67620300	-0.47775700	-1.28110300
H	-4.06031100	-0.21062600	-1.94766800
C	-5.04463100	-3.25812600	-1.60922300
H	-3.07997500	-2.35152800	-1.80654800
H	-3.28686200	-3.30818300	-0.34196700
N	-3.46495500	1.05408400	0.60273800
C	-5.35998800	2.07807800	-0.43340600
H	-5.53621400	-2.61628000	-2.34669400
H	-4.77337600	-4.18992400	-2.11472800
H	-5.77211500	-3.50474700	-0.82785500
C	-3.24457800	2.17863700	1.29864600
C	-5.13013500	3.24699300	0.28600100
H	-6.19141100	1.99872100	-1.12607800
H	-2.38895300	2.15185900	1.96590800
C	-4.05394300	3.29932400	1.16951400
H	-5.78547000	4.10368800	0.16216300
H	-3.84229200	4.18935600	1.75154400
N	-0.98015100	0.23980000	1.81346300
N	0.15064500	0.37488800	1.48082600
N	1.27143500	0.52338300	1.18511300
Cu	2.37350600	0.65863600	-0.71926900
N	2.11462700	2.38814500	-1.57437500
N	1.10864400	2.81772300	-2.06859500
N	0.16144300	3.27432800	-2.55963700
N	4.04021100	1.39030700	0.23473700
C	4.63065400	0.29236400	1.01365100
C	3.79306900	2.61779100	1.02149300
H	4.67306200	1.62723600	-0.52980400
C	4.50058800	-0.99827700	0.25128400
H	5.67645300	0.47805500	1.28073100
H	4.06077400	0.21026600	1.94754200
C	5.04405200	3.25814400	1.60983800
H	3.28606600	3.30804600	0.34288100
H	3.07970300	2.35088600	1.80720800
N	3.46527900	-1.05388500	-0.60311200
C	5.36079400	-2.07763300	0.43239600
H	5.53595200	2.61623000	2.34703900
H	5.77133300	3.50520900	0.82842200
H	4.77260300	4.18971100	2.11566200
C	3.24508500	-2.17831100	-1.29928000
C	5.13112800	-3.24641900	-0.28728000
H	6.19233100	-1.99822800	1.12492500
H	2.38933400	-2.15159000	-1.96638100
C	4.05478100	-3.29881100	-1.17059900
H	5.78672500	-4.10296500	-0.16379700
H	3.84326500	-4.18874600	-1.75282600
N	0.98011800	-0.23986300	-1.81334600
N	-0.15057400	-0.37547100	-1.48057500
N	-1.27125800	-0.52448200	-1.18475500

(1) Cu_2 (Azide: End on) : E = -2999387.49535079 a.u.
(S= 2/2)

N	0.69813700	2.08373300	1.94801800
N	-0.40661600	2.45513500	2.23692900
N	-1.45160800	2.85286800	2.54780000
Cu	1.23906700	0.63833700	0.75221800
N	2.86966800	1.75984300	0.21776300
C	3.83733900	0.90588400	-0.48728400
C	2.54941500	3.02381500	-0.48073900
H	3.25440900	2.00524800	1.13072400
C	3.80836200	-0.48374700	0.09283500
H	4.85441600	1.31137900	-0.45974800
H	3.53554100	0.85708000	-1.54109900
C	3.72272800	3.98683300	-0.61063300
H	2.15659300	2.76246200	-1.46742900
H	1.73808400	3.48271200	0.08991100
N	2.64049000	-0.85148100	0.64629200
C	4.89699300	-1.34883400	0.03172200
H	4.52816400	3.58138100	-1.23051900
H	3.38319200	4.91554400	-1.07890200
H	4.13722500	4.24200300	0.37088800
C	2.51016800	-2.09111900	1.13934500
C	4.76254600	-2.63419400	0.54795400
H	5.82886800	-1.01672000	-0.41404900
H	1.53831700	-2.32954200	1.55802500
C	3.54629900	-3.01485100	1.11070200
H	5.59667100	-3.32818500	0.51308200
H	3.39879400	-4.00711400	1.52217500
N	-0.24558100	-0.58830600	1.21574700
N	-0.71295200	-0.73399600	2.31858100
N	-1.18085700	-0.90817800	3.36027900
Cu	-1.23907300	-0.63851000	-0.75142600
N	-0.69929800	-2.08447800	-1.94721200
N	0.40506200	-2.45878800	-2.23343100
N	1.44966700	-2.85917900	-2.54186700
N	-2.87090900	-1.75841100	-0.21731700
C	-3.83898500	-0.90324100	0.48571600
C	-2.55231500	-3.02190700	0.48279700
H	-3.25471500	-2.00450800	-1.13049300
C	-3.80826700	0.48592100	-0.09533500
H	-4.85620000	-1.30805900	0.45703200
H	-3.53870600	-0.85386600	1.53985400
C	-3.72657900	-3.98381300	0.61269300
H	-1.74086800	-3.48210200	-0.08666500
H	-2.16015500	-2.75987400	1.46959500

N	-2.63933600	0.85247000	-0.64727700
C	-4.89644200	1.35174700	-0.03659500
H	-4.53200500	-3.57722500	1.23191400
H	-4.14082200	-4.23931900	-0.36889500
H	-3.38807100	-4.91248600	1.08178500
C	-2.50745000	2.09164600	-1.14098600
C	-4.76038200	2.63661800	-0.55352500
H	-5.82922600	1.02057400	0.40788700
H	-1.53477700	2.32903400	-1.55833100
C	-3.54301100	3.01607800	-1.11457400
H	-5.59413200	3.33114900	-0.52051400
H	-3.39422200	4.00793100	-1.52650000
N	0.24630200	0.58721100	-1.21536400
N	0.71507300	0.73082700	-2.31786600
N	1.18437000	0.90308600	-3.35925100

(2) Cu_2 (SCN^-: Side on) : E = -3819768.60380838 a.u. (S= 2/2)

N	-2.56398800	2.20965200	-0.53982600
C	-2.23402100	3.33744600	-0.66891600
S	-1.81707500	4.89980800	-0.85336100
Cu	-2.75101300	0.29770500	-0.37244700
N	-4.51204300	0.51428800	0.61407800
C	-5.09369100	-0.82067500	0.84368900
C	-4.48441100	1.36993300	1.82658800
H	-5.08476100	0.99405200	-0.08249900
C	-4.77301700	-1.71515300	-0.32061600
H	-6.17388100	-0.77837500	1.01339500
H	-4.63496900	-1.23331600	1.75065700
C	-5.85839500	1.67606200	2.40667600
H	-3.84877500	0.86875000	2.56196000
H	-3.97689600	2.29196500	1.53607000
N	-3.66543900	-1.38164300	-1.00517800
C	-5.53582700	-2.82812200	-0.65934300
H	-6.36043800	0.78249700	2.78896100
H	-5.74841900	2.37346300	3.24214500
H	-6.50967600	2.14868600	1.66346000
C	-3.27441700	-2.13975500	-2.04122300
C	-5.12967700	-3.61741100	-1.73084100
H	-6.42896700	-3.06666000	-0.09162400
H	-2.37279800	-1.81768700	-2.54963800
C	-3.97996100	-3.26741000	-2.43594500
H	-5.70653000	-4.49187100	-2.01524000
H	-3.63249600	-3.85331300	-3.27923200
N	-1.12782400	-0.08075300	-1.33131300
C	-0.01672900	-0.24839800	-1.68102200
S	1.51299500	-0.51206700	-2.19592100
Cu	2.82788300	-0.39986800	0.43175700
N	4.59702800	-0.21321500	-0.54411800
C	4.66390500	1.12999900	-1.14800400
C	4.93997200	-1.30814800	-1.48471100
H	5.26939000	-0.25149400	0.22410500
C	3.97483300	2.11804000	-0.25022100
H	5.69213700	1.44168600	-1.35401300
H	4.12920600	1.08921300	-2.10483900
C	6.36875400	-1.25737100	-2.00791300
H	4.76167700	-2.24087300	-0.94603700
H	4.22248100	-1.26592500	-2.30926300
N	3.02002100	1.59762600	0.54022500
C	4.26250800	3.47895900	-0.25075200
H	6.55907900	-0.37195700	-2.62129000
H	7.09391200	-1.27385700	-1.18713200
H	6.55487200	-2.13604600	-2.63215700
C	2.31419800	2.40589000	1.34600000
C	3.52996800	4.31903000	0.58236500
H	5.04503100	3.86728500	-0.89399900
H	1.55701600	1.92396900	1.95405600
C	2.53833800	3.77428300	1.39564400
H	3.73314200	5.38519100	0.59918500
H	1.94633400	4.39403300	2.05922400
N	3.34025100	-2.12560300	1.11994800
C	3.40667600	-3.22468500	1.55124100
S	3.53654200	-4.73036600	2.15353500
N	1.11161600	-0.41129700	1.29684000
C	-0.01066200	-0.58050900	1.60746600
S	-1.56760500	-0.79438100	2.05938300

(2) Cu_2 (SCN^-: End on) : E = -3819767.95399887 a.u. (S= 2/2)

N	0.04058300	-2.64987600	-1.05888100
C	-0.70927900	-3.55223100	-1.20486700
S	-1.71408400	-4.81418900	-1.42264200
Cu	1.01113400	-1.03787000	-0.63639700
N	2.62033400	-2.13096100	-0.04203200
C	3.74755300	-1.21861600	0.21707600
C	2.37266400	-3.09931100	1.05414300
H	2.83086000	-2.67048300	-0.88313700
C	3.69009000	-0.05416000	-0.73158300
H	4.71424900	-1.72674300	0.14592700
H	3.64861300	-0.84715400	1.24461600
C	3.52548000	-4.06123400	1.30839500
H	2.14653400	-2.52023200	1.95388200
H	1.47050100	-3.64929500	0.77899100
N	2.46845300	0.24253700	-1.20991600
C	4.81155100	0.69900700	-1.06544700
H	4.42353600	-3.55086500	1.66822500
H	3.22904400	-4.78387200	2.07412000
H	3.78340000	-4.62247600	0.40376500
C	2.32031600	1.30360500	-2.01849800
C	4.65760100	1.79765500	-1.90456800
H	5.78385200	0.42660200	-0.66868400
H	1.31227500	1.49962900	-2.36383800
C	3.38884400	2.10730000	-2.38911800
H	5.51652600	2.40239300	-2.17802900
H	3.22364500	2.95511100	-3.04410400
N	-0.45798700	0.12813700	-1.33963500
C	-1.04618100	0.08450100	-2.38228900
S	-1.84857200	0.06449600	-3.77543900
Cu	-1.01111300	1.03785000	0.63634700
N	-2.62029000	2.13097100	0.04198100
C	-3.74754000	1.21865700	-0.21709700

C	-2.37260600	3.09929800	-1.05421100
H	-2.83078600	2.67051000	0.88308200
C	-3.69009800	0.05421300	0.73157700
H	-4.71421900	1.72681400	-0.14594300
H	-3.64862600	0.84717700	-1.24463300
C	-3.52537500	4.06128800	-1.30841900
H	-1.47040000	3.64923200	-0.77910100
H	-2.14654800	2.52020100	-1.95395500
N	-2.46846400	-0.24251600	1.20989500
C	-4.81157700	-0.69891500	1.06546800
H	-4.42348200	3.55096800	-1.66819000
H	-3.78320900	4.62256200	-0.40378600
H	-3.22893500	4.78389300	-2.07417400
C	-2.32034900	-1.30357900	2.01848700
C	-4.65765000	-1.79755800	1.90460100
H	-5.78387500	-0.42648500	0.66871600
H	-1.31230900	-1.49962900	2.36381600
C	-3.38889600	-2.10723600	2.38913400
H	-5.51658900	-2.40226400	2.17808300
H	-3.22371200	-2.95504300	3.04412800
N	-0.04055000	2.64984800	1.05884600
C	0.70927600	3.55221100	1.20492900
S	1.71403600	4.81417900	1.42281500
N	0.45798100	-0.12817100	1.33961300
C	1.04616400	-0.08456100	2.38227200
S	1.84853800	-0.06459400	3.77543200