Supporting Information for "Preparation and Luminescence Properties of a M_{16} Heterometallic Coinage Metal Chalcogenide Cluster"

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General Considerations

All syntheses described were conducted under an atmosphere of high-purity dry nitrogen using standard double-manifold Schlenk line techniques. Non-chlorinated solvents (tetrahydrofuran, pentane, hexanes) were dried and collected using an MBraun MB-SP Series solvent purification system and stored over 3Å molecular sieves. Deuterated chloroform was purchased from Caledon and dried over P_2O_5 by refluxing under N_2 prior to collecting by distillation and stored over 3Å molecular sieves. Diethyl ether was dried and distilled over sodium benzophenone ketyl radical and stored over 3Å molecular sieves. [(IPr)AuSSiMe$_3$],[1] Cu(OAc),[2] and E(SiMe$_3$)$_2$[3] were prepared following literature procedures. Other chemicals were used as received from commercial sources (Alfa Aesar and Aldrich).

NMR spectra were recorded on Inova 400 and Inova 600 spectrometers. ^{1}H and ^{13}C{^{1}H} chemical shifts are referenced to SiMe$_4$. Elemental analysis was performed by Laboratoire d'analyse élémentaire at the Université de Montréal, Montreal, Canada. Samples were dried under dynamic vacuum (< 10 mTorr) for at least 12 hours prior to shipment.

Photoluminescence measurements for solid samples of **1** were performed on a Horiba JobinYvon Fluorolog-3 spectrometer equipped with Hamamatsu R9110 and R5509 vis-NIR photomultipliers (covering respectively emission ranges of ~300-850 and ~500 – 1400 nm) and an optical close-cycle cryostat (Leybold) for measurements at cryogenic temperatures down to ca. 15 K. Solid state spectra were measured in back-scattering geometry transmission for samples which were prepared as micron-sized crystalline powders dispersed in a mineral oil layer between two quartz plates. The emission spectra were corrected for the wavelength-dependent response of the spectrometer and detector (in relative photon flux units). Emission decay traces were recorded by connecting the photomultiplier to an oscilloscope (typically with a 500 or 50 Ohm load) and using a N_2-laser for pulsed excitation at 337 nm (~2 ns, ~5μJ per pulse). Quantum yield determination for **1** was performed at ambient temperature using an integrating sphere by the method of Friend *et al.*[4]

X-ray measurements were made on a Nonius KappaCCD Apex2 with Cu Kα_1 (λ=1.5418 Å) radiation at a temperature of 110 K. The sample was mounted on a Mitegen polyimide micromount with a small amount of Paratone N oil. The collection strategy was a number of ω and φ scans with data collected up to >50° (2θ). The frame integration was performed using SAINT.[5] The resulting raw data was scaled and absorption corrected using a multi-scan averaging of symmetry equivalent data using SADABS.[6] The structure was solved by using a dual space methodology using the SHELXT program.[7] All non-hydrogen atoms were obtained from the initial solution. The hydrogen atoms were introduced at idealized positions and were allowed to ride on the parent atom. The structural model was fit to the data using full matrix least-squares based on F^2. The calculated structure factors included corrections for anomalous dispersion from the usual tabulation. The structures were refined using the SHELXLE program from the SHELXTL suite of crystallographic software.[8] Unless otherwise stated, all non-hydrogen atoms were refined anisotropically. A disordered THF molecule was refined with a split occupancy model over two positions and all atoms were refined isotropically using the SADI command to constrain the C-C

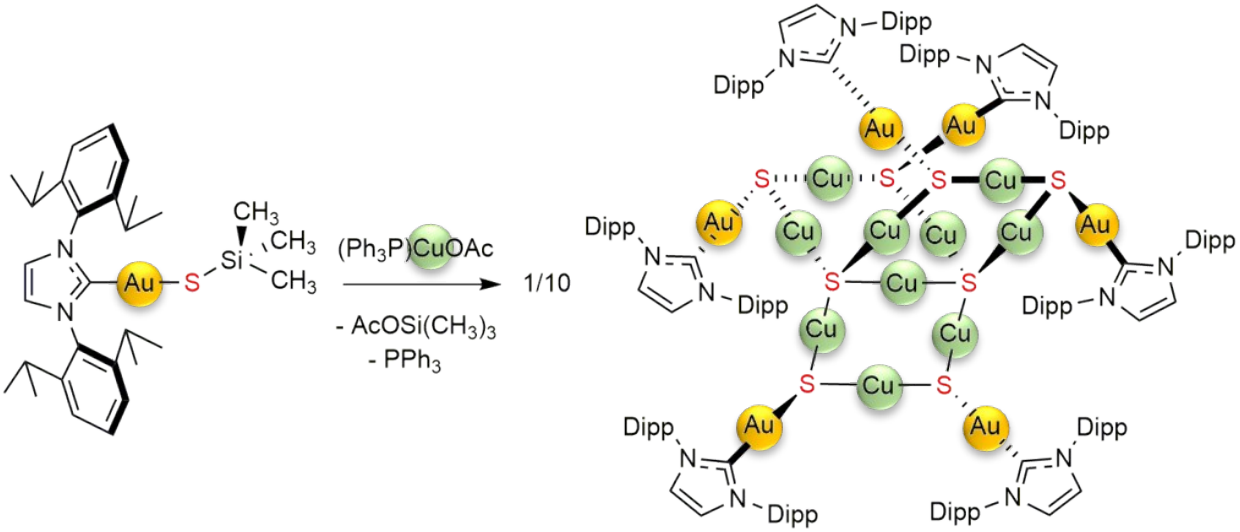
and C-O bond lengths. Additional (unresolved) solvent contributions were calculated using the PLATON SQUEEZE program.[9] CCDC 1853267 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Center via www.ccdc.cam.ac.uk/data_request/cif.

Quantum chemical calculations were done with TURBOMOLE[10,11] employing the functional B3LYP,[12] def2-SV(P) bases[13], within the RI approximation.[14]

Synthesis

Synthesis of $[Au_6Cu_{10}S_8(IPr)_6]$ (1)

$(Ph_3P)CuOAc$ was generated by the addition of PPh_3 (15 mg, 0.0579 mmol in 3 mL THF) to solid CuOAc followed by stirring until the solution is golden coloured. $[(IPr)AuSSiMe_3]$ (40 mg, 0.0579 mmol) was dissolved in 2 mL THF and both solutions were cooled to -78°C. The solutions were combined and the resulting clear yellow mixture was allowed to warm to -25°C with stirring and then held at this temperature overnight. The solution was then layered with 30 mL hexanes and stored at room temperature for two days, at which point colourless block crystals and yellow oil formed in solution. The crystals were removed and washed with Et_2O to afford the title complex as a pure white solid. Yield was increased by recrystallizing the mother liquor of the original reaction from THF/hexanes (9 mg, 32% based on Cu). **^{1}H NMR** ($CDCl_3$, 25°C, 599.301 MHz) δ7.37-7.41 (4H, BC portion of ABC, δ_B = 7.389 ppm, δ_C = 7.399 ppm, J_{BC} = 6.87 Hz, from simulation), 7.28-7.30 (2H, A portion of ABC, δ_A = 7.290 ppm, J_{AB} = 6.57 Hz, J_{AC} = 2.33 Hz, from simulation), 7.04 (2H, s, CH_{imid}), 2.61 (sept, $J_{H\text{-}H}$ = 7.0 Hz, $CH(CH_3)_2$), 2.58 (sept, $J_{H\text{-}H}$ = 7.0 Hz, $CH(CH_3)_2$); overlapping signals at 2.61 and 2.58 integrate to 4H in total; 1.40 (d, $J_{H\text{-}H}$ = 7.0 Hz, $CH(CH_3)_2$), 1.38 (d, $J_{H\text{-}H}$ = 7.0 Hz, $CH(CH_3)_2$); overlapping signals at 1.40 and 1.38 integrate to 12H in total; 1.17 (d, $J_{H\text{-}H}$ = 7.0 Hz, $CH(CH_3)_2$); 1.13 (d, $J_{H\text{-}H}$ = 7.0 Hz, $CH(CH_3)_2$); overlapping signals at 1.17 and 1.13 integrate to 12H in total. **^{13}C{^{1}H} NMR** ($CDCl_3$, 25°C, 150.78 MHz) δ190.2 (s, C-Au), 145.3 (s, C_{Ar}), 145.0 (s, C_{Ar}), 134.4 (s, C_{Ar}), 130.8 (s, C_{Ar}), 125.0 (s, C_{Ar}), 124.2 (s, C_{Ar}), 121.9 (s, C_{imid}), 28.9 (s, $CH(CH_3)_2$), 28.9 (s, $CH(CH_3)_2$), 25.6 (s, $CH(CH_3)_2$), 25.5 (s, $CH(CH_3)_2$), 24.3 (s, $CH(CH_3)_2$), 24.1 (s, $CH(CH_3)_2$). **Anal. Calcd** for $C_{162}H_{216}Au_6Cu_{10}N_{12}S_8 \cdot C_4H_8O$: C, 44.53; H, 5.04; N, 3.75; S, 5.73. Found C, 44.89; H, 5.15; N, 3.58; S, 5.47. The presence of 1 molecule of THF per molecule of the title cluster is determined by the integration of the THF signals in the ^{1}H NMR spectrum after vacuum drying.



NMR Data

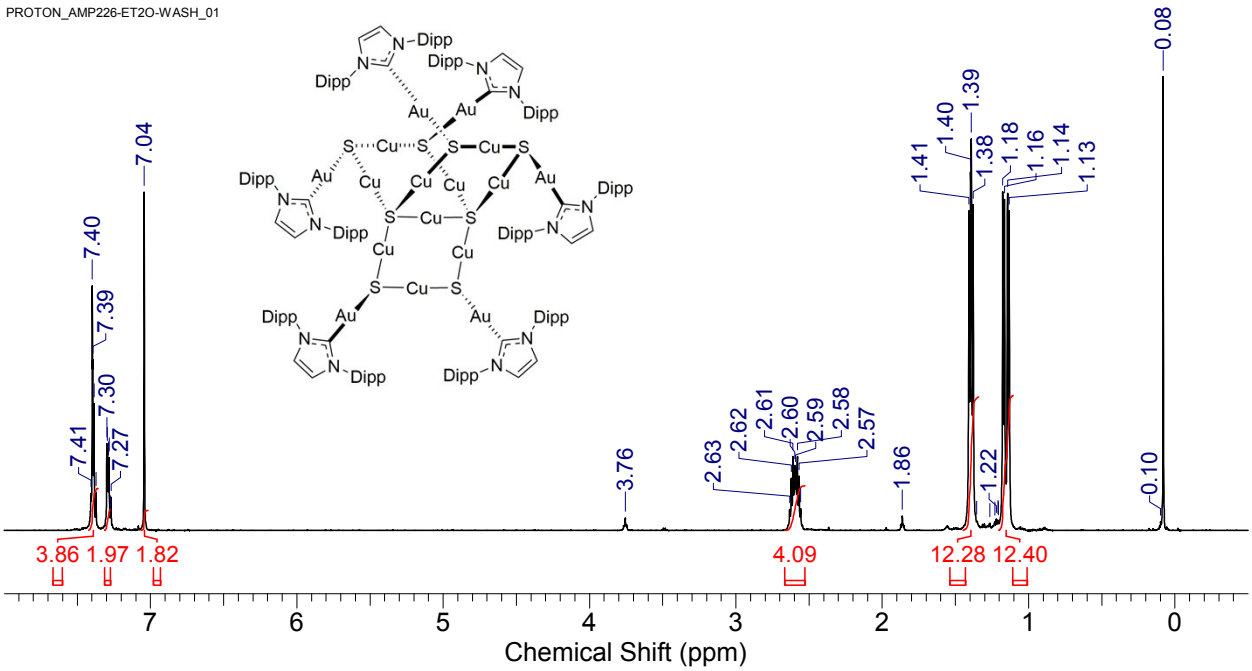


Figure S1 ^{1}H NMR spectrum of **1** in $CDCl_3$ at 298K

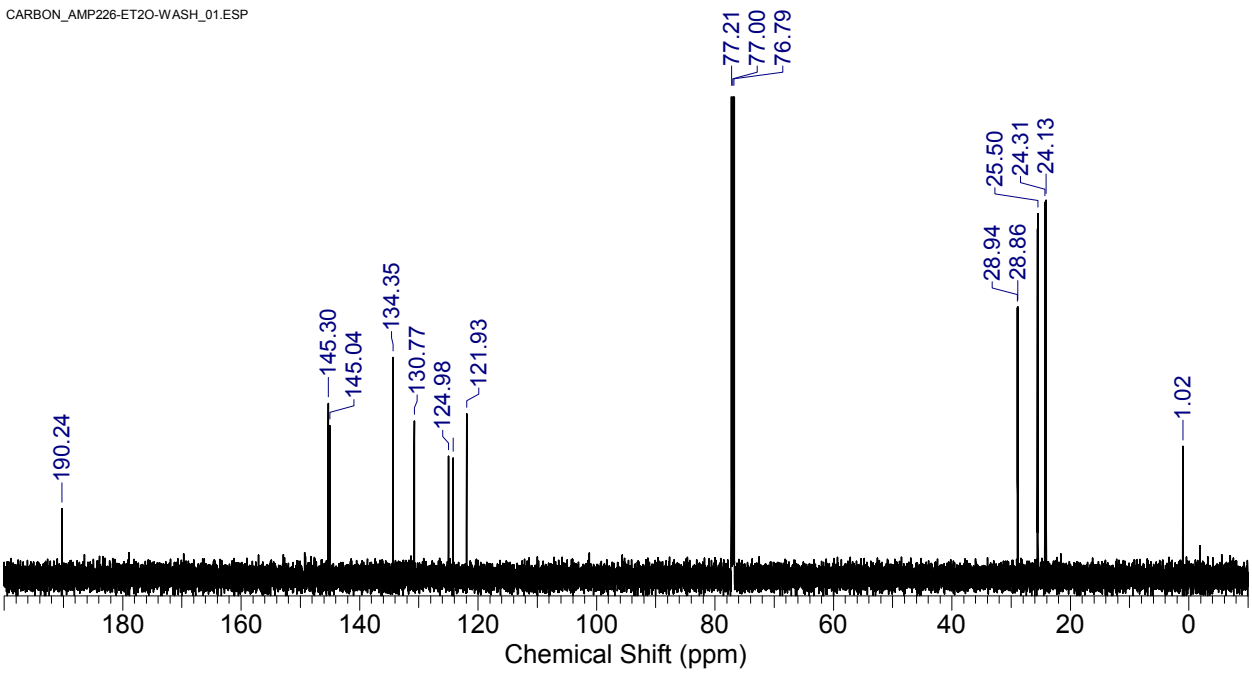


Figure S2 $^{13}C\{^{1}H\}$ NMR spectrum of 1 in $CDCl_3$ at 298K

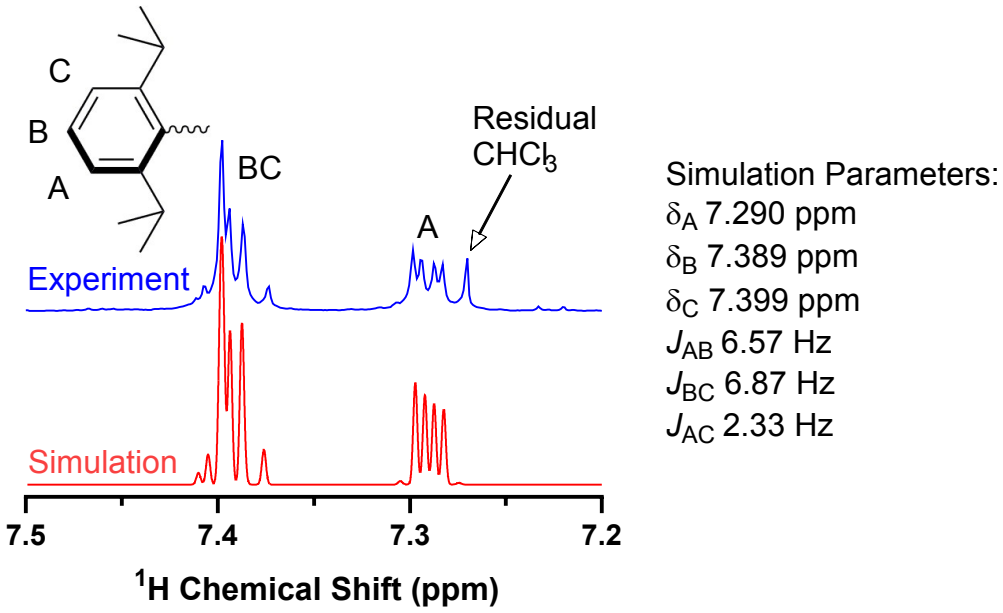


Figure S3 Simulated (lower, red) and experimental (upper, blue) ^{1}H NMR spectra for the aromatic region of **1**. The spectrum was simulated as an ABC spin system with the parameters given on the right. The ^{1}H NMR spectrum of 1 in $CDCl_3$ contains what at first appears to be two overlapping sets of signals for two chemically inequivalent carbene ligands (Figures S1 and S3). However, the presence of only one signal for the imidazole-2-ylidene backbone conflicts with this interpretation. Instead, all six ligands are chemically equivalent, and the apparent doubling of signals is instead due to a loss of symmetry in the 2,6-diisopropylphenyl moiety. The normal AB_2 spin system for the aromatic protons is reduced to an ABC system. Spectral simulation of the aromatic region of the ^{1}H NMR spectrum supports this (Figure S3), as does the presence of six, rather than four signals in the aromatic region of the $^{13}C\{^{1}H\}$ NMR spectrum for a fully asymmetric C_6 ring (Figure S2).

Crystallographic Data

	1·$(OC_4H_8)_3$
Molecular Formula	$C_{162}H_{216}Au_6Cu_{10}N_{12}S_8 \cdot 3C_4H_8O$
Formula Weight	4621.44
Crystal Habit	Colourless Prism
Crystal System	Trigonal
Space Group	$R\bar{3}_c$
Temperature (K)	110
λ (Å)	1.54178
a (Å)	28.6657(8)
b (Å)	28.6657(8)
c (Å)	52.375(2)
α (deg)	90
β (deg)	90
γ (deg)	120
V (Å^3)	37271(3)
Z	6
μ (mm^{-1})	8.285
$\rho_{calc.}$ (g cm^{-3})	1.235
$2\theta_{max}$	131.232
Reflections collected	118487
Ind. Reflections	7124
R_{merge}	0.1361
R_1, wR_2 [$I > 2\sigma(I)$]	0.0537, 0.1743
R_1, wR_2 (all data)	0.0403, 0.0972
GOF	0.0696, 0.1172
Max, min residual electron density (e^-/Å^3)	1.034
	0.878, -1.313

$R_1 = \Sigma(|F_o| - |F_c|) / \Sigma F_o$

$wR_2 = [\Sigma(w(F_o^2 - F_c^2)^2) / \Sigma(w F_o^4)]^{½}$

GOF = $[\Sigma(w(F_o^2 - F_c^2)^2) / (\text{No. of reflns.} - \text{No. of params.})]^{½}$

Table S1 Crystallographic data for **1**·$(OC_4H_8)_3$

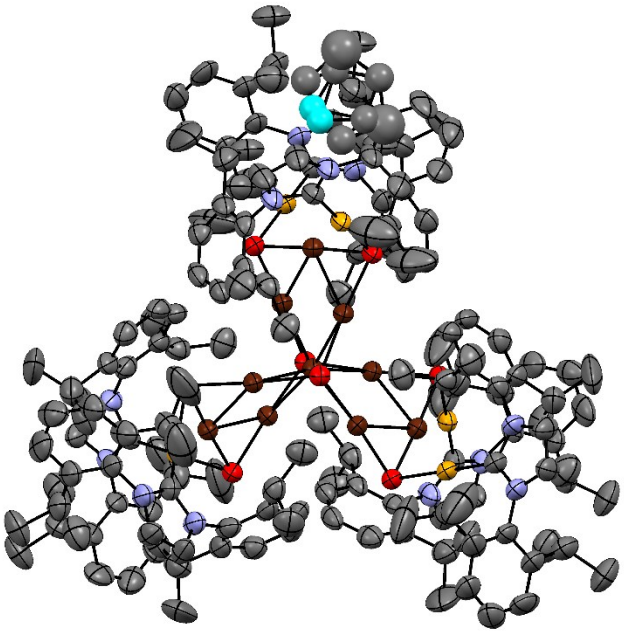


Figure S4 Thermal ellipsoid plot of **1**·$(OC_4H_8)_3$ (50% probability level; hydrogen atoms omitted). Spheres are used to represent the atoms of an isotropically refined, disordered THF molecule. Colour scheme: Cu – brown, Au – yellow, S – red, N – blue, C – gray, O – cyan.

Quantum chemical calculations

Table S2. Energies of the electronic states S0, T1 and S1 (rows) for structure parameters of S0, T1 and S1 (columns) relative to the ground state (S0 for structure parameters S0). For instance, the energy of the electronic ground state (S_0) for the structure parameters of the first excited triplet state (T_1) amounts to 0 .60054 eV.

		Structure parameters		
		S_0	T_1	S_1
Electronic state	S_0	0.0	0 .60054	0 .59423
	T_1	3.21543	2.49258	2.49704
	S_1	3.26685	2.68806	2.68374

Table S3: Lowest ten excitations for the ground state (S0) structure parameters. Oscillator strengths (spatial part) are given in the velocity representation. Note that for the triplet excitations they have no physical meaning, as in the approximation without spin-orbit coupling these transitions are spin-forbidden. In the column "Largest contribution", H denotes the highest occupied and L the lowest unoccupied orbital, the number in parentheses is the relative contribution of the listed orbital pair to the excitation in percent.

	Singlet excitations			Triplet excitations		
	Energy / eV	Oscillator strength	Largest Contribution	Energy / eV	Oscillator strength	Largest Contribution
1	3.26685	0.03658	H → L+1 (41)	3.21543	0.09717	H → L (25)
2	3.26889	0.01145	H → L (24)	3.21656	0.12030	H → L+1 (24)
3	3.27174	0.00534	H → L+3 (46)	3.22242	0.08920	H → L+2 (23)
4	3.27428	0.00938	H → L+2 (35)	3.22381	0.10066	H → L+3 (25)
5	3.27773	0.02092	H → L+4 (42)	3.23054	0.08229	H → L+5 (25)
6	3.27872	0.00050	H → L+5 (42)	3.23098	0.09545	H → L+4 (24)
7	3.30906	0.00020	H → L+7 (37)	3.30446	0.00166	H → L+4 (16)
8	3.30924	0.00004	H → L+6 (60)	3.30540	0.00048	H → L+7 (22)
9	3.31235	0.00005	H-1 → L (22)	3.30616	0.00200	H → L+8 (14)
10	3.32163	0.00181	H → L+2 (41)	3.30733	0.00234	H → L+6 (20)

Table S4: Lowest ten excitations for the S1 structure parameters. The energy of the electronic S_0 state for these structure parameters is 0 .59423 eV above that for the S_0 structure parameters. For further details see table S3.

	Singlet excitations			Triplet excitations		
	Energy / eV	Oscillator strength	Largest Contribution	Energy / eV	Oscillator strength	Largest Contribution
1	2.08951	0.00052	H → L (93)	1.90281	0.01321	H → L (93)
2	2.77595	0.02948	H-1 → L (62)	2.43044	0.40868	H-6 → L (53)
3	2.82036	0.03657	H-2 → L (69)	2.46216	0.18030	H-1 → L (51)
4	2.89335	0.00568	H-3 → L (43)	2.81433	0.02040	H-3 → L (53)
5	2.93143	0.00482	H → L+7 (89)	2.90365	0.01617	H → L+8 (82)
6	2.93244	0.00840	H → L+8 (91)	2.90446	0.04348	H → L+7 (82)
7	2.95834	0.00082	H → L+11 (97)	2.93741	0.19648	H-4 → L (30)
8	2.96419	0.00014	H → L+12 (95)	2.95619	0.00570	H → L+10 (67)
9	2.99130	0.00003	H → L+1 (78)	2.95968	0.02585	H → L +10(30)
10	2.99353	0.00059	H → L+2 (88)	2.96348	0.00041	H → L+11 (95)

Table S5: Lowest ten excitations for the T1 structure parameters. The energy of the electronic S_0 state for these structure parameters is 0 .60054 eV above that for the S_0 structure parameters. For further details see table S3.

	Singlet excitations			Triplet excitations		
	Energy / eV	Oscillator strength	Largest Contribution	Energy / eV	Oscillator strength	Largest Contribution
1	2.08752	0.00035	H → L (93)	1.89204	0.01251	H → L (93)
2	2.76876	0.02827	H-1 → L (59)	2.40653	0.40203	H-6 → L (52)
3	2.80496	0.03669	H-2 → L (64)	2.45131	0.17009	H-1 → L (47)
4	2.88078	0.00415	H-3 → L (45)	2.80249	0.01239	H-3 → L (52)
5	2.92927	0.00689	H → L+7 (77)	2.90223	0.01670	H → L+7 (47)
6	2.93133	0.00629	H → L+8 (73)	2.90479	0.03921	H → L+8 (44)
7	2.95830	0.00080	H → L+11 (97)	2.93303	0.18240	H-4→ L (31)
8	2.96432	0.00016	H → L+12 (94)	2.94956	0.02776	H-7 → L (27)
9	2.98769	0.00003	H → L+1 (73)	2.95757	0.00446	H → L+11 (92)
10	2.99010	0.00052	H → L+2 (81)	2.96358	0.00031	H → L+12 (94)

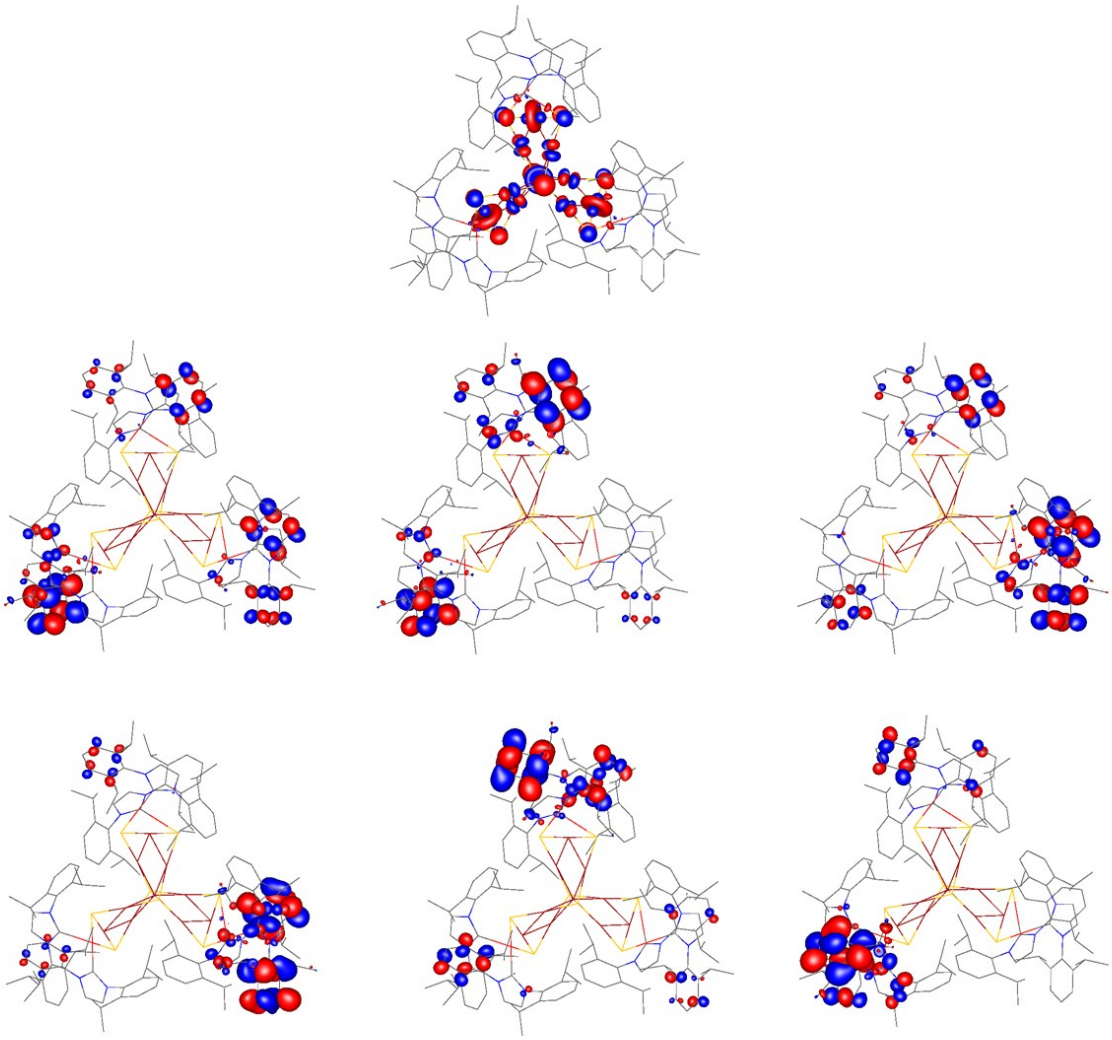


Figure S5. Orbitals involved in the lowest five transitions (S0→S1, S0→S2,…) for the S0 structure. First row: HOMO, second row: LUMO…LUMO+2, third row: LUMO+3…LUMO+5. Contours are drawn at ±0.03 a.u.

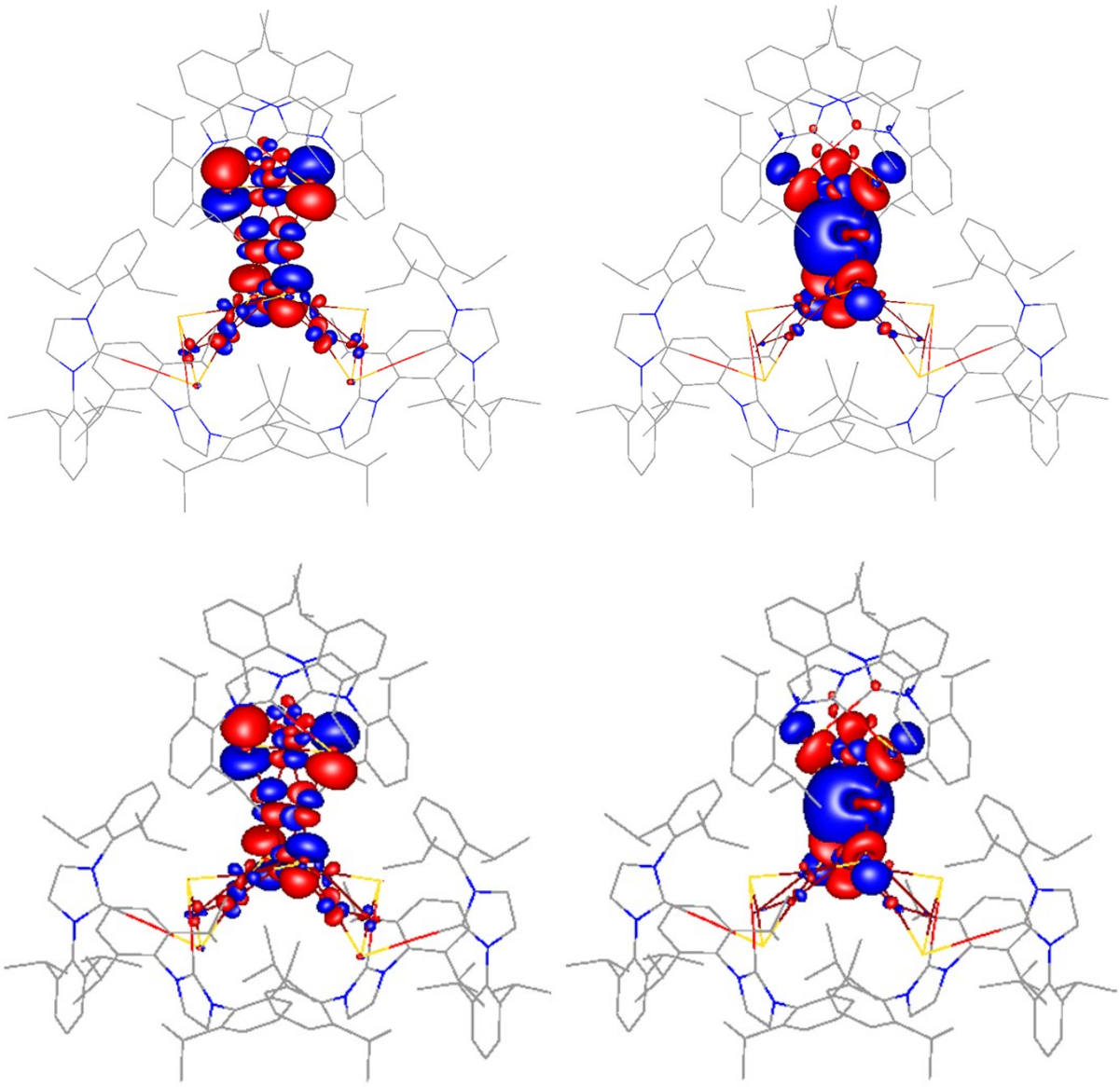


Figure S6. HOMO (left) and LUMO (right) for the S1 structure(top) and for the T1 structure (bottom). Contours are drawn at ±0.03 a.u.

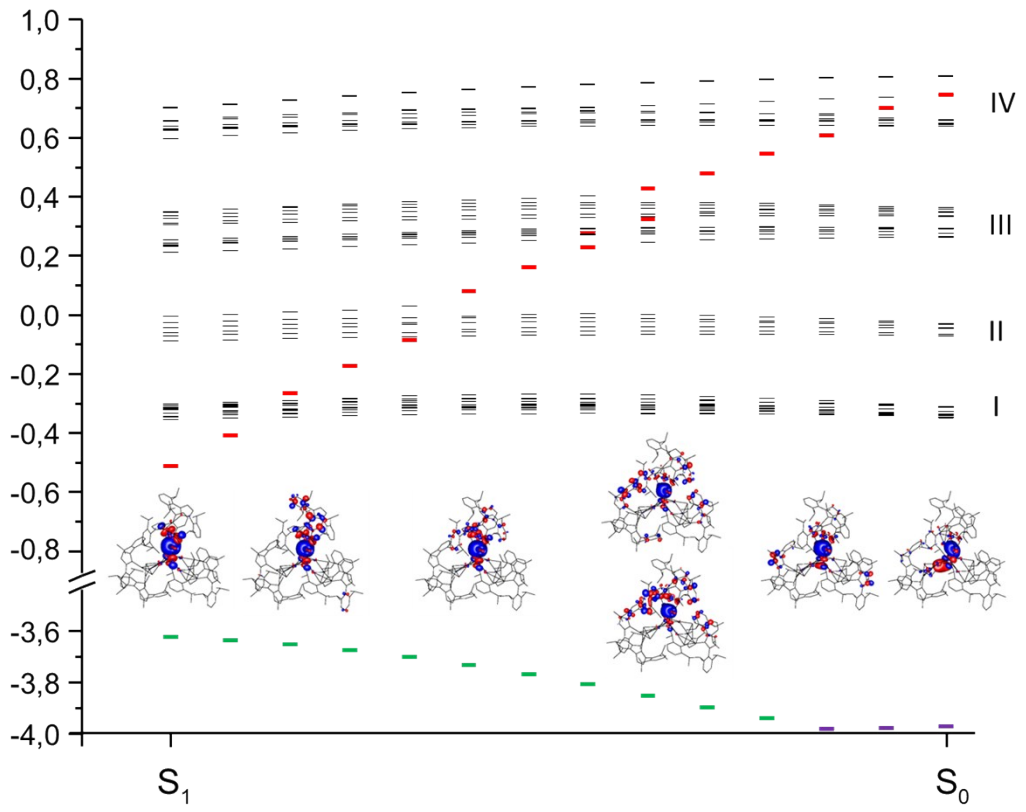


Figure S7. Scheme of the electronic structure (HOMO (green/pink), LUMO, LUMO+1,… LUMO+38 (black)) for the S1 and the S0 structure as well as for 12 interpolated structures. The energies of orbitals do not show a significant dependence on the structure parameters, except of the MO plotted and marked by a red bar in the scheme. This MO is mainly located at Cu2 and Cu3 (see main text, Figure 1) and their neighbors. The other unoccupied orbitals may be divided into four energetically well separated groups (I to IV). The MOs of groups I and III are located at the ligands only, some of those in groups II and IV show contributions also from cluster core atoms other than Cu2 and Cu3. The shape of the HOMO for most interpolated structures has the shape of that in the S_1 structure (see figure S6), which is marked in green in the scheme, only for the two interpolated structures next to S_0 the shape of the HOMO of the S_0 structure (see figure S5) is maintained (pink).

Table S6. Cartesian coordinates, in Å, for the states S_0, S_1 and T_1.

	S_0, *E*=-27352.202465 Ha			S_1, *E*=-27352.103840 Ha			T_1, *E*=-27352.110865 Ha		
	x	y	Z	X	Y	Z	X	Y	z
Au	-2.3803918	-4.6699165	-2.9995336	-2.5038394	-4.5664683	-2.9087745	-2.5145882	-4.5617163	-2.9236252
Cu	-2.0286030	-3.4888294	-0.0110050	-1.9045952	-3.5238514	0.1218401	-1.9097440	-3.5307580	0.1136166
Cu	-0.4111541	-2.1495423	-1.7387301	-0.4559670	-2.1658956	-1.7186116	-0.4633463	-2.1653064	-1.7222179
Cu	-0.0196684	0.0042728	0.0016903	0.0317462	-0.0516362	-0.0117336	0.0444481	-0.0780174	-0.0143028
S	-0.5867752	-4.3601583	-1.4847941	-0.6141044	-4.3824075	-1.4888698	-0.6243077	-4.3828931	-1.5040067
S	-0.0226762	-0.0009901	-2.2540699	-0.1346870	-0.0447476	-2.3223233	-0.1352378	-0.0438629	-2.3247932
N	-4.9863921	-4.0909034	-4.5035637	-5.0562802	-3.8384672	-4.4798753	-5.0699785	-3.8239251	-4.4840636
N	-4.1580917	-5.9623423	-5.1901488	-4.4465667	-5.8602135	-4.9271656	-4.4602737	-5.8416625	-4.9492083
C	-3.9382457	-4.9405891	-4.3117375	-4.1091817	-4.7709452	-4.1756587	-4.1215793	-4.7582701	-4.1899369
C	-5.8426260	-4.5682549	-5.4851214	-5.9630689	-4.3331107	-5.4069552	-5.9791602	-4.3116895	-5.4123447
H	-6.7371376	-4.0243559	-5.7792567	-6.7903845	-3.7316767	-5.7757241	-6.8075881	-3.7076103	-5.7742470
C	-5.3234255	-5.7489658	-5.9187964	-5.5817960	-5.6079951	-5.6890502	-5.5979528	-5.5841125	-5.7056782
H	-5.6679082	-6.4549796	-6.6707401	-6.0050634	-6.3565554	-6.3545989	-6.0226673	-6.3275455	-6.3760438
C	-5.1840410	-2.8605098	-3.7681869	-5.1348589	-2.5150085	-3.9004014	-5.1462636	-2.5051613	-3.8935813
C	-4.5515454	-1.6863156	-4.2315396	-4.3793105	-1.4718862	-4.4790289	-4.3936285	-1.4573104	-4.4673534
C	-4.7240285	-0.5205964	-3.4722509	-4.4611618	-0.2077355	-3.8776643	-4.4706079	-0.1986506	-3.8537976
H	-4.2266159	0.4074146	-3.7660914	-3.8649370	0.6233535	-4.2631873	-3.8751185	0.6354160	-4.2342081
C	-5.4969907	-0.5233665	-2.3110835	-5.2758069	0.0125805	-2.7674322	-5.2784942	0.0121084	-2.7368743
H	-5.5778425	0.3978212	-1.7266255	-5.2933321	1.0065971	-2.3105444	-5.2906510	1.0013754	-2.2696109
C	-6.1265268	-1.6943829	-1.8904035	-6.0304898	-1.0328017	-2.2351922	-6.0315550	-1.0373609	-2.2102135
H	-6.7211120	-1.6846329	-0.9724588	-6.6647269	-0.8471396	-1.3639314	-6.6608495	-0.8589746	-1.3338871
C	-5.9826018	-2.8928262	-2.6045836	-5.9703978	-2.3241691	-2.7779600	-5.9755521	-2.3238051	-2.7648733
C	-3.7153248	-1.6510450	-5.5085468	-3.5151804	-1.6729292	-5.7215804	-3.5342939	-1.6472412	-5.7150092
H	-3.6000938	-2.6864608	-5.8688573	-3.4739479	-2.7535273	-5.9353588	-3.5146514	-2.7232615	-5.9537450
C	-2.2987470	-1.1019506	-5.2647296	-2.0658380	-1.2010992	-5.5124950	-2.0761300	-1.2091736	-5.4932808
H	-1.6970487	-1.1714835	-6.1904270	-1.4485333	-1.4670504	-6.3910563	-1.4631704	-1.4614523	-6.3789537
H	-1.7782467	-1.6652981	-4.4715733	-1.6136562	-1.6622086	-4.6184077	-1.6338227	-1.7044065	-4.6125897
H	-2.3089351	-0.0433771	-4.9507918	-2.0009740	-0.1070280	-5.3771843	-1.9909352	-0.1211391	-5.3252401
C	-4.4399560	-0.8639581	-6.6188928	-4.1534920	-0.9908020	-6.9492161	-4.1572697	-0.9248771	-6.9272330
H	-3.8513453	-0.8818533	-7.5554178	-3.5477109	-1.1773890	-7.8558835	-3.5552623	-1.1052324	-7.8376558
H	-4.5817637	0.1932471	-6.3300172	-4.2197861	0.1036278	-6.8068684	-4.1997182	0.1675199	-6.7621429
H	-5.4373601	-1.2899009	-6.8344495	-5.1761044	-1.3662864	-7.1389116	-5.1877036	-1.2740623	-7.1247417
C	-6.6753912	-4.1638727	-2.1173691	-6.7953109	-3.4551095	-2.1658322	-6.7981712	-3.4597576	-2.1588427
H	-6.3213480	-5.0024014	-2.7395294	-6.4337338	-4.4047315	-2.5936642	-6.4381865	-4.4057817	-2.5959452
C	-6.3146860	-4.5075842	-0.6608725	-6.6203170	-3.5613093	-0.6397858	-6.6172688	-3.5789002	-0.6344707
H	-6.7513753	-5.4852820	-0.3821307	-7.1237498	-4.4716123	-0.2639747	-7.1189264	-4.4925360	-0.2644131
H	-6.7011291	-3.7550867	0.0491006	-7.0713536	-2.7005571	-0.1133580	-7.0662814	-2.7227377	-0.0989255
H	-5.2224977	-4.5550685	-0.5139661	-5.5568071	-3.6088808	-0.3481853	-5.5525802	-3.6282586	-0.3475704
C	-8.2029456	-4.0722819	-2.3085555	-8.2853241	-3.3214634	-2.5423704	-8.2896211	-3.3234175	-2.5287591
H	-8.4713164	-3.8851432	-3.3647195	-8.4322240	-3.3111756	-3.6378617	-8.4405812	-3.3043654	-3.6235879
H	-8.6327270	-3.2515191	-1.7053404	-8.7134351	-2.3845763	-2.1403038	-8.7164026	-2.3898727	-2.1175975
H	-8.6920579	-5.0131748	-1.9934901	-8.8696037	-4.1646022	-2.1284229	-8.8722077	-4.1699997	-2.1194415
C	-3.3141068	-7.1216407	-5.3548174	-3.7377285	-7.1174387	-4.9462284	-3.7501589	-7.0979475	-4.9808202
C	-2.2823082	-7.0787433	-6.3177972	-2.7378844	-7.3157621	-5.9233988	-2.7538441	-7.2873627	-5.9633807
C	-1.4942613	-8.2286526	-6.4753326	-2.0844083	-8.5569189	-5.9396315	-2.0996455	-8.5279240	-5.9925275
H	-0.6810781	-8.2277044	-7.2073188	-1.2996748	-8.7424065	-6.6791022	-1.3177543	-8.7067650	-6.7366443
C	-1.7238110	-9.3709405	-5.7088624	-2.4115705	-9.5559350	-5.0231021	-2.4221115	-9.5345583	-5.0826719
H	-1.0948310	-10.2565501	-5.8459684	-1.8863657	-10.5161827	-5.0509575	-1.8965082	-10.4942492	-5.1206968
C	-2.7491376	-9.3850465	-4.7635851	-3.4016461	-9.3317104	-4.0668388	-3.4080160	-9.3186780	-4.1201866
H	-2.9139110	-10.2850831	-4.1637529	-3.6433336	-10.1212303	-3.3490550	-3.6455137	-10.1138985	-3.4073159
C	-3.5674439	-8.2632995	-4.5631366	-4.0882848	-8.1098970	-4.0047240	-4.0953398	-8.0979399	-4.0452950
C	-1.9942256	-5.8381140	-7.1591690	-2.3412197	-6.2334615	-6.9243243	-2.3612042	-6.1962007	-6.9563055
H	-2.7397322	-5.0703789	-6.8983573	-2.9970309	-5.3636073	-6.7616439	-3.0161974	-5.3277462	-6.7831511
C	-2.1420724	-6.1186822	-8.6669773	-2.5493289	-6.6897018	-8.3810951	-2.5755210	-6.6394488	-8.4161965
H	-1.3992150	-6.8566832	-9.0215618	-1.8951088	-7.5418283	-8.6419226	-1.9227585	-7.4894996	-8.6872568
H	-1.9906317	-5.1898923	-9.2471811	-2.3143655	-5.8650553	-9.0789522	-2.3431343	-5.8087566	-9.1077207
H	-3.1463967	-6.5114033	-8.9093700	-3.5940167	-7.0017820	-8.5626067	-3.6210724	-6.9495171	-8.5961520
C	-0.6110177	-5.2468181	-6.8270791	-0.8975997	-5.7533091	-6.6820552	-0.9164959	-5.7183338	-6.7158575
H	0.2035615	-5.9489839	-7.0836347	-0.1654263	-6.5647791	-6.8490745	-0.1851018	-6.5282425	-6.8934876
H	-0.5312251	-5.0077961	-5.7517306	-0.7719532	-5.3867138	-5.6478792	-0.7863677	-5.3611889	-5.6789467
H	-0.4434390	-4.3155062	-7.3984632	-0.6454168	-4.9267209	-7.3714701	-0.6672835	-4.8853696	-7.3986667
C	-4.6702626	-8.3056020	-3.5082437	-5.1572479	-7.8923640	-2.9366316	-5.1594784	-7.8896073	-2.9705386
H	-5.1964664	-7.3381361	-3.5285574	-5.5773015	-6.8839132	-3.0776435	-5.5811748	-6.8805351	-3.1020085
C	-5.7156430	-9.3951777	-3.8152120	-6.3220716	-8.8909728	-3.0802945	-6.3239488	-8.8883129	-3.1162910
H	-6.1616158	-9.2574127	-4.8170850	-6.7796776	-8.8383498	-4.0850430	-6.7864122	-8.8284764	-4.1184064
H	-6.5331261	-9.3636894	-3.0715346	-7.1094125	-8.6719038	-2.3357104	-7.1079804	-8.6758172	-2.3663350
H	-5.2740505	-10.4081698	-3.7813951	-5.9910378	-9.9331563	-2.9171157	-5.9910388	-9.9313582	-2.9627118
C	-4.0851149	-8.4647778	-2.0918752	-4.5518801	-7.9287379	-1.5201521	-4.5474174	-7.9359566	-1.5571704
H	-3.5580504	-9.4299905	-1.9760593	-4.1286185	-8.9230025	-1.2847899	-4.1215542	-8.9313524	-1.3314678

H	-4.8922872	-8.4290543	-1.3367647	-5.3282679	-7.7057429	-0.7652164	-5.3206456	-7.7199760	-0.7969429
H	-3.3696045	-7.6551286	-1.8644537	-3.7471479	-7.1803561	-1.4117065	-3.7433790	-7.1871071	-1.4467273
Au	5.1896427	0.2783530	-2.9911837	5.0834133	-0.0388427	-3.2142257	5.0819524	-0.0446862	-3.2121306
Cu	4.0040378	0.0045827	0.0000002	4.0160711	-0.1057842	-0.1387358	4.0184327	-0.1036063	-0.1319739
Cu	2.0332972	0.7326615	-1.7354579	1.9728721	0.5814055	-1.8703800	1.9711430	0.5796412	-1.8690501
S	4.0339454	1.6866610	-1.4776772	4.0226680	1.4641023	-1.7246400	4.0217071	1.4600169	-1.7240535
N	6.0239286	-2.2819691	-4.4593006	5.9134933	-2.6852009	-4.5315710	5.9122703	-2.6917932	-4.5278592
N	7.2016955	-0.6194896	-5.1726015	6.9516996	-1.0424370	-5.4700749	6.9544362	-1.0498853	-5.4634893
C	6.2101764	-0.9422770	-4.2914156	6.0428076	-1.3294564	-4.4926899	6.0423489	-1.3361179	-4.4888527
C	6.8787759	-2.7868550	-5.4283998	6.7243053	-3.2361297	-5.5135480	6.7258892	-3.2434417	-5.5071045
H	6.8754230	-3.8387766	-5.7038017	6.7554814	-4.3076607	-5.6960257	6.7568384	-4.3150006	-5.6893642
C	7.6236724	-1.7409034	-5.8786116	7.3811100	-2.2021832	-6.1059177	7.3853071	-2.2100600	-6.0975300
H	8.4084457	-1.6851935	-6.6293187	8.1070505	-2.1783892	-6.9152206	8.1140670	-2.1869448	-6.9043050
C	5.0658205	-3.0731369	-3.7178464	5.0379361	-3.4509200	-3.6717723	5.0339040	-3.4571556	-3.6706245
C	3.7340059	-3.1330647	-4.1827200	3.6881915	-3.6101951	-4.0540529	3.6846223	-3.6144410	-4.0555142
C	2.8188814	-3.8712853	-3.4191963	2.8534704	-4.3279407	-3.1863381	2.8478195	-4.3331419	-3.1905709
H	1.7671217	-3.9192775	-3.7132349	1.7909102	-4.4463127	-3.4137175	1.7855657	-4.4502583	-3.4200306
C	3.2150680	-4.5269208	-2.2536862	3.3455006	-4.8705491	-2.0000325	3.3374040	-4.8788734	-2.0046912
H	2.4635875	-5.0631514	-1.6667301	2.6563236	-5.3954074	-1.3322945	2.6467774	-5.4049284	-1.3393931
C	4.5429627	-4.4673837	-1.8317560	4.6881107	-4.7130308	-1.6576772	4.6795427	-4.7230312	-1.6596485
H	4.8377113	-4.9784254	-0.9108415	5.0584480	-5.1345228	-0.7186482	5.0481008	-5.1470321	-0.7210152
C	5.5001473	-3.7350120	-2.5489429	5.5664128	-3.9934354	-2.4808253	5.5597771	-4.0021679	-2.4796031
C	3.2766602	-2.4431635	-5.4657796	3.1197098	-3.0359960	-5.3493339	3.1184387	-3.0372956	-5.3505398
H	4.1112057	-1.8262887	-5.8374499	3.9205047	-2.4714377	-5.8548936	3.9208928	-2.4740167	-5.8548646
C	2.0898662	-1.4933345	-5.2265265	1.9703306	-2.0476998	-5.0815570	1.9712926	-2.0465803	-5.0817043
H	1.8388533	-0.9520410	-6.1581006	1.6024666	-1.6172504	-6.0319904	1.6054309	-1.6130000	-6.0314606
H	2.3201721	-0.7480418	-4.4462720	2.2950761	-1.2168856	-4.4319012	2.2976338	-1.2180512	-4.4299268
H	1.1838389	-2.0316006	-4.8971469	1.1154530	-2.5306831	-4.5766018	1.1147138	-2.5287222	-4.5788045
C	2.9567813	-3.4786844	-6.5625356	2.6857770	-4.1600644	-6.3109190	2.6818724	-4.1588027	-6.3139031
H	2.6702596	-2.9722220	-7.5034275	2.3278983	-3.7344746	-7.2671600	2.3255442	-3.7308728	-7.2696658
H	2.1172463	-4.1314715	-6.2621520	1.8624053	-4.7594525	-5.8825234	1.8566111	-4.7565293	-5.8867869
H	3.8269065	-4.1270171	-6.7753382	3.5219923	-4.8480806	-6.5349961	3.5163228	-4.8487491	-6.5386321
C	6.9472281	-3.6784046	-2.0634090	7.0266450	-3.8147602	-2.0709346	7.0188322	-3.8232870	-2.0654011
H	7.4746175	-2.9173281	-2.6620197	7.5005896	-3.1323911	-2.7956657	7.4938140	-3.1378693	-2.7865783
C	7.0598014	-3.2424201	-0.5915938	7.1631166	-3.1580078	-0.6848836	7.1508364	-3.1709203	-0.6767965
H	8.1225861	-3.1026052	-0.3177449	8.2269063	-2.9465110	-0.4662158	8.2137628	-2.9585910	-0.4547134
H	6.6366362	-3.9957539	0.0963843	6.7794171	-3.8092948	0.1203030	6.7661852	-3.8255513	0.1252538
H	6.5206999	-2.2982599	-0.4053978	6.5977236	-2.2124252	-0.6280055	6.5839595	-2.2263139	-0.6180963
C	7.6652115	-5.0222722	-2.3032745	7.7949282	-5.1499555	-2.1375058	7.7889924	-5.1572928	-2.1343240
H	7.6450608	-5.3117402	-3.3701302	7.7469618	-5.5978276	-3.1472751	7.7447495	-5.6017157	-3.1457967
H	7.1878279	-5.8371324	-1.7283844	7.3800420	-5.8873762	-1.4259083	7.3728608	-5.8977300	-1.4265694
H	8.7233706	-4.9610026	-1.9865020	8.8604170	-4.9990466	-1.8814250	8.8535099	-5.0059440	-1.8744590
C	7.7486732	0.7015020	-5.3705420	7.3960906	0.2812323	-5.8349817	7.4011651	0.2733911	-5.8270661
C	7.1882617	1.5219888	-6.3740185	6.7127148	0.9600567	-6.8680281	6.7239685	0.9512046	-6.8648649
C	7.7543623	2.7912145	-6.5648332	7.1772408	2.2351405	-7.2231099	7.1897020	2.2265516	-7.2174797
H	7.3405257	3.4556521	-7.3292167	6.6679875	2.7922857	-8.0151163	6.6849977	2.7830359	-8.0128743
C	8.8302745	3.2247919	-5.7905963	8.2729673	2.8086699	-6.5781332	8.2809283	2.8011577	-6.5658513
H	9.2542725	4.2209534	-5.9535193	8.6171987	3.8064988	-6.8688662	8.6259859	3.7993071	-6.8545401
C	9.3627534	2.3942985	-4.8048879	8.9274748	2.1162059	-5.5598041	8.9297182	2.1094338	-5.5433472
H	10.2021185	2.7494184	-4.1995794	9.7811099	2.5808243	-5.0573943	9.7799124	2.5748352	-5.0358548
C	8.8367368	1.1148849	-4.5709835	8.5061331	0.8380286	-5.1633214	8.5069559	0.8310090	-5.1490675
C	5.9960554	1.0858058	-7.2220322	5.4981140	0.3667069	-7.5783147	5.5146597	0.3563944	-7.5829894
H	5.7343367	0.0548521	-6.9359514	5.3273984	-0.6430282	-7.1730594	5.3423685	-0.6535022	-7.1787779
C	6.3343992	1.0654490	-8.7250076	5.7364636	0.2100537	-9.0924995	5.7629637	0.1998714	-9.0955909
H	6.5746873	2.0752800	-9.1053512	5.8796234	1.1875688	-9.5886678	5.9082416	1.1774904	-9.5909303
H	5.4739487	0.6875744	-9.3072844	4.8676917	-0.2801806	-9.5690894	4.8978520	-0.2913770	-9.5777639
H	7.2012351	0.4130519	-8.9362462	6.6308078	-0.4052125	-9.3005551	6.6593176	-0.4144080	-9.2978127
C	4.7583627	1.9560712	-6.9323417	4.2244402	1.1831099	-7.2879880	4.2382518	1.1714732	-7.3010989
H	4.9276874	3.0110506	-7.2161754	4.2997881	2.2107766	-7.6882432	4.3151864	2.1992342	-7.7007623
H	4.4978804	1.9281110	-5.8595105	4.0366995	1.2537846	-6.2021116	4.0431866	1.2418662	-6.2164956
H	3.8867023	1.5901187	-7.5055437	3.3450102	0.7028399	-7.7554123	3.3624243	0.6903842	-7.7744220
C	9.4352905	0.2364863	-3.4751820	9.2355245	0.1125578	-4.0353521	9.2304889	0.1061695	-4.0168997
H	8.8863216	-0.7184886	-3.4681542	8.7537742	-0.8682745	-3.8963250	8.7476473	-0.8743572	-3.8794487
C	10.9149579	-0.0938885	-3.7514629	10.7118451	-0.1541408	-4.3876638	10.7083642	-0.1614107	-4.3619835
H	11.0445008	-0.5817354	-4.7347533	10.8069462	-0.7290123	-5.3269020	10.8077387	-0.7372036	-5.3002194
H	11.3066092	-0.7791860	-2.9773170	11.1999848	-0.7340157	-3.5827865	11.1924961	-0.7407317	-3.5542979
H	11.5460912	0.8138079	-3.7422918	11.2799466	0.7862124	-4.5115166	11.2773275	0.7786647	-4.4840387
C	9.2468322	0.8693781	-2.0831390	9.1000178	0.8696554	-2.7000725	9.0888266	0.8643193	-2.6828234
H	9.7905636	1.8282642	-1.9954021	9.5812948	1.8641968	-2.7465216	9.5707756	1.8586070	-2.7275790
H	9.6312908	0.1914719	-1.2985977	9.5836808	0.2993470	-1.8856380	9.5682113	0.2943272	-1.8656075
H	8.1794657	1.0609419	-1.8748529	8.0383224	1.0138782	-2.4321110	8.0259130	1.0091987	-2.4201079
Au	-2.8470783	4.3797859	-2.9639075	-2.2197292	4.8227529	-3.2073300	-2.2095220	4.8143666	-3.2037590
Cu	-2.0301316	3.4953823	0.0185525	-2.0894108	3.6081249	-0.0068347	-2.1044674	3.6377701	-0.0050038
Cu	-1.6805315	1.4148827	-1.7216721	-1.3822922	1.6384984	-1.2503411	-1.3702195	1.6380183	-1.2249728
S	-3.5013978	2.6755083	-1.4551617	-3.1342803	3.0634527	-1.9439210	-3.1296389	3.0601560	-1.9366118

N	-1.0418498	6.4080485	-4.3909573	-0.1628039	6.8318587	-4.2608021	-0.1592047	6.8206908	-4.2805541
N	-3.0512449	6.5500203	-5.1667560	-2.0532217	7.1358335	-5.2576783	-2.0609633	7.1254420	-5.2553506
C	-2.2889829	5.8751340	-4.2574614	-1.4415008	6.3662960	-4.3115049	-1.4387521	6.3557913	-4.3159581
C	-1.0226679	7.3941938	-5.3665664	0.0248398	7.8715582	-5.1601465	0.0183097	7.8603967	-5.1821008
H	-0.1130260	7.9346416	-5.6174679	0.9846130	8.3716819	-5.2662398	0.9769891	8.3600964	-5.2994029
C	-2.2888665	7.4866670	-5.8564430	-1.1663712	8.0656551	-5.7893617	-1.1800277	8.0549205	-5.7973878
H	-2.7196582	8.1242069	-6.6248373	-1.4675474	8.7710122	-6.5602758	-1.4898355	8.7602938	-6.5648608
C	0.1046571	6.0066984	-3.6047180	0.8617741	6.3084496	-3.3837913	0.8762320	6.2966351	-3.4169698
C	0.8714428	4.9040959	-4.0398170	1.6275373	5.2063232	-3.8220969	1.6337948	5.1923495	-3.8640007
C	1.9448050	4.5070707	-3.2299640	2.5921400	4.7000228	-2.9405182	2.6101777	4.6861866	-2.9954285
H	2.5486666	3.6369338	-3.5004422	3.1858889	3.8239405	-3.2134799	3.1980284	3.8083189	-3.2750851
C	2.2433776	5.1827893	-2.0470983	2.7850532	5.2685468	-1.6824413	2.8229639	5.2573580	-1.7418018
H	3.0660560	4.8206423	-1.4234083	3.5229426	4.8239823	-1.0086969	3.5697177	4.8126386	-1.0779813
C	1.4820562	6.2834617	-1.6550966	2.0211299	6.3635269	-1.2796909	2.0670422	6.3547618	-1.3305702
H	1.7214979	6.7977369	-0.7200464	2.1730798	6.7903800	-0.2836431	2.2353782	6.7845357	-0.3384087
C	0.3920103	6.7209375	-2.4213389	1.0362999	6.9074730	-2.1172850	1.0702761	6.8980400	-2.1544275
C	0.5778747	4.1540664	-5.3369784	1.4324025	4.5471698	-5.1850532	1.4170416	4.5301214	-5.2222041
H	-0.3497123	4.5661393	-5.7675331	0.6153899	5.0728087	-5.7068642	0.5921583	5.0548722	-5.7323099
C	0.3340988	2.6535568	-5.0974358	1.0044956	3.0731851	-5.0457795	0.9903123	3.0568260	-5.0728004
H	0.0637511	2.1521317	-6.0458508	0.8251845	2.6300550	-6.0435405	0.7950921	2.6114738	-6.0665594
H	-0.4833377	2.4880484	-4.3749776	0.0752571	2.9815274	-4.4564431	0.0702659	2.9674626	-4.4688988
H	1.2258967	2.1450784	-4.6907828	1.7728523	2.4633546	-4.5378771	1.7659345	2.4475135	-4.5754313
C	1.6972397	4.3843032	-6.3719383	2.6923350	4.6916279	-6.0612317	2.6630769	4.6720471	-6.1184059
H	1.4527572	3.8813431	-7.3263865	2.5158691	4.2611187	-7.0646818	2.4713795	4.2379941	-7.1175332
H	2.6609271	3.9779411	-6.0153501	3.5550757	4.1628716	-5.6176510	3.5328357	4.1452669	-5.6863440
H	1.8426723	5.4605028	-6.5803101	2.9768904	5.7525317	-6.1895103	2.9451158	5.7326215	-6.2547468
C	-0.4314871	7.9240625	-1.9659172	0.1917519	8.0857434	-1.6367837	0.2351222	8.0793076	-1.6649182
H	-1.2987772	8.0159835	-2.6403597	-0.5683202	8.2950230	-2.4074539	-0.5435439	8.2796395	-2.4192127
C	-0.9913646	7.7463893	-0.5430851	-0.5680284	7.7571727	-0.3375327	-0.4932023	7.7627890	-0.3448583
H	-1.6631217	8.5886538	-0.2910693	-1.2448594	8.5902226	-0.0693355	-1.1670108	8.5963625	-0.0709146
H	-0.1899815	7.7188194	0.2161741	0.1181489	7.5982464	0.5133198	0.2131072	7.6175444	0.4919760
H	-1.5558131	6.8038124	-0.4456193	-1.1712361	6.8389533	-0.4411600	-1.0951317	6.8412038	-0.4236355
C	0.3770766	9.2313846	-2.0897689	1.0415100	9.3628231	-1.4825745	1.0863373	9.3590581	-1.5434612
H	0.7338111	9.3937644	-3.1236290	1.5463276	9.6319717	-2.4286500	1.5670327	9.6204109	-2.5041948
H	1.2639175	9.2176738	-1.4297952	1.8237295	9.2353041	-0.7118312	1.8878413	9.2390188	-0.7914773
H	-0.2429123	10.1011870	-1.8019054	0.4079010	10.2169605	-1.1785243	0.4593241	10.2151478	-1.2312631
C	-4.4594806	6.3369357	-5.4008416	-3.4316796	7.0145816	-5.6690780	-3.4442753	7.0048512	-5.6503130
C	-4.8482351	5.4171950	-6.3993816	-3.7452894	6.1539066	-6.7439893	-3.7706781	6.1466124	-6.7234001
C	-6.2222724	5.2513124	-6.6283741	-5.0885767	6.0773817	-7.1410842	-5.1185226	6.0713041	-7.1050235
H	-6.5591011	4.5422365	-7.3904452	-5.3687736	5.4152422	-7.9657142	-5.4083016	5.4121010	-7.9287147
C	-7.1673970	5.9680436	-5.8948634	-6.0752891	6.8227970	-6.4962313	-6.0976138	6.8146751	-6.4463231
H	-8.2350156	5.8208430	-6.0876645	-7.1179278	6.7458314	-6.8212547	-7.1441783	6.7377772	-6.7585430
C	-6.7552887	6.8660966	-4.9107345	-5.7378422	7.6595922	-5.4327813	-5.7476173	7.6485708	-5.3846501
H	-7.5072556	7.4149972	-4.3360708	-6.5233241	8.2303096	-4.9285067	-6.5271478	8.2175948	-4.8693396
C	-5.3943830	7.0721045	-4.6394120	-4.4107953	7.7748572	-4.9926277	-4.4153894	7.7631464	-4.9602026
C	-3.8391881	4.5989619	-7.2012637	-2.6931095	5.3039595	-7.4523506	-2.7268698	5.2986747	-7.4464483
H	-2.8283726	4.9046307	-6.8882586	-1.7124098	5.5401352	-7.0098244	-1.7412823	5.5323045	-7.0135635
C	-3.9463456	4.8717059	-8.7138231	-2.6016439	5.6329558	-8.9547226	-2.6514194	5.6335857	-8.9484094
H	-4.9248987	4.5553566	-9.1195227	-3.5392463	5.3874557	-9.4865221	-3.5951105	5.3913223	-9.4708694
H	-3.1641164	4.3138604	-9.2607508	-1.7899680	5.0491942	-9.4265338	-1.8456287	5.0508457	-9.4314585
H	-3.8207139	5.9458931	-8.9418150	-2.3919385	6.7050973	-9.1228531	-2.4423214	6.7061610	-9.1145389
C	-3.9668935	3.0959324	-6.8881094	-2.9377211	3.8006530	-7.2153505	-2.9700545	3.7946123	-7.2128217
H	-4.9511160	2.6991077	-7.1980474	-3.8965545	3.4704949	-7.6563917	-3.9336591	3.4667234	-7.6450499
H	-3.8459487	2.9054397	-5.8069963	-2.9591300	3.5698739	-6.1354813	-2.9802351	3.5595194	-6.1337312
H	-3.1893482	2.5227634	-7.4256912	-2.1305192	3.2029757	-7.6775324	-2.1681898	3.1982228	-7.6858372
C	-4.9783040	8.0492078	-3.5426539	-4.0786247	8.6767150	-3.8061573	-4.0689505	8.6635551	-3.7766905
H	-3.8776064	8.0687186	-3.5054565	-2.9883590	8.6459854	-3.6515075	-2.9769240	8.6323598	-3.6351086
C	-5.4464399	9.4854553	-3.8470178	-4.4551320	10.1462183	-4.0757225	-4.4480950	10.1334913	-4.0403466
H	-5.0674209	9.8365583	-4.8241157	-3.9618711	10.5302410	-4.9872449	-3.9658980	10.5181311	-4.9575192
H	-5.0806041	10.1816467	-3.0699511	-4.1457698	10.7836344	-3.2270444	-4.1280507	10.7700404	-3.1949780
H	-6.5492361	9.5611170	-3.8688527	-5.5455591	10.2733965	-4.2060471	-5.5399928	10.2612270	-4.1571665
C	-5.4630989	7.5767188	-2.1582780	-4.7280913	8.1542671	-2.5095064	-4.7028859	8.1400932	-2.4727657
H	-6.5671635	7.5548227	-2.1001803	-5.8319188	8.1764810	-2.5719477	-5.8073822	8.1619151	-2.5221288
H	-5.0978438	8.2606304	-1.3697811	-4.4263250	8.7804271	-1.6494818	-4.3912614	8.7659815	-1.6160677
H	-5.0881344	6.5632836	-1.9306423	-4.4179937	7.1149263	-2.3012871	-4.3898544	7.1008270	-2.2685755
Au	-2.8355947	-4.3735824	2.9721373	-2.4939107	-4.4086945	3.1956905	-2.4889030	-4.4156249	3.1923572
Cu	-1.6780614	-1.4085053	1.7276657	-1.4863725	-1.4122583	1.8504494	-1.4900338	-1.4170625	1.8414304
S	-3.4984070	-2.6707629	1.4652329	-3.2749140	-2.7456488	1.7030266	-3.2757376	-2.7554436	1.6992282
S	-0.0205952	0.0083488	2.2573686	0.1133190	0.0950283	2.2988684	0.1069745	0.0903874	2.2969169
N	-1.0257845	-6.4085634	4.3849777	-0.6162086	-6.4615854	4.4954046	-0.6068191	-6.4658320	4.4907607
N	-3.0293237	-6.5419689	5.1771992	-2.5409172	-6.5077522	5.4705633	-2.5320627	-6.5170221	5.4645657
C	-2.2715895	-5.8700774	4.2618695	-1.8484621	-5.8806579	4.4751416	-1.8398919	-5.8867580	4.4708915
C	-1.0029707	-7.3950529	5.3601028	-0.5383782	-7.4325968	5.4834787	-0.5281270	-7.4388546	5.4768012
H	-0.0935825	-7.9393990	5.6033350	0.3703272	-8.0050792	5.6536727	0.3812961	-8.0103846	5.6462843
C	-2.2654588	-7.4821198	5.8604415	-1.7514372	-7.4645594	6.0989838	-1.7415533	-7.4739987	6.0913771

H	-2.6922936	-8.1175161	6.6328399	-2.1274014	-8.0702405	6.9201557	-2.1171445	-8.0820787	6.9109360
C	0.1161297	-6.0124947	3.5894431	0.4751094	-6.1029244	3.6163066	0.4843563	-6.1043199	3.6126581
C	0.8922520	-4.9144231	4.0188725	1.3076604	-5.0230624	3.9824652	1.3143461	-5.0227024	3.9795528
C	1.9602496	-4.5218078	3.1998353	2.3379954	-4.6752272	3.0978902	2.3452674	-4.6733283	3.0962510
H	2.5705105	-3.6547178	3.4653534	2.9859151	-3.8214047	3.3124636	2.9918519	-3.8187325	3.3117738
C	2.2452526	-5.1981394	2.0140681	2.5346272	-5.3798720	1.9110920	2.5445813	-5.3777958	1.9097821
H	3.0644893	-4.8398330	1.3836557	3.3284871	-5.0596686	1.2302832	3.3387404	-5.0564101	1.2298858
C	1.4756520	-6.2951731	1.6280414	1.7074904	-6.4539042	1.5841149	1.7196071	-6.4532263	1.5818365
H	1.7052537	-6.8102067	0.6909570	1.8657191	-6.9898009	0.6437542	1.8800712	-6.9892244	0.6418852
C	0.3900810	-6.7276014	2.4034480	0.6528226	-6.8381232	2.4247668	0.6645221	-6.8391367	2.4212005
C	0.6146969	-4.1651462	5.3198826	1.1256247	-4.2376742	5.2788350	1.1285379	-4.2363701	5.2748577
H	-0.3101105	-4.5742224	5.7592522	0.2398938	-4.6366091	5.8002641	0.2429666	-4.6368120	5.7954147
C	0.3744812	-2.6634413	5.0843326	0.8582598	-2.7454883	5.0115069	0.8579099	-2.7451138	5.0051607
H	0.1170840	-2.1614355	6.0360351	0.6940914	-2.2062809	5.9634780	0.6899083	-2.2053319	5.9561172
H	-0.4505327	-2.4943192	4.3713581	-0.0341149	-2.6020717	4.3784477	-0.0334621	-2.6049282	4.3699547
H	1.2636471	-2.1584311	4.6676454	1.7003714	-2.2588741	4.4887834	1.7001250	-2.2567962	4.4841442
C	1.7437429	-4.4016887	6.3429036	2.3293849	-4.4361199	6.2210624	2.3313995	-4.4305535	6.2191217
H	1.5109822	-3.8997945	7.3008223	2.1618270	-3.9089849	7.1789776	2.1613872	-3.9019850	7.1757960
H	2.7052055	-3.9981760	5.9772741	3.2577270	-4.0346944	5.7765521	3.2595491	-4.0279343	5.7752529
H	1.8874267	-5.4788897	6.5475053	2.4980009	-5.5059029	6.4447078	2.5019204	-5.4995668	6.4450204
C	-0.4421710	-7.9276662	1.9563804	-0.2544716	-8.0020493	2.0322042	-0.2414943	-8.0034204	2.0264983
H	-1.3070986	-8.0118435	2.6348030	-1.0726405	-8.0567348	2.7691787	-1.0598913	-8.0600310	2.7630622
C	-1.0075029	-7.7530880	0.5355083	-0.9082476	-7.7874327	0.6547376	-0.8951623	-7.7867830	0.6492207
H	-1.6855897	-8.5923504	0.2906147	-1.6388342	-8.5926169	0.4496659	-1.6249638	-8.5922412	0.4423628
H	-0.2095754	-7.7341144	-0.2276476	-0.1639826	-7.7953507	-0.1611894	-0.1506849	-7.7924084	-0.1665359
H	-1.5665901	-6.8074414	0.4365762	-1.4303357	-6.8170340	0.6021460	-1.4182100	-6.8167946	0.5982912
C	0.3599697	-9.2387041	2.0828947	0.4993329	-9.3457432	2.0924113	0.5131309	-9.3467342	2.0846639
H	0.7188236	-9.3988342	3.1163892	0.9230666	-9.5306583	3.0967911	0.9362344	-9.5333232	3.0890059
H	1.2450852	-9.2318565	1.4205195	1.3348004	-9.3697867	1.3687218	1.3491256	-9.3690430	1.3615348
H	-0.2651457	-10.1065281	1.8002149	-0.1799139	-10.1842182	1.8490176	-0.1654235	-10.1851669	1.8392336
C	-4.4346566	-6.3224972	5.4225069	-3.8978578	-6.2084926	5.8603930	-3.8895644	-6.2206163	5.8546497
C	-4.8107167	-5.4058107	6.4285590	-4.1100577	-5.2633060	6.8883603	-4.1029941	-5.2810457	6.8875267
C	-6.1820132	-5.2327806	6.6683320	-5.4357882	-5.0046796	7.2669241	-5.4290679	-5.0261052	7.2674150
H	-6.5090691	-4.5256758	7.4364801	-5.6375470	-4.2731507	8.0550686	-5.6317800	-4.2996762	8.0600330
C	-7.1367025	-5.9395257	5.9375119	-6.5023415	-5.6584875	6.6499916	-6.4948224	-5.6773621	6.6463902
H	-8.2019985	-5.7865839	6.1384800	-7.5296299	-5.4397272	6.9590270	-7.5224433	-5.4610542	6.9560976
C	-6.7370287	-6.8347296	4.9456269	-6.2633191	-6.5858261	5.6361865	-6.2546075	-6.5985265	5.6272345
H	-7.4963520	-7.3756859	4.3730697	-7.1095518	-7.0854682	5.1553307	-7.1002224	-7.0964763	5.1435308
C	-5.3793486	-7.0477938	4.6636575	-4.9579093	-6.8832098	5.2167083	-4.9487873	-6.8922884	5.2064020
C	-3.7907938	-4.5980169	7.2271743	-2.9642700	-4.5178995	7.5691593	-2.9580722	-4.5378715	7.5722631
H	-2.7842524	-4.9046302	6.9016581	-2.0178789	-4.8932711	7.1491763	-2.0113075	-4.9083118	7.1487603
C	-3.8842542	-4.8840837	8.7381391	-2.9224520	-4.7877449	9.0855768	-2.9142178	-4.8181710	9.0867517
H	-4.8584537	-4.5693816	9.1553335	-3.8252451	-4.4044412	9.5957420	-3.8176314	-4.4408593	9.6002724
H	-3.0957914	-4.3329119	9.2828988	-2.0470166	-4.2885274	9.5401444	-2.0397063	-4.3198865	9.5441190
H	-3.7589552	-5.9605918	8.9551499	-2.8485714	-5.8689275	9.3030268	-2.8373309	-5.9006477	9.2965830
C	-3.9161481	-3.0919402	6.9280130	-3.0176227	-3.0087102	7.2647460	-3.0147689	-3.0267601	7.2783492
H	-4.8958999	-2.6940400	7.2504233	-3.9306225	-2.5423460	7.6782251	-3.9283090	-2.5649966	7.6957469
H	-3.8047189	-2.8928469	5.8474027	-3.0031278	-2.8217901	6.1765200	-3.0015355	-2.8323472	6.1914320
H	-3.1314992	-2.5259025	7.4628760	-2.1453500	-2.4956011	7.7101082	-2.1431636	-2.5149595	7.7265188
C	-4.9766480	-8.0224646	3.5596977	-4.7311108	-7.8914183	4.0930221	-4.7206612	-7.8952166	4.0782063
H	-3.8764327	-8.0436366	3.5110403	-3.6449580	-7.9810824	3.9327345	-3.6344596	-7.9814518	3.9163863
C	-5.4440375	-9.4587134	3.8652456	-5.2505890	-9.2928558	4.4683281	-5.2361977	-9.2994503	4.4485765
H	-5.0544949	-9.8135811	4.8368208	-4.7864498	-9.6606966	5.4015763	-4.7697358	-9.6700413	5.3795774
H	-5.0884812	-10.1531980	3.0818837	-5.0188265	-10.0161374	3.6648793	-5.0039621	-10.0189167	3.6418502
H	-6.5466704	-9.5321575	3.8994653	-6.3464588	-9.2981533	4.6145709	-6.3318217	-9.3078568	4.5965391
C	-5.4746467	-7.5462407	2.1813583	-5.3391866	-7.3989935	2.7654584	-5.3313187	-7.3991556	2.7531946
H	-6.5791725	-7.5209595	2.1345650	-6.4387466	-7.3029273	2.8334339	-6.4310525	-7.3060628	2.8224819
H	-5.1197693	-8.2302190	1.3881306	-5.1133446	-8.1134136	1.9523557	-5.1044906	-8.1098623	1.9371021
H	-5.0988851	-6.5336417	1.9513495	-4.9253158	-6.4154294	2.4806562	-4.9200795	-6.4135372	2.4717293
Au	-2.3822911	4.6756859	3.0062790	-3.0719523	4.3181727	3.1986842	-3.0628159	4.2962769	3.2025723
Cu	-0.4108097	2.1568996	1.7434774	-0.7339336	2.0117850	1.2322829	-0.7367246	1.9992545	1.2036641
S	-0.5879070	4.3675884	1.4917832	-1.0941774	4.2390284	1.9300407	-1.0881195	4.2297116	1.9276719
N	-4.9900262	4.0947197	4.5064242	-5.8444009	3.5433843	4.2442534	-5.8331661	3.5264320	4.2613386
N	-4.1629867	5.9653463	5.1965656	-5.1586715	5.3259165	5.2503361	-5.1397931	5.3107179	5.2590067
C	-3.9414950	4.9445662	4.3174299	-4.7983524	4.4132242	4.3023005	-4.7845434	4.3937163	4.3130739
C	-5.8481527	4.5710633	5.4867504	-6.8408924	3.9020672	5.1405351	-6.8261475	3.8911295	5.1591767
H	-6.7431234	4.0267867	5.7787060	-7.7568647	3.3245732	5.2407791	-7.7433705	3.3164766	5.2641189
C	-5.3297360	5.7512347	5.9227153	-6.4112011	5.0268518	5.7752412	-6.3915781	5.0169038	5.7886685
H	-5.6753832	6.4561278	6.6751456	-6.8722843	5.6399978	6.5459542	-6.8488376	5.6340403	6.5584625
C	-5.1873088	2.8659988	3.7682343	-5.9036566	2.3970883	3.3636720	-5.8984535	2.3763923	3.3862807
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C	-4.7292104	0.5263756	3.4679083	-5.3789261	0.0946621	2.9151010	-5.3817875	0.0703830	2.9470398
H	-4.2338242	-0.4029963	3.7609342	-4.9192239	-0.8590418	3.1864671	-4.9236376	-0.8831791	3.2214559
C	-5.4990512	0.5329201	2.3047165	-5.9619945	0.2174214	1.6548709	-5.9702462	0.1882578	1.6888734
H	-5.5793462	-0.3867668	1.7178320	-5.9448664	-0.6415206	0.9781870	-5.9577728	-0.6739403	1.0162080

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H	-6.7175774	1.6989787	0.9650471	-6.9659438	1.5148512	0.2563501	-6.9781212	1.4808941	0.2887353
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C	-3.7221301	1.6510892	5.5081066	-4.6740429	1.0135553	5.1655783	-4.6649676	0.9990162	5.1899496
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H	-1.7015611	1.1786105	6.1890018	-2.7141712	0.5755640	6.0305784	-2.7019585	0.5628019	6.0487980
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H	-5.4436688	1.2662966	6.8277655	-6.4956859	0.2765532	6.1584598	-6.4831151	0.2687779	6.1941730
C	-6.6737468	4.1750357	2.1174783	-7.0959089	3.8748106	1.6158906	-7.0973681	3.8478823	1.6379187
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C	-6.3077568	4.5226735	0.6632700	-6.4203929	4.3729603	0.3240860	-6.4387795	4.3333839	0.3326724
H	-6.7407704	5.5024399	0.3860295	-6.8007621	5.3767684	0.0562932	-6.8174267	5.3376161	0.0641184
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H	-5.2149762	4.5673391	0.5202381	-5.3244926	4.4353509	0.4371864	-5.3408968	4.3902354	0.4283530
C	-8.2019482	4.0846251	2.3040069	-8.6257125	3.7812791	1.4494023	-8.6298404	3.7589094	1.4942054
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H	-8.6315017	3.2668727	1.6965305	-8.9019560	3.0447725	0.6726069	-8.9196965	3.0159430	0.7285576
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H	-5.2779184	10.4110379	3.7817951	-6.0812848	9.9282687	4.1954899	-6.0565849	9.9104281	4.1857955
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Au	5.1907537	-0.2652492	2.9898946	5.1999553	-0.1015427	2.9122142	5.1967529	-0.0811897	2.9257223
Cu	2.0352972	-0.7238855	1.7364882	2.1139048	-0.6803596	1.6966002	2.1130668	-0.6753352	1.6976374
S	4.0363863	-1.6770377	1.4783933	4.1162591	-1.6466942	1.4776795	4.1206523	-1.6346505	1.4939479
N	6.0289125	2.2992629	4.4492016	5.8275137	2.4783627	4.4802399	5.8227446	2.5134700	4.4703672
N	7.2004052	0.6361722	5.1716607	7.2675531	0.9417326	4.9537309	7.2481608	0.9739133	4.9771677
C	6.2113683	0.9582658	4.2873706	6.1641932	1.1897342	4.1881721	6.1539603	1.2193286	4.1977004
C	6.8836835	2.8055798	5.4176463	6.6993423	3.0220916	5.4133042	6.6888729	3.0634617	5.4049744
H	6.8838203	3.8587752	5.6881783	6.5884974	4.0416528	5.7743728	6.5807568	4.0880261	5.7524002
C	7.6245348	1.7592893	5.8736127	7.6092124	2.0559821	5.7117595	7.5894998	2.0954300	5.7244911
H	8.4074107	1.7042247	6.6263251	8.4616653	2.0522525	6.3868762	8.4351496	2.0947497	6.4080880
C	5.0760502	3.0911457	3.7015125	4.7255948	3.2037900	3.8860222	4.7298316	3.2369893	3.8575477
C	3.7429555	3.1589089	4.1618739	3.4396911	3.0746770	4.4549932	3.4391536	3.1240943	4.4188462
C	2.8337068	3.8984201	3.3925831	2.3910002	3.7743717	3.8409952	2.3986170	3.8185404	3.7851807
H	1.7813097	3.9525227	3.6830711	1.3700186	3.6770140	4.2189461	1.3737902	3.7317003	4.1554719
C	3.2363412	4.5472137	2.2254542	2.6167866	4.5827240	2.7272654	2.6371697	4.6073524	2.6603109
H	2.4888893	5.0843321	1.6340508	1.7683617	5.0917064	2.2601312	1.7946532	5.1118748	2.1778913
C	4.5651423	4.4797683	1.8076923	3.9035742	4.7095457	2.2041336	3.9287819	4.7200515	2.1456675
H	4.8650940	4.9852241	0.8853506	4.0669431	5.3455747	1.3297389	4.1022265	5.3412441	1.2626124
C	5.5167997	3.7462887	2.5311745	4.9873372	4.0152393	2.7602396	5.0046176	4.0294604	2.7213232
C	3.2778380	2.4761664	5.4460855	3.1721123	2.2344391	5.7014537	3.1548235	2.3024330	5.6739454
H	4.1071720	1.8542963	5.8211809	4.0820975	1.6520181	5.9200726	4.0712574	1.7464530	5.9313792
C	2.0844966	1.5344052	5.2075266	2.0307823	1.2233368	5.4965781	2.0442668	1.2608974	5.4517572
H	1.8275183	0.9983208	6.1404888	1.9466174	0.5611135	6.3786831	1.9399812	0.6180401	6.3460360

H	2.3107272	0.7844916	4.4305963	2.1993561	0.5950093	4.6059715	2.2613602	0.6155833	4.5840834
H	1.1830342	2.0780703	4.8743842	1.0548571	1.7213774	5.3584977	1.0645328	1.7335418	5.2620386
C	2.9631692	3.5170533	6.5393438	2.9056567	3.1375762	6.9234620	2.8298306	3.2200851	6.8704641
H	2.6724778	3.0151726	7.4813977	2.7570692	2.5261220	7.8333529	2.6716177	2.6208747	7.7868328
H	2.1279313	4.1740660	6.2360542	1.9965281	3.7491343	6.7753230	1.9093870	3.8044214	6.6867755
H	3.8370095	4.1606268	6.7513234	3.7476383	3.8293741	7.1110918	3.6479716	3.9371462	7.0685536
C	6.9646695	3.6807792	2.0490442	6.3843011	4.1600981	2.1588546	6.4072503	4.1581068	2.1294327
H	7.4907062	2.9289819	2.6603808	7.0211652	3.3725005	2.5943767	7.0357078	3.3725391	2.5806288
C	7.0779643	3.2205779	0.5845730	6.4008998	3.9507504	0.6335387	6.4350186	3.9281283	0.6073020
H	8.1409380	3.0785121	0.3126551	7.4439571	3.9293133	0.2662382	7.4808701	3.8945614	0.2489969
H	6.6521787	3.9607500	-0.1159493	5.8859972	4.7704851	0.1002572	5.9300560	4.7439031	0.0586748
H	6.5410047	2.2721243	0.4147907	5.9116711	3.0055294	0.3410556	5.9412118	2.9825931	0.3237383
C	7.6839474	5.0274425	2.2682913	7.0125058	5.5175545	2.5364792	7.0409870	5.5165382	2.4941757
H	7.6613418	5.3345013	3.3301861	7.0680100	5.6531805	3.6320666	7.0893601	5.6659458	3.5883065
H	7.2097139	5.8334586	1.6785254	6.4198327	6.3563747	2.1268346	6.4564338	6.3535650	2.0694612
H	8.7429155	4.9592335	1.9556581	8.0384298	5.5992024	2.1309894	8.0703305	5.5868031	2.0952173
C	7.7421193	-0.6857245	5.3781922	7.9989290	-0.3020676	4.9916934	7.9695276	-0.2746394	5.0402483
C	7.1770712	-1.4976569	6.3861148	7.6610207	-1.2553528	5.9771062	7.6141477	-1.2105835	6.0361362
C	7.7380277	-2.7678139	6.5859060	8.4045076	-2.4443981	6.0107639	8.3493347	-2.4037242	6.0963805
H	7.3201933	-3.4263485	7.3532497	8.1649988	-3.2080745	6.7567315	8.0968063	-3.1541211	6.8514971
C	8.8139223	-3.2100088	5.8165047	9.4382830	-2.6741621	5.1032110	9.3911891	-2.6542887	5.2036832
H	9.2340880	-4.2066144	5.9864582	10.0034514	-3.6109496	5.1445991	9.9496020	-3.5939844	5.2655732
C	9.3511333	-2.3878143	4.8264678	9.7493025	-1.7157086	4.1390766	9.7187112	-1.7131836	4.2280020
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C	8.8299104	-1.1082131	4.5830204	9.0395082	-0.5081939	4.0595462	9.0182362	-0.5022261	4.1223428
C	5.9849145	-1.0511504	7.2288320	6.5187578	-1.0435306	6.9676216	6.4624503	-0.9760291	7.0105209
H	5.7299462	-0.0199789	6.9375694	6.0973507	-0.0413028	6.7911426	6.0485503	0.0252921	6.8125462
C	6.3182007	-1.0259427	8.7328443	7.0073362	-1.0770039	8.4283870	6.9350127	-0.9872749	8.4768983
H	6.5500383	-2.0355057	9.1190890	7.4135859	-2.0678375	8.7029022	7.3337460	-1.9751903	8.7722011
H	5.4581206	-0.6393543	9.3099256	6.1712750	-0.8583772	9.1179260	6.0925714	-0.7534942	9.1535871
H	7.1885585	-0.3783092	8.9442863	7.8006718	-0.3285113	8.6075125	7.7297754	-0.2393860	8.6522108
C	4.7431878	-1.9155046	6.9390477	5.3801389	-2.0530034	6.7280860	5.3207499	-1.9831069	6.7756024
H	4.9058146	-2.9701860	7.2278072	5.7127023	-3.0919222	6.9082024	5.6451287	-3.0206379	6.9772604
H	4.4858490	-1.8906234	5.8653674	5.0070885	-1.9883870	5.6907024	4.9594768	-1.9342698	5.7332039
H	3.8720357	-1.5420410	7.5082063	4.5338261	-1.8487431	7.4094510	4.4680991	-1.7622406	7.4437894
C	9.4329451	-0.2398174	3.4816970	9.3977390	0.5142352	2.9838894	9.3947232	0.5010908	3.0349477
H	8.8867092	0.7166304	3.4664875	8.7355925	1.3854366	3.1100721	8.7367888	1.3781831	3.1405357
C	10.9130968	0.0884067	3.7578250	10.8450843	1.0210844	3.1357145	10.8434906	1.0014023	3.1947047
H	11.0424654	0.5834399	4.7375476	11.0202085	1.4534419	4.1377605	11.0103671	1.4484040	4.1917258
H	11.3079022	0.7666729	2.9790644	11.0581768	1.8042636	2.3850258	11.0696580	1.7714365	2.4343083
H	11.5416350	-0.8211660	3.7565793	11.5812440	0.2095944	2.9876970	11.5761331	0.1832208	3.0675228
C	9.2452203	-0.8830538	2.0942262	9.1378749	-0.0417918	1.5705292	9.1463678	-0.0750817	1.6275345
H	9.7876346	-1.8434174	2.0146079	9.7857647	-0.9105808	1.3501351	9.7902048	-0.9518597	1.4278611
H	9.6316259	-0.2118372	1.3049286	9.3436832	0.7335096	0.8096562	9.3662774	0.6867668	0.8570347
H	8.1778429	-1.0747824	1.8861035	8.0869344	-0.3608226	1.4554198	8.0943831	-0.3882329	1.5058288

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