

Supporting Information

Modulation of Metallophilic Bonds: Solvent-Induced Isomerization and Luminescence Vapochromism of a Polymorphic Au-Cu Cluster

Igor O. Koshevoy,^{*a} Yuh-Chia Chang,^b Antti J. Karttunen,^a Matti Haukka,^a Tapani Pakkanen,^a Pi-Tai Chou^{*b}

^a Department of Chemistry, University of Eastern Finland, Joensuu, 80101, Finland;

^b National Taiwan University, [#] Department of Chemistry, Taipei 106, Taiwan

E-mail: igor.koshevoy@uef.fi, chop@ntu.edu.tw

Experimental

General comments

Au(tht)Cl (tht = tetrahydrothiophene)¹ was obtained according to the literature method. Other reagents and solvents were used as received. The solution ¹H NMR spectra were recorded on Bruker Avance 400 spectrometer. Mass spectra were measured on a Bruker APEX-Qe ESI FT-ICR instrument in the negative mode. Microanalyses were carried out in the analytical laboratory of the University of Eastern Finland.

{AuCu(C₂C₅H₉O)₂}_n (1)

Au(tht)Cl (100 mg, 0.312 mmol) was dissolved in CH₂Cl₂ (10 cm³) and a solution of HC₂OHC₅H₈ (70 mg, 0.64 mmol) in CH₂Cl₂ (5 cm³) was added, followed by neat NEt₃ (70 mg, 0.69 mmol) and a solution of Cu(NCMe)₄PF₆ (117 mg, 0.314 mmol) in CH₂Cl₂ (5 cm³). The reaction mixture was stirred for 1 h in the absence of light resulting in formation of a pale yellowish suspension. It was evaporated and methanol (3 cm³) was added causing fast precipitation of white microcrystalline solid as very thin needles. The solid was collected by centrifugation, washed with methanol (2×3 cm³), pentane (3×4 cm³) and vacuum dried to give form **a** (139 mg, 93 %). Recrystallization from EtOH gave yellow block crystals (form **b**). Recrystallization from toluene gave nearly colorless small block crystals (form **c**). Recrystallization from ethyl acetate or diethyl ether gave bright orange needles (form **d**). ¹H NMR (CD₂Cl₂, 298 K; δ): 4.95 (s, OH, 1H), 2.10 (m, 2H), 2.04 (m, 2H), 1.79 (m, 4H); (ethanol-d₆, 298 K; δ): 2.05 (m, 4H), 1.79 (m, 4H). Anal. Calc. for AuC₁₄CuH₁₈O₂: C, 35.12; H, 3.79. Found: C, 35.00; H, 3.80.

Photophysical measurements.

Steady-state emission measurements in the solid state were measured by an Edinburgh (FS920) fluorometer. Both the wavelength-dependent excitation and emission response of the fluorometer

have been calibrated. Solid state quantum yields were determined with a calibrated integrating sphere system. The uncertainty of the quantum yield measurement was in the range of <2% (an average of four replica). Lifetime studies were performed with an Edinburgh FL 900 photon-counting system using a hydrogen-filled lamp as the excitation source. The emission decays were fitted by the sum of exponential functions with a temporal resolution of ~300 ps by the deconvolution of instrument response function.

Computational details. The Au-Cu alkynyl clusters **1b-d** were studied using the hybrid PBE0 density functional.² The gold and copper atoms were described by a triple-valence-zeta quality basis set with polarization functions (def2-TZVP).³ Scalar relativistic effects were taken into account by applying a 60-electron relativistic effective core potential for Au.⁴ A split-valence basis set with polarization functions on non-hydrogen atoms was used for all the other atoms.⁵ The multipole-accelerated resolution-of-the-identity technique was used to speed up the calculations.⁶ The geometries of the complexes were taken from the solid state X-ray structures. In the clusters **1b** and **1c**, the positions of the C, O, and H atoms were allowed to relax. In the case of the polymeric form **1d**, which shows independent disorder of the two different {Au₄Cu₄} blocks **A** and **B** (see Figure 2 in the main text), we applied a finite structural model consisting of two {Au₄Cu₄} blocks and investigated all four possible structural conformations. The excited state characteristics were found to be practically identical for all conformations and only the energetically most favorable conformation is discussed here. The excited states were investigated with the Time-Dependent DFT approach.⁷ All electronic structure calculations were carried out with the TURBOMOLE program package (version 6.3).⁸

X-ray structures determination. The crystals of **1b-1d** were immersed in cryo-oil, mounted in a Nylon loop, and measured at a temperature of 100 K. The X-ray diffraction data were collected on a Bruker Kappa Apex II Duo diffractometer using MoK α radiation ($\lambda = 0.71073$ Å). The APEX2⁹ program package was used for cell refinements and data reductions. The structures were solved by direct methods using the SHELXS-97¹⁰ programs with the WinGX¹¹ graphical user interface. A semi-empirical absorption correction (SADABS)¹² was applied to all data. Structural refinements were carried out using SHELXL-97.¹⁰ One ethanol crystallization molecule in **1b** was disordered over two sites with occupancies of 0.60 and 0.40. Both geometric and displacement constraints and restraints were applied to the disordered moieties. Also, all their atoms were restrained so that their U_{ij} components approximate to isotropic behavior. The same restraints were applied to the carbon atoms C42, C45 and C46 due to disorder of the cyclopentyl ring (C42-C46). The carbon atoms C11 and C12 were constrained to have equal anisotropic displacement parameters. In **1c** the displacement constraints were applied to the selected carbon atoms of the cyclopentyl rings C17-C21, C22-C26, C27-C31, C32-C36, C37-C41, C73-C77,

C78-C82, C83-C87, C93-C97, C103-C107. These constraints were also applied to the carbon atoms of alkynyl triple bonds (C1, C2, C9, C10, C13, C14, C57, C58, C63-C68). Additionally, the U_{ij} components of the carbon atoms C2, C24, C25, C37, C40, C54, C59, C82, C92 and of some atoms of crystallization toluene molecules (C118, C120, C121, C127-C129) were restrained to approximate to isotropic behavior. The metal atoms of both Au_2Cu_2 units were disordered over two sites with occupancies 0.86/0.14 and 0.43/0.57, respectively. Due to disorder of the cyclopentyl rings (C17-CC21, C27-C31, C42-C46, C47-C51) both geometric and displacement constraints and restraints were applied to most of these carbon atoms, which were also restrained so that their U_{ij} components approximate to isotropic behavior. The positions of the OH hydrogens for oxygen atoms O1-O8 in **1b** and for oxygen atoms O1-O16 in **1c** were estimated with *HYDROGEN*¹³ program and constrained to ride on their parent atom with $U_{iso} = 1.5$ (parent atom). All other hydrogen atoms were positioned geometrically and constrained to ride on their parent atoms, with O-H = 0.84 Å, C-H = 0.95-0.99 Å.

References

1. Uson, R.; Laguna, A.; Laguna, M. *Inorg. Synth.* **1989**, 26, 85-91.
2. (a) Perdew, J. P.; Burke, K.; Ernzerhof, M. *Phys. Rev. Lett.* **1996**, 77, 3865-3868; (b) Adamo, C.; Barone, V. *J. Chem. Phys.* **1999**, 110, 6158-6170.
3. Weigend, F.; Ahlrichs, R. *Phys. Chem. Chem. Phys.* **2005**, 7, 3297-3305.
4. Andrae, D.; Häußermann, U.; Dolg, M.; Stoll, H.; Preuß, H. *Theor. Chem. Acc.* **1990**, 77, 123-141.
5. Schäfer, A.; Horn, H.; Ahlrichs, R. *J. Chem. Phys.* **1992**, 97, 2571-2577.
6. (a) Eichkorn, K.; Treutler, O.; Öhm, H.; Häser, M.; Ahlrichs, R. *Chem. Phys. Lett.* **1995**, 240, 283-290; (b) Sierka, M.; Hogeamp, A.; Ahlrichs, R. *J. Chem. Phys.* **2003**, 118, 9136-9148; (c) Eichkorn, K.; Weigend, F.; Treutler, O.; Ahlrichs, R. *Theor. Chem. Acc.* **1997**, 97, 119-124; (d) Weigend, F. *Phys. Chem. Chem. Phys.* **2006**, 8, 1057-1065.
7. (a) Furche, F.; Rappoport, D., Density Functional Methods for Excited States: Equilibrium Structure and Electronic Spectra. In *Computational Photochemistry*, Olivucci, M., Ed. Elsevier: Amsterdam, 2005; pp 93-128; (b) Furche, F.; Ahlrichs, R. *J. Chem. Phys.* **2002**, 117, 7433-7447; (c) van Wüllen, C. *J. Comput. Chem.* **2011**, 32, 1195-1201.
8. Ahlrichs, R.; Bär, M.; Häser, M.; Horn, H.; Kölmel, C. *Chem. Phys. Lett.* **1989**, 162, 165-169.
9. *APEX2 - Software Suite for Crystallographic Programs*, Bruker AXS, Inc.: Madison, WI, USA, 2009.
10. Sheldrick, G. M. *Acta Crystallogr., Sect. A* **2008**, A64, 112-122.
11. Farrugia, L. J. *J. Appl. Cryst.* **1999**, 32, 837-838.
12. Sheldrick, G. M. *SADABS-2008/1 - Bruker AXS area detector scaling and absorption correction*, Bruker AXS: Madison, Wisconsin, USA, 2008.
13. Nardelli, M. *J. Appl. Cryst.* **1999**, 32, 563-571.

Table S1. Crystal data and structure refinement for **1b–1d**.

Identification code	1b		1c		1d	
Empirical formula	$\text{C}_{60}\text{H}_{84}\text{Au}_4\text{Cu}_4\text{O}_{10}$		$\text{C}_{133}\text{H}_{168}\text{Au}_8\text{Cu}_8\text{O}_{16}$		$\text{C}_{56}\text{H}_{72}\text{Au}_4\text{Cu}_4\text{O}_8$	
Formula weight	2007.30		4106.73		1915.16	
Temperature	100(2) K		100(2) K		100(2) K	
Wavelength	0.71073 Å		0.71073 Å		0.71073 Å	
Crystal system	Triclinic		Triclinic		Triclinic	
Space group	$P \bar{1}$		$P \bar{1}$		$P \bar{1}$	
Unit cell dimensions	$a = 10.5462(7)$ Å	$\alpha = 82.413(2)^\circ$	$a = 15.3186(12)$ Å	$\alpha = 98.870(4)^\circ$	$a = 14.2646(13)$ Å	$\alpha = 113.804(2)^\circ$
	$b = 10.8009(7)$ Å	$\beta = 83.268(3)^\circ$	$b = 20.9450(17)$ Å	$\beta = 110.220(4)^\circ$	$b = 14.3128(7)$ Å	$\beta = 103.210(3)^\circ$
	$c = 27.5951(17)$ Å	$\gamma = 89.393(3)^\circ$	$c = 21.9478(16)$ Å	$\gamma = 90.562(4)^\circ$	$c = 16.4962(8)$ Å	$\gamma = 103.317(3)^\circ$
Volume	3094.3(3) Å ³		6513.8(9) Å ³		2796.3(3) Å ³	
Z	2		2		2	
Density (calculated)	2.154 Mg/m ³		2.094 Mg/m ³		2.275 Mg/m ³	
Absorption coefficient	10.845 mm ⁻¹		10.304 mm ⁻¹		11.992 mm ⁻¹	
F(000)	1912		3916		1808	
Crystal size	0.69 x 0.27 x 0.09 mm ³		0.25 x 0.24 x 0.13 mm ³		0.30 x 0.07 x 0.05 mm ³	
θ range for data collection	1.94 to 25.50°		1.52 to 25.05°		1.71 to 25.53°	
Index ranges	-11 ≤ h ≤ 12, -10 ≤ k ≤ 13, -33 ≤ l ≤ 33		-18 ≤ h ≤ 18, -24 ≤ k ≤ 24, -26 ≤ l ≤ 26		-17 ≤ h ≤ 15, -17 ≤ k ≤ 17, -19 ≤ l ≤ 19	
Reflections collected	39821		97658		27281	
Independent reflections	11427 [R(int) = 0.0367]		22798 [R(int) = 0.0632]		10031 [R(int) = 0.0368]	
Completeness to θ	$\theta = 25.50^\circ$, 99.2 %		$\theta = 25.05^\circ$, 98.9 %		$\theta = 25.53^\circ$, 96.0 %	
Absorption correction	Numerical		Multi-scan		Numerical	
Max. and min. transmission	0.4419 and 0.0499		0.3477 and 0.1827		0.5854 and 0.1234	
Refinement method	Full-matrix least-squares on F ²		Full-matrix least-squares on F ²		Full-matrix least-squares on F ²	
Data / restraints / parameters	11427 / 59 / 707		22798 / 100 / 1252		10031 / 126 / 641	
Goodness-of-fit on F ²	1.056		1.154		1.042	
Final R indices [I > 2σ(I)]	R1 = 0.0672, wR2 = 0.1660		R1 = 0.0852, wR2 = 0.1901		R1 = 0.0568, wR2 = 0.1067	
R indices (all data)	R1 = 0.0815, wR2 = 0.1766		R1 = 0.1084, wR2 = 0.2010		R1 = 0.0917, wR2 = 0.1243	
Largest diff. peak and hole	9.125 and -3.705 e.Å ⁻³		8.714 and -6.138 e.Å ⁻³		2.900 and -2.320 e.Å ⁻³	

Table S2. Selected bond lengths (Å) for **1b–1d**.

1b	1c		1d
	<i>molecule 1</i>	<i>molecule 2</i>	
Au(2)-Au(4) 3.1943(8)	Au(1)-Cu(1) 2.993(3)	Au(5)-Cu(5) 2.962(3)	Cu(1)-Au(1) 2.938(2)
Au(2)-Cu(3) 2.899(2)	Au(1)-Cu(2) 2.966(3)	Au(5)-Cu(8) 2.978(3)	Cu(1)-Au(2) 3.0235(19)
Au(2)-Cu(2) 2.905(2)	Au(2)-Cu(1) 2.942(3)	Au(5)-Cu(6) 2.991(3)	Cu(2)-Au(2) 2.9373(19)
Au(4)-Cu(1) 2.9444(17)	Au(2)-Cu(2) 3.042(3)	Au(5)-Au(8) 3.2870(12)	Cu(2)-Au(1) 3.017(2)
Au(4)-Cu(4) 2.9553(18)	Au(2)-Au(3) 3.3194(12)	Au(6)-Cu(6) 2.975(3)	Au(2)-Au(1') 3.264(2)
	Au(3)-Cu(4) 2.969(3)	Au(6)-Cu(5) 2.990(3)	Au(2)-Au(3) 3.0244(21)
	Au(3)-Cu(1) 2.973(3)	Au(7)-Cu(7) 2.961(3)	Cu(3)-Au(3) 2.900(4)
	Au(3)-Cu(3) 2.998(3)	Au(7)-Cu(8) 2.975(3)	Cu(3)-Au(4') 3.047(6)
	Au(4)-Cu(3) 2.987(3)	Au(8)-Cu(8) 2.948(3)	Au(3)-Au(4) 3.143(6)
	Au(4)-Cu(4) 2.993(3)	Au(8)-Cu(7) 3.027(3)	Cu(4)-Au(4) 2.720(8)
			Cu(4)-Au(3) 2.764(4)
			Au(3)-Au(3') 3.297(3)

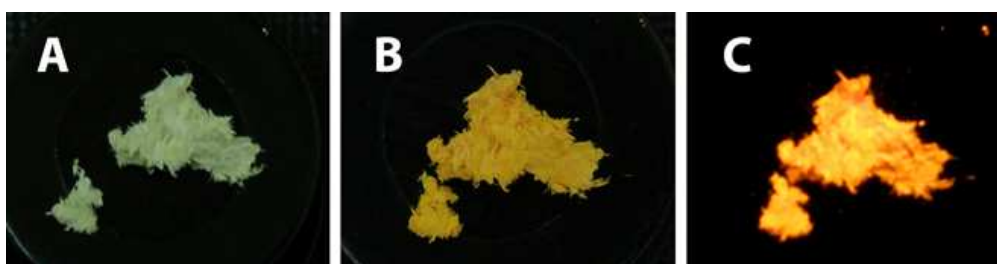


Figure S1. Form **1a** under ambient light (A); **1a** after being treated with Et₂O vapors for 30 min. (B) under ambient light and under UV excitation (C, max λ_{exc} = 365 nm). The same effect is achieved by vapors of ethyl acetate. Vapors were generated by natural evaporation of the solvents at room temperature in a closed vessel.



Figure S2. Form **1c** before (A) and after (B) being heated at 115 °C for 2 min. (under ambient light).

Cartesian coordinates of the structures used in the computational studies (PBE0-DFT, atomic units)

1b

0.31438236853521	0.73348812284480	7.38151373679926	c
2.21378148048029	1.23478706971995	8.67450838868990	c
-6.25808729207857	-0.70059114478573	4.04682930163012	c
-8.38224877090868	-1.33158829071011	3.25747411517232	c
3.55103425536416	3.71845408533821	1.38016288952836	c
5.72212504971816	3.69019534136509	2.27297324419685	c
-3.03719422633602	-2.72000208593746	-2.26242423041825	c
-4.97150318342048	-3.21142635195509	-3.49666842543251	c
3.90945082560586	1.74322680461688	10.82023348567275	c
3.96970191199905	4.57399474047274	11.48041307633865	c
4.25073413239396	5.77237831823436	9.80163798033138	h
5.59759787421076	4.88223589552072	12.75949602520091	h
1.47225506933529	5.03876992826274	12.86941627773869	c
1.66196919969767	6.54391052126080	14.29613435058797	h
0.01294512137664	5.66588493240069	11.52303139962526	h
0.72033830869878	2.45803174362985	14.04883564635629	c
0.54474806795935	2.55137932034935	16.12207165859346	h
-1.12810106959125	1.83909428564033	13.31689365250577	h
2.78797635814929	0.59522724121015	13.24956693468561	c
2.12112795779066	-1.35555929368650	12.96508995231618	h
4.32601795584304	0.54012172624021	14.66784138135706	h
-11.08299240239034	-2.01471602791739	2.91623395530556	c
-12.71978841629397	-0.37460344780719	4.69288558140459	c
-12.23459671189004	1.64960387312429	4.59131934538357	h
-14.68069706794164	-0.60028832514699	4.01436392651101	h
-12.37090375842640	-1.53346371387358	7.32123626010021	c
-10.82238680541229	-0.57655042640755	8.33577059429060	h
-14.08095559016904	-1.30872945438193	8.49083107099687	h
-11.69252018061604	-4.34947509573759	6.85493383213087	c
-13.07637616810958	-5.64911457709453	7.71395877968556	h
-9.84493356753947	-4.79910959983007	7.70662195574249	h
-11.59318463266170	-4.67187135085465	3.97913523672888	c
-13.44730933831800	-5.23800938559871	3.20628615312655	h
-10.18530745079701	-6.06169368004872	3.32964906734953	h
8.45723348975113	3.84872392140776	2.80714206891884	c
9.84334471319558	5.54599873871509	0.90460099085727	c
8.75566499466369	7.30765874608656	0.67073621891192	h
9.97056538016772	4.62494406206120	-0.95930070870621	h
12.40820994179423	6.04027719610316	2.16682674956405	c
13.80388312547566	4.63300406006090	1.53180220781905	h
13.15589479251695	7.91510264400532	1.64998649972170	h
11.93938343452463	5.77988826612876	5.04601145411531	c
12.42429261886510	7.51527459992861	6.09212527466512	h
13.11332769480952	4.25117929704317	5.83199131926836	h
9.12434360817773	5.13117326599301	5.32729336370091	c
8.69578900193796	3.89809866497831	6.95262440395545	h
7.96443902152727	6.85405987021377	5.52474008288724	h
-6.96445714554364	-3.93892475649749	-5.29989220898874	c
-5.94551778170694	-5.51980609015541	-7.51648739236911	c
-4.82406938462281	-4.36445245208988	-8.84070386107659	h
-4.67476860608098	-6.98023636619279	-6.74566907418478	h
-8.32796546428718	-6.70118552356064	-8.68211639792057	c
-9.01703583074553	-5.53667623142934	-10.26605774983251	h
-7.91974704407406	-8.58904403882491	-9.46363710128772	h
-10.30965844755185	-6.78344052104076	-6.52783963122688	c
-11.01483298388611	-8.71078539760881	-6.17096796536164	h
-11.96158200298571	-5.61599901911372	-7.01632421418978	h
-8.98153839493614	-5.69748895075413	-4.18994555614386	c
-8.00835184755251	-7.19457454515047	-3.11202052940421	h
-10.24260854476897	-4.68626017688099	-2.87387526672161	h
-2.83149118230621	0.04297520685102	5.44239935743601	au
0.03182109835166	3.64800461672128	-0.00019917713441	au
-0.02071328814256	-2.38399949869617	-0.00019917713441	au
2.60335966409199	1.99449481736418	4.65665160932739	cu
-5.41739166665647	-1.61393628851789	0.48186977039211	cu
6.33008216958731	0.74685616063534	10.20964764439269	o
9.62378073526919	1.44790821357563	2.67369496339797	o
-8.24547989639716	-1.76321961486174	-6.24331601401652	o
-11.83330293968043	-1.91404436150702	0.38411762643158	o
-0.30157120863305	0.77193086740076	-7.39912456101070	c
-2.19918338853820	1.28584028630513	-8.68920390800219	c
6.25157127541095	-0.67936066542018	-4.03592151006212	c

8.37317167052844	-1.32179445521974	-3.24983441714475	c
-3.48986671301603	3.74238035492799	-1.37172301394961	c
-5.66624658180036	3.72116788188241	-2.25173213240754	c
3.00286020774856	-2.73983102496682	2.24956894746701	c
4.94285347512123	-3.23995674197495	3.47202127784943	c
-3.89918145194594	1.81976180348544	-10.82496961554939	c
-3.95593284814675	4.65776996085210	-11.45410970084573	c
-4.22966811744500	5.83826254450700	-9.76150335550864	h
-5.58709287201848	4.98292998813694	-12.72483847310311	h
-1.46198300820006	5.13320188129860	-12.84560166025518	c
-1.65302512646403	6.65461479150157	-14.25476579908448	h
0.00261334424285	5.74236934947200	-11.49672145908715	h
-0.71878894560526	2.56437175439778	-14.05601492448809	c
-0.55101272816765	2.68028552085778	-16.12876603045463	h
1.13155462274126	1.93466433168788	-13.33823044259438	h
-2.78654165415627	0.69603034949756	-13.26969011598978	c
-2.12150748617769	-1.25850195714829	-13.00781205951359	h
-4.32907440946621	0.65773378477923	-14.68353051357592	h
11.07186002717794	-2.01839712376717	-2.91905698595079	c
12.71201190385060	-0.36293045458741	-4.67867557179951	c
12.23435769173023	1.66169944580507	-4.55248330409227	h
14.67300302959911	-0.60367991552172	-4.00552827975706	h
12.35581192196488	-1.48895333743873	-7.32035906854187	c
10.81086056973974	-0.51328665413586	-8.32236668269760	h
14.06605864346287	-1.25786561853094	-8.48846457153603	h
11.66551743446261	-4.30729516489730	-6.88693218963127	c
13.04141693972857	-5.60275285253269	-7.76485510449495	h
9.81393359470841	-4.73786266393226	-7.73982461499964	h
11.57069962211903	-4.66426718543876	-4.01509763366661	c
13.42438407475456	-5.24607240304589	-3.25283288790289	h
10.15920659533120	-6.05697436709392	-3.37981146559537	h
-8.40498120946316	3.88543893953588	-2.76566780814543	c
-9.77620832538988	5.57045708290153	-0.84166693985087	c
-8.68685365484438	7.33071890500756	-0.60495669477598	h
-9.888912862484569	4.63724862404921	1.01713271202983	h
-12.35061065619899	6.07226446587320	-2.08118001610228	c
-13.74051373313882	4.65923741625660	-1.44614785201438	h
-13.09585500777415	7.94265760362977	-1.54512683892363	h
-11.90291333985465	5.83315482919839	-4.96559051107390	c
-12.39385716407560	7.57684671088539	-5.99495483494748	h
-13.08403397455398	4.31159066835790	-5.75471222303730	h
-9.09038172480591	5.18447856573105	-5.27224427183020	c
-8.67497315992101	3.96199750219452	-6.90901696127792	h
-7.93074480656390	6.90778455836695	-5.46730819100384	h
6.93816970982175	-3.99297245200425	5.26275076065878	c
5.91735993848073	-5.58947501305808	7.46733786480073	c
4.80624938215696	-4.44070937080126	8.80596687326918	h
4.63611088642048	-7.03533436825127	6.68652383421288	h
8.29664206363194	-6.79537919379114	8.61430780594080	c
8.99672871283489	-5.65084074651731	10.20791792876782	h
7.88017128683495	-8.68880836154543	9.37781414358366	h
10.27165636445436	-6.86687539914006	6.45357239163102	c
10.96618343498164	-8.79415351835973	6.07608229513361	h
11.93077962426071	-5.71238944118986	6.94843900910755	h
8.94248230662965	-5.75173988979903	4.13016370560627	c
7.95801440940470	-7.23336876290538	3.04113944174245	h
10.20532448068844	-4.73485432501875	2.82015572375486	h
2.83277241662431	0.07472260588350	-5.44260892806415	au
-2.56825233199524	2.02170687367774	-4.65686117995553	cu
5.38938214591484	-1.61110169931856	-0.48207934102025	cu
-6.32020810852060	0.82156983177078	-10.21872919331044	o
-9.57147989752969	1.48385024391604	-2.63903345901165	o
8.23348840228824	-1.83352199018705	6.22301309204354	o
11.82632801670666	-1.95138597727979	-0.38759972078646	o
7.48305671996369	1.06197568399484	11.60051743622548	h
7.27777997935210	-1.04464065151067	7.61314198753409	h
9.07735122765662	0.31988953145400	4.08147910504535	h
11.10050601251761	-0.46873816581317	0.47738545409602	h
-7.47735676205230	1.15898389188922	-11.60087462105340	h
-7.28244219222381	-0.96948780367872	-7.62559936682793	h
-9.05040056814917	0.37129483025388	-4.06857707612721	h
-11.08854616853270	-0.43231662923877	-0.46553509909689	h

1c

7.45516853230119	11.91101560413295	33.79583456688025	c
6.94318352180951	10.25815357320180	35.38075260935344	c

9.45077241782423	17.44711060237928	29.05736297261257	c
10.01153501733250	19.08615305103768	27.46576034345906	c
14.60593895612744	9.37179924751867	33.91805274919160	c
14.14217701880436	8.65689547416581	36.09970113090557	c
15.64137371668465	13.57368020340584	27.73424458928253	c
16.2091191523592	15.16481269126576	26.08622047978712	c
10.89822655449663	5.13246747845705	30.92857851708323	c
11.51665378674296	3.27568308631432	32.22484161948118	c
9.22466995392739	10.75826359169920	26.17512331713561	c
8.61054986547969	12.20213125843778	24.42566191765155	c
18.11414533612616	5.24209015038116	28.86325502843319	c
18.75042078797431	4.20135051139396	30.86785772211109	c
15.64744882720864	8.98655278556211	22.79596482396226	c
14.88976717464514	10.26646177227581	20.97594397347657	c
5.82412910552182	8.46117997501977	37.22412008580751	c
4.93455308818040	6.04890250540618	35.85087388549078	c
2.50909612566098	6.82341319181412	34.47286559643128	c
1.40713251037475	9.06209425594568	36.01398716273620	c
3.29132201894864	9.54442070992204	38.15940477848170	c
10.30791157952103	20.98768827251273	25.44523633650989	c
12.02399685032379	23.22261431007380	26.11160131988113	c
11.42303393708485	25.20275501887610	24.08078102238177	c
8.67854072261814	24.64839097605910	23.22787587789319	c
7.82443000133268	22.33964064795539	24.76465567123077	c
13.91709842602993	7.62901292443153	38.67481725055217	c
16.4409689462003	6.58051265270144	39.68177226567555	c
15.94921783708059	6.26606818532138	42.51754892319212	c
14.01245171218589	8.34924637362596	43.20380019296262	c
13.26692900930269	9.61080677556641	40.69366835312784	c
17.43073375216804	16.70874437126043	24.08066207659512	c
19.70492033164868	15.26680626482644	22.99284060957351	c
21.79176494530875	15.56377027818867	24.97846219301065	c
21.15208253171524	18.01651470263530	26.45019289912412	c
18.73103927394485	19.04194845333270	25.23560332377372	c
11.88396760243087	1.09010072402627	33.91312364889440	c
12.83338512912110	-1.30688362569553	32.57598916268505	c
12.32429419035005	-3.42821821982858	34.49099103369657	c
10.14437813878663	-2.46196617439135	36.18924199711562	c
9.43789952603419	0.15396701965933	35.15456134712602	c
7.27199874046234	13.86414078673477	22.62399891751602	c
5.87264575406582	12.405142644410629	20.53095411318866	c
4.02608291623004	14.35683165270009	19.44764330844394	c
3.42702057981968	16.17595221857026	21.66027903217387	c
5.07969315579414	15.29376224556701	23.87772045745207	c
20.22489721282963	3.15724635073278	32.98360432729722	c
22.48876153612950	1.63832644859817	31.96311599133002	c
24.40278804660630	3.65087540129358	31.14618086364148	c
23.79990579526301	6.02670383618487	32.76128897885452	c
21.557007298868540	5.29628395116877	34.44195987021692	c
14.31129395794224	11.67578143078494	18.63691094775571	c
12.54208561987424	10.26799582609906	16.82572154833394	c
12.80631786683638	11.71870026848882	14.33279089559405	c
15.50656430719346	12.84798547163339	14.37148729090261	c
16.63683701433427	12.11574660627032	16.94556077497207	c
7.39912313935995	8.01287355520482	39.29371145764345	o
11.34507184982446	19.81459566016995	23.25720669316243	o
12.02789507693310	5.73403705695502	38.77584722926488	o
15.71809014587918	17.32588786038720	22.13203615202391	o
13.56260111022521	1.73475984390549	35.92019822710646	o
8.90770637202126	15.67996172644522	21.51708437159807	o
18.58094429734733	1.67591295484158	34.51210816192023	o
13.14963912936440	14.02975548253629	19.20464745647442	o
8.57897869807424	14.57337896420079	31.38400469712490	au
15.02086611246811	11.18491103532354	30.64190924474071	au
16.77944525173149	7.08666197093445	25.87110664965761	au
10.16351406049885	8.08519325955123	28.68264119016487	au
10.89578293699204	10.40672181380124	33.74861900720471	cu
12.80308352291352	16.20912590482661	27.78842278408338	cu
14.71869890381970	5.27290282859081	30.53967506095159	cu
12.43496487222740	10.54316004059558	24.18433710344389	cu
6.39551230242037	5.26218502408139	34.58952880832670	h
4.54126785834315	4.64769446684957	37.34862226027565	h
1.17689217165992	5.22886698566477	34.31490020196444	h
2.95031070702563	7.43126368264685	32.52890613038593	h
1.21958842690365	10.75095381765899	34.80826296711177	h
-0.49426868185469	8.64927019261980	36.76022184822586	h
3.44789649757150	11.54170299418376	38.72397841007336	h
2.81867349235715	8.43702658468810	39.86343276559294	h
11.50524615631783	23.90073686498256	28.01302945484442	h

14.02752194431417	22.65720170383840	26.16597767958432	h
12.73225298255495	25.00216497919187	22.47552529940741	h
11.65482101639866	27.13774652480786	24.81650902567808	h
7.40696892130789	26.26907085128958	23.53759513332391	h
8.62664756850270	24.21882945354385	21.19224377987844	h
6.87243665532909	22.90983222760748	26.53037177372611	h
6.52673701448026	21.07921479210234	23.73168582565308	h
16.98749180972200	4.82188700765034	38.70548663512509	h
17.93774295452491	7.98895241135554	39.32302048983166	h
15.14180478677270	4.38324846494115	42.88609469301060	h
17.71117315954988	6.40545171108617	43.62212324953379	h
14.80273317617199	9.74611834094587	44.53259630977990	h
12.34228466158800	7.51849712910767	44.12541586071855	h
11.25807475809049	10.14371409984665	40.59120333748230	h
14.41248491462195	11.31362365814893	40.33079389119614	h
19.24685374447802	13.28678641368152	22.54472682638336	h
20.20442254346047	16.24493621673897	21.21746623268794	h
21.80345857947444	13.92576523005962	26.26567601392669	h
23.67314769028407	15.63760972883821	24.08762434182594	h
22.68965303300395	19.41974252428358	26.37373111645804	h
20.82981606153295	17.58986376980039	28.46368392643385	h
19.16126581819793	20.31720043965308	23.64044534318816	h
17.50358903625898	20.07135819822249	26.56862236410867	h
14.83428976253995	-1.13263689440950	32.01855182059159	h
11.71923393390201	-1.57174122331864	30.83392157517602	h
14.024312237363189	-3.80059319545721	35.63418595678468	h
11.850222576170570	-5.21264000999897	33.52645540513998	h
8.50330702564852	-3.74494679902719	36.18611241434167	h
10.78222554639221	-2.29759689496669	38.16320802448929	h
8.77050522081846	1.48501980876092	36.60962238019145	h
7.96165924317076	0.02403313165259	33.68947551057250	h
7.18842370003264	11.62076769885405	19.11917283793842	h
4.86220057447283	10.80278961999847	21.40249770206864	h
2.31976294008266	13.44564465617623	18.67478814215074	h
4.92346863293129	15.39575888803559	17.88321321494416	h
3.88322102039022	18.13903266276332	21.13372782034108	h
1.40956162618432	16.15074081602000	22.17975692452379	h
4.05145295805696	13.95340425867226	25.09690770502721	h
5.77873223735627	16.82089050296366	25.10390596253156	h
23.23968535918852	0.50920862467481	33.55767667013048	h
21.93786937026131	0.31496161544803	30.45491667259030	h
24.17450679111268	4.07629633888424	29.12033186072409	h
26.36016535862225	2.98671513969156	31.40219313038088	h
25.42914567551221	6.65103903413489	33.89837048322721	h
23.27954414898857	7.62378043225703	31.53053091473604	h
22.22151657394593	4.49149849371742	36.25633972046339	h
20.26859260314697	6.87154063575311	34.87851275514225	h
13.22404810552014	8.30722466843475	16.64179558745394	h
10.59636288841483	10.18915252714168	17.56162973244244	h
12.47887028448035	10.47946198837752	12.69069284534828	h
11.38945902061923	13.24049008495586	14.23959145713370	h
16.68427255504109	12.13564746112777	12.80775427849658	h
15.42964673011270	14.91843493949250	14.17379199738286	h
17.89975881613846	13.56318466677001	17.75056997418217	h
17.71871666495136	10.33757624015934	16.82416698645374	h
8.92412142331345	7.06112209101275	38.80218626766939	h
10.22421211781173	18.40317209766987	22.70979337724227	h
12.56368967624161	4.27175314062562	37.73045159538160	h
14.33408073954712	18.42846796560635	22.76647256123272	h
15.29703056352124	1.87780227738427	35.25510576887477	h
10.26421483784817	14.82136697001516	20.54106380907370	h
19.56202960388493	0.96374689310944	35.88902933348544	h
14.31747295143185	15.11290116154296	20.20759237878552	h

1d

-13.97680620330183	5.24707394682175	3.27772997749015	c
-13.63117529359705	5.80624390954261	5.45960777051991	c
-8.38170506905402	0.60363889309514	3.64225814852379	c
-8.19802368893753	1.13616371734232	5.86759964260992	c
-3.36126965181673	4.49288424718709	-0.35318981423633	c
-4.07993250015314	6.61391285873793	-0.77497668709640	c
-3.25998033109406	-2.98608486893442	0.46543954652973	c
0.20710020491123	-5.14207341394365	6.64862345333156	c
0.46448090421025	4.64954254360331	5.63176182122579	c
0.32520808821658	6.93856780836768	5.39384530109549	c
0.42687535416583	-2.86665417733605	6.48100474534460	c

-3.77493070230540	-5.16437218231171	0.57920105972945	c
-13.45108439313305	7.02341651173425	7.99713202175875	c
-15.86105213040211	8.58792077715028	8.38698252297306	c
-16.34501099303412	8.67163564483711	10.19223789771872	h
-17.29214173083640	7.91083190373735	7.39015198787588	h
-14.98705379394250	11.18232578498897	7.38712842606327	c
-15.25293826083951	11.28361510571164	5.53803140503467	h
-15.96706576645699	12.55143236826462	8.20273422501671	h
-12.31668179556180	11.44896614233914	7.97577811645715	c
-12.10522144129189	12.33675947956881	9.60887944049692	h
-11.46290352872406	12.44882023924893	6.64503297367908	h
-11.14977590850491	8.78860969246273	8.12790107015444	c
-9.98664947371380	8.48266303154855	6.69492174358726	h
-10.2153063579296	8.55598440550451	9.73190061174777	h
-7.40792919277805	1.51089640949354	8.53702677792418	c
-5.63215354570541	-0.56799130929396	9.49436203684405	c
-4.39419395605202	-1.07954017346610	8.18837230640678	h
-6.57701661214823	-2.07145742061777	10.08320069985121	h
-4.33958087081163	0.85799603058155	11.72990805204777	c
-5.29068003349297	0.54543532820227	13.31028601698003	h
-2.59687543106449	0.21775681675990	11.96158847593954	h
-4.27230662048090	3.55690289356883	11.20834363937133	h
-2.51712898825671	4.11588388367640	10.88236588144855	c
-4.94618295946792	4.52066322134050	12.66343276169327	h
-5.92392726062295	3.98076846517508	8.85941405619447	c
-7.08591985973434	5.42414128547313	9.11717270072007	h
-4.86397987268740	4.31921841557489	7.35538102703079	h
-5.52387223829106	8.94318929013278	-1.31260377190237	c
-6.54016695255696	10.23727374593287	1.12004067896132	c
-5.95567465965543	9.32151246193648	2.64297096945386	h
-5.94358041240496	12.00756918722013	1.21925130093782	h
-9.37248848052596	10.15053531643341	0.93201292873920	c
-10.04088461372761	8.64328975284383	1.81621578631639	h
-10.12648920754733	11.67951273055119	1.70264324572996	h
-9.93524892289931	10.03941941981974	-1.61269228180461	c
-9.83849494489556	11.74603109042876	-2.37311807767779	h
-11.66472627971625	9.37253506752439	-1.86572661099800	h
-7.94517833235744	8.23869938779301	-2.87257269459947	c
-7.72823777230216	8.61305413471766	-4.69275690579492	h
-8.40702739923469	6.43873524621943	-2.65714391545050	h
-0.14571166409852	-7.82283890605523	7.37522315142609	c
-2.62824488487039	-8.16128885645505	8.96202618521016	h
-3.36674985760210	-6.50210931178145	9.41083614177050	h
-3.89795187355626	-9.15566274757947	8.01395058434144	h
-1.76652976827454	-9.56724509932197	11.30528658998836	c
-3.07554306052442	-10.79140968820528	11.84177983911460	h
-1.46889790234505	-8.36462338835354	12.70708543536293	h
0.72979845326740	-10.97830360274767	10.62819771657544	c
1.73966809868148	-11.41898773693661	12.13997862288395	h
0.43386734085751	-12.50293464675981	9.58525786383585	h
1.87421659934294	-8.82458272909791	9.12926694797054	c
2.45549635781856	-7.47191676317836	10.28370064255038	h
3.34234483198180	-9.43345248911366	8.14245196137766	h
0.16136883249540	9.69359953750167	5.71585463413921	c
-2.02353252234698	10.38089293203217	7.40715952307186	c
-3.41078047649834	9.13386265694094	7.26467417265228	h
-2.68436975101709	12.08410309560200	7.00408093892735	h
-0.78028169952152	10.31475251738117	10.12458570216141	c
-1.70889312122152	11.42515559306478	11.30982193270729	h
-0.76667567136474	8.57374783115363	10.80923348010588	h
1.63176473649372	11.17760146965676	9.74966403739690	c
2.77372623859651	10.39468793280224	11.00803266928545	h
1.67466151971022	13.03066691556442	10.00421014749659	h
2.52295958076259	10.58328260086422	7.21289567661121	c
3.81231972123046	9.22891588142509	7.27053232366422	h
3.27733825301053	12.09581939762590	6.41089590581455	h
-5.04841714325704	-7.66769239054532	0.560492777101388	c
-6.68416408388284	-8.10591988076150	-1.78805886693640	c
-5.64632649170205	-8.62710634821136	-3.25486429128223	h
-7.65964071367841	-6.57354095960453	-2.23592396043029	h
-8.45275877165052	-10.28156157755274	-0.89818683096055	c
-10.17618900484223	-10.02663752222646	-1.58000001970569	h
-7.80968496862954	-11.92524536793667	-1.51839494777361	h
-8.51644254232877	-10.27022322075542	1.88689154368631	c
-7.83651907971651	-11.87951399552084	2.55661048518099	h
-10.27464373636557	-10.06972327805626	2.49368260495589	h
-6.87842793034349	-8.03222056157896	2.78375556635384	c
-7.91626552252429	-6.50154239394159	3.06702551367340	h
-5.95888719408134	-8.45155079046628	4.35827538027416	h

-13.44636007780083	5.14786332484525	9.96131336428009	o
-12.17967665092759	4.20621279282833	9.79067109448052	h
-9.61456239814861	1.60708346965742	10.16389200572543	o
-10.42071956643763	0.24496887307345	10.04294953322075	h
-3.89549522958350	10.61824253432261	-2.66375795691560	o
-4.67444034155897	11.96108192435115	-2.99521592062374	h
-0.41235202144869	-9.43609810569970	5.20921905791256	o
0.88834647581650	-9.32800577089864	4.30574099377994	h
-0.09544494896376	10.96821981413303	3.35388594064544	o
1.17388409449552	10.66737541377764	2.44946301344637	h
-3.12165237816683	-9.66021962505994	0.59866523889817	o
-2.22063095800696	-9.49997084899124	1.89558428389759	h
-11.15298844293082	2.97335546373374	3.96710207076683	cu
-11.28583619057268	1.82742553675189	-4.50699682693226	cu
-14.20735279151388	4.50573438489071	-0.40950365299632	au
-8.50472624030487	-0.05700936296168	-0.08825021040576	au
-1.84514237540258	4.17862279128820	-3.26639162069283	cu
0.76834886637827	4.26347149465477	1.86534866577142	cu
-2.91642812013545	0.70662896733741	0.83582586857532	au
0.48300022031253	0.85724014012840	5.70432730472860	au
-14.05598572826974	4.23758224663424	-4.16420050642680	c
-13.82203763301850	4.20129950488283	-6.44339919530018	c
-13.90783119945151	4.67127439413149	-9.20542291112583	c
-16.38356140614499	6.20667687710108	-9.79256082061340	c
-17.76891963416345	5.78904740173335	-8.60675767222766	h
-16.96351835632759	5.96063453459937	-11.55416352168940	h
-15.40827374896271	8.69147776923241	-9.38154538671078	c
-16.17833714811361	9.82191194192460	-10.65767744424845	h
-16.00769487831403	9.26652143146951	-7.70516933422792	h
-12.58540085165813	9.08095032522014	-9.47149635063613	c
-12.08991465961552	10.24350984217139	-10.85080745502936	h
-11.92248492424185	9.72421310085441	-7.84463112283488	h
-11.70195388453409	6.34009154208280	-9.99419459899230	c
-10.17505516916250	5.93493425919212	-8.99188385810976	h
-11.31153646547992	6.10595447421827	-11.80870963178910	h
-14.02045887697149	2.41059502136039	-10.59002524869114	o
-12.72618544855811	1.54169894545958	-10.29031468401548	h
-8.42951514021603	-0.43098616465975	-3.85749795505946	c
-8.39342137107791	-0.51848048461235	-6.16825507035203	c
-7.93478483862657	-0.95538516653551	-8.86848474163232	c
-6.29469152789512	1.10989652409521	-10.07488590486652	c
-7.36200884774893	2.44007474903341	-10.84381546833769	h
-5.17370598586735	1.89602259537564	-8.80007665562186	h
-4.72659678282661	-0.27678451221628	-12.12334903291456	c
-2.91642812013545	0.17882845842245	-11.99824916291753	h
-5.34245852953404	0.15161640210890	-13.83714166282855	h
-5.12665180515850	-3.11704288994340	-11.55340763123625	c
-3.47219657581712	-3.98934047288341	-11.50881009450015	h
-6.15825330110077	-3.89183060442651	-12.90815229590196	h
-6.36631214833148	-3.41202913928685	-9.19446249955510	c
-7.48049467628085	-4.91492833277080	-9.21222592520422	h
-5.12343927073260	-3.59627743724320	-7.80834838108348	h
-10.18563763550665	-1.10542942148663	-10.31714879510246	o
-11.07437583580277	-2.31050777642781	-9.79067109448052	h
13.97680620330183	-5.24707394682175	-3.27772997749015	c
13.63117529359705	-5.80624390954261	-5.45960777051991	c
8.38170506905402	-0.60363889309514	-3.64225814852379	c
8.19802368893753	-1.13616371734232	-5.86759964260992	c
3.36126965181673	-4.49288424718709	0.35318981423633	c
4.07993250015314	-6.61391285873793	0.77497668709640	c
3.25998033109406	2.98608486893442	-0.46543954652973	c
-0.20710020491123	5.14207341394365	-6.64862345333156	c
-0.46448090421025	-4.64954254360331	-5.63176182122579	c
-0.32520808821658	-6.93856780836768	-5.39384530109549	c
-0.42687535416583	2.86665417733605	-6.48100474534460	c
3.77493070230540	5.16437218231171	-0.57920105972945	c
13.45108439313305	-7.02341651173425	-7.99713202175875	c
15.86105213040211	-8.58792077715028	-8.38698252297306	c
16.34501099303412	-8.67163564483711	-10.19223789771872	h
17.29214173083640	-7.91083190373735	-7.39015198787588	h
14.98705379394250	-11.18232578498897	-7.38712842606327	c
15.25293826083951	-11.28361510571164	-5.53803140503467	h
15.96706576645699	-12.55143236826462	-8.20273422501671	h
12.31668179556180	-11.44896614233914	-7.97577811645715	c
12.10522144129189	-12.33675947956881	-9.60887944049692	h
11.46290352872406	-12.44882023924893	-6.64503297367908	h
11.14977590850491	-8.78860969246273	-8.12790107015444	c
9.98664947371380	-8.48266303154855	-6.69492174358726	h
10.21530633579296	-8.55598440550451	-9.73190061174777	h

7.40792919277805	-1.51089640949354	-8.53702677792418	c
5.63215354570541	0.56799130929396	-9.49436203684405	c
4.39419395605202	1.07954017346610	-8.18837230640678	h
6.57701661214823	2.07145742061777	-10.08320069985121	h
4.33958087081163	-0.85799603058155	-11.72990805204777	c
5.29068003349297	-0.54543532820227	-13.31028601698003	h
2.59687543106449	-0.21775681675990	-11.96158847593954	h
4.27230662048090	-3.55690289356883	-11.20834363937133	c
2.51712898825671	-4.11588388367640	-10.88236588144855	h
4.94618295946792	-4.52066322134050	-12.66343276169327	h
5.92392726062295	-3.98076846517508	-8.85941405619447	c
7.08591985973434	-5.42414128547313	-9.11717270072007	h
4.86397987268740	-4.31921841557489	-7.35538102703079	h
5.52387223829106	-8.94318929013278	1.31260377190237	c
6.54016695255696	-10.23727374593287	-1.12004067896132	c
5.95567465965543	-9.32151246193648	-2.64297096945386	h
5.94358041240496	-12.00756918722013	-1.21925130093782	h
9.37248848052596	-10.15053531643341	-0.93201292873920	c
10.04088461372761	-8.64328975284383	-1.81621578631639	h
10.12648920754733	-11.67951273055119	-1.70264324572996	h
9.93524892289931	-10.03941941981974	1.61269228180461	c
9.83849494489556	-11.74603109042876	2.37311807767779	h
11.66472627971625	-9.37253506752439	1.86572661099800	h
7.94517833235744	-8.23869938779301	2.87257269459947	c
7.72823777230216	-8.61305413471766	4.69275690579492	h
8.40702739923469	-6.43873524621943	2.65714391545050	h
0.14571166409852	7.82283890605523	-7.37522315142609	c
2.62824488487039	8.16128885645505	-8.96202618521016	c
3.36674985760210	6.50210931178145	-9.41083614177050	h
3.89795187355626	9.15566274757947	-8.01395058434144	h
1.76652976827454	9.56724509932197	-11.30528658998836	c
3.07554306052442	10.79140968820528	-11.84177983911460	h
1.46889790234505	8.36462338835354	-12.70708543536293	h
-0.72979845326740	10.97830360274767	-10.62819771657544	c
-1.7396680986148	11.41898773693661	-12.13997862288395	h
-0.43386734085751	12.50293464675981	-9.58525786383585	h
-1.87421659934294	8.82458272909791	-9.12926694797054	c
-2.45549635781856	7.47191676317836	-10.28370064255038	h
-3.34234483198180	9.43345248911366	-8.14245196137766	h
-0.16136883249540	-9.69359953750167	-5.71585463413921	c
2.02353252234698	-10.38089293203217	-7.40715952307186	c
3.41078047649834	-9.13386265694094	-7.26467417265228	h
2.68436975101709	-12.08410309560200	-7.00408093892735	h
0.78028169952152	-10.31475251738117	-10.12458570216141	c
1.70889312122152	-11.42515559306478	-11.30982193270729	h
0.76667567136474	-8.57374783115363	-10.80923348010588	h
-1.63176473649372	-11.17760146965676	-9.74966403739690	c
-2.77372623859651	-10.39468793280224	-11.00803266928545	h
-1.67466151971022	-13.03066691556442	-10.00421014749659	h
-2.52295958076259	-10.58328260086422	-7.21289567661121	c
-3.81231972123046	-9.22891588142509	-7.27053232366422	h
-3.27733825301053	-12.09581939762590	-6.41089590581455	h
5.04841714325704	7.66769239054532	-0.56049277101388	c
6.68416408388284	8.10591988076150	1.78805886693640	c
5.64632649170205	8.62710634821136	3.25486429128223	h
7.65964071367841	6.57354095960453	2.23592396043029	h
8.45275877165052	10.28156157755274	0.89818683096055	c
10.17618900484223	10.02663752222646	1.58000001970569	h
7.80968496862954	11.92524536793667	1.51839494777361	h
8.51644254232877	10.27022322075542	-1.88689154368631	c
7.83651907971651	11.87951399552084	-2.55661048518099	h
10.27464373636557	10.06972327805626	-2.49368260495589	h
6.87842793034349	8.03222056157896	-2.78375556635384	c
7.91626552252429	6.50154239394159	-3.06702551367340	h
5.95888719408134	8.45155079046628	-4.35827538027416	h
13.44636007780083	-5.14786332484525	-9.96131336428009	o
12.17967665092759	-4.20621279282833	-9.79067109448052	h
9.61456239814861	-1.60708346965742	-10.16389200572543	o
10.42071956643763	-0.24496887307345	-10.04294953322075	h
3.89549522958350	-10.61824253432261	2.66375795691560	o
4.67444034155897	-11.96108192435115	2.99521592062374	h
0.41235202144869	9.43609810569970	-5.20921905791256	o
-0.88834647581650	9.32800577089864	-4.30574099377994	h
0.09544494896376	-10.96821981413303	-3.35388594064544	o
-1.17388409449552	-10.66737541377764	-2.44946301344637	h
3.12165237816683	9.66021962505994	-0.59866523889817	o
2.22063095800696	9.49997084899124	-1.89558428389759	h
11.15298844293082	-2.97335546373374	-3.96710207076683	cu
11.28583619007268	-1.82742553675189	4.50699682693226	cu

14.20735279151388	-4.50573438489071	0.40950365299632	au
8.50472624030487	0.05700936296168	0.08825021040576	au
1.84514237540258	-4.17862279128820	3.26639162069283	cu
-0.76834886637827	-4.26347149465477	-1.86534866577142	cu
2.91642812013545	-0.70662896733741	-0.83582586857532	au
-0.48300022031253	-0.85724014012840	-5.70432730472860	au
14.05598572826974	-4.23758224663424	4.16420050642680	c
13.82203763301850	-4.20129950488283	6.44339919530018	c
13.90783119945151	-4.67127439413149	9.20542291112583	c
16.38356140614499	-6.20667687710108	9.79256082061340	c
17.76891963416345	-5.78904740173335	8.60675767222766	h
16.96351835632759	-5.96063453459937	11.55416352168940	h
15.40827374896271	-8.69147776923241	9.38154538671078	c
16.17833714811361	-9.82191194192460	10.65767744424845	h
16.00769487831403	-9.26652143146951	7.70516933422792	h
12.58540085165813	-9.08095032522014	9.47149635063613	c
12.08991465961552	-10.24350984217139	10.85080745502936	h
11.92248492424185	-9.72421310085441	7.84463112283488	h
11.70195388453409	-6.34009154208280	9.99419459899230	c
10.17505516916250	-5.93493425919212	8.99188385810976	h
11.31153646547992	-6.10595447421827	11.80870963178910	h
14.02045887697149	-2.41059502136039	10.59002524869114	o
12.72618544855811	-1.54169894545958	10.29031468401548	h
8.42951514021603	0.43098616465975	3.85749795505946	c
8.39342137107791	0.51848048461235	6.16825507035203	c
7.93478483862657	0.95538516653551	8.86848474163232	c
6.29469152789512	-1.10989652409521	10.07488590486652	c
7.36200884774893	-2.44007474903341	10.84381546833769	h
5.17370598586735	-1.89602259537564	8.80007665562186	h
4.72659678282661	0.27678451221628	12.12334903291456	c
2.91642812013545	-0.17882845842245	11.99824916291753	h
5.34245852953404	-0.15161640210890	13.83714166282855	h
5.12665180515850	3.11704288994340	11.55340763123625	c
3.47219657581712	3.98934047288341	11.50881009450015	h
6.15825330110077	3.89183060442651	12.90815229590196	h
6.36631214833148	3.41202913928685	9.19446249955510	c
7.48049467628085	4.91492833277080	9.21222592520422	h
5.12343927073260	3.59627743724320	7.80834838108348	h
10.18563763550665	1.10542942148663	10.31714879510246	o
11.07437583580277	2.31050777642781	9.79067109448052	h