Supporting Information for

First example of structurally characterized "molecular brass"

Kerstin Freitag,[a] Hung Banh,[a] Christian Gemel,[a] Rüdiger W. Seidel[a] Samia Kahlal[b], Jean-Yves Saillard,[b] and Roland A. Fischer[a,*]

[a] Inorganic Chemistry II, Ruhr-University Bochum, Universitätsstraße 150, 44801 Bochum, Germany. E-mail: roland.fischer@rub.de

[b] Institut des Sciences Chimiques de Rennes - UMR 6226 Université de Rennes 1, 35042 Rennes Cedex, France. E-mail: jean-yves.saillard@univ-rennes1.fr

Materials and Methods

Spectroscopy. NMR spectra were recorded on a Bruker Avance DPX-250 spectrometer (^{1}H, 250.1 MHz; ^{13}C, 62.9 MHz) in C_6D_6 at 298 K unless otherwise stated. Chemical shifts are given relative to TMS and were referenced to the residual solvent peak as internal standards. Chemical shifts are reported in parts per million, downfield shifted from TMS, and are consecutively reported as position (δ_H or δ_C), relative integral, multiplicity (s = singlet, d = doublet, sept = septet, m = multiplet), coupling constant (J in Hz) and assignment. IR spectra were recorded on a Bruker Alpha-P Fourier transform spectrometer. FT-IR spectra were measured in an ATR setup with a Bruker Alpha FTIR spectrometer under an inert gas atmosphere in a glove-box.

Spectrometry. Mass spectrometry was measured with a Waters LCT; Ionisation method: liquid injection field desorption ionization (LIFDI; special ionization cell obtained from Linden CMS GmbH, Leeste, Germany; http://www.linden-cms.de), solvent: toluene.

X-ray crystallography. The X-ray intensity data of **1a**/**1b** were collected on an Oxford Diffraction Xcalibur2 diffractometer with a Sapphire2 CCD. A dark red cubic crystal of **1a**/**1b** was selected from the crude product with the aid of an optical microscope. The crystal was coated with a perfluoropolyether, picked up with a glass fiber and immediately mounted in the nitrogen cold gas stream of the diffractometer. The diffraction data were processed with CrysAlisPro [17]. An absorption correction based on multiple-scanned reflections was carried out with ABSPACK in CrysAlisPro. The crystal structure was solved by direct methods using SHELXS-97 and refined with SHELXL-2013 [18]. The crystal structure was described as a 1:1 solid solution of **1a** and **1b**. In the crystal, the molecules are located on a -43*m* special position. Anisotropic displacement parameters were introduced only for Cu1 and Zn1. For ring and terminal carbon atoms of the Cp/Cp* ligands, each one isotropic displacement

parameter was refined by means of a free variable. Cp/Cp* ligands were treated as rigid groups and appropriate geometric restraints were applied to the *tert*-butyl-isonitrile ligand. Hydrogen atoms were placed at geometrically calculated positions and refined with the appropriate riding model. The structure was refined as an inversion twin, affording a Flack x parameter of 0.38(16) [19]. The crystal structure contains large solvent-accessible voids of 1633 $Å^3$. These voids are most likely occupied by severely disordered toluene molecules of crystallization. The resulting electron density was found to be uninterpretable. The solvent contribution to the scattering was not removed, since this did not markedly improve the overall refinement results. The formula mass and density do not take account of the solvent. Figure S1 shows the disorder model of **1a**/**1b**. Table S1 lists relevant crystal data and refinement details. CCDC 985016 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

DFT Calculations. Density functional theory (DFT) geometry optimizations have been carried out on the $[(CuCNMe)_4(ZnCp)_4]$ and $[(ZnCNMe)_4(CuCp)_4]$ model, using the Gaussian 09 package [20], with the PBE0 functional [21] and the Def2-TZVP (triple-ζ polarized) basis set from the EMSL Basis Set Exchange Library [22]. All the stationary points were fully characterized as true minima via analytical frequency calculations. Because the Cp ligands are not compatible with 3-fold symmetry, the highest symmetry possible for the computed clusters is D_{2d}. However, both optimized structures exhibit a very strong T_d pseudo-symmetry. Whereas $[(ZnCNMe)_4(CuCp)_4]$ energy minimum maintains the highest D_{2d} symmetry, $[(CuCNMe)_4(ZnCp)_4]$ was found to be very slightly distorted to S_4 symmetry, due to rotations of methyl groups induced by weak steric interactions. The natural orbital analysis was performed with the NBO 5.0 program [23]. The MO interaction diagram of Figure S8 was built up from data obtained by a single-point calculation at the PBE0/TZVP level on the D_{2d} structure of $[(CuCNMe)_4(ZnCp)_4]$ using the ADF 2013 program [24]. Molecular orbital plots were obtained using the Molekel4.3 code [25].

Additional References

[17] Agilent Technologies, (2011), CrysAlisPro Software system, version 1.171.35.19, Agilent Technologies UK Ltd, Oxford, UK.

[18] G. M. Sheldrick, Acta Cryst. 2008, A64, 112-122.

[19] H. D. Flack, Acta Cryst. 1983, A39, 876-881.

[20] Gaussian 09, Revision D 01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[21] (a) C. Adamo, and V. Barone, *J. Chem. Phys.* 1999, **110**, 6158. (b) M. Ernzerhof, M and G. E. Scuseria, *J. Chem. Phys.* 1999, **110**, 5029.

[22] F. Weigend, and R. Ahlrichs, *Phys. Chem. Chem. Phys.* 2005, **7**, 3297.

[23] E. D. Glendening, J. K. Badenhoop, A. E. Reed, J. E. Carpenter, J. A. Bohmann, C. M. Morales and F. Weinhold, F. *NBO 5.0*; Theoretical Chemistry Institute, University of Wisconsin: Madison, WI, 2001; http://www.chem.wisc.edu/~nbo5.

[24] (a) G. te Velde, F.M. Bickelhaupt, S.J.A. van Gisbergen, C. Fonseca Guerra, E.J. Baerends, J.G. Snijders and T. Ziegler, *Journal of Comput. Chem*. 2001, 22, 931. (b) E.J. Baerends, T. Ziegler, J. Autschbach, D. Bashford, A. Bérces, F.M. Bickelhaupt, C. Bo, P.M. Boerrigter, L. Cavallo, D.P. Chong, L. Deng, R.M. Dickson, D.E. Ellis, M. van Faassen, L. Fan, T.H. Fischer, C. Fonseca Guerra, M. Franchini, A. Ghysels, A. Giammona, S.J.A. van Gisbergen, A.W. Götz, J.A. Groeneveld, O.V. Gritsenko, M. Grüning, S. Gusarov, F.E. Harris, P. van den Hoek, C.R. Jacob, H. Jacobsen, L. Jensen, J.W. Kaminski, G. van Kessel, F. Kootstra, A. Kovalenko, M.V. Krykunov, E. van Lenthe, D.A. McCormack, A. Michalak, M. Mitoraj, S.M. Morton, J. Neugebauer, V.P. Nicu, L. Noodleman, V.P. Osinga, S. Patchkovskii, M. Pavanello, P.H.T. Philipsen, D. Post, C.C. Pye, W. Ravenek, J.I. Rodríguez, P. Ros, P.R.T. Schipper, G. Schreckenbach, J.S. Seldenthuis, M. Seth, J.G. Snijders, M. Solà, M. Swart, D. Swerhone, G. te Velde, P. Vernooijs, L. Versluis, L. Visscher, O. Visser, F. Wang, T.A. Wesolowski, E.M. van Wezenbeek, G. Wiesenekker, S.K. Wolff, T.K. Woo and A.L. Yakovlev. *ADF2013*, SCM, Theoretical Chemistry, Vrije Universiteit, Amsterdam, The Netherlands, http://www.scm.com.

[25] P. Flukiger, H. P. Luthi, S. Portmann and J. Weber, *MOLEKEL 4.3*; Swiss Center for Scientific Computing: Manno, Switzerland, 2000, http://www.cscs.ch/

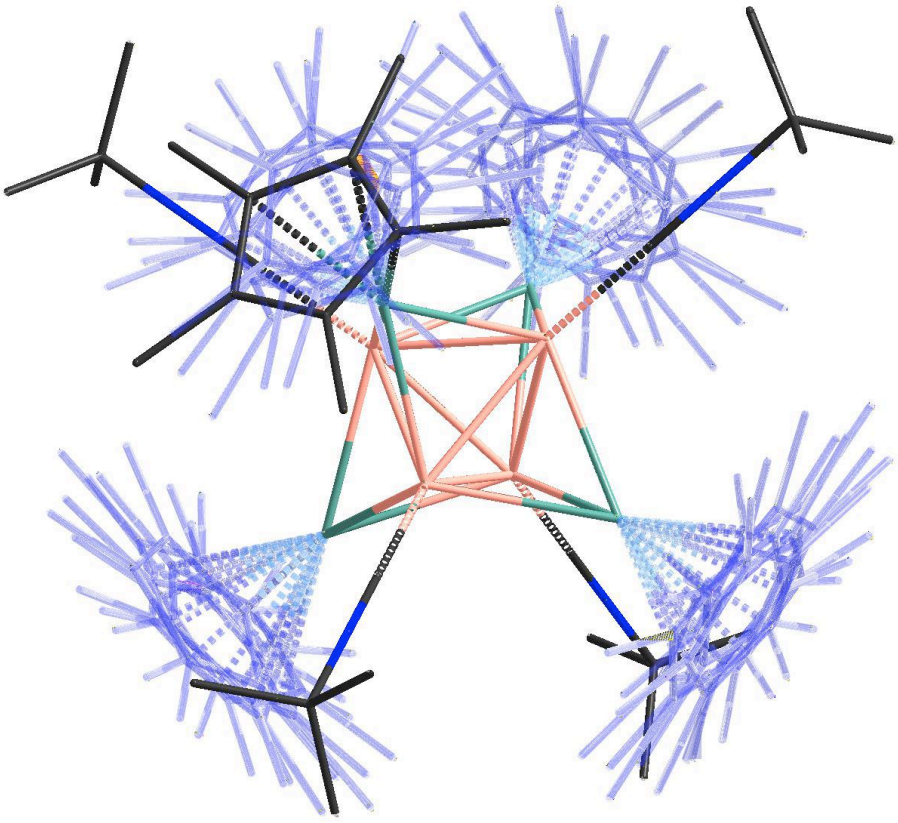

Figure S1. Disorder model of **1a**/**1b** in the crystal.

Table S1. Crystallographic data and refinement details for **1a**/**1b**

Empirical formula	$C_{57.5}H_{91}N_4Cu_4Zn_4$
M_r	1353.98
T (K)	110(2)
λ (Å)	0.71073
Crystal size (mm^3)	0.23 × 0.09 × 0.08
Crystal system	Cubic
Space group	*I*-43*m*
a (Å)	16.8803(5)
V ($Å^3$)	4810.0(4)
Z	2
$\rho_{calc.}$ (g cm^{-3})	0.935
μ (mm^{-1})	1.869
F (000)	1400
$2\theta_{max}$(°)	57.74
Reflections collected	17012
Reflections unique	1141
R_{int}	0.1838
Reflections observed [$I>2\sigma(I)$]	518
Parameters / restraints	25 / 5
Goodness-of-fit on F^2	1.045
R_1 [$I>2\sigma(I)$]	0.0678
wR_2 (all data)	0.2042
Residuals (e $Å^{-3}$)	0.359 / -0.478

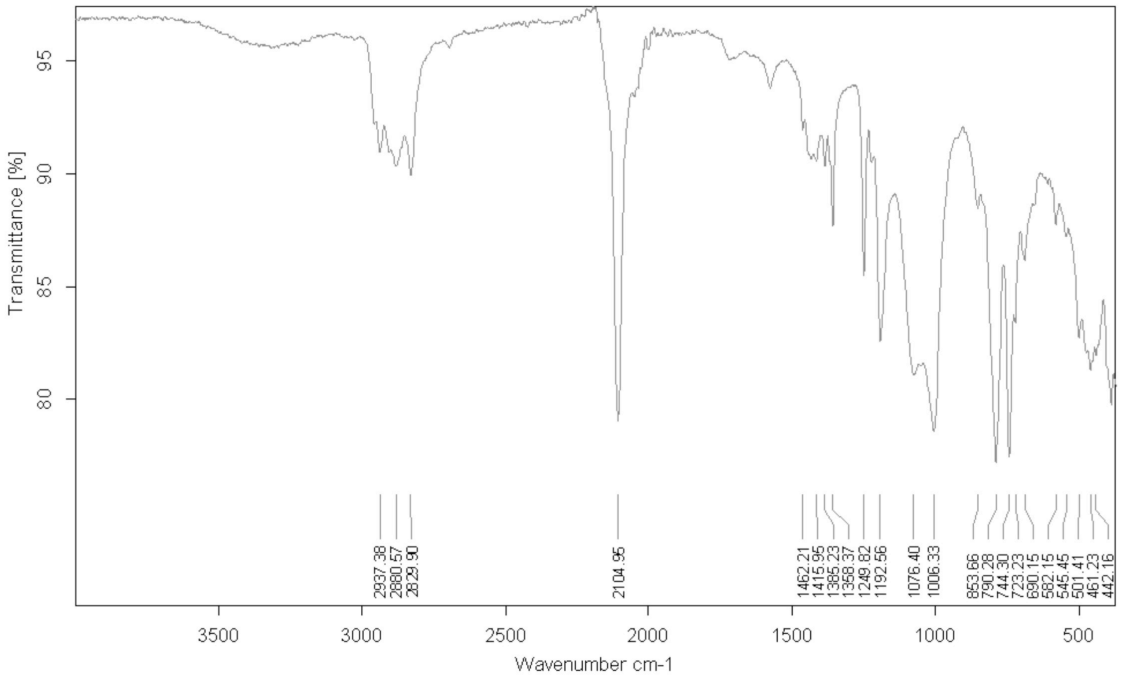

Figure S2. IR Spectrum of **1**.

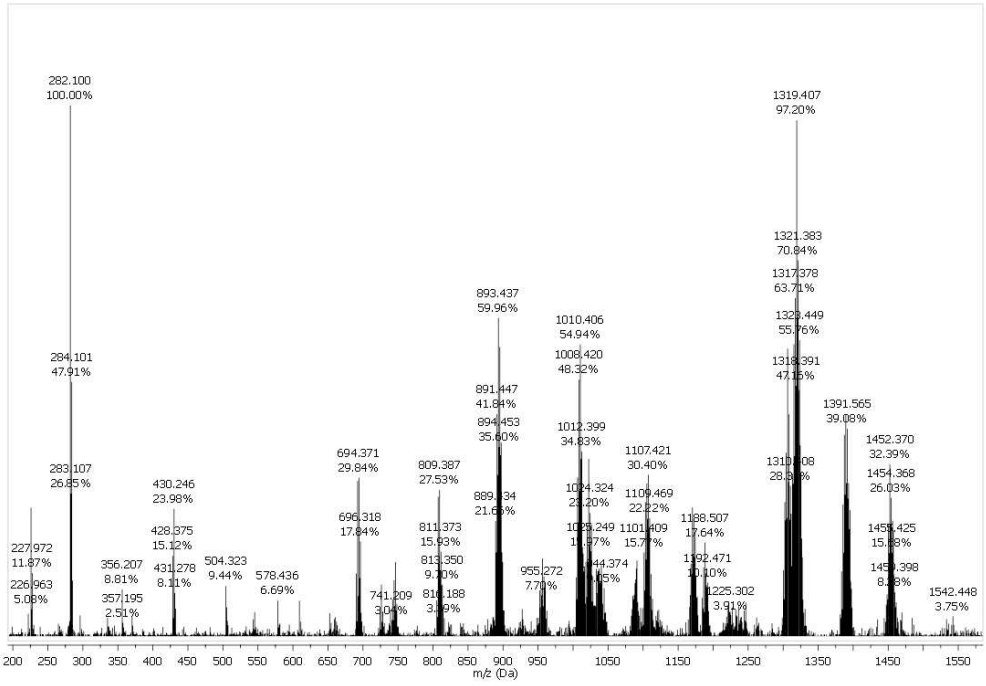

Figure S3. LIFDI-MS Spectrum of **1**, and list of signals:

m/z	fragment
1452	[**1a** + Cu]$^+$
1389	[**1a**]$^+$
1319	[**1b**]$^+$
1306	[**1a** – CN^{t}Bu]$^+$
1188	[**1a** – ZnCp*]$^+$ [**1b** – ZnCp]$^+$
1170	[**1a** – CN^{t}Bu – Cp*]$^+$
1091	[**1b** – Cu(CN^{t}Bu) – CN^{t}Bu)]$^+$
1040	[**1a** – Cu(CN^{t}Bu) – ZnCp*]$^+$ [**1b** – Cu(CN^{t}Bu) – ZnCp]$^+$
1022	[**1b** – Cu(CN^{t}Bu) – CN^{t}Bu – Cp]$^+$
956	[**1b** – Cu(CN^{t}Bu) - CN^{t}Bu – ZnCp]$^+$
893	[**1a** – 2Cu(CN^{t}Bu) – ZnCp*]$^+$ [**1b** – 2Cu(CN^{t}Bu) – ZnCp]$^+$
809	[**1b** – Cu(CN^{t}Bu) – 2CN^{t}Bu – ZnCp*]$^+$
746	[**1a** – 3Cu(CN^{t}Bu) – ZnCp*]$^+$ [**1b** – 3Cu(CN^{t}Bu) – ZnCp]$^+$
694	[**1a** – 2Cu(CN^{t}Bu) – 2ZnCp*]$^+$ [**1b** – 2Cu(CN^{t}Bu) – ZnCp* - ZnCp]$^+$
282	[Cp*CuCN^{t}Bu]$^+$

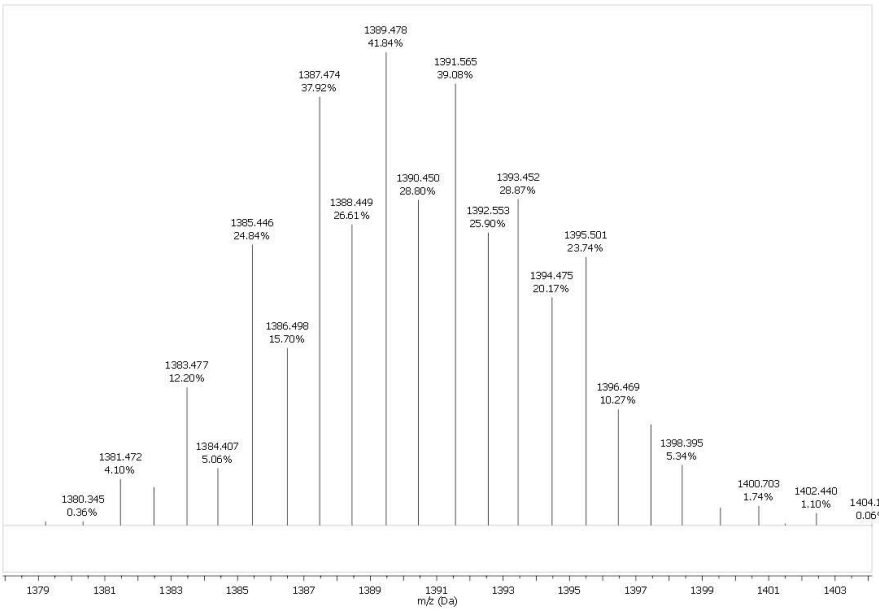

Figure S4. Isotopic pattern of the molecular [M]$^+$ ion peak of **1a**

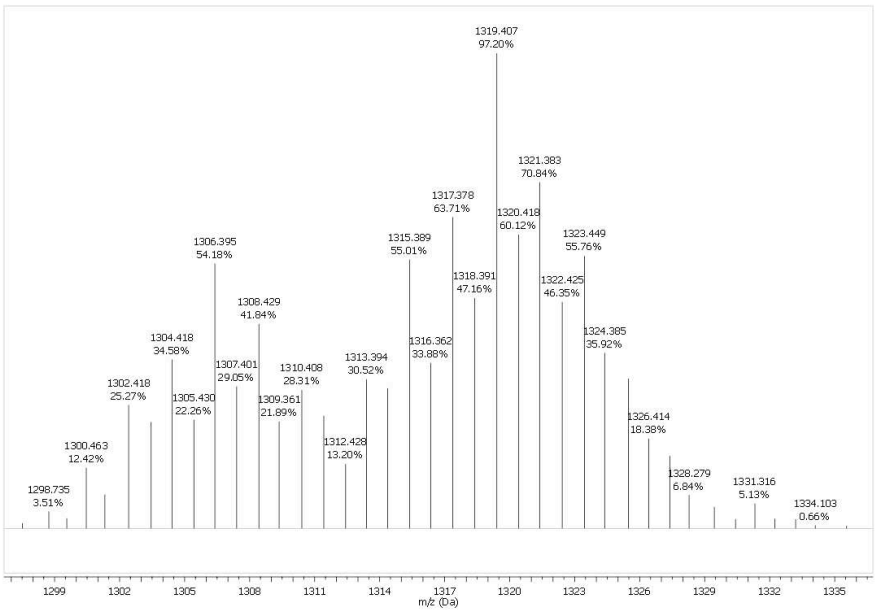

Figure S5. Isotopic Pattern of the molecular $[M]^+$ ion peak of **1b**, superimposing with [**1a**-$CN^tBu]^+$

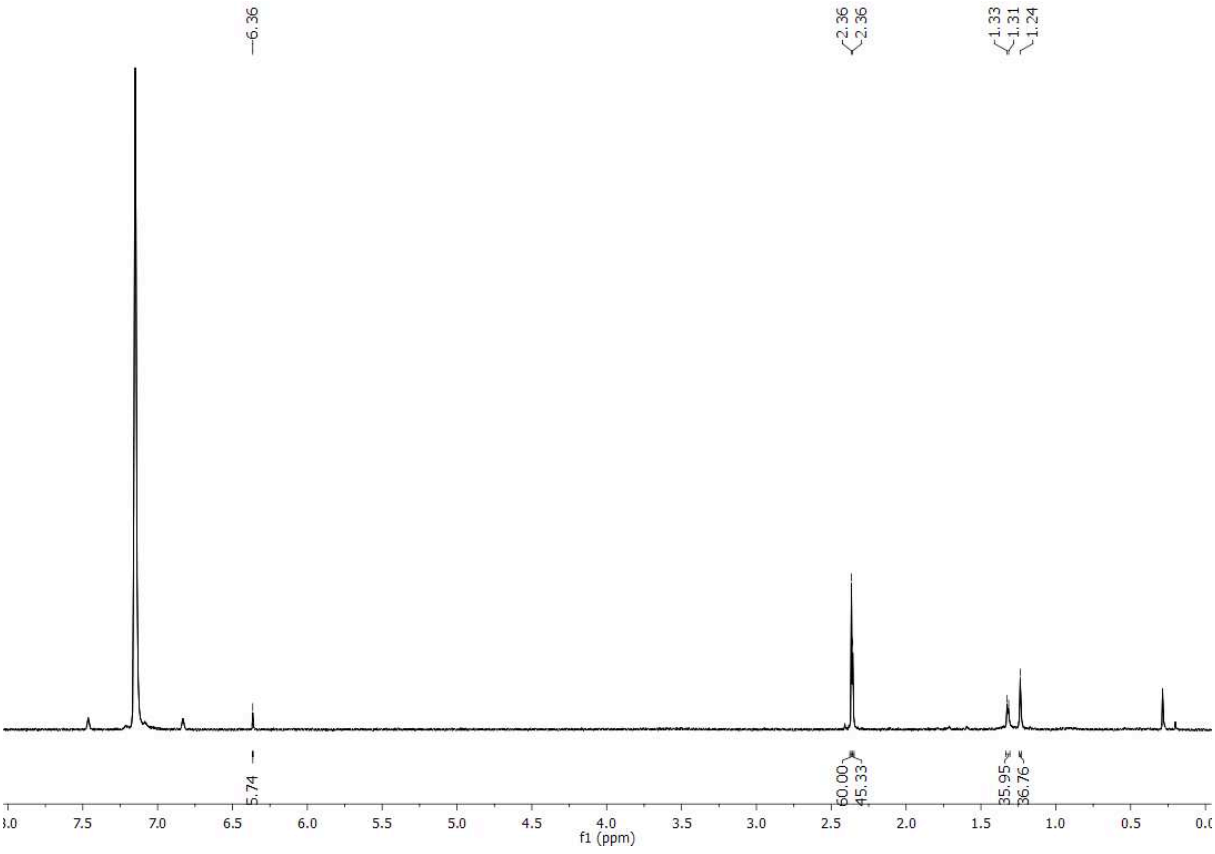

Figure S6. ^{1}H-NMR spectrum of **1**, recorded at room temperature in C_6D_6.

Results of the DFT Calculations

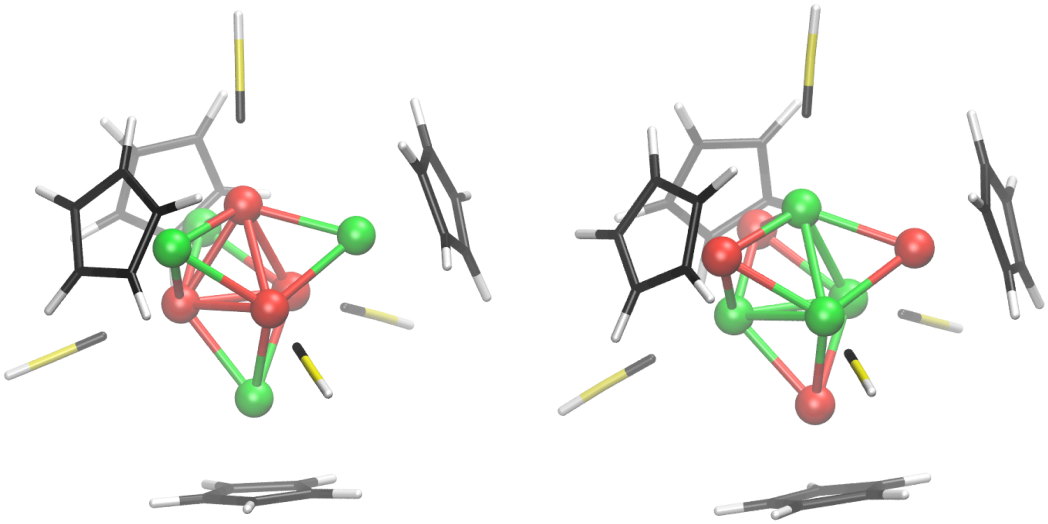

Figure S7. Illustration of the structures of the two simplified models **[(CuCNH)$_4$(ZnCp)$_4$]** (left) and **[(CuCp)$_4$(ZnCNH)$_4$]** (right) are shown for comparison (Cp* is substituted by Cp and CN^{t}Bu is substituted by CNH). Atom coloring: Cu red, Zn green, C black, N yellow, H white.

Table S2. Relevant computed data for the relevant models **[(MCNMe)$_4$(M'Cp)$_4$]** (M = Cu, M' =Zn and M = Zn, M' = Cu) with Cp* substituted by Cp and CN^{t}Bu substituted by CNMe.

	[(CuCNMe)$_4$(ZnCp)$_4$] **(S_4)**	**[(ZnCNMe)$_4$(CuCp)$_4$]** **(D_{2d})**
Relative energy (eV)[a]	0.00	2.05
HOMO-LUMO gap (eV)	*3.57*	*3.47*
Bondn distances (Å)[b] and Wiberg indices in parenthesis :		
M-M	2.513 (0.102)	2.562 (0.104)
M-M'	2.574 (0.151)	2.531 (0.179)
M-C	1.891 (0.316)	2.051 (0.166)
M'-(Cp centroid)	2.040	1.921

Natural atomic charges:		
M	*0.21*	*0.73*
M’	0.73	0.16
υ(CN) (cm^{-1})	2268	2317

[a] Including ZPVE contribution

[b] Averaged over very similar values (pseudo-T_d symmetry)

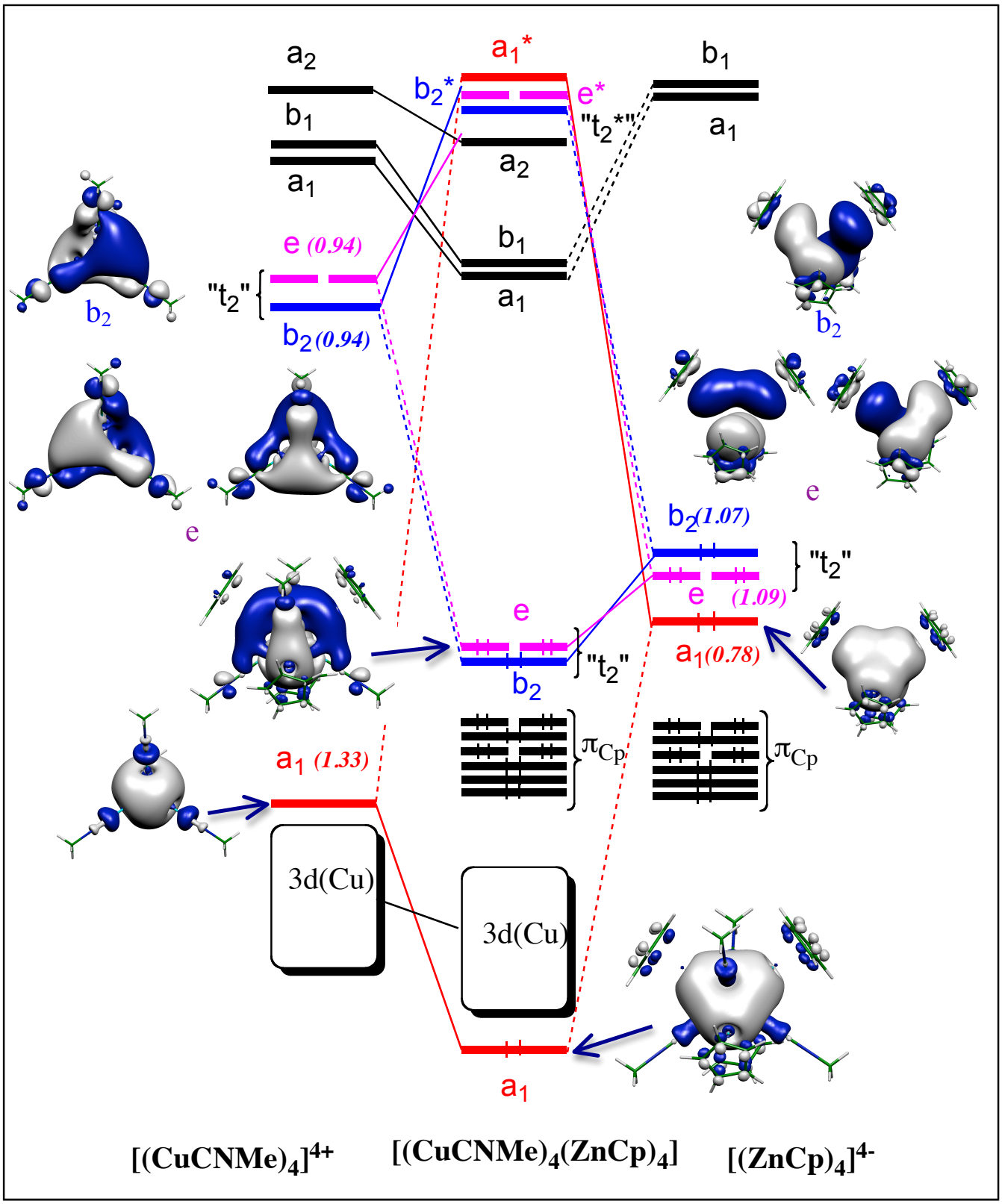

Figure S8. MO interaction diagram of $[(CuCNMe)_4(ZnCp)_4]$ in D_{2d} symmetry (from ADF calculations). The *e* (pink) and b_2 (blue) irreducible representations correspond to t_2 in the T_d pseudosymmetry. The four $[(CuCNMe)_4]^{4+}$ skeletal orbitals [a_1 (bonding) + "t_2"

(antibonding)] interact with the four non-bonding $[(ZnCp)_4]^{4-}$ combinations (a_1 + "t_2") giving rise to four occupied bonding skeletal orbitals (a_1 +"t_2") and four antibonding vacant ones (a_1* +"t_2*"). Values in parentheses indicate the occupation of the $[(CuCNMe)_4]$ and $[(ZnCp)_4]$ fragment orbitals in the $[(CuCNMe)_4(ZnCp)_4]$ cluster. The MO plots are those of the above-discussed orbitals. Only one of the occupied "t_2" component of $[(CuCNMe)_4(ZnCp)_4]$ is shown for clarity.

Table S3. Cartesian coordinates of the optimized geometries

$[(CuCNMe)_4(ZnCp)_4]$ PBE0/Def2TZVP; D_{2d} symmetry; Energy = -14981.9780265 a. u.

Atom	X	Y	Z (Angstrom)
Zn	2.158921	0.000000	1.516765
Zn	-2.158921	0.000000	1.516765
Zn	0.000000	2.158921	-1.516765
Zn	0.000000	-2.158921	-1.516765
C	3.144819	0.000000	3.668787
C	3.620488	1.143356	2.986865
C	4.389568	0.706840	1.883861
C	4.389568	-0.706840	1.883861
C	3.620488	-1.143356	2.986865
C	-3.144819	0.000000	3.668787
C	-3.620488	-1.143356	2.986865
C	-4.389568	-0.706840	1.883861
C	-4.389568	0.706840	1.883861
C	-3.620488	1.143356	2.986865
C	-0.706840	4.389568	-1.883861
C	-1.143356	3.620488	-2.986865
C	0.000000	3.144819	-3.668787
C	1.143356	3.620488	-2.986865
C	0.706840	4.389568	-1.883861
C	0.706840	-4.389568	-1.883861
C	1.143356	-3.620488	-2.986865
C	0.000000	-3.144819	-3.668787
C	-1.143356	-3.620488	-2.986865
C	-0.706840	-4.389568	-1.883861
H	2.526277	0.000000	4.554583
H	3.431101	2.171307	3.260009
H	4.888908	1.343260	1.167740
H	4.888908	-1.343260	1.167740
H	3.431101	-2.171307	3.260009
H	-2.526277	0.000000	4.554583
H	-3.431101	-2.171307	3.260009
H	-4.888908	-1.343260	1.167740
H	-4.888908	1.343260	1.167740
H	-3.431101	2.171307	3.260009
H	-1.343260	4.888908	-1.167740
H	-2.171307	3.431101	-3.260009

12

H	0.000000	2.526277	-4.554583
H	2.171307	3.431101	-3.260009
H	1.343260	4.888908	-1.167740
H	1.343260	-4.888908	-1.167740
H	2.171307	-3.431101	-3.260009
H	0.000000	-2.526277	-4.554583
H	-2.171307	-3.431101	-3.260009
H	-1.343260	-4.888908	-1.167740
Cu	1.255333	0.000000	-0.890417
Cu	-1.255333	0.000000	-0.890417
Cu	0.000000	1.255333	0.890417
Cu	0.000000	-1.255333	0.890417
C	2.796587	0.000000	-1.985928
N	3.744109	0.000000	-2.660279
C	4.889728	0.000000	-3.475174
H	5.787322	0.000000	-2.854251
H	4.895213	0.888564	-4.108948
H	4.895213	-0.888564	-4.108948
C	-2.796587	0.000000	-1.985928
N	-3.744109	0.000000	-2.660279
C	-4.889728	0.000000	-3.475174
H	-5.787322	0.000000	-2.854251
H	-4.895213	-0.888564	-4.108948
H	-4.895213	0.888564	-4.108948
C	0.000000	2.796587	1.985928
N	0.000000	3.744109	2.660279
C	0.000000	4.889728	3.475174
H	0.000000	5.787322	2.854251
H	0.888564	4.895213	4.108948
H	-0.888564	4.895213	4.108948
C	0.000000	-2.796587	1.985928
N	0.000000	-3.744109	2.660279
C	0.000000	-4.889728	3.475174
H	0.000000	-5.787322	2.854251
H	-0.888564	-4.895213	4.108948
H	0.888564	-4.895213	4.108948

[(CuCNMe)$_4$(ZnCp)4] PBE0/Def2TZVP; S$_4$ symmetry; Energy = -14981.9780316 a. u.

Atom	**X**	**Y**	**Z (Angstrom)**
Zn	2.159200	0.000027	1.516745
Zn	-2.159200	-0.000027	1.516745
Zn	-0.000027	2.159200	-1.516745
Zn	0.000027	-2.159200	-1.516745
C	3.160114	-0.008046	3.660116
C	3.629378	1.139448	2.980565
C	4.392651	0.709523	1.871006
C	4.395422	-0.704015	1.864395
C	3.633865	-1.147294	2.969877
C	-3.160114	0.008046	3.660116
C	-3.629378	-1.139448	2.980565

13

C	-4.392651	-0.709523	1.871006
C	-4.395422	0.704015	1.864395
C	-3.633865	1.147294	2.969877
C	-0.709523	4.392651	-1.871006
C	-1.139448	3.629378	-2.980565
C	0.008046	3.160114	-3.660116
C	1.147294	3.633865	-2.969877
C	0.704015	4.395422	-1.864395
C	0.709523	-4.392651	-1.871006
C	1.139448	-3.629378	-2.980565
C	-0.008046	-3.160114	-3.660116
C	-1.147294	-3.633865	-2.969877
C	-0.704015	-4.395422	-1.864395
H	2.547432	-0.013287	4.549961
H	3.439922	2.165678	3.260001
H	4.886113	1.350255	1.154659
H	4.891230	-1.336070	1.141984
H	3.448317	-2.176881	3.239424
H	-2.547432	0.013287	4.549961
H	-3.439922	-2.165678	3.260001
H	-4.886113	-1.350255	1.154659
H	-4.891230	1.336070	1.141984
H	-3.448317	2.176881	3.239424
H	-1.350255	4.886113	-1.154659
H	-2.165678	3.439922	-3.260001
H	0.013287	2.547432	-4.549961
H	2.176881	3.448317	-3.239424
H	1.336070	4.891230	-1.141984
H	1.350255	-4.886113	-1.154659
H	2.165678	-3.439922	-3.260001
H	-0.013287	-2.547432	-4.549961
H	-2.176881	-3.448317	-3.239424
H	-1.336070	-4.891230	-1.141984
Cu	1.254845	-0.000216	-0.891167
Cu	-1.254845	0.000216	-0.891167
Cu	0.000216	1.254845	0.891167
Cu	-0.000216	-1.254845	0.891167
C	2.799969	0.000216	-1.980922
N	3.751167	0.000837	-2.650094
C	4.901876	0.002348	-3.457853
H	5.790314	0.137627	-2.838515
H	4.845936	0.816139	-4.182992
H	4.981881	-0.945591	-3.992842
C	-2.799969	-0.000216	-1.980922
N	-3.751167	-0.000837	-2.650094
C	-4.901876	-0.002348	-3.457853
H	-5.790314	-0.137627	-2.838515
H	-4.845936	-0.816139	-4.182992
H	-4.981881	0.945591	-3.992842
C	-0.000216	2.799969	1.980922
N	-0.000837	3.751167	2.650094

C	-0.002348	4.901876	3.457853
H	-0.137627	5.790314	2.838515
H	0.945591	4.981881	3.992842
H	-0.816139	4.845936	4.182992
C	0.000216	-2.799969	1.980922
N	0.000837	-3.751167	2.650094
C	0.002348	-4.901876	3.457853
H	0.137627	-5.790314	2.838515
H	-0.945591	-4.981881	3.992842
H	0.816139	-4.845936	4.182992

[(ZnCNMe)4(CuCp)4] PBE0/Def2TZVP

D2d symmetry

Energy = -14981.9018933 a. u.

Atom	**X**	**Y**	**Z (Angstrom)**
Cu	2.107488	0.000000	1.482082
Cu	-2.107488	0.000000	1.482082
Cu	0.000000	2.107488	-1.482082
Cu	0.000000	-2.107488	-1.482082
C	2.992584	0.000000	3.569696
C	3.468894	1.144868	2.887006
C	4.239457	0.707552	1.782559
C	4.239457	-0.707552	1.782559
C	3.468894	-1.144868	2.887006
C	-2.992584	0.000000	3.569696
C	-3.468894	-1.144868	2.887006
C	-4.239457	-0.707552	1.782559
C	-4.239457	0.707552	1.782559
C	-3.468894	1.144868	2.887006
C	-0.707552	4.239457	-1.782559
C	-1.144868	3.468894	-2.887006
C	0.000000	2.992584	-3.569696
C	1.144868	3.468894	-2.887006
C	0.707552	4.239457	-1.782559
C	0.707552	-4.239457	-1.782559
C	1.144868	-3.468894	-2.887006
C	0.000000	-2.992584	-3.569696
C	-1.144868	-3.468894	-2.887006
C	-0.707552	-4.239457	-1.782559
H	2.386740	0.000000	4.464292
H	3.297035	2.172920	3.171692
H	4.752790	1.344293	1.076698
H	4.752790	-1.344293	1.076698
H	3.297035	-2.172920	3.171692
H	-2.386740	0.000000	4.464292
H	-3.297035	-2.172920	3.171692
H	-4.752790	-1.344293	1.076698
H	-4.752790	1.344293	1.076698
H	-3.297035	2.172920	3.171692

15

H	-1.344293	4.752790	-1.076698
H	-2.172920	3.297035	-3.171692
H	0.000000	2.386740	-4.464292
H	2.172920	3.297035	-3.171692
H	1.344293	4.752790	-1.076698
H	1.344293	-4.752790	-1.076698
H	2.172920	-3.297035	-3.171692
H	0.000000	-2.386740	-4.464292
H	-2.172920	-3.297035	-3.171692
H	-1.344293	-4.752790	-1.076698
Zn	1.281193	0.000000	-0.905880
Zn	-1.281193	0.000000	-0.905880
Zn	0.000000	1.281193	0.905880
Zn	0.000000	-1.281193	0.905880
C	2.932900	0.000000	-2.121870
N	3.854475	0.000000	-2.819831
C	4.974016	0.000000	-3.673530
H	5.887358	0.000000	-3.077464
H	4.952307	0.890064	-4.303544
H	4.952307	-0.890064	-4.303544
C	-2.932900	0.000000	-2.121870
N	-3.854475	0.000000	-2.819831
C	-4.974016	0.000000	-3.673530
H	-5.887358	0.000000	-3.077464
H	-4.952307	-0.890064	-4.303544
H	-4.952307	0.890064	-4.303544
C	0.000000	2.932900	2.121870
N	0.000000	3.854475	2.819831
C	0.000000	4.974016	3.673530
H	0.000000	5.887358	3.077464
H	0.890064	4.952307	4.303544
H	-0.890064	4.952307	4.303544
C	0.000000	-2.932900	2.121870
N	0.000000	-3.854475	2.819831
C	0.000000	-4.974016	3.673530
H	0.000000	-5.887358	3.077464
H	-0.890064	-4.952307	4.303544
H	0.890064	-4.952307	4.303544