Inorganic Chemistry
including bioinorganic chemistry
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Table S1. Crystal data and structure refinement for 1.

Identification code	frt
Empirical formula	$C_8 H_{16} Cu N_6 O_4$
Formula weight	323.81
Temperature	293(2) K
Wavelength	0.71069 Å
Crystal system	monoclinic
Space group	P 2(1)/n (No. 14)
Unit cell dimensions	a = 10.0116(10) Å α = 90 deg
	b = 5.6665(8) Å β = 99.71(2) deg
	c = 11.6338(12) Å γ = 90 deg
Volume	650.53(13) $Å^3$
Z	2
Density (calculated)	1.653 Mg/m^3
Absorption coefficient	1.700 mm^{-1}
F(000)	334
Crystal size	0.057 × 0.255 × 0.770 mm
Theta range for data collection	2.49 to 29.98 deg.
Index ranges	$-14 \le h \le 14, -7 \le k \le 1, -16 \le l \le 16$
Reflections collected	4249
Independent reflections	1884 [R(int) = 0.0134]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1883 / 0 / 120
Goodness-of-fit on F^2	1.082
Final R indices [$I>2\sigma$ (I)]	R1 = 0.0259, wR2 = 0.0719
R indices (all data)	R1 = 0.0352, wR2 = 0.0804
Largest diff. peak and hole	0.393 and -0.363 e. $Å^{-3}$

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($Å^2 \times 10^3$) for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Cu(1)	5000	0	0	35(1)
N(2)	3390(1)	1950(3)	-103(1)	43(1)
C(3)	3177(2)	3643(3)	599(1)	36(1)
N(4)	4035(1)	4564(3)	1487(1)	38(1)
C(5)	5264(2)	3656(3)	1788(1)	37(1)
N(6)	5801(2)	1853(3)	1352(1)	45(1)
O(7)	1918(1)	4590(2)	400(1)	45(1)
C(8)	1614(2)	6400(4)	1177(2)	52(1)
O(9)	6069(1)	4734(2)	2701(1)	48(1)
C(10)	5516(2)	6742(4)	3209(2)	59(1)

Table S3. Bond lengths (Å) and angles (deg) for 1.

Cu(1)-N(2)	1.9416(14)	C(5)-O(9)	1.364(2)
Cu(1)-N(2)#1	1.9416(14)	N(6)-H(6)	0.78(2)
Cu(1)-N(6)#1	1.9478(14)	O(7)-C(8)	1.434(2)
Cu(1)-N(6)	1.9478(14)	C(8)-H(81)	0.97(3)
N(2)-C(3)	1.300(2)	C(8)-H(82)	0.93(2)
N(2)-H(2)	0.71(2)	C(8)-H(83)	0.85(3)
C(3)-N(4)	1.333(2)	O(9)-C(10)	1.436(2)
C(3)-O(7)	1.354(2)	C(10)-H(101)	0.96(3)
N(4)-C(5)	1.325(2)	C(10)-H(102)	0.88(3)
C(5)-N(6)	1.297(2)	C(10)-H(103)	0.88(3)
N(2)-Cu(1)-N(2)#1	180.0	C(5)-N(6)-H(6)	111(2)
N(2)-Cu(1)-N(6)#1	91.87(6)	Cu(1)-N(6)-H(6)	123(2)
N(2)#1-Cu(1)-N(6)#1	88.13(6)	C(3)-O(7)-C(8)	117.78(14)
N(2)-Cu(1)-N(6)	88.13(6)	O(7)-C(8)-H(81)	110(2)
N(2)#1-Cu(1)-N(6)	91.87(6)	O(7)-C(8)-H(82)	106.1(14)
N(6)#1-Cu(1)-N(6)	180.0	H(81)-C(8)-H(82)	102(2)
C(3)-N(2)-Cu(1)	127.10(11)	O(7)-C(8)-H(83)	114(2)
C(3)-N(2)-H(2)	108(2)	H(81)-C(8)-H(83)	118(3)
Cu(1)-N(2)-H(2)	125(2)	H(82)-C(8)-H(83)	106(2)
N(2)-C(3)-N(4)	128.53(14)	C(5)-O(9)-C(10)	117.19(14)
N(2)-C(3)-O(7)	115.51(13)	O(9)-C(10)-H(101)	109(2)
N(4)-C(3)-O(7)	115.96(14)	O(9)-C(10)-H(102)	107(2)
C(5)-N(4)-C(3)	120.10(14)	H(101)-C(10)-H(102)	105(3)
N(6)-C(5)-N(4)	129.02(14)	O(9)-C(10)-H(103)	113(2)
N(6)-C(5)-O(9)	115.34(13)	H(101)-C(10)-H(103)	117(3)
N(4)-C(5)-O(9)	115.62(14)	H(102)-C(10)-H(103)	106(3)
C(5)-N(6)-Cu(1)	126.81(11)		

Symmetry transformations used to generate equivalent atoms: #1 -x+1,-y,-z

Table S4. Anisotropic displacement parameters (Å × 10^3) for 1. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2a^2U_{11} + ... + 2hkabU_{12}]$

	U11	U22	U33	U23	U13	U12
Cu(1)	29(1)	41(1)	34(1)	-6(1)	-2(1)	3(1)
N(2)	32(1)	50(1)	43(1)	-11(1)	-9(1)	6(1)
C(3)	30(1)	40(1)	36(1)	2(1)	1(1)	3(1)
N(4)	34(1)	43(1)	35(1)	-5(1)	-1(1)	3(1)
C(5)	33(1)	43(1)	31(1)	-3(1)	-2(1)	-2(1)
N(6)	31(1)	53(1)	44(1)	-12(1)	-9(1)	8(1)
O(7)	33(1)	53(1)	46(1)	-7(1)	-4(1)	11(1)
C(8)	44(1)	57(1)	55(1)	-7(1)	5(1)	15(1)
O(9)	39(1)	56(1)	42(1)	-16(1)	-9(1)	3(1)
C(10)	55(1)	58(1)	58(1)	-24(1)	-4(1)	3(1)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for 1.

	x	y	z	U(eq)
H(2)	2782(23)	1792(40)	-515(20)	53(6)
H(6)	6518(25)	1596(40)	1698(21)	56(6)
H(81)	2066(26)	7854(46)	1026(22)	69(7)
H(82)	703(26)	6778(41)	937(20)	58(6)
H(83)	1678(30)	5961(62)	1879(29)	89(9)
H(101)	5316(32)	7953(56)	2624(28)	95(10)
H(102)	6177(31)	7341(53)	3726(26)	87(9)
H(103)	4869(31)	6361(53)	3598(25)	78(9)

Table S6. Calculated bonding and atomic characteristics for **1**[a)]

	QR-INDO/1			*ab initio*		
Bond A-B	R_{A-B}	W_{A-B}	E_{A-B}	P_{A-B}[b)]		
Cu1-N2	1.930	0.75	-24.5	0.13		
N2-C3	1.293	1.43	-57.1	0.89		
C3-N4	1.343	1.30	-56.3	0.88		
C3-O7	1.353	1.03	-44.5	0.67		
O7-C8	1.427	1.02	-41.5	0.37		
C8-H81	1.100	0.97	-28.4	0.78		
N2-H21	1.044	0.92	-27.9	0.64		
	QR-INDO/1		*ab initio*			
Atom A	Q_A	N_z	Q_A^{Mul}	Q_A^{SEN-2}	Q_A^{SEN-n}	N_z
N2	-0.29	1.49	-0.87	-0.64	-0.56	1.59
C3	+0.60	0.82	+0.84	+0.58	+0.60	0.75
N4	-0.54	1.44	-0.74	-0.66	-0.62	1.53
O7	-0.22	1.81	-0.64	-0.44	-0.43	1.87
C8	+0.03	1.01	-0.01	+0.15	+0.12	1.10
H81	+0.03		+0.14	+0.09	+0.05	
H21	+0.16		+0.27	+0.17	+0.14	

[a)] Numbering of atoms according to Fig.1. Distances in Å, energies in eV, charges in e.

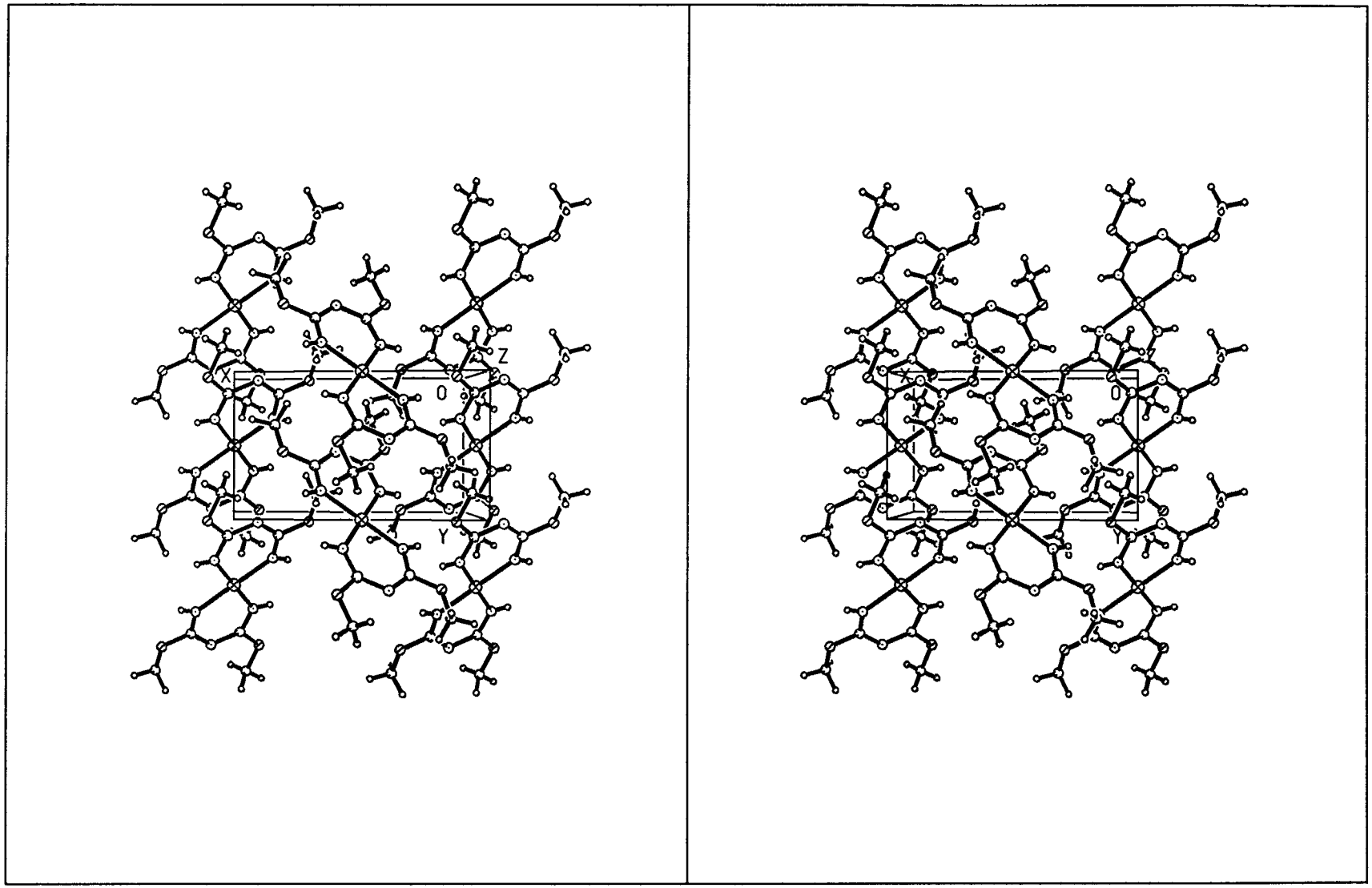
[b)] P_{A-B} - Mulliken overlap population.

Table S7. Total molecular energies

System	Basis set [a]	Geometry [b]	Version	Energy/eV
$N(CN)_2^-$	dzp	1(o)	RHF	-6505.41
			+MP2	-6526.56
		2(f)	RHF	-6499.24
CH_3OH	dzp	3(o)	RHF	-3129.90
			+MP2	-3139.82
$L=N(C(NH)OCH_3)_2^-$	dzp	4(f)	RHF	-12764.86
		5(o)	RHF	-12765.11
			+MP2	-12806.44
Cu	dz		RHF	-44568.23
$[Cu(N(CN)_2)_2]$	dz/dzp	IV(f)	UHF	-57593.64
[CuL2]	dz/dz	III(f)	UHF	-70114.20
[CuL2]	dz/dz	III(f)	RHF	-70114.14
$[CuL2]^-$	dz/dz	III(f)	RHF	-70110.54
$[CuL2]^+$	dz/dz	III(f)	RHF	-70105.02
[CuL2]	dz/dzp	III(f)	RHF	-70127.02

[a] Basis set extent: metal/ligand.

[b] o - optimized geometry, f - fixed.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