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Structure and Magnetic Behavior of a New 1-D Compound with Simultaneous End-On Azido and Carboxylato Bridges. Unexpected Strong Ferromagnetic Coupling for a Cu−N−Cu Bond Angle of 111.9° as a Consequence of Ligand HOMOs Countercomplementarity

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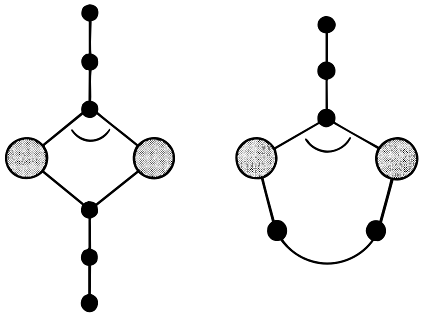
The X-ray structure of the μ-carboxylate$-\mu_{1,1}$-azido-bridged compound $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$ has been determined (Hpht = hydrogen phthalate). Crystal data: formula $C_8H_7CuN_3O_5$, monoclinic, $P2_1/m$ (No. 11), $a = 7.383(3)$ Å, $b = 6.568(4)$ Å, $c = 10.659(4)$ Å, $\beta = 93.38(3)°$, $Z = 2$. The compound is found to be a system formed by chains of copper atoms bridged simultaneously by *syn*−*syn* carboxylato and end-on azido bridges. The copper chains are linked by a second carboxylato bridge, giving a 2-D compound. Magnetic measurements indicate strong ferromagnetic coupling, which affords a good example of unexpected magnetic properties due to the countercomplementarity of the superexchange pathways of the two ligands.

Introduction

Polynuclear compounds bridged by the azido ligand show different magnetic behaviors according to the coordination mode of the bridge: generally, end-to-end ($1,3$-μ-N_3) allows antiferromagnetic interactions whereas the end-on ($1,1$-μ-N_3) bridge allows ferromagnetic interactions.[1] In the past few years the end-to-end coordination mode has been exhaustively studied and the dependence of the antiferromagnetic component of J on structural parameters has been established for Cu and Ni[2] and even the predicted ferromagnetic behavior for large M−N−N bond angles has been experimentally found.[3] Correlations of this kind have recently been extended to the Mn(II)−1,3-azido system.[4]

For the end-on azido bridge, the most common kind of compound shows two azido bridges with M−N−M bond angles in the 100−106° range for M = Cu, Ni and Mn(II).[5] Recently, some larger Cu−N−Cu angles have been reported by Thompson, (up to 122.5°), in series of dinuclear compounds with two simultaneous bridges, one end-on azido bridge and one pyridazine bridge.[6]

From magnetic measurements performed on compounds of this kind it has been proposed that the accidental orthogonality in the end-on azido bridge occurs at Cu−N−Cu bond angles close to 108°, and so antiferromagnetic interaction should be found for greater Cu−N−Cu bond angles. Following the characterization of the magnetic properties of large M−N−M end-on azido compounds, in this paper we present the synthesis and structural characterization of the end-on azido-bridged compound $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$ which shows a Cu−N−Cu bond angle of 111.9(1)°. The title compound was obtained following the strategy of mixing different potential bridging ligands with the copper salt. The most interesting property was the very strong ferromagnetic coupling attributable to the countercomplementarity of the ligands HOMO. The magnetic properties of the title compound were compared with the copper−μ-diazine−μ-azido system and the global magnetic



Cu-N-Cu = 100-106° **Cu-N-Cu up to 120°**

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Table 1. Crystallographic Data and Processing Parameters for the $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$ Complex

formula	$C_8H_7CuN_3O_5$	V, Å^3	516.0(4)
fw	288.71	Z	2
space group	monoclinic $P2_1/m$	T, °C	25
	(No. 11)	λ(Mo Kα), Å	0.71069
a, Å	7.383(3)	μ(Mo Kα), mm^{-1}	2.13
b, Å	6.568(4)	D_{calc}/D_{obs} (g/cm^{-3})	1.858/1.85(3)
c, Å	10.659(4)	$R(F)^a$	0.028
β, deg	93.38(3)	$R_w(F)^a$	0.029

^{a} $R(F) = \Sigma\{|F_o| - |F_c|\}/\Sigma F_o$. $R_w(F) = [w\Sigma(|F_o| - |F_c|)^2/\Sigma wF_o^2]^{1/2}$.

properties are explained in terms of complementary−counter-complementary interactions.

Experimental Section

Synthesis. A 20 mL aliquot of an aqueous solution of copper nitrate, (3 mmol, 0.72 g), was mixed with an ethanolic solution (20 mL) of phthalic acid (4.3 mmol, 0.71 g) followed by the addition of a concentrated solution of sodium azide (3 mmol, 0.39 g). The final clear green mixture was left to stand at room temperature. Green crystals were collected after several weeks. The IR spectrum shows the characteristic bands attributable to the phthalate and strong bands at 2085 cm^{-1} (υ_{as} N$_3$) and 1307−1279 cm^{-1} (υ_s N$_3$), which suggest an asymmetric azido ligand. Anal. Calcd (Found) for $C_8H_7CuN_3O_5$: C, 33.28 (33.4); H, 2.44 (2.6); N 14.55 (14.2); Cu 22.00 (22.3).

X-ray Crystallography. A prismatic crystal (0.50 × 0.35 × 0.25 mm) was selected and mounted in a modified STOE four-circle diffractometer. Orientation matrix and lattice parameters were obtained by least-squares refinement of the diffraction data from 32 reflections in the 2θ range 10−26°. The intensities collected were corrected for Lorentz polarization and absorption[7] effects. Selected crystallographic data are given in Table 1. The structure was solved by Patterson superposition methods and subsequent Fourier analyses. Anisotropic displacement parameters were applied to the non-hydrogen atoms in full-matrix least-squares refinements. Hydrogen positions were obtained from ΔF maps and included in the final refinement cycles by geometrical constraints. The programs DIFABS,[7] SHELX-76,[8] SHELX-86,[9] PLATON,[10] and THE XRAY SYSTEM[11] were used for computations. Analytical expressions of neutral-atom scattering factors were used and anomalous dispersion corrections were incorporated.[12] Atomic coordinates are given in Table 2 and selected bond angles and distances are given in Table 3.

Results and Discussion

Description of the Structure of $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$. An ORTEP plot of the basic unit of $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$ is shown in Figure 1. The structure consists of neutral two-dimensional sheets of $[Cu(Hpht)(N_3)]$ complexes. Coordination around the copper atoms is an elongated octahedron in which the short distances correspond to two *trans* Cu(1)−O(1) bonds at 1.975(2) Å and to two *trans* Cu(1)−N(11) bonds at 1.982(2) Å, whereas the two large axial distances correspond to two Cu(1)−O(2) bonds at 2.570(4) Å. The azido ligand acts as a bridge between neighboring copper atoms in the μ_2-1,1 coordination mode. The deprotonated carboxylate group acts as a *syn*−*syn* carboxylato bridge, whereas the protonated carboxylate also acts as a bridge through the O(1) oxygen atom, the protonated O(3) atom remaining uncoordinated. The hydrogenphthalate anion shows the two carboxylate planes tilted 90°. Then, three kinds of simultaneous bridge are present in the compound, Figure 1. The C(8)−O(3) bond distance 1.304(5)

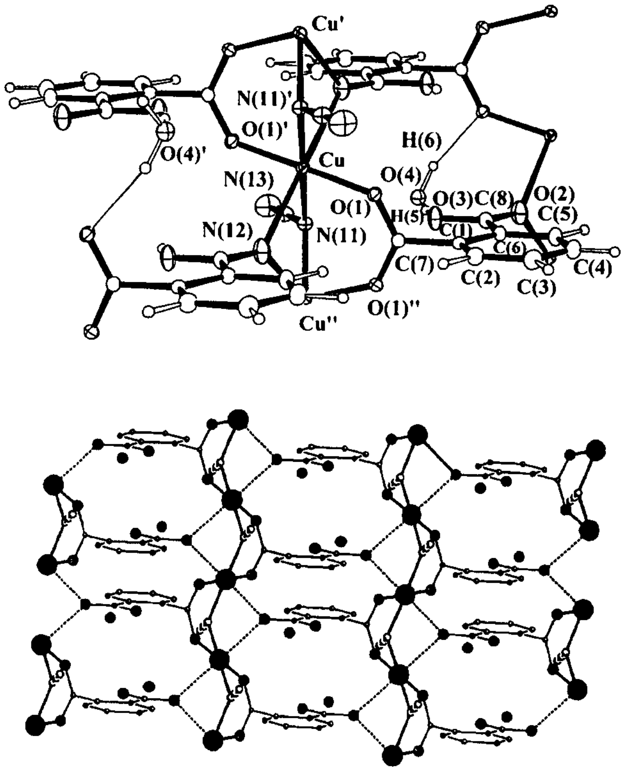

Figure 1. ORTEP (50% probability) labeled plot of $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$ and a view of a sheet of $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$ showing the three simultaneous bridges between the copper atoms and the general structure of chains weakly linked by the phthalate anions.

Table 2. Atomic Coordinates (×10^4) and U_{eq} values (Å^2 × 10^3) of Non-Hydrogen Atoms of $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$

atom	x/a	y/b	z/c	U_{eq}
Cu(1)	0	5000	0	20(0)
N(11)	673(4)	2500	−904(3)	22(1)
N(12)	709(4)	2500	−2049(3)	29(2)
N(13)	759(7)	2500	−3115(4)	60(2)
O(1)	1629(2)	4215(2)	1456(2)	24(1)
O(2)	7804(3)	2500	975(3)	45(2)
O(3)	4865(3)	2500	356(3)	40(1)
C(1)	3778(4)	2500	2802(3)	22(1)
C(2)	3325(5)	2500	4058(4)	31(2)
C(3)	4673(6)	2500	5023(4)	39(2)
C(4)	6473(6)	2500	4749(4)	41(2)
C(5)	6939(5)	2500	3516(4)	34(2)
C(6)	5615(4)	2500	2526(3)	24(2)
C(7)	2242(4)	2500	1805(3)	20(1)
C(8)	6192(4)	2500	1220(4)	28(2)
O(4)	5963(3)	2500	−1880(3)	32(1)

Table 3. Selected Bond Distances (Å) and Bond Angles (deg) for $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$

Cu(1)···Cu(1a)	3.284(2)	O(2)−C(8)	1.233(4)
Cu(1)−O(1)	1.975(2)	O(3)−C(8)	1.304(5)
Cu(1)−O(2)	2.570(4)	N(11)−N(12)	1.222(4)
Cu(1)−N(11)	1.982(2)	N(12−-N(13)	1.139(5)
O(1)−C(7)	1.262(2)		

O(1)−Cu(1)−N(11)	90.4(1)	Cu(1)−N(11)−Cu(1a)	111.9(1)
O(2)−Cu(1)−N(11)	81.4(1)	N(11)−N(12)−N(13)	179.3(6)
O(1)−Cu(1)−O(2)	83.4(1)	O(1)−C(7)−O(1a)	126.5(3)
Cu(1)−N(11)−N(12)	120.4(1)	O(2)−C(8)−O(3)	123.0(4)

Hydrogen Bond Distances

O(3)−H(5)	0.94(3)	O(4)−H(6)	0.93(3)
H(5)···O(4)	1.63(3)	H(6)···O(1)	1.94(3)
O(3)−H(5)···O(4)	1.73(4)	O(4)−H(6)···O(1)	1.57(4)
O(3)···O(4)	2.563(4)	O(4)···O(1)	2.815(3)

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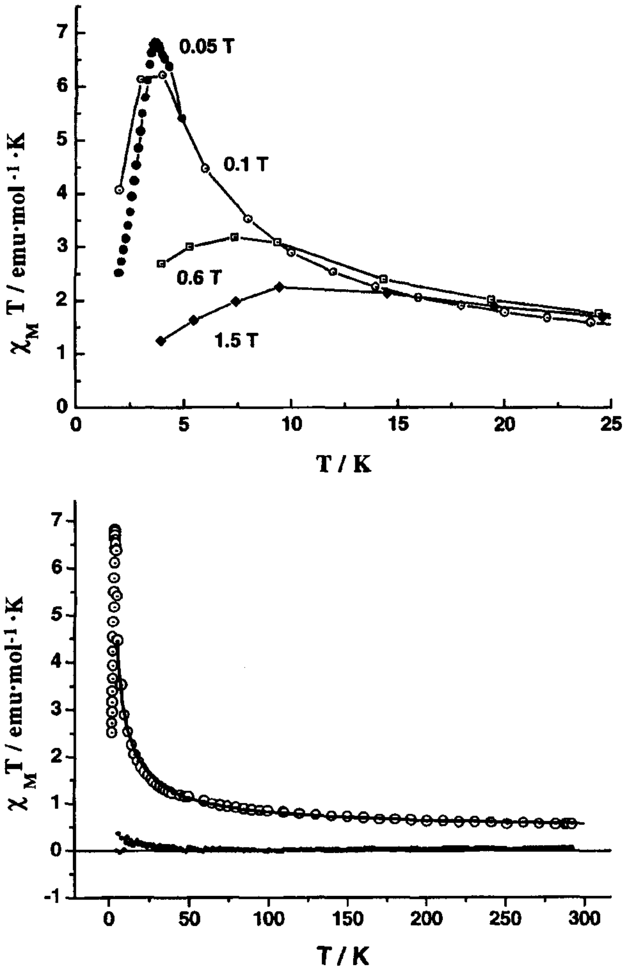

Figure 2. (**a**) $\chi_M T$ vs T plots between 25 and 2 K for $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$ measured under different fields. (b) $\chi_M T$ vs T plot between 300 and 2 K measured at 0.05 T. Solid line shows the fit up to 10 K for the measurement performed at 0.05 T.

Å, is greater than the C(8)−O(2), 1.233(4) Å, or C(7)-O(1), 1.262(2) Å, bond distances; the N(11)−N(12) bond distance, 1.222(4) Å, is also larger than the N(12)−N(13) distance, 1.139(5) Å, as is common for end-on azido bridges. The water molecule forms a set of hydrogen bonds that involves the O(1) and O(3) oxygen atoms: O(3)−H(5) = 0.94(3) Å, H(5)−O(4) = 1.63(3) Å, O(4)−H(6) = 0.93(3) Å, and finally H(6)−O(1) = 1.94(3) Å. O(3)−O(4) and O(4)−O(1) distances are 2.563(4) and 2.815(3) Å, respectively. From the magnetic point of view, the most appropriate description of the structure is as quasi-isolated chains of copper atoms bridged simultaneously by one end-on azido and one *syn*−*syn* carboxylato bridge, with a Cu−Cu distance of 3.282(2) Å. Superexchange through the pathway provided by the large axial bonds to O(2) atoms can be expected not relevant due to the low unpaired electronic density along the d_{z^2} atomic orbital in the octahedral coordination around the copper atoms.

Magnetic Behavior. The $\chi_M T$ value increased when the temperature decreased, indicating ferromagnetic behavior. The high $\chi_M T$ value at low temperature indicates that the compound acts as a ferromagnetic chain, consistent with the structural data. The plots of $\chi_M T$ vs T, measured at several fields between 1.5 and 0.05 T are given in Figure 2. The dependence of the plot on the applied magnetic fields confirms the ferromagnetic interaction. The superexchange parameter $J = 75$ cm^{-1} was obtained from the expansion series expression proposed by Baker[13] based on the Hamiltonian $-{}^1/_2 J\sum S_i\cdot S_j - (\mu H)\sum S_{zi}$ and assuming $g = 2.16$, from experimental EPR data

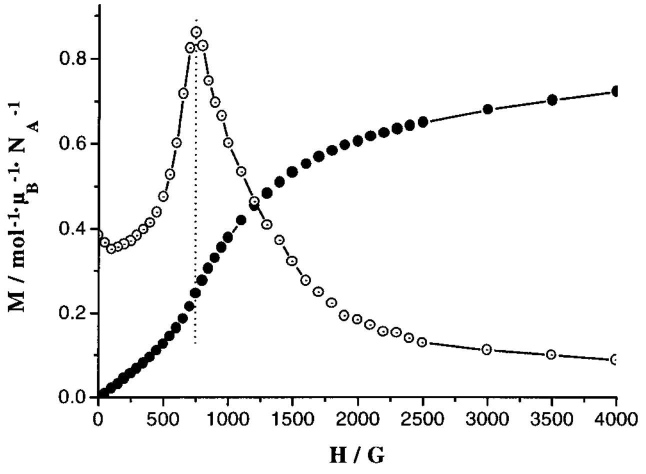

Figure 3. Magnetization measurement for $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$ (magnetization, solid circles; first derivative, open circles), showing the metamagnetic behavior at very low fields, pointing out the very low interchain antiferromagnetic coupling.

$$\chi_M = N_A g^2\beta^2/4kT[\mathrm{NM/DN}]^{2/3}$$

where

$$\mathrm{NM} = 1.0 + 5.79799x + 16.902653x^2 + 29.376885x^3 + 29.832959x^4 + 14.036918x^5$$

$$\mathrm{DN} = 1.0 + 2.79799x + 7.008678x^2 + 8.6538644x^3 + 4.5743114x^4$$

and $x = J/2kT$.

The decay at low temperatures, due to antiferromagnetic interactions in the 2-D sheets, was evaluated from a magnetization experiment as $J' = -0.07$ cm^{-1} (Figure 3). EPR measurements performed at variable temperature show well-defined signals at $g_{\parallel} = 2.32$ and $g_{\perp} = 2.09$ between 300 and 15 K. Below this temperature the intensity of the signal decreases continuously due probably to a saturation effect due to an increase in the relaxation time. Shift of the resonance field[14] at low temperature found for strongly ferromagnetic coupled copper(II) chains[15] was not observed for the title compound.

According to the structural data, the strong ferromagnetic interaction corresponds to the superexchange through the carboxylato−azido-bridged chains, whereas the very weak antiferromagnetic interaction may be propagated by the poorly efficient phthalato ligand which links the chains at long distance.

Magnetostructural Correlations. The net superexchange constant coupling found between the copper atoms in the title compound corresponds to the combined interactions due to the single *syn*−*syn* carboxylato and the end-on azido bridges. Compounds derived from the copper acetate structure show typical J values close to −300 cm^{-1} for four simultaneous bridges,[16] but less efficient superexchange was found in compounds with one or two carboxylato bridges, as a function of the structural parameters that may reduce the overlap between

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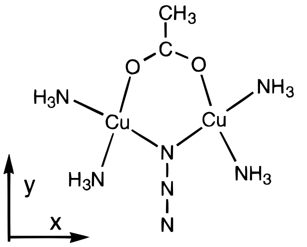
the atomic orbitals of the copper atoms and the appropiatete MOs of the carboxylato bridge. A parametric approach to the J values has been pointed out by Wieghardt[17] by means of the relationship between J/n and the Cu−O−C bond angle in which n is the number of carboxylate bridges. Taking into account the large Cu−O(1)−C(7) bond angle of the single carboxylato bridge (131°) in the title compound, a moderately weak antiferromagnetic behavior should be expected.

Thompson et al.[6] have proposed that the accidental orthogonality for the 1,1-azido bridge takes place at a Cu−N−Cu bond angle close to 108°, on the basis of measurements performed on series of diazine-azido bridged compounds. For larger angles the antiferromagnetic behavior of the 1,1-azide bridge increases to the maximum $J = -921$ cm^{-1} value found for the [$Cu_2(PPD35Me)(\mu_2\text{-}N_3)Br_3(CH_3OH)$] compound, (Cu−N−Cu 122.5°).[6] From these considerations, a moderately antiferromagnetic behavior should also be expected for the azido bridge of the title compound taking into account the Cu−N−Cu bond angle of 111.9°.

To explain the apparently anomalous net ferromagnetic behavior of $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$ we chose a dimeric fragment under C_{2v} symmetry which models the superexchange pathway of the chain:



In this model the coordination sites of the copper atoms not involved in the bridging region have been replaced by NH_3 molecules. The MO calculations were performed by means of the CACAO program.[18]

In the above dimeric fragment, the magnetically active atomic orbitals of the copper atoms are the $d_{x^2-y^2}$ orbitals, which allows the symmetric ϕ_S and the antisymmetric ϕ_A combinations (A_1 and B_2 respectively under C_{2v}). From the proposal of Hoffmann,[19] the square of the gap between the two antibonding ϕ_S and ϕ_A, named Δ^2, is proportional to the antiferromagnetic component of the J constant coupling. To transmit the antiferromagnetic coupling, the most useful molecular orbitals of the two bridges are the highest filled MOs, which have A_1 symmetry for the acetate and B_2 for the azido ligands. The antibonding character of ϕ_S is then enhanced by the overlap with the appropiate MO of the acetate bridge, whereas ϕ_A overlaps with the Π_{xy} MO of the azido group as is shown in Figure 4a. The gap between the two MOs ϕ_S and ϕ_A should be lower than the interaction with the two "antiferromagnetic" ligands due to the **countercomplementarity** of the ligand HOMOs. Incidentally, if this countercomplementary interaction of the bridging ligands allows a very low Δ value, it is possible to find a net ferromagnetic interaction from two ligands which commonly allow antiferromagnetic coupling. MO extended Hückel calculations for the above model give $\Delta^2 = 0.005$ eV^2, ($E(\phi_S) = -11.544$ eV and $E(\phi_A) = -11.614$ eV), e.g., quasi-degenerate ϕ_S and ϕ_A levels.

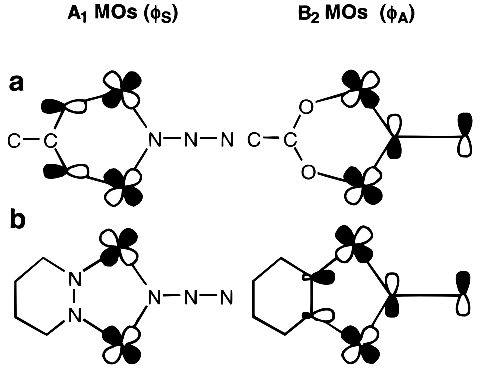


Figure 4. Bridging HOMOs complementarity and noncomplementarity for the pyridazine−azido and the carboxylato−azido systems. (a) Each ligand interacts with one of the two A_1 or B_2 combinations of the atomic $d_{x^2-y^2}$ orbitals, giving a low Δ value. (b) The two HOMOs of the ligands interact with the same combination B_2, giving large Δ and J_{AF} values.

Table 4. Bond Magnetic Data for a Set of Mixed Bridged Copper Compounds with Similar Cu−N−Cu Bond Angles[a]

compound	Cu−N−Cu	J (cm^{-1})	interaction
[$Cu_2(PAP)(\mu_{1,1}\text{-}N_3)Br_3$]	108.7	−241	C
[$Cu_2(PAP6Me)(\mu_{1,1}\text{-}N_3)(\mu\text{-}Br)Br_2$]	110.9	−234	C
[$Cu_2(PAP6Me)(\mu_{1,1}\text{-}N_3)(\mu\text{-}H_2O)\text{-}(NO_3)_2]^+$	111.7	−187	C
[$Cu_2(PAN)(\mu_{1,1}\text{-}N_3)(\mu\text{-}NO_3)(NO_3)_2$]	111.1	−220	C
$\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$	111.9	+75	counter-C

[a] Data for PAP and PAN phthalazines were taken from ref 6). Notations C and counter-C refer to the complementary or counter-complementary kind of interaction between the ligand HOMOs and the active atomic orbitals of the copper atoms.

It is interesting to compare the magnetic properties of $\{[Cu(Hpht)(N_3)]\cdot H_2O\}_n$ with the pyridazine-1,1-azido system described by Thompson: using the same C_{2v} symmetry, the HOMO of the pyridazine has B_2 symmetry, as occurs with the Π_{xy} of the azido bridge: in this case ϕ_A MO results strongly unstabilized due the **complementary** antibonding overlap, allowing a high Δ and consequently a high J_{AF}, Figure 4b. The magnetic data for a homogeneous group of copper compounds with the Cu−N−Cu bond angle between 108.7 and 111.9° are shown in Table 4.

The copper-azido vs. carboxylate or diazine bridges described above is a new example of an unusual kind of complementary−countercomplementary magnetic system, pointed out by McKee[20] for the [$Cu_2(L\text{-}Et)(\mu\text{-}L)]^{2+}$ series of complexes, (HL-Et = *N*,*N*,*N′*,*N′*-tetrakis(2-(1-ethylbenzimidazolyl)-2-hydroxy-1,3-diaminopropane), in which countercomplementarity was found for the acetate derivative, $J = +24$ cm^{-1}, whereas the complementary systems with μ-L = $\mu_{1,3}$-N_3 and μ-NO_2 bridges show values of $J = -1100$ and -278 cm^{-1}, respectively.

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Supporting Information Available: Text giving details of the structure determination and tables of crystallographic data, complete bond lengths and angles, atom coordinates, thermal parameters, and hydrogen atom coordinates (7 pages). Ordering information is given on any current masthead page.

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