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Structural and Magnetic Studies on a Bromine-Bridged Copper(II) Dimer with 5,7-Dimethyl[1,2,4]triazolo[1,5-*a*]pyrimidine

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The crystal structure of the compound bis(μ-bromo)bis[bromobis(dmtp)copper(II)] dihydrate (where dmtp = 5,7-dimethyl[1,2,4]triazolo[1,5-*a*]pyrimidine) has been determined from single-crystal X-ray diffraction methods. The crystal belongs to the triclinic system, space group $P\bar{1}$, with $a = 9.614(4)$ Å, $b = 12.370(6)$ Å, $c = 9.645(4)$ Å, $\alpha = 99.01(3)°$, $\beta = 60.17(3)°$, $\gamma = 79.61(4)°$, $Z = 2$, $D_{\mathrm{calcd}} = 1.906$ g·cm^{-3}, $R = 0.053$ for 2188 observed reflections. The structure of the complex consists of dimeric molecules $[\mathrm{Cu(dmtp)_2Br_2}]_2$ in which copper atoms are bridged by bromine ligands. The geometry at copper is a distorted trigonal bipyramid with bromine atoms occupying equatorial positions and N3-coordinated dmtp ligands in apical posistions. The Cu−Cu separation is 3.603(3) Å, and Cu−bridging Br distances are 2.588(2) and 2.706(2) Å. The magnetic susceptibility of a powdered sample has been measured in the 4.1−250.5 K temperature range and the data have been fitted to the modified Bleany−Bowers equation for exchange coupled copper(II) dimers indicating an antiferromagnetic coupling with a singlet-triplet separation of approximately 20 cm^{-1}. A comparison to other bis(μ-bromine)-bridged five-coordinated copper dimers has been made, showing that the magnetic interaction strength can be correlated to the arrangement of bromine atoms around the copper.

Introduction

Metal−metal interactions in metal dimeric complexes can be studied through experimental results or theoretical treatments. Bulk magnetic susceptibility measurements constitute the principal means by which metal−metal interactions between paramagnetic transition metal ions have been identified and studied, although in most cases there is not a clear understanding of the real origin of this coupling, δ bond, σ bond, and superexchange and what kind of superexchange.

The search of empirical relationships relating structural characteristic of bis(μ-hydroxo)- and bis(μ-chloro)-bridged copper(II) complexes to their magnetic properties has been an intensively studied field, as evidenced by numerous recent papers.[1−7] Thus Marsh *et al.*,[3] in their studies on five-coordinated dimeric bis(μ-chloro)copper(II) complexes of the type $[\mathrm{CuA_2Cl_2}]_2$ and $[\mathrm{CuLCl_2}]_2$ (where A and L are monodentate and bidentate ligands, respectively), have found a strong correlation between the 2J value and the structural parameter ϕ/R (ϕ is the Cu−Cl−Cu′ bridging angle and R is the longer Cu-Cl' bridge bond distance). However, in the case of the bis(μ-bromo)copper(II) dimers, Landee and Greeney[6] have shown that the dominant factor controlling the superexchange strength is not related to the bridging angle but instead to the amount of distortion within the copper basal plane.

Previous crystal structure determinations of metal compounds containing the ligand 5,7-dimethyl[1,2,4]triazolo[1,5-*a*]pyrimidine (dmtp) have revealed that binding principally occurs via the N3 position of this ligand[8,9] although a bidentate coordination mode via N3 and N4 has been observed in the tetranuclear copper(I) complex $[\mathrm{Cu_4(dmtp)_4Cl_2}][\mathrm{Cu_2Cl_4}]$[10] in which two $\mathrm{Cu_2(dmtp)_2}$ units are bridged by two chloro ligands.

Experimental Section

Starting Materials. 5,7-Dimethyl[1,2,4]triazolo[1,5-*a*]pyrimidine (dmtp) was purchased from Aldrich Chem. Co. and used as received. Chemical reagents were supplied from commercial sources. All preparative manipulations were carried out at room temperature in an open atmosphere.

Synthesis of $[\mathrm{Cu(dmtp)_2Br_2}]_2{\cdot}2\mathrm{H_2O}$. A clear solution of dmtp (0.296 g, 2 mmol) in *ca.* 15 mL of water was added to a sky-blue solution of $\mathrm{CuBr_2}$ (0.447 g, 2 mmol) in *ca.* 15 mL of $\mathrm{H_2O}$ at room temperature. By slow evaporation of the solvent in air over several days dark green crystals of the compound were obtained; yield 0.453 g (84%). Anal. Calcd for $\mathrm{C_{14}H_{18}N_8OBr_2Cu}$: C, 31.26; H, 3.35; N, 20.84. Found: C, 31.21; H, 3.35; N, 20.88. Molar conductivity: 60 Ω^{-1}·cm^2·M^{-1} (DMF).

Physical Measurements. Microanalysis of C, H, and N were performed with a Perkin Elmer 240C analyzer by the Technical Services of the University of Granada. The infrared spectrum was recorded in the 4000−180 cm^{-1} range on a Perkin Elmer

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Table 1. Crystallographic Data

chem formula: $C_{14}N_{18}N_8Br_2CuO$	fw = 537.7
$a = 9.614(4)$ Å	cryst syst: triclinic
$b = 12.370(6)$ Å	space group: $P\bar{1}$
$c = 9.645(4)$ Å	temp = 18 °C
$\alpha = 99.01(3)°$	$\lambda = 0.710\,69$ Å (Mo Kα)
$\beta = 60.17(3)°$	$\varrho_{calc} = 1.906$ grcm^{-3}
$\gamma = 79.61(4)°$	$\mu = 54.5$ cm^{-1}
$V = 937.1(7)$ Å^3	$R = 0.053^a$
$Z = 2$	$R_w = 0.066^b$

[a] $R = \Sigma(||F_o| - |F_c||)/\Sigma|F_o|$. [b] $R_w = \Sigma(||F_o| - |F_c||w^{1/2})/\Sigma(|F_o|w^{1/2})$; $w = (\sigma^2(F) + 0.04F^2)^{-1}$.

983G spectrophotometer, using KBr and polyethylene pellets. The diffuse reflectance spectrum was obtained in a Schimadzu MPC-3100 refractometer. TG and DSC diagrams were obtained on a Mettler TA-3000 equipment provided with a Mettler TG-50 thermobalance and a DSC-20 differential scanning calorimeter at a heating rate of 10 K·min^{-1}, using an atmosphere of pure air (100mL·min^{-1}).

Magnetic measurements in the 4.1–250.5 K temperature range were recorded on a Manics DSM-8 equipment. Diamagnetic correction term (Pascal) and temperature independent paramagnetism were taken as was -543×10^{-6} and 120×10^{-6}emu·(mol of dimer)$^{-1}$. EPR spectra were measured at room temperature on a Varian E-9 (X-band *ca.* 9.5 GHz) and a Bruker 200D-SRC (Q-band, *ca.* 34 GHz) spectrophotometers. Both spectra indicate axial-type structure with $g_{\parallel} = 2.22$ and $g_{\perp} = 2.05$.

Crystal Structure Determinations. Relevant crystallographic data are presented in Table 1. A crystal, dimensions 0.17 × 0.27 × 0.12 mm was mounted on a Stoe-Siemens AED-2 diffractometer. A total of 4077 unique reflection intensities were measured in the range $3 < 2\theta < 65°$. The intensity data were corrected for Lorentz and polarization effects and empirically (ψ scans) for absorption (transmission ranges are 0.46–0.25). 2188 reflections with $F > 5\sigma(F)$ were considered as observed. The structure was solved by the heavy atom method, and non-hydrogen atoms were refined anisotropically by full-matrix least squares. Hydrogen atoms were refined isotropically. Maximum peak in the final ΔF map was 1.02 e·Å^{-3}. Maximum Δ/σ in the last cycle = 0.30. Goodness of fit was 0.46. Calculations were made in a Microvax II computer with the SHELXTL PLUS program package.[11] Final atomic coordinates have been collected in Table 2.

Results and Discussion

Infrared spectra of free dmtp and the complex are virtually identical above 300 cm^{-1}, differing only by the presence of absorption bands at 3508 and 3468 cm^{-1} associated with ν(OH) of water molecules. Far-infrared absorptions at 244 and 197 cm^{-1} have been assigned to terminal and bridging bromine groups, respectively. The electronic spectrum (diffuse reflectance) at room temperature has a major absorption with a low energy shoulder (12 600, 10 500 cm^{-1}) typical of a distorted trigonal-bipyramidal copper(II) complex.[12] The ligand-to-metal charge-transfer transition occurs at 21 700 cm^{-1}. This band has been considered to be characteristic of the bridging system since it does not appear in other monomeric copper(II) complexes of dmtp.[13]

Table 2. Atomic Coordinates (×10^4) and Equivalent Isotropic Displacement Coefficients (Å^2 × 10^3) for $[CuBr_2(DMTP)_2]_2{\cdot}2H_2O$

	x	y	z	U(eq)^a
Cu	24(2)	3539(1)	4387(1)	32(1)
Br1	−429(2)	1730(1)	3636(1)	41(1)
Br2	2149(1)	4380(1)	4732(1)	33(1)
N1A	1627(11)	4021(8)	−327(8)	31(4)
C2A	544(13)	4220(9)	1303(9)	35(4)
N3A	1189(10)	3576(8)	2006(8)	30(3)
C3aA	2774(12)	2904(8)	735(9)	31(4)
N4A	3913(12)	2134(8)	729(10)	38(4)
C5A	5342(12)	1633(9)	−724(11)	31(4)
C51A	6624(15)	732(11)	−789(14)	45(5)
C6A	5682(13)	1891(10)	−2185(10)	38(4)
C7A	4483(15)	2715(10)	−2187(11)	39(5)
C71A	4678(16)	3084(15)	−3650(12)	61(7)
N8A	3014(11)	3202(9)	−689(8)	36(4)
N1B	−3212(10)	4037(9)	9537(8)	35(4)
C2B	−2760(11)	4219(9)	8087(9)	28(4)
N3B	−1165(10)	3551(8)	6797(8)	34(3)
C3aB	−599(12)	2894(8)	7498(9)	27(4)
N4B	860(11)	2046(8)	6807(9)	36(4)
C5B	1026(14)	1545(10)	7818(11)	39(5)
C51B	2557(16)	597(13)	7091(14)	50(6)
C6B	−201(15)	1843(12)	9585(12)	49(6)
C7B	−1685(13)	2732(10)	10256(9)	37(4)
C71B	−3070(17)	3115(14)	12050(11)	56(6)
N8B	−1869(10)	3217(8)	9175(8)	33(4)
O1W	3988(15)	1231(12)	3369(11)	74(7)

[a] Equivalent isotropic U defined as one-third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor.

The thermal behavior has been deduced from its TG and DSC curve. An outstanding feature in the latter is a small endothermic peak that can be seen in the 35–65 °C temperature range (maximum at 47 °C), which has been assigned to a phase transition, TG analysis showing no weight change at this point. The ΔH value of *ca.* 8.6 kJ·mol^{-1} is in good agreement with those previously found for other crystalline phase transitions.[14] The powder X-ray diffraction pattern has been recorded immediately below and above the phase transition temperature, the patterns of both phases being significantly different. Many of the diffraction lines of the room temperature phase diagram are reproduced in the high-temperature one with just a small shift to lower Bragg angles but with notorious changes in the intensity of a few lines. It seems to indicate that there is a change in the internal structure but without a major change in the unit cell. On the basis of these results and taking into account that the triclinic structure of the compound is not so far away from monoclinic symmetry (see below), we propose that a triclinic–monoclinic transition takes place when the sample is heated around 60 °C. The proposed monoclinic form is thermally stable up to 120 °C, a dehydration process starting at this temperature and overlapping with the fusion of the sample (total ΔH for the two processes, 136 kJ·mol^{-1}). Immediately after this point, the pyrolytic decomposition starts, and it finishes around 750 °C.

Description of the Structure. The molecular structure of the complex is shown in Figure 1. Crystal data are collected in Table 1, atomic coordinates are found in Table 2, and selected interatomic distances and angles are listed in Table 3. The structure consists of centrosymmetric dimeric $[Cu(dmtp)_2Br_2]_2{\cdot}2H_2O$ units, in which two bromine atoms bridge the copper atoms forming a four membered ring. Earlier results with $CuBr_2$ and the unsubstituted ligand 1,2,4-triazolo[1,5-*a*]pyrimidine (tp)[15] have shown that the complex, with molecular formula $[Cu(tp)_2Br_2{\cdot}H_2O]$, consists of monomeric molecules in which

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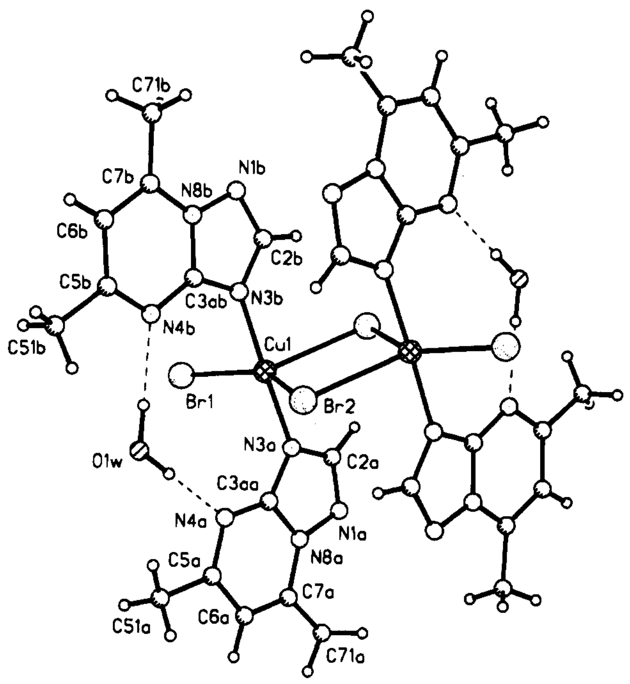

Figure 1. Molecular structure of $[Cu(dmtp)_2Br_2]_2 \cdot 2H_2O$ (I).

Table 3. Selected Bond Distances and Angles for $[Cu(dmtp)_2Br_2]_2 \cdot 2H_2O$

	Bond Distances (Å)		
Cu–N3A	2.006(8)	Cu–Br2	2.588(2)
Cu–N3B	2.012(7)	Cu–Br2′	2.706(2)
Cu–Br1	2.425(2)		
	Hydrogen Bonds (Å)		
O1W–N4A	2.963(9)	O1W–N4B	2.999(8)
	Bond Angles (deg)		
N3A–Cu–N3B	178.4(4)	N3B–Cu–Br2′	89.7(3)
N3A–Cu–Br1	91.0(3)	Br1–Cu–Br2	141.9(1)
N3A–Cu–Br2	89.8(3)	Br1–Cu–Br2′	124.0(1)
N3A–Cu–Br2′	88.8(2)	Br2–Cu–Br2′	94.1(1)
N3B–Cu–Br1	90.4(3)	Cu–Br2–Cu′	85.9(1)
N3B–Cu–Br2	89.6(3)		

the copper atom is surrounded by two N3 atoms of two tp ligands, two Br atoms, and the oxygen atom of the water molecule in a trigonal bipyramidal geometry. In our case, copper(II) atoms exhibit the same geometry, but the coordination sphere is formed by three equatorial Br atoms (one terminal and two bridging) and two apical N3 atoms of the dmtp ligands.

The Cu–N distances (see Table 3) are in good agreement with those reported in the literature for other copper(II) complexes of the dmtp ligand.[13,16,17] The terminal Cu–Br1 distance (2.425(2) Å) is within the range of values (2.37–2.43 Å) reported for the other structurally similar compounds listed in Table 4, as well as the angles within the four member ring Cu–Br2–Cu′ and Br2–Cu–Br2′. On the other hand, the bridging Cu–Br2 and Cu–Br2′ distances are less dissimilar than those in the other compounds in Table 4, in which there is a short distance in the range 2.42–2.56 Å and a longer one in the range 2.71–3.87 Å.

The four bromine atoms together with the two copper atoms of the dimer are coplanar, the major deviation from the mean plane of ±0.002 Å being exhibited by the metal ions. Water oxygen is also placed very close of this plane (0.099 Å), hydrogen-bond linked to the N4 atoms of the two ligands. The dimer exhibits a point symmetry very close to $2/m$ and the whole structure is not too far away from monoclinic symmetry, supergroup $C2/c$.

The two dmtp moieties are planar as in other triazolopyrimidine complexes,[8–10,13,16,17] deviations from the respective mean planes being below 0.05 Å. The metal atom is displaced from these planes 0.008 and 0.069 Å. The two dmtp molecules are nearly coplanar, the dihedral angle between their planes being 2.5°, and they are almost perpendicular to the Cu_2Br_4 plane (dihedral angles, 90.1 and 91.4°).

Several complexes of types $[CuA_2Br_2]_2$ and $[CuLBr_2]_2$ with CuN_2Br_3 chromophores have been reported in the literature (Table 4). A precise description of the geometry of these complexes can be obtained by application of Muertterties and Guggenberger's presciption involving dihedral angles between the various faces of the polyhedron.[18] However, these are rarely tabulated in the literature. By this reason we have calculated for these systems the structural index τ to show the relative amount of trigonality (square pyramid $\tau = 0$; trigonal bipyramid $\tau = 1$), defined by Addison *et. al*[19] as $\tau = (\beta - \alpha)/60$, where α and β are the two largest angles around the central atom. The results of these calculations are also shown in Table 4, in which the compound $[Cu(TMSO)_2Br_2]_2$ (chromophore CuO_2Br_3) has also been included by structural similarity. The distortion of the coordination polyhedron of our compound has been also calculated by quantification[20] of the Muertterties and Guggenberger description.[18] The value obtained, $\Delta = 0.26$ (Table 5) is also indicative of a geometry nearer to trigonal bipyramid ($\Delta = 0$, trigonal bipyramid; $\Delta = 1$, tetragonal pyramid).

Magnetic Studies. Susceptibility values per mole of dimer as a function of the temperature have been plotted in Figure 2. The dominant features of the data are a maximum near 20 K and a rapid decrease to zero at lower temperatures, indicating antiferromagnetism within a cluster compound. The solid curve in Figure 2 is the best fit of the data to the modified Bleaney–Bowers equation for exchange-coupled copper(II) dimers:

$$\chi_M = \frac{(2Ng^2\mu^2)}{k(T - \Theta)\left(3 + \exp\left(\frac{-2J}{kT}\right)\right)}(1 - \varrho) + \frac{Ng^2\mu^2}{2kT}\varrho$$

which results from a consideration of the eigenvalues of $H = -2JS_1S_2$, the Heisenberg exchange Hamiltonian. In this expression χ_M represents the susceptibility per mole of dimer corrected for diamagnetism and temperature independent paramagnetism $-2J$ is the exchange coupling constants and the parameter Θ accounts for the interdimer coupling of spins throughout the lattice. The last term in the expression is a correction for the presence of a monomeric impurity suggested by the very low T points (ϱ is the proportion of such impurity).

An attempt to fit the data to the isolated dimer (Bleaney–Bowers model, $\Theta = 0$) gave a poor fit in the region around the maximum of χ_M. This suggests that interdimer interaction has certain importance. The parameters J, g, Θ, and ϱ were taken as adjustable parameters in a least-squares fitting procedure that led to the values $2J = -30.4$ K (-21.1 cm^{-1}), $g = 2.17$, $\Theta =$

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Table 4. Structural Indices for Bis(μ-bromo)-Bridged Cu(II) Dimers

compd[a]	α, deg	β, deg	τ[b]	ΔR,[c] Å	2J, cm^{-1}	geometry	struct type[d]	refs
$[Cu(2\text{-pic})_2Br_2]_2$	176.2	176.2	0	1.446(8)	−5	TP	AE	22
$[Cu(DMG)Br_2]_2$	166.0	167.5	0.025	0.496	−3	TP	AE	23
$[Cu(4\text{-metz})_2Br_2]_2$	171.9	169.2	0.045	0.541(2)	−2.48	TP	AE	24
$[Cu(dmen)Br_2]_2$	166.2	172.9	0.11	0.405(4)	−2	TP	AE	25
$[Cu(tmen)Br_2]_2$	173.2	158.3	0.25	0.78	−4	TP	AE	26
$[Cu(4\text{-meox})_2Br_2]_2$	157.2	172.7	0.26	0.154(2)	−15.2	TP	EE	27
$[Cu(DPM)Br_2]_2$	176.5	154.8	0.36	0.316(2)	+2.6	TP	AE	7, 28
$[Cu(TMSO)_2Br_2]_2$	139.6	169.9	0.505	0.520	−33.8	TBP	EE	6
$[Cu(MAEP)Br_2]_2$	172.8	141.6	0.52	0.334(6)	−4.2	TBP	AE	29
$[Cu(dmtp)_2Br_2]_2{\cdot}2H_2O$	141.7	179.0	0.62	0.118(4)	−21.1	TBP	EE	this work

[a] Abbreviations: 2-pic = 2-methylpyridine; DMG = dimethylglyoxime; 4-metz = 4-methylthiazole; dmen = *N,N*-dimethylethylenediamine; tmen = *N,N,N',N'*-tetramethylethylenediamine; 4-meox = 4-methyloxazole; DPM = 2-pyridylmethane; TMSO = tetramethylene sulfoxide; MAEP = 2-(2-(methylamino)ethyl)pyridine; dmtp = 5, 7 dimethyl-1,2,4-triazolo[1,5-*a*]pyrimidine. [b] Trigonality index defined as $\tau = |\beta - \alpha|/60$ ($\tau = 0$ for a tetragonal pyramid, TP and $\tau = 1$ for a trigonal bipyramid, TBP). α and β are the largest X−Cu−X angles. [c] Difference between the two Cu−bridging Br distances. [d] See text for definitions of AE and EE structural types.

Table 5. Dihedral angles (deg) and distortion (Δ) for the Coordination Polyhedron of $[Cu(dmtp)_2Br_2]_2{\cdot}2H_2O$, As Proposed by Galy *et al.*[20] Compared to Ideal Trigonal Bipyramid (TBP) and Regular Tetragonal Pyramid (TP) Structures[a]

dihedral angles	TBP	compound I	TP
δa_1	101.5	108.4	119.8
δa_3	101.5	108.9	119.8
δa_4	101.5	93.3	119.8
δa_6	101.5	93.9	119.8
δe_1	53.1	61.4	75.7
δe_2	53.1	83.2	75.7
δa_2	101.5	96.0	75.7
δa_5	101.5	95.4	75.7
δe_3	53.1	45.2	0
Δ	0	0.264	1

[a] Dihedral angles are defined in ref 18. Distortion parameter is defined as $\Delta = |\delta a_1 + \delta a_3 + \delta a_4 + \delta a_6 - 406|/164.7 + |\delta e_1 + \delta e_2 - 106.2|/203.4 + |203 - \delta a_2 - \delta a_5|/232.2 + |53.1 - \delta e_3|/477.9$

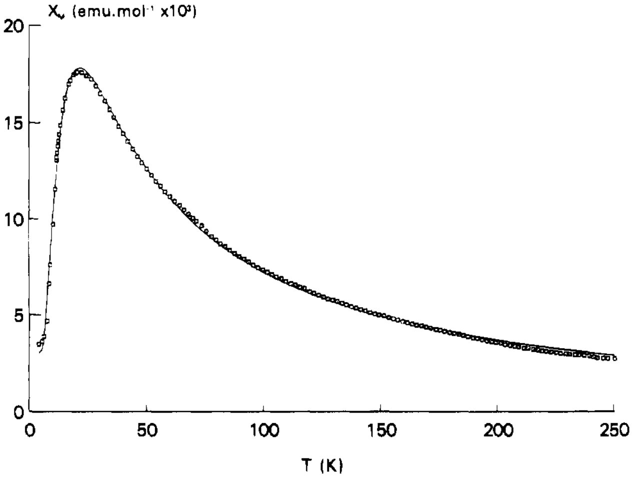

Figure 2. Magnetic susceptibility per mole of dimer of $Cu_2(dmtp)_4Br_4{\cdot}2H_2O$ plotted as a function of temperature. The solid line corresponds to the theoretical prediction for the data based on modified Bleany−Bowers equation (see text) with best-fit parameters $2J = -30.4$ K, $g = 2.17$, $\Theta = -6.3$ K, and $\varrho = 0.0155$.

-6.3 K and $\varrho = 0.0155$. The agreement factor R defined as $\Sigma(\chi_{Mcalc}\text{-}\chi_{Mobserv})^2/\chi_{Mobs}{}^2$. is then equal to 5.86×10^{-4}.

The obtained value of Θ is surprisingly high, since the shortest distance between atoms in neighbouring Cu_2Br_6 units is 5.508(3) Å (Br1−Br1($-x$, $-y$, $1 - z$)) and other clear interdimer interaction that could justify this value has not been found. However, it must be emphasized that a strong correlation of J with Θ is present, and so the uncertainty in both values is quite large. Likewise, it should be concluded only that in this complex the first triplet state lies approximately 20 cm^{-1} higher in energy over the ground singlet state.

Since Cu−Cu distance within the dimer is 3.606(3) Å, direct metal orbital overlap between the two copper can be ruled out and we may assume that the exchange is supported by the bromine bridging ligands. In Table 4, we have collected structural and magnetic data reported in the literature for five-coordinated dimeric copper(II) complexes with bromine bridging ligands. A correlation may be established between the arrangement of the ligands around the metal and the value of $2J$, considering the geometry in all cases as trigonal bipyramids, even if very distorted (a tetragonal pyramid can be considered as the limit case of distortion of a trigonal bipyramid via the Berry rearrangement mechanism). According to this, the compounds in Table 4 can be divided into two groups, those with one bridging bromine atom in axial and the other in equatorial position (type AE) and those with the two bridging bromine atoms in equatorial position (type EE). It is important to emphasize that types AE and EE are not interchangeable via a Berry mechanism. It is observed in Table 4 that the compounds type EE display significantly larger exchange constants than those type AE.

Another possible correlation could be found looking to bond distances instead of bond angles. Table 4 also shows that the magnetic interaction is bigger for the compounds in which the two Cu−bridging Br distances are less different to each other ($[Cu(4\text{-meox})_2Br_2]_2$ and $[Cu(dmtp)_2Br_2]_2$) though the compound $[Cu(TMSO)_2Br_2]_2$, the only one with oxygen instead of nitrogen atoms in the non-bromine positions, clearly does not follow this rule.

Antimicrobial Studies. The determination of minimum inhibitory concentration (MIC) of the dmtp ligand and its complex against *Pseudomonas* sp., *Escherichia coli*, *Proteus*

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sp., *Salmonella* sp., *Micrococcus* sp., *Staphylococcus* sp., *Bacillus* sp., and *Candida* sp. was performed according to a technique described elsewhere.[21] The growth-inhibitory activity of the compounds tested toward above microorganisms clearly indicate that in the experimental conditions used, the ligand dmtp is inactive against all assayed microorganisms in concentrations up to 2000 $\mu g \cdot cm^{-3}$. However, the copper compound shows a considerable biological activity toward some Gram(−) bacteria (*E. coli*, *Proteus* sp., and *Salmonella* sp.; MIC lower than 50 $\mu g \cdot cm^{-3}$) and MIC's in the range 100−500 $\mu g \cdot cm^{-3}$ for the other microorganisms.

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Supplementary Material Available: Tables of anisotropic thermal parameters, bond distances and angles, H-atom coordinates, and magnetic susceptibility data (5 pages). Ordering information is given on any current masthead page.