

Correction to Highly Organized Structures and Unusual Magnetic Properties of Paddlewheel Copper(II) Carboxylate Dimers Containing the π - π Stacking, 1,8-Naphthalimide Synthons [*Inorganic Chemistry* 2009, 48, 8911–8924 DOI: 10.1021/ic901138h]. Daniel L. Reger,* Agota Debreczeni, Bryn Reinecke, Vitaly Rassolov, Mark D. Smith, and Radu F. Semeniuc

Page 8911. The last sentence of the Abstract should read: Magnetic measurements show that the compounds are strongly antiferromagnetically coupled with J values ranging from -270 to -341 cm^{-1} , values typical for these types of dimers.

Page 8913. The assumption made in this paper that the gelatin capsules used to hold the samples in the SQUID measurements “make a negligible contribution to the overall magnetization” is

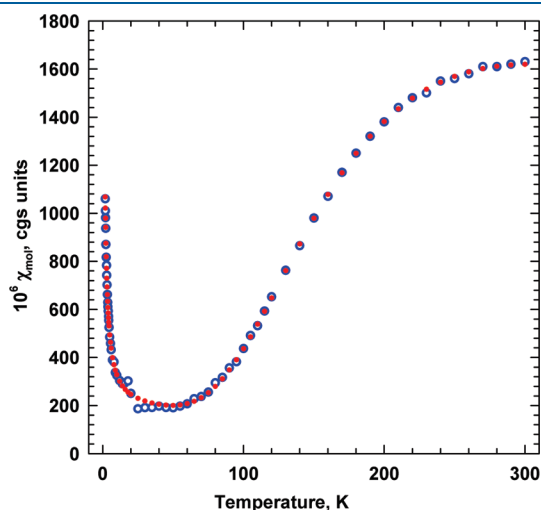


Figure 18. Magnetic susceptibility of **2**. Blue circles are data points, and red dots indicate the total fit for $J = -341\text{ cm}^{-1}$ and $g = 2.175$.

incorrect for the $3d^9$, strongly antiferromagnetically coupled copper(II) compounds reported in this paper. New data sets (the magnetic susceptibility has been remeasured using a MPMS-XL-5 SQUID magnetometer at the Faculty of Chemistry, Wrocław University, Wrocław, Poland), in which the susceptibility of the sample container was measured independently and the data were corrected appropriately, have been collected and analyzed.

Page 8921. The Magnetic Properties section should read as follows:

Magnetic Properties. The magnetic susceptibilities of **1**, **2**, and **3** were investigated and show antiferromagnetic behavior, as expected.¹² The magnetic behavior of **2** is typical and is illustrated in Figure 18 (page 9823, Figure corrected as shown here). The values, using the Hamiltonian $\mathcal{H} = -JS_1 \cdot S_2$, are, for **1**, $J = -321\text{ cm}^{-1}$ and $g = 2.169$, for **2**, $J = -341\text{ cm}^{-1}$ and $g = 2.175$, and for **3**, $J = -270\text{ cm}^{-1}$ and $g = 2.175$ (the g values were verified by EPR analysis: Ozarowski, A., unpublished results). The values for compound **4** could not be remeasured due to the formation of a mixture of polymorphs, but reevaluation of the earlier data (measured on the polymorph reported in the manuscript) indicates that the values for this compound are similar to those reported above. The copper(II) ions in these compounds are strongly antiferromagnetically coupled, but not to the degree indicated in the original paper.

Page 8923. The last three paragraphs of the Discussion section should be replaced with the following: Complexes that contain the paddlewheel $\text{Cu}_2(\text{O}_2\text{CCH}_3)_4$ building unit are known to possess very strong antiferromagnetic interaction between the unpaired electrons of the Cu(II) centers.¹² This interaction is mediated by superexchange via the four bridging carboxylates and leads to a singlet ground state and a thermally populated triplet excited state.¹² The singlet–triplet energy gap is characterized by the J parameter, which expresses the magnitude of the intramolecular exchange interaction. This exchange interaction is known to be influenced by several factors, including the stereochemistry of the Cu(II) ions, the bridging mode of the ligand, the bond angles at the bridging

Table 4. Structural Parameters of Carboxylato-Bridged Cu(II) Compounds

compound	Cu–Cu (Å)	Cu–O (basal) (Å)	Cu–L (axial) (Å)	O–C (Å)	Cu–O–C (deg)	O–C–O (deg)	$-J$ (cm^{-1})
$\text{Cu}_2(\text{CH}_3\text{COO})_4(\text{py})_2^a$	2.630(3)	1.981(10)	2.126(10)	1.239(18)	123.4(7)	125.1(9)	325
$\text{Cu}_2(\text{CH}_3\text{COO})_4(\text{py})_2^b$	2.645(3)	1.955(8)	2.186(8)	1.244(18)	123.4	125.6	
$\text{Cu}_2(\text{CH}_3\text{COO})_4(2\text{-pic}^c)_2$	2.671	1.975(10)	2.240(12)	1.244(14)	121.7(10)	125.9(14)	318
$[\text{Cu}_2(\text{CH}_3\text{COO})_4(4,4'\text{-bipy})]_n \cdot \text{DMF}$	2.6037(8)	1.969	2.169(3)	1.247	123.45	124.6	
$[\text{Cu}_2(\text{fum}^d)_2(4,4'\text{-bipy})] \cdot 0.5\text{H}_2\text{O}$	2.675(1)	1.970	2.144	1.258	123.9	124.1	296
$\text{Cu}_2(\text{C}_3\text{H}_7\text{COO})_4$	2.584(1)	1.961		1.255	123.5	124.6	322
$\{[\text{Cu}_2(\text{glu}^e)_2(\text{bpmp}^f)](\text{H}_2\text{O})_4\}_n$	2.6513(7)	1.9697	2.179(2)	1.258	123.63	124.85	283(8)
$[\text{Cu}_2(\text{L}_{\text{C}2})_4(\text{py})_2](\text{CH}_2\text{Cl}_2)_2(\text{CH}_3\text{OH})$ (1)	2.6572(6)	1.9691	2.164(2)	1.258	123.06	125.55	321
$[\text{Cu}_2(\text{L}_{\text{C}3})_4(\text{py})_2](\text{CH}_2\text{Cl}_2)_2$ (2)	2.6632(5)	1.9718	2.1796(18)	1.258	123.65	125.15	341
$[\text{Cu}_2(\text{L}_{\text{C}2})_4(4,4'\text{-bipy})] \cdot \text{unknown solvent}$ (3)	2.6870(9)	1.9808	2.120(3)	1.257	123.28	125.1	270
$[\text{Cu}_2(\text{L}_{\text{C}3})_4(4,4'\text{-bipy})](\text{CH}_2\text{Cl}_2)_{3.37}(\text{CH}_3\text{OH})_2$ (4)	2.6147(8)	1.9725	2.150(3)	1.257	123	124.9	

^a Monoclinic. ^b Orthorhombic. ^c pic = picoline. ^d fum = fumarate. ^e glu = glutarate. ^f bpmp = N,N' -bis(4-pyridyl)piperazine.

atoms, and the copper–bridge ligand bond lengths. Table 4 (page 8924, Table corrected as shown here) shows the structural parameters and J values for the new complexes reported here and similar $\text{Cu}_2(\text{O}_2\text{CR})_4(\text{L})_2$ -type compounds.^{12,22} The structural parameters for the new complexes and the J values are very similar to those reported previously, with the exception of compound 3, where the $\text{Cu}\cdots\text{Cu}$ distance is longer and the absolute J value somewhat lower. As mentioned earlier, the geometry in 3 is also more distorted toward trigonal-bipyramidal, as indicated by an increase in the τ parameter. Rodriguez-Fortea et al.¹⁷ concluded that for these types of complexes an increase of the τ parameter leads to a decrease of the anti-ferromagnetic coupling, as observed with 3.

Page 8924. The last sentence of the Conclusion section should be changed to the following: These new complexes all show antiferromagnetic interactions that are typical of this class of compounds.

The following additional text should be added to the Acknowledgment: The authors thank Dr. Julia Jezierska of the Faculty of Chemistry, Wroclaw University, Wroclaw, Poland, for collecting the magnetic data and Dr. Andrew Ozarowski of the National High Magnetic Field Laboratory, The Florida State University, Tallahassee, FL, for his analysis of the data and supplying the EPR results prior to publication.

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