ADDENDA AND ERRATA

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Structure of Bis(2,2′-bipyridyl)(saccharinato-*N*)copper(II) Saccharinate Dihydrate. Addendum

ORHIDEJA GRUPČE,[a] GLIGOR JOVANOVSKI,[a] BOJAN ŠOPTRAJANOV[a] AND ANTONIJA HERGOLD-BRUNDIĆ[b]

[a]*Institut za hemija, PMF, Univerzitet 'Sv. Kiril i Metodij', PO Box 162, 91001 Skopje, Macedonia, and* [b]*Laboratory of General and Inorganic Chemistry, Faculty of Science, University of Zagreb, PO Box 153, 41001 Zagreb, Croatia. E-mail: gligor@robig.pmf.ukim.edu.mk*

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Abstract

The crystal structures of bis(2,2′-bipyridyl)(saccharinato-*N*)copper(II) saccharinate dihydrate [Hergold-Brundić *et al.* (1991). *Acta Cryst.* C**47**, 2659–2660] and bis(2,2′-bipyridine)(saccharinato-*N*)copper(II) saccharinate trihydrate [Li *et al.* (1991). *Polyhedron*, **10**, 403–407] are compared. It is concluded that the subject of both papers is likely to be the same compound and that the reported water content in the trihydrate is in error.

Comment

Our determination of the crystal structure of a 2,2′-bipyridine saccharinato complex of copper (Hergold-Brundić *et al.*, 1991) gave the formula of the complex as $[Cu(bpy)_2(sac)](sac).2H_2O$, where bpy is 2,2′-bipyridyl and sac is a saccharinate anion. Almost simultaneously, the crystal structure of a complex with the formula given as $[Cu(bpy)_2(sac)](sac).3H_2O$ was published (Li *et al.*, 1991). Although, in principle, the existence of two different hydrates of a given complex is indeed possible, the quite pronounced structural similarities of these complexes suggested that the compounds studied might be identical. Therefore, we compared the two structures more closely.

Even a quick comparison of the data presented in the two papers shows that the conditions for data collection and all relevant structural parameters are very similar, with the exception of the different choice of axes and, consequently, the values for the fractional atomic coordinates†. As no table of atomic coordinates was given in the paper by Li *et al.* (1991), the coordinates were obtained from the Cambridge Structural Database (1992). However, the list of coordinates was incomplete (even for non-H atoms), since only one water O atom was given. It should also be noted, particularly in terms of the formulae of the compounds studied, that the unit-cell volume for $[Cu(bpy)_2(sac)](sac).3H_2O$ with, apparently, 24 water molecules in the unit cell is unexpectedly smaller (V = 6881 Å^3) than that of the dihydrate, which contains 16 water molecules in the unit cell (V = 6947 Å^3).

As discussed by Hergold-Brundić *et al.* (1991), in the structure of $[Cu(bpy)_2(sac)](sac).2H_2O$, two O atoms belonging to two crystallographically different water molecules occupy special positions (on twofold axes) while the third water O atom is located at a general position. This makes the complex a dihydrate, even though three distinct water-molecule sites are present. On the other hand, in the complex described as $[Cu(bpy)_2(sac)](sac).3H_2O$ (Li *et al.*, 1991), the position of only one of the O atoms [O(7)] of the water molecules is given. This O atom occupies a general position; the positions of the remaining two water O atoms [denoted O(8) and O(9)] are not discussed, except that in Table 1 of the paper by Li *et al.* (1991), two unreasonably short distances [O(8)···O(8′) 0.46 (4) and O(9)···O(9′) 0.25 (7) Å] are mentioned. These distances are not discussed further. The crystal packing is similar in both cases and features pairs of symmetry-related saccharinate anions linked to water molecules by O*W*—H···O or O*W*—H···N hydrogen bonds (Table 1).

In order to verify the number of water molecules present in the complex studied in our laboratory, thermogravimetric and differential thermal analyses were carried out. These gave 2.17 molecules of water per formula unit and confirmed the formula $[Cu(bpy)_2(sac)](sac).2H_2O$.

On the basis of the discussion above, it seems certain that the compound studied by us is a dihydrate. The pronounced structural similarities between the trihydrate and the dihydrate, the short O*W*···O*W* distances reported for the trihydrate and the relative unit-cell volumes make it very likely that the compound studied by Li *et al.* (1991) is not properly formulated and is, in fact, identical to the dihydrate we studied.

† The atomic coordinates for $[Cu(bpy)_2(sac)](sac).2H_2O$ and for $[Cu(bpy)_2(sac)](sac).3H_2O$ are related by symmetry according to $x_1 = x_2$, $y_1 = 1/2 - x_2$ and $z_1 = 3/4 - z_2$, where x_1, y_1 and z_1 correspond to the dihydrate, and x_2, y_2 and z_2 correspond to the trihydrate.

Table 1. *Hydrogen bonds (Å) in [Cu(bpy)$_2$(sac)](sac).2H$_2$O and [Cu(bpy)$_2$(sac)](sac).3H$_2$O*

	[Cu(bpy)$_2$(sac)](sac).2H$_2$O[a]	[Cu(bpy)$_2$(sac)](sac).3H$_2$O[b]
OW1···O	2.873 (8) (OW1···O11)	2.82 [O(9)···O(6)]
	2.873 (8) (OW1···O11^{i})	2.89 [O(9)···O(6′)]
OW2···O	2.828 (8) (OW2···O13)	2.64 [O(8)···O(4)]
	2.828 (8) (OW2···O13^{i})	2.94 [O(8)···O(4′)]
OW3···N	2.969 (10) (OW3···N^{i})	2.97 [O(7)···N(6)]
OW3···*X*	> 3.5	not available

Symmetry code: (i) x, $1-y$, $1-z$.

References: (*a*) Hergold-Brundić *et al.* (1991); (*b*) Li *et al.* (1991).

Supplementary data for this paper are available from the IUCr electronic archives (Reference: CF1234). Services for accessing these data are described at the back of the journal. Thermal analysis data have also been deposited.

References

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