Acta Crystallographica Section C
Crystal Structure Communications
ISSN 0108-2701

Comment on $\mu_{1,3}$-azido-diazido-tetrakis(1,10-phenanthroline)-dicopper(II) azide tetrahydrate

Ponraj Prabakaran†

RIKEN Tsukuba Institute, 3-1-1 Koyadai, Tsukuba, Ibaraki 305-0074, Japan
Correspondence e-mail: praba@rtc.riken.go.jp

Received 2 January 2002
Accepted 14 January 2002
Online 12 March 2002

The supramolecular structure of the title dimeric azido complex of copper(II), $[Cu_2(\mu_{1,3}\text{-}N_3)(N_3)_2(phen)_4](N_3)\cdot 4H_2O$ (phen is 1,10-phenanthroline, $C_{12}H_8N_2$) [Cheng, Hu, Wang & Ye (2002). *Acta Cryst.* C**58**, m12–m13], which was originally described in terms of hydrogen-bonded chains, has been re-interpreted as two-dimensional hydrogen-bonded sheets built from $R_6^4(12)$ and $R_{10}^{10}(28)$ rings, taking into account the complete hydogen-bonding pattern.

Comment

In a recent paper, Cheng *et al.* (2002) reported a dimeric azido complex of copper(II), *viz*. $[Cu_2(\mu_{1,3}\text{-}N_3)(N_3)_2(phen)_4](N_3)\cdot 4H_2O$. Although the correct formula was given, the molecular unit was described as being comprised of a dimeric cation, two azide anions and four water molecules. However, re-examination of the structure using the deposited coordinates shows that the molecular unit possesses a dimeric cation along with only one azide anion and four water molecules. This is evident from the fact that both the central N2 and N11 atoms of the two azide ions lie on the special positions at $(0,0,\frac{1}{2})$ and (0,0,0), respectively.

The authors also showed that there were hydrogen-bonding and aromatic π–π interactions producing, respectively, a one-dimensional chain and a two-dimensional supramolecular array. However, re-examination using *PLATON* (Spek, 2001) clearly reveals further relatively strong hydrogen bonds that were overlooked in the original report, namely the O1*W*—H1*WA*$\cdots$O2*W*^{i} and O2*W*—H2*WA*$\cdots$N10^{i} hydrogen bonds [symmetry code: (i) $1-x$, $-y$, $-z$]. These intermolecular hydrogen bonds are involved in the formation of a two-dimensional sheet consisting of $R_6^4(12)$ and $R_{10}^{10}(28)$ rings (Fig. 1) (Etter, 1990; Bernstein *et al.*, 1995). The $R_6^4(12)$ rings adopt a chair conformation and if the weak O1*W*—H1*WA*$\cdots$O2*W*^{i} component of the nearly planar three-centre hydrogen-bonding system is also considered, then this ring is itself divided into three smaller rings (Fig. 1), one of the $R_4^4(8)$ type and two of the $R_2^2(4)$ type.

Thus, the structure is now correctly described with a complete hydrogen-bonding pattern which dominates the overall structure and plays an important role in the crystal packing (Jeffrey, 1997).

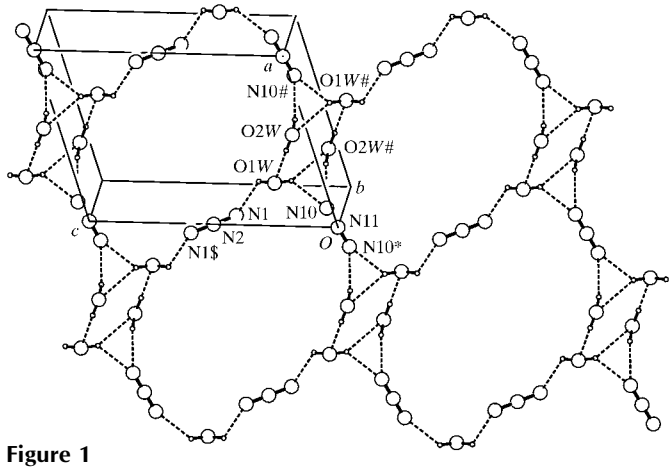

Figure 1
Part of the crystal structure depicting a two-dimensional sheet built from large and small hydrogen-bonded rings. Atoms labelled with an asterisk (*), hash (#) and dollar sign ($) are at the symmetry positions $(-x, -y, -z)$, $(1-x, -y, -z)$ and $(-x, -y, 1-z)$, respectively.

Table 1
Hydrogen-bonding geometry (Å, °).

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O1*W*—H1*WA*$\cdots$N10	0.94	2.25	2.792 (7)	116
O1*W*—H1*WA*$\cdots$O2*W*^{i}	0.94	2.53	3.369 (6)	149
O1*W*—H1*WB*$\cdots$N1	0.94	2.24	2.908 (6)	128
O2*W*—H2*WA*$\cdots$N10^{i}	0.94	2.33	3.245 (8)	163
O2*W*—H2*WB*$\cdots$O1*W*	0.94	1.92	2.857 (6)	178

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

The author wishes to thank the referees for their helpful suggestions.

Supplementary data for this paper are available from the IUCr electronic archives (Reference: GD1188). Services for accessing these data are described at the back of the journal.

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Cheng, Y.-Q., Hu, M.-L., Wang, S. & Ye, M.-D. (2002). *Acta Cryst.* C**58**, m12–m13.
Etter, M. C. (1990). *Acc. Chem. Res.* **23**, 120–126.
Jeffrey, G. A. (1997). *An Introduction to Hydrogen Bonding*. New York: Oxford University Press Inc.
Spek, A. L. (2001). *PLATON*. University of Utrecht, The Netherlands.

† The author is currently a postdoctoral fellow.