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Re-reporting the Crystal Structure of Copper Complex from Another Point of View

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Abstract

We faced an example of re-reporting of the crystal structure, which was studied from another perspective. With the development of data-driven science, the efficiency of all researchers may be improved if the rules of data "reuse", which are different from "novelty", are established. In this context, the crystal structure of a copper(II) complex with 2,6-pyridine dicarboxylic acid, $C_{14}H_8O_8CuN_2.H_2O$ (monohydrate), was re-determined by us again. It has a different number of crystalline water molecules in a crystal of the same copper(II) complex previously reported (trihydrate). Interestingly, both crystal structures have been reported again and again by many researchers for a long time. What's novelty for each report?

Keywords: Crystal structure analysis, Hirshfeld surface analysis, Hydrate, Intermolecular interaction, Copper complex

Introduction

With the development of data-driven science, the efficiency of all researchers may be improved if the rules of data "reuse", which are different from "novelty", are established along with the new era. Indeed, Aims and Scopes of *Scientific Data* published by publisher of *Nature* stated "*Scientific Data* is a peer-reviewed, open-access journal for descriptions of scientifically valuable datasets, and research that advances the sharing and reuse of scientific data. We aim to promote wider data sharing and reuse, and to credit those that share" [1].

Recently, we faced an example of his re-reporting of the crystal structure, which was studied from another perspective. To be honest, the cause was an omission when searching the database for previous studies. Regarding the contents of crystal structure analysis and the latest intramolecular interaction analysis, several previous studies were pointed out in the paper review, and publication was refused. Curiously, it turns out that the same crystal structure has been reported over and over again (monohydrate 5 and trihydrate 3 and other co-crystals a few times, respectively).

Discussion (from our point of view)

Metal complexes incorporating tridentate coordinated to mersites called pincer complexes are important for their potential applications for catalytic reactions [2]. Besides catalysis, some copper(II) complexes having two types of tridentate ligands were reported as a precursor of copper oxide materials derived from electrosynthesis [3]. Herein, in order to discuss intermolecular interactions, we determined and investigated the crystal structure of the same complex crystallized in *P*nma containing one crystalline water molecule abbreviated as "monohydrate" (**Figure 1**) (our deposition was CCDC 2115891; the first available report is [4], which was originally prepared as a starting metal complex for further reactions by accident. The previously reported crystal of the same complex has three crystalline water molecules abbreviated as "trihydrate" (the first available report is [5], in which both monohydrate and trihydrate were reported and compared for discussion of solvent [6]).

Originally, we have investigated angles between two characteristic mean planes (**Figure 2** and **Figure 3**). In addition, Hirshfeld surface analysis has been carried out for the first time [7]. For monohydrate (**Figure 4**), there were close contacts with H atoms inside the surface and H atoms outside: (H-H)=16.4%, H-O=16.8%, O-H=18.5%, C-C =11.4%, and N-C=7.3%. For trihydrate (**Figure 5**), the molecule A with dihedral angle is of 88.01(2)°: H-H=16.4%, H-O=19.1%, O-H= 30.6%, C-H=8.8%, and C-O=7.6%, and another molecule B with dihedral angle of 88.90(2)°: H-H=16.9%, H-O=18.9%, O-H=28.5%, C-H=10.0%, and H-C=3.4% [5].

Concluding Remarks

In general, crystalline water is an important factor or phenomenon related to the phase transition of crystals. This new study of intermolecular interaction is worth reporting in that it is due to the different numbers of crystalline water, as many researchers have been reported identical crystal structures repeatedly. To discuss the intermolecular interaction, we now used Hirshfeld surface analysis, which may be relativity new or current methods for crystal chemistry. This new aspect of our study (except for crystal structure report), at least, will be expected to be applied to computational chemistry prediction of crystal structure, which is currently being researched. Therefore, it was a case where we felt that research rules that could use past data with a limited range of novelty were required.

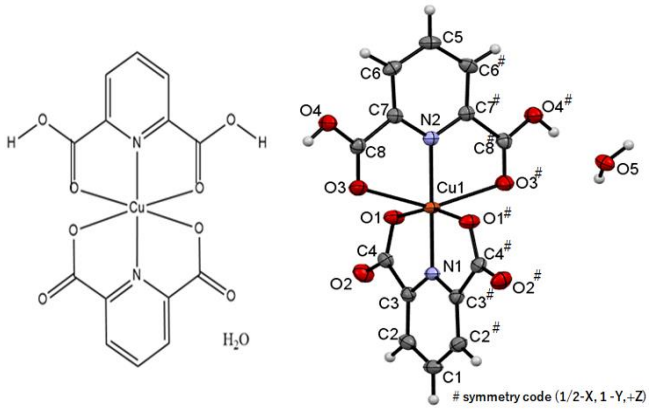

Figure 1: Chemical structure of the copper(II) complex.

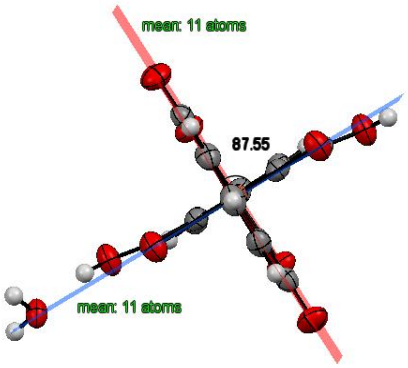

Figure 2: Angle between mean-planes for monohydrate.

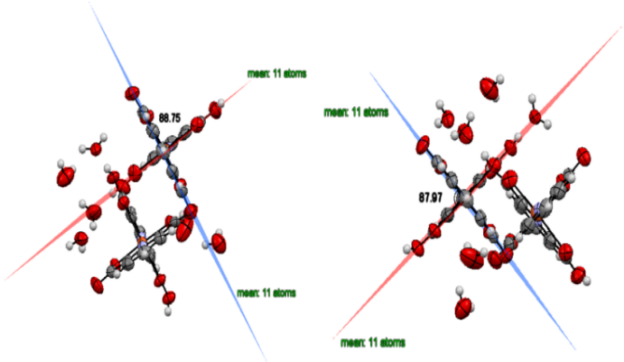

Figure 3: The angle between mean-planes for trihydrate for two molecules (A: right, B: left) in an asymmetric unit.

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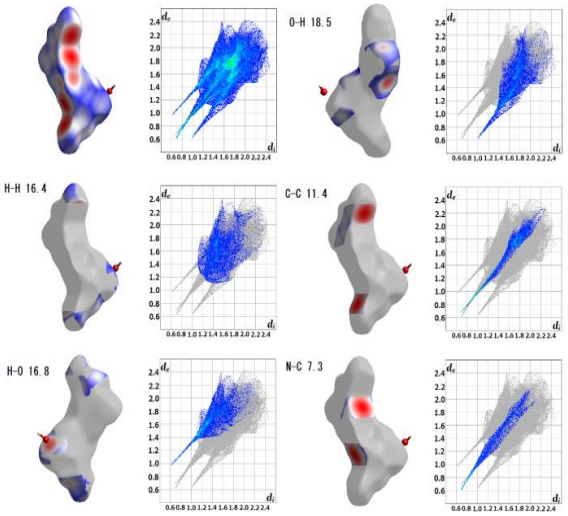
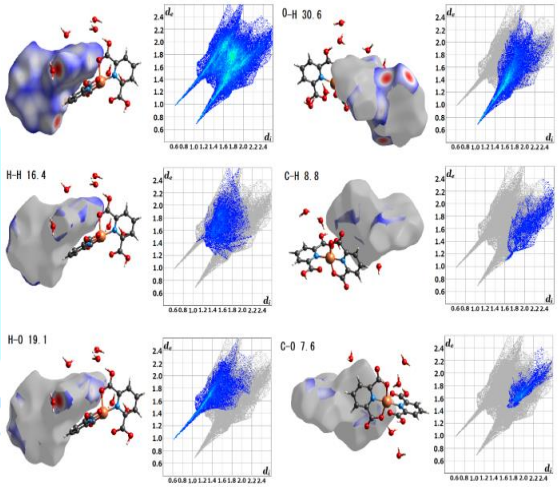
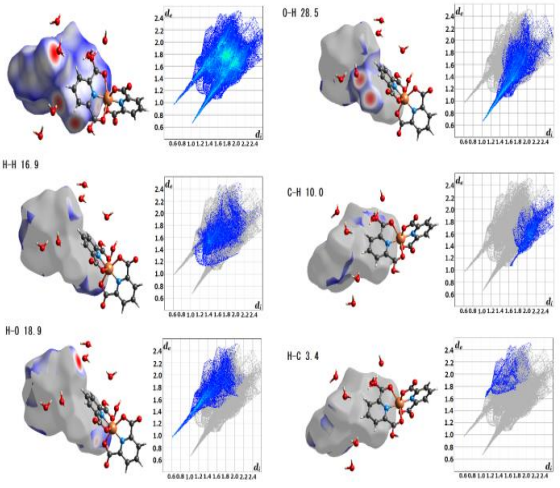


Figure 4: Hirshfeld surface analysis of monohydrate.



A



B

Figure 5: Hirshfeld surface analysis of trihydrate for two molecules in the asymmetric unit.

References

1. https://www.nature.com/sdata/publish/for-authors
2. Morisako S and Yamashita M. Chemistry of pincer complexes possessing x-type boron ligand (2019) Bull Jpn Soc Coord Chem 74: 29-45. https://doi.org/10.4019/bjscc.74.29
3. Zhu Q, Sun X, Yang D, Ma J, Kang X, et al. Carbon dioxide electroreduction to C_2 products over copper-cuprous oxide derived from electrosynthesized copper complex (2019) Nat Commun 10: 3851. https://doi.org/10.1038/s41467-019-11599-7
4. Sarchet C and Loiseleur L. Structure cristalline du [(pyridine-2,6 di-carboxylato) (acide pyridine-2,6 di-carboxylique)]cuivre(II) hydraté (1973) Acta Cryst B29: 1345-1351. https://doi.org/10.1107/S0567740873004486
5. Sileo EE, Blesa MA, Rigotti G, Rivero BE and Castellano EE. The crystal chemistry of copper(II) dipicolinates (1996) Polyhedron 15: 4531-4530. https://doi.org/10.1016/0277-5387(96)00189-1
6. Akitsu T and Einaga Y. trans-Bis(2,2-diphenyl-ethyl-amine-[kappa]N)bis-(5,5-diphenyl-hydantoinato-[kappa]N_3) copper(II) and its chloro-form disolvate (2005) Acta Crystallogr 61: m183-m186. https://doi.org/10.1107/S010827010500209X
7. Spackman MA and Sayatilaka D. Hirshfeld surface analysis (2009) Cryst Eng Comm 11: 19-32. https://doi.org/10.1039/B818330A