水素結合を有する銅二核錯体[Cu(Eta)(Heta)(NO_3)]$_2$の結晶構造と磁性における重水素置換効果

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Crystal Structures, Magnetic Properties, and their Deuterium Substitution Effects of Hydrogen-bonded Dinuclear Copper Complexes, [Cu(Eta)(Heta)(NO_3)]$_2$ ([1]*Faculty of Marine Engineering, Tokyo University of Marine Science and Technology*, [2]*Graduate School of Science, Nagoya City University*) Tasuku Murai,[1] Shinobu Aoyagi[2], ○Wataru Fujita[1]

The title compound, [Cu(II)(Eta)(Heta)(NO_3)]$_2$ (Eta = $H_2NCH_2CH_2O^-$, Heta = $H_2NCH_2CH_2OH$) (the hydrogen derivative **H**), reported by Bertrand et al.,[1)] has the copper dimer structure via O•••H–O strong hydrogen bonds, as shown in Fig. 1. In the dimer, an antiferromagnetic interaction works via the hydrogen bonds. In this presentation, crystal structures, magnetic properties, and their deuterium substitution effects of the complex were studied.

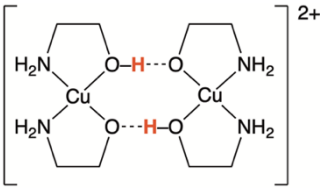

Fig. 1. Molecular structure of **H**.

The derivative **D** with the deuterated hydroxy and amino groups was prepared by mixing of $Cu(NO_3)_2$•$3D_2O$ and $D_2NCH_2CH_2OD$ in MeOD, and was identified by IR spectroscopy. Xray structure analyses revealed that the **D** derivative was isostructural with **H**. We found that these derivatives showed structural phase transitions to the low temperature phases at 118 K for **H**, and 126 K for **D**. Magnetic measurements revealed that the *g*-factors and the magnetic coupling constants $2J/K_B$, estimated from the Bleany-Bowers model, were 2.024 and –51.9 K for **H**, and, 2.039 and –51.3 K for **D**, respectively. It is concluded that there was little difference in magnetism between **H** and **D**. We will show the detailed data at the presentation venue.

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表題の物質 [Cu(Eta)(Heta)(NO_3)]$_2$ (Eta = $H_2NCH_2CH_2O^-$, Heta = $H_2NCH_2CH_2OH$)（**H**）は、Fig. 1 に示すように、２つの単核錯体が水素結合を介して二量体構造を形成し、この二量体間には水素結合を介して磁気的相互作用が働くことが知られている[1)]。本研究ではこの物質について、結晶構造の温度依存性、磁気測定、さらには水素結合部位の重水素置換を行った際の構造物性への影響について検討を行った。重水素置換体（**D**）は $Cu(NO_3)_2$•$3D_2O$ と $D_2NCH_2CH_2OD$ とを重メタノール中で混合することによって、調製した。**H** と **D** の結晶構造を検討したところ、**H** は 118 K 以下で、**D** は 126 K 以下でそれぞれ低温相へ相転移を示すことを発見した。一方、これらの磁気的性質を検討したところ、有意な差は認められなかった。詳細は当日報告する。

1) J. A. Bertrand et al. *Inorg. Chem*. **1980**, *19*, 2022.