

parallel to the aromatic ring plane. Attractive interaction energies, obtained from ab initio calculations, are significant and consistent with the observed crystal structures. The most stable parallel alignment interactions are not above C-H region of the aromatic ring, but for larger offset distances.

The most stable model system of all those considered has one O-H bond parallel to benzene ring at horizontal displacement of 2.6 Å (B set), $\Delta E_{\text{CCSD(T)}(\text{limit})} = -2.45$ kcal/mol. These interactions are somewhat weaker than O-H \cdots π (-3.19 kcal/mol) but quite stronger than C-H \cdots O interactions (-1.41 kcal/mol). The calculated energies of the parallel alignment interactions are comparable with the energy for the slipped-parallel benzene-benzene dimer ($\Delta E_{\text{CCSD(T)}(\text{limit})} = -2.45$ kcal/mol).

[1] G. V. Janjić, D. Ž. Veljković, S.D. Zarić, *Crystal Growth & Design*, 2010, submitted.

Keywords: Water/aromatic interactions, Crystal structures, Ab initio calculations.

L.A.36

Acta Cryst. (2011) A67, C823

A Copper(II) Complex with Neutral Carboxylic Acid Ligand
Hiroshi Miyamae, Kazuki Ito, Goro Hihara, *Department of Chemistry, Josai University, Keyakidai 1-1, Sakado-Shi, Saitama 350-0295 (Japan)*. E-mail: miya@josai.ac.jp

A large number of dimeric copper(II) carboxylate adducts, $[\text{Cu}(\text{RCOO})_2 \cdot \text{L}]_2$, were studied and characterized the structure being copper(II) acetate type by many groups.[1] When $\text{Cu}(\text{OH})_2$ (0.99 g, 10 mmol) were added to ethanol solution (20 ml) of pivalic acid (Hpiv: 2,2-dimethylpropionic acid) (3.27 g, 32 mmol) and kept for a week in a refrigerator, deep green crystals were grown from the solution, in which the axial position of square-pyramidal coordination geometry around the Cu is occupied by an O atom at C=O of the neutral pivalic acid molecule. Thus the formula is $[\text{Cu}(\text{piv})_2 \cdot \text{Hpiv}]_2$. The O-H group of the pivalic acid molecule forms an intramolecular H-bond (O...O distance of 2.692(5) Å).

X-ray structure determination showed that the crystal exhibits disorder in the position of tertial butyl group at one of the bridging ligands at ambient temperature. However, at 123K, all the carbon atoms can fixed at suitable positions.

Crystal data . $[\text{Cu}_2(\text{C}_5\text{H}_9\text{O}_2)_4(\text{C}_5\text{H}_{10}\text{O}_2)_2]$, Mr = 735.86

For 296K: monoclinic, $P2_1/c$, a = 9.505(5), b = 17.965(12), c = 11.642(8) Å, $\beta = 99.42(2)^\circ$, V = 1961.2(21) Å³, Z = 2, $D_x = 1.246$ Mg m⁻³.

For 123K: monoclinic, $P2_1/c$, a = 9.561(5), b = 17.514(11), c = 11.323(6) Å, $\beta = 99.739(19)^\circ$, V = 1868.7(18) Å³, Z = 2, $D_x = 1.308$ Mg m⁻³.

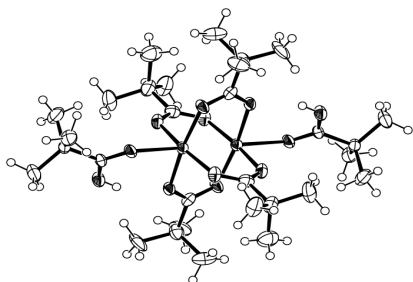


Fig. 1. Molecular structure of $[\text{Cu}_2(\mu\text{-piv})_4(\text{Hpiv})_2]$ at 123 K.

[1] For example, Y. Kani, M. Tsuchimoto, S. Ohba, H. Matsushima, & T. Tokii. (2000), *Acta Cryst.* C56, 923-925.

Keywords: copper(II)_carboxylate, intramolecular_H-bond