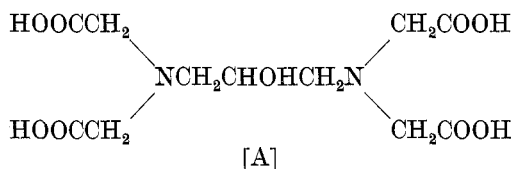


DIHYDROGEN 1,3-DIAMINO-2-HYDROXYPROPANE-
N,N,N',N'-TETRAACETATOCOPPER(II)*

By C. H. L. KENNARD†

Dihydrogen 1,3-diamino-2-hydroxypropane-*N,N,N',N'*-tetraacetatocopper(II) was synthesized by treating freshly prepared copper(II) hydroxide with a saturated aqueous solution of complexing agent [A]:



This produced a deep blue solution which on evaporation gave a similarly coloured crystalline precipitate. The hydrated compound was recrystallized from hot water, washed with cold water, and alcohol (Found: C, 32.9; H, 4.6; N, 6.8; Cu, 15.6. Calc. for $\text{C}_{11}\text{H}_{18}\text{N}_2\text{O}_{10}\text{Cu}$: C, 32.9; H, 4.5; N, 7.0; Cu, 15.8%).

TABLE I
CRYSTAL DATA

$\text{C}_{11}\text{H}_{18}\text{CuN}_2\text{O}_{10}$: mol. wt. 401.82; monoclinic; $a = 13.92 \pm 0.01$ Å, $b = 7.00 \pm 0.01$ Å, $c = 15.59 \pm 0.01$ Å; $\beta = 97 \pm 1^\circ$; d_m 1.77 g cm⁻³ (by flotation method); $U = 1502.9$ Å³; $Z = 4$; d_c 1.78 g cm⁻³; space group, $P2_{1/c}$ (hkl all present; $h0l$: $l = 2n$; $0k0$: $k = 2n$). Radiation: copper unfiltered, single crystal oscillation, equi-inclination Weissenberg and precession photographs. Comparison with isomorphous compounds: X-ray diffraction data with a, b, c in Å; d_c and d_m in g cm⁻³

Compound	<i>a</i>	<i>b</i>	<i>c</i>	β	d_c	d_m	Space Group	<i>Z</i>
Ni(OH ₂)H ₂ EDTA ²	11.71	6.94	16.65	91.2°	1.80	1.80	$P2_{1/c}$	4
Cu(OH ₂)H ₂ EDTA ²	11.61	7.00	16.50	92.0°	1.84	1.82	$P2_{1/c}$	4
Cu(OH ₂)H ₂ A	13.92	7.00	15.54	97.0°	1.77	1.77	$P2_{1/c}$	4

Infrared studies, using a Beckman 21 infrared spectrophotometer, on the solid in potassium bromide pressed plates, gave peaks at 1770 and 1247 cm⁻¹. Morris and Busch¹ characterized two peaks at 1745 and 1228 cm⁻¹ in sodium hydrogen ethylenediaminetetraacetatocobaltate(III) monohydrate as being due to a free carboxylic acid. Consequently a similar result is indicated in this complex.

* Manuscript received January 10, 1967.

† Department of Chemistry, University of Queensland, Brisbane.

¹ Morris, M. L., and Busch, D. H., *J. Am. chem. Soc.*, 1956, **78**, 5178.

² Smith, G. S., and Hoard, J. L., *J. Am. chem. Soc.*, 1959, **81**, 556.

Single crystal X-ray diffraction studies listed in Table I show that this compound is isomorphous and probably isostructural with dihydrogen ethylenediaminetetraacetatoquo-copper(II) and -nickel(II). In the case of the last compound, Smith and Hoard² have shown that ethylenediaminetetraacetic acid wraps itself around the metal ion as a pentadentate leaving one carboxylic acid uncomplexed. A water molecule completes the distorted octahedral coordination surrounding the metal ion. A similar structure is indicated in the case of dihydrogen 1,3-diamino-2-hydroxypropane-*N,N,N',N'*-tetraacetatocopper(II).

Acknowledgment

This work, carried out at Cornell University in 1961, was financed by a National Science Foundation Grant No. G 23470.