09.4-06 CRYSTAL STRUCTURE OF AN ACTIVE-SITE MODEL FOR CARBONIC ANHYDRASE: \([\text{TRIS}+2(4,5-\text{DIISOPROPYLMETHYLIDAZO} \\
\text{DYL})\text{PHOSPHINE}][\text{DICHLOROZINC}]\text{NC}(\text{II})\]. 2[Zn,(N=O)IMETHYLFORMamide \text{H}] \cdot 3\text{H}2\text{O}]

The active site of the enzyme carbonic anhydrase includes a Zn(II) atom, which is coordinated to the N atoms of three histidine residues and to a solvent molecule (Kannan et al., Proc. Natl. Acad. Sci. USA 72: 51-55 [1975]). The title compound was synthesized as a structural analogue to this portion of the carbonic anhydrase active site. In fact, it shows a small catalytic activity toward CO2 hydration. (Brown et al., submitted to J. Am. Chem. Soc.)

09.4-07 TWO Cd(II) WITH DIFFERENT COORDINATION NUMBERS IN THE CRYSTAL STRUCTURE OF HEXAMETHYLENETETRAMINE-CADMIUMIODIDE-WATER (2/5/4). By Thomas C.H. Mak, Department of Chemistry, The Chinese University of Hong Kong, Shatin, New Territories, Hong Kong.

As part of our investigation of the coordination properties of hexamethylenetetramine, \((\text{CH}_2)\text{N}_4\), we have prepared the title compound and determined its crystal structure. Crystals of stoichiometry \(2Cd\text{II}\cdot(\text{CH}_2)\text{N}_4\cdot3\text{H}2\text{O}\) are monoclinic, space group \(P2_1/\text{c}\), with \(a=8.114(1)\), \(b=10.482(2)\), \(c=19.133(2)\) Å, \(\beta=107.06(4)\)°, \(Z=2\). The structure was solved by direct methods using 3404 diffractometer measured \((\text{MoK}\alpha)\) observed reflections and refined by full-matrix anisotropic least-squares to \(R=0.042\).

The hexamethylenetetramine molecule makes full use of its four nitrogen lone pairs: N(1) and N(4) are coordinated to Cd(1) and Cd(2), respectively; and N(2) and N(3) accept protons from water oxygen atoms O(1) and O(2), respectively. Atom Cd(1) is situated at a center of symmetry and octahedrally coordinated by N(1), O(1), I(1), and atoms related to them by the inversion center. The configuration around Cd(2) is distorted tetrahedral, with coordination sites occupied by N(4), I(1), I(2) and I(3). Zigzag chains composed of Cd(1) coordination octahedra, Cd(2) coordination tetrahedra, and hexamethylenetetramine groups are cross-linked by hydrogen bonds involving water molecules to form a three-dimensional network.