X-Ray Crystal Structure of Hexakis(imidazole)cadmium(II) Carbonate Pentahydrate, $[Cd(C_3H_4N_2)_6]CO_3,5H_2O$, a Supposed Hydroxy-nitrate

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Summary The crystal structure of $[Cd(C_3H_4N_2)_6]CO_3,5H_2O$ has been determined and the complex has been shown to be identical with that previously reported as $[Cd(C_3H_4N_2)_6](OH)(NO_3),4H_2O$.

When aqueous solutions of cadmium(II) chloride and imidazole in a molar ratio of 1 : 10 are mixed and allowed to evaporate, two types of crystal are obtained, one type with and one type without chloride. The crystals that do not contain chloride are isomorphous with $[Co(C_3H_4N_2)_6]CO_3,5H_2O$,[1] which indicated a molecular formula of $[Cd(C_3H_4N_2)_6]CO_3,5H_2O$.†

Recently, a structure supposed to be $[Cd(C_3H_4N_2)_6](OH)(NO_3),4H_2O$ has been described by Mighell and

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† Verified by N and CO_3^{2-} analyses.

Santoro.[2] Its cell parameters show a remarkable resemblance to those of $[Cd(C_3H_4N_2)_6]CO_3,5H_2O$.

Crystal Data: $a = 9{\cdot}0426(5)$, $c = 21{\cdot}720(5)$Å, $U = 1538{\cdot}07$ Å^3, $Z = 2$, $D_c = 1{\cdot}45$ g cm^{-3}, $D_m = 1{\cdot}46$ g cm^{-3}, space group $P6_3/m$.

The atomic parameters are almost the same. The fact that we obtained crystals free from chloride in a medium containing chloride, and the resemblance between the crystal data for the two complexes led us to believe that the reported structure of $Cd(C_3H_4N_2)_6(OH)(NO_3),4H_2O$ is wrong. Mighell and Santoro reported that the N–O bond lengths (1·286 Å) were longer than expected (1·24 Å). They claimed that this increase arose from hydrogen bonding to water molecules. A distance of 1·286 Å is in fact normal for C–O bond lengths. We have found a C–O bond length of 1·285 Å in the carbonate ion. Thus we believe that the two compounds are identical and contain carbonate and not nitrate.

The Co^{II} compound was obtained from the preparation described by Strandberg and Lundberg[1] and also from the reaction of $CoCl_2$ with imidazole as described for the cadmium analogue. The carbonate ions in these cases can come only from dissolved CO_2. This means that the solubility products are very low for these compounds.

The intensities from the crystals of $[Cd(C_3H_4N_2)_6]CO_3,5H_2O$ were collected and measured by using an automatic linear diffractometer, PAILRED, and Mo-K_α radiation. Correction for Lorentz and polarisation factors was carried out in the usual way,[3] and correction for absorption was also made. Least-squares refinements are in progress using anisotropic temperature factors for all atoms. The conventional R-value is 0·050; the satisfactory refinement supports the formulation, $[Cd(C_3H_4N_2)_6]CO_3,5H_2O$. Our aim is to locate the positions of the hydrogen atoms, especially those in the carbonate–water layers, since there are indications that the carbonate ions are hydrated.

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