SHORT COMMUNICATIONS

CRYSTAL STRUCTURE OF DIAQUABISGLYCINECOBALT(II) BROMIDE

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A SYSTEMATIC crystallographic investigation of the complexes of glycine[1] with many inorganic salts is in progress in our laboratory. In this preliminary note, we report the structure of diaquabisglycinecobalt(II) bromide.

Single crystals of the above complex, $(NH_2CH_2COOH)_2\ CoBr_2 \cdot 2H_2O$, were grown from a saturated aqueous solution containing stoichiometric amounts of glycine and $CoBr_2$. The crystal data are as follows: $a = 8.822(1)$, $b = 6.0552(4)$, $c = 11.771(1)$ Å, $\beta = 111.53(5)°$, $V = 584.9$ Å^3, F. W. = 404.75, $d_{expt} = 2.29$ g.cm^{-3}, $d_{cal} = 2.295$ g.cm^{-3}, $Z = 2$ and the space group is $P2_1/a$. The density was determined by flotation method using a liquid mixture of bromoform and carbon tetrachloride. The molecular formula was confirmed from the elemental analysis data for C, H and N.

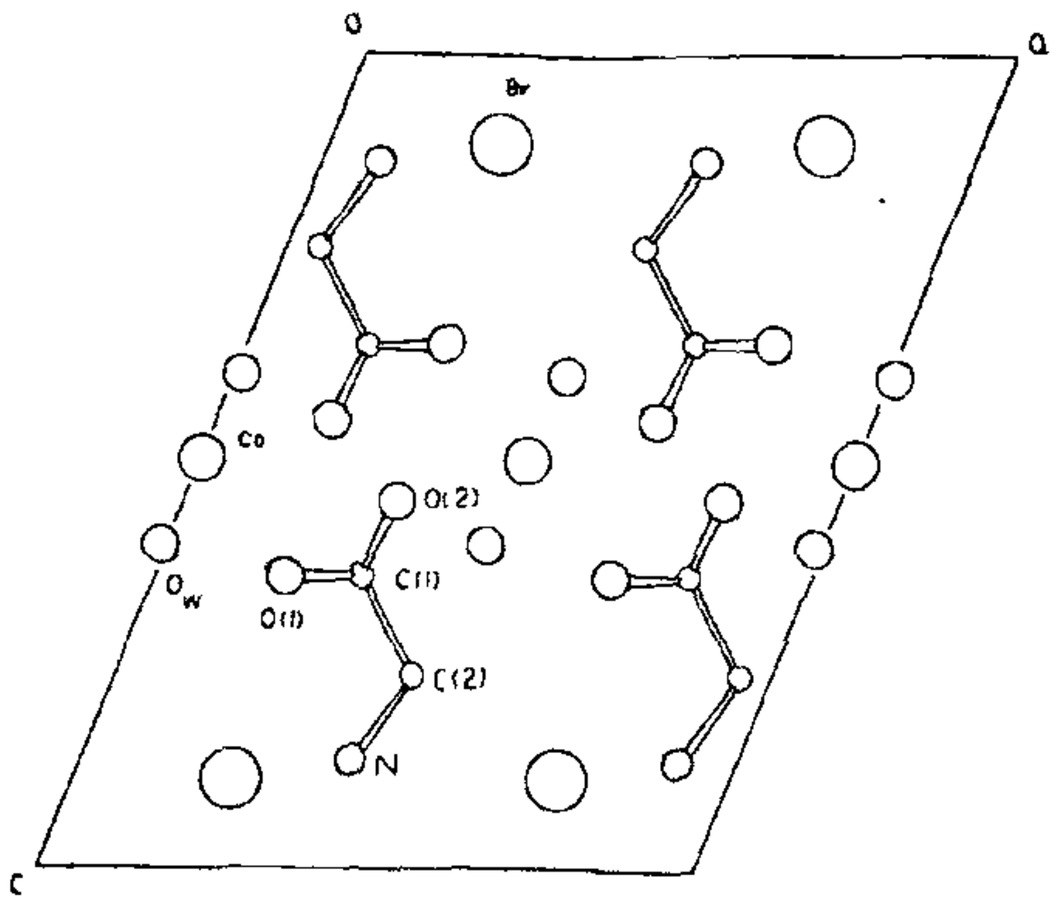

Figure 1. *Projection* of the structure of diaquabisglycinecobalt(II) bromide down the *b*-axis.

The three-dimensional intensity data were collected using a CAD-4 diffractometer, with graphite monochromatised MoK α radiation using ω scan technique. The reflection data were collected upto 65° in 2θ giving 1595 unique reflections with $0 < h < 12$, $0 < k < 8$, $-16 < l < 16$. 1338 reflections had $I_{net} > 2.5\sigma(I_{net})$ based on counting statistics. Lorentz and polarisation corrections were applied on this intensity data. From a three-dimensional Patterson synthesis, the positions of the bromine and cobalt atoms were determined.

Thereafter, successive Fourier and difference Fourier syntheses revealed the atoms in the glycine and water molecules. Structure-factor least-squares refinement using the block-diagonal approximation was carried out on an IBM 1130 computer. With isotropic thermal parameters for all the non-hydrogen atoms, the *R* index at present is about 0.09 for 1338 reflections. Anomalous dispersion corrections were applied to bromine and cobalt[2]. Further refinement is under progress. A view of the structure looking down the *b*-axis is shown in figure 1.

Cobalt is coordinated by six oxygen atoms, four of them belonging to glycine molecules and the other two of the water molecules. The Co-O distance range from 2.065 to 2.108 Å. The glycine molecule exists in the zwitterionic form. Bromine ions are hydrogen bonded to the nitrogens of the two glycine molecules and another oxygen of the water molecule.

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2. Cromer, D. T. and Libermann, D., *J. Chem. Phys.*, 1970, **53**, 1891.