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X-Ray Crystal Structure of a Glycine Platinum(II) Compound of Formula $2Pt(NH_2CH_2CO_2)_2 \cdot H_2C_2O_4 \cdot 2H_2O$

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The anti-tumour activity of *cis*-$Pt(NH_3)_2Cl_2$ and some related complexes has stimulated efforts to obtain other drugs of this type. As part of a programme with this objective, a series of platinum(II) complexes with amino acids has been prepared.

During the course of this work it was found that *cis*-$[PtL_2]$ (where L = glycine (gly) or alanine (an) anions) gave, on reaction with oxalic acid in water, colourless crystals of stoichiometry $Pt_2L_4(H_2C_2O_4) \cdot 2H_2O$ (*Anal.* L = gly, Found, C, 14.59; H, 2.59; N, 6.78; O, 27.37; Pt, 47.98; Calc. C, 14.78; H, 2.73; N, 6.89; O, 27.57; Pt, 48.02%. L = an, Found, C, 19.09; H, 3.27; N, 6.46; O, 25.54; Calc. C, 19.36; H, 3.48; N, 6.45; O, 25.79%). As it was found that the i.r. spectra of the compounds did not permit a clear decision to be made concerning the coordination of the ligand about the platinum atoms we have determined the structure of the glycine complex by X-ray diffraction methods.

Colourless crystals of the title compound are monoclinic, with a = 5.551(1), b = 17.596(1), c = 10.169(1) Å, β = 106.88(1)° (at 12 °C), space group $P2_1/c$ and Z = 2. Intensity data were collected on a Siemens off-line four-circle automatic diffractometer to θ = 70°. A total of 1815 independent reflections were measured, of which 54 were judged to be 'unobserved'. The structure was solved by Patterson and Fourier methods, and full-matrix least-squares refinement has now reached R = 0.037.

The crystal structure consists essentially of *cis*-bis(glycinato)platinum(II) complex molecules, and of oxalic acid dihydrate, with these components linked together by hydrogen bonds involving the water molecules. In the complex molecule, the platinum is bound by two bidentate glycine ligands in a slightly distorted square-planar *cis* configuration, as shown in Fig. 1. Molecules of formula $Pt(gly)_2$ are known to exist in both the *cis* [1] and the *trans* [2] forms, however, the structure of the former has been determined with only moderate accuracy (R = 0.11).

Mean Pt–O bond length in the title compound is 2.015 Å, while the mean Pt–N is 2.013. By comparison, in the accurately determined structure of *trans*-$Pt(gly)_2$ [2] the mean values are 2.002 and 2.039 Å respectively. Freeman observed [3] that in amino acid complexes a linear relationship exists between the mean metal–ligand bond length and the angle subtended by the donor atoms at the metal. The mean N–Pt–O angle of 83.0° in the title compound is in excellent agreement with the value of 83° predicted for a mean metal–ligand bond of 2.0 Å. Within the ligands the bond lengths are very similar to those found in free glycine [4], except that the two C–O bonds are asymmetric, with a mean of 1.296 Å for the coordinated C–O bond, and 1.215 Å for the free bond.

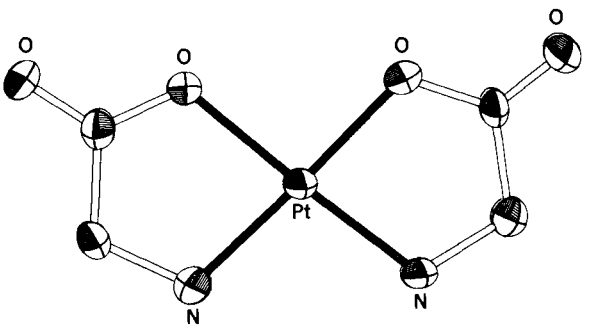

Fig. 1. Structure of the *cis*-$Pt(gly)_2$ moiety.

Oxalic acid molecules, which lie on centres of symmetry, have strong hydrogen bonds connecting them to water molecules. The length of these bonds, O...O of 2.50 Å, is typical of those found for carboxylic acids. Each water molecule then uses its own hydrogen atoms to form two weaker hydrogen bonds, of length 2.70 and 2.77 Å, to the uncoordinated glycine oxygen atoms on neighbouring complex molecules.

The results of preliminary tests show that the activity of the title compound against L-1210 leukemia is similar to that of *cis*-$Pt(gly)_2$, which is now explicable in the light of the fact that the oxalate groups are not coordinated.

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