

### X-Ray Crystal Structure of a Platinum-9-Methyladenine Complex

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(Received November 11, 1974)

The discovery by Rosenberg and collaborators of the activity of certain platinum compounds as anti-tumor agents<sup>1</sup> stimulated greatly research in this area.

In our studies<sup>2-4</sup> of the anti-tumor properties of complexes of platinum(II) and their interactions

with purines, nucleosides and nucleotides, we noted that 9-methyladenine reacted with potassium chloroplatinate ( $K_2PtCl_4$ ) in water yielding a deep yellow colored compound. Suitable crystals for X-ray work were obtained by slow evaporation of the acid (3N HCl) solution. We report here the results of the crystal structure analysis of the compound formed having the formula,  $Pt(9\text{-methyladenine})Cl_3H^+$  (*Anal. Found*: C, 16.33; H, 1.78; N, 15.96; Pt, 42.76; Cl, 23.01. *Calc.* C, 15.93; H, 1.77; N, 15.47; Pt, 43.21; Cl, 23.57).

The crystals are triclinic, space group  $P\bar{1}$ ,  $a = 9.495 \pm 0.002$ ,  $b = 9.924 \pm 0.002$ ,  $c = 6.961 \pm 0.001$  Å,  $\alpha = 104.57 \pm 0.03^\circ$ ,  $\beta = 93.48 \pm 0.03^\circ$ ,  $\gamma = 114.94 \pm 0.03^\circ$ ,  $Z = 2$ ,  $D_c = 2.607$  g cm<sup>-3</sup>,  $D_m = 2.63$  (by flotation).

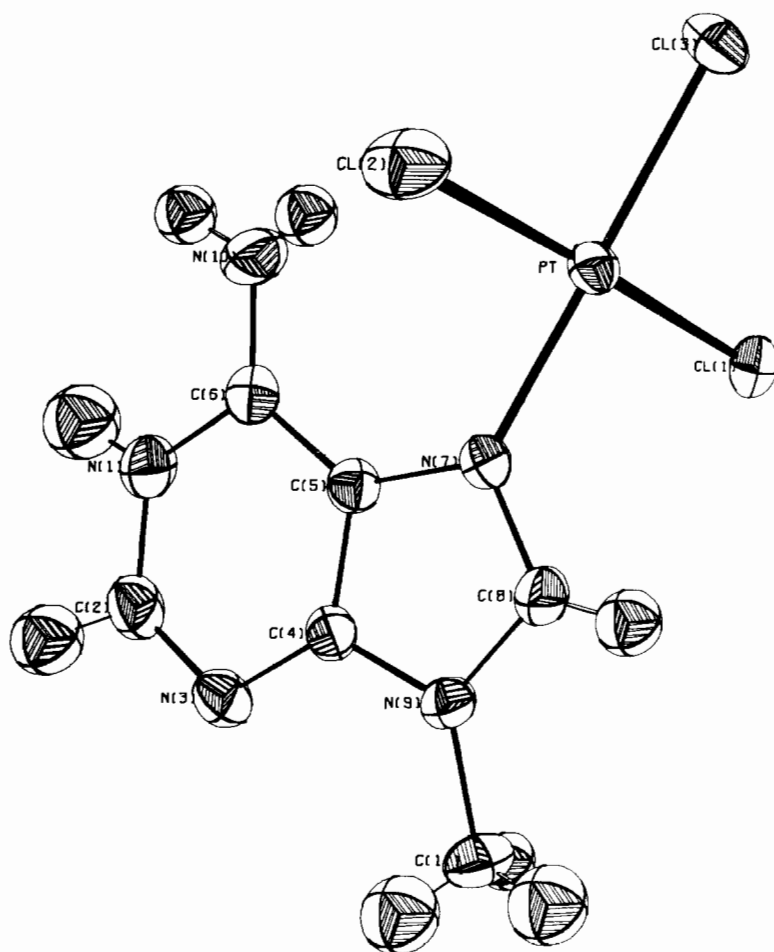


Fig. 1. Molecular structure of  $Pt(9\text{-methyladenine})Cl_3H^+$ .

The intensities were measured on a Picker automatic diffractometer using graphite-monochromated Mo-radiation ( $\lambda = 0.7107 \text{ \AA}$ ) and a  $\theta-2\theta$  scan mode out to a  $2\theta$  value of  $55^\circ$ . The position of the platinum was located from a three-dimensional Patterson synthesis. All atoms, including the hydrogens, were located by two Fourier syntheses. Using block-diagonal least-squares refinements, anisotropic temperature factors for the non-hydrogen atoms and isotropic for the hydrogens the  $R$  index converged to a present value of 0.025.

As can be seen in the Figure the Platinum is coordinated to the  $N_7$  site and the  $N_1$  hydrogen is involved in a hydrogen bond with the Cl(1) of a centrosymmetrically related molecule, forming in this way weakly bonded dimers which are held together by Van der Waals forces.

We believe that the platinum-9-methyladenine structure is the first to show coordination of a

platinum ion to the  $N_7$  site<sup>3</sup>. This site is a potential target for interaction with platinum ions in DNA<sup>5</sup> whereas the  $N_1$  site is directly involved in hydrogen bonding.

#### Acknowledgement

We thank the Ministry of Education of the Province of Quebec for support of this Research.

#### References

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