

## The Structure of an Acetylene Complex of Platinum(II)

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IN describing the preparations and properties of several complexes of substituted acetylenes with platinum(II), Chatt, Guy, and Duncanson<sup>1</sup> observed that they are exactly analogous to olefin complexes of similar general formula. They therefore suggested that their structures are similar, with the acetylenic triple bond perpendicular to the co-ordination plane and joined by a three-centre or  $\pi$ -type bond to the platinum atom.

In the course of our studies of complexes of unsaturated hydrocarbons with transition metals, we have determined the structure by X-ray methods of  $[(\text{Bu}^t\text{C}\equiv\text{CBu}^t)(p\text{-toluidine})\text{PtCl}_2]$ . The crystals are monoclinic;  $a = 9.81$ ,  $b = 9.79$ ,  $c = 10.61$  Å,  $\beta = 95.3^\circ$ ; Space group  $P2_1/m$ ,  $Z = 2$ , molecular symmetry,  $m$ ;  $D_m = 1.67$ ,  $D_c = 1.66$ . The intensities of 1680 reflections were measured by a Picker automatic diffractometer, and ten cycles of least-squares refinement of the structure have reduced the mean discrepancy  $R$  to 0.056; further refinement is now in progress. The results show that the molecule has the predicted structure (see Figure). The two acetylenic carbon atoms C(9) and C(10) are equidistant from the platinum atom, and lie on a line perpendicular to the co-ordination plane. The dimensions of the

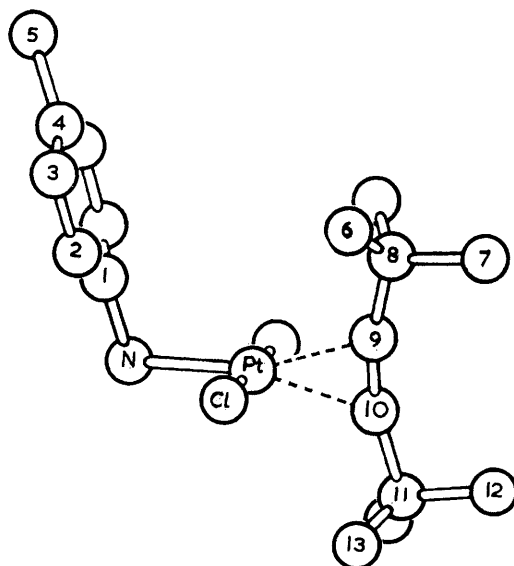


FIGURE. General view of the molecule. The atoms bearing numbers only are carbon atoms, and the unlabelled atoms are C(3'), C(2'), C(1'), C(6'), C(13'), related by a plane of symmetry to the corresponding labelled atoms.

molecule show that the triple bond has been modified by co-ordination to the metal atom, and is intermediate between a triple and a double bond. Thus the angles C(8)-C(9)-C(10) and C(9)-C(10)-C(11) are approximately 165° instead of 180°, and the C(9)-C(10) bond-length is 1.27 Å (e.s.d. 0.03 Å), mid-way between the usual values for double and triple bonds. The acetylenic ligand is symmetrically arranged, within experimental error, about the co-ordination plane of the platinum atom. Unlike the complex  $[(\text{CH}_2=\text{CH}_2)(\text{NHMe}_2)\text{PtCl}_2]$

which has a crystallographic symmetry plane coinciding with the co-ordination plane,<sup>2</sup> this molecule has a crystallographically determined plane of symmetry perpendicular to the co-ordination plane. This symmetry plane contains the atoms C(7)-C(12) of the acetylene ligand, as well as the Pt atom and the N, C(1), C(4), and C(5) atoms of the *p*-toluidine ligand.

Full details of the structure will be published when refinement has been completed.

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<sup>1</sup> J. Chatt, R. G. Guy, and L. A. Duncanson, *J. Chem. Soc.*, 1961, 827.

<sup>2</sup> P. R. H. Alderman, P. G. Owston, and J. M. Rowe, *Acta Cryst.*, 1960, **13**, 149.