Molecular Structure of Bis(triphenylphosphine)alleneplatinum

By MINORU KADONAGA, NORITAKE YASUOKA, and NOBUTAMI KASAI*
(*Department of Applied Chemistry, Faculty of Engineering, Osaka University, Yamadakami, Suita, Osaka, 565, Japan*)

Summary *X*-Ray structure analysis of $Pt(PPh_3)_2(C_3H_4)$ shows that, unlike in other transition-metal–allene complexes in which allene is perpendicular to the co-ordination plane, allene is *in* the co-ordination plane.

THE molecular structures of several allene complexes with transition-metal ions have been determined by *X*-ray diffraction,[1] and the results are consistent with a structure in which allene is perpendicular to the co-ordination plane. We report that $Pt(PPh_3)_2(C_3H_4)$ has a different type of the structure.

Crystal data: $C_{39}H_{34}P_2Pt$, $M = 759{\cdot}7$, $a = 10{\cdot}515(11)$, $b = 10{\cdot}209(9)$, $c = 17{\cdot}892(10)$ Å, $\alpha = 104{\cdot}64(9)°$, $\beta = 87{\cdot}91(12)°$, $\gamma = 119{\cdot}24(7)°$; space group $P\bar{1}$, $Z = 2$, $D_m = 1{\cdot}57$ (by flotation), $D_c = 1{\cdot}50$ g cm^{-3}. Unit cell dimensions were determined on a G.E. single-crystal orienter equipped with a Rigaku SG-2 goniometer. Using Cu-K_α radiation, a total of 4112 independent reflexions were collected by multiple-film equi-inclination Weissenberg photographs mainly around the *c* axis. Corrections for the usual Lorentz and polarization factors and for the shape effect were made. The structure was solved by the heavy-atom method, and refined by block-diagonal least-squares with anisotropic thermal parameters for Pt and P ($R = 0{\cdot}099$ for non-zero reflexions).

The molecular geometry around the platinum atom is shown in the Figure. The co-ordination around platinum is approximately square-planar; two phosphorus atoms and two carbon atoms of the allene molecule lie on the co-ordination plane. Allene is co-ordinated to platinum atom as a bidentate ligand; the co-ordinated bond, C(1)–C(2) [1·48(5) Å] is longer than the unco-ordinated bond, C(2)–C(3) [1·31(5) Å]. The allene molecule is not linear; the unco-ordinated carbon atom, C(3), is located away from the platinum atom, and the angle C(1)–C(2)–C(3) is 142(3)°. The dihedral angle between planes formed by P(1)PtP(2) and C(1)PtC(2) is 9°. The present complex is isostructural with $Pt(PPh_3)_2(CS_2)$[2] and $Pd(PPh_3)_2(CS_2)$.[3]

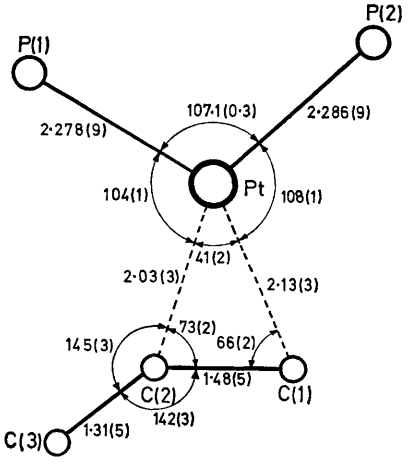

FIGURE. *Molecular geometry around platinum in* $Pt(PPh_3)_2(C_3H_4)$.

We thank Professor Sei Otsuka and his co-workers for crystals.

(*Received, October 4th*, 1971; *Com.* 1737.)

[1] T. G. Hewitt and J. J. DeBoer, *J. Chem. Soc.* (*A*), 1971, 817; P. Racanelli, G. Pantini, A. Immirzi, G. Allegra, and L. Porri, *Chem. Comm.*, 1969, 361; T. Kashiwagi, N. Yasuoka, N. Kasai, and M. Kakudo, *ibid.*, p. 317.
[2] M. Baird, G. Hartwell, R. Mason, A. I. M. Rae, and G. Wilkinson, *Chem. Comm.*, 1967, 92.
[3] T. Kashiwagi, N. Yasuoka, T. Ueki, N. Kasai, M. Kakudo, S. Takahashi, and N. Hagihara, *Bull. Chem. Soc. Japan*, 1968, **41**, 296.