The Crystal Structure of $Ru_6C(CO)_{17}$

By A. SIRIGU*

(*Laboratorio di Chimica Generale, Istituto Chimico, Università di Napoli*, 80134 *Napoli, Italy*)

and M. BIANCHI and E. BENEDETTI

(*Istituto di Chimica Organica Industriale, Università di Pisa, Italy*)

CONTROLLED thermal decomposition of $[Ru(CO)_4]_3$ gave[1] a cluster ruthenium carbonyl complex, assigned the structure $Ru_6(CO)_{18}$ from analytical data. Johnson, Johnston, and Lewis[2] independently synthesized what appeared to be the same compound and some of its arene derivatives; on the basis of mass spectral data they assigned it the structure $Ru_6C(CO)_{17}$. A preliminary account of the structure of the mesitylene derivative $Ru_6C(CO)_{14}(C_6H_3Me_3)$ has been given by Mason and Robinson.[3] The formulation of the compound as a carbide was confirmed.

We have now determined the structure of the ruthenium carbonyl prepared by Piacenti *et al.* and show that the correct structure is $Ru_6C(CO)_{17}$ (Figure). The crystals are monoclinic with $a = 24{\cdot}06 \pm 0{\cdot}10$ Å, $b = 9{\cdot}36 \pm 0{\cdot}04$ Å, $c = 17{\cdot}70 \pm 0{\cdot}08$ Å, $\beta = 96°22' \pm 30'$, space group $P2/c$ or Pc, $Z = 6$.

The structure was determined by direct Sayre–Zachariasen and Patterson methods. The refinement was carried out for 3070 observed reflections (Weissenberg–photographic data, visual estimation of the intensities) by the block-diagonal least-squares method in the space group $P2/c$. The present value of R is 0·139.

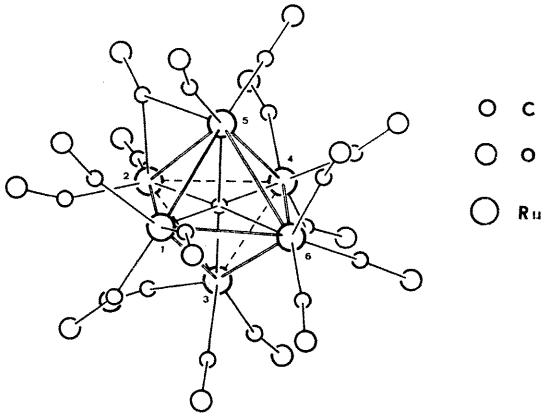

FIGURE. *Only the molecule located at the general position in the unit cell is shown; the molecule at the special position, along a twofold axis, is not substantially different. The carbon atom is at the centre of the octahedral metal cluster. Mean* Ru–C *distance* 2·05 Å [maximum deviation 0·07 Å, σ (Ru–C) = 0·05 Å]: Ru(1)–Ru(2) = 2·885(6), Ru(1)–Ru(3) = 2·951(6), Ru(1)–Ru(5) = 2·827(5), Ru(1)–Ru(6) = 2·927(5), Ru(2)–Ru(3) = 2·897(5), Ru(2)–Ru(4) = 2·969(5), Ru(2)–Ru(5) = 2·855(6), Ru(3)–Ru(4) = 2·917(6), Ru(3)–Ru(6) = 2·840(6), Ru(4)–Ru(5) = 2·858(6), Ru(4)–Ru(6) = 2·872(7), Ru(5)–Ru(6) = 3·034(5) (σ *values in parentheses.*)

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[1] F. Piacenti, M. Bianchi, and E. Benedetti, *Chem. Comm.*, 1967, 775.
[2] B. F. G. Johnson, R. D. Johnston, and J. Lewis, *Chem. Comm.*, 1967, 1057.
[3] R. Mason and W. R. Robinson, *Chem. Comm.*, 1968, 468.