The Structure of Methylmethoxycarbenetriphenylphosphinetetracarbonylchromium

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THE molecular structure of phenylmethoxycarbenepentacarbonylchromium (I) was recently reported.[1] Substitution of one carbonyl group by triphenylphosphine is accompanied by an increase in stability towards atmospheric oxidation.[2] We have now analysed the crystal structure of methylmethoxycarbenetriphenylphosphinetetracarbonylchromium (II) to see whether the increase in stability is associated with any substantial change in structure, to obtain a second value for the chromium–carbene distance and to determine whether the triphenylphosphine group is *cis* or *trans* to the carbene group. We thank Professor E. O. Fischer for supplying us with crystals of the compound.[3]

$Me(MeO)C(Ph_3P)Cr(CO)_4$ crystallises in space group $P2_1/n$ with $a = 9{\cdot}29$, $b = 22{\cdot}61$, $c = 11{\cdot}60$Å, $\beta = 92{\cdot}57°$ and $Z = 4$. The structure was determined by Fourier methods from 833 reflexions collected on precession photographs taken with molybdenum K_α radiation ($R = 8{\cdot}2\%$). The structure shown in the Figures confirms the basic geometry found for (I).

The chromium–carbene distance, 2·04 Å, is the same as in (I) and is significantly longer than the remaining Cr–C distances (average 1·84 Å). Some differences, however, are found. One minor change is that the normal to the plane of the substituted carbene in (II) lies approximately at 65° to one of the principal axes of the chromium octahedron as compared with 45° in (I). We conclude that the replacement of the phenyl group in (I) by methyl is not accompanied by large

differences in arrangement. One interesting difference, however, does occur. In (II) the methoxy-group is bent away from the chromium atom whereas in (I) the reverse occurs. Additionally the angle subtended at the carbene carbon atom by the substituents is increased from 104° in (I) to 115° in (II).

The triphenylphosphine group is *cis* and the Cr–P distance 2·42 Å. The P–C distances, average 1·82 Å, compare well with those found in triphenylphosphine itself (average 1·828 Å).[4]

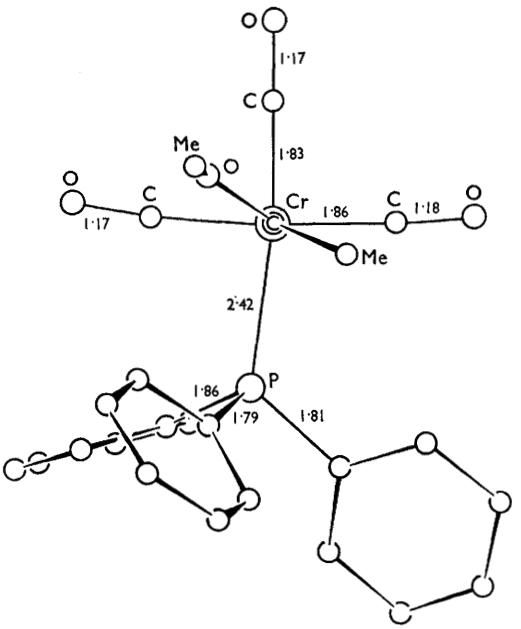

FIGURE 1.

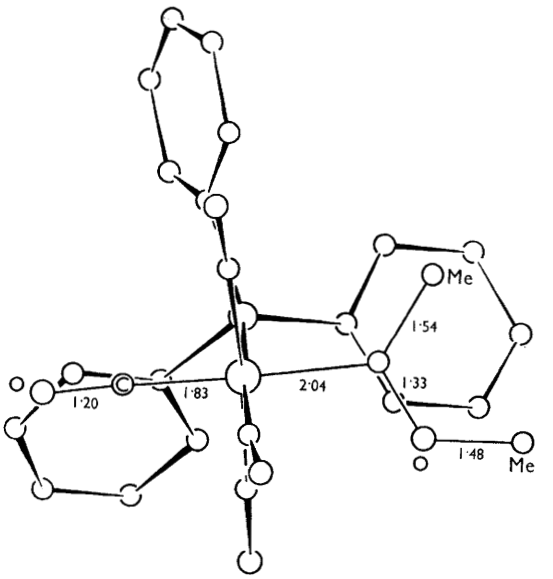

FIGURE 2. *The structure in Figure* 1 *rotated through* 90°.

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[1] O. S. Mills and A. D. Redhouse, *Angew. Chem.*, 1965, **77**, 1142; *Angew. Chem. Internat. Edn.*, 1965, **4**, 1082.
[2] E. O. Fischer, Chemical Society Lecture, Nottingham, September 1965.
[3] E. O. Fischer and R. Aumann, unpublished results.
[4] J. J. Daly, *J. Chem. Soc.*, 1964, 3799.