

The Structure of a Cumulene Metal Carbonyl Complex

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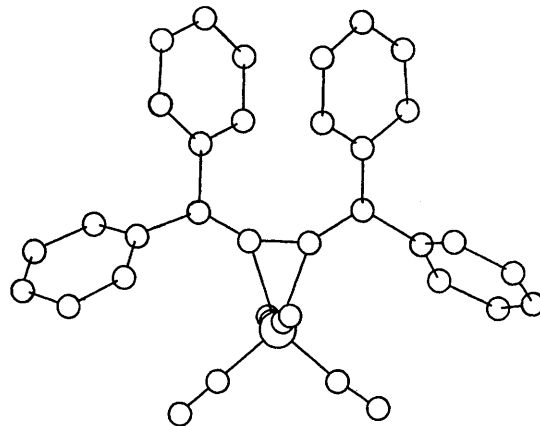
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A NUMBER of iron complexes of cumulenes have been prepared by Joshi.¹ We report the crystal structure determination of tetraphenylbutatriene-tetracarbonyliron. The pale yellow crystals are monoclinic with $a = 12.64$, $b = 10.25$, $c = 20.17$ Å and $\beta = 93.25^\circ$. Systematic absences are consistent with the space-group $P2_1/c$. There are four molecules per cell and the asymmetric unit contains 37 atoms excluding hydrogen. 1426 unique reflections were estimated visually from precession photographs which were taken with Mo radiation. The structure was found by Fourier methods and refined by least-squares ($R = 12.9\%$).

The iron atom is co-ordinated exclusively to the central bond of the cumulated double-bond system and the metal co-ordination is trigonal bipyramidal. A sketch of the molecule, projected on to the equatorial plane, is shown in the Figure. It is apparent that the cumulene chain is no longer linear but is symmetrically deformed at the central carbon atoms and bent away from the co-ordinating metal atom.

The arrangement of the carbonyl groups and the co-ordinated double bond around the iron atom is

similar to that found in acrylonitriletetracarbonyliron.² However, although the metal-equatorial carbon distances are comparable with the acrylonitrile complex, we find no indication of the lengthening of the apical Fe-C distances reported for that compound.



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¹ K. K. Joshi, personal communication; and *J. Chem. Soc., (A)*, 1966, 594, 598.

² A. R. Luxmoore and M. R. Truter, *Acta Cryst.*, 1962, 15, 1117.