

## Crystal Structure of a Bis(tricarbonyliron) Complex of 3, $\alpha$ -Dimethylstyrene

By F. H. HERBSTEIN\* and M. G. REISNER

(Department of Chemistry, Technion—Israel Institute of Technology, Haifa, Israel)

**Summary** Crystal structure analysis shows that the molecules of a bis(tricarbonyliron) complex of 3, $\alpha$ -dimethylstyrene consist of two, linked, planar tricarbonyliron-isoprene units, inclined to one another at an angle of 37.4°.

SAREL *et al.*<sup>1</sup> have prepared two isomeric tricarbonyliron complexes of 3, $\alpha$ -dimethylstyrene. Chemical properties and spectroscopic data show that these complexes do not have any aromatic character, trapping of Kekulé structures being inferred. To test this proposal we have determined the crystal structure of one of them.

The crystals are orange-red monoclinic needles,  $a = 9.217(3)$ ,  $b = 7.00(1)$ ,  $c = 13.021(3)$  Å,  $\beta = 93.1(2)^\circ$ , space group  $P2_1$ ,  $Z = 2$ . Intensities of 1981 reflections (224 with zero intensity) were measured on a Stoe semi-automatic Weissenberg diffractometer using graphite-monochromatized Mo- $K_\alpha$  radiation. Structure solution and refinement were by standard methods; the current  $R$ -factor is 12% (anisotropic temperature factors for all non-hydrogen atoms) and the e.s.d. of C—C bond lengths is 0.03 Å.

The molecule has a *trans* configuration of tricarbonyliron groups with respect to the ligand, thus resembling the bis(tricarbonyliron) complexes of *m* and *p*-divinylbenzene<sup>2</sup> and of many other ligands. Molecular dimensions are shown in the Figure. The following groups of carbon atoms are planar: I: C(6), C(1), C(7), C(8), C(9), C(5), C(2); II: C(2), C(3), C(4), C(5), C(10); III: C(1), C(6), C(3), C(4). The angle between planes I and II is 37.4°. Atoms C(2) C(5) are on the *same* side of plane III and 0.43 and 0.36 Å respectively from it; thus the six-membered ring has a boat conformation.

The molecule can be described as consisting of two tricarbonyliron complexes of isoprene, with an angle of 37.4°

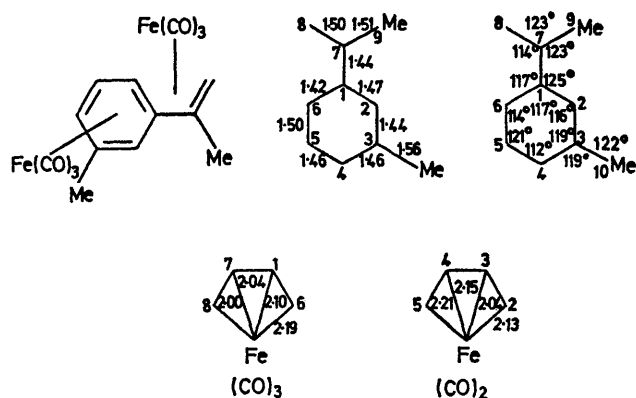


FIGURE. Bond lengths and angles in a bis(tricarbonyliron)-3, $\alpha$ -dimethylstyrene complex.  $d(\text{Fe} \cdots \text{Fe}) = 4.67$  Å. Average  $d(\text{Fe-carbonyl C}) = 1.78$  Å (range 1.73—1.83 Å). Average  $d(\text{C}=\text{O}) = 1.15$  Å (range 1.12—1.18 Å).

between their planes and having atoms C(2) and C(5) in common. Hydrogen positions have not been determined and therefore no statement about the hybridisation at these carbon atoms is possible. It appears that the lack of aromatic properties in the benzene ring should be ascribed to the formation of two isoprene type complexes, appreciably isolated from one another, rather than to bond-fixation in the ring.

We thank Prof. S. Sarel, Dr. R. Victor, and Dr. R. Ben-Shoshan for suggesting this study and for providing the crystals used.

(Received, 9th August, 1972; Com. 1402.)

<sup>1</sup> R. Victor, R. Ben-Shoshan, and S. Sarel, *Chem. Comm.*, 1970, 1680; R. Victor, R. Ben-Shoshan, and S. Sarel, *Tetrahedron Letters*, 1970, 4257.

<sup>2</sup> R. E. Davis and R. Pettit, *J. Amer. Chem. Soc.*, 1970, 92, 716.