A Gas-phase Electron-diffraction Investigation of Trimethylenemethaneiron Tricarbonyl, $C(CH_2)_3Fe(CO)_3$

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TRIMETHYLENEMETHANEIRON TRICARBONYL has been synthesized by Emerson *et al.*[1] We report the results of a gas-phase electron-diffraction investigation of the compound.

The scattering pattern from the gas at about 50° was recorded on the Oslo electron-diffraction unit.[2] The final modified molecular-intensity points extended from $s = 2{\cdot}50$ to $s = 38{\cdot}75$ Å^{-1}. [$s = (4\pi\sin\theta)/\lambda$, where θ is half the scattering angle and λ the electron wavelength].

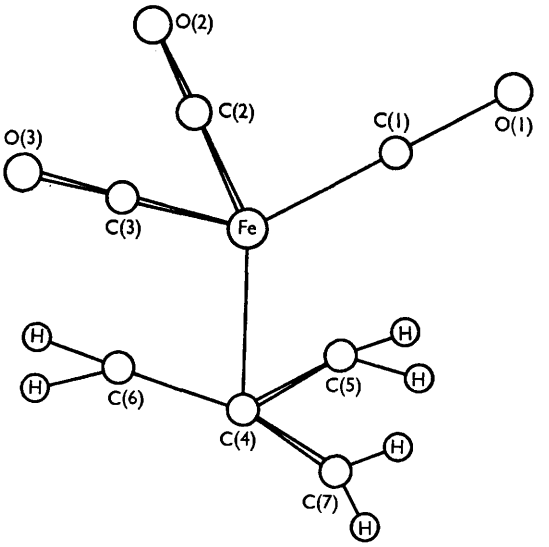
It was clear from the experimental o.r.d. curve that the three distances Fe–C(5), Fe–C(6), and Fe–C(7) were essentially equal. Hence the kind of valence tautomerism discussed by Emerson *et al.* could be ruled out.

There are two possible molecular models of C_{3v} symmetry. In one, the six carbon atoms form a trigonal prism around the iron atom, in the other (shown in the Figure) they form a trigonal antiprism. It was found that the prismatic model was incompatible with the experimental data.

The antiprismatic C_{3v} model was refined by least-squares calculations[3] on the intensity data. The most important structure parameters and their standard deviations are given in the Table.

The Fe–C(4) bond is found to be significantly shorter than the distance from the iron atom to the four carbon atoms in the cyclobutadiene ring of tetraphenylcyclobutadiene irontricarbonyl[3] (2·067 ± 0·012 Å) while the Fe–C(5) distance is significantly longer. In fact the Fe–C(4) distance is roughly equal to the two Fe–C(alkyl) distances found in $H_2Fe_2(CO)_6(CH_3COCH_3)$[4] (1·946 ± 0·007 Å).

However, since the bonding in the $FeC(CH_2)_3$



FIGURE

Structure parameters for trimethylenemethane irontricarbonyl

	Å
Fe–C(1)	= 1·810 (0·003)
Fe–C(4)	= 1·938 (0·005)
Fe–C(5)	= 2·123 (0·005)
C(1)–O	= 1·153 (0·002)
C(4)–C(5)	= 1·437 (0·003)
C(5)–H	= 1·111 (0·009)
∠ Fe–C(4)–C(5)	= 76·4° (0·2°)
∠ C(4)–Fe–C(1)	= 118·4° (1·3°)

(The angles have not been corrected for shrinkage.)

fragment is almost certainly highly strained, we believe it would be unwise to draw any conclusions regarding the relative strength of the Fe–C(4) and Fe–C(5) bonds from these comparisons.

We are indebted to Professor Emerson for a sample of the compound.

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