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NOTE

THE STRUCTURE OF THE IRON-ACETYLENE COMPLEX $Fe_2(CO)_7(C_2Ph_2)_2$

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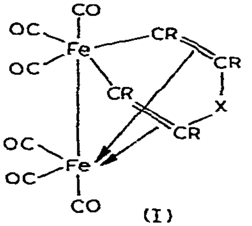
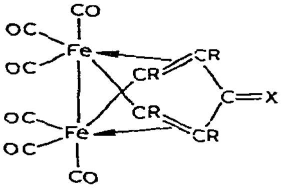
Among the numerous complexes of acetylenes first reported by Hübel and coworkers[1,2] and by Schrauzer[3] were two compounds to which the structures (I; X=C=O; R=Ph) and (I; X=C=CH_2; R=H) were initially assigned. This formulation was based on analogy to the ferracyclopentadiene complexes (I; no X) whose structures appear firmly established[4,5]. Subsequently X-ray examination[6] led to the reformulation of one of the compounds, the "triacetylene" complex, as (II; X=CH_2; R=H). Hence there exists an equally good analogy for regarding the complex "$Fe_2(CO)_7(C_2Ph_2)_2$" as (II; X=O; R=Ph) rather than (I; X=CO; R=Ph). Nevertheless recent publications have continued to use the latter formulation[7]. We have now examined the Mössbauer spectrum of this substance. The result shown in Fig. 1 is a spectrum with only two peaks having (within experimental error) equal line-widths, Γ; this clearly indicates equivalence of the two metal atoms. Structure (II; X=O; R=Ph) with equivalent iron atoms, is therefore preferred and the former representa-



(I)



(II)

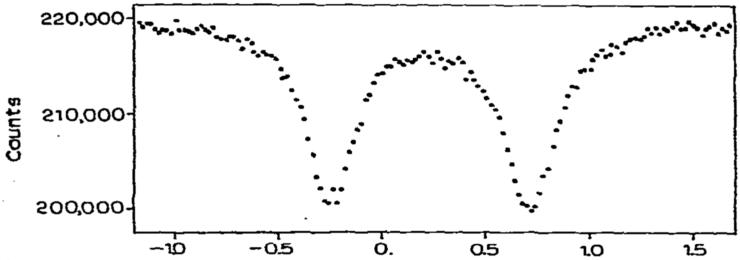


Fig. 1. Mössbauer spectrum of $Fe_2(CO)_7(C_2Ph_2)_2$.

tion (I; X=CO; R=Ph) is considered to be ruled out for this compound. When two different iron environments are known to be present [*e.g.* (I; R=H, no X)] the Mössbauer spectrum is more complex and the two iron atoms show differing chemical isomer shifts, δ, and quadrupole splittings, Δ[8]. The observed values for the Mössbauer parameters of $Fe_2(CO)_7(C_2Ph_2)_2$ at 80°K were: δ (with respect to sodium nitroprusside at room temperature) 0.246 ± 0.010 mm/sec; Δ 0.995 ± 0.010 mm/sec, $\Gamma = 0.31 \pm 0.02$ mm/sec.

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