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SHORT COMMUNICATIONS

A revised structure for the butatriene iron carbonyl complexes

We have reported the formation of butatriene di-iron pentacarbonyl, C₄H₄-Fe_a(CO)₅ (I), and related complexes¹. The mass spectrum of I now showed the correct composition of I to be $C_1H_1Fe_2(CO)_8^+$. The parent peak (M⁺) appeared at m/e 332 (calcd. for C₄H₄Fe₂(CO)₆, 332). The presence of six CO groups was indicated by the appearance of six similarly-shaped groups of peaks at the interval of m/e 28, i.e. at $M^{\pm} - 28 \cdot n$ (n = 1, 2, ...6). The previous elemental analysis also conformed to the hexacarbonyl structure. (Found: C, 35.85; H, 1.27. C₁₀H₄Fe₂O₆ calcd.: C, 36.19; H, 1.21 %.) The infrared pattern of the metal carbonyl stretching region is similar to that of the other di-iron hexacarbonyl compounds, e.g. (RC=CR)₂Fe₂(CO)₆², in which the disposition of Fe₂(CO)₆ moiety will presumably be similar to I. Therefore, the composition of the substituted butatriene iron carbonyl complexes³ previously reported probably have the similar di-iron hexacarbonyl structure.

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^{*} The same mass spectral result was also reported by R. B. King, J. Am. Chem. Soc., 88 (1966) 2075.

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