A New Complex of Iron containing a Delocalized, Heterocyclic Bidentate Ligand

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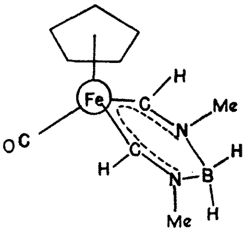
Summary The reaction of $C_5H_5Fe(CO)(CNMe)_2^+$ and BH_4^- proceeds with B–H addition to the two C≡N groups, yielding $C_5H_5Fe(CO)(CNMe)_2BH_4$, for which a delocalized structure is suggested.

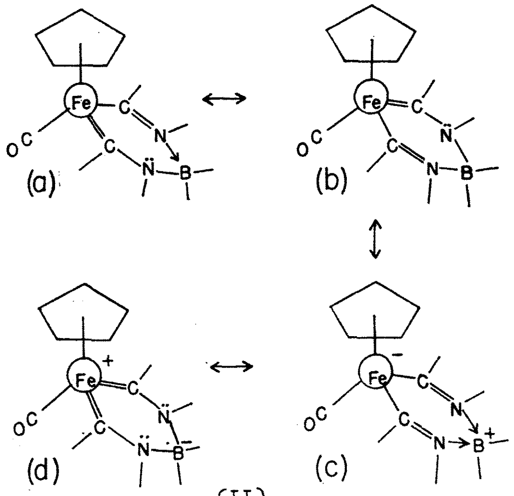
IN the course of our work on nucleophilic reactions of cationic metal carbonyl complexes[1] we have investigated the reaction of $C_5H_5Fe(CO)(CNMe)_2^+PF_6^-$ [2] with sodium borohydride. From this reaction, run in tetrahydrofuran at 0° for 15 hr., we have isolated in 50% yield a stable yellow covalent complex of empirical formula consistent with $C_5H_5Fe(CO)(CNMe)_2BH_4$, m.p. 123—124°.† It was separated by chromatography on alumina and could be purified by crystallization or sublimation.



(I)

The significant features of this compound are: in the i.r. spectrum, a single carbonyl stretching frequency at 1950 cm.$^{-1}$, BH stretching frequencies around 2300 cm.$^{-1}$, and lack of any C≡N stretching modes around 2200 cm.$^{-1}$; and in the ^1H n.m.r. spectrum, a singlet C_5H_5 proton resonance at τ 5·2 (intensity, 5), a singlet methyl resonance at τ 6·7 (intensity, 6), and a somewhat broad singlet peak of intensity 2 at τ −3·0. The ^{11}B spectrum shows a triplet, δ +5·9 relative to BF_3,OEt_2 [J_{BH} 96 c./sec.). The unusually low-field proton resonance at τ −3·0 is associated with the unique C–H protons, and the hydrogens on the boron atom (predictably) are not seen in dilute solution, owing to their broadness and expected multiplicity.

Of the several bonding pictures that can be drawn for this geometry which allow both C–H and N–Me groups to be equivalent, we prefer the structure (I), which implies delocalization over the two nitrogens, two carbons, and the iron atom. The boron atom is co-ordinately saturated and is presumably not a part of the delocalized system. There are six electrons associated with delocalized π-system. In valence-bond notation we consider the possible resonance structures below (II a—d) as all contributing to the bonding.



(II)

It is difficult to distinguish which of these structures, if any, predominates, from the data at hand, although the fairly high solubility of the complex in pentane suggests that the more polar forms are less appropriate.

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† Satisfactory elemental analyses have been obtained. The mass spectrum of this compound shows a parent peak at *m/e* 246.

[1] P. M. Treichel and R. L. Shubkin, *Inorg. Chem.*, 1967, **6**, 1328.

[2] C. E. Coffey, *J. Inorg. Nuclear Chem.*, 1963, **25**, 179.