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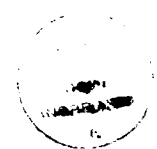
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Synthesis and Structural Characterization of Mononuclear
Iron (II) Ferracarboranes

by

Sharon S. Lee, Carolyn Knobler, and M. Frederick Hawthorne*



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19. ABSTRACT (Continue on reverse if necessary and identify by block number) Neutral iron(II) ferracarboranes of the type [closo-3-CO-3-L-3-L'-3,1,2-FeC ₂ B ₉ H ₁₁] (3, L = CO, L' = PPh ₃ ; 4, L = PPh ₃ , L' = CH ₃ CN; 5, L = CO, L' = CH ₃ CN; 6, L = CO, L' = P(OCH ₃) ₃ ; 7, L = L' = P(OCH ₃) ₃ ; 8, L = L' = CO) have been prepared by the Cu(I) oxidation of the dimeric iron dicarbollide complex [closo-3-CO-3,3'-(μ-CO)-3,1,2'-FeC ₂ B ₉ H ₁₁] ₂ ²⁺ (2) in the presence of the designated monodentate ligands. Complexes 3, 4, 7, and 8 have been structurally characterized by single-crystal X-ray diffraction. Crystallographic parameters are as follows (compound: crystal system; space group; crystal parameters; Z; unique data (I > 3σ(I)); R, R _w). 3: monoclinic; A2/a; a = 18.384 (3) Å, b = 12.762 (2) Å, c = 23.059 (3) Å, β = 104.081 (4)°; 8: 1780; 7.4, 8.8. 4: monoclinic; C2/c; a = 28.050 (2) Å, b = 11.5715 (9) Å, c = 19.042 (2) Å, β = 116.846 (2)°; 8: 1702; 6.5, 7.7. 7: orthorhombic; Pbnm (standard setting Pnma); a = 10.397 (2) Å, b = 14.419 (3) Å, c = 15.092 (3) Å; 4: 1051; 7.1, 8.9. 8: monoclinic; P2 ₁ /n; a = 6.971 (4) Å, b = 15.900 (9) Å, c = 11.237 (7) Å, β = 91.42 (2)°; 4: 1108; 6.2, 7.4. The closo 12-vertex icosahedral geometry comprising a polyhedral (d ⁶ Fe)C ₂ B ₉ framework and the pseudooctahedral coordination exhibited by the iron atom are common structural features displayed by all four ferracarboranes.				
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Synthesis and Structural Characterization of Mononuclear Iron(II) Ferracarboranes

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Neutral iron(II) ferracarboranes of the type [*closo*-3-CO-3-L-3-L'-3,1,2-FeC₂B₉H₁₁] (3, L = CO, L' = PPh₃; 4, L = PPh₃, L' = CH₃CN; 5, L = CO, L' = CH₃CN; 6, L = CO, L' = P(OCH₃)₃; 7, L = L' = P(OCH₃)₃; 8, L = L' = CO) have been prepared by the Cu(I) oxidation of the dimeric iron dicarbollide complex [*closo*-3-CO-3,3'-(μ-CO)-3,1,2-FeC₂B₉H₁₁]₂²⁻ (2) in the presence of the designated monodentate ligands. Complexes 3, 4, 7, and 8 have been structurally characterized by single-crystal X-ray diffraction. Crystallographic parameters are as follows (compound: crystal system; space group; crystal parameters; Z; unique data (*I* > 3σ(*I*)); *R*, *R*_w). 3: monoclinic; *A*2/*a*; *a* = 18.384 (3) Å, *b* = 12.762 (2) Å, *c* = 23.059 (3) Å, β = 104.081 (4)°; 8; 1780; 7.4, 8.8. 4: monoclinic; *C*2/*c*; *a* = 28.050 (2) Å, *b* = 11.5715 (9) Å, *c* = 19.042 (2) Å, β = 116.846 (2)°; 8; 1702; 6.5, 7.7. 7: orthorhombic; *Pbnm* (standard setting *Pnma*); *a* = 10.397 (2) Å, *b* = 14.419 (3) Å, *c* = 15.092 (3) Å; 4; 1051; 7.1, 8.9. 8: monoclinic; *P*2₁/*n*; *a* = 6.971 (4) Å, *b* = 15.900 (9) Å, *c* = 11.237 (7) Å, β = 91.42 (2)°; 4; 1108; 6.2, 7.4. The *closo* 12-vertex icosahedral geometry comprising a polyhedral (d⁶Fe)C₂B₉ framework and the pseudooctahedral coordination exhibited by the iron atom are common structural features displayed by all four ferracarboranes.

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