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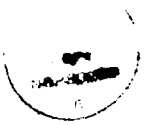
Synthesis and Molecular Structure of

closo-3-(η^6-C_6H_6)-3,1,2-$FeC_2B_9H_{11}$

by

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



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The mixed-sandwich complex, closo-3-(η^6-C_6H_6)-3,1,2-$FeC_2B_9H_{11}$ (2), has been prepared in high yield by the photolysis of closo-3,3,3-$(CO)_3$-3,1,2-$FeC_2B_9H_{11}$ (1) in benzene. The molecular structure of 2 has been determined by an X-ray diffraction study. Compound 2 crystallized in the orthorhombic space group Pmcn (standard setting Pnma) with a 7.693(1) Å, b 9.001(2) Å, c 18.420(3) Å, V 1276 Å^3, and Z = 4 (8 half molecules related by a mirror plane at x = 1/4). The structure was solved by heavy atom methods to a final discrepancy index of R = 0.053, R_w = 0.067 for 861 independent reflections.

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Abstract

The mixed-sandwich complex, *closo*-3-(η^6-C_6H_6)-3,1,2-$FeC_2B_9H_{11}$ (**2**), has been prepared in high yield by the photolysis of *closo*-3,3,3-$(CO)_3$-3,1,2-$FeC_2B_9H_{11}$ (**1**) in benzene. The molecular structure of **2** has been determined by an X-ray diffraction study. Compound **2** crystallized in the orthorhombic space group *Pmcn* (standard setting *Pnma*) with a 7.693(1) Å, b 9.001(2) Å, c 18.420(3) Å, V 1276 Å^3, and $Z = 4$ (8 half molecules related by a mirror plane at $x = 1/4$). The structure was solved by heavy atom methods to a final discrepancy index of $R = 0.053$, $R_w = 0.067$ for 861 independent reflections.

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