Redetermination of Bis(\(\eta^4\)-1,3-cyclohexadiene)monocarbonyliron

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The crystal structure of bis(\(\eta^4\)-1,3-cyclohexadiene)monocarbonyliron has been redetermined by X-ray data. The compound crystallizes in the enantiomorphic, orthorhombic space group \( P2_12_12_1 \) with one complete molecule in the asymmetric unit. For concordance to the originally reported structure, which was determined under ambient conditions, the redetermination has been carried out at room temperature and at low temperature (\( T = 293 \) K: \( a = 7.618(2) \), \( b = 8.522(2) \), \( c = 17.138(4) \) Å, \( V = 1112.6(5) \) Å\(^3\), \( R_1 = 0.0226 \), \( wR_2 = 0.0539 \); \( T = 120 \) K: \( a = 7.509(2) \), \( b = 8.417(3) \), \( c = 16.778(6) \) Å, \( V = 1060.3(6) \) Å\(^3\), \( R_1 = 0.0242 \), \( wR_2 = 0.0533 \)). The redetermination proved this complex to have non-crystallographic \( C_{2v} \) point group symmetry. Correlation effects to the atomic coordinates and displacement parameters introduced problems during the structure refinement caused by pseudo-symmetry of the molecule. All bond lengths, angles, and torsion angles appear in this revised crystal structure in the normal range for \( \pi \)-coordinated diene transition metal complexes.