**Experimental and Theoretical Charge Densities of $Fe(CO)_3(\eta^4\text{-}C_4H_6)$**

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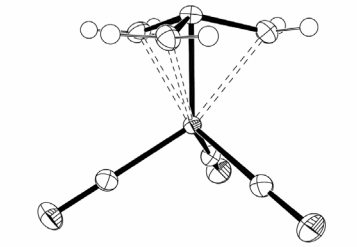
Topological analysis of the experimental charge density of $Fe(CO)_3(\eta^4\text{-}C_4H_6)$ (1) based on high resolution X-ray diffraction data collected at 100K is presented. The nature of the metal-ligand interaction is examined using the Atoms in Molecules (AIM) approach. The interaction between the iron atom and the carbon atoms of the trimethylenemethane ligand has been explored in depth. Theoretical DFT studies on the molecule calculated at the B3LYP/6-311++G(2p,2d) level show close agreement with the experimental results.



ORTEP diagram of $Fe(CO)_3(\eta^4\text{-}C_4H_6)$

**Keywords: experimental charge density, DFT, carbonyl**