COMPLETE STRUCTURE DETERMINATION OF ETHYLENEIRONTETRACARBONYL FROM THE ROTATIONAL SPECTRUM

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Microwave spectra of seven isotopomers of tetracarbonylethyleneiron were recorded using Fourier transform microwave spectroscopy. Rotational transitions for a $'c'$ dipole moment were measured in the 4 - 12 GHz range. The moments of inertia of the seven isotopomers were used in a Kraitchman analysis, and also in two different least squares fitting analyses to determine the molecular structure of the compound. The ethylene ligand exhibits significant structural changes upon complexation to iron, primarily an increase in C-C bond length and movement of the hydrogen atoms away from the metal center.