

## Theoretical study of 3-penten-2-one complexes of iron and chromium subgroup metals with various modes of the enone coordination

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### Abstract

The calculated parameters of the steric and electronic structure and shielding constants of  $\eta^2$ -(3-penten-2-one)Fe(CO)<sub>4</sub>,  $\eta^2$ -(3-penten-2-one)M(CO)<sub>5</sub>,  $\eta^4$ -(3-penten-2-one)Fe(CO)<sub>3</sub>, and  $\eta^4$ -(3-penten-2-one) · M(CO)<sub>4</sub> (M = Cr, Mo, W) nicely agree with the experiment. Coordination of the  $\alpha$ -enone with transition metals significantly distorts the conjugation between the C=C and C=O bonds.

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