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Study of mediborol by density functional theory

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Abstract

Quantum-chemical calculations of the mediborol in the gas phase and in solution by using the density functional with use all-electron basis set 6-31G(d) on GAUSSIAN'03 and TZ2P+ on Amsterdam density functional program. It is shown that the possibility of the mediborol reaction with iron chloride, the analysis of orbital interactions was carried out. It is provided the thermodynamic impossibility of this reaction.