An ab initio approach to the structure and EPR parameters of formaldiminoxy radical.

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Streszczenie

The structures and hyperfine coupling constants of formaldiminoxyl are investigated using ab initio methods. Geometries have been obtained at the UHF, UMP2 and UQCISD levels in combination with different basis sets of 6-31G and 6-311G type. The effect of the C□N□O bond angle on the hyperfine parameters of the radical is discussed. The isotropic hyperfine constants, calculated using UQCISD and UQCISD(T) methods with a variety of basis sets, including D95(d,p), IGLO-III, 6-311 + G(d,p), 6-311 + G(2df,p), DZP + D of Chipman, [742|52] of van Duijneveldt, are generally in a good agreement with the experimental data. The analysis of direct, spin polarization and correlation contributions to the hyperfine constants is made using ROHF, UHF, UCCD, UQCISD, UQCISD(T), UQCISD(TQ) models combined with [421|21] and [742|52] basis sets.

Adres publiczny

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