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The halogen derivatives of nitromethane: calculation, force fields in X_{δ}^{0} coordinates

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Abstract

This article deals with the electronic structure of compounds that are halogen derivatives of nitromethane. The matrix of the force coefficients in Cartesian coordinate system and in X_{δ}^{0} coordinates were calculated with the help of hybrid density functional theory. The generalized force constants of couple vectors obtained in X_{δ}^{0} coordinates when selected system of couple vectors coincides with the traditional chemical bonds in compounds are presented here.