

Quantum-chemical research of force field of nitromethane in X_8^0 coordinates

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Keywords: *force field, nitromethane, X_8^0 coordinates, quantum-chemical calculations.*

Abstract

In the frames of DFT method for the first time the matrix of force coefficient of nitromethane in X_8^0 coordinates was calculated. The peculiarities of the given approach in relation to traditional ones are presented.