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Theoretical estimation of the force field of tetrafluorohydrazine

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Abstract

For the first time the force field of tetrafluorohydrazine molecule in coordinates X_δ^0 has been obtained. For this purpose there were carried out quantum-chemical calculations B3LYP 6-311G++ (3df, 3pd) and the obtained matrix of force constants was translated from the Cartesian coordinates to internal coordinates. As a result there appeared the opportunity of the analysis of force constants. Frequencies of normal vibrations were calculated and their assignments was carried out. Normal frequencies were calculated and their assignment was performed.