OBTAINING INFORMATION ON JAHN-TELLER ACTIVE SYSTEMS THROUGH ASYMMETRIC ISOTOPIC SUBSTITUTION: CASE OF CHD_2O AND CH_2DO METHOXY RADICALS

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As for vibrational analyses of molecules in non-degenerate electronic states, isotopic substitution can enhance the set of parameters determinable from vibrational spectra of Jahn-Teller active systems. In comparison with molecular systems in non-degenerate electronic states, the vibronic Hamiltonian of Jahn-Teller active systems includes additional parameters - linear and higher-order Jahn-Teller coupling constants. Asymmetric isotopic substitution lowers the original vibrational symmetry of the problem, and thus, drastically modifies the observed vibrational spectrum. This modification allows determination of parameters of the vibronic Hamiltonian of Jahn-Teller active systems with greater confidence than is possible using the symmetric isotopomers alone. SEP spectra of CHD_2O and CH_2DO are presented and analysis of the patterns of spin-vibronic states is attempted. A spin-vibronic Hamiltonian is used that considers simultaneous effects of linear Jahn-Teller and spin-orbit interactions. Connections between the Jahn-Teller interaction parameters of the isotopomers are discussed.

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