ON ISOTOPE EFFECT IN THE EXPANDED LOCAL MODE APPROACH: XY_2 (C_{2v}) MOLECULES

O. N. ULENIKOV, I .M. OLEKHNOVITCH, AND R. N. TOLCHENOV, *Tomsk State University, Tomsk, Russia*.

Earlier[a], "expanded" local mode method was derived, which allows one to considerably move apart frameworks of efficient in chemical physics local mode approach. In present paper this method is further derived, and influence of isotope substitutions of light atoms on properties of Hamiltonians, spectroscopic parameters, etc., of different isotopic species is considered. It is shown that analysis of properties of transformation coefficients allows one to obtain sets of new nontrivial relations between different spectroscopic parameters of different isotopic species. XY_2 (C_{2v} symmetry) molecules are considered as an example. As an illustration, H_2Se – HDS – D_2S species are considered.

[a] O. N. Ulenikov, R. N. Tolchenov, and Q.-S. Zhu, *Spectr. Acta*, **52A**,1829-1841(1996).