ISOTOPIC EFFECTS IN LINE INTENSITIES AND DYNAMICS OF THE OZONE MOLECULE: AB INITIO CALCULATIONS

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Anomalous isotopic effects in the ozone formation are still far from being fully understood. A recent progress in the theoretical studies, which could pave the way towards a solution of these challenging problem will be discussed. This will include ab initio line intensity calculations for ro-vibrational bands of isotopologues containing both boson ^{18}O and fermion ^{17}O oxygen atoms that result to significant changes in the inter-mode couplings and in the resonance intensity transfer. Theoretical spectra for the full set of all eighteen ozone isotopic species together with the interpretation of observed perturbations in available experimental data will be overviewed in this work for the first time. At high energy range near the dissociation threshold, the interaction between the three potential wells that occur due to Jahn-Teller effect results to a delocalization of wave functions. In this context, the lifetimes of the metastable states above the D_0 threshold and a classification of scattering resonances and dissociation channels for symmetric and asymmetric isotopic species will be discussed. The role of the mass-dependent contributions to the band origins and rotational patterns beyond the Born-Oppenheimer approximation will be also reviewed. The work of the Tomsk group was supported by the RSF grant 19-12-00171-P.

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