WAVE FUNCTIONS AND LIFETIMES OF OZONE METASTABLE STATES ABOVE THE DISSOCIATION THRESHOLD : IMPACT ON THE DYNAMICS

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The new potential energy surface of ozone recently developed[1,2] is used to determine energies of vibrational bound states and predissociation resonances of O_3. For the vibrational state calculations, the hyperspherical coordinates and the methods of slow-variable discretization with a complex absorbing potential are used[3]. Results obtained in this study perfectly agree with previous calculations and reproduce the experimental energies up to the 8000 cm^{-1} region. Coupling between the three potential wells of the ozone molecule is taken into account, which is important for the correct description of excited vibrational levels and resonances. Symmetric and asymmetric isotopologues can be treated. For symmetric isotopologues, states of all possible irreducible representations have been calculated and widths of the resonances in the region 0-3000 cm^{-1} above dissociation determined. The widths are mostly between 0.1 cm^{-1} and 10 cm^{-1}, depending on the nature of the short-range part of the resonance wave functions: Resonances may differ by the degree of vibrational excitation and also by the relative angular momentum of the dissociating O-O_2 system, which can also be viewed as motion between the three potential wells. Wave functions of the predissociation resonances obtained for asymmetric molecules provide information about the exchange reaction $^{x}O + {}^{y}O^{z}O \rightarrow {}^{y}O + {}^{x}O^{z}O$ or $^{x}O + {}^{y}O^{y}O \rightarrow {}^{y}O + {}^{x}O^{y}O$. A possible impact on the dynamics will be discussed. This work is supported by the Conseil Régional Champagne-Ardenne (ESRI/Sdel/OD-20130604), National Science Foundation, Grant No PHY-10-68785 and French-Russian LIA SAMIA.

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