Abstract Submitted
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Several levels of theory for description of isotope effects in ozone
DMITRI BABIKOV, Marquette University — We developed a multi-level theory for description of the intricate isotope effect in ozone. At 0th level of theory the role of molecular symmetry is taken into account. Although the important factors of 1/2 appear in seven different places in the formalism, this level of theory does not lead to any isotope effect. At the 1st level the effect of atomic masses is introduced to elucidate the roles of vibrational zero-point energies and rotational excitations. It is found that averaging over thermal distribution smooths isotopic differences and leads to a small net effect. At the 2nd level the process is assumed to proceed through independent diabatic ro-vibrational channels, which permits to determine contribution of shape resonances populated by tunnelling. Resultant isotope effects do not look like experiment and the rate coefficient is too small. At the 3rd level the role of Feshbach resonances is determined, by accurate close-coupling calculations using hyper-spherical coordinates, adaptive grids, sequential diagonalization truncation technique and complex absorbing potential. Comparison with experiment is presented. Refs: J. Phys. Chem. A 122, 9177 (2018); J. Chem. Phys. 149, 164302 (2018).

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