

[CITATION] [Several levels of theory for description of anomalous isotope effect in ozone](#)

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We developed a rigorous multi-level theory for description of ozone formation, with particular emphasis on the isotope effect. At 0th level of theory the role of molecular symmetry is accurately outlined, and it is shown that it does not lead to any isotope effect. At the 1st level of theory, equivalent to the statistical description of the recombination process, the effect of atomic masses is taken into account to elucidate the roles of vibrational zero-point energies and rotational excitations. A relatively small isotope effect is obtained, insufficient to explain experiments. At the 2nd level of theory, the reaction is assumed to proceed through the independent diabatic ro-vibrational channels, which permits to determine contribution of shape-type resonances, populated by tunneling and trapped behind the centrifugal barrier. The resultant isotope effects do not look like experimental data. At the 3rd level of theory 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 available experimental data is presented.



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