

**[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 0<sup>th</sup> 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 1<sup>st</sup> 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 2<sup>nd</sup> 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 3<sup>rd</sup> 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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