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Calculation of scattering resonances in ozone using stabilization method ELIZAVETA GRUSHNIKOVA, DMITRI BABIKOV, Marquette University — Study of the formation mechanism for atmospheric ozone helps to understand development of planetary atmosphere. We focus on anomalous mass-independent isotope effect. To understand the nature of isotope effect we consider all stages of ozone formation with commonly used mechanism at the low pressure regime - energy transfer (Lindemann) mechanism which involves metastable intermediate state O3*. O3* is described by scattering resonance in quantum mechanics. Particularly, scattering resonances can be calculated using of stabilization method of Clary. Stabilization approach implies that eigenvalues change as a functions of stabilization parameter (extension of the grid boundary). Based on quantum mechanical calculations of scattering resonances, kinetic rate coefficients were computed. Found resonance states were used for calculation of kinetics rate coefficients such as equilibrium and recombination coefficients for three pressure regimes (0.3, 30 and 3000 atm). Influence of pressure was estimated as well as contributions of other kinetic parameters - stabilization constant weight of each resonance, rotational, vibrational and electronic partition functions for molecule ^{686}O3.

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