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LOW TEMPERATURE QUANTUM DYNAMICS OF OXYGEN EXCHANGE REACTIONS INVOLVING 17O

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Context: Molecular oxygen is peculiar of Earth's atmosphere and the precursor of stratospheric ozone which absorbs most of the Sun UV radiations. Oxygen isotopic analysis allows one to trace back the origin of elements constituting Solar system primitive materials, like meteorites and comets. O_2 and O_3 formed from ^{16}O isotope are dominant, thereby giving a reference for any process involving oxygen. A strong enrichment, about 10% greater than that following usual fractionation rules, of O_3 in both ^{18}O and ^{17}O, the so-called mass-independent fractionation (MIF), has first been observed decades ago in primitive chondrites and stratosphere [1,2], and since reproduced in laboratory experiments [3]. However, its proper quantum mechanical explanation has never been attained. Ozone is the stabilized form of the oxygen exchange reaction O + $O_2 \rightarrow O_3^* \rightarrow$ O_2 + O intermediate O_3^*. The study of the latter with ^{17}O-enriched isotopomers of O_2 is thus important for a full understanding of heavy O_3 formation. The $^{34}O_2$ species has already been investigated in collision with He [4], in the context of buffer gas cooling and subsequent magnetic trapping allowed by its $S = 1$ electronic spin. Furthermore, the nonzero nuclear spin of ^{17}O, $I = 5/2$, makes it a suitable candidate for further study at ultra-low temperatures, in the presence of a magnetic field.

Methodology: We have used a high quality ab initio potential energy surface [5] to perform computationally intensive full quantum investigation of the dynamics of this scattering process.

Results: We shall present cross sections and rate constants [6,7,8] for the ^{17}O + $^{32}O_2$, ^{16}O + op$^{34}O_2$ and ^{17}O + op$^{34}O_2$ reactions. We will discuss observed isotope effects, and the importance of symmetry in relation to nuclear spin and ortho-para conversions [8].

References:

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