

"Mass-independent isotope fractionation in ozone"

P. Reinhardt (UPMC), F. Robert (MNHN)

Laboratoire de Chimie Théorique
Université Pierre et Marie Curie
tour 12-13, 4e étage, bureau 402
4, place Jussieu, case courrier 137
F - 75252 Paris CEDEX 05

The origin of this effect is supposed to be linked to the quantum mechanical principle according to which it is not permitted, in a scattering process, to separate the probabilities describing the recoil from the incident particle, if the two particles are indistinguishable. We ascribe the mass independent isotopic fractionation factor to the lifetime ratio of the complexes formed by reactions involving dis- and indistinguishable isotopes.

In order to illustrate the consequences of this principle, all the accompanying scattering calculations of $O+O_2 \rightarrow O_3^* \rightarrow O+O_2$ were performed in a thermal gas with oxygen isotopes having the same mass (16 amu). It is numerically shown that the origin of the experimentally observed mass-independent isotope fractionation in ozone is well accounted for within this single assumption.

Including masses explicitly has only little influence on the results. More important seems to consider differences in zero-point energies of the O_2 moieties in the intermediate O_3 complex in a collision process. All together allow to reproduce the experimental results to a reasonable precision.