Atmospheric chemistry hinges on better physics model

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New theoretical physics models could help us better grasp the atmospheric chemistry of ozone depletion. Indeed, understanding photoabsorption of nitrous oxide (N2O) - a process which involves the transfer of the energy of a photon to the molecule - matters because a small fraction of N2O reacts with oxygen atoms in the stratosphere to produce among others nitric oxide (NO). The latter participates in the catalytic destruction of ozone (O3). Now, new theoretical work unveils the actual dynamic of the photoabsorption of nitrous oxide molecules.

These findings by Mohammad Noh Daud from the University of Malaya, Kuala Lumpur in Malaysia, have just been published in the *European Physical Journal D*. The work has led to new calculations of the probability of an absorption process taking place, also referred to as absorption cross section. These calculations confirm experimental results.

In this study, the author introduces improvements in an established calculation approach, referred to as the ab initio time-dependent method. It helps calculate the absorption cross section, or spectrum, of nitrous oxide. The advantage of this approach is that it immediately yields the energy dependence of a cross section or spectrum from a single calculation. By taking into account key factors such as the correct angular momentum coupling of the molecule and the component of the transition dipole moment vector, the theoretical model of calculated spectrum has produced better results than previously obtained and more closely matches experimental observations.

Daud's calculation thus provides an improved theoretical prediction of how nitrous oxide evolves and breaks down over time, thus contributing to the nitrous oxide photoabsorption process. As such processes occur in a small gap between the absorption band of oxygen and that of ozone, the predicted major dissociation pathway allows us to understand the involvement of nitrous oxide in the formation of ozone at the molecular level.

More information: Daud, M. N. (2014). "Accurate treatment of total photoabsorption cross sections by an ab initio time-dependent method." *European Physical Journal D*. DOI: 10.1140/epjd/e2014-50400-4

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