

## T19 (OC)

### AB INITIO STUDY OF ICE, NAM, NAD AND NAT CRYSTALS

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Polar Stratospheric Clouds (PSC's) are mixtures of ice and nitric acid-ice crystals that form over Antarctica during the winter and catalyze the destruction of the chlorine reservoir species to form chlorine active substances, which are responsible for ozone depletion. In this work we present a theoretical, quantum mechanical study of these crystals as a first step in the process of understanding the mechanisms implied in the reactions taking place there.

We have studied crystals of ice and nitric acid hydrates with one, two and three water molecules (NAM, NAD and NAT respectively), which are the three known forms of nitric ice crystals. Our model supposes they are perfect periodic crystals that can be studied using the solid state approximations. We have used a density functional formulation (DFT), with a generalized gradient approximation (GGA) for the exchange-correlation potential. We have also used norm conserving pseudopotentials. The basis set has been numerical LCAO. All the calculations have been performed using the SIESTA program (acronym for Spanish Initiative for Electronic Simulation with Thousands of Atoms).[1] It is a method that scales linearly with the number of atoms in the simulation cell.

The results obtained concern the optimized crystal structures at temperatures relevant for the atmospheric conditions, as well as the infrared frequencies of every solid. They have been compared with experimental measurements and with results of other different theoretical models and calculations. The conclusion is that the technique we have selected is able to give good results in this type of crystals and can be used in the next steps of our study, which are the geometry and forces responsible for the adsorption and further reaction of the chlorine reservoir species.

1. P. Ordejon, *Physica Status Solidi (b)* 217, 335 (2000), see also <http://www.uam.es/siesta>.