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Theoretical study of atmospheric clusters: HNO3:HCl:H2O

PC Gomez (1), RM Escribano (2), and O Galvez (2)

(1) Dept. Quimica-Fisica, Universidad Complutense and Unidad Asociada UCM-CSIC, Madrid, Spain (pgomez@quim.ucm.es,T:+34 913944279), (2) Inst. Estructura de la Materia, CSIC, Molecular Physics, Madrid, Spain

Water, nitric acid and hydrogen chloride play an important role in several atmospheric processes, as individual species, and also interacting in the complex reactions related to ozone depletion in polar stratospheric clouds (PSC). The atmospheric importance of the ternary system HCl:HNO3:H2O was recognized long ago [1]. It is also known that HCl attaches to the surface of PSC particles formed by nitric acid hydrates in what can be considered the first step of the heterogeneous reactions leading to the release of the active chlorine molecule [2]. Recently, HCl was detected dissolved in liquid particles with HNO3/H2O by in situ measurements in the Artic stratosphere [3].

The study of simple models including these three species at a high level of theory can be the first step towards the understanding of all possible kinds of bonding and structures that can arise among these molecules, and can constitute the embryo of more complex mixtures with higher amounts of water or variable proportions of their constituents. This kind of calculations have been successfully performed in the past [4,5].

We present in this contribution our results on the structure and spectroscopical properties of the many different ways that these molecules can be bonded in what are predicted to be thermodynamically stable species. The calculations are performed by density functional methods (B3LYP) using Dunning's quadruple-zeta augmented correlated consisted basis sets (aug-cc-pVQZ).

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