



## Quantum chemical study of ternary mixtures of: $\text{HNO}_3\text{:H}_2\text{SO}_4\text{:H}_2\text{O}$

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Water, nitric acid and sulfuric acid are important atmospheric species as individual species and as hydrogen-bonded aggregates involved in many physical-chemical processes both superficial and bulk. The importance of heterogeneous chemical reactions taking place on ice surfaces, either solid water or solid water plus nitric or sulfuric acid, is well established now in relation to the ozone-depleting mechanisms. Also the importance of liquid droplets formed by  $\text{HNO}_3\text{:H}_2\text{SO}_4\text{:H}_2\text{O}$  as components of PSC was soon recognized [1-3]. Finally the physical properties of finely divided aqueous systems is an interesting and active field of research in which theoretical information on the microphysical domain systems may help to understand and rationalize the wealth of experimental information. This can also be the initial step in the study 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].

We present here our results on the structure and spectroscopic and thermodynamic properties of the energy-lowest lying structures among those thermodynamically stable formed by linking the acids plus water. The calculations have been carried out by means of DFT methods (in particular the successful B3LYP) using different basis sets that contain appropriate sets of polarization and diffuse functions up to quadruple-Z quality (Dunning's aug-cc-pVQZ). Careful assessment of the dependability of the methodology used has been carried out.

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### References:

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