Theoretical Characterization and Identification of Electrides

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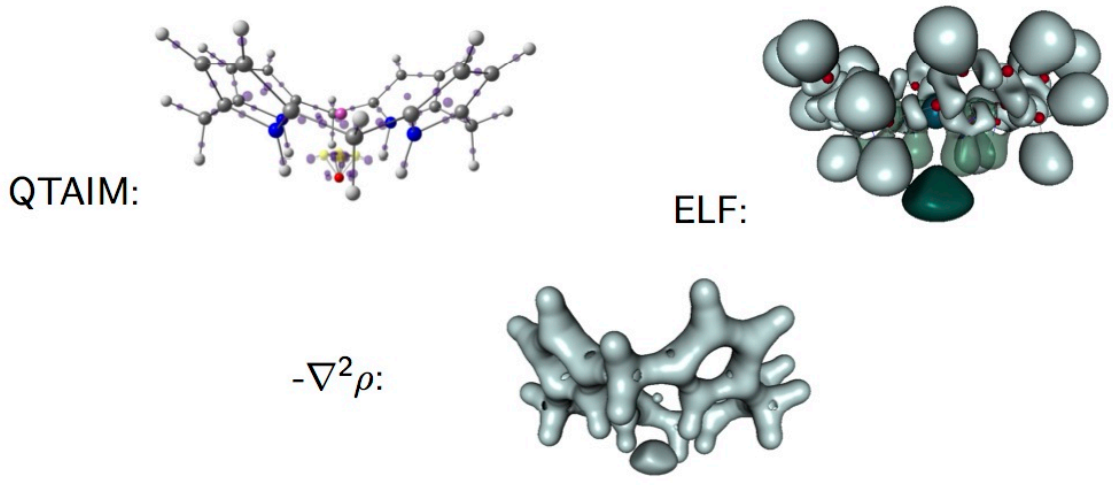
The electrides[1-2] are intriguing chemical species with an electron not formally assigned to any atom. This situation is, however, completely different to that given in a metal where the electrons are delocalized between positively charged metal ions. The electron in an electride acts as a formal anion, which is bonded to positively charged species in the molecule. This particular feature of electrides prompts very particular chemical and physical properties: they are powerful reducing reagents, exhibit exalted electric linear and non-linear optical properties as well as a particular magnetic behavior.

In this work, we analyze the electronic structure and the identification of several electride structures by means of the Quantum Theory of Atoms in Molecules (QTAIM) and the Electron Localization Function (ELF).[3] Our results show that these tools make possible the classification of candidate species as electrides or not. It was already proved that one could distinguish the electride behavior in insulating high-pressure forms of alkali metals from ELF analysis[4] but now we show that with QTAIM and ELF is possible to characterize the electride behavior in all sorts of molecules.



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2.- Dye, J. L. *Science*, **1990**, *247*, 663
3.- Matito, E.; Solà, M. *Coord. Chem. Rev.,* **2009**, *253*, 647-665
4.- Marqués et al., Phys Rev. Lett. **2009**, 103, 115501