Atoms that bond to C:
QTAIM analysis of the electron density and beyond

D. Menéndez-Crespo[1], *A. Otero-de-la-Roza*[2] *and* *Víctor Luaña*

1. Departamento de Química Física y Analítica, Facultad de Química, Universidad de Oviedo, E-33006 Oviedo, Spain
2. National Institute of Nanotechnology, National Research Council of Canada, 11421 Saskatchewan Drive, Edmonton, Alberta T6G 2M9, Canada;

In a previous work [1] we have shown that the distance evolution of the CC couple is a good predictor for this atomic graph (two binded atoms with a nolecule) [2] in molecules an solids. Our intention now is to extend this analysis to other CX graphs. Combinations that have not been exhaustively studied by experimental synthesis groups are particularly interesting, like the CS case. Our traditional tools, $\rho(\bm{r})$ and $\nabla^2\rho(\bm{r})$, are now extended to the topology of the electrostatic potential [3] and the NCI index [4,5].

References:

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