Electron localization function as a measure of electron delocalization and aromaticity

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The Electron Localization Function (ELF) has played in the last time an important role in understanding the special characteristics of the chemical bond. The chemical interpretation of the ELF as an indicator of the regions of the space where it is most probable to find a localized electron pair has been of great value in order to understand some complex chemical bonds. In this work, the ELF has been used to study the delocalization and aromatic character of a diversity of molecules. It is shown that whereas the analysis of the total ELF does not provide clear information about aromaticity, the separation of the function on its ? and ? parts yields indeed valuable information about it. Moreover, it is possible to construct a quantitative scale of aromaticity. It is also shown that the use of the ELF to understand aromaticity is complementary to other methodologies. The study includes mono substituted benzene derivatives, cyclic organic compounds, borazine molecule and the mechanism of