



Quantum chemical topology study on the electronic structure of *cis*- and *trans*-FONO.

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Streszczenie

The electronic structure of *cis*- and *trans*-FONO has been studied using topological analysis of the electron localization function at the B3LYP/aug-cc-pVTZ computational level. In *cis*-FONO with "normal" F-O bond length (1.428-1.441 Å), a protocovalent F-O bonding has been found. The central N-O bond is "drained off" with the electron density (0.40e and 0.42e) and the terminal N-O bond resembles an electron-rich single bond (2.13e-2.14e). The F...ONO form with a long F...O bond (1.719 and 1.696 Å) has a diradical character and consists of F and NO(2) subunits without clear indications of the covalent bond in the F...O region.

Adres publiczny

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