FONO: a difficult case for theory. The ELF and ELI–D topological studies on the chemical bonding using correlated wavefunctions.

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Streszczenie

The complicated nature of the chemical bonding in cis and trans isomers of F–O–N=O is discussed based on the results obtained from the topological analysis of electron localization function (η) (ELF), electron localizability index (YσD), and electron density (ρ). The calculations have been performed for correlated wavefunctions using the CCSD and CASSCF methods. The F–O1 bond with non-bonding basins, V(F) and V$^{\prime}$(O1), belongs to the protocovalent type (η,YσD) and its total population ranges between 0.2 and 0.4e. The central N–O1 bond in the cis form is protocovalent (η, YσD) with two basins, V(N) and V(O1). The total population oscillates between 0.7 and 0.9e. In the trans isomer, topology of ELF depends on used method. At the CCSD level only one non-bonding basin, V(N), is observed (η). Its population is about 0.5e. According to the definition of a heteronuclear charge-shift (CS) bond, only N–O1 bond in *trans*-FONO belongs to the CS class. A relation between η- and ρ-topology and N–O1 bond length is discussed.

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