Diversity of the nature of the nitrogen-oxygen bond in inorganic and organic nitrites in the light of topological analysis of electron localisation function (ELF).

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Streszczenie

The electronic structure of nitrite group (–ONO) has been studied for 21 inorganic and organic nitrites using topological analysis of Electron Localisation Function (ELF) for the DFT(B2PLYP)/aug-cc-pVTZ and DFT(B3LYP)/aug-cc-pVTZ optimised geometrical structures. The N–O bonds exhibit populations smaller than 2e, thus including the N+O−, N−O+ Lewis-type structures in the description of electron density delocalisation is of great importance. The main focus of the ELF analysis was formally single N–O bond in the nitrite group (–O–NO). The results have yielded four different types of local topology: (a) single local maximum V(N,O) with the disynaptic bonding basin, (b) two local maxima V(N), V(O) with monosynaptic non-bonding basins, (c) single local maximum V(N) with monosynaptic non-bonding basin, (d) absence of the local maxima in the N–O bond. Analysis of relationships between basin population values, calculated for the V(N,O), V(N) and V(O) basins, and the N–O bond length, has shown overall trends that can be qualitatively described by the catastrophe theory.

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