# Quantum chemical topology: the electronic structure of the alkaline nitrites MONO (M = Li, Na, K) studied by means of topological analysis of the electron localization function.

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Rok wydania

2010

Czasopismo

International Journal of Quantum Chemistry

Numer woluminu

110

Strony

1890-1900

DOI

10.1002/qua.22383

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

In the search of the protocovalent bonding, previously recognized in the nitrous acid (HONO), a nature of the chemical bonds in the alkaline nitrites MONO (M = Li, Na, K) has been studied by means of the topological analysis of the Electron Localization Function (ELF) and Electron Localizability Indicator (ELI-D). Calculations carried out with the B3LYP and MP2(full) methods, in conjunction with the aug-cc-pVTZ and 6-311++G(3df,3pd) basis sets, revealed the *cis* ($C_{2v}$, more stable) and *trans* ($C_s$) isomers as minima on PES. Alkaline nitrites consist of the alkali metal cation $M^{\delta+}$ interacting, mainly via electrostatic forces, with the nitrite anion $[ONO]^{\delta-}$ ($\delta \approx 1e$). The covalent N▯O bonds are characterized by disynaptic basins V(N,O) with the basin populations: 1.58÷1.62e for *cis*-$M^{\delta+}[ONO]^{\delta-}$ but 1.39÷1.49e for single N▯O bond and 1.81÷1.87e for formally double N⌡O bond in *trans* $M^{\delta+}$[O▯N⌡O]$^{\delta-}$. The protocovalent nitrogen–oxygen bond has not been observed. The N▯O bonds are slightly polarized towards the nitrogen atom with the polarity index $p_{NO} \leq 0.12$. Two different sets of the hybrid (Lewis) structures are compared leading to different pictures of the bonding. According to NBO data there is a delocalization between the single N▯O and double N⌡O type bonds, meanwhile results of the ELF analysis emphasize an electron delocalization between the single N▯O and ionic $O^{-}N^{+}$ hybrids. © 2009 Wiley Periodicals, Inc. Int J Quantum Chem, 2010

Słowa kluczowe

electron localization function, chemical bond, B3LYP, MP2, DFT

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https://doi.org/10.1002/qua.22383