

Protocovalent N–O bonding in methyl nitrite (CH_3ONO) and ethyl nitrite ($\text{C}_2\text{H}_5\text{ONO}$).
Topological analysis of the electron localization function (ELF) and electron localizability
indicator (ELI-D) functions.

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Streszczenie

Topological analysis of the ELF and ELI-D functions has been carried out using DFT and CASSCF methods for cis- and trans-isomers of methyl nitrite (CH_3ONO), as well as three conformers of ethyl nitrite ($\text{C}_2\text{H}_5\text{ONO}$). The N–O central bond is of protocovalent type and is represented by the $V(\text{N})$ and $V(\text{O})$ attractors (basins), with a population of 0.79/1.15e in CH_3ONO and 1.08/1.12e in $\text{C}_2\text{H}_5\text{ONO}$. The correspondence between the protocovalent N–O bond and the most favourable dissociation channel, previously observed for nitrous acid (HONO) [9], has been confirmed.

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