

The view on the C=N-O group in the RHC=NO (R=H, BH₂, CH₃, NH₂, OH, F) iminoxy radicals by means of electron localisation function (ELF).

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Streszczenie

The topological analysis of the electron localisation function (ELF) for a variety of RHC=NO iminoxy radicals shows that *Z* to *E* isomerisation results in a redistribution of electron density from the N and O lone electron pairs to the N–O and C=N bonds. Substitution of R by more electronegative group is associated with increase of $\langle S \rangle$ for $V_1(O) \cup V_2(O)$ and decrease for $V(N)$. The mean electron population of $V(R,C)$ basin decreases with growing electronegativity of R. Dependence of hyperfine coupling on the R substituent may be explained as a consequence of an electron density delocalisation between the C–H and C–R bonds: $V(C,H) \Leftrightarrow V(C,R)$.

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