

Relationship between electron difference-density distribution, planarity of the >N-O groups and intermolecular hydrogen bond systems in crystals of stable nitroxide radicals.

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The electron density distribution calculated for 2,2,6,6-tetramethyl-1-piperidinyloxy (**1**), 4-hydroxy-2,2,6,6-tetramethyl-1-piperidinyloxy (**2**) and 3-carbamoyl-2,2,5,5-tetramethyl-3-pyrrolin-1-yloxy (**3**) free radicals on the basis of low-temperature X-ray single crystal diffraction experiments revealed some differences in region of the >N-O groups. Generally, the experimental bonding density along the axis of the N-O bond is relatively low and asymmetric in cases of the pyramidal geometry of the aminoxyl group (**1** and **2**) and almost symmetrical for the planar geometry (**3**). The shape and distribution of electron densities in the region of the oxygen lone-pairs suggest that this atom is sp^3 hybridized but the spatial orientation of these maxima depends on hydrogen bond interactions ($>N-O\cdots H$) in studied crystals. Also the relation between the direction of the relatively strong hydrogen bonds ($O\cdots H < 2.2 \text{ \AA}$) and the geometry of aminoxyl groups analysed for crystal structures collected in the Cambridge Structural Database showed that these interactions can affect the aminoxyl group geometry.

Adres publiczny

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