Aromaticity of overcrowded nitroanilines.

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Streszczenie

For a series of 2,4,6-trinitroanilines substituted with bulky groups, the influence of intramolecular hydrogen bonds, electronic substituents effect, and steric hindrance on aromaticity of the molecules in crystals and their analogues optimized at the B3LYP/6-311++G** level were studied. The HOMA index was used as a measure of the aromaticity, while the parameter ΔP was a description of the distortion of the benzene ring from planarity. Conformation of the nonplanar ring in crystal and optimized structures was also described using the puckering parameters. A comparison of the data for crystal and optimized structures showed an important effect of the intermolecular interactions on aromaticity of the overcrowded nitroanilines. The packing effects were analyzed using the simplified PCM model of solvents. NBO analysis illustrated the changes of orbitals upon dearomatisation

Adres publiczny

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Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html