

The conformational analysis of 2-hydroxyaryl Schiff thiosemicarbazones.

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Streszczenie

X-Ray measurements and quantum-mechanical (B3LYP and MP2) calculations of 2-hydroxyaryl Schiff thiosemicarbazones were performed to describe the tautomeric and conformational equilibrium. The structures of five N-alkyl- and N-aryl-thiosemicarbazone derivatives were determined by single-crystal X-ray diffraction at 100 K. The conformational schemes for determining the various states of the compounds were calculated by the DFT (B3LYP/6-31+G(d,p)) method. The difference between the phenolic and heterocyclic derivatives with respect to the $\text{OH} \rightleftharpoons \text{HN}$ tautomeric equilibrium is shown. The influence of the environment's polarity on $\text{C}[\text{double bond, length as m-dash}]\text{S} \rightleftharpoons \text{S}[\text{double bond, length as m-dash}]\text{C}$ conformational equilibrium was determined by DFT calculations. The potential energy curves for rotating particular fragments of the thiosemicarbazone moiety were calculated to estimate the rotational energetic barriers.

Adres publiczny

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Strona internetowa wydawcy

<https://www.rsc.org/>