Steric and aromatic impact on intramolecular hydrogen bonds in *o*-hydroxyaryl ketones and ketimines.

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Streszczenie

X-ray measurements at 100 K and quantum-mechanical calculations showed a domination of the enol (OH) form in o-hydroxyaryl ketones [6-methoxy-2-hydroxyacetophenone (6OMeK), 4-methoxy-2-hydroxyacetophenone (4OMeK), 5-chloro-4-methyl-2-hydroxybenzophenone (5Cl4MeK) and 2-hydroxyacetonaphthone (o-HAN)], whereas a prevailing proton-transfer (NH) form was found in o-hydroxyacetonaphthylimine [2-(N-methyl-α-iminoethyl)naphthol (o-HIN)]. The effective mechanism of the reduction in hydrogen bridge length due to steric repulsion in the o-hydroxyaryl ketones is presented. The following phenomena were found: a decrease in phenol ring aromaticity caused by the proton-transfer process, dependence of the HOMA index of aromaticity on the HOSE index defining the destabilization of the chelate ring and a dependence of the HOMA index on the lengths of the carbonyl bonds. Moreover, a correlation between phenol ring aromaticity [HOMA(phenol)] and the pseudo-aromatic ring [HOSE(chelate)] is shown. Correlations between structural parameters of the chelate ring [d(C—O), d(Caryl—Calkyl)] and aromatic rings [HOMA(phenol)] of the o-hydroxyaryl ketimines and ketones are presented.

Adres publiczny

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