Structures and energetic properties of 4-halobenzamides.

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Streszczenie

The amide bond represents one of the most fundamental functional groups in chemistry. The properties of amides are defined by amidic resonance ($n_N \rightarrow \pi^*_{C=O}$ conjugation), which enforces planarity of the six atoms comprising the amide bond. Despite the importance of 4-halo-substituted benzamides in organic synthesis, molecular interactions and medicinal chemistry, the effect of 4-halo-substitution on the properties of the amide bond in N,N-disubstituted benzamides has not been studied. Herein, we report the crystal structures and energetic properties of a full series of 4-halobenzamides. The structures of four 4-halobenzamides (halo = iodo, bromo, chloro and fluoro) in the N-morpholinyl series have been determined, namely 4-[(4-halophenyl)carbonyl]morpholine, $C_{11}H_{12}XNO_2$, for halo = iodo (X = I), bromo (X = Br), chloro (X = Cl) and fluoro (X = F). Computations have been used to determine the effect of halogen substitution on the structures and resonance energies. 4-Iodo-N-morpholinylbenzamide crystallized with a significant distortion of the amide bond ($\tau + \chi_N = 33°$). The present study supports the correlation between the Ar-C(O) axis twist angle and the twist angle of the amide N-C(O) bond. Comparison of resonance energies in synthetically valuable N-morpholinyl and N-piperidinyl amides demonstrates that the O atom of the morpholinyl ring has a negligible effect on amidic resonance in the series.

Słowa kluczowe

amide bonds, crystal structure, morpholinyl amides, resonance energies, twisted amides

Adres publiczny

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