

Neutral pyrrole nitrogen atom as a π - and mixed n,π -donor in hydrogen bonding.

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Rok wydania

2019

Czasopismo

Journal of Organic Chemistry

Numer woluminu

84

Strony

726-737

DOI

10.1021/acs.joc.8b02562

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

9-Dimethylaminobenzo[*g*]indoles **3–6** and 1-dimethylamino-8-(pyrrolyl-1)naphthalene **7** were examined as possible models for establishing the ability of the pyrrole nitrogen atom to participate in $[\text{NHN}]^+$ hydrogen bonding as a proton acceptor. Indoles **3–5** (to a lesser extent **6**) form rather stable tetrafluoroborates, with the proton mostly located on the NMe_2 group but simultaneously engaged in the formation of a charged intramolecular $[\text{NHN}]^+$ hydrogen bond (IHB) with the pyrrole N atom. The theoretically estimated energies of IHB in salts **3H⁺BF₄[−]–6H⁺BF₄[−]** vary between 7.0–10.7 and 6.2–7.0 kcal mol^{−1} in vapor and MeCN, respectively. The pyrrole N atom undergoes a perceptible pyramidalization but still remains involved in the 6 π -electron aromatic system, suggesting that the hydrogen bonding in salts **3H⁺BF₄[−]–6H⁺BF₄[−]** represents a previously unknown mixed $\text{NH}\cdots\text{N}(n,\pi)$ interaction. Despite the favorable orientation of the N–H bond and the pyrrole ring in salt **7H⁺BF₄[−]**, no signs of $\text{NH}\cdots\text{N}(n)$ bonding in it were noticed, and the existing interaction was classified as pure $\text{NH}\cdots\text{N}(\pi)$. The results obtained may be useful in studies of secondary protein structures, especially those α -helix sections which contain tryptophan residues.

Adres publiczny

<https://doi.org/10.1021/acs.joc.8b02562>

Strona internetowa wydawcy

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Plik został wygenerowany dnia 2026-10-11 02:52:20

Adres w repozytorium <https://old.chem.uni.wroc.pl/pl/repozytorium/1LRSa8e>.