

Calculations of the - NH₂ group vibrations and intensities in aromatic amines by classical VFF and quantum chemical methods.

Autorzy

V. E. Borisenko

A. V. Baturin

Małgorzata Przesławska

Aleksander Koll

Rok wydania

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The equilibrium NH bond lengths, $\gamma(\text{HNH})$ angles, dipole moments and derivatives of the dipole moment with respect to the NH bond length $\partial\mu/\partial r_{\text{NH}}$ were calculated by semiempirical MINDO/3, MNDO, AM1 and PM3 methods, for aniline and its 12 mono-substituted -CH₃, -F, -Cl and -Br derivatives. The results of the calculations were compared with analogous values obtained with the help of VFF and ab initio MP2/6-31G** procedures. All methods give a reasonable reproduction of the structure and dipole moments of the studied compounds. The results of $\partial\mu/\partial r_{\text{NH}}$ derivative calculations with MNDO, AM1 and PM3 procedures properly describe the experimental tendencies, but numerical values obtained by molecular orbital and VFF methods can differ in value or even in sign.

Adres publiczny

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