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Dipole moments of 2,4-diketopyrimidines: Part II: Uracil, thymine  
and their derivatives

I. Kulakowska<sup>a</sup> ... K.L. Wierzchowski<sup>a</sup>

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Abstract

The dipole moments of uracil, thymine and of 29 of their variously substituted derivatives were experimentally determined in dioxane. A vector scheme of calculations was applied to evaluate the effects of alkyl and halogen substituents on the dipole moment of uracil. The dipole moments of a number of diketopyrimidines studied were also calculated quantum mechanically by the CNDO2 method. General agreement between the experimental and calculated values was obtained. The substituent-induced electron charge redistributions are discussed in terms of  $\dot{\rho}_f$ - and  $\dot{\rho}_\pi$ -populations.



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