

Prediction of Dipole Moment (μ) for Antifine substituted, Calculation theory and (QSPR) Techniques.

Kawkaib A. Hussain

Department of Chemistry – College of Education Pure Science
University of Basrah – Iraq

Abstract

Calculated theory for dipole moment (μ), of aniline substituted have been conducted. The study was done by using molecular modeling. The calculation was performed by different methods PM3, PM6, and MM2 at 6-31G(d,p) basis set and predicted dipole moment (μ) by QSPR. The relationship analysis between dipole moment (μ), and physicochemical properties understudy was done by multiple linear regression (MLR) analysis to produce the equation that relates the structural features to the dipole moment (μ), properties. The results show good models with one and two parameters linear equations. The best model predicted in this study was the eq 6, with excellent statistical fit as evident from its $R^2 = 0.972$, $F = 41.455$, $S = 0.329$, and $RA^2 = 0.949$, the model including the descriptors [LogP, surface(A), surface(G), T.E, REIT and E.GAP], which showed insignificant role in the dipole moment (μ), of compounds. And this could potentially offer a new opportunity in the design of novel properties or extended to other compounds.

Keywords Aniline substituted predicted dipole moment(μ) (QSPR) Model

الخلاصة