



## Solvatochromic Study of Organic Dyes: A Qualitative Approach using Semiempirical (ZINDO-IEFPCM) Method

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### Abstract

The present investigation accounts for determining computationally the solvatochromic behavior of Coumarin dyes (C478, C519 and C523) in series of alcohols. Experimentally observed positive and negative solvatochromism are accounted for and their behavior is well explained by computational results. The semi empirical  $E_T(30)$  scale has been adopted to define the polarity dependent solvent-solute interaction. The ZINDO/PCM method follows the observed experimental trends for all the Coumarin dyes. The small discrepancies with experimental values are discussed in detail. Computational results suggest that ZINDO/PCM values lie in closer proximity to the experimental values depending on the polarity of Coumarin molecules. Switching between positive and negative solvatochromism in polarity scale referred as polarity switch is discussed.

**Keywords:** Polarity scale, Positive and negative solvatochromism, ZINDO/PCM, Polarity switch.

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