

## Solvatochromic reversal: is it really possible?

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**Abstract:** Several theoretical and experimental studies have shown that organic dyes may show solvatochromic reversal in the visible region with respect to the solvent polarity. This controversial non-monotonic behavior is still not well understood. This has been analyzed here using the merocyanine of Brooker as the working example. Sometimes the solvatochromic reversal is attributed to self-aggregation.[1] In spite of this, some works discard the aggregation origin and point to structural changes of resonance hybrid between the neutral (quinoid) and the zwitterionic (benzenoid) canonical structures.[2,3,4,5,6]. Also it is argued that the flow direction of the charge transfer in the merocyanine dye plays an important role.[7] A better understanding of the real possibility of solvatochromic reversal is both timely and relevant. Considering an electric field to model the solvent polarity a solvatochromic reversal is obtained with a single solute without aggregation. Thus the reversal behavior is obtained as the result of a competition between structural changes and intramolecular charge transfer. [8] This change of regime, held responsible for the solvatochromic reversal, affects in a similar way the <sup>13</sup>C magnetic shielding constant. [8]

**Key-words**: Solvatochromic reversal, Merocyanine of Brooker, Absorption spectrum, Solvent effect.

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