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Title:	Rhodamine 6G interaction with solvents studied by vibrational spectroscopy and density functional theory
Authors:	Mhahajan, C.G. (/jspui/browse?type=author&value=Mhahajan%2C+C.G.)
Keywords:	Density functional theory calculations Infrared spectra Raman spectra Rhodamine 6G Solvent effect Atoms
Issue Date:	2009
Publisher:	Elsevier B.V.
Citation:	Journal of Molecular Structure, 931 (1-3), pp. 10-19.
Abstract:	We report Raman and infrared spectra of rhodamine 6G dye in different experimental conditions. Positions of some of the observed vibrational bands show noticeable change in the solvents. The bands, which shift, have contributions from the vibrational motion of nitrogen atoms of the ethoxyamine groups, oxygen atom of the ethoxycarbonyl group attached to the phenyl ring and the atoms of the xanthene ring. These shifts arise due to simultaneous interaction of a number of solvent molecules at nitrogen and hydrogen atoms of ethoxyamine, oxygen atom of ethoxycarbonyl and the central oxygen atom of the xanthene ring of the dye molecule. Density functional theory calculations of molecular parameters and atomic charge densities of rhodamine 6G and most probable rhodamine 6G-methanol complexes also support these interactions. Methanol and dimethylformamide also interact electrostatically with the positively charged nitrogen atom of the dye molecule.
Description:	Only IISERM authors are available in the record.
URI:	<a href="http://dx.doi.org/10.1016/j.molstruc.2009.05.015">http://dx.doi.org/10.1016/j.molstruc.2009.05.015</a> ( <a href="http://dx.doi.org/10.1016/j.molstruc.2009.05.015">http://dx.doi.org/10.1016/j.molstruc.2009.05.015</a> ) <a href="http://www.sciencedirect.com/science/article/pii/S0022286009002993">http://www.sciencedirect.com/science/article/pii/S0022286009002993</a> ( <a href="http://www.sciencedirect.com/science/article/pii/S0022286009002993">http://www.sciencedirect.com/science/article/pii/S0022286009002993</a> )
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