

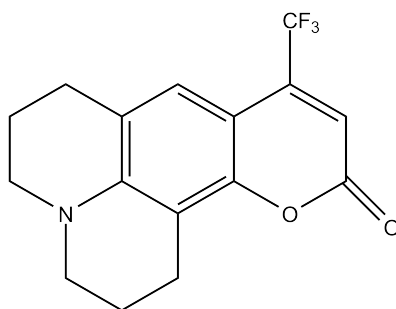
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Solvent Effects on Electronic Structures of Coumarin 153: RISM-SCF Analysis

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Solvent fluctuation plays an essential role to express functions in proteins or biological systems. A part of the present authors have studied solvation dynamics by fs-ps transient hole-burning spectroscopy,[1,2] dynamic fluorescence Stokes-shift measurements,[2] and RISM/mode-coupling theory.[3] In these experimental and theoretical studies, the electronic structure of solute is assumed to be stationary throughout the solvation process. In reality, dynamic rearrangements of solvent can alter solute electronic properties.

In our present works, we have applied RISM-SCF theory to describe electronic structures of a dye molecule, coumarin 153 (C153), in the ground and excited states, immersed in solvents with various polarity and chemical structures. RISM-SCF theory allows us to consider the solvent effects on the electronic structure of solvated molecule as well as solvent distribution around it, which is free from empirical parametrizations as appeared in the usual models based on the dielectric continuum picture. [4,5]



Coumarin 153

In this contribution, we provide a detail of theoretical method and analysis. Vertical $S_0 \rightarrow S_1$ transition energies for the ground state equilibrium geometry and those for the 1st excitation state as well as point dipole moment of c153 in each electronic state in various solvent such as water, THF, THP, acetone, acetonitrile, methanol and ethanol. The solvent distributions are also shown in terms of radial distribution functions between solute and solvent interaction sites.

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