Calculation of resonance Raman intensities using sum-over-state expressions

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Vibrational resonance Raman (RR) spectroscopy is a useful tool to provide information on structures and properties of molecular excited states [1]. Therefore, an accurate simulation of absorption and RR spectra, by quantum chemistry methods, can help in the interpretation of experimental data as well as in the design of new compounds for specific applications e.g. in dye-sensitized solar cells or as photocatalysts [2-4].

In this contribution, simplified sum-over-state expressions are presented to calculate RR intensities, which allow inclusion of Franck-Condon and Herzberg-Teller effects. The molecular properties are calculated with density functional theory or wavefunction-based approaches. The methods are applied to organic dyes and transition metal complexes and comparison with experimental results is provided to assess the methods. In particular, the inclusion of Herzberg-Teller vibronic couplings is described in the case of Rhodamine 6G [5-7].

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