

The molecular spectroscopy which works in the wavelength regions of UV-Vis have various applications. For quantitative determination species in mixtures, characterization of pure compound, identification of the presence or absence of a particular species in a mixture or certain functional groups in a compound. It also used to study self-association, hetero-association and thermodynamic properties of compound. Thus, in this research, the contents of caffeine and chlorogenic acids in coffee beans have been investigated by spectroscopic and theoretical methods. In addition, the optical transition properties of caffeine, caffeic and 5-caffeoylquinic acids were determined in different solvents by integrating the absorption coefficients. Moreover, the concentration dependent self-association of caffeic, 5-caffeoylquinic acids and their hetero-association were analyzed by dimer model and Benesi-Hildebrand approaches. The thermodynamic parameters, enthalpy, Gibbs free energy and entropy of dimerization reactions were calculated from vant Hoff equation.

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