Structural assignment of adenine aggregates in CDCl₃

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We reinvestigated the self-association of 9-substituted adenine derivatives in CDCl₃ solutions and present the infrared spectra of 9-ethyladenine and N-methyl-9-ethyladenine and its aggregates in the spectral regions between 1500 and 1800 cm⁻¹ and between 2700 and 3600 cm⁻¹. Wavelength dependent absolute extinction coefficients of the monomer and dimers are presented on the basis of a simple deconvolution method. Comparison of the deconvoluted dimer spectra with quantum chemical calculations allows for a structural assignment of the two dimer structures that coexist in 9-ethyladenine/CDCl₃ solutions. In contrast, the dimer spectrum of N-methyl-9-ethyladenine is dominated by a single isomer. © 2008 American Institute of Physics. [DOI: 10.1063/1.2912064]