

T03. The study of the interaction between dimethyl formamide and water in binary mixtures by means of Raman spectroscopy and chemometric techniques

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In both liquid dimethyl formamide (DMF) and water, some self-association between the molecules takes place. When the two liquids are mixed, some of this association is expected to change, and instead some interaction between the two liquids is anticipated.

The interaction between DMF and water has been investigated by recording Raman spectra of DMF-water mixtures over the entire composition range. Interaction between DMF and water seems likely, because the maxima of several of the bands in the spectra shift as the composition of the mixtures is varied; the shapes of several of the bands change as well. Such a changes are particularly evident for the -C=O stretching vibration of DMF. The plot of the band maximum of this vibrational band versus mixture composition exhibits unusual features: first it shifts to a lower wavenumber, then to a higher wavenumber as the water component of the mixture increases. The exact positions of the band maxima have been determined by evaluating the second derivative of the Raman spectra.

The spectra of the binary mixtures have been analysed using chemometric techniques, in particular multivariate curve resolution, to validate the observations of the spectral shifts. The results which were obtained assisted in the elucidation of some of the unusual behaviour which has been observed, and some explanations will be presented.