RAMAN SPECTRA AND INTERMOLECULAR HYDROGEN BONDS OF QUINOLINE IN SOLUTIONS

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S u m m a r y

The half-widths of the 1014- and 1033-cm^{-1} bands of the Raman spectrum of quinoline at its dilution in neutral solvents (benzene, CCl_4) are narrowed by 1.3-1.5 times at high dilutions. This effect is associated with the increased time of the vibrational relaxation. For the 520-cm^{-1} band in pure liquid quinoline, the parallel polarized component at 20 °C is asymmetric in the high-frequency region. The shape of the perpendicular polarized component is complicated. A non-coincidence of the peak frequencies of the parallel and perpendicular polarized components is observed (~ 2 cm^{-1}). Quantum-chemical calculations showed that, in the region of 520 cm^{-1} for a monomer molecule, we should really have two near located lines with the wavenumbers 530 and 527 cm^{-1} (scaling factor 0.97), and with the depolarization ratios 0.61 and 0.26. In the solutions with propan-2-ol, the 1033.8-cm^{-1} band becomes of a doublet character. The resolution of the doublet becomes better by the dilution of a binary quinoline-alcohol solution with a large amount of a neutral solvent (benzene). The wavenumbers of bands in the triple mixture are 1033 cm^{-1} and 1039 cm^{-1}. The doublet nature of the band in the binary and triple mixtures is associated with the presence of monomer molecules and quinoline-propan-2-ol aggregates (the high-frequency line) in the liquid mixture. Quantum-chemical calculations showed that the hydrogen bonds with a length of 1.958 Å and an energy gain of 22.0 kJ/mole can be formed between molecules of quinoline and alcohol. The formation of aggregates can be also detected in the 820-cm^{-1} band of propan-2-ol. A similar picture is observed for the 667-cm^{-1} band of chloroform in its solution with quinoline.