STRUCTURE OF COLD, MIXED PARAHYDROGEN-DEUTERIUM CLUSTERS

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Vibrational spectra of para-H₂ molecules in clusters consisting of para-H₂ or para-H₂/D₂ seeded in He have been obtained using coherent anti-Stokes Raman spectroscopy. The Q₁(0) line of para-H₂, obtained upon expansion of neat para-H₂/D₂, exhibits a high frequency vibrational shift of about 2.6 cm⁻¹ with change of D₂ concentration from 0 to 98%. This shift is assigned to a decrease of the para-H₂ vibron band width in mixed clusters, similar to that previously observed in bulk H_2/D_2 solid. 1% para-H₂/D₂ clusters in He are liquid and show a much smaller shift of about 0.5 cm⁻¹ and indicate phase separation into a predominantly D₂ core and H₂ shell. The onset of phase separation in para-H₂/D₂ mixtures is predicted at approximately 3 K providing further evidence of super-cooled liquid hydrogen clusters previously studied.