SH-STRETCHING INTENSITIES AND INTRAMOLECULAR HYDROGEN BONDING IN ALKANETHIOLS

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The SH-stretching overtone transitions of tert-butylthiol and ethanethiol are observed using FT-IR, NIR and photoacoustic spectroscopies. The intensities of these are compared with OH-stretching overtones from the corresponding alcohols. We explain the paucity of SH-stretching intensity using an anharmonic oscillator local mode model. SH- and OH-stretching overtone spectra of 1,2-ethanedithiol and 2-mercaptoethanol are recorded to observe the different effects that hydrogen bonding involving SH - - - S, SH - - - O and OH - - -S have on the spectra. We discuss these effects with the help of high level ab initio calculations.