

INFRARED SPECTROSCOPY PROBING OF BLUE-SHIFTING CHO HYDROGEN-BONDED COMPLEXES BETWEEN CYCLIC KETONES AND HALOFORMS

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Non-bonded interactions between a weakly acidic CH group and an oxygen atom of a functional group belonging to the same or of a different molecule are categorized as weak hydrogen bonds. Recently, our group has studied a number of dimeric molecular complexes by infrared spectroscopy, where CH–O hydrogen bonding has been invoked to be the dominant binding force for stability of those complexes in ground electronic state. An intriguing spectroscopic attribute of such hydrogen bonding, identified though in a handful of favourable cases, is spectral blue shifting of the donor CH stretching fundamental. Citing examples of the complexes between various cyclic ketones and haloforms studied by our group, the correlation that has been understood partly between the spectral blue shifts and geometries of the complexes will be discussed. An important issue here is whether such hydrogen bonds are stabilized by cooperative interaction, an underlying feature for excess stability of interconnected classical hydrogen bonds, and the spectral manifestation of this effect for the complexes we have studied will be presented. IR spectroscopy measurements have been performed in the gas phase, in carbontetrachloride solution at different temperatures and by isolating the complexes in cold inert gas matrixes.