DUAL FREQUENCY 2DIR SPECTROSCOPIC STUDIES ON WEAK IR MODES.

SRI RAM G NARAHARISETTY^a, VALERIY M. KASYANENKO, IGOR V RUBTSOV, Tulane University, Dept. of Chemistry, New Orleans, LA 70118-5636, USA.

Dual frequency two-dimensional infrared spectroscopy (DF-2DIR) has proven its capability of accessing structural constraints in molecules. The quality of 2DIR structural measurements depends on availability of localized IR modes, labels, which can be accessed selectively. Weak IR modes in various spectral regions that can serve as such labels are the target of this study. DF-2DIR measurements on several weak IR modes, such as CD, CN, and the modes in the fingerprint region, and their interactions with strong modes are presented for several compounds, including Boc-leucine- d_{10} . The applicability of these IR labels for structural measurements in peptides is discussed. The relaxation-assisted 2DIR spectroscopy method was used for assigning different CD transitions of Leu- d_{10} .

^aSupport by NSF, CHE-075415, and Louisiana Board of Regents RCS grants is gratefully acknowledged.