MOLECULAR STRUCTURES OF DIFLUOROBENZALDEHYDES AND THEIR HYDRATED COMPLEXES CHARACTERIZED BY CP-FTMW SPECTROSCOPY

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Difluorobenzaldehydes are used as the starting substrate for the synthesis of high-efficiency pesticides and pharmaceutical bioactive materials. The rotational spectra of difluorobenzaldehydes and of their hydrated complexes are measured by using a new-build 2–8 GHz chirped-pulse Fourier transform microwave (CP-FTMW) spectroscopy at Fudan University. Their precise structures have been determined from the rotational constants of the parent species combined with that of the 13C,18O and deuterated isotopologues. These results can benchmark theoretical methods for the structural optimization of weakly bound complexes. The effect of halogen substituents on intermolecular interactions is also discussed.