STARK SPECTRUM SIMULATION OF X_2Y_4 ASYMMETRIC MOLECULES: APPLICATION TO ETHYLENE IN A MFI-TYPE HOST ZEOLITE

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We present the $D_{2h}TDS - ST$ ($D_{2h} - STARK$ Top Data System) program suite developed to simulate Stark spectra of any IR active rovibrational polyad of X_2Y_4 (D_{2h}) asymmetric-top molecules. It is based on the $D_{2h}TDS$ package, released for studying any rovibrational band or polyad in the abscence of an electric field [a,b]. The $D_{2h}TDS - ST$ suite consists in a series of FORTRAN programs called by a script. For calculation of Stark spectra we obtained the expressions of the dipole moment and polarizability operators of X_2Y_4 molecules, using a tensorial formalism [c] analogous to the one developed for tetrahedral and octahedral molecules [d]. The developed program suite was used to estimate an effective average field in a cavity of a MFI-type host zeolite by comparison, with vibrational absorption spectra of ethylene in MFI-zeolite that have been recorded.

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[b] Ch. Wenger, V. Boudon, M. Rotger, J.-P. Champion and M. Sanzharov, *J. Mol. Spectrosc.* 251 (2005) 102-113.

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[d] V. Boudon, J.-P. Champion, T. Gabard, M. Loëte, F. Michelot, G. Pierre, M. Rotger, Ch. Wenger and M. Rey, *J. Mol. Spectrosc.* 228 (2004) 620-634.