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

M. SANZHAROV, V. BOUDON, M.LOËTE, N. ZVEREVA-LOËTE, A. BALLANDRAS, G. WEBER, *Laboratoire Interdisciplinaire Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, 9 avenue Alain Savary, B.P. 47870, F-21078 Dijon Cedex, France*; M. ROTGER, *Groupe de Spectrométrie Moléculaire et Atmosphérique (GSMA), CNRS UMR 6089, Moulin de la Housse, BP 1039, Cases 16-17, F-51687 Reims Cedex 2, France*.

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.

[a] Ch. Wenger, W. Raballand, M. Rotger and V. Boudon, *J. Quant. Spectrosc. Radiat. Transfer* 95 (2005) 521-538.
[b] Ch. Wenger, V. Boudon, M. Rotger, J.-P. Champion and M. Sanzharov, *J. Mol. Spectrosc.* 251 (2005) 102-113.
[c] W. Raballand, M. Rotger, V. Boudon and M. Loëte, *J. Mol. Spectrosc.* 217 (2003) 239-248.
[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.