NEW TORSION-ROTATION FITTING PROGRAM FOR MOLECULES WITH A SIX-FOLD BARRIER

VADIM V. ILYUSHIN, *Institute of Radio Astronomy of NASU, Chervonopraporna 4, 61002 Kharkov, Ukraine*; ZBIGNIEW KISIEL, LECH PSZCZÓLKOWSKI, *Institute of Physics, Polish Academy of Sciences, Al. Lotników 32/46, 02-668 Warszawa, Poland*; HEINRICH MÄDER, *Institut für Physikalische Chemie, Christian-Albrechts Universität zu Kiel, Olshausenstrasse 40, D-24098, Kiel, Germany*; JON T. HOUGEN, *Optical Technology Division, National Institute of Standards and Technology, Gaithersburg, MD 20899-8441*.

Most torsion-rotation fitting programs consider an expansion of the internal rotation barrier in cos3$n\alpha$, where $\alpha$ is the internal rotation angle and $n = 1, 2, ...$, since such an expansion applies to the large class of molecules (like acetaldehyde) where the frame (CHO) has a plane of symmetry. The present program is designed for molecules like toluene, where the frame ($C_6H_5$) has $C_{2v}$ symmetry. This requires expanding the internal rotation barrier in cos6$n\alpha$, and using the permutation-inversion group $G_{12}$, together with its symmetry species $A_1$, $A_2$, $B_1$, $B_2$, $E_1$ and $E_2$, to set up the symmetry-adapted basis set and chose symmetry-allowed terms for the Hamiltonian. The first application of the program is planned for toluene itself, using the published and rather extensive unpublished data, since fits of these data using other torsion-rotation programs have not been very successful. Details of the $G_{12}$ group theory and the allowed torsion-rotation terms in the program, a comparison with terms in the usual $G_6$ programs (e.g., BELGI), and details of the toluene fit will be presented in this talk.