IMPROVED ANALYSIS OF THE ROTATION SPECTRUM OF META-CHLOROTOLUENE USING A FREE ROTOR BASIS AND NON-PERTURBATIVE HYPERFINE TREATMENT

J. H. WESTERFIELD, S E WORTHINGTON-KIRSCH, KYLE N. CRABTREE, *Department of Chemistry, University of California, Davis, Davis, CA, USA*.

Using the soon to be publicly available westerfit package, the rotational spectrum of meta-chloro-toluene has been re-examined. This program allows for treatment of a C_s molecule with an arbitrary-fold internal rotor and a single strong spin source which makes meta-chloro-toluene a promising test case for the code. Unlike other programs designed for internal rotation with spin effects, westerfit includes matrix elements off-diagonal in N rather than the perturbative treatment of the spin-rotation and quadrupole interactions. This allows fitting of all symmetrically allowed terms in both the spin-rotation and the quadrupole tensors as well as inclusion of any higher order terms coupling the large amplitude motion to the spin angular momentum. Meta-chloro-tolune is a particularly challenging case for internal rotor packages due to the low V_3 term coupled to a large V_6 term as well as the spin 3/2 nucleus. Previous attempts to fit this molecule[a] were complicated by XIAM's limitations at very low barrier heights and perturbative quadrupole treatment. This work presents a more complete treatment of the meta-chloro-toluene spectrum and demonstrates comparisons between westerfit and other programs.

[a]Nair et al, J. Mol. Spec. 361 (2019), p1-7