THE LATEST REVISION OF THE ERHAM CODE

P. GRONER, *Department of Chemistry, University of Missouri-Kansas City, Kansas City, MO 64110-2499*.

ERHAM is a program based on the Effective Rotational Hamiltonian for molecules with two periodic large-amplitude internal motions that can also be used for molecules with just one internal rotor.[a] A new version of the program is now available on the PROSPE web site.[b] The recent modifications including a correction and some new features are described in this presentation. They are:

1. The relative intensities have been corrected and now are calculated as $I_{rel} = S * \mu^2 * exp(-E_l/kT) * (1 - exp(-h\nu/kT)) * \nu$. The intensity threshold for printing now applies to I_{rel} as given above instead to $S * \mu^2$.
2. There is a new option to generate an additional file containing the predictions in the JPL catalog file format.
3. During the prediction, the program automatically acquires the rotational partition function by summation if the minimum of the range of J is 0, but only up to the maximum of the range. This required a revised definition of the - signs printed for some energy levels during the prediction to ensure that the partition function acquisition works with the correct spin weights.
4. Scaling factors for the spectroscopic parameters are used during the least-squares fit to help alleviate problems that occasionally affected the inversion of the normal matrix. This feature has improved the convergence of the least-squares fit in some cases.
5. The upper limit of the number of tunneling parameters per state has been increased to 37 (up from 31). The dimensions of arrays have been increased to allow to order up to 140000 predicted transitions (up from 50000).

[a] P. Groner, *J. Chem. Phys.* 107, 4483 (1997); *J. Mol. Spectrosc.* 278, 52 (2012).
[b] Z. Kisiel, http://www.ifpan.edu.pl/∼kisiel/prospe.htm