Supporting Information: Deciphering the Complexity in the Rotational Spectrum of Deuterated Ethylene Glycol

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1 List of files provided

The following files are provided as Supporting Information:

1. `ODOH_OHOD_aGg.pi`: combined fit of the aGg' conformer of the mono-deuterated species CH_2OD-CH_2OH and CH_2OH-CH_2OD;
2. `ODOD_aGg.pi`: fit of the aGg' conformer of the doubly-deuterated species CH_2OD-CH_2OD;
3. `ODOH_gGg.pi`: fit of the gGg' conformer of the mono-deuterated species CH_2OD-CH_2OH;
4. `OHOD_gGg.pi`: fit of the gGg' conformer of the mono-deuterated species CH_2OD-CH_2OH.

Each file consists of a reformatted version of the standard SPFIT output file (*.fit) using the PIFORM code available on the PROSPE website (Programs for ROtational SPEctroscopy, `http://info.ifpan.edu.pl/~kisiel/asym/asym.htm\#piform`)

The files are composed by several blocks containing:

- The list of assigned transitions

  Each line contains quantum numbers for the upper and lower states (J', K'_a, K'_c, v', J, K_a, K_c, v; see below for more details about the meaning of v), observed frequency in MHz, difference between observed and calculated frequency (obs.-calc.) in MHz, measurement uncertainty in MHz, and two optional columns in case of blended lines (obs.-calc. value with respect to the frequency of the blend and the relative weight of line within the blend);

- Fitted parameters with their uncertainties;

- Fit statistics, such as the root-mean-square (rms) error, the weighted rms, the number of distinct parameters and lines in the fit, and so on;

- Fitted parameters with their standard errors;

- A list of worst fitted constants;

- Correlations between parameters;

- A list of largest correlation coefficients;

- A list of worst fitting lines.

The v quantum number has the following meaning:

1. `ODOH_OHOD_aGg.pi`: $v = 0$ stands for the ODOH species and $v = 1$ for the OHOD species;

2. `ODOD_aGg.pi`: v refers to the tunnelling substate which can take the value of 0 or 1, with the $v = 1$ state being higher in energy than the $v = 0$ state;

3. `ODOH_gGg.pi` and `OHOD_gGg.pi`: no use of v;