Using H_2O and/or CO as projectiles

In cometary comas and in some protoplanetary and debris disks, collisional excitation can be dominated by H_2O and/or CO molecules. Just like H_2, water molecules exist in two isomeric forms: para-water with total nuclear spin $I = 0$ and ortho-water with $I = 1$. The rotational energy levels of H_2O are labeled by three numbers, the angular momentum j and the pseudo-quantum numbers k_a and k_c (corresponding to the projection of j along the principal inertia a and c axes). In the ground electronic and vibrational state[1], the rotational levels of para-H_2O have even values of $k_a + k_c$ while the levels of ortho-H_2O have odd values of $k_a + k_c$. The rotational energy levels of CO are labelled by the angular momentum j.

In contrast to H_2, even in cold environments where the kinetic temperature T_k is lower than 50 K, several rotational states of H_2O and CO can be significantly populated due to the relatively small rotational spacings in these species (compared to those of para- and ortho-H_2). As a result, several excited levels of H_2O and CO must be considered as collision partners in radiative transfer calculations.

EMAA provides de-excitation rate coefficients (in cm^3s^{-1}) due to collisions with 'para-H_2O', 'ortho-H_2O' and 'CO' which in practice correspond (for each species) to 'thermalized' rate coefficients, *i.e.* **summed over all possible final states and averaged over a thermal distribution (at the kinetic temperature) of initial states (see Faure et al. 2020 and Żółtowski et al. 2023).**

Note: H_2O and CO are not handled as colliding partners in the public version of the `RADEX`[2] code. In order to use `RADEX` with para-H_2O and/or ortho-H_2O as projectiles, please select 'pH2' and/or 'oH2' as collision partners in the `RADEX` input file (corresponding to id=2 and id=3 respectively, where 'id' is the code of collision partner). This is obviously only possible if H_2 and H_2O are not simultaneous collision partners. In order to use `RADEX` with CO as projectile, please select 'H' as collision partners (id=5) in the input file. Again, this is only possible if H and CO are not simultaneous collision partners.

References

Faure A., Lique F., Loreau J., *MNRAS* **493** 776-782 (2020)
Żółtowski, M., Lique F., Loreau J, Faure A., Cordiner M., *MNRAS* **520** 3887-3894 (2023)

[1] The first vibrational level of H_2O opens at 1594.7 cm^{-1}.
[2] https://home.strw.leidenuniv.nl/∼moldata/radex.html.