TH07: A SIMULTANEOUS FIT OF THE TORSION-WAGGING-ROTATIONAL LEVELS FROM THE EXCITED (v_t = 0, 1 and 2) STATES OF METHYLAMINE USING A HYBRID (TUNNELING AND NON-TUNNELING) HAMILTONIAN FORMALISM

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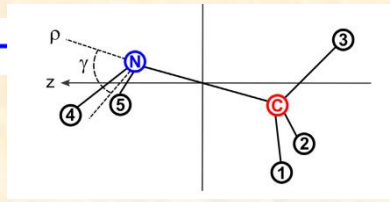


An Hybrid program for methylamine-type molecules.

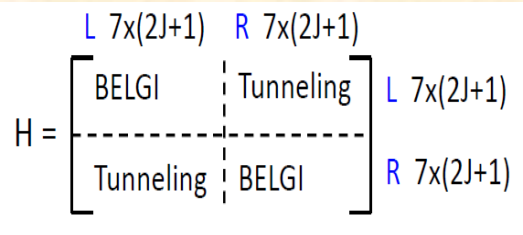
- What is a "methylamine-like molecule"?

= A molecule with 2 Large Amplitude Motions: 1 internal rotation motion (rotatory) + 1 back-and-forth motion (oscillatory)

CH_3-NH_2: Internal rotation = methyl-group rotation, Back-and-forth motion = amino-group inversion

- What are the deficiencies of the "traditional" tunneling approach (Ohashi and Hougen, JMS 1987) we would like to fix with this hybrid code?

-Treat torsional states near or above the top of the barrier
-Use one set of parameters for all the torsional states
-Treat the intertorsional interactions



Kleiner and Hougen JMS 2020

BREAKTHROUGH : NEW FIR AND (sub)MM DATASET FOR v_t=1 and in v_t=2

REPORT OUR LATEST RESULTS OF THE HYBRID FIT