ANALYSIS OF THE CH_2OH RADICAL SPECTRUM WITH AN IAM TUNNELING APPROACH

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Early *ab initio* calculations[a] revealed that the hydroxymethyl radical (CH_2OH) is a non-rigid species exhibiting a complicated potential energy surface. It displays 4 C_1 non-superimposable, energetically equivalent, equilibrium configurations and 4 C_s maxima, approximately 300 and 1500 cm^{-1} above the equilibrium configurations. The large amplitude motion of the radical can be pictured as an internal rotation of the CH_2 group with respect to the OH group. The axis of internal rotation is the CO bond and the two-fold symmetry hindering potential is characterized by a barrier height of 1500 cm^{-1}. Aided by new *ab initio* results, the torsional levels associated with this torsional motion were computed. The energy levels display a tunneling splitting which, for the ground torsional level, was found to be smaller than 0.1 cm^{-1}.

As the large amplitude motion of the hydroxymethyl radical seems to be well described by the high barrier approximation, the tunneling IAM water dimer formalism[b] was used to derive a fitting approach aimed at accounting for its rotation-tunneling energy. The effects of the fine spin-rotation and hyperfine spin-spin couplings were also included since there is an unpaired electron.

In the paper, the analysis with the IAM approach[b] of already available[c,d] and newly measured sub-millimeter wave spectroscopic data will be reported. The fitted value of the tunneling splitting will be compared to that retrieved from the torsional energy level calculation. The rotational dependence of the tunneling splitting will be discussed.

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[a] Saebø, Radom, and Schaefer, *J. Chem. Phys.* **78** (1983) 845; Marenich and Boggs, *J. Chem. Phys.* **119** (2003) 3098; and Ibid., *J. Chem. Phys.* **119** (2003) 10105

[b] Hougen, *J. Mol. Spectrosc.* **114** (1985) 395; and Coudert and Hougen, *J. Mol. Spectrosc.* **130** (1988) 86

[c] Bermudez, Bailleux, and Cernicharo, *A&A* **598** (2017) A9

[d] Chitarra, Martin-Drumel, Gans, Loison, Spezzano, Lattanzi, Müller, and Pirali, *A&A* **644** (2020) A123