THE ROTATION-TUNNELING SPECTRUM OF 3-HYDROXYPROPENAL, HOCHCHCHO

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3-Hydroxypropenal is the lower energy tautomeric form of propanedial, also known as malonaldehyde. It has two equivalent minima separated by a modest barrier which leads to two tunneling states separated by 647 GHz. Its rotational spectrum was analyzed in several studies, most recently through its a-type rotation-tunneling spectrum near 650 GHz.[1]

3-Hydroxypropenal was identified tentatively within the framework of the Protostellar Interferometric Line survey (PILS) toward the prototypical solar-type Class 0 young stellar system IRAS 16293−2422 carried out with the Atacama Large Millimeter/submillimeter Array (ALMA).[2] The conclusions drawn from this study were severely limited by the fact that the rest frequencies of many potentially observable transitions were so uncertain that they could not be identified unambiguously. We have analyzed spectral recordings of 3-hydroxypropenal taken in Lille[3] that cover large parts of the 150−660 GHz region to overcome these limitations. Moderately large rotational parameters, the asymmetry of the molecule, and a plethora of rotation-tunneling interactions give rise to a very rich and quite complex spectrum. We will also present the astronomical implications.

[1] doi: 10.1063/1.478296, T. Baba et al., J. Chem. Phys. **110** 1999, 4131.

[2] doi: 10.1051/0004-6361/202243038, A. Coutens et al., Astron. Astrophys. **660** 2022, L6.

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