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A global study of the conformers of 1,2-propanediol and new vibrationally excited states

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ABSTRACT

The astrochemically relevant molecule 1,2-propanediol was investigated at room temperature between 75 and 110 GHz with the aims of providing accurate global rotational constants for its numerous conformers and vibrationally excited states. This was performed with our segmented chirped-pulse millimeter-wave spectrometer. In the spectrum, six previously observed conformers were assigned and treated in global fits, and three vibrationally excited states of the molecule were identified and assigned. The provided transition frequencies of the ground states and vibrationally excited states will aid in the astronomical detection of 1,2-propanediol, specifically in the Atacama Large Millimeter/submillimeter Array Band 3 regime as it overlaps with the frequency range of our spectrometer.

1. Introduction

Since the detection of formaldehyde, H_2CO, in 1969 by radio observations [1], organic molecules have continued to be detected with increasing complexity within the interstellar medium (ISM). They range considerably - from simple organic molecules such as methanol, CH_3OH [2], to larger unsaturated examples such as cyanotriacetylene, HC_7N [3], to molecular C_{60} [4]. These species make up the chemical inventory of the ISM, which has grown significantly over time, with approximately 200 molecules having been detected to date.[1] The continued search for new complex organic molecules (COMs) is driven by the desire to characterize the chemical complexity of the ISM and to understand the chemical reactions that result in their formation, ultimately with the hope that fundamental questions in astrobiology will be answered. Many of the already detected species are COMs and have been identified through the parallel use of radio astronomy observatories and laboratory spectroscopy. This synergy between laboratory experiments and radio astronomy will continue to play an important role as new facilities of unprecedented sensitivity, such as the Atacama Large Millimeter/submillimeter Array (ALMA), release new data sets. However, the large throughput of data from the new astronomy facilities is creating the need for high-resolution laboratory data to help characterize these datasets completely and, in particular, laboratory spectroscopic studies of increasingly complex molecules.

Many features in astronomical datasets cannot presently be identified because of the observed line density. Among others, these emissions can be attributed to low-lying vibrationally excited states and isotopologue species [5]. In particular, vibrationally excited states play an important role in warmer regions of the ISM - they can act as temperature probes of the surrounding environment and can be involved in chemical reactions [6]. They are important to characterize so that we may learn about their interstellar abundances and roles in astrochemical reactions. Vibrationally excited states and isotopologue species can also be considered as 'weeds' [7] or a hindrance to identifying new COMs, so their elimination from astronomical datasets is an additional result of investigations into these species.

The molecules that comprise the family of alcohols are of general interest due to the importance of terrestrial oxygen chemistry. Oxygen-containing compounds are typically precursors to prebiotic molecules and through a series of reactions can be incorporated into larger COMs that are important for sustaining life, such as amino acids and nucleobases. The alcohols are an extensive family of molecules that have been studied, with methanol and

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[1] Cologne Database for Molecular Spectroscopy, see www.astro.uni-koeln.de/cdms/molecules.

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0022-2852/

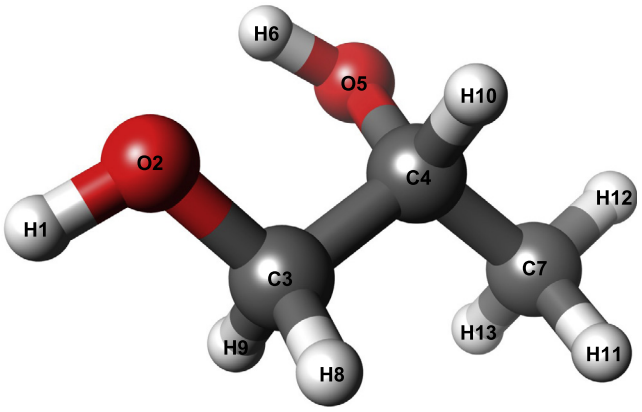

Fig. 1. The equilibrium structure, optimized at the MP2/aug-cc-pVTZ level of theory, of the lowest energy conformer of 1,2-propanediol (tG′g) with atom labels. The labels are in keeping with Vázquez et al. [16].

ethanol having already been detected in the ISM [2,8,9]. The concept that smaller organic molecules can undergo reactions to form more biologically relevant COMs can be applied to interstellar environments, and reactions that explain the constituents of particular environments can be outlined. However, in many cases the proposed reactions fail to account for the presence of particular species that have been observed in that environment. It can also be that one of the proposed reactants/products has yet to be detected - this is the case for 1,2-propanediol, $C_3H_8O_2$. This molecule can evolve into larger prebiotic molecules, and it is a chiral molecule. Chiral molecules have an important role in terrestrial life, and the homochirality of biomolecules has been referred to as a 'signature of life' [10]. Previously, 1,2-propanediol has been searched for, but it has yet to be detected in any interstellar environment. Based on the column density predicted by their calculations, Lovas et al. explain that instrumentation with increased sensitivity would be required to observe 1,2-propanediol [11]. The plausibility of 1,2-propanediol being in interstellar environments comes from the fact that one of its possible precursors, 1,2-ethanediol, has already been detected in Sgr B2(N-LMH) [12]. The ethane analogue (also known as ethylene glycol, $HOCH_2CH_2OH$) could react with the methyl radical, among others, to form 1,2-propanediol. The presence of 1,2-propanediol in this region would then allow us to consider reactions with other smaller abundant molecules present in such an environment. This, in turn, could result in the formation of important and complex hydroxyl-containing species, such as glycerol, lactic acid, and pyruvic acid.

Because of the biological and astrochemical importance of this molecule and due to its structural complexity, it has already been

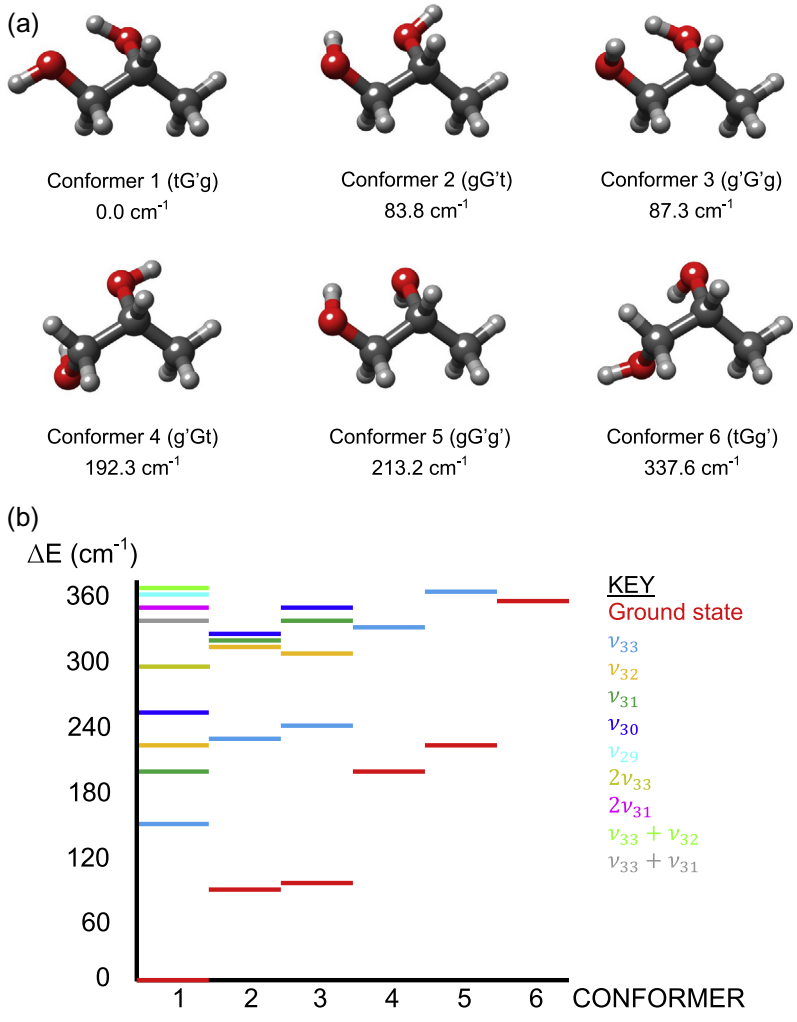

Fig. 2. (a) The structures of six vibronic ground state conformers of 1,2-propanediol optimized at the MP2/aug-cc-pVTZ level of theory, and their energies with respect to the lowest energy conformer. (b) Diagram illustrating the energies of the conformers and selected vibrationally excited states up to 360 cm^{-1}, also calculated at the MP2/aug-cc-pVTZ level of theory.

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