A Search for Interstellar Monohydric Thiols

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Abstract

It has been pointed out by various astronomers that a very interesting relationship exists between interstellar alcohols and the corresponding thiols (sulfur analog of alcohols) as far as the spectroscopic properties and chemical abundances are concerned. Monohydric alcohols such as methanol and ethanol are widely observed and 1-propanol was recently claimed to have been seen in Orion KL. Among the monohydric thiols, methanethiol (chemical analog of methanol) has been firmly detected in Orion KL and Sgr B2(N2) and ethanethiol (chemical analog of ethanol) has been observed in Sgr B2(N2), though the confirmation of this detection is yet to come. It is very likely that higher order thiols could be observed in these regions. In this paper, we study the formation of monohydric alcohols and their thiol analogs. Based on our quantum chemical calculation and chemical modeling, we find that the Tg conformer of 1-propanethiol is a good candidate of astronomical interest. We present various spectroscopically relevant parameters of this molecule to assist in its future detection in the interstellar medium.

Key words: astrochemistry – evolution – ISM: abundances – ISM: molecules – methods: numerical – techniques: spectroscopic

Supporting material: tar.gz file

1. Introduction

Starting from the detection of the first carbon containing molecule, the methylidyne radical (CH) in 1937 (Swings & Rosenfeld 1937), almost 200 molecules including neutrals, radicals, and ions have been observed in the interstellar medium (ISM) or in circumstellar shells, and almost 60 molecules have been observed in comets. A mismatch between the cosmic abundance of sulfur and observed abundances of S-bearing species is well known (Palumbo et al. 1997). Particularly around the dense cloud regions, this inequality is pronounced (Tieftrunk et al. 1994; Palumbo et al. 1997). Around the diffuse cloud and highly ionized regions, sulfur related species roughly resemble the cosmic abundance $\sim 10^{-5}$ (Savage & Sembach 1996; Howk et al. 2006). Earlier, Millar & Herbst (1990) and Jansen et al. (1995) suggested that S, SO, CS, and H_2S may explain the missing sulfur problem, though our knowledge of the CS related species is very limited. Recently, Müller et al. (2016) suggested that at 400 K more than 50% of the sulfur budget is shared by CS and H_2CS and that a remainder resides in the form of SO and SO_2 for hot source Sgr B2(N). Several experiments were carried out to determine the abundant S-bearing species on interstellar grains. The proposed outcome of these experiments is that OCS (Garozzo et al. 2010), CS_2 (Ferrante et al. 2008), and hydrated sulfuric acid (Scappini et al. 2003) would act as a sink for the interstellar sulfur. To date, only two sulfur related molecules (OCS and SO_2) have been detected on grain surfaces with full confidence, thus the exact reservoir of sulfur is not yet known with certainty (Palumbo et al. 1995; Boogert et al. 1997; Woods et al. 2015).

Among the monohydric alcohols, methanol (CH_3OH) is the simplest alcohol that is widely observed in both the gas and solid phases (Tielens & Allamandola 1987) of the ISM. A major portion of the interstellar grain mantle is found to be covered with methanol (Gibb et al. 2004; Das et al. 2008a, 2010; Das & Chakrabarti 2011; Das et al. 2016). The gas-phase abundance of methanol relative to H_2 is found to be in the range from 10^{-9} in cold dark clouds to 10^{-6} in hot molecular cores (Charnley et al. 1995). The presence of ethanol (C_2H_5OH) (the second alcohol in this homologous series) is observed in star-forming regions in the range of 10^{-8} – 10^{-6} (Millar et al. 1988; Turner 1991). Propanol is the next alcohol in the series of monohydric alcohols which may appear in two different forms: normal(n)-propanol ($CH_3CH_2CH_2OH$) and 2-propanol ($CH_3CHOHCH_3$). Recently n-propanol (1-propanol) was claimed to be detected toward Orion KL by Tercero et al. (2015) with a column density of $\leqslant(1.0 \pm 0.2 \times 10^{15})$ cm^{-2}, whereas the presence of 2-propanol has not yet been verified.

It is now confirmed that methanol and ethanol are mainly produced on dust grains during the cold phase, and evaporate from warm dust grains in later stages of evolution. Following this trend, even higher order alcohols would be produced on interstellar grains. In the case of thiols, sulfur takes the place of oxygen in the hydroxyl group of an alcohol. Like their alcohol analogs, these thiols are mainly produced on the grain surface and are evaporated in suitable time. A tentative detection of methanethiol (CH_3SH) in Sgr B2 was done by Turner (1977). Later this claim was confirmed by Linke et al. (1979) and showed that the CH_3SH/CH_3OH ratio is close to the cosmic S/O ratio. Recently, Majumdar et al. (2016) detected CH_3SH in IRAS 16293-2422, and Kolesniková et al. (2014) reported the detection of C_2H_5SH in the hot core of Orion KL, but very recent observations by Müller et al. (2016) suggested that the detection of C_2H_5SH in Orion KL is uncertain. The presence of higher order thiols is yet to be seen.

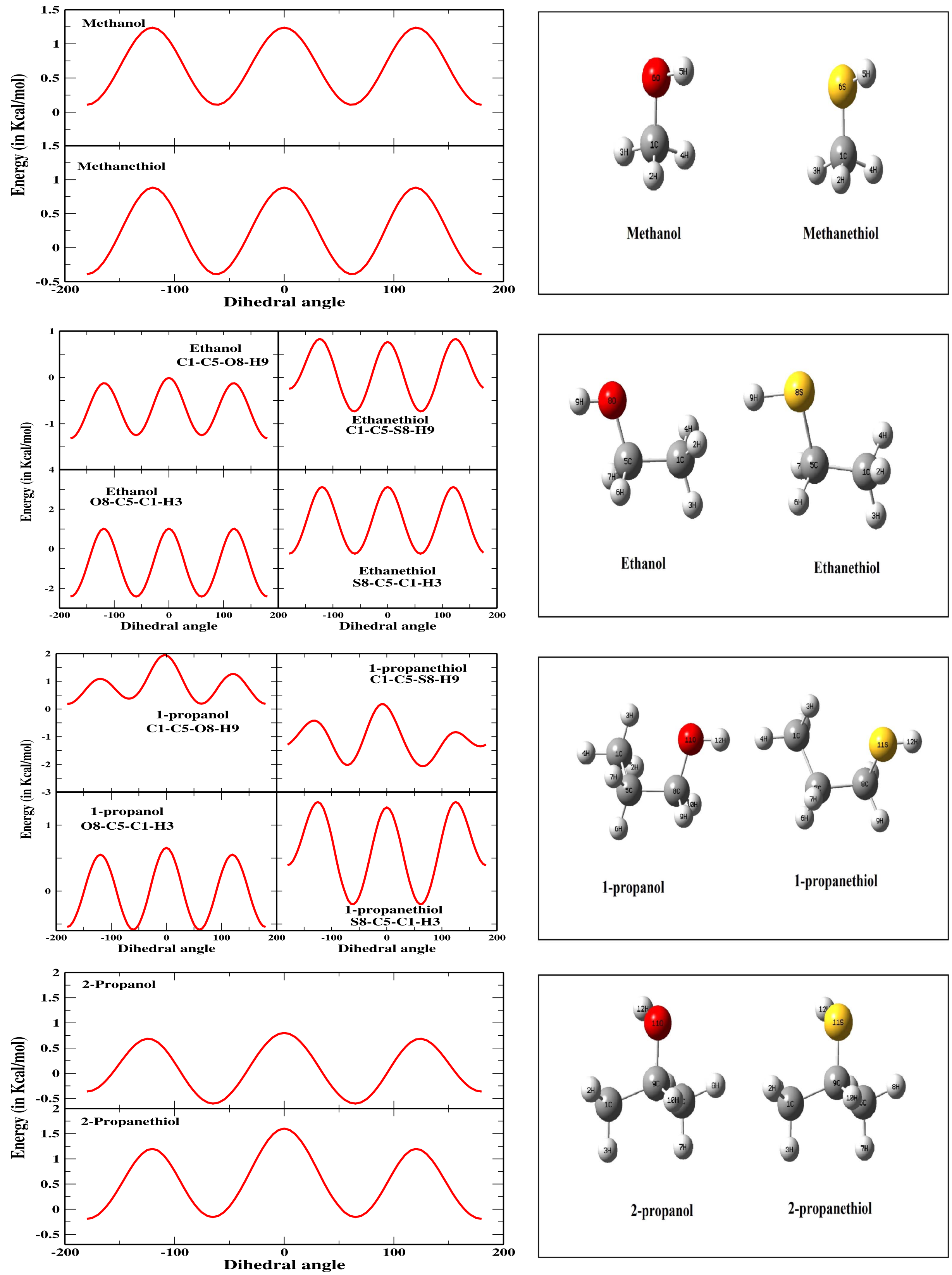

Figure 1. Relaxed potential energy surface scan of the dihedral angle of monohydric alcohols and their thiol analogs using the MP2/cc-pVTZ level of theory.

In this paper, we discuss the formation of monohydric alcohols and their thiol analogs. First, we identify the most stable conformers of alcohols and their thiols. Then we develop a chemical network to study the formation of all these species. From the outcome of our chemical modeling, the most probable new candidate for the astronomical detection is determined. Moreover, a detailed spectroscopic study is carried out to set a guideline for observing this species in the near future. This