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Wentao Song - Rotational spectroscopic study of cysteamine

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Cysteamine (NH2CH2CH2SH) is a molecule that is potentially of interest to astrobiology, but it has not yet been detected in the interstellar medium. Its rotational spectrum was investigated in the 18-40 GHz frequency region and two conformers and their vibrational satellites were characterized [1], but the sparse frequency coverage prevents their accurate predictions in higher frequency ranges. We have calculated the conformational potential energy scans at the B3LYP-GD3(BJ)/def2-TZVP level which suggest the existence of more stable conformers. To fill the lack of its spectroscopic knowledge, we have investigated the pure rotational spectrum of cysteamine by means of a Pulsed Jet Fourier transform microwave spectrometer and a Stark modulated free-jet millimeter-wave absorption spectrometer with frequency ranges of 6.5-18 GHz (46.12-16.66 mm) and 59.6-110.0 GHz (5.03-2.72 mm), respectively. According to theoretical predictions, five conformers, belonging to the gauche skeletal arrangement (∠NCCS≈60◦) have been observed, and for three of them also the 34S isotopologues were observed in natural abundance. Some of the detected lines shown a hyperfine structure ($\Delta\nu \leq 1$ MHz) due to the nuclear quadrupole interaction of the 14N atom. Altogether, 336 transition lines of the five parent species and 63 lines of the three 34S isotopologues conformers were assigned to fit the rotational constants, quartic centrifugal distortion constants and the 14N nuclear quadrupole coupling constants. New laboratory data on cysteamine provided very precise values of the spectroscopic constants that can be used to search for cysteamine in astronomical surveys. Based on the predicted spectra, a search of the different conformers of cysteamine was performed toward the G+0.693-0.027 molecular cloud, where its O-bearing analog (ethanolamine) was detected. The search was unfruitful, and no transitions of cysteamine were found. We computed the upper limit of the ratio of ethanolamine to cysteamine, which is >0.8−5.3, in agreement with the OH/SH ratios found previously in other molecules [2]. References [1] Nandi, R. N., Boland, M. F., & Harmony, M. D. (1982). Microwave spectral studies of rotational isomerism in substituted ethanethiols: 2-Aminoethanethiol and 2-chloroethanethiol. Journal of Molecular Spectroscopy, 92(2), 419-430. [2] Rodríguez-Almeida, L. F., Jiménez-Serra, I., Rivilla, V. M., Martín-Pintado, J., Zeng, S., Tercero, B., Vicente, P., Colzi, L., Rico-Villas, F., & Requena-Torres, M. A. (2021). Thiols in the Interstellar Medium: First Detection of HC(O)SH and Confirmation of C2H5SH. The Astrophysical Journal Letters, 912(1), L11.

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