MICROWAVE STUDY OF THE TRIOSE ($C_3H_6O_3$) SUGAR SYSTEM: GLYCERALDEHYDE AND 1,2-DIHYDROXY-2-PROPANONE

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Recently, the simplest sugar, glycolaldehyde was identified in the Sgr B2 molecular cloud by Hollis, Lovas, and Jewell [a]. As a result of this discovery, we became interested in studying the next larger sugars characterized as trioses. The triose sugars consist of the aldehyde form, glyceraldehyde, and the ketone form, 1,3-dihydroxy-2-propanone. The microwave spectra were obtained with the NIST Fourier-transform pulsed-nozzle microwave spectrometer that was equipped with a heated nozzle located in one mirror. A few tenths of a gram of solid sample was placed in the nozzle base, which was heated to between 100 °C and 135 °C and pressurized with Ne. Broad survey scans were run from 10 GHz to 26 GHz in both samples. In the glyceraldehyde study, three conformers of the parent species were identified as well as 1,3-dihydroxy-2-propanone. In addition three decomposition products were also identified: formic acid, $trans$-methyl glyoxal, and a previously unknown product 2-hydroxy-2-propen-1-al. $Ab\ initio$ calculations were carried out with the Gaussian 98 program at the MP2/6-311++G** level to aid in the identification of each of the new species. The survey scan from 1,3-dihydroxy-2-propanone confirmed the identification of this species initially assigned in the glyceraldehyde study, and also exhibited spectra from the three decomposition products. However, the three conformers of glyceraldehyde were not present. Details of the measurements, assignments and $ab\ initio$ results will be presented.

[a] J.M. Hollis, F.J. Lovas, and P.R. Jewell, Astrophys. J. (Letters) 540, L107 (2000).