FOURIER TRANSFORM MICROWAVE SPECTRA OF 1-PENTANETHIOL

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Rotational spectra of the 1-pentanethiol (1-C_5SH) were observed using a Fourier transform microwave spectrometer. Eight sets of the 1-C_5SH were assigned by combined with the quantum chemical calculations. The four Sets 1-4 of *a*-type *R*-branch transitions of 1-C_5SH were observed in diluted Ar. Another four Sets 5-8 of *a*-type transition were observed near the four Sets 1-4 in diluted Ne instead of Ar. The Set 1 has the most intense spectrum and small splittings due to the torsional motion of the SH group and the internal rotation of the CH_3 group of the *TTTg* conformer of the 1-C_5SH. In the case of 1-C_5SH there are four operations; the first generating operation is the relative orientation of CH_3 groups around the C(5)H_3C(4)H_2-C(3)H_2C(2)H_2C(1)H_2SH axis, leading to *gauche* and *trans* conformers, *G* or *T*, the second is around C(3)-C(2) axis and the third is around C(2)-C(1) axis, leading to *gauche* and *trans* conformers, *G*, *G'* or *T*, and the fourth is around C(1)-SH also leading to *gauche* and *trans* orientations, *g*, *g'* or *t*. For Set 2, *a*-, *b*-, and *c*-type transitions were observed and assigned as to *TTGg'* conformer. Only *a*-type transitions of the Sets 3 and 4 were observed. The obtained rotational constants of the Sets 3 and 4 agreed with the calculated values of the *TGTg*/*TGTg'* and *GTTg*/*GTTg'*, respectively. Comparing the obtained rotational constants with the quantum chemical calculations, the Sets 5 and 6 were assigned as to be *TTTt* and *TTGg*, respectively. Similarly Sets 3, 7, 4 and 8 were assigned as *TGTg'*, *TGTg*, *GTTg* and *GTTg'*, respectively.