COUPLED LARGE AMPLITUDE MOTIONS: THE EFFECTS OF TWO METHYL INTERNAL ROTATIONS AND ^{14}N QUADRUPOLE COUPLING IN 4,5-DIMETHYLTHIAZOLE

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The molecular jet Fourier-transform microwave spectrum of 4,5-dimethylthiazole has been recorded between 2.0 and 26.5 GHz, revealing torsional splittings arising from two inequivalent methyl internal rotations with relatively low hindering barriers and nitrogen quadrupole hyperfine structures. Two global fits of 97 rotational transitions with 315 torsional and 1009 hyperfine components involving 5 torsional species were performed using the program *XIAM* [a] and *BELGI-C_s-2Tops-hyperfine*, an extended version of the *BELGI-C_s-2Tops* code [b] which includes the effect of the ^{14}N quadrupole coupling, giving a root-mean-square deviation of 399.8 kHz and 4.2 kHz, respectively. Compared to the monomethyl substituted thiazole derivatives, the barriers to internal rotation are drastically lower. This is also in contrast to chemical intuition which suggests high barriers due to steric hindrance. Because of the strong interaction between the methyl groups, strong top-top couplings in both the potential energy and kinetic parts of the Hamiltonian were observed.

[a] H. Hartwig, H. Dreizler, Z. Naturforsch. 51a, 923–932, 1996.

[b] M. Tudorie, I. Kleiner, J.T. Hougen, S. Melandri, L.W. Sutikdja, W. Stahl,J. Mol. Spectrosc.269, 211-225, 2011.