MICROWAVE SPECTROSCOPIC AND QUANTUM CHEMICAL INVESTIGATIONS ON ACETYLTHIOPHENES AND 2-ACETYLFLURAN

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It is known that the torsional barrier of an acetyl methyl group strongly depends on the substituent attached to the other side of the carbonyl group, especially if double bonds or π conjugated systems are present. Although several molecules of this type have been investigated, such as allyl acetone\textsuperscript{1}, methyl vinyl ketone\textsuperscript{2} or 2-acetyl-5-methylfurane\textsuperscript{3}, no apparent trends for the torsional barrier of the acetyl methyl group have been found. This work will present the influence of sulfur- and oxygen-containing five membered aromatic rings on the torsional barrier of the acetyl methyl group.

The microwave spectra of 2-acetylthiophene, 2-acetylfuran and 2-acetyl-4-methylthiophene were recorded using a pulsed molecular jet Fourier transform microwave spectrometer operating in the frequency range from 2 to 26.5 GHz. Conformational analyses carried out at the MP2/6-311++G(d,p) level of theory yielded two stable conformers (syn and anti) for all three molecules. While the syn-conformers of the thiophenes are energetically more stable, the anti-conformer is more stable in the case of 2-acetylfuran. This shows that the conformational stability depends on the hetero atom in the ring.

Both, the syn- and the anti- conformers were assigned in the microwave spectra of 2-acetylthiophene and 2-acetylfuran. The torsional barriers of the acetyl methyl group in syn- and anti-2-acetylthiophene are 333.602(14) cm\textsuperscript{-1} and 298.600(14) cm\textsuperscript{-1}, respectively. The respective barriers for syn- and anti-2-acetylfuran are 238.406(49) cm\textsuperscript{-1} and 319.417(24) cm\textsuperscript{-1}.

In 2-acetyl-4-methylthiophene a second rotor is present in the system. The assignment of the spectrum is in progress. Currently, the (00), (01) and (10) species of the syn-conformer have been assigned.