Acetyl- and nitrogen containing substances play an important role in chemical, physical, and especially biological systems. This applies in particular for acetamides, which are structurally related to peptide bonds. In this work, N-methyldiacetamide, CH$_3$N(COCH$_3$)$_2$, was investigated by a combination of molecular beam Fourier transform microwave spectroscopy and quantum chemical calculations.

In N-methyldiacetamide, at least three large amplitude motions are possible: (1) the internal rotation of the methyl group attached to the nitrogen atom and (2, 3) the internal rotations of both acetyl methyl groups. This leads to a rather complicated torsional fine structure of all rotational transitions with additional quadrupole hyperfine splittings caused by the $^{14}$N nucleus.

Quantum chemical calculations were carried out at the MP2/6-311++G(d,p) level of theory to support the spectral assignment. Conformational analysis was performed by calculating a full potential energy surface depending on the orientation of the two acetyl groups. This yielded three stable conformers with a maximum energy difference of 35.2 kJ/mol.

The spectrum of the lowest energy conformer was identified in the molecular beam. The quadrupole hyperfine structure as well as the internal rotation of two methyl groups could be assigned. For the N-methyl group and for one of the two acetyl methyl groups, barriers to internal rotation of 147 cm$^{-1}$ and of 680 cm$^{-1}$, respectively, were determined. The barrier of the last methyl group seems to be so high that no additional splittings could be resolved.

Using the XIAM program, a global fit with a standard deviation on the order of our experimental accuracy could be achieved.