The microwave spectra of two conformers, trans and cis, of the title compound were recorded using two molecular beam Fourier transform microwave spectrometers operating in the frequency range 2 GHz to 40 GHz, and aimed at analysis of their $^{14}\text{N}$ quadrupole hyperfine structures. Rotational constants, centrifugal distortion constants, and nuclear quadrupole coupling constants (NQCCs) $\chi_{aa}$ and $\chi_{bb} - \chi_{cc}$, were all determined with very high accuracy. Two fits including 176 and 117 hyperfine transitions were performed for the trans and cis conformers, respectively. Standard deviations of both fits are close to the measurement accuracy of 2 kHz. The NQCCs of the two conformers are almost exactly the same, and are compared with values found for other saturated and unsaturated formamides.

Complementary quantum chemical calculations - MP2/6-311++G(d,p) rotational constants, MP2/cc-pVTZ centrifugal distortion constants, and B3PW91/6-311+G(d,p)/MP2/6-311++G(d,p) nuclear quadrupole coupling constants - give spectroscopic parameters in excellent agreement with the experimental parameters. B3PW91/6-311+G(d,p) calculated electric field gradients, in conjunction with $eQ/h = 4.599(12)$ MHz/a.u., yields more reliable NQCCs for formamides possessing conjugated $\pi$-electron systems than does the B3PW91/6-311+G(df,pd) model recommended in Ref. $^a$, whereas this latter performs better for aliphatic formamides.$^b$ We conclude from this that f-polarization functions on heavy atoms hinder rather than help with modeling of conjugated $\pi$-electron systems.


$^b$W. C. Bailey, Calculation of Nuclear Quadrupole Coupling Constants in Gaseous State Molecules, http://nqcc.wcbailey.net/index.html