THE LOW-LYING CCN BENDING MODE OF THE CLOSE-TO-LINEAR MOLECULE NCCNO

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The band system of the low-lying CCN bending mode ν_7 of the pseudohalofulminate NCCNO around $85\,\mathrm{cm}^{-1}$ has been recorded by high resolution FTIR spectroscopy to supplement our previous investigation of the pure rotational spectrum, which had revealed some slight, but significant indications of quasilinearity[a]. Besides rovibrational transitions of the fundamental band, rovibrational transitions belonging to the first, second, third, and fourth hot band could be assigned. Using a conventional linear-molecule type Hamiltonian[b], these rovibrational transitions have been analyzed together with the pure rotational transitions. The results of this analysis confirm a moderate anharmonicity in the CCN bending potential. To quantify this anharmonicity, the combined data have been subjected to a *semirigid bender* analysis, which resulted in a rather flat bending potential with a significant quartic contribution.

[a] H. Lichau, B. P. Winnewisser, M. Winnewisser, C. W. Gillies, and J. Z. Gillies, *53rd Int. Symposium*, talk TH09 (1998)
[b] K. M. T. Yamada, F. W. Birss, and M. R. Aliev, *J. Mol. Spectrosc.* **112**, 347–356 (1985)