ANALYSIS OF THE ROTATIONAL STRUCTURE IN THE HIGH-RESOLUTION INFRARED SPECTRA OF cis, cis- AND $trans, trans$-1,4-DIFLUOROBUTADIENE-1-d_1 AND $trans, trans$-1,4-DIFLUOROBUTADIENE-1,4-d_2

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Samples of *cis,cis*- and *trans,trans*-1,4-difluorobutadiene-1-d_1 (DFBD) and *trans,trans*-DFBD-1,4-d_2 have been synthesized and investigated with high-resolution (0.0015 cm^{-1}) infrared spectroscopy. For the first two species the rotational structure in more than one band has been analyzed. For the 1,4-d_2 species the spectrum of only one C-type band was available in an isotopic mixture. Ground state rotational constants are reported for all three molecules. It is proposed that quartic centrifugal distortion constants computed with a B3LYP/cc-pVTZ model can be used to assess the quality of observed rotational constants. The favorable comparison of predicted and observed ground state rotational constants for all four ^{13}C species of *cis,trans*-DFBD, which is MW active,[a] demonstrates that the ground state rotational constants for the ^{13}C species of the *cis,cis* and *trans,trans* isomers can be successfully predicted with high accuracy. Rotational constants for a full set of isotopologues will be used to determine accurate semiexperimental equilibrium structures of the *cis,cis* and *trans,trans* species of DFBD.

[a] N. C. Craig, C. M. Oertel, D. C. Oertel, M. J. Tubergen, R. J. Lavrich, A. M Chaka J. Phys. Chem. A 106, 4230-4235 (2002).