ANALYSIS OF THE ROTATIONAL STRUCTURE IN A C-TYPE BAND IN THE HIGH-RESOLUTION INFRARED SPECTRUM OF trans,trans-1,4-DIFLUOROBUTADIENE-1-d1

NORMAN C. CRAIG, CHRISTOPHER F. NEESE, and DEACON J. NEMCHICK, Department of Chemistry and Biochemistry, Oberlin College, Oberlin, OH 44074; MICHAEL LOCK, Physikalisch-Chemisches Institut der Justus Liebig Universität, Heinrich-Buff Ring 58, D-35392, Giessen, Germany.

A mixture of deuterium isotopomers of trans,trans-1,4-difluorobutadiene (ttDFBD) was prepared by partial exchange with NaOD/D2O. A prominent component of the mixture was the 1-d1 species. The rotational structure in a C-type band of this species centered at 920.5 cm⁻¹ was analyzed in the high-resolution (0.002 cm⁻¹) infrared spectrum. The analysis of this band was compromised by large contributions from a C-type band at 893 cm⁻¹ in the spectrum of ttDFBD-1,4-d2. Provisional ground state rotational constants for ttDFBD-1-d1 are reported. We have recently shown that 1-fluoroethylene can be exchanged with NaOD/D2O to give 1-fluoroethylene-1-d1, which can be used in known chemistry to make pure DFBD-1-d1. An improved high-resolution infrared spectrum of ttDFBD-1-d1 will be obtained. This method will also yield cis,cis-DFBD-1-d1 for investigation. Rotational constants for ttDFBD-1-d1 and ccDFBD-1-d1 are needed for determining the semi-experimental equilibrium structures of the two nonpolar isomers of DFBD.