FOURIER-TRANSFORM FAR-INFRARED SPECTRA OF $^{13}CD_3OH$ IN THE 10 TO 800 cm^{-1} RANGE: RITZ AND GLOBAL ANALYSIS

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The FIR spectrum of $^{13}CD_3OH$ has been recorded through 10 to 800 cm^{-1} on two high-resolution FT instruments, one at NRC, Ottawa, and the other in Giessen. The subband analyses for the first three torsional levels (i.e. ν_t=0,1,2) have largely been previously published. The present report goes beyond these to the more complete Ritz energy level analysis which reduces previously ungrouped families of transitions down to the minimum number of separate entities. Ideally, one would aim for a family number of unity for each of the distinct A/E torsional symmetry species. In the present work, we have compiled the following data statistics and degrees of reduction for the $^{13}CD_3OH$ FTFIR spectra: A: 9679 lines, 3486 levels, 106 sequences, 4 families; E: 15582 lines, 5096 levels, 196 sequences, 4 families (Note data listed here contains several vibrational bands as well).

One of the motivations in studying different isotopomers of methanol is to obtain information on the mass-dependence of the molecular parameters. With this in mind, global fitting is underway for $^{13}CD_3OH$ for the first two torsional levels (ν_t=0,1) up to J_{max}=20. The data range chosen here is consistent with previous global fits for other methanol isotopomers in order to permit ready inter-comparison of parameters. At the present time, we are working on fitting globally only to the FT data dealt with in this talk. In the future, however, as with the previously published global fits for CH_3OH, $^{13}CH_3OH$ and CD_3OH, we will include all known measurements for microwave transitions in the data set.

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