THE $\nu_{12} + \nu_6 - \nu_6$ AND $\nu_{11} - \nu_{12}$ BANDS OF $^{12}CH_3^{13}CH_3$: A FREQUENCY ANALYSIS INCLUDING DATA FROM THE FOUR LOWEST VIBRATIONAL STATES

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High-resolution infrared spectra of the $\nu_{12} + \nu_6 - \nu_6$ (around 820 cm^{-1}) and $\nu_{11} - \nu_{12}$ (around 370 cm^{-1}) bands of $^{12}CH_3^{13}CH_3$ are assigned. Frequencies from these bands together with data from the ν_{12} and ν_5 fundamentals and the torsional bands were analysed in a 4-state fit to determine the torsion mediated Coriolis and Fermi interactions. As compared to normal ethane this lower symmetry isotopologue shows more complicated vibrational couplings. The combined data set includes more than 6800 frequencies and was fitted to within experimental accuracy using a 77-parameter Hamiltonian. The first determination of molecular parameters for the ν_{11} state of $^{12}CH_3^{13}CH_3$ has been made and using this Hamiltonian we have provided lower state energies and partition functions between 100 and 330 K in increment of 10 K for planetary data analysis.[a] A comparison with a 4-state fit of similar data for $^{12}CH_3^{12}CH_3$ will be made.

[a] N. Moazzen-Ahmadi, J. Norooz Oliaee, and V.-M. Horneman, *JQSRT*, submitted.