

METHOXYETHANOL, ETHOXYETHANOL, AND SPECTRAL COMPLEXITY

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Over the last few years, we have been working to improve the AUTOFIT program^a and extend it to work on more complex spectra, especially spectra collected near room temperature. In this talk, we will discuss the problem of spectral complexity and the challenges it poses for moving to increasingly complicated systems. This will be highlighted by the cases of methoxyethanol, in which AUTOFIT was able to easily extract contributions from the ground state and four vibrationally excited states, and ethoxyethanol, in which AUTOFIT had difficulty identifying more than the ground vibrational state without the assistance of additional double resonance measurements.

^aSeifert, N.A., Finneran, I.A., Perez, C., Zaleski, D.P., Neill, J.L., Steber, A.L., Suenram, R.D., Lesarri, A., Shipman, S.T., Pate, B.H., J. Mol. Spec. 312, 13-21 (2015)