

A GLOBAL RAM METHOD FOR FITTING INFRARED AND FAR-INFRARED DATA FOR SMALL VOLATILE ORGANIC COMPOUNDS: APPLICATION TO TOLUENE

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Producing spectroscopic data in the infrared range for a number of VOCs (volatile organic compounds) to be used for detecting and measuring their abundance with remote sensing is highly needed to control air pollution and air quality. Toluene is one of the important VOCs and abundant hydrocarbon in the Earth's atmosphere and it is a major anthropogenic pollutant emitted by various sources. The ultimate goal of our study is twofold: (i) develop an offspring of the RAM36 code^a capable of simultaneous fitting torsion-rotation spectra in several vibrational states of a molecule with C_{3v} internal rotor and C_{2v} frame, and (ii) build an infrared database for toluene in the spectral range 600-800 cm^{-1} for remote sensing purposes. For the second goal new data were recorded using the JET-AILES experiment at the SOLEIL synchrotron around the band ν_{36} at 729 cm^{-1} . In order to account for possible hot bands in the infrared spectrum we also performed a search for the transitions belonging to the lowest vibration state of toluene ν_{38} at 204 cm^{-1} . The details of the new code and the first assignments of the torsion-rotation spectrum for the lowest vibrational state of toluene in the microwave range will be presented.^b

^aV. V. Ilyushin, Z. Kisiel, L. Pszczólkowski, H. Mäder, J. T. Hougen, *J. Mol. Spectrosc.* 259, 26 (2010)

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