ISOTOPOLOGUE-SENSITIVE DETECTION USING CHIRPED-PULSE FT-MW SPECTROSCOPY: MINOR SPECIES OF PROPOFOL

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The capabilities of chirped-pulse FT-microwave spectroscopy to achieve full-bandwidth (11 GHz) isotopologue-sensitive detection have been tested on the 13-heavy atoms molecule of propofol (2,6-diisopropylphenol). The analysis of the rotational spectrum using moderate signal averaging (10 k FIDs) had previously detected the presence of two conformers arising from the combined internal rotations of the hydroxyl and the two isopropyl groups[a]. In the new experiment reported here 600 k FIDs were coherently averaged, using three pulsed nozzle sources and reading multiple FIDs per sample injection cycle to reduce the total acquisition time and sample consumption. The new spectrum revealed a very large number of weak transitions, suggesting that full-band ^{13}C sensitivity had been surpassed. The new data have resulted in the assignment of a third conformer of propofol, followed by all twelve ^{13}C-monosubstituted species in natural abundance for the most stable conformer. The isotopic information confirmed the molecular structure for the preferred conformation of propofol, validating the *ab initio* predictions for this compound. The potential function for the OH internal rotation has been determined using a flexible model.

[a] A. Lesarri, S. T. Shipman, G. G. Brown, L. Alvarez-Valtierra, R. D. Suenram and B. H. Pate, *63rd OSU Int. Symp. On Mol. Spectrosc.*, Columbus, OH, 2008, RH07