ROTATIONAL SPECTRA OF HALOGENATED ETHERS USED AS VOLATILE ANAESTHETICS

ALICIA VEGA-TORIBIO and ALBERTO LESARRI, *Departamento de Química Física y Química Inorgánica, Facultad de Ciencias, Universidad de Valladolid, E-47011 Valladolid, Spain*; RICHARD D. SUENRAM, *Department of Chemistry, University of Virginia, Charlottesville, VA 22904, USA*; JENS-UWE GRABOW, *Institut für Physikalische Chemie und Elektrochemie, Leibniz Universität Hannover, Callinstraße 3 - 3A, D-30167 Hannover, Germany*.

Following previous microwave investigations by Suenram *et al.*[a] we will report on the rotational spectrum of several halogenated ethers used as volatile anaesthetics, including sevoflurane ($(CF_3)_2CH\text{-}O\text{-}CH_2F$), isoflurane ($CF_3CHCl\text{-}O\text{-}CHF_2$), enflurane ($CHFClCF_2\text{-}O\text{-}CHF_2$) and methoxyflurane ($CHCl_2CF_2\text{-}O\text{-}CH_3$). This study has been conducted in the 6-18 GHz centimetre-wave region using Balle-Flygare-type FT-microwave spectroscopy. The results will include the analysis of the rotational spectra of minor species in natural abundance (^{13}C and ^{18}O in some cases), structural calculations and auxiliary *ab initio* modelling. The conformational and structural conclusions will be compared with previous gas-phase electron diffraction and solid-state X-ray diffraction analysis.

[a] R. D. Suenram, D. J. Brugh, F. J. Lovas and C. Chu, *51st OSU Int. Symp. On Mol. Spectrosc.*, Columbus, OH, 1999, RB07