

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 ((CF₃)₂CH-O-CH₂F), isoflurane (CF₃CHCl-O-CHF₂), enflurane (CHFClCF₂-O-CHF₂) and methoxyflurane (CHCl₂CF₂-O-CH₃). 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 (¹³C and ¹⁸O 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.

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