

SIFT-MS measurement of distribution coefficients for volatile organic compounds in human blood constituents

Paul F. Wilson¹, **Colin G. Freeman**¹, Murray J. McEwan¹, Randall A. Allardyce² and Geoffrey M. Shaw³

- 1 Department of Chemistry, University of Canterbury, Christchurch, New Zealand
- 2 Department of Surgery, Christchurch School of Medicine, New Zealand
- 3 Department of Intensive Care Medicine, Christchurch Hospital, New Zealand

The new technique of selected ion flow tube - mass spectrometry (SIFT-MS) has been applied to the determination of Henry's Law constants for the volatile organic chemicals (VOCs) o-xylene and trichloroethylene, both of which have very low solubility in aqueous solvents.

The operation of the SIFT-MS technique is described. This technique provides an absolute concentration measurement of VOCs in gas mixtures without the need for calibration using known concentrations of the analyte. Results are presented which have been derived from the measurement of equilibrium headspace concentrations of the above VOCs over water at 298 and 309 K as well as the human body fluids: urine; saline; whole blood; red cells in saline; and plasma (all at 309 K). The dimensionless distribution coefficients for these VOCs vary markedly in the different fluids. For o-xylene values range from $k_H = 0.12 - 0.15$ in water, saline and urine; 0.53 for red cells in saline; 1.9 for whole blood; to 2.4 in plasma. In the case of trichloroethylene the distribution coefficients range from $k_H = 0.070 - 0.091$ in water, saline and urine; 0.28 for red cells in saline; 0.35 for plasma; to 0.48 in whole blood. The widely different solubilities of organic solvents in body fluids may influence the uptake of solvents in individuals exposed to VOCs and some of the implications of this are discussed briefly.
