Title: Accuracy of reduced mobilities and measurement of instrumental parameters in ion mobility spectrometry

Author: Roberto Fernández-Maestre

PII: S1387-3806(17)30064-7
DOI: http://dx.doi.org/doi:10.1016/j.ijms.2017.05.018
Reference: MASPEC 15809

To appear in: *International Journal of Mass Spectrometry*

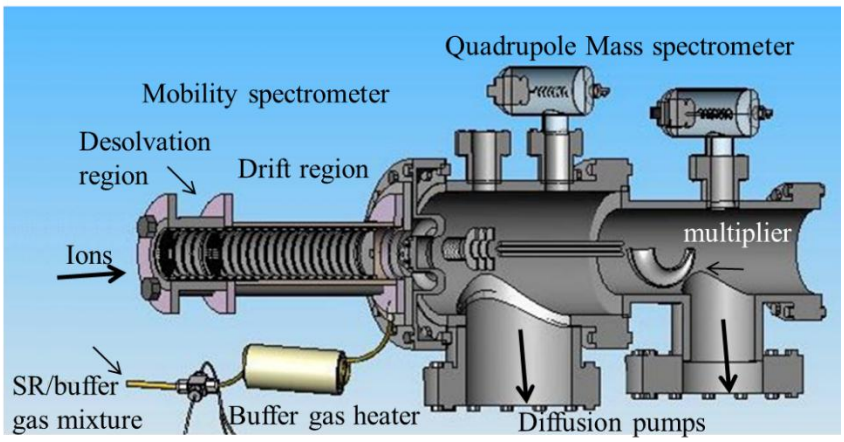
Received date: 9-2-2017
Revised date: 3-5-2017
Accepted date: 29-5-2017

Please cite this article as: Roberto Fernández-Maestre, Accuracy of reduced mobilities and measurement of instrumental parameters in ion mobility spectrometry, International Journal of Mass Spectrometryhttp://dx.doi.org/10.1016/j.ijms.2017.05.018

Accuracy of reduced mobilities and measurement of instrumental parameters in ion mobility spectrometry

Roberto Fernández-Maestre
Universidad de Cartagena, Campus de San Pablo, Programa de Química, Cartagena, Colombia

Graphical Abstract



Accuracy of reduced mobilities and measurement of instrumental parameters in ion mobility spectrometry
Roberto Fernández-Maestre
Universidad de Cartagena, Campus de San Pablo, Programa de Química, Cartagena, Colombia

Highlights

IMS-MS was used to obtain mobilities (K_0) of amino acids and chemical standards

Buffer gas temperature and calibration with two chemical standards were used

Reproducibilities from 0.3 to 0.6% and repeatability of 0.17% for K_0 were found

Small changes in instrument parameters produced important drift times variations

We recommend K_0 to be obtained from calibration with chemical standards.

ABSTRACT

Ion mobility spectrometry (IMS) separates gas-phase ions drifting under an electric field according to their size to charge ratio. We used electrospray ionization-drift tube IMS coupled to quadrupole mass spectrometry to obtain the mobilities of common amino acids, amines, valinol, atenolol, and the chemical standards tetramethylammonium ion (TMA), tetraethylammonium ion (TEA), tetrapropylammonium ion (TPA), and tetrabutylammonium (TBA) ions, 2,4-lutidine and 2,6-di-tert-butyl pyridine (DTBP). The mobilities were obtained in pure nitrogen or when shift reagents (SR) such as ammonia, 2-butanol, ethyl lactate, methanol, methyl 2-chloropropionate, nitrobenzene, 1-phenyl ethanol, trifluoromethyl benzyl alcohol, and water were introduced in the buffer gas. We found important differences in the buffer gas temperature between different regions of the drift tube and differences between the buffer gas and drift tube temperatures, which is normally used instead of the buffer gas temperature in reduced mobility calculations. Therefore, we used the buffer gas temperature instead of the drift tube temperature and a calibration method with two types of chemical standards, finding excellent precision, reproducibilities from 0.3 to 0.6% for reduced mobilities (K_0) of the chemical standards during nine months. Repeatability during this period was 0.17% for the drift times of all the analytes. We also show that the changes in instrumental parameters such as temperature, pressure and voltage that produce important variations in drift times are small; for this, we recommend to calculate K_0 from calibration with chemical standards instead of replacing instrumental parameters in the IMS fundamental equations.