Analytical Performance of an Ion Trap Mass Spectrometer Using Air as the Buffer Gas

Stephen A. Lammert, Roosevelt Merriweather, and Marcus B. Wise*
Oak Ridge National Laboratory, P.O. Box 2008, Oak Ridge, TN 37831-6120

Ion trap mass spectrometers are typically operated using helium as the buffer gas in order to kinetically cool the ion population to the center of the device prior to mass analysis. In a laboratory setting, the use of helium poses no serious limitations other than cost. However in field analysis (using transportable instruments) the need carrying compressed gases for analysis hinders the transportation of the instrument and adds complexity to the instrument setup. Under these circumstances, the elimination of the need for compressed gases is desirable.

We have previously shown that the performance of ion traps (sensitivity and mass resolution) is not only dependent on the type and pressure of buffer gas, but also the ejection q_z-value.[1,2] It has been shown that when using helium, a q_z-value of *ca.* 0.85 will provide better resolution and peak intensities than will a q_z-value of 0.906 (the standard value for most Finnigan-MAT type ion traps). This previously presented data was obtained by directly admitting both the samples (perfluorotributylamine and krypton) and the buffer gas (helium and air). It remained to further apply this technique to practical analytical problems such as the direct sampling analysis of volatile organic compounds (VOC's) in water.

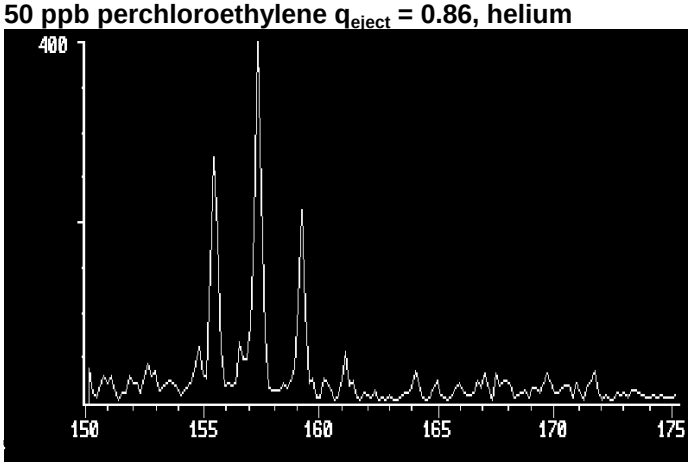
Experiments comparing helium performance at q_{eject}-values of 0.906 vs. 0.84 were performed on a Finnigan-MAT ITMS™ using the direct sampling water purge interface developed at ORNL.[3] Forty milliliter samples of water spiked with one of eight VOC's was purged for 3 minutes and the areas of resulting mass chromatograms were integrated over this time period. The lower q_{eject}-value was effected by setting the axial modulation mass to a value of 0.908/0.84*X where X is the first mass of the mass analysis scan and 0.908 is the q-value of the stability boundary. Several concentrations of VOC's were examined in triplicate in order to calculate and compare (see Table 1) the method detection limits (MDL / 99% confidence interval) for both q_z-values of 0.906 and 0.84 when using helium as the buffer gas. MDL values using a q_{eject}-value of 0.84 are significantly lower than those using the traditional q_{eject}-value of 0.906.

TABLE 1

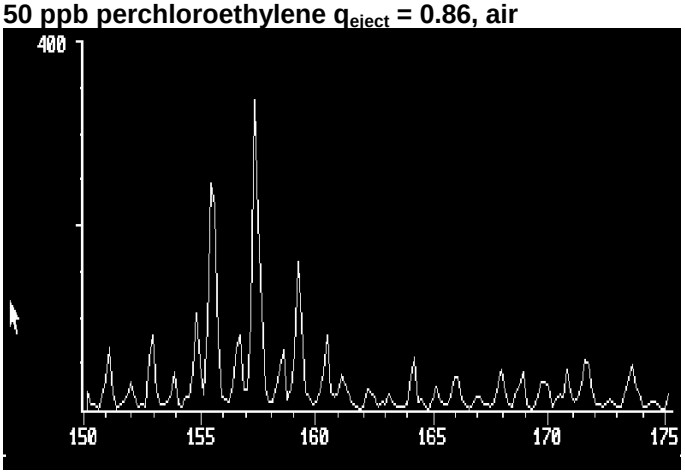
COMPOUND	MDL (ppb) q_{eject}=0.906	MDL (ppb) q_{eject}=0.84
carbon tetrachloride	0.23	0.06
chloroform	0.15	0.04
trichloroethylene	0.20	0.15
perchloroethylene	0.14	0.10
1,1-dichloroethane	0.35	0.18
cis -1,2 dichloroethylene	0.31	0.06
1,2 dichloropropane	0.35	0.14
dibromochloromethane	0.17	0.20

Experiments comparing air and helium at a q_{eject}-value of 0.86 were performed on a different Finnigan-MAT ITMS, similarly configured with the exception that the Teflon conductance spacers were removed from the ion trap analyzer electrode assembly. Mass profiles were acquired during the direct purge in order to show both peak intensity as well as mass resolution. When air was used as the buffer gas, it was also used as the purge gas. The figures below compare the results obtained for the direct sampling of a water sample containing 50 ppb perchloroethylene when using helium vs. air as the buffer gas. As is shown, at a q_{eject}-value of 0.86, similar mass resolution and peak intensity is obtained for both buffer gas types. The mass peaks for perchloroethylene are displayed at their mass-range-extended values (0.86/0.906*m/z).

50 ppb perchloroethylene q_{eject} = 0.86, helium



50 ppb perchloroethylene q_{eject} = 0.86, air



References

1) Lammert, S.A., and Wells, J.M., Presented at the 43rd ASMS Conference on Mass Spectrometry and Allied Topics, Atlanta, GA, 21-26 May 1995.
2) Lammert, S.A., and Wells, J.M., *Rapid Commun. Mass Spectrom.* **10(3)** (1996) 361-371.
3) Wise, M.B., Thompson, C.V., Buchanan, M.V., Merriweather, R., Guerin, M.R., *Spectroscopy* **2(5)** (1993) 14-22.

Acknowledgments

This research is sponsored by the US Department of Energy, Office of Research and Development. Oak Ridge National Laboratory, managed by Lockheed Martin Energy Research Corp. for the US Department of Energy under contract number DE-AC05-96OR224