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SHORT COMMUNICATION

Optimization of Fast Atom Bombardment (FAB) Mass Spectra of Arsenobetaine and Arsenocholine

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Optimized FAB mass spectra of arsenobetaine and arsenocholine may be obtained when the matrices glycerol and thioglycerol are used.

Keywords: fast atom bombardment; mass spectroscopy; arsenobetaine; arsenocholine

INTRODUCTION AND DISCUSSION

Arsenobetaine (AB) and arsenocholine (AC) are believed to be widely distributed in seawater, marine animals and plants. Fast atom bombardment (FAB) mass spectrometry has been used for the study of synthetic AB and AC[1] as well as for the identification of these organoarsenic compounds in fish, shellfish and shrimp extracts.[2–7]

Considering the importance of these species in the environment and the important role played by the matrix in FAB mass spectra, we decided to investigate the behaviour of these compounds under FAB conditions, using matrices with different physical and chemical properties such as glycerol, thioglycerol, *m*-nitrobenzyl alcohol, diethanolamine and triethanolamine.

The experiments were performed on an AEI MS 9 mass spectrometer updated by VG Analytical. The compounds were synthesized according to known procedures.[8] The spectra were obtained by bombardment of the sample on the probe target with a xenon beam with an energy of 7 keV and a gun current of 1 mA.

The results obtained for AB are presented in Fig. 1. With glycerol, characteristic fragment ions

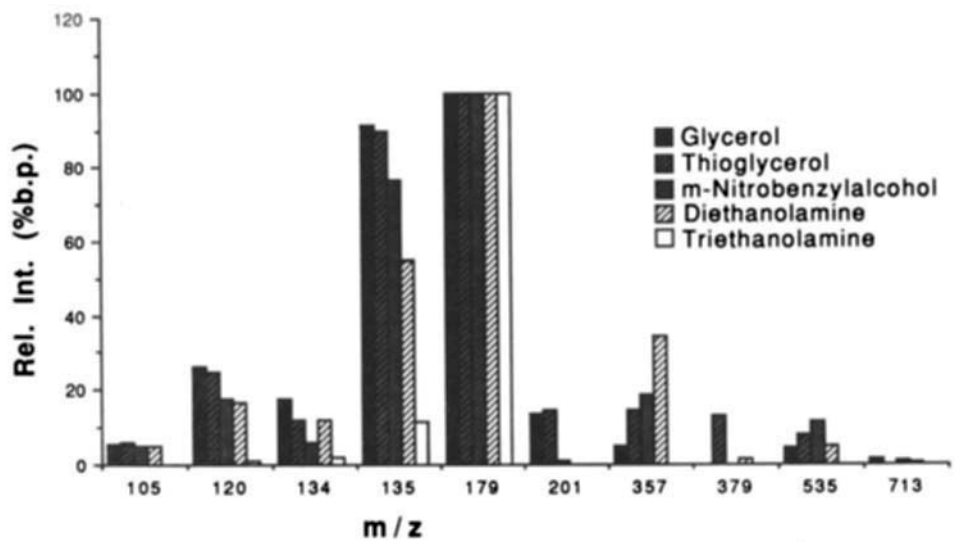

Figure 1 Abundances of the most characteristic ions in the FAB mass spectra of arsenobetaine (AB), obtained with different matrices.

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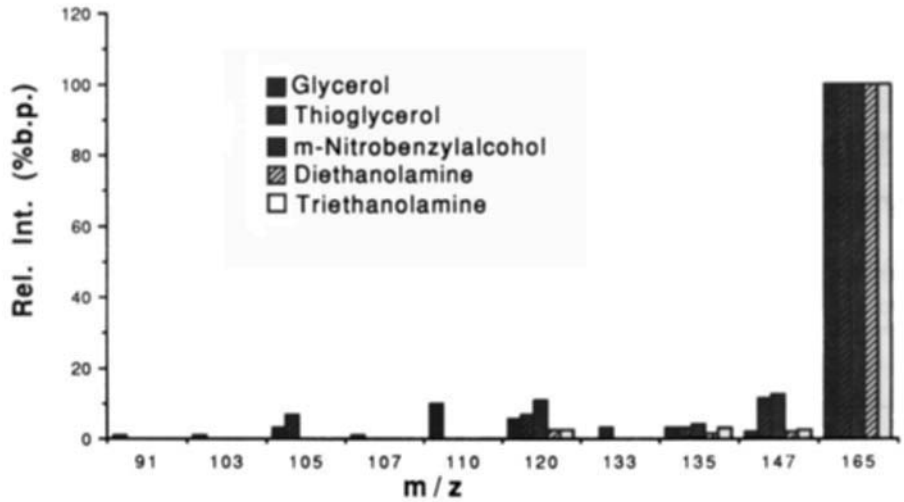

Figure 2 Abundances of the most characteristic ions in the FAB mass spectra of arsenocholine (AC), obtained with different matrices.

at *m/z* 135, 134, 120 and 105, along with the presence of the protonated molecule at *m/z* 179 and adduct ions at *m/z* 201, 357, 535 and 713, closely resembling literature spectra[1–7] may be observed. Using thioglycerol, *m*-nitrobenzyl alcohol or diethanolamine the same characteristic ions were observed. With triethanolamine, however, only *m/z* 179, 135, 134 and 120 are apparent. Best results seem to be obtained when glycerol and thioglycerol are used, which may be attributed to the higher hydrophobic character of these compounds.[9] With glycerol, slightly more abundant fragment ions are obtained, while the matrix thioglycerol seems to favour the formation of adduct ions.

The FAB mass spectra of AC (Fig. 2) present an abundant molecular ion at *m/z* 165 besides some rather low-abundant fragment ions at *m/z* 147, 135, 120, 110 and 105, in agreement with previous reports.[1,2,4] Similarly to the observations for arsenobetaine, optimized mass spectra concerning significant fragment ions may be obtained for arsenocholine when glycerol and thioglycerol are used as matrices.

REFERENCES

1. H. Norin, R. Ryhage, A. Christakopoulos and M. Sandstrom, *Chemosphere* **12**, 299 (1983).
2. B.P.-Y. Lau, P. Michalik, C.J. Porter and S. Krolik, *Biomed. Environm. Mass Spectrom.* **14** 723 (1987).
3. J. B. Luten, G. Riekwel-Booy, J. v. d. Greef and M. C. ten Noever de Brauw, *Chemosphere* **12**, 131 (1983).
4. J. F. Lawrence, P. Michalik, G. Tam and H. B. S. Conacher, *J. Agric. Food Chem.* **34**, 315 (1986).
5. K. Hanaoka and S. Tagawa, *Bull. Jpn. Soc. Sci. Fish.* **51**(4), 681 (1985).
6. K. Shiomi, Y. Kakehashi, H. Yamanaka and T. Kikuchi, *Appl. Organomet. Chem.* **1**, 177 (1987).
7. W. R. Cullen and M. Todd, *Appl. Organomet. Chem.* **3**, 79 (1989).
8. L. Goetz and H. Norin, *Int. J. Appl. Radiat. Isot.* **34** (11), 1509 (1983).
9. A. Santos, M. F. Duarte, M. H. Florêncio and B. Saramago, *J. Chem. Soc., Faraday Trans.* submitted.