

MS Quali e Quanti - 12

**STUDY OF SUPRAMOLECULE COMPLEXATION BY ESI/MS/MS.
THE CASE OF P-TERT-BUTYLCALIX[6]ARENE COMPLEXATION
WITH AMMONIUM HYDROXIDE, AND AMMONIUM AND SODIUM
IONS.**

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The formation of complexes involving p-tert-butylcalix[6]arene with neutral and charged species has been investigated by tandem mass spectrometry combined with electrospray ionization. Complexes of p-tert-butylcalix[6]arene with NH_4^+ ions were observed in the ratios 1:1, 2:1, and 3:1 together with the complexes of p-tert-butylcalix[6]arene with NH_4OH and Na^+ ions in the ratios 1:1:1, 2:1:1, and 3:1:1. A single 1:1 complex of p-tert-butylcalix[6]arene with Na^+ ions was observed. In addition, a doubly-charged complex of p-tert-butylcalix[6]arene with NH_4OH , Na^+ , and NH_4^+ ions in the ratio 6:1:1:1 was observed. The identity of each complex was determined by mass analysis of fragment ions formed by the application of a declustering potential over the range 20 – 220 V and by observation of product ion mass spectra where in the collision energy was varied from 5 – 50 eV. Fragmentation of the complexes is characterised by the facile loss of the sodium ion as sodium hydroxide, loss of neutral p-tert-butylcalix[6]arene, and successive neutral losses of C_4H_8 from the six tert-butyl groups in each p-tert-butylcalix[6]arene molecule.

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