

Thematic course: Synthesis, structure, properties and agrochemical use of new potentially biologically active derivatives of triethanolamine. Part 2.

Synthesis, properties and structural characteristics of aromatic carboxylic acid (2-hydroxyethyl)ammonium salts

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Abstract

Aromatic carboxylic acid salts with (2-hydroxyethyl)ammonium derivative cations (monoethanolamine, diethanolamine, *N*-methyldiethanolamine and triethanolamine) were synthesized and characterized. The parent acid functional group electronic feature and spatial surrounding effects on stability and physical properties were shown. As in the case of aliphatic carboxylic acids tris(2-hydroxyethyl)ammonium cations were found to selectively exist in endo or exo-conformations (so-called protatranic and quasiprotatranic ones, respectively).

Formerly accepted characteristic empirical criterion for aliphatic tris(2-hydroxyethyl)ammonium salts (dissociation constant logarithm difference) was declared invalid for acid salt synthesis possibility prediction in aromatic carboxylic acids derivatives, since all fulfilled the criterion phthalic acids were found to form exceptionally normal salts during our research treats.

As opposed to electron acceptor functional group-containing acid derivatives (nitrogroup, carboxyl) some functional group introduction (halogen, hydroxyl or aminogroup) to the anion structure was described to decrease melting points and phase transition to liquid or amorphous states.

Cationic structure complication from monoethanol to di- and triethanolamines is accompanied by systemless compound thermal stability changes, i.e. transition to more sterically developed cations may possibly induce either increasing or decreasing product melting point. Since that, such pattern of change indicates on the key role of electrostatic and steric anion and cation properties combination in each case and low impact of quantitative carbon skeleton atomic changes. Opposed to aliphatic triethanolamine salts the greater number of crystallographic parameter variations were described. The existence of monoclinic, orthorhombic and hexagonal crystal families, *Pbca*, *P2₁/n*, *P1*, *C2/c* space group causes was discovered. Such behavior is presumably caused by significant anion functional group affecting compared to chain length increase in aliphatic triethanolamine salts.

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