Synthesis, structure, and properties of azatriangulenium salts

A general synthetic route to novel nitrogen-bridged heterocyclic carbenium ions of the acridinium and triangulenium type has been developed and investigated. The synthetic method is based on nucleophilic aromatic substitution (SNAr) on the tris(2,6-dimethoxyphenyl)carbenium ion (1) with primary amines and, by virtue of its stepwise and irreversible nature, provides a powerful tool for the preparation of a wide variety of novel heterocyclic carbenium salts. Several derivatives of the three new oxygen- and/or nitrogen-bridged triangulenium salts, azadioxa- (6), diazaoxa- (7), and triazatriangulenium (4), have been synthesized and their physicochemical properties have been investigated. Crystal structures for compounds 2 b-PF6: 2d-PF6, 4b-BF4, 4c-BF4, 6e-BF4, and 8 are reported. The different packing modes found for the triazatriangulenium salts are discussed in relation to the electrostatic and space-filling requirements of the ions. The stabilities of the cations 6a, 7b, and 4a, as expressed by their pK(R+) values, have been determined in strongly basic nonaqueous solution by use of the C- acidity function; the values obtained were 14.5, 19.4, and 23.7, respectively. This study further implied that the C- scale in its present form is unsuitable for the precise determination of pK(R+) values beyond 22.

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