SYNTHESIS, REACTION AND MASS SPECTRA OF DISUBSTITUTED PYRAZINE DERIVATIVES

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Pyrazines exist in some species of mold as 2,5-disubstituted pyrazinols or N-oxides (e.g. aspergillic acid, neoaspergillic acid, pulcherrimic acid) and some of them were already synthesized by the authors. During the course of an investigation of these syntheses, it became desirable to clarify the reactivity of disubstituted pyrazines. On this ground were prepared 2,3-, 2,5- and 2,6-disubstituted pyrazines (R,R'=Me and/or Ph) and investigated reactivity and mass spectra of these compounds.

N-Oxidation of most disubstituted pyrazines, except two 2,6-disubstituted pyrazines (R=R'=Ph; R=Me, R'=Ph), with per-acetic or maleic acid gave a mixture of 1-, 4- and di-oxides. The pyrazine N-oxides prepared were treated with phosphorylchloride and acetic anhydride to chlorinated and acetoxylated pyrazines, and the reaction mechanism of these reactions was discussed with relation to the MO-calculation.

It was found that mass spectra of substituted pyrazine N-oxides are characteristic of the fragment ion peak of M-16 or M-17 (in the case of 2-alkyl compounds) and a correlation exists between the intensity of M-16 and the N-O bond order.