A COMPARISON OF THE MASS SPECTRA OF 2,3-POLYMETHYLENE-1,2,3,4-TETRAHYDROQUINAZOLIN-4-ONES

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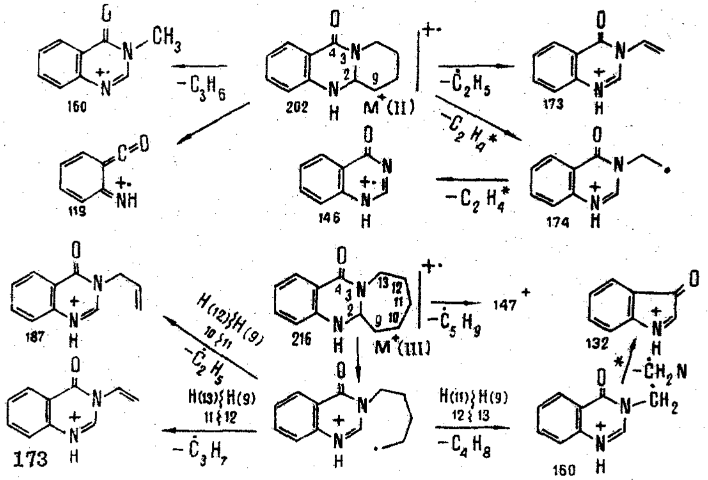
The fragmentation of 2,3-trimethylene-1,2,3,4-tetrahydroquinazolin-4-one (I) (dihydrodeoxyvasicinone) has been studied previously [1]. It has been established that the main mode of decomposition of the acyclic ring C is the elimination of a molecule of ethylene accompanying the cleavage of C_2—C_9 bond. When the size of this ring is increased, the contribution of the processes involving the elimination of its element rises, as can be seen from the spectra of tetra- and pentamethylenetetrahydroquinazolin-4-one (II and III), respectively, obtained from the corresponding 2,3-polymethylene-3,4-dihydroquinazolin-4-ones by reduction with sodium tetrahydroborate in ethanol. In spite of the fact that qualitatively any of the directions of fragmentation of compounds (I-III) can be explained, the intensities of the individual peaks change in what is at first sight a complex manner.



We have turned our attention to the fact that the contributions of the processes of the detachment of various members of ring C coincide fairly strictly with those of the corresponding alicyclic hydrocarbons. Thus, in the decomposition of the molecular ions of cyclopentane and cyclohexane the elimination of the two-carbon chain (in the form of an ethylene molecule) takes place with the greatest intensity [2]. We have also observed the predominant elimination of a chain of two carbon atoms both in the case of (I) and in the case of a compound with a six-membered ring C (II). It is also necessary to take into account the fact that the reduction in the height of the peak of the $(M - 28)^+$ ion in the last-mentioned case is caused by its decomposition leading to a fragment with m/e 146 (Scheme).

For the molecular ion of cyclopentane, the most characteristic elimination is that of a chain including three or four carbon atoms, and the elimination of a chain of two or five carbon atoms is less important. A similar distribution of intensities is observed in the spectrum of (III) (Fig. 1).

Hirota and Niwa [3], having calculated by the MO method the relative probabilities of the degradation of each of the C—C bonds after the initial equiprobable cleavage of one of the bonds of the skeleton in the molecular ions of cycloalkanes, found a good agreement of these values with the relative intensities of the peaks of the ions formed as the result of the cleavage of the corresponding bonds. Since, however, for the molecular ions of compounds

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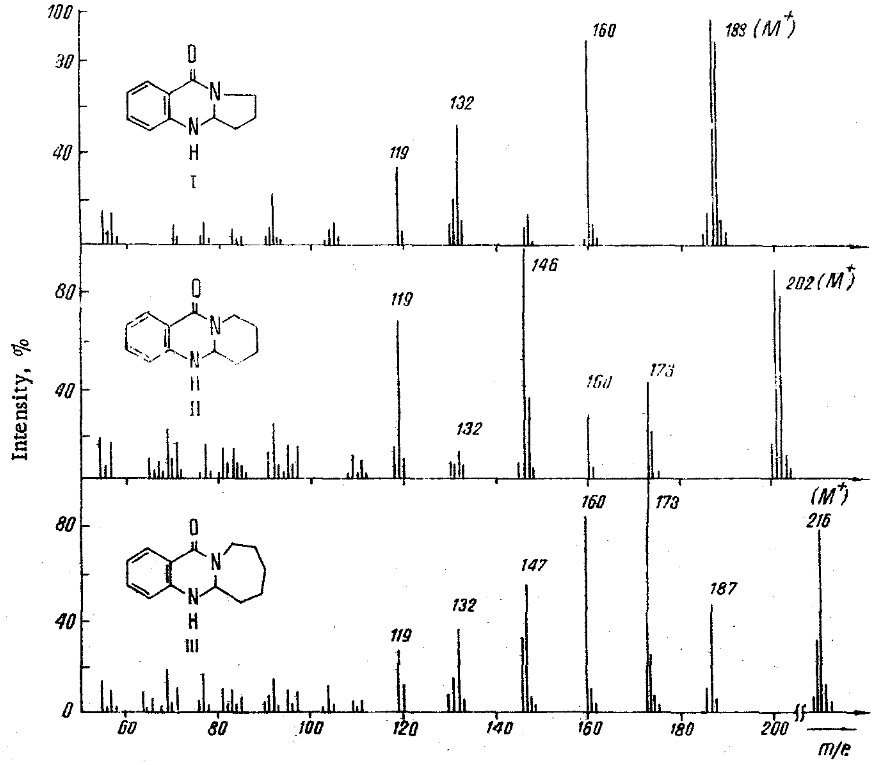

Fig. 1

(I-III) the equal probability of cleavage of the bonds of ring C is excluded, the reason for the observed analogies with the spectra of the cycloalkanes may be the predominant tendency of any particular one of the bonds to be cleaved first. This condition is satisfied by the C_2—C_9 bonds in all three compounds.

LITERATURE CITED

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