RELATIONSHIP BETWEEN THE NITRATION PRODUCTS, MASS SPECTRA AND ELECTRONIC STRUCTURE OF MONONITROQUINOLINE

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Seven kinds of mononitroquinolines (2-,3-,4-,5-,6-,7- and 8-nitroquinolines) were investigated as systems possessing 13 orbitals and 14π-electrons, and their electronic distribution and π-bond order were calculated by the simple Hückel method. These mononitroquinolines were nitrated to dinitroquinolines and in all cases the second nitro group was introduced onto the carbon atom which possesses the largest electron density. It was also found that a certain relation exists between the intensity of m/e 128 (M^+-NO_2) and the π-bond order of mononitroquinolines, so that the greater the π-bond order, the stronger the intensity of m/e 128.