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Structure-mutagenicity correlation of nitrobenzanthrones by molecular orbital calculations

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The mutagenic activity of nitrobenzanthrones(NBAs) , depends significantly on the position of their nitro groups. 3-NBA shows the highest activity among NBAs, 9-NBA almost 40% activity of 3-NBA, and 11-NBA extremely low activity. To elucidate this large difference in the mutagenicity, molecular orbital calculations were carried out for the three NBAs and their metabolites produced in the activation pathways. The LUMO energies of the parent molecules were found to correlate with their mutagenicities; the energy decreases with increasing mutagenicity. This indicates that the electrophilicity of the parent molecules is an important factor in their mutagenicity and 3-NBA is the most electrophilic reagent. In the binding reaction of nitrenium ions, final metabolites of NBAs, to guanine, the activation energy (*Ea*) was almost the same and no correlations were found between *Ea* and mutagenicity. This suggests that the production rate and stability of nitrenium ions are more important in determining the mutagenicity than the binding reaction rate.