

Division of the History of Chemistry American Chemical Society

Citation for Chemical Breakthrough



Journal of Chemical Physics 1952, 20, 722-725.

A Molecular Orbital Theory of Reactivity in Aromatic Hydrocarbons

Kenichi Fukui, Teljiro Yonezawa, and Haruo Shingu Faculty of Engineering, Kyoto University, Kyoto, Japan (Received October 29, 1951)

In the present paper it is shown that on the ground of the latter method, if we distinguish the pair of π -electrons in the highest occupied orbital in the ground state from the others and assume that this pair of π -electrons plays a decisive role in the reaction in question, we can obtain an illuminating explanation of the difference of reactivity at each position in a molecule.

In the first place we will report on the treatment of nonsubstituted aromatic hydrocarbons. The orienting effect of substituents in aromatic nuclei will be treated in the next publication.

Presented to the Faculty of Engineering, Kyoto University, 2021.