

Comment

Comment concerning the review article: The Diels-Alder reaction and biopolymer catalysis by T. M. Tarasow and B. E. Eaton

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Notwithstanding the surprising opinion of the second referee, who finds the two schemes very helpful for the reader in visualizing the mechanism and understanding the orbital model of Diels-Alder chemistry and the authors' reply, in which they claim that the scheme may have been confusing because, for the sake of simplicity, only the four electrons in the two HOMO orbitals have been shown, I maintain that this oversimplification is inadequate and hardly acceptable. At best, the left part of the scheme can be taken as an example of the frontier orbital approach advocated by Fukui, which predicts that a concerted chemical reaction is allowed when there is a crossed symmetry fit between the HOMOs-LUMOs of the two reacting partners. The main issue, however, is the following: the dotted lines in the two schemes seem to refer to a mixing of the corresponding orbitals during the course

of the reaction and such a mixing is explicitly mentioned in the text of the same page; as a result of the oversimplification, an innocent reader gets the impression that the mixing of the HOMO-LUMO pair with A-symmetry results exclusively in the formation of an empty antibonding orbital in the product and wonders accordingly what has happened to the original pair of electrons. The statement in the text that this pair has been used (together with another pair) for creating α -bonds does not make the attempted correlation any clearer and the right parts of the two schemes might as well have been dropped. Unfortunately, the situation is not improved by the wrong placing of the orbitals in the product of the reaction in scheme 2 (the residual double bond in this compound is no longer conjugated with the nitrile group, as shown correctly in scheme 3).