

Erratum

Classification of Chemical Reactions: Potential, Possibilities, and Continuing Relevance [*J. Chem. Inf. Comput. Sci.* 31, 212–216 (1991)] By DAVID BAWDEN. City University, Northampton Square, London EC1V 0HB, England

In a recent paper,¹ I gave an overview of the nature of, and methods for, classifying chemical reactions. The choice of references, as stated in the paper, was deliberately selective rather than comprehensive; perhaps overselective, as it has been suggested that some important material was omitted. This corrects this failing.

One approach which did not receive mention in the original paper was that due to Fujita, the approach based on "imaginary transition structures". The latter are structural formulas, with nodes linked by formal bonds, including those formed or broken in reaction, as well as those remaining unchanged. One single formula may therefore represent a reaction or a reaction sequence.² Subgraphs of these representations may be used to give a systematic hierarchical classification.^{3,4} An example is dechlorination – dehalogenation – reductive elimination – elimination – double bond formation – and more general terms.

In the cited papers, the author compares the imaginary transition-structure approach with both IUPAC nomenclature and with other reaction classification schemes.

In the original review,¹ mention was made of the work of Zefirov on the derivation of general hierarchical classifications of reactions. It should be noted that this has been directly utilized in a system allowing the exhaustive generation of equations describing all possible forms of structural change from given precursors.⁵ Similarly, the formal classification

schemes of Ugi and co-workers were described in the original review. These have been incorporated in a system for synthetic analysis, so that desired individual reactions may be identified, from the output for a reaction generator, by a selection procedure using a hierarchical classification of reactions based on minimum chemical distance.⁶

Finally, I should note that Kvasnicka⁷ has presented a classification of reactions, based on the Ugi model of the reaction centre, and incorporating a precise and formal definition of the "reaction core".

REFERENCES AND NOTES

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