A new electronic theory of pericyclic chemistry and aromaticity is proposed: The Cplex-isoelectronic theory. Consistent with Santilli's hadronic chemistry

Martin O. Cloonan

Caherfourvase, Craughwell, Galway, Republic of Ireland

Received 21 April 2005; revised 18 March 2006; accepted 21 March 2006. Available online 7 July 2006.

Abstract

A new electronic theory of pericyclic chemistry and aromaticity, in line with the Robinson/Ingold electronic theory, is proposed. It is referred to as the Cplex-isoelectronic theory. This represents the first successful theory that is not based on quantum mechanics. There are three assumptions in this theory (1) ADEP, (2) SDEP and (3) SDSE. The ADEP assumption refers to isoelectron pairs moving in an antiperiplanar mode in relation to the plane of the molecule. SDEP relates to isoelectron pairs moving in a synperiplanar mode and SDSE refers to single isoelectrons moving in a synperiplanar mode. These assumptions are deduced from nucleophilic, radical addition, S_N2 and S_N2' reactions and the anomeric effect. Application of the ADEP concept to pericyclic reactions is supported by Complexity theory and backed up by direct empirical evidence from 1,3-dipolar cycloaddition reactions involving nitronates and by its ability to

predict the experimental data. The heavy atom effect provides experimental evidence for the SDSE mode in pericyclic reactions. The HOMO Diels–Alder is consistent with the SDEP concept. Evidence for the assumptions in aromatic compounds is found in the observation of a diamagnetic ring current in the presence of an applied field and in the applicability of the Biot–Savart law. The Cplex-isoelectronic theory makes different predictions from the present quantum chemical methods in some cases, namely the existence of suprafacial concerted thermal [2+2], [4+4], [6+2] and [6+6] cycloadditions, suprafacial concerted photochemical [4+2] and [6+4] cycloadditions, stepwise [2+2+2] cycloadditions of ethyne, diamagnetic ring currents for some cyclic systems with $4n\pi$ electrons. The available empirical evidence is consistent with these predictions. This finding is consistent with Santilli's hadronic chemistry which proposes that the present quantum chemical theories require the addition of a small correction factor for molecules with two or more electrons.

Keywords: Electronic theory; Pericyclic; Aromaticity; Hadronic chemistry; Complexity; Quantum chemistry

Abbreviations: ADEP, antiperiplanar dynamics of isoelectron pairs; AFS, acceptor at the final facial selectivity site; ASIED, acceptor site of initial electron dynamics; DFS, donor at the final facial selectivity site; DSIED, donor site of initial electron dynamics; FSED, final facial selectivity of electron density; RCEDGD, rate of continuous electron dynamics greater

than delocalisation; SEADEF, substituent electronic assistance in the direction of the electron flow; SDSE, synperiplanar dynamics of single isoelectrons; SDEP, synperiplanar dynamics of isoelectron pairs

Tel.: +353 091 846 290.