Extended characteristic polynomial estimating the electrochemical behaviour of azulene thiophen–vinyl–pyridines

Eleonora-Mihaela Ungureanu[1], Amalia Stefaniu[2], Oana Ciocirlan[3], Cornelia Musina[3], Magdalena-Rodica Bujduveanu[3], Lorentz Jäntschi[4]

[1]Doctoral School of Chemical Engineering and Biotechnologies,
National University of Science and Technology POLITEHNICA, Bucharest, Romania
[2]National Institute of Chemical, Pharmaceutical Research and Development, Bucharest, Bucharest, Romania
[3]Faculty of Chemical Engineering and Biotechnologies,
National University of Science and Technology POLITEHNICA, Bucharest, Romania
[4]Department of Physics and Chemistry, Technical University of Cluj-Napoca, Cluj-Napoca, Romania

A series of 6 azulene thiophen–vinyl–pyridine ligands for which two electrochemical properties (oxidation (E_a) and reduction (E_c) potentials) were collected in a recent study (see Table 3 in [1]) was subjected to (i) raw molecular modelling with Merck molecular force field (MMFF, see [2]), followed by (ii) computational analysis using families of molecular descriptors. Two descriptor families were considered in this analysis, Fragmental Matrix Property Indices (FMPI, as seen in [3] and [4]) and Extended Characteristic Polynomial (EChP, as seen in [5] and [6]). The results show that EChP is able to well distinguish between ligands as well as to provide a high estimation capability ($R^2 > 0.9990$ for E_a; $R^2 > 0.9998$ for E_c). As it is known, MMFF method is a very good first level of approximation for molecular geometry. Thus, further investigation is required in order to validate these preliminary results. The results with FMPI are not spectacular - they are inferior to those with EChP, and this suggests that the nature of the property - the reduction and oxidation potentials - is localized. A functional group or a position in the structure is more suitable to express an electrochemical property. Figures 1 and 2 give estimates of the association between the chemical structure and the electrochemical potentials by means of the individuals "RDCN0940" and "LEGN0705" members of the family of extended characteristic polynomials.
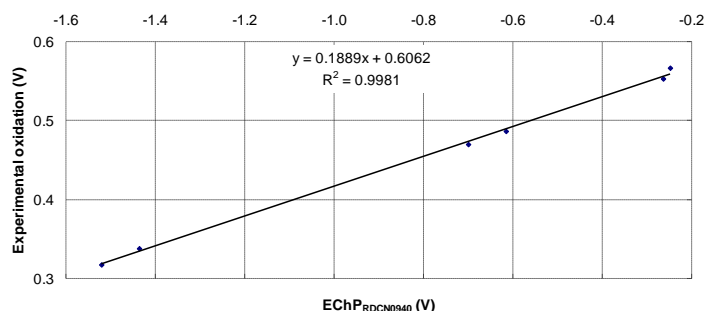

Figure 1. Oxidation as linear function of RDCN0940 extended characteristic polynomial
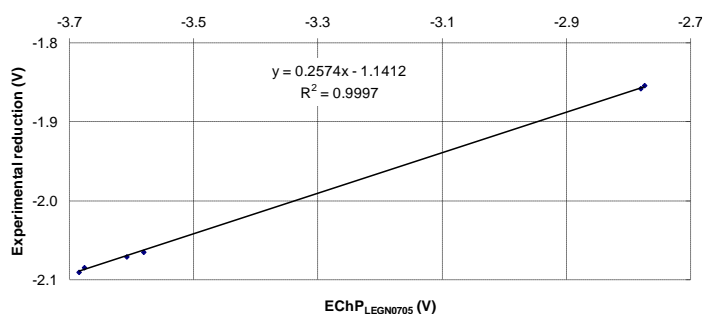

Figure 2. Reduction as linear function of LEGN0705 extended characteristic polynomial

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