

Weller correlation

Empirical correlation for the energy of full charge-transfer exciplex relative to the ground state in *n*-hexane as a function of the electrochemical one electron standard reduction potential of the cation radical produced upon electron donation and standard reduction potential of the acceptor measured in a polar solvent for the donor (D) and the acceptor (A) involved

$$\Delta H(D^+A^-, \text{hexane}) = e [E^0(D^{+\bullet} / D) - E^0(A / A^{-\bullet})] + e \Delta E$$

with $E^0(D^{+\bullet} / D)$ and $E^0(A / A^{-\bullet})$ the standard electrode potentials of the donor and acceptor, respectively.

Notes:

1. In the case diethylaniline as donor and aromatic hydrocarbons as acceptors, the last term on the right, i.e., $e \Delta E = (0.15 \pm 0.10)$ eV. This equation assumes a constant Coulomb term and a constant entropy change within a particular series of partners. e is the elementary charge.
2. The IUPAC recommendations for the sign and symbols of standard potentials are used in the equation as written above.
3. Although not complying with the IUPAC recommended nomenclature for the standard electrode potentials, traditionally the equation has been written as:

$$\Delta H(D^+A^-, \text{hexane}) = e [E_{\text{ox}}^0 - E_{\text{red}}^0] + (0.15 \pm 0.10) \text{ eV}$$

with E_{ox}^0 the standard electrode potential at which the oxidation occurs, and E_{red}^0 the standard electrode potential at which the reduction occurs. This writing of the first term within the square brackets is misleading and not recommended.

Source:

PAC, 2007, 79, 293 (*Glossary of terms used in photochemistry, 3rd edition (IUPAC Recommendations 2006)*) on page 439