

**FEATURES OF CALCULATION OF STANDARD RedOx POTENTIALS
BY THE SEMI-EMPIRICAL METHODS AM1, RM1 PM7**

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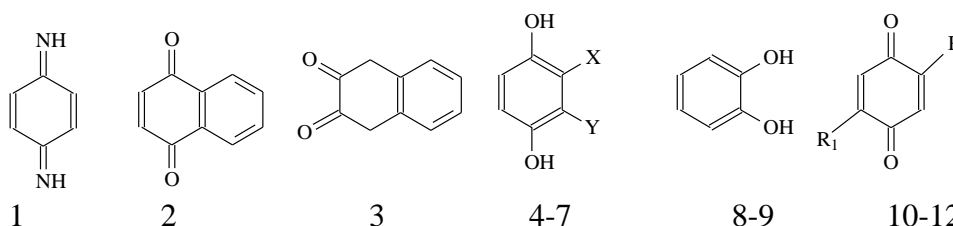
We calculated the standard RedOx potentials the semi-empirical methods AM1, RM1 and PM7. RedOx potential calculation is based on the following equation¹:

$$\Delta G(X_{vs}NHE) = \Delta G_{solv}^0(X^+) - \Delta G_{solv}^0(X) - 4.44eV \quad (1)$$

$$E^0 = -\Delta G/F \quad (2)$$

4.44 eV – change of energy of Gibbs in hydrogen reduction reaction, $F = 1 \text{ eV}$, Faraday constant. Solvation effects was considered by the continual model PCM.

We calculated the standard RedOx potentials for the anylines, quinones and their analogs containing nitrogen (12):



(4) X=Cl; (5) X=Cl; (6) X=Y=CN; (7) X=Y=CN; (10) R=R₁=CH₃; (11) R= CH₃; (12) R=OH, R=OH

Comparison of average absolute errors of calculation of $E_{Red/Ox}$ of the potentials calculated through the total energies (E_{tot}) and heat of formation (ΔH_f^0) is presented in Table.

Table. Accuracy of calculation of $E_{Red/Ox}$ on all set of compounds

Method	MUE	
	$E_{Red/Ox}^{E_{tot}}$	$E_{Red/Ox}^{\Delta H_f}$
AM1	1.39	1.45
RM1	1.24	1.24
PM7	1.56	1.61

All methods approximately on 1B systematically overestimates value Red/Ox potential. The average absolute mistake concerning an experiment is 1.39 V for AM1, 1.56 V for PM7. 1.24 V for RM1. The most precise is the RM1 method. Specified approximations gives an identical average absolute error of calculation for both considered schemes of calculation.