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-emperical methods AM1, RM1 and PM7. RedOx potential calculation is based on the following equation:

\[ \Delta G(X_{vs}NHE) = \Delta G^0_{solv}(X^+)-\Delta G^0_{solv}(X) - 4.44 \text{eV} \ (1) \]

\[ E^0 = -\Delta G/F \ (2) \]

4.44 eV – change of energy of Gibbs in hydrogen reduction reaction, F = 1 eV, Faraday constant. Solvation effects was considered by the continial model PCM.

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

1 2 3 4-7 8-9 10-12
(4) X=Cl; (5) X=Cl; (6) X=Y=CN; (7) X=Y=CN; (10) R=R_1=CH_3; (11) R= CH_3; (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 (\( \Delta H^0_f \)) is presented in Table.

<table>
<thead>
<tr>
<th>Method</th>
<th>MUE</th>
<th>( E_{Red/Ox}^{E_{tot}} )</th>
<th>( E_{Red/Ox}^{\Delta H_f} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>AM1</td>
<td>1.39</td>
<td>1.45</td>
<td></td>
</tr>
<tr>
<td>RM1</td>
<td>1.24</td>
<td>1.24</td>
<td></td>
</tr>
<tr>
<td>PM7</td>
<td>1.56</td>
<td>1.61</td>
<td></td>
</tr>
</tbody>
</table>

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.