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**Andrew S. Dutton, Jon M. Fukuto, and Kendall N. Houk\*:**  
Theoretical Reduction Potentials for Nitrogen Oxides from CBS-QB3 Energetics and (C)PCM Solvation Calculations

Page 4027. The reference to the experimental reduction potential of cysteine, 0.9 V, should be as follows: Surdhar, P. S.; Armstrong, D. A. *J. Phys. Chem.* **1986**, *90*, 5915–5917.

Page 4025. In the computation of reduction potentials in aqueous solution, the free energies of water reactants or products should have been computed for 55 M H<sub>2</sub>O, instead of 1 M. We thank David Stanbury and Michael McKee (Auburn University) for pointing out these errors to us.

The correct correlations between computed and experimental reduction potentials are as follows:

With the PCM solvation model:  $E_{\text{exp}}^{\circ}(\text{V}) = 0.94E_{\text{calc}}^{\circ}(\text{V}) + 0.08 \text{ V}$  [ $R^2 = 0.93$ , MAD = 0.19 V, max dev = 0.45 V].

With the CPCM solvation model:  $E_{\text{exp}}^{\circ}(\text{V}) = 0.96E_{\text{calc}}^{\circ}(\text{V}) + 0.16 \text{ V}$  [ $R^2 = 0.97$ , MAD = 0.13 V, max dev = 0.37 V].

These new correlations result in new computed values of the reduction potentials. The computed  $E^{\circ}$  values are given below in a revised version of Table 1. Several predicted values in Tables 2–4 are changed by as much as 0.2 V, as shown in the revised tables given below.  $E_{\text{pred,Old}}^{\circ}(\text{V})$  refers to the predicted values printed in the original manuscript. These should now be replaced by  $E_{\text{pred}}^{\circ}(\text{V})$ . In addition, the following are corrected predicted reduction potentials ( $\pm 0.3 \text{ V}$ ) that appear in the text and the abstract: NO<sub>2</sub>/NO<sub>2</sub><sup>-</sup> (0.7 V), NO<sub>3</sub>/NO<sub>3</sub><sup>-</sup> (2.2 V), N<sub>2</sub>O<sub>3</sub><sup>-</sup>/N<sub>2</sub>O<sub>3</sub><sup>2-</sup> (0.6 V), HN<sub>2</sub>O<sub>3</sub>/HN<sub>2</sub>O<sub>3</sub><sup>-</sup> (1.1 V), HONNO,H<sup>+</sup>/HONNOH (1.8 V), 2NO,H<sup>+</sup>/HONNO (0.1 V), 2NO/ONNO<sup>-</sup> (-0.1 V), ONNO<sup>-</sup>/ONNO<sup>2-</sup> (-0.4 V), HNO,H<sup>+</sup>/H<sub>2</sub>NO (0.7 V), H<sub>2</sub>NO,H<sup>+</sup>/H<sub>2</sub>NOH (1.1 V), HNO,2H<sup>+</sup>/H<sub>2</sub>NOH (0.9 V), and HNO/HNO<sup>-</sup> (-0.7 V).

Revised Table 1

reaction couple	PCM $E_{\text{calc}}^{\circ}$ (V)	CPCM $E_{\text{calc}}^{\circ}$ (V)	$E_{\text{exp}}^{\circ}$ (V)	PCM $E_{\text{pred}}^{\circ}$ (V)
H <sub>2</sub> N <sub>2</sub> O <sub>2</sub> + 2H <sub>3</sub> O <sup>+</sup> + 2e <sup>-</sup> /N <sub>2</sub> + 4H <sub>2</sub> O	2.63	2.53	2.65	2.55
O <sub>3</sub> + 2H <sub>3</sub> O <sup>+</sup> + 2e <sup>-</sup> /O <sub>2</sub> + 3H <sub>2</sub> O	2.03	1.98	2.076	1.99
H <sub>2</sub> O <sub>2</sub> + 2H <sub>3</sub> O <sup>+</sup> + 2e <sup>-</sup> /4H <sub>2</sub> O	1.66	1.56	1.776	1.64
N <sub>2</sub> O + 2H <sub>3</sub> O <sup>+</sup> + 2e <sup>-</sup> /N <sub>2</sub> + 3H <sub>2</sub> O	1.73	1.67	1.766	1.71
2HOCl + 2H <sub>3</sub> O <sup>+</sup> + e <sup>-</sup> /Cl <sub>2</sub> + 4H <sub>2</sub> O	1.56	1.50	1.611	1.55
2NO + 2H <sub>3</sub> O <sup>+</sup> + 2e <sup>-</sup> /N <sub>2</sub> O + 3H <sub>2</sub> O	1.64	1.60	1.591	1.62
HO <sub>2</sub> + H <sub>3</sub> O <sup>+</sup> + e <sup>-</sup> /H <sub>2</sub> O <sub>2</sub> + H <sub>2</sub> O	1.54	1.64	1.495	1.53
HOCl + H <sub>3</sub> O <sup>+</sup> + e <sup>-</sup> /Cl <sup>-</sup> + 2H <sub>2</sub> O	1.48	1.38	1.482	1.47
2HNO <sub>2</sub> + 4H <sub>3</sub> O <sup>+</sup> + 4e <sup>-</sup> /N <sub>2</sub> O + 7H <sub>2</sub> O	0.82	0.80	1.297	0.85
ClO <sub>2</sub> + H <sub>3</sub> O <sup>+</sup> + e <sup>-</sup> /HClO <sub>2</sub> + H <sub>2</sub> O	1.08	1.07	1.277	1.10
O <sub>3</sub> + H <sub>2</sub> O + 2e <sup>-</sup> /O <sub>2</sub> + 2HO <sup>-</sup>	1.30	1.09	1.24	1.30
3O <sub>2</sub> + 4H <sub>3</sub> O <sup>+</sup> + 4e <sup>-</sup> /6H <sub>2</sub> O	0.93	0.89	1.229	0.95
N <sub>2</sub> O <sub>4</sub> + 2H <sub>3</sub> O <sup>+</sup> + 2e <sup>-</sup> /2HNO <sub>2</sub> + 2H <sub>2</sub> O	1.12	1.01	1.065	1.13
N <sub>2</sub> O <sub>4</sub> + 4H <sub>3</sub> O <sup>+</sup> + 4e <sup>-</sup> /2NO + 6H <sub>2</sub> O	0.62	0.56	1.035	0.66
HNO <sub>2</sub> + H <sub>3</sub> O <sup>+</sup> + e <sup>-</sup> /NO + 2H <sub>2</sub> O	0.93	0.93	0.983	0.95
NO <sub>3</sub> <sup>-</sup> + 4H <sub>3</sub> O <sup>+</sup> + 3e <sup>-</sup> /NO + 6H <sub>2</sub> O	0.70	0.63	0.957	0.74
NO <sub>3</sub> <sup>-</sup> + 3H <sub>3</sub> O <sup>+</sup> + 2e <sup>-</sup> /HNO <sub>2</sub> + 4H <sub>2</sub> O	0.96	0.89	0.934	0.98
HO <sub>2</sub> <sup>-</sup> + H <sub>2</sub> O + 2e <sup>-</sup> /3HO <sup>-</sup>	1.32	0.91	0.878	1.32
N <sub>2</sub> O <sup>+</sup> + 2e <sup>-</sup> /2NO <sub>2</sub>	0.65	0.61	0.867	0.69
2HNO <sub>2</sub> + 4H <sub>3</sub> O <sup>+</sup> + 4e <sup>-</sup> /H <sub>2</sub> N <sub>2</sub> O <sub>2</sub> + 6H <sub>2</sub> O	0.42	0.42	0.86	0.47
<sup>1</sup> O <sub>2</sub> + e <sup>-</sup> /O <sub>2</sub> <sup>-</sup>	0.70	0.76	0.83	0.74
ClO + H <sub>2</sub> O + 2e <sup>-</sup> /Cl + 2HO <sup>-</sup>	1.22	0.96	0.81	1.23
2NO + H <sub>2</sub> O + 2e <sup>-</sup> /N <sub>2</sub> O + 2HO <sup>-</sup>	0.91	0.72	0.76	0.94
<sup>3</sup> O <sub>2</sub> + 2H <sub>3</sub> O <sup>+</sup> + 2e <sup>-</sup> /H <sub>2</sub> O <sub>2</sub> + 2H <sub>2</sub> O	0.92	0.92	0.695	0.94
<sup>3</sup> O <sub>2</sub> + 2H <sub>2</sub> O + 4e <sup>-</sup> /4HO <sup>-</sup>	0.61	0.41	0.401	0.65
(CN) <sub>2</sub> + 2H <sub>3</sub> O <sup>+</sup> + 2e <sup>-</sup> /2HCN + 2H <sub>2</sub> O	0.06	0.12	0.373	0.14
2NO <sub>2</sub> + 3H <sub>2</sub> O + 4e <sup>-</sup> /N <sub>2</sub> O + 6HO <sup>-</sup>	0.49	0.19	0.15	0.54
NO <sub>3</sub> <sup>-</sup> + H <sub>2</sub> O + 2e <sup>-</sup> /NO <sub>2</sub> <sup>-</sup> + 2HO <sup>-</sup>	0.04	-0.20	0.01	0.12
<sup>3</sup> O <sub>2</sub> + H <sub>2</sub> O + 2e <sup>-</sup> /HO <sub>2</sub> <sup>-</sup> + HO <sup>-</sup>	-0.29	-0.28	-0.076	-0.19
<sup>3</sup> O <sub>2</sub> + 2H <sub>2</sub> O + 2e <sup>-</sup> /H <sub>2</sub> O <sub>2</sub> + 2HO <sup>-</sup>	0.10	-0.06	-0.146	0.17
<sup>3</sup> O <sub>2</sub> + e <sup>-</sup> /O <sub>2</sub> <sup>-</sup>	-0.54	-0.48	-0.16	-0.43
CO <sub>2</sub> + 2H <sub>3</sub> O <sup>+</sup> + 2e <sup>-</sup> /HCOOH + 2H <sub>2</sub> O	-0.10	-0.11	-0.199	-0.01
NO <sub>2</sub> <sup>-</sup> + H <sub>2</sub> O + e <sup>-</sup> /NO + 2HO <sup>-</sup>	-0.35	-0.74	-0.46	-0.25
2NO <sub>3</sub> + 2H <sub>2</sub> O + 2e <sup>-</sup> /N <sub>2</sub> O <sub>4</sub> + 4HO <sup>-</sup>	-0.56	-1.00	-0.85	-0.45
NO + e <sup>-</sup> /3NO <sup>-</sup>	-1.11	-1.00	-0.81	-0.96
CO <sub>2</sub> + e <sup>-</sup> /CO <sub>2</sub> <sup>-</sup>	-2.11	-1.98	-1.8	-1.90

## ADDITIONS AND CORRECTIONS

Revised Table 2

reaction couple	$E_{\text{pred}}^{\circ}$ (V)	$E_{\text{exp}}^{\circ}$ (V)	$E_{\text{pred,Old}}^{\circ}$ (V)
$2\text{NO} + \text{e}^-/\text{ONNO}^-$	$-0.1 \pm 0.3$	$0.38^b$	$-0.1 \pm 0.3$
$\text{ONNO}^- + \text{e}^-/\text{ONNO}^{2-}$	$-0.4 \pm 0.3$	$0.96^b$	$-0.4 \pm 0.3$
$2\text{NO} + \text{H}_3\text{O}^+ + \text{e}^-/\text{HONNO} + \text{H}_2\text{O}$	$0.1 \pm 0.3$	$-0.06^b$	$0.0 \pm 0.3$
$\text{HONNO} + \text{H}_3\text{O}^+ + \text{e}^-/\text{HONNOH} + \text{H}_2\text{O}$	$1.8 \pm 0.3$	$1.75^b$	$1.6 \pm 0.3$
$\text{NO} + \text{e}^-/\text{NO}^-$	$-1.0 \pm 0.3$	$-0.81^a$	$-0.9 \pm 0.3$

Revised Table 3

reaction couple	$E_{\text{pred}}^{\circ}$ (V)	$E_{\text{exp}}^{\circ}$ (V)	$E_{\text{pred,Old}}^{\circ}$ (V)
$\text{HNO} + \text{H}_3\text{O}^+ + \text{e}^-/\text{H}_2\text{NO} + \text{H}_2\text{O}$	$0.7 \pm 0.3$		$0.6 \pm 0.3$
$\text{H}_2\text{NO} + \text{H}_3\text{O}^+ + \text{e}^-/\text{H}_2\text{NOH} + \text{H}_2\text{O}$	$1.1 \pm 0.3$		$0.9 \pm 0.3$
$\text{HNO} + 2\text{H}_3\text{O}^+ + 2\text{e}^-/\text{H}_2\text{NOH} + 2\text{H}_2\text{O}$	$0.9 \pm 0.3$	$-0.7^b$	$0.8 \pm 0.3$
$\text{HNO} + \text{e}^-/\text{HNO}^-$	$-0.7-0.4-0.3$		$-0.7 \pm 0.3$
$3\text{O}_2 + \text{e}^-/\text{O}_2^-$	$-0.4 \pm 0.3$	$-0.33^a$	$-0.4 \pm 0.3$
${}^3\text{O}_2 + \text{H}_3\text{O}^+ + \text{e}^-/\text{HO}_2 + \text{H}_2\text{O}$	$-0.3 \pm 0.3$	$-0.076^c$	$-0.3 \pm 0.3$

Revised Table 4

reaction couple	$E_{\text{pred}}^{\circ}$ (V)	$E_{\text{pred,Old}}^{\circ}$ (V)
$\text{N}_2\text{O}_3^- + \text{e}^-/\text{N}_2\text{O}_3^{2-}$	$0.6 \pm 0.3$	$0.5 \pm 0.3$
$\text{HN}_2\text{O}_3 + \text{e}^-/\text{HN}_2\text{O}_3^-$	$1.1 \pm 0.3$	$0.9 \pm 0.3$

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