ADDITIONS AND CORRECTIONS

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Patrik Johansson: Intrinsic Anion Oxidation Potentials

Page 12077. In the original paper[1] prediction of anion limiting oxidation potentials (E_{ox}) was made by computing the vertical transition energy (ΔE_v) as the electronic energy difference between the anion and the corresponding neutral radical. In addition, the vertical free energy difference (ΔG_v) was computed via addition of ΔG_{solv} and further strengthened as a necessary improvement of ΔE_v by an empirical correction vs experimental data using the anion volume as a parameter (ΔG_v*). However, an incorrect data correction was made using the Li^+/Li^0 vs SHE (−3.04 V) rather than the Li^+/Li^0 counter electrode value (−1.46 V). Thus the computed data in ref 1 should be corrected by 1.58 V. A new Table 1 and Figures 2−4 are presented here. The change is uniform and thus does not change any interanionic comparisons, but clearly the comparison vs experimental data is now more favorable for the ΔE_v measure than in the original paper (Figure 3). The smallest standard deviation of ΔE_v vs E_{ox} is obtained for the VSXC functional, but clearly the freeenergy correction term ΔG_{solv} must now be severely reduced in size and in the present Figure 4 the default medium water[1] has been replaced by a solvent with a dielectric constant of 5.0 and a radius of 6.0 Å. Yet, as seen in Figure 4, the role of the free energy correction is dubious—the standard deviation in fact increases, although a smaller rms error is obtained. A volume correction does not have any substantial effect. To conclude, for a prediction of intrinsic anion oxidation potentials, the direct use of vertical transition energy (ΔE_v) as a measure seems agreeable if an acceptable computational level is used, e.g., the

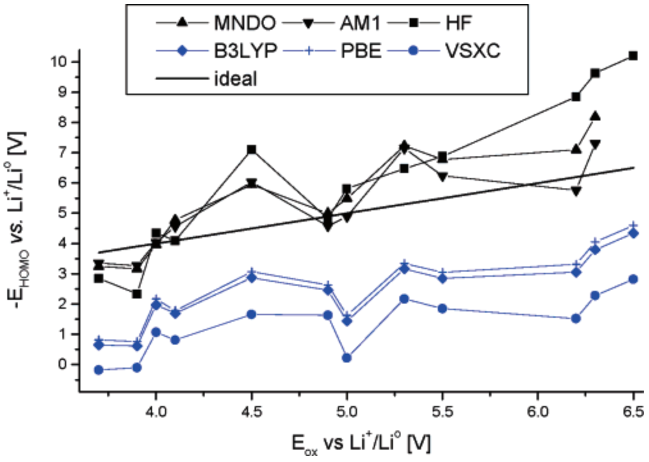

Figure 2. Updated $-E_{HOMO}$ vs E_{ox} for different computational levels.

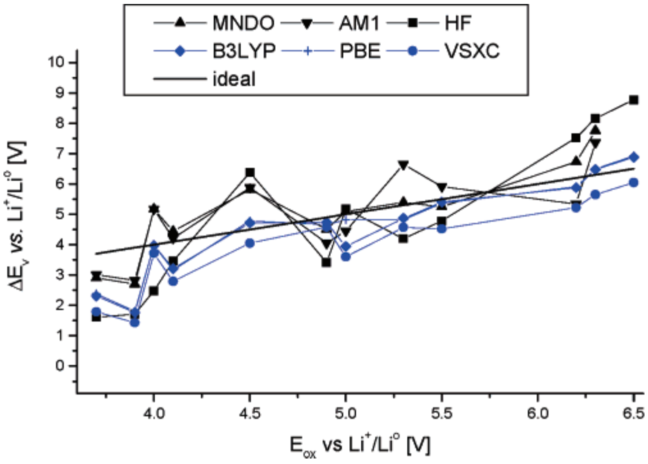

Figure 3. Updated ΔE_v vs E_{ox} for different computational levels.

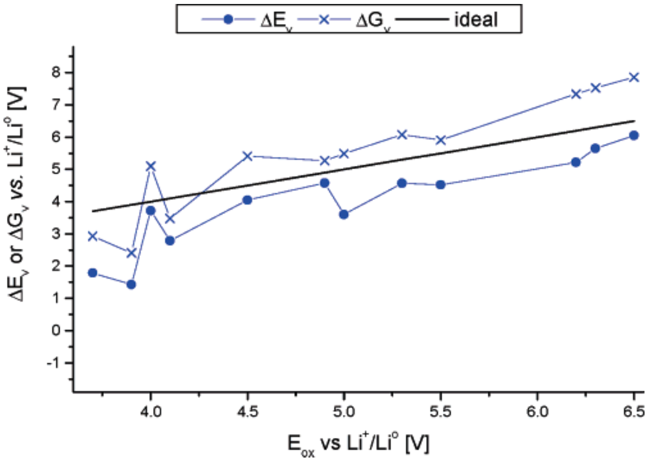

Figure 4. Updated ΔE_v and ΔG_v vs E_{ox} using the VSXC functional.

TABLE 1:

			E_{HOMO} vs Li^+/Li^0 (V)						ΔE_v vs Li^+/Li^0 (V)					
anion	E_{ox} vs Li^+/Li^0 (V)	ref	MNDO	AM1	HF	B3LYP	PBE	VSXC	MNDO	AM1	HF	B3LYP	PBE	VSXC
AsF_6^-	6.5−6.8	5, 9	n/a	n/a	−10.21	−4.34	−4.60	−2.82	n/a	n/a	8.77	6.88	6.93	6.05
PF_6^-	6.3−6.8	5, 9	−8.19	−7.31	−9.63	−3.80	−4.05	−2.28	7.75	7.36	8.16	6.47	6.49	5.65
BF_4^-	6.2−6.6	5, 9	−7.10	−5.76	−8.85	−3.05	−3.31	−1.52	6.73	5.34	7.52	5.88	5.91	5.22
$TFSI^-$	6.1−6.3, 5.3	5, 9, 10	−6.78	−6.24	−6.88	−2.85	−3.05	−1.85	5.25	5.91	4.78	5.40	5.36	4.52
$TriTFSM^-$	6.1,5.5	9, 10	−7.23	−7.15	−6.48	−3.16	−3.34	−2.17	5.39	6.65	4.20	4.87	4.83	4.57
Tf^-	5.9−6.0, 5.0	5, 9, 10	−5.49	−4.89	−5.82	−1.44	−1.63	−0.22	5.09	4.45	5.18	3.94	4.82	3.60
Id^-	4.9	13	−5.00	−4.58	−4.83	−2.46	−2.63	−1.63	4.51	4.05	3.41	4.73	4.66	4.58
BOB^-	>4.5	16	−5.95	−6.03	−7.10	−2.87	−3.07	−1.66	5.82	5.88	6.38	4.72	4.78	4.05
$4F\text{-}BBB^-$	4.1	33	−4.78	−4.56	−4.10	−1.69	−1.78	−0.81	4.44	4.21	3.46	3.21	3.17	2.79
$TADC^-$	>4.0	15	−3.96	−4.04	−4.35	−1.97	−2.17	−1.07	5.17	5.17	2.48	3.98	3.97	3.72
BNB^-	3.9	33	−3.17	−3.27	−2.34	−0.61	−0.76	0.10	2.70	2.82	1.71	1.77	1.81	1.43
BBB^-	3.7	33	−3.24	−3.35	−2.85	−0.65	−0.81	0.18	2.91	3.01	1.61	2.31	2.38	1.79

6-311+G(2df,p) basis set and the VSXC functional, and the use of (ΔG_v) does not seem entirely necessary.

Supporting Information Available: Updated Table 1S. This material is available free of charge via the Internet at http://pubs.acs.org.

References and Notes

(1) Johansson, P. *J. Phys. Chem. A* **2006**, *110*, 12077−12080.

10.1021/jp070202i