Supplementary Information for

Transient Methods for Understanding the Properties of Strongly Oxidizing Radicals

Dmitry E. Polyansky

Chemistry Division, Brookhaven National Laboratory, Upton, NY 11973-5000, USA.

*email: dep@bnl.gov

Table S1. Data used for plotting Figure 2.

Compound	Ip, V	E°, V
mesitylene	8.87	1.47
p-xylene	8.8	1.47
1,2,4-trimethylbenzene	8.69	1.49
durene	8.2	1.35
naphthalene	8.15	1.26
m-terphenyl	8.01	1.39
hexamethylbenzene	7.9	1.2
biphenyl	7.89	1.33
triphenylene	7.86	1.26
phenanthrene	7.85	1.22
fluorene	7.78	1.13
9-anthraldehyde	7.69	1.18
chrysene	7.59	1.13
9,10-dibromoanthracene	7.58	1.09
anthracene	7.45	0.94
pyrene	7.41	0.85
coronene	7.29	0.82
9-anthracenemethanol	7.21	0.75

Table S2. Data used for plotting Figure 6.

$E°$(equilibrium), V	Compound	$E°_{min}$(echem)	$E°_{max}$(echem)	$E°_{av}$(echem)	Standard deviation($E°$_echem)
1.254	indole	1.12	1.61	1.365	0.34648
1.184	N-methylindole	1.1	1.58	1.34	0.33941
1.146	4-cyano-N,N-dimethylaniline	1.05	1.18	1.115	0.09192
1.108	4-trifluoromethyl-N,N-dimethylaniline	1.11	1.11	1.11	0
1.106	2-methylindole	0.9	1.25	1.075	0.24749
1.085	3-methylindole	0.95	1.26	1.105	0.2192
1.058	4-methylcarboxy-N,N-dimethylaniline	0.98	0.98	0.98	0
1.038	aniline	0.8	1.28	1.04	0.33941
0.954	diphenylmethylamine	0.8	1.05	0.925	0.17678
0.928	N-methylaniline	0.59	1.03	0.81	0.31113
0.916	4-bromo-N,N-dimethylaniline	0.86	0.96	0.91	0.07071
0.851	N,N-dimethylaniline	0.64	1.01	0.825	0.26163

Table S3. Data used for plotting Figure 7A. Hammett parameters σ_p^+ are sourced from C. Hansch, A. Leo and R. W. Taft, *Chem. Rev.*, 1991, 91, 165-195.

$\Sigma\sigma_p^+$	Compound	$E^{o\prime}$, V	$E^{o\prime}$, V	$E^{o\prime}$, V
0	benzene	2.48		
0.11	Cl benzene	2.46		
-0.26	tBu benzene		2.28	
-0.31	toluene	2.26		
-0.62	m-xylene	2.1		
-0.62	o-xylene	2.09		
-0.52	1,4 di tBu benzene		2.06	
-0.93	mesitylene	2.05		
-0.78	1,3,5 tri tBu benzene		2.04	
-0.62	p-xylene	2.01		
-0.93	1,2,4-trimethylbenzene	1.905		
-1.24	1,2,3,4-tetramethylbenzene	1.825		
-1.24	1,2,3,5-tetramethylbenzene	1.82		
-1.24	durene	1.75		
-1.86	hexamethylbenzene	1.59		
-1.55	pentamethylbenzene	1.71		
-0.78	methoxybenzene			1.77
-1.56	1,3-dimethoxybenzene			1.55
-2.34	1,3,5-trimethoxybenzene			1.54
-1.56	1,2-dimethoxybenzene			1.42
-2.34	1,2,3-trimethoxybenzene			1.39
-1.87	1,2-dimethoxy-4-methylbenzene			1.29
-1.56	1,4-dimethoxybenzene			1.23
-3.12	1,2,3,5-tetramethoxybenzene			1.09
-2.34	1,2,4-trimethoxybenzene			1.08

Table S4. Data used for plotting Figure 7B. Hammett parameters σ^{+}_{p} are sourced from C. Hansch, A. Leo and R. W. Taft, *Chem. Rev.*, 1991, 91, 165-195.

$\Sigma\sigma^{+}_{p}$	Compound	$E^{o\prime}$, V	$E^{o\prime}$, V	$E^{o\prime}$, V	$E^{o\prime}$, V
0	biphenyl	1.95			
1.09	4-CO2Bu, 4'-CF3			2.35	
0.96	4-CO2Bu, 4'-CO2Bu			2.28	
0.49	4-CO2Me			2.1	
0.42	3-CO2H			2.06	
0.3	4-Br, 4'-Br				1.98
-0.19	4-OCOMe			1.81	
-0.31	4-Me	1.795			
-0.62	3-Me, 3'-Me	1.85			
-0.62	4-Me, 4'-Me	1.66			
-0.93	3,4,4′-trimethyl	1.62			
-1.24	3,3′,4,4′-tetramethyl	1.581			
-1.56	2,2′-dimethoxybiphenyl		1.6		
-0.78	4-methoxybiphenyl		1.5		
-1.09	4-methoxy-4′-methylbiphenyl		1.43		
-1.56	3,4-dimethoxybiphenyl		1.3		
-1.56	4,4′-dimethoxybiphenyl		1.27		
-1.87	3,4-dimethoxy-4′-methylbiphenyl		1.25		
-2.34	3,4,4′-trimethoxybiphenyl		1.16		
-3.12	3,3′,4,4′-tetramethoxybiphenyl		1.11		

Table S5. Data used for plotting Figure 8.

benzenes	$E^{o\prime}$, V	biphenyls	$E^{o\prime}$, V
H	2.48	H	1.95
1-Me	2.26	4-Me	1.796
1,4-(Me)2	2.01	4,4’-(Me)2	1.67
1-MeO	1.773	4-MeO	1.503
1,2-(MeO)2	1.415	3,4-(MeO)2	1.303
1,2-(MeO)2-4-Me	1.286	3,4-(MeO)2-4’-Me	1.252
1,4-(MeO)2	1.278	4,4’-(MeO)2	1.266
1,2,4-(MeO)3	1.08	3,4,4’-(MeO)3	1.161

Table S6. Data used for plotting Figure 9.

Compound	Ip, V	$E^{o\prime}$, eV	Compound	Ip, V	$E^{o\prime}$, eV
benzene	9.24	2.1	acetonitrile	12.2	4.14728
toluene	8.828	1.88	carbon tetrachloride	11.47	3.64183
p-xylene	8.44	1.63	dichloromethane	11.33	3.54489
biphenyl	8.16	1.57	dichloroethane	11.07	3.36487
durene	8.06	1.37	hexane	10.13	2.71401
HMB	7.85	1.2	benzonitrile	9.73	2.43705
acetanilide	8.3	1.3	THF	9.4	2.20856
1,2,4-trimethylbenzene	8.69	1.49	DMF	9.13	2.02161
durene	8.2	1.35	cyclohexane	9.88	2.54091
naphthalene	8.15	1.26	methanol	10.84	3.20562
m-terphenyl	8.01	1.39	acetic acid	10.65	3.07406
hexamethylbenzene	7.9	1.2	water	12.6	4.42424
biphenyl	7.89	1.33			
triphenylene	7.86	1.26			
phenanthrene	7.85	1.22			
fluorene	7.78	1.13			
9-anthraldehyde	7.69	1.18			
chrysene	7.59	1.13			
9,10-dibromoanthracene	7.58	1.09			
anthracene	7.45	0.94			
pyrene	7.41	0.85			
coronene	7.29	0.82			
9-anthracenemethanol	7.21	0.75			
N,N-dimethylaniline	7.12	0.47			
aniline	7.72	0.658			
indole	7.76	0.874			
triphenylamine	6.8	0.516			

3-methylindole	7.5	0.7			
2-methylindole	7.671	0.726			
diphenylmethylamine	7	0.574			
N-methylaniline	7.32	0.548			