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Computational Electrochemistry: Prediction of Liquid-Phase Reduction Potentials

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Supporting Information

Table 1. Calculated and experimental adiabatic ionization energies (in electron volts).[a]

	Expt	G3(MP2,CC)(+)[b]	G3MP2B3	ROCBS-QB3	B3LYP[b,c]	BMK[b,c]	B971[b,c]	M05-2X[b,c]	M06-2X[b,c]
isopentane	10.32	10.08 (240)	10.06 (259)	10.03 (288)	9.58 (740)	9.75 (570)	9.52 (800)	9.72 (600)	9.86 (460)
difluorodichloromethane	12	11.77 (230)	11.78 (222)	11.74 (263)	11.47 (530)	11.65 (350)	11.37 (630)	11.79 (210)	11.78 (220)
dichloromethane	11.33	11.12 (210)	11.15 (180)	11.08 (247)	10.9 (430)	11.04 (290)	10.82 (510)	11.1 (230)	11.13 (200)
methylamine	8.9	9.06 (160)	9.07 (166)	9.05 (148)	8.91 (10)	8.89 (10)	8.82 (80)	9.01 (110)	9.04 (140)
difluoromethane	12.71	12.82 (110)	12.83 (116)	12.77 (63)	12.41 (300)	12.52 (190)	12.26 (450)	12.76 (50)	12.64 (70)
cis-2-butene	9.11	9.21 (100)	9.21 (96)	9.17 (61)	8.79 (320)	8.82 (290)	8.71 (400)	8.85 (260)	8.9 (210)
trans-2-butene	9.1	9.21 (110)	9.21 (108)	9.17 (74)	8.79 (310)	8.81 (290)	8.71 (390)	8.85 (250)	8.9 (200)
bicyclo[1.1.0]butane	8.7	8.82 (120)	8.83 (132)	8.77 (67)	8.6 (100)	8.42 (280)	8.45 (250)	8.73 (30)	8.85 (150)
1-methyl-1,3-cyclopentadiene	8.4	8.22 (180)	8.25 (153)	8.17 (232)	7.81 (590)	7.85 (550)	7.73 (670)	7.91 (490)	7.99 (410)
chlorotrifluoromethane	12.6	12.47 (130)	12.45 (151)	12.55 (46)	12.25 (350)	12.47 (130)	12.2 (400)	12.54 (60)	12.46 (140)
tetrachloromethane	11.47	11.62 (150)	11.53 (62)	11.35 (116)	10.99 (480)	11.4 (70)	10.95 (520)	11.54 (70)	11.58 (110)
o-dichlorobenzene	9.06	9.13 (70)	9.15 (91)	9.14 (75)	8.81 (250)	8.97 (90)	8.74 (320)	9.03 (30)	9.08 (20)
trichloromethane	11.37	11.35 (20)	11.42 (53)	11.32 (50)	10.97 (400)	11.31 (60)	10.92 (450)	11.4 (30)	11.45 (80)
fluorotrichloromethane	11.68	11.69 (10)	11.69 (14)	11.60 (84)	11.21 (470)	11.95 (270)	11.15 (530)	11.68 (0)	11.72 (40)
acetylene	11.4	11.43 (30)	11.45 (46)	11.43 (32)	11.26 (140)	11.24 (160)	11.17 (230)	11.28 (120)	11.28 (120)
hydrogen cyanide	13.6	13.61 (10)	13.61 (8)	13.63 (28)	13.49 (110)	13.51 (90)	13.38 (220)	13.55 (50)	13.52 (80)
carbon monoxide	14.014	14.03 (16)	14.03 (19)	14.05 (37)	14.18 (166)	14.27 (256)	14.11 (96)	14.41 (396)	14.12 (106)
formaldehyde	10.88	10.88 (0)	10.90 (21)	10.92 (37)	10.81 (70)	10.79 (90)	10.7 (180)	10.89 (10)	10.9 (20)
propene	9.73	9.81 (80)	9.81 (83)	9.78 (45)	9.46 (270)	9.46 (270)	9.38 (350)	9.48 (250)	9.51 (220)
carbon dioxide	13.777	13.76 (17)	13.77 (6)	13.79 (8)	13.74 (37)	13.91 (133)	13.63 (147)	14.08 (303)	13.97 (193)
ethylene oxide	10.56	10.57 (10)	10.59 (26)	10.62 (59)	10.41 (150)	10.46 (100)	10.31 (250)	10.58 (20)	10.59 (30)
acetaldehyde	10.229	10.24 (11)	10.25 (20)	10.26 (34)	10.08 (149)	10.09 (139)	9.97 (259)	10.21 (19)	10.21 (19)
formic acid	11.33	11.31 (20)	11.32 (10)	11.37 (35)	11.2 (130)	11.21 (120)	11.08 (250)	11.31 (20)	11.28 (50)
fluoroethene	10.36	10.4 (40)	10.40 (38)	10.38 (24)	10.17 (190)	10.13 (230)	10.06 (300)	10.19 (170)	10.17 (190)
methanethiol	9.439	9.44 (1)	9.44 (2)	9.43 (4)	9.33 (109)	9.36 (79)	9.27 (169)	9.36 (79)	9.41 (29)
chloromethane	11.26	11.26 (0)	11.26 (2)	11.27 (7)	11.09 (170)	11.18 (80)	11.02 (240)	11.2 (60)	11.22 (40)
cyanogen chloride	12.36	12.32 (40)	12.30 (57)	12.36 (3)	12.09 (270)	12.28 (80)	12.01 (350)	12.3 (60)	12.33 (30)
chloroethene	9.99	10.03 (40)	10.03 (36)	10.01 (19)	9.76 (230)	9.83 (160)	9.69 (300)	9.81 (180)	9.85 (140)

carbonic difluoride	13.04	13 (40)	13.00 (44)	13.07 (32)	12.9 (140)	12.99 (50)	12.75 (290)	13.09 (50)	13.02 (20)
1-buten-3-yne	9.58	9.64 (60)	9.66 (84)	9.60 (19)	9.24 (340)	9.29 (290)	9.16 (420)	9.35 (230)	9.41 (170)
2-propenenitrile	10.91	10.98 (70)	10.99 (81)	10.94 (29)	10.57 (340)	10.67 (240)	10.49 (420)	10.75 (160)	10.77 (140)
cyclobutene	9.43	9.52 (90)	9.52 (88)	9.49 (56)	9.15 (280)	9.17 (260)	9.07 (360)	9.19 (240)	9.23 (200)
methyloxirane	10.22	10.25 (30)	10.26 (35)	10.29 (68)	10.03 (190)	10.1 (120)	9.93 (290)	10.23 (10)	10.24 (20)
oxetane	9.65	9.72 (70)	9.73 (79)	9.73 (83)	9.4 (250)	9.48 (170)	9.3 (350)	9.65 (0)	9.62 (30)
acetic acid	10.65	10.64 (10)	10.65 (0)	10.69 (37)	10.44 (210)	10.48 (170)	10.32 (330)	10.61 (40)	10.58 (70)
1,1-difluoroethene	10.29	10.33 (40)	10.33 (36)	10.34 (46)	10.13 (160)	10.12 (170)	10 (290)	10.22 (70)	10.18 (110)
1-penten-3-yne	9	9.05 (50)	9.07 (73)	8.99 (6)	8.58 (420)	8.66 (340)	8.5 (500)	8.73 (270)	8.8 (200)
1,3-cyclopentadiene	8.57	8.64 (70)	8.67 (99)	8.59 (21)	8.27 (300)	8.3 (270)	8.19 (380)	8.35 (220)	8.42 (150)
2-methyl-1-buten-3-yne	9.25	9.3 (50)	9.31 (63)	9.26 (7)	8.85 (400)	8.93 (320)	8.78 (470)	9 (250)	9.05 (200)
pyrrole	8.207	8.25 (43)	8.27 (68)	8.24 (36)	8.1 (107)	8.12 (87)	8.02 (187)	8.17 (37)	8.24 (33)
furan	8.88	8.92 (40)	8.95 (65)	8.91 (30)	8.73 (150)	8.74 (140)	8.63 (250)	8.79 (90)	8.84 (40)
1H-imidazole	8.81	8.86 (50)	8.86 (51)	8.85 (39)	8.72 (90)	8.73 (80)	8.64 (170)	8.77 (40)	8.84 (30)
tetrahydrofuran	9.4	9.48 (80)	9.49 (89)	9.49 (94)	9.14 (260)	9.21 (190)	9.04 (360)	9.4 (0)	9.36 (40)
neopentane	10.3	10.23 (70)	10.22 (81)	10.19 (112)	9.76 (540)	9.92 (380)	9.71 (590)	9.88 (420)	10.01 (290)
pentane	10.28	10.26 (20)	10.25 (25)	10.20 (77)	9.84 (440)	9.85 (430)	9.71 (570)	9.96 (320)	10.02 (260)
carbon disulfide	10.073	10.06 (13)	10.11 (39)	10.05 (20)	10.03 (43)	10.11 (37)	10.01 (63)	10.13 (57)	10.15 (77)
benzene	9.24	9.32 (76)	9.34 (100)	9.33 (87)	9.06 (184)	9.11 (134)	8.99 (254)	9.16 (84)	9.21 (34)
pyridazine	8.74	8.78 (40)	8.80 (61)	8.68 (55)	8.52 (220)	8.59 (150)	8.45 (290)	8.67 (70)	8.69 (50)
thiophene	8.86	8.92 (60)	8.94 (84)	8.91 (47)	8.71 (150)	8.75 (110)	8.64 (220)	8.83 (30)	8.89 (30)
hexane	10.13	10.07 (60)	10.06 (70)	9.93 (204)	9.61 (520)	9.65 (480)	9.49 (640)	9.78 (350)	9.83 (300)
2,5-norbornadiene	8.38	8.45 (70)	8.48 (97)	8.38 (4)	8.06 (320)	8.11 (270)	7.96 (420)	8.22 (160)	8.31 (70)
toluene	8.828	8.91 (82)	8.95 (118)	8.91 (84)	8.59 (238)	8.65 (178)	8.52 (308)	8.72 (108)	8.78 (48)
aniline	7.72	7.8 (80)	7.86 (136)	7.75 (30)	7.55 (170)	7.57 (150)	7.47 (250)	7.69 (30)	7.74 (20)
phenol	8.49	8.59 (100)	8.62 (131)	8.58 (86)	8.31 (180)	8.34 (150)	8.22 (270)	8.46 (30)	8.49 (0)
1,1-dichloroethene	9.81	9.85 (40)	9.84 (33)	9.83 (22)	9.53 (280)	9.65 (160)	9.46 (350)	9.64 (170)	9.67 (140)
cis-1,2-dichloroethene	9.66	9.68 (20)	9.67 (6)	9.65 (7)	9.38 (280)	9.52 (140)	9.31 (350)	9.5 (160)	9.55 (110)
trans-1,2-dichloroethene	9.64	9.65 (10)	9.63 (6)	9.62 (21)	9.33 (310)	9.48 (160)	9.26 (380)	9.46 (180)	9.51 (130)
tetrafluoroethene	10.14	10.14 (0)	10.13 (14)	10.15 (5)	9.88 (260)	9.88 (260)	9.69 (450)	10.06 (80)	10 (140)

styrene	8.464	8.54 (76)	8.62 (154)	8.52 (53)	8.16 (304)	8.24 (224)	8.09 (374)	8.33 (134)	8.4 (64)
chlorobenzene	9.07	9.14 (70)	9.18 (111)	9.13 (65)	8.84 (230)	8.95 (120)	8.77 (300)	9.01 (60)	9.06 (10)
m-difluorobenzene	9.33	9.4 (70)	9.42 (93)	9.41 (75)	9.14 (190)	9.19 (140)	9.03 (300)	9.33 (0)	9.34 (10)
o-difluorobenzene	9.29	9.36 (70)	9.38 (93)	9.38 (92)	9.09 (200)	9.14 (150)	8.98 (310)	9.28 (10)	9.29 (0)
p-difluorobenzene	9.1589	9.22 (61)	9.24 (78)	9.24 (79)	8.95 (209)	8.98 (179)	8.83 (329)	9.13 (29)	9.12 (39)
chlorotrifluoroethene	9.81	9.85 (40)	9.83 (18)	9.84 (31)	9.56 (250)	9.63 (180)	9.42 (390)	9.74 (70)	9.71 (100)
trichloroethene	9.46	9.5 (40)	9.48 (24)	9.47 (10)	9.17 (290)	9.34 (120)	9.1 (360)	9.33 (130)	9.37 (90)
m-dichlorobenzene	9.1	9.21 (110)	9.23 (135)	9.20 (102)	8.86 (240)	9.03 (70)	8.8 (300)	9.09 (10)	9.14 (40)
p-dichlorobenzene	8.92	9.01 (90)	9.02 (97)	9.00 (80)	8.67 (250)	8.83 (90)	8.6 (320)	8.89 (30)	8.93 (10)
tetrachloroethene	9.326	9.35 (24)	9.33 (6)	9.31 (11)	9 (326)	9.2 (126)	8.93 (396)	9.19 (136)	9.23 (96)
1,2,4-trichlorobenzene	9.04	9.08 (40)	9.09 (51)	9.07 (33)	8.72 (320)	8.92 (120)	8.66 (380)	8.97 (70)	9.01 (30)
dimethylamine	8.24	8.36 (115)	8.36 (121)	8.34 (96)	8.14 (100)	8.13 (110)	8.06 (180)	8.27 (30)	8.31 (70)
piperidine	8.03	8.09 (55)	8.08 (51)	8.03 (5)	7.81 (220)	7.81 (220)	7.72 (310)	7.97 (60)	8 (30)
indole	7.7602	7.83 (65)	7.91 (153)	7.79 (34)	7.58 (180)	7.65 (110)	7.51 (250)	7.78 (20)	7.83 (70)
MAD		64	74	61	258	187	343	124	105
AD_{max}		240	260	288	740	570	800	600	460

[a] Absolute deviations in parentheses (mV) [b] A modified version of G3(MP2)-RAD where calculations involving the 6-31G(d) basis set is replaced with the 6-31+G(d) basis set. [c] DFT calculations were carried out using the 6-311+G(3df,2p) basis set.

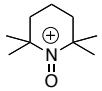
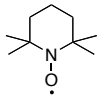
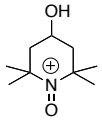
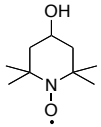
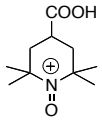
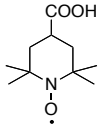
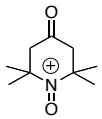
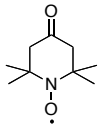
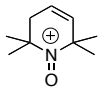
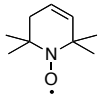
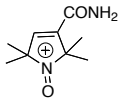
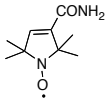
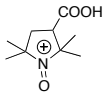
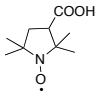
Table 2. Calculated and experimental adiabatic electron affinities (in electron volts).[a]

Molecule	Expt	G3(MP2,CC)(+)[b]		G3MP2B3		ROCBS-QB3		B3LYP[b,c]		BMK[b,c]		B971[b,c]		M05-2X[b,c]		M06-2X[b,c]	
allyl radical	0.481	0.48	(1)	0.54	(64)	0.43	(48)	0.52	(39)	0.42	(61)	0.44	(41)	0.47	(11)	0.57	(89)
propionic acid radical	3.43	3.34	(90)	3.33	(100)	3.31	(119)	3.17	(260)	3.3	(130)	3.06	(370)	3.53	(100)	3.44	(10)
ethylperoxy radical	1.186	1.17	(16)	1.19	(1)	1.20	(12)	1.08	(106)	0.96	(226)	0.92	(266)	1.03	(156)	1.03	(156)
ethylthio radical	1.953	2.00	(47)	1.99	(39)	1.98	(25)	1.89	(63)	1.89	(63)	1.83	(123)	1.91	(43)	1.92	(33)
perfluoro-tert-butyl radical	3.55	3.54	(10)	3.54	(14)	3.56	(12)	3.57	(20)	3.48	(70)	3.39	(160)	3.67	(120)	3.54	(10)
methanoic acid radical	3.47	3.29	(180)	3.30	(173)	3.28	(195)	3.14	(330)	3.27	(200)	3.02	(450)	3.5	(30)	3.41	(60)
methoxy radical	1.572	1.53	(42)	1.56	(13)	1.56	(14)	1.5	(72)	1.37	(202)	1.39	(182)	1.44	(132)	1.43	(142)
methylperoxyl radical	1.161	1.18	(19)	1.17	(8)	1.18	(21)	0.96	(201)	0.78	(381)	0.79	(371)	0.88	(281)	1.01	(151)
methyl thiyl radical	1.867	1.90	(33)	1.89	(27)	1.88	(13)	1.81	(57)	1.82	(47)	1.76	(107)	1.82	(47)	1.84	(27)
amidogen radical	0.771	0.68	(91)	0.74	(29)	0.70	(73)	0.7	(71)	0.56	(211)	0.59	(181)	0.63	(141)	0.6	(171)
hydroxy radical	1.827	1.68	(147)	1.79	(34)	1.76	(70)	1.76	(67)	1.6	(227)	1.62	(207)	1.65	(177)	1.58	(247)
tert-butoxy radical	1.909	1.93	(21)	1.98	(69)	1.96	(51)	1.83	(79)	1.69	(219)	1.73	(179)	1.78	(129)	1.78	(129)
ter-butyl thiyl radical	2.07	2.22	(150)	2.17	(100)	2.14	(75)	2.03	(40)	2.03	(40)	1.98	(90)	2.06	(10)	2.07	(0)
nitrogen dioxide	2.273	2.29	(15)	2.29	(12)	2.26	(10)	2.23	(43)	2.31	(37)	2.09	(183)	2.36	(87)	2.31	(37)
nitrogen trioxide	3.937	4.05	(113)	3.99	(58)	3.92	(14)	3.88	(57)	4.24	(303)	3.75	(187)	4.46	(523)	4.38	(443)
phenoxyl radical	2.253	2.18	(69)	2.42	(166)	2.24	(10)	2.22	(33)	2.2	(53)	2.14	(113)	2.32	(67)	2.33	(77)
phenylthiyl radical	2.46	2.41	(51)	2.77	(307)	2.74	(277)	2.71	(250)	2.72	(260)	2.66	(200)	2.74	(280)	2.74	(280)
hydroperoxy radical	1.078	1.01	(65)	1.06	(17)	1.06	(19)	0.97	(108)	0.83	(248)	0.78	(298)	0.9	(178)	0.87	(208)
cyanogen radical	3.862	3.91	(44)	3.90	(34)	3.89	(31)	4.05	(188)	4.19	(328)	3.95	(88)	4.26	(398)	4.07	(208)
2,3-dichloro-napthoquinone	2.21	2.21	(0)	2.24	(31)			2.42	(210)	2.34	(130)	2.31	(100)	2.46	(250)	2.39	(180)
2,6-dichlorobenzonitrile	0.698	0.67	(28)	0.66	(41)	0.71	(10)	0.83	(132)	0.74	(42)	0.74	(42)	0.79	(92)	0.78	(82)
2,6-dichlorobenzoquinone	2.48	2.43	(50)	2.47	(11)	2.53	(50)	2.7	(220)	2.62	(140)	2.59	(110)	2.75	(270)	2.65	(170)
5f-benzonitrile	1.08	1.06	(20)	1.06	(22)	1.11	(31)	1.09	(10)	0.94	(140)	0.92	(160)	1.09	(10)	1	(80)
acetophenone	0.334	0.25	(84)	0.26	(70)	0.29	(44)	0.43	(96)	0.25	(84)	0.32	(14)	0.36	(26)	0.34	(6.1)
benzaldehyde	0.39	0.35	(40)	0.35	(39)	0.40	(12)	0.56	(170)	0.39	(0)	0.44	(50)	0.49	(100)	0.47	(80)
benzonitrile	0.256	0.07	(186)	0.14	(112)	0.10	(159)	0.26	(4)	0.12	(136)	0.16	(96)	0.19	(66)	0.19	(66)
benzoquinone	1.86	1.87	(10)	1.90	(42)	1.97	(110)	2.18	(320)	2.04	(180)	2.05	(190)	2.2	(340)	2.11	(250)

maleic anhydride	1.44	1.43	(10)	1.44	(2)	1.48	(45)	1.71	(270)	1.56	(120)	1.57	(130)	1.71	(270)	1.62	(180)
1-trifluoromethyl-3-nitrobenzene	1.41	1.37	(40)	1.28	(130)	1.48	(73)	1.68	(270)	1.62	(210)	1.53	(120)	1.67	(260)	1.6	(190)
1-chloro-3-nitrobenzene	1.28	1.25	(30)	1.15	(126)	1.35	(66)	1.54	(260)	1.5	(220)	1.41	(130)	1.53	(250)	1.47	(190)
methylbenzoquinone	1.85	1.81	(40)	1.84	(7)	1.90	(52)	2.08	(230)	1.94	(90)	1.96	(110)	2.1	(250)	2.02	(170)
1-fluoro-3-nitrobenzene	1.206	1.19	(16)	1.11	(99)	1.28	(71)	1.48	(274)	1.43	(224)	1.33	(124)	1.48	(274)	1.41	(204)
1,2-dinitrobenzene	1.66	1.5	(160)	1.49	(172)	1.65	(6)	2.04	(380)	1.89	(230)	1.9	(240)	1.84	(180)	1.77	(110)
1-chloro-2-nitrobenzene	1.16	1.14	(20)	0.99	(174)	1.20	(36)	1.42	(260)	1.35	(190)	1.26	(100)	1.41	(250)	1.32	(160)
1-fluoro-2-nitro-benzene	1.08	1.06	(20)	0.96	(119)	1.15	(72)	1.35	(270)	1.29	(210)	1.2	(120)	1.34	(260)	1.27	(190)
1,4-dicyanotetrafluorobenzene	1.89	1.84	(50)	1.84	(54)	1.93	(36)	2.1	(210)	2	(110)	1.96	(70)	2.14	(250)	2.05	(160)
phthalic anhydride	1.245	1.2	(45)	1.22	(25)	1.26	(13)	1.42	(175)	1.27	(25)	1.3	(55)	1.4	(155)	1.34	(95)
1,3-dinitrobenzene	2	1.95	(50)	1.93	(72)	2.09	(88)	2.43	(430)	2.35	(350)	2.29	(290)	2.31	(310)	2.24	(240)
sulphur dioxide	1.107	1.11	(3)	1.10	(3)	1.18	(73)	1.39	(283)	1.21	(103)	1.22	(113)	1.43	(323)	1.29	(183)
tetrachloromethane	1.14	1.18	(40)	1.00	(135)	1.06	(78)	1.47	(330)	0.76	(380)	1.27	(130)	0.66	(480)	1.13	(10)
carbon dioxide	-0.6	-0.56	(35)	-0.61	(12)	-0.55	(50)	-0.34	(260)	-0.59	(10)	-0.54	(60)	-0.5	(100)	-0.57	(30)
MAD			53		67		57		174		162		155		187		134
AD_{max}			186		308		277		430		381		450		523		443

[a] Absolute deviations in parentheses (mV) [b] A modified version of G3(MP2)-RAD where calculations involving the 6-31G(d) basis set is replaced with the 6-31+G(d) basis set. [c] DFT calculations were carried out using the 6-311+G(3df,2p) basis set.

Table 3. Calculated[a] and experimental one-electron standard reduction potentials of nitroxides and related compounds in aqueous solution at 298 K with respect to the standard hydrogen electrode (SHE).[b]

Ox	**Red**	Expt	UAKS	UAHF	SMD	COSMO-RS
$NH_2OH^{+\cdot}$	NH_2OH	1.3[1]	1.00 (0.30)	0.92 (0.38)	1.60 (0.30)	1.11 (0.19)
		0.74[2]	0.78 (0.04)	0.58 (0.16)	0.62 (0.12)	0.90 (0.16)
		0.825[2]	0.76 (0.06)	0.56 (0.26)	0.66 (0.16)	1.00 (0.17)
		0.805[3]	0.80 (0.01)	0.57 (0.23)	0.69 (0.12)	1.01 (0.20)
		0.918[3]	0.93 (0.01)	0.70 (0.21)	0.75 (0.17)	1.15 (0.23)
		0.795[3]	0.81 (0.06)	0.61 (0.19)	0.67 (0.12)	0.94 (0.15)
		0.955[3]	1.02 (0.06)	0.79 (0.17)	0.80 (0.16)	1.10 (0.15)
		0.87[3]	0.93 (0.06)	0.70 (0.17)	0.77 (0.10)	1.09 (0.22)
		MAD	0.04	0.20	0.13	0.18
		AD_{max}	0.06	0.26	0.17	0.23

[a] Based on cycle A in Figure 2. Gas phase calculations were carried out on the G3(MP2,CC)(+) level of theory and solvation free energies were obtained using solution-phase optimized geometries.
[b] All calculations reported are based on the reference value of E°_{abs}(SHE) = 4.28 V with the exception of CPCM-UAHF model where E°_{abs}(SHE) = 4.47 V. Absolute deviations in parentheses (V).

Table 4. Calculated[a] and experimental one-electron standard reduction potentials of phenols and related compounds in aqueous solution at 298 K with respect to the standard hydrogen electrode (SHE).[b]

Ox	**Red**	Expt	UAKS	UAHF	SMD	COSMO-RS
$PhO^{\cdot}$	PhO^{-}	0.79[4]	0.42 (0.37)	0.53 (0.26)	0.32 (0.47)	0.60 (0.19)
4F-$PhO^{\cdot}$	4F-PhO^{-}	0.76[4]	0.32 (0.44)	0.43 (0.33)	0.21 (0.55)	0.52 (0.24)
4CN-$PhO^{\cdot}$	4CN-PhO^{-}	1.12[4]	0.95 (0.17)	0.97 (0.15)	0.78 (0.34)	1.16 (0.04)
4$COCH_3$-$PhO^{\cdot}$	4$COCH_3$-PhO^{-}	1.00[4]	0.83 (0.17)	0.92 (0.08)	0.72 (0.28)	1.10 (0.10)
4NO_2-$PhO^{\cdot}$	4NO_2-PhO^{-}	1.22[4]	0.96 (0.26)	0.95 (0.27)	0.86 (0.36)	1.24 (0.02)
4NMe_2-$PhO^{\cdot}$	4NMe_2-PhO^{-}	0.174[5]	-0.12 (0.29)	0.19 (0.01)	-0.22 (0.40)	-0.02 (0.19)
4MeO-$PhO^{\cdot}$	4MeO-PhO^{-}	0.54[4]	0.26 (0.28)	0.45 (0.09)	0.15 (0.39)	0.41 (0.13)
4OH-$PhO^{\cdot}$	4OH-PhO^{-}	0.45[4]	0.22 (0.23)	0.42 (0.03)	0.15 (0.30)	0.39 (0.06)
1-naphthol$^{\cdot}$	1-naphthol^{-}	0.59[6]	0.33 (0.26)	0.45 (0.14)	0.21 (0.38)	0.42 (0.17)
$PhOH^{\cdot+}$	PhOH	1.5[7]	2.02 (0.52)	1.82 (0.32)	1.88 (0.38)	1.95 (0.45)
4MeO-$PhOH^{\cdot+}$	4MeO-PhOH	1.1[7]	1.45 (0.35)	1.28 (0.18)	1.36 (0.26)	1.45 (0.35)
OH-$PhOH^{\cdot+}$	OH-Ph-OH	1.1[7]	1.45 (0.35)	1.28 (0.18)	1.41 (0.31)	1.39 (0.29)
$PhS^{\cdot}$	PhS^{-}	0.69[8]	0.56 (0.13)	0.53 (0.16)	0.26 (0.43)	0.26 (0.43)
4MeO-$PhS^{\cdot}$	4MeO-PhS^{-}	0.57[8]	0.38 (0.19)	0.45 (0.12)	0.06 (0.51)	0.08 (0.49)
4NH_2-$PhS^{\cdot}$	4NH_2-PhS^{-}	0.36[8]	0.15 (0.21)	0.35 (0.01)	-0.13 (0.49)	-0.14 (0.50)
$HS^{\cdot}$	HS^{-}	1.15[9]	0.97 (0.18)	0.86 (0.29)	0.64 (0.51)	0.71 (0.44)
$CH_3S^{\cdot}$	CH_3S^{-}	0.73[5]	0.49 (0.24)	0.41 (0.32)	0.09 (0.64)	0.13 (0.60)
Semiquinone ($HQ^{\cdot}$)	$HQ^{\cdot-}$	0.099[10]	-0.31 (0.41)	-0.46 (0.56)	-0.28 (0.38)	0.22 (0.12)
Me-HQ	Me-$HQ^{\cdot-}$	0.023[10]	-0.39 (0.41)	-0.52 (0.55)	-0.34 (0.36)	0.13 (0.11)
235Me_3HQ	235Me3$HQ^{\cdot-}$	-0.165[10]	-0.57 (0.41)	-0.70 (0.53)	-0.51 (0.35)	-0.11 (0.05)
Tetramethyl-HQ	Tetramethyl-$HQ^{\cdot-}$	-0.235[11]	-0.68 (0.45)	-0.80 (0.57)	-0.62 (0.38)	-0.28 (0.04)
2-methyl-14-naphthalene-diol	2-methyl-14-naphthalene-diol$^{\cdot-}$	-0.203[11]	-0.60 (0.39)	-0.72 (0.51)	-0.54 (0.34)	-0.16 (0.05)
2,3-dimethyl-14-	2,3Me2-14-	-0.24[10, 12]	-0.69 (0.45)	-0.81 (0.57)	-0.63 (0.39)	-0.30 (0.06)

naphthalene-diol	naphthalene-diol$^{\bullet-}$					
Ascorbate$^{\bullet}$	Ascorbate^{-}	0.72[12, 13]	0.61 (0.11)	0.59 (0.13)	0.73 (0.01)	1.02 (0.30)
PhCOS$^{\bullet}$	PhCOS^{-}	1.21[14]	1.05 (0.16)	0.87 (0.34)	1.00 (0.21)	1.18 (0.03)
4MePhCOS$^{\bullet}$	4MePhCOS^{-}	1.19[15]	1.03 (0.16)	0.85 (0.34)	0.98 (0.21)	1.17 (0.02)
4MeOPhCOS$^{\bullet}$	4MePhCOS^{-}	1.17[15]	1.12 (0.05)	0.85 (0.32)	0.98 (0.19)	1.16 (0.01)
EtCOS$^{\bullet}$	EtCOS^{-}	1.22[16]	1.04 (0.18)	0.84 (0.38)	0.95 (0.27)	1.18 (0.04)
$Me_2COHO^{\bullet}$	Me_2COHO^{-}	1.45[17]	0.93 (0.52)	1.00 (0.45)	1.00 (0.45)	1.44 (0.01)
MeHCOHO$^{\bullet}$	MeHCOHO^{-}	1.47[17]	1.03 (0.44)	1.15 (0.32)	0.99 (0.48)	1.44 (0.03)
MAD			0.29	0.28	0.37	0.18
AD_{max}			0.52	0.57	0.64	0.60

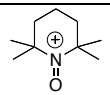
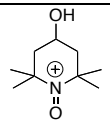
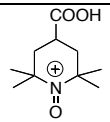
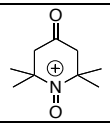
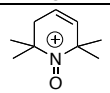
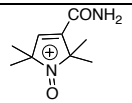
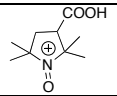
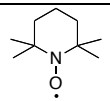
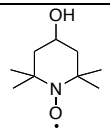
[a] Based on cycle A in Figure 2. Gas phase calculations were carried out on the G3(MP,CC)(+) level of theory and solvation free energies were obtained using solution-phase optimized geometries.
[b] All calculations reported are based on the reference value of E°_{abs}(SHE) = 4.28 V with the exception of CPCM-UAHF model where E°_{abs}(SHE) = 4.47 V. Absolute deviations in parentheses (V).

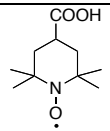
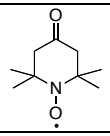
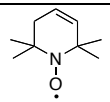
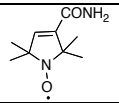
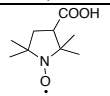
Table 5. Calculated[a] and experimental one-electron standard reduction potentials of anilines and related compounds in aqueous solution at 298 K with respect to the standard hydrogen electrode (SHE).[b]

Ox	**Red**	**Expt**	UAKS	UAHF	SMD	COSMO-RS
$Me_2NH^{\cdot+}$	Me_2NH	1.27[18]	1.25 (0.02)	1.04 (0.23)	1.23 (0.04)	1.29 (0.02)
$Et_2NH^{\cdot+}$	Et_2NH	1.36[18]	1.23 (0.13)	1.01 (0.35)	1.23 (0.13)	1.39 (0.03)
Piperidine$^{\cdot+}$	Piperidine	1.34[18]	1.27 (0.07)	1.00 (0.34)	1.27 (0.07)	1.41 (0.07)
$PhNH_2^{\cdot+}$	PhNH2	1.02[19]	1.28 (0.26)	1.10 (0.08)	1.17 (0.15)	1.12 (0.10)
4OH-$PhNH_2^{\cdot+}$	4OH-$PhNH_2$	0.76[19]	0.89 (0.13)	0.68 (0.08)	0.85 (0.09)	0.77 (0.01)
4NH_2-Ph-$NH_2^{\cdot+}$	4NH_2-Ph-NH_2	0.59[19]	0.52 (0.07)	0.42 (0.17)	0.50 (0.09)	0.39 (0.20)
4Me-$PhNH_2^{\cdot+}$	4Me-$PhNH_2$	0.92[19]	1.12 (0.20)	0.92 (0.00)	1.01 (0.09)	1.00 (0.08)
4MeO-$PhNH_2^{\cdot+}$	4MeO-$PhNH_2$	0.79[19]	0.90 (0.11)	0.65 (0.14)	0.82 (0.03)	0.83 (0.04)
4COCH3-$PhNH_2^{\cdot+}$	4COCH3-$PhNH_2$	1.14[19]	1.50 (0.36)	1.25 (0.11)	1.36 (0.22)	1.48 (0.34)
4CN-$PhNH_2^{\cdot+}$	4CN-$PhNH_2$	1.32[19]	1.72 (0.40)	1.41 (0.09)	1.52 (0.20)	1.58 (0.26)
4CF_3-$PhNH_2^{\cdot+}$	4CF3-$PhNH_2$	1.28[19]	1.55 (0.27)	1.31 (0.03)	1.38 (0.10)	1.42 (0.14)
$Ph_2NH^{\cdot+}$	Ph_2NH	1.0[18]	1.17 (0.17)	0.94 (0.06)	1.05 (0.05)	1.16 (0.16)
Indole$^{\cdot+}$	Indole	1.24[20]	1.49 (0.25)	1.26 (0.02)	1.35 (0.11)	1.42 (0.18)
3-methyl-indole$^{\cdot+}$	3-methyl-indole	1.07[20]	1.25 (0.18)	1.03 (0.04)	1.11 (0.04)	1.21 (0.14)
2,3-dimethyl-indole$^{\cdot+}$	2,3-dimethyl-indole	0.93[20]	1.08 (0.15)	0.88 (0.05)	0.93 (0.00)	1.06 (0.13)
MAD			0.18	0.12	0.09	0.12
AD_{max}			0.40	0.35	0.22	0.34

[a] Based on cycle A in Figure 2. Gas phase calculations were carried out on the G3(MP2,CC)(+) level of theory and solvation free energies were obtained using solution-phase optimized geometries.
[b] All calculations reported are based on the reference value of E°_{abs}(SHE) = 4.28 V with the exception of CPCM-UAHF model where E°_{abs}(SHE) = 4.47 V. Absolute deviations in parentheses (V).

Table 6. G3(MP2,CC)(+) Gibbs free energies (Hartree) and continuum solvent solvation free energies[a] (kJ mol^{-1}) at 298 K.

	Compounds	G^{o}_{298}(gas)	ΔG^{*}_{solv}(UAKS)	ΔG^{*}_{solv}(UAHF)	ΔG^{*}_{solv}(SMD)	ΔG^{*}_{solv}(C-RS)
N1	$NH_2OH^{+\cdot}$	-131.2346875	-417.12	-406.29	-348.22	-397.25
N2		-482.65521	-192.95	-191.23	-211.32	-184.86
N3		-557.7997745	-234.54	-232.55	-244.94	-208.35
N4		-671.0256968	-242.17	-241.17	-250.52	-215.71
N5		-556.6005745	-230.08	-229.61	-256.21	-208.25
N6		-481.4450986	-194.36	-192.79	-210.44	-184.65
N7		-610.7123941	-218.83	-220.25	-249.83	-217.03
N8		-631.7917804	-227.97	-227.81	-242.59	-210.17
N1-red	NH_2OH	-131.5742523	-38.87	-38.43	-27.27	-29.35
N2-red		-482.9093551	-18.01	-14.67	-20.71	-20.74
N3-red		-558.0577998	-47.28	-44.42	-48.28	-43.68

N4-red		-671.2850729	-54.54	-50.5	-52.66	-48.62
N5-red		-556.8678299	-34.55	-30.78	-43.74	-34.32
N6-red		-481.7009198	-17.48	-14.65	-20.26	-20.65
N7-red		-610.9725039	-50.76	-48.06	-60.39	-57.23
N8-red		-632.0523854	-49.73	-46.4	-49.55	-48.04
P1	PhO$^{\cdot}$	-306.3715739	-24.00	-17.53	-26.61	-26.53
P2	4F-PhO$^{\cdot}$	-405.5380747	-25.82	-20.16	-25.24	-24.79
P3	4CN-PhO$^{\cdot}$	-398.5002168	-29.47	-24.28	-31.64	-29.01
P4	4COCH$_3$-PhO$^{\cdot}$	-458.8065561	-31.23	-25.63	-40.19	-34.05
P5	4NO$_2$-PhO$^{\cdot}$	-510.6656379	-29.29	-24.98	-28.59	-27.06
P6	4NMe$_2$-PhO$^{\cdot}$	-440.1162418	-53.28	-29.76	-59.99	-64.40
P7	4MeO-PhO$^{\cdot}$	-420.7449989	-36.90	-26.24	-39.91	-41.65
P8	4OH-PhO$^{\cdot}$	-381.5245668	-60.15	-47.15	-55.5	-60.45
P9	1-naphthol$^{\cdot}$	-459.7653352	-23.14	-16.08	-30.79	-31.46
P10	PhOH$^{\cdot+}$	-306.6929737	-247.22	-249.62	-255.56	-246.17
P11	4MeO-PhOH$^{\cdot+}$	-421.091758	-232.55	-233.38	-236.5	-223.91
P12	OH-PhOH$^{\cdot+}$	-381.8635725	-274.29	-274.05	-268.97	-266.97
P13	PhS$^{\cdot}$	-628.9906196	-6.17	-8.91	-9.38	-10.99
P14	4MeO-PhS$^{\cdot}$	-743.366514	-20.43	-14.72	-22.58	-20.43
P15	4NH$_2$-PhS$^{\cdot}$	-684.2826015	-50.58	-25.05	-47.03	-46.93
P16	HS$^{\cdot}$	-398.3190947	-2.39	-2.34	-6.6	0.17

P17	$CH_3S^{\cdot}$	-437.5564996	-4.33	-4.26	-6.68	-2.95
P18	Hydroquinone (HQ)	-380.9361062	-30.52	-36.01	-32.81	-25.11
P19	Me-HQ	-420.1820779	-27.31	-32.05	-31.28	-24.86
P20	$235Me_3HQ$	-498.6701599	-20.21	-23.87	-27.62	-23.15
P21	Tetramethyl-HQ	-537.9123823	-16.04	-19.03	-24.35	-21.38
P22	2-methyl-14-naphthalene-diol	-573.5864507	-21.61	-26.23	-31.38	-27.40
P23	2,3-dimethyl-14-naphthalene-diol	-612.8293592	-17.53	-21.41	-27.61	-24.37
P24	Ascorbate$^{\cdot}$	-683.3114692	-130.38	-123.92	-110.23	-87.95
P25	$PhCOS^{\cdot}$	-742.1861246	-11.42	-10.96	-16.8	-12.51
P26	$4MePhCOS^{\cdot}$	-781.4297369	-12.08	-10.58	-16.93	-13.40
P27	$4MeOPhCOS^{\cdot}$	-856.5599743	-12.09	-18.81	-25.26	-19.74
P28	$EtCOS^{\cdot}$	-589.9980992	-15.56	-13.21	-15.97	-6.46
P29	$Me_2COHO^{\cdot}$	-268.5548524	-29.77	-29.47	-33.81	-21.50
P30	$MeHCOHO^{\cdot}$	-229.3111462	-42.43	-39.35	-34.87	-23.92
P1-red	PhO^-	-306.4511506	-272.33	-294.47	-265.1	-292.34
P2-red	$4F\text{-}PhO^-$	-405.6170932	-266.07	-289.52	-254.18	-284.00
P3-red	$4CN\text{-}PhO^-$	-398.6149935	-236.03	-251.58	-222.03	-256.45
P4-red	$4COCH_3\text{-}PhO^-$	-458.9144254	-244.6	-266.49	-243.28	-273.50
P5-red	$4NO_2\text{-}PhO^-$	-510.7852131	-224.42	-237.32	-214.68	-249.08
P6-red	$4NMe_2\text{-}PhO^-$	-440.1870717	-272.38	-296.94	-268.96	-293.09
P7-red	$4MeO\text{-}PhO^-$	-420.8188149	-285.12	-310.68	-277.32	-304.04
P8-red	$4OH\text{-}PhO^-$	-381.5992195	-302.23	-327.09	-290.94	-318.33
P9-red	1-naphthol$^-$	-459.8508719	-246.6	-269.88	-243.24	-263.70
P10-red	PhOH	-307.0077484	-31.94	-34.23	-26.88	-24.83
P11-red	4MeO-PhOH	-421.3773722	-39.36	-42.18	-34.01	-30.77
P12-red	OH-Ph-OH	-382.1574184	-58.94	-60.71	-50.05	-45.92
P13-red	PhS^-	-629.0785082	-245.73	-264.63	-220.53	-221.59
P14-red	$4MeO\text{-}PhS^-$	-743.4481718	-259.19	-278.54	-231.07	-230.68
P15-red	$4NH_2\text{-}PhS^-$	-684.3601527	-278.47	-290.51	-247.78	-246.80

P16-red	HS^-	-398.4050778	-287.1	-294.17	-259.4	-259.38
P17-red	CH_3S^-	-437.6255193	-287.18	-297.55	-250.42	-251.20
P18-red	$HQ^{\cdot-}$	-381.0052272	-235.29	-245.41	-240.95	-281.12
P19-red	Me-$HQ^{\cdot-}$	-420.2486888	-231.52	-241.73	-240.46	-279.48
P20-red	235Me3$HQ^{\cdot-}$	-498.7316633	-220.17	-230.13	-233.42	-267.58
P21-red	Tetramethyl-$HQ^{\cdot-}$	-537.9712141	-212.48	-221.84	-226.81	-256.91
P22-red	2-methyl-14-naphthalene-$diol^{\cdot-}$	-573.649818	-214.44	-225.57	-229.23	-262.52
P23-red	2,3Me2-14-naphthalene-$diol^{\cdot-}$	-612.8900977	-208	-218.4	-223.55	-252.50
P24-red	$Ascorbate^-$	-683.4414082	-264.72	-275.03	-256.29	-261.65
P25-red	$PhCOS^-$	-742.2986009	-234.22	-234.61	-234.67	-247.92
P26-red	4Me$PhCOS^-$	-781.5407078	-237.12	-236.6	-237.11	-251.80
P27-red	4Me$PhCOS^-$	-856.6703348	-246.63	-245.66	-246.87	-258.56
P28-red	$EtCOS^-$	-590.1047726	-252.5	-248.76	-244.65	-256.85
P29-red	Me_2COHO^-	-268.6418518	-307.28	-332.25	-318.36	-349.10
P30-red	$MeHCOHO^-$	-229.3963286	-334.42	-361.76	-323.55	-356.07
A1	$Me_2NH^{\cdot+}$	-134.6308532	-283.29	-285.15	-282.97	-267.63
A2	$Et_2NH^{\cdot+}$	-213.1169985	-263.82	-266.39	-259.96	-235.69
A3	$Piperidine^{\cdot+}$	-251.1645559	-264.32	-271.9	-258.1	-238.58
A4	$PhNH_2^{\cdot+}$	-286.8549254	-239.72	-235.04	-246.41	-248.77
A5	4OH-$PhNH_2^{\cdot+}$	-362.0204558	-261.69	-260.36	-258.14	-261.84
A6	4NH_2-Ph-$NH_2^{\cdot+}$	-342.1720523	-244.09	-227.25	-240.22	-247.77
A7	4Me-$PhNH_2^{\cdot+}$	-326.1071232	-227.95	-225.9	-233.98	-234.36
A8	4MeO-$PhNH_2^{\cdot+}$	-401.2467483	-224.48	-228.03	-228.58	-224.41
A9	4COCH3-$PhNH_2^{\cdot+}$	-439.2910708	-253.07	-250.71	-268.27	-254.17
A10	4CN-$PhNH_2^{\cdot+}$	-378.9738436	-267.84	-270.31	-278.1	-277.41
A11	4CF_3-$PhNH_2^{\cdot+}$	-623.5979675	-254.02	-253.71	-265.98	-261.58
A12	$Ph_2NH^{\cdot+}$	-517.5261119	-200.11	-202.74	-209.89	-200.66
A13	$Indole^{\cdot+}$	-362.9478852	-222.78	-224.15	-228.65	-224.58
A14	3-methyl-$indole^{\cdot+}$	-402.199972	-215.18	-215.2	-221.63	-216.20

A15	2,3-dimethyl-indole$^{\cdot+}$	-441.4522281	-207.95	-206.51	-216.16	-207.52
A1-red	Me_2NH	-134.9349783	-21.81	-21.64	-19.61	-10.51
A2-red	Et_2NH	-213.4135307	-20.48	-20.25	-16.36	-7.94
A3-red	Piperidine	-251.4608469	-25.66	-25.58	-19.55	-13.67
A4-red	PhNH2	-287.1415194	-27.45	-24.00	-23.33	-21.49
A5-red	4OH-$PhNH_2$	-362.2910444	-53.63	-50.64	-46.3	-42.52
A6-red	4NH_2-Ph-NH_2	-342.4246542	-48.08	-39.71	-41.55	-39.17
A7-red	4Me-$PhNH_2$	-326.3840139	-25.88	-22.42	-21.14	-20.71
A8-red	4MeO-$PhNH_2$	-401.5109978	-34.61	-31.45	-30.36	-27.62
A9-red	4COCH3-$PhNH_2$	-439.5833785	-46.81	-38.58	-48.44	-46.52
A10-red	4CN-$PhNH_2$	-379.2792316	-48.74	-39.93	-39.68	-44.45
A11-red	4CF3-$PhNH_2$	-623.8995145	-28.28	-23.26	-23.75	-23.45
A12-red	Ph_2NH	-517.7956937	-22.32	-20.66	-20.38	-21.52
A13-red	Indole	-363.2348393	-29.42	-27.03	-21.9	-25.31
A14-red	3-methyl-indole	-402.4764456	-26.55	-23.97	-19.28	-23.51
A15-red	2,3-dimethyl-indole	-441.7202703	-25.21	-22.54	-19.25	-22.65

[a] Solvation free energies were computed on solution-phase optimized geometries. For the COSMO-RS model, the calculations were carried out on the B3LYP/6-31+G(d) gas phase optimized geometries. All electronic structure calculations were carried out using Gaussian09[21] and Molpro[22, 23] suite of programs. COSMO-RS calculations were carried in ADF.[24]

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