

Computational Electrochemistry: Prediction of Liquid-Phase Reduction Potentials

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Supporting Information

Table	Contents	Page
1	Calculated and experimental adiabatic ionization energies	S2
2	Calculated and experimental adiabatic electron affinities	S5
3	Calculated reduction potentials of nitroxides and derivatives	S7
4	Calculated reduction potentials of phenols and derivatives	S8
5	Calculated reduction potentials of anilines and derivatives	S10
6	G3(MP2,CC)(+) Gibbs energies and calculated solvation free energies	S11
7	References	S16

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)
fluorotrchloromethane	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)
phenoxy 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^+	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 $E_{\text{abs}}^{\square}(\text{SHE}) = 4.28 \text{ V}$ with the exception of CPCM-UAHF model where $E_{\text{abs}}^{\square}(\text{SHE}) = 4.47 \text{ V}$. 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 [•]	PhO ⁻	0.79 ⁴	0.42 (0.37)	0.53 (0.26)	0.32 (0.47)	0.60 (0.19)
4F-PhO [•]	4F-PhO ⁻	0.76 ⁴	0.32 (0.44)	0.43 (0.33)	0.21 (0.55)	0.52 (0.24)
4CN-PhO [•]	4CN-PhO ⁻	1.12 ⁴	0.95 (0.17)	0.97 (0.15)	0.78 (0.34)	1.16 (0.04)
4COCH ₃ -PhO [•]	4COCH ₃ -PhO ⁻	1.00 ⁴	0.83 (0.17)	0.92 (0.08)	0.72 (0.28)	1.10 (0.10)
4NO ₂ -PhO [•]	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 [•]	4NMe ₂ -PhO ⁻	0.174 ⁵	-0.12 (0.29)	0.19 (0.01)	-0.22 (0.40)	-0.02 (0.19)
4MeO-PhO [•]	4MeO-PhO ⁻	0.54 ⁴	0.26 (0.28)	0.45 (0.09)	0.15 (0.39)	0.41 (0.13)
4OH-PhO [•]	4OH-PhO ⁻	0.45 ⁴	0.22 (0.23)	0.42 (0.03)	0.15 (0.30)	0.39 (0.06)
1-naphthol [•]	1-naphthol ⁻	0.59 ⁶	0.33 (0.26)	0.45 (0.14)	0.21 (0.38)	0.42 (0.17)
PhOH ^{+•}	PhOH	1.5 ⁷	2.02 (0.52)	1.82 (0.32)	1.88 (0.38)	1.95 (0.45)
4MeO-PhOH ^{+•}	4MeO-PhOH	1.1 ⁷	1.45 (0.35)	1.28 (0.18)	1.36 (0.26)	1.45 (0.35)
OH-PhOH ^{+•}	OH-Ph-OH	1.1 ⁷	1.45 (0.35)	1.28 (0.18)	1.41 (0.31)	1.39 (0.29)
PhS [•]	PhS ⁻	0.69 ⁸	0.56 (0.13)	0.53 (0.16)	0.26 (0.43)	0.26 (0.43)
4MeO-PhS [•]	4MeO-PhS ⁻	0.57 ⁸	0.38 (0.19)	0.45 (0.12)	0.06 (0.51)	0.08 (0.49)
4NH ₂ -PhS [•]	4NH ₂ -PhS ⁻	0.36 ⁸	0.15 (0.21)	0.35 (0.01)	-0.13 (0.49)	-0.14 (0.50)
HS [•]	HS ⁻	1.15 ⁹	0.97 (0.18)	0.86 (0.29)	0.64 (0.51)	0.71 (0.44)
CH ₃ S [•]	CH ₃ S ⁻	0.73 ⁵	0.49 (0.24)	0.41 (0.32)	0.09 (0.64)	0.13 (0.60)
Semiquinone (HQ [•])	HQ ⁻	0.099 ¹⁰	-0.31 (0.41)	-0.46 (0.56)	-0.28 (0.38)	0.22 (0.12)
Me-HQ	Me-HQ ⁻	0.023 ¹⁰	-0.39 (0.41)	-0.52 (0.55)	-0.34 (0.36)	0.13 (0.11)
235Me ₃ HQ	235Me ₃ HQ ⁻	-0.165 ¹⁰	-0.57 (0.41)	-0.70 (0.53)	-0.51 (0.35)	-0.11 (0.05)
Tetramethyl-HQ	Tetramethyl-HQ ⁻	-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 ⁻	-0.203 ¹¹	-0.60 (0.39)	-0.72 (0.51)	-0.54 (0.34)	-0.16 (0.05)
2,3-dimethyl-14-	2,3Me ₂ -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 ⁻					
Ascorbate [·]	Ascorbate ⁻	0.72 ^{12, 13}	0.61 (0.11)	0.59 (0.13)	0.73 (0.01)	1.02 (0.30)
PhCOS [·]	PhCOS ⁻	1.21 ¹⁴	1.05 (0.16)	0.87 (0.34)	1.00 (0.21)	1.18 (0.03)
4MePhCOS [·]	4MePhCOS ⁻	1.19 ¹⁵	1.03 (0.16)	0.85 (0.34)	0.98 (0.21)	1.17 (0.02)
4MeOPhCOS [·]	4MeOPhCOS ⁻	1.17 ¹⁵	1.12 (0.05)	0.85 (0.32)	0.98 (0.19)	1.16 (0.01)
EtCOS [·]	EtCOS ⁻	1.22 ¹⁶	1.04 (0.18)	0.84 (0.38)	0.95 (0.27)	1.18 (0.04)
Me ₂ COHO [·]	Me ₂ COHO ⁻	1.45 ¹⁷	0.93 (0.52)	1.00 (0.45)	1.00 (0.45)	1.44 (0.01)
MeHCOHO [·]	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 $E_{\text{abs}}^{\square}(\text{SHE}) = 4.28$ V with the exception of CPCM-UAHF model where $E_{\text{abs}}^{\square}(\text{SHE}) = 4.47$ V. Absolute deviations in parentheses (V).

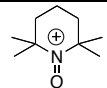
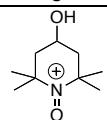
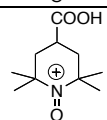
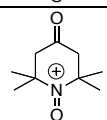
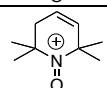
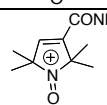
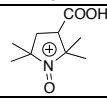
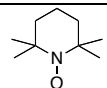
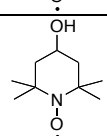
Table 5. Calculated^a and experimental one-electron standard reduction potentials of anilines and related compounds in aqueous solution at 298 K with respect to the standard hydrogen electrode (SHE).^b

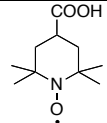
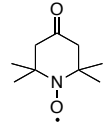
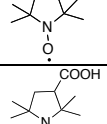
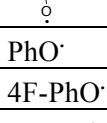
Ox	Red	Expt	UAKS	UAHF	SMD	COSMO-RS
Me ₂ NH ⁺	Me ₂ NH	1.27 ¹⁸	1.25 (0.02)	1.04 (0.23)	1.23 (0.04)	1.29 (0.02)
Et ₂ NH ⁺	Et ₂ NH	1.36 ¹⁸	1.23 (0.13)	1.01 (0.35)	1.23 (0.13)	1.39 (0.03)
Piperidine ⁺	Piperidine	1.34 ¹⁸	1.27 (0.07)	1.00 (0.34)	1.27 (0.07)	1.41 (0.07)
PhNH ₂ ⁺	PhNH ₂	1.02 ¹⁹	1.28 (0.26)	1.10 (0.08)	1.17 (0.15)	1.12 (0.10)
4OH-PhNH ₂ ⁺	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 ⁺	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 ⁺	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 ⁺	4MeO-PhNH ₂	0.79 ¹⁹	0.90 (0.11)	0.65 (0.14)	0.82 (0.03)	0.83 (0.04)
4COCH ₃ -PhNH ₂ ⁺	4COCH ₃ -PhNH ₂	1.14 ¹⁹	1.50 (0.36)	1.25 (0.11)	1.36 (0.22)	1.48 (0.34)
4CN-PhNH ₂ ⁺	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 ⁺	4CF ₃ -PhNH ₂	1.28 ¹⁹	1.55 (0.27)	1.31 (0.03)	1.38 (0.10)	1.42 (0.14)
Ph ₂ NH ⁺	Ph ₂ NH	1.0 ¹⁸	1.17 (0.17)	0.94 (0.06)	1.05 (0.05)	1.16 (0.16)
Indole ⁺	Indole	1.24 ²⁰	1.49 (0.25)	1.26 (0.02)	1.35 (0.11)	1.42 (0.18)
3-methyl-indole ⁺	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 ⁺	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

^aBased 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.

^bAll calculations reported are based on the reference value of $E_{\text{abs}}^{\square}(\text{SHE}) = 4.28$ V with the exception of CPCM-UAHF model where $E_{\text{abs}}^{\square}(\text{SHE}) = 4.47$ 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 ⁰ _{298(gas)}	ΔG [*] _{solv(UAKS)}	ΔG [*] _{solv(UAHF)}	ΔG [*] _{solv(SMD)}	ΔG [*] _{solv(C-RS)}
N1	NH ₂ OH ⁺	-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 ₂ OH	-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·	-306.3715739	-24.00	-17.53	-26.61	-26.53
P2	4F-PhO·	-405.5380747	-25.82	-20.16	-25.24	-24.79
P3	4CN-PhO·	-398.5002168	-29.47	-24.28	-31.64	-29.01
P4	4COCH ₃ -PhO·	-458.8065561	-31.23	-25.63	-40.19	-34.05
P5	4NO ₂ -PhO·	-510.6656379	-29.29	-24.98	-28.59	-27.06
P6	4NMe ₂ -PhO·	-440.1162418	-53.28	-29.76	-59.99	-64.40
P7	4MeO-PhO·	-420.7449989	-36.90	-26.24	-39.91	-41.65
P8	4OH-PhO·	-381.5245668	-60.15	-47.15	-55.5	-60.45
P9	1-naphthol·	-459.7653352	-23.14	-16.08	-30.79	-31.46
P10	PhOH ⁺	-306.6929737	-247.22	-249.62	-255.56	-246.17
P11	4MeO-PhOH ⁺	-421.091758	-232.55	-233.38	-236.5	-223.91
P12	OH-PhOH ⁺	-381.8635725	-274.29	-274.05	-268.97	-266.97
P13	PhS·	-628.9906196	-6.17	-8.91	-9.38	-10.99
P14	4MeO-PhS·	-743.366514	-20.43	-14.72	-22.58	-20.43
P15	4NH ₂ -PhS·	-684.2826015	-50.58	-25.05	-47.03	-46.93
P16	HS·	-398.3190947	-2.39	-2.34	-6.6	0.17

P17	CH ₃ S [·]	-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 ₃ HQ	-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 [·]	-683.3114692	-130.38	-123.92	-110.23	-87.95
P25	PhCOS [·]	-742.1861246	-11.42	-10.96	-16.8	-12.51
P26	4MePhCOS [·]	-781.4297369	-12.08	-10.58	-16.93	-13.40
P27	4MeOPhCOS [·]	-856.5599743	-12.09	-18.81	-25.26	-19.74
P28	EtCOS [·]	-589.9980992	-15.56	-13.21	-15.97	-6.46
P29	Me ₂ COHO [·]	-268.5548524	-29.77	-29.47	-33.81	-21.50
P30	MeHCOHO [·]	-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-PhO [·]	-405.6170932	-266.07	-289.52	-254.18	-284.00
P3-red	4CN-PhO [·]	-398.6149935	-236.03	-251.58	-222.03	-256.45
P4-red	4COCH ₃ -PhO [·]	-458.9144254	-244.6	-266.49	-243.28	-273.50
P5-red	4NO ₂ -PhO [·]	-510.7852131	-224.42	-237.32	-214.68	-249.08
P6-red	4NMe ₂ -PhO [·]	-440.1870717	-272.38	-296.94	-268.96	-293.09
P7-red	4MeO-PhO [·]	-420.8188149	-285.12	-310.68	-277.32	-304.04
P8-red	4OH-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-PhS [·]	-743.4481718	-259.19	-278.54	-231.07	-230.68
P15-red	4NH ₂ -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 ₃ S ⁻	-437.6255193	-287.18	-297.55	-250.42	-251.20
P18-red	HQ ⁻	-381.0052272	-235.29	-245.41	-240.95	-281.12
P19-red	Me-HQ ⁻	-420.2486888	-231.52	-241.73	-240.46	-279.48
P20-red	235Me3HQ ⁻	-498.7316633	-220.17	-230.13	-233.42	-267.58
P21-red	Tetramethyl-HQ ⁻	-537.9712141	-212.48	-221.84	-226.81	-256.91
P22-red	2-methyl-14-naphthalene-diol ⁻	-573.649818	-214.44	-225.57	-229.23	-262.52
P23-red	2,3Me2-14-naphthalene-diol ⁻	-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	4MePhCOS ⁻	-781.5407078	-237.12	-236.6	-237.11	-251.80
P27-red	4MePhCOS ⁻	-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 ₂ COHO ⁻	-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 ₂ NH ⁺	-134.6308532	-283.29	-285.15	-282.97	-267.63
A2	Et ₂ NH ⁺	-213.1169985	-263.82	-266.39	-259.96	-235.69
A3	Piperidine ⁺	-251.1645559	-264.32	-271.9	-258.1	-238.58
A4	PhNH ₂ ⁺	-286.8549254	-239.72	-235.04	-246.41	-248.77
A5	4OH-PhNH ₂ ⁺	-362.0204558	-261.69	-260.36	-258.14	-261.84
A6	4NH ₂ -Ph-NH ₂ ⁺	-342.1720523	-244.09	-227.25	-240.22	-247.77
A7	4Me-PhNH ₂ ⁺	-326.1071232	-227.95	-225.9	-233.98	-234.36
A8	4MeO-PhNH ₂ ⁺	-401.2467483	-224.48	-228.03	-228.58	-224.41
A9	4COCH3-PhNH ₂ ⁺	-439.2910708	-253.07	-250.71	-268.27	-254.17
A10	4CN-PhNH ₂ ⁺	-378.9738436	-267.84	-270.31	-278.1	-277.41
A11	4CF ₃ -PhNH ₂ ⁺	-623.5979675	-254.02	-253.71	-265.98	-261.58
A12	Ph ₂ NH ⁺	-517.5261119	-200.11	-202.74	-209.89	-200.66
A13	Indole ⁺	-362.9478852	-222.78	-224.15	-228.65	-224.58
A14	3-methyl-indole ⁺	-402.199972	-215.18	-215.2	-221.63	-216.20

A15	2,3-dimethyl-indole ⁺	-441.4522281	-207.95	-206.51	-216.16	-207.52
A1-red	Me ₂ NH	-134.9349783	-21.81	-21.64	-19.61	-10.51
A2-red	Et ₂ NH	-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	PhNH ₂	-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	4COCH ₃ -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	4CF ₃ -PhNH ₂	-623.8995145	-28.28	-23.26	-23.75	-23.45
A12-red	Ph ₂ NH	-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 Gaussian09²¹ and Molpro^{22, 23} suite of programs. COSMO-RS calculations were carried in ADF.²⁴

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