Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting Information: Method for the Accurate Prediction of Electron Transfer Potentials using an Effective Absolute Potential

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Summary of Test Set for Benchmarking

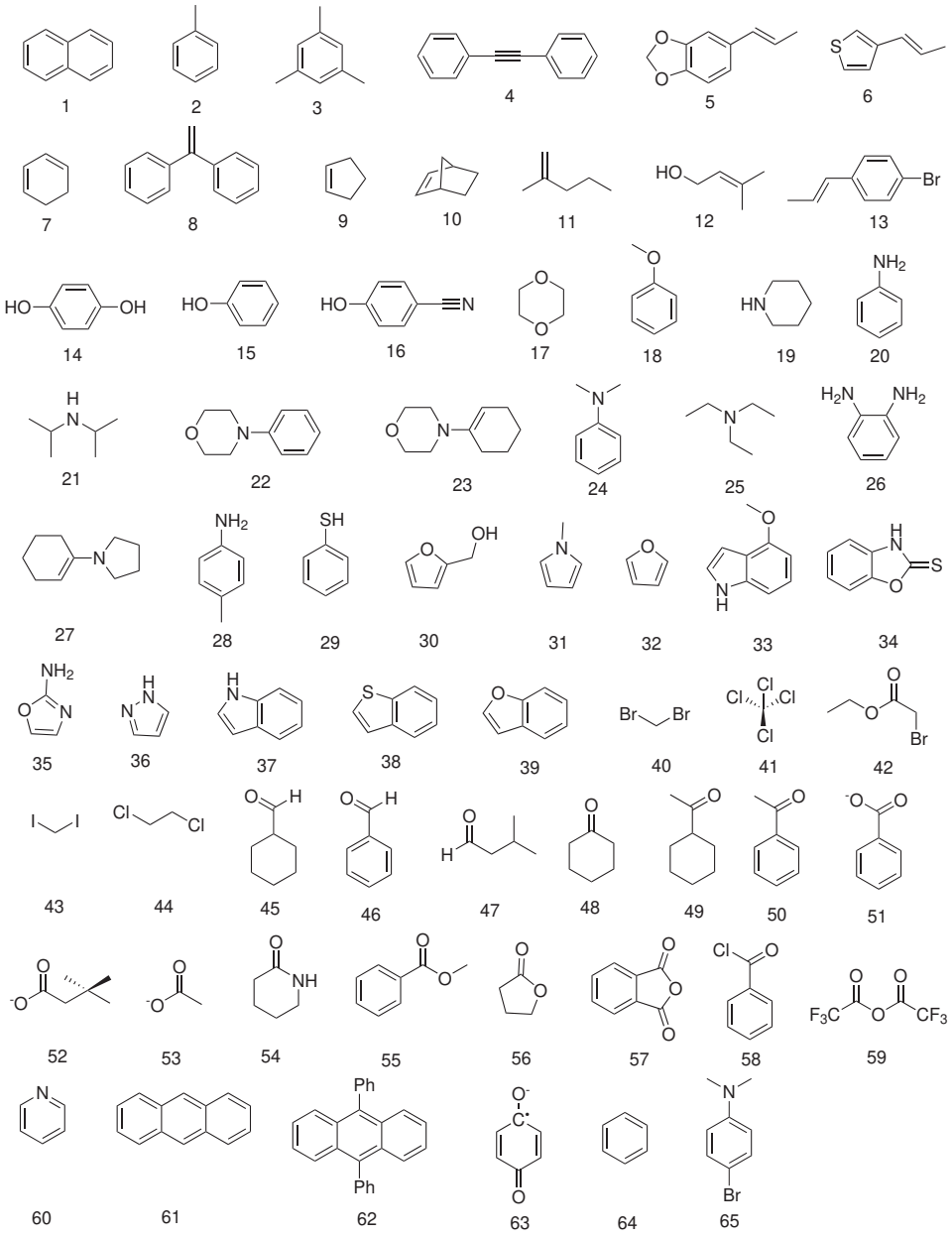

Figure S1: Summary of organic molecules used for benchmarking DFT functionals.

Comparison of CCSD(T) and DFT with Experiment

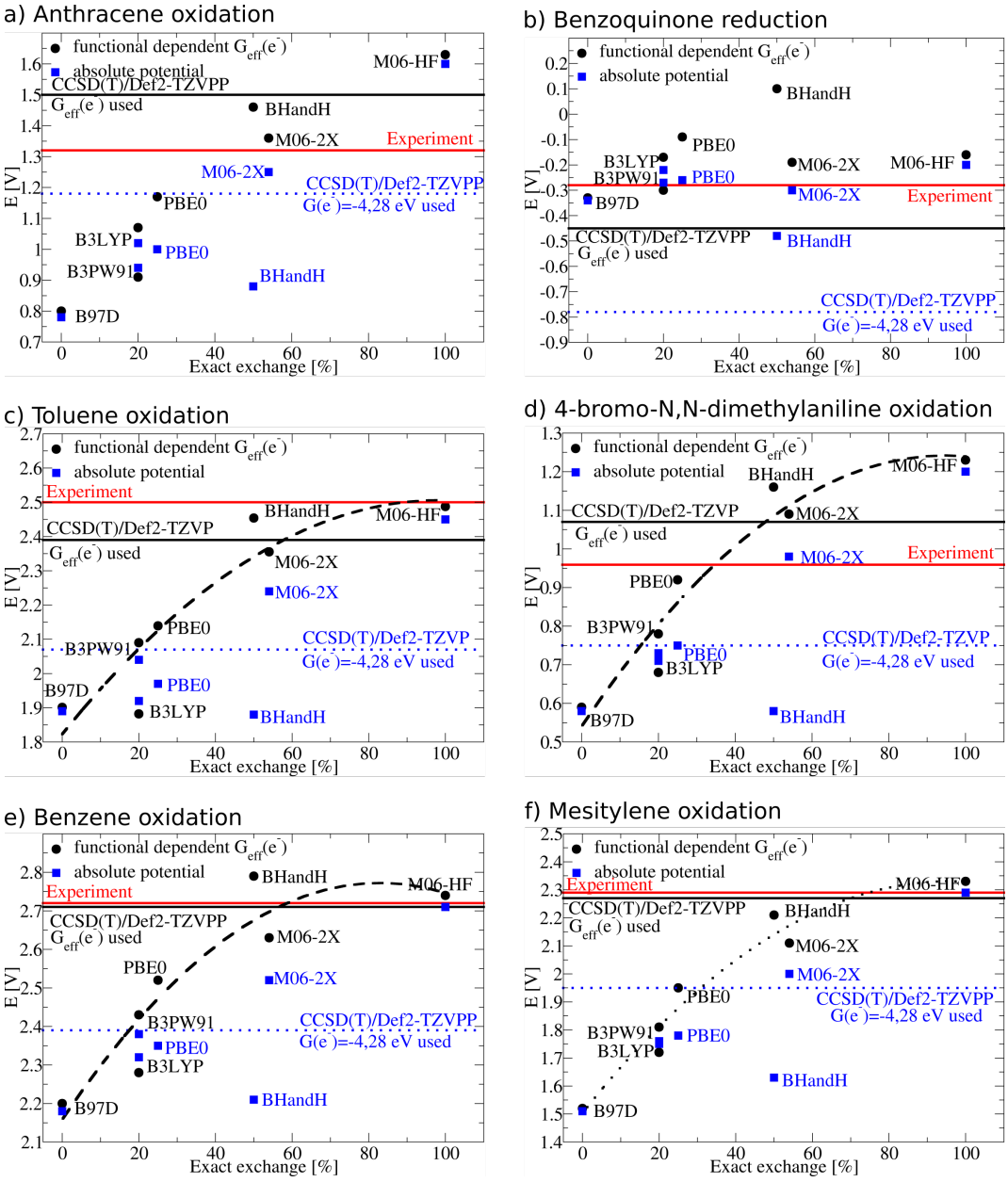

Figure S2: Comparison of electron transfer potentials obtained with CCSD(T)/Def2-TZVPP/SMD and different DFT functionals with experiment.

Convergence Tests

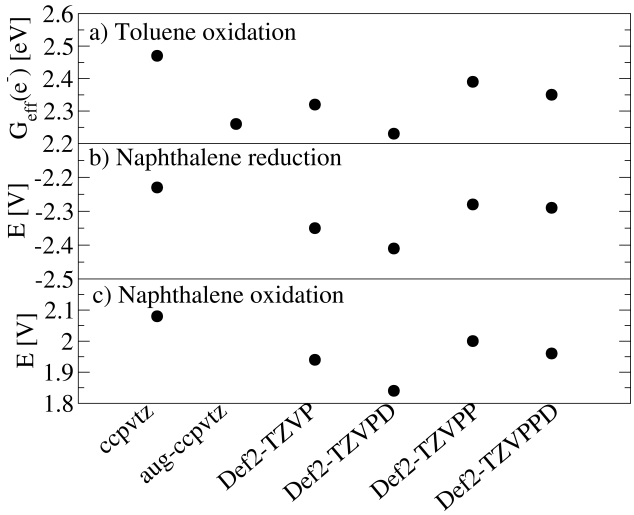

Figure S3: Convergence of CCSD(T)/SMD with respect to the basis set for toluene oxidation (a) and naphthalene reduction (b) and naphthalene oxidation (c).

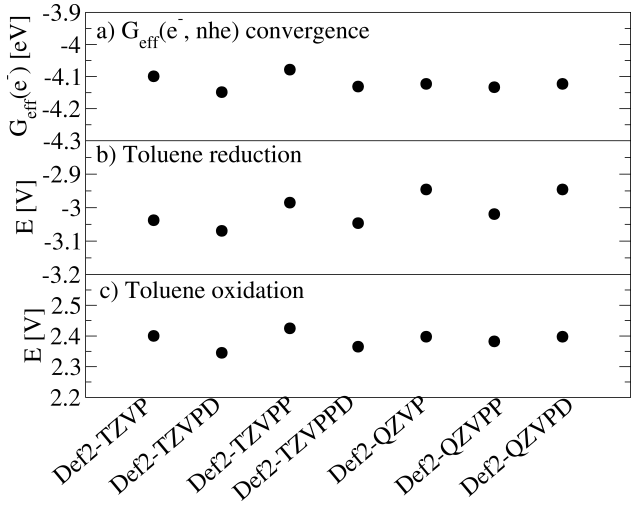

Figure S4: Convergence of DFT/M06-2X/SMD calculations with respect to the basis set for the effective electron energy (a), toluene reduction (b) and toluene oxidation (c).

Summary of Experimental Reference Potentials

The experimental electron transfer (ET) potentials for mesytilene and benzoquinone have been converted to the normal hydrogen electrode (NHE) in water. For both systems the potential value of standard calomel electrode (SCE) in water was used in the calculation of potentials. It is unclear in the cited references if the aqueous SCE was separated by a salt bridge from the organic solvent. In case of direct contact, the liquid junction potential will influence the potential value.[S1,S2] However, the liquid potential depends on the system and is not available in the cited references. Efforts have been made to estimate the potential for the SCE electrode in different solvents[S3] and for acetonitrile the potential for SCE was found to be 0.141 V vs. SHE. If this value was to be used instead of the potential in water, 0.241 V vs, SHE, the potential values for mesitylene and benzoquinone should be 0.1 V more negative. This change in potential will not influence the general conclusion in the paper.

Table S1: Summary of the experimental reference electron transfer potentials in acetonitrile.

Compound	Name	E [V] vs. nhe	source
65	4-bromo-N,N-dimetylaniline	0.959	[S4]
61	Anthracene	1.328	[S5]
64	Benzene	2.721	[S6]
2	Toluene	2.501	[S6]
3	Mesitylene	2.291	[S6]
63	Benzoquinone	-0.281	[S7]

References

(S1) Gritzner, G. In *Handbook of Reference Electrodes*; Inzelt, G., Lewenstam, A., Scholz, F., Eds.; Springer Berlin Heidelberg: Berlin, Heidelberg, 2013; Chapter 2, pp 25–31.

(S2) Izutsu, K. In *Handbook of Reference Electrodes*; Inzelt, G., Lewenstam, A., Scholz, F., Eds.; Springer Berlin Heidelberg: Berlin, Heidelberg, 2013; Chapter 6, pp 145–187.

(S3) Isse, A.; Gennaro, A. Absolute Potential of the Standard Hydrogen Electrode and the Problem of Interconversion of Potentials in Different Solvents. *J. Phys. Chem. B* **2010**, *114*, 7894–7899, PMID: 20496903.

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(S5) Ahlberg, E.; Parker, V. Kinetics of Rapid Reactions Coupled to Charge Transfer at Electrodes. Reactions of Anthracene Cation Radicals with Pyridine. *Acta Chem. Scand. B* **1980**, *34*, 97–102.

(S6) Merkel, P.; Luo, P.; Dinnocenzo, J.; Farid, S. Accurate Oxidation Potentials of Benzene and Biphenyl Derivatives via Electron-Transfer Equilibria and Transient Kinetics. *J. Org. Chem.* **2009**, *74*, 5163–5173, PMID: 19588891.

(S7) Sasaki, K.; Kashimura, T.; Ohura, M.; Ohsaki, Y.; Ohta, N. Solvent Effect in the Electrochemical Reduction of p-Quinones in Several Aprotic Solvents. *J Electrochem Soc* **1990**, *137*, 2437.

Summary of Effective Absolute Potentials

Table S2: Summary of the effective absolute potentials versus nhe in water.

Method	Basis set	Solvation	Reference	E_{eff}(nhe) [V]
CCSD(T)	ccpvtz	SMD	HCOOH	3.849
CCSD(T)	ccpvqz	SMD	HCOOH	4.039
CCSD(T)	Aug-ccpvtz	SMD	HCOOH	4.119
CCSD(T)	Aug-ccpvqz	SMD	HCOOH	4.141
CCSD(T)	Def2-TZVP	SMD	HCOOH	4.009
CCSD(T)	Def2-TZVPP	SMD	HCOOH	3.958
CCSD(T)	Def2-QZVP	SMD	HCOOH	4.862
CCSD(T)	Def2-TZVPPD	SMD	HCOOH	4.075
CCSD	ccpvtz	SMD	HCOOH	3.818
CCSD	ccpvqz	SMD	HCOOH	3.988
CCSD	Aug-ccpvtz	SMD	HCOOH	4.057
CCSD	Aug-ccpvqz	SMD	HCOOH	4.075
CCSD	Def2-TZVP	SMD	HCOOH	3.965
CCSD	Def2-TZVPP	SMD	HCOOH	3.919
CCSD	Def2-QZVP	SMD	HCOOH	4.027
CCSD	Def2-TZVPPD	SMD	HCOOH	4.018
MP2	ccpvtz	SMD	HCOOH	3.854
MP2	ccpvqz	SMD	HCOOH	4.046
MP2	Aug-ccpvtz	SMD	HCOOH	4.126
MP2	Aug-ccpvqz	SMD	HCOOH	4.152
MP2	Def2-TZVP	SMD	HCOOH	4.017
MP2	Def2-TZVPP	SMD	HCOOH	3.968
MP2	Def2-QZVP	SMD	HCOOH	4.094
MP2	Def2-TZVPPD	SMD	HCOOH	4.082
B97D	6-311++G**	SMD	HCOOH	4.265
B3LYP	6-311++G**	SMD	HCOOH	4.315
B3PW91	6-311++G**	SMD	HCOOH	4.228
PBE0	6-311++G**	SMD	HCOOH	4.110
BhandH	6-311++G**	SMD	HCOOH	3.702
M06-2X	6-311++G**	SMD	HCOOH	4.201
M06-HF	6-311++G**	SMD	HCOOH	4.248
ωB97X-D	6-311++G**	SMD	HCOOH	4.194
HSE06	6-311++G**	SMD	HCOOH	4.129
M06-2X	6-311++G**	PCM	HCOOH	4.037
M06-2X	6-311++G**	PCM	Pentafluorothiophenol	4.503

Electron Transfer Potentials - CCSD(T)

Table S3: Summary of the computed electron transfer potentials at the CCSD(T)/Def2-TZVPP/SMD level of theory. The HCOOH/$HCOO^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.28	2.00	-2.60	1.68	-2.76	1.52
2	-3.01	2.39	-3.33	2.07	-3.49	1.91
3	-3.24	2.27	-3.56	1.95	-3.72	1.79
4	-2.14	2.16	-2.46	1.84	-2.62	1.68
5	-2.68	1.49	-3.00	1.17	-3.16	1.01
6	-2.84	1.88	-3.16	1.56	-3.32	1.40
7	-2.66	1.78	-2.98	1.45	-3.14	1.29
8	-2.32	2.19	-2.64	1.87	-2.80	1.71
9	-3.56	2.37	-3.88	2.05	-4.04	1.89
10	-3.34	2.30	-3.66	1.97	-3.82	1.81
11	-3.49	2.50	-3.81	2.18	-3.97	2.02
12	-3.32	2.30	-3.65	1.98	-3.81	1.82
13	-2.37	2.10	-2.69	1.78	-2.85	1.62
14	-2.80	1.58	-3.12	1.26	-3.28	1.10
15	-2.89	2.13	-3.21	1.81	-3.37	1.65
16	-2.35	2.50	-2.68	2.18	-2.84	2.02
17	-5.77	2.50	-6.09	2.17	-6.25	2.01
18	-2.98	2.00	-3.30	1.68	-3.46	1.52
19	-4.56	1.43	-4.88	1.11	-5.04	0.95
20	-2.97	1.33	-3.30	1.01	-3.46	0.85
21	-4.81	1.44	-5.13	1.12	-5.29	0.96
22	-3.06	1.09	-3.38	0.77	-3.54	0.61
23	-3.85	0.68	-4.17	0.35	-4.33	0.19
24	-3.12	1.06	-3.44	0.74	-3.60	0.58
25	-4.26	1.06	-4.59	0.74	-4.75	0.58
26	-3.24	0.93	-3.56	0.60	-3.72	0.44
27	-3.86	0.56	-4.18	0.23	-4.34	0.07
28	-2.99	1.18	-3.31	0.86	-3.47	0.70
29	-2.77	2.13	-3.09	1.81	-3.25	1.65
30	-3.27	2.05	-3.59	1.72	-3.75	1.56
31	-3.80	1.55	-4.12	1.22	-4.28	1.06
32	-3.39	2.19	-3.71	1.87	-3.87	1.71
33	-3.10	1.35	-3.42	1.03	-3.58	0.87
34	-1.81	2.39	-2.13	2.07	-2.29	1.91
35	-4.16	1.67	-4.49	1.35	-4.65	1.19
36	-3.41	2.53	-3.73	2.21	-3.89	2.05

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
37	-2.88	1.57	-3.20	1.25	-3.36	1.09
38	-2.63	2.06	-2.95	1.74	-3.11	1.58
39	-2.64	2.04	-2.96	1.72	-3.12	1.56
40	unstable	4.10	unstable	3.78	unstable	3.62
41	unstable	5.05	unstable	4.72	unstable	4.56
42	unstable	3.98	unstable	3.66	unstable	3.50
43	unstable	2.33	unstable	2.01	unstable	1.85
44	unstable	4.95	unstable	4.63	unstable	4.47
45	-2.75	3.00	-3.07	2.68	-3.23	2.52
46	-1.80	2.94	-2.12	2.62	-2.28	2.46
47	-2.75	3.12	-3.07	2.80	-3.23	2.64
48	-2.90	2.73	-3.23	2.41	-3.39	2.25
49	-2.98	2.78	-3.30	2.46	-3.46	2.30
50	-1.98	3.00	-2.30	2.67	-2.46	2.51
51	-3.02	1.55	-3.34	1.23	-3.50	1.07
52	-4.92	0.58	-5.24	0.26	-5.40	0.10
53	-5.28	1.41	-5.60	1.08	-5.76	0.92
54	-3.39	2.58	-3.71	2.26	-3.87	2.10
55	-2.14	2.96	-2.46	2.63	-2.62	2.47
56	-3.23	3.61	-3.55	3.29	-3.71	3.13
57	-1.21	3.46	-1.53	3.13	-1.69	2.97
58	-1.53	2.59	-1.85	2.27	-2.01	2.11
59	-1.13	5.05	-1.45	4.72	-1.61	4.56
60	-2.49	2.74	-2.81	2.42	-2.97	2.26
61	-1.74	1.50	-2.06	1.18	-2.22	1.02
62	–	–	–	–	–	–
63	-1.43	-0.45	-1.75	-0.77	-1.91	-0.93
64	-2.93	2.72	-3.26	2.39	-3.42	2.23
65	–	1.07	–	0.75	–	0.59

Electron Transfer Potentials - CCSD

Table S4: Summary of the computed electron transfer potentials at the CCSD/Def2-TZVPP/SMD level of theory. The HCOOH/$HCOO^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.34	2.03	-2.70	1.67	-2.86	1.51
2	-3.02	2.35	-3.38	1.99	-3.54	1.83
3	-3.26	2.23	-3.62	1.86	-3.78	1.70
4	-2.24	2.21	-2.60	1.85	-2.76	1.69
5	-2.72	1.52	-3.08	1.16	-3.24	1.00
6	-2.87	1.88	-3.24	1.52	-3.40	1.36
7	-2.69	1.75	-3.06	1.39	-3.22	1.23
8	-2.40	2.20	-2.76	1.84	-2.92	1.68
9	-3.57	2.30	-3.93	1.94	-4.09	1.78
10	-3.35	2.24	-3.71	1.87	-3.87	1.71
11	-3.49	2.43	-3.85	2.07	-4.01	1.91
12	-3.36	2.23	-3.72	1.87	-3.88	1.71
13	-2.41	2.09	-2.77	1.73	-2.93	1.57
14	-2.79	1.62	-3.15	1.26	-3.31	1.10
15	-2.90	2.11	-3.26	1.75	-3.42	1.59
16	-2.38	2.49	-2.74	2.13	-2.90	1.97
17	-5.86	2.67	-6.22	2.31	-6.38	2.15
18	-2.98	1.98	-3.35	1.62	-3.51	1.46
19	-4.58	1.41	-4.94	1.05	-5.10	0.89
20	-2.98	1.32	-3.34	0.96	-3.50	0.80
21	-4.88	1.40	-5.24	1.04	-5.40	0.88
22	-3.07	1.11	-3.43	0.75	-3.59	0.59
23	-3.89	0.64	-4.25	0.28	-4.41	0.12
24	-3.13	1.07	-3.49	0.71	-3.65	0.55
25	-4.88	1.02	-5.24	0.65	-5.40	0.49
26	-3.24	0.92	-3.60	0.55	-3.76	0.39
27	-3.90	0.52	-4.26	0.16	-4.42	0.00
28	-3.00	1.16	-3.36	0.80	-3.52	0.64
29	-2.78	2.15	-3.14	1.79	-3.30	1.63
30	-3.31	2.00	-3.67	1.64	-3.83	1.48
31	-3.82	1.50	-4.18	1.14	-4.34	0.98
32	-3.42	2.15	-3.78	1.79	-3.94	1.63
33	-3.13	1.38	-3.50	1.02	-3.66	0.86
34	-2.31	2.33	-2.67	1.97	-2.83	1.81
35	-4.16	1.66	-4.52	1.30	-4.68	1.14
36	-3.41	2.46	-3.78	2.10	-3.94	1.94

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
37	-2.91	1.56	-3.27	1.20	-3.43	1.04
38	-2.67	2.09	-3.03	1.73	-3.19	1.57
39	-2.68	2.04	-3.04	1.68	-3.20	1.52
40	unstable	4.19	unstable	3.82	unstable	3.66
41	unstable	5.19	unstable	4.83	unstable	4.67
42	unstable	4.20	unstable	3.84	unstable	3.68
43	unstable	2.42	unstable	2.06	unstable	1.90
44	unstable	5.16	unstable	4.80	unstable	4.64
45	-2.75	3.07	-3.11	2.71	-3.27	2.55
46	-1.83	2.89	-2.19	2.53	-2.35	2.37
47	-2.75	3.15	-3.11	2.79	-3.27	2.63
48	-2.91	2.77	-3.27	2.41	-3.43	2.25
49	-2.98	2.84	-3.35	2.48	-3.51	2.32
50	-2.02	2.99	-2.38	2.63	-2.54	2.47
51	-3.03	1.67	-3.39	1.31	-3.55	1.15
52	-5.00	0.54	-5.37	0.18	-5.53	0.02
53	-5.31	1.53	-5.67	1.17	-5.83	1.01
54	-3.39	2.57	-3.75	2.21	-3.91	2.05
55	-2.16	2.91	-2.52	2.55	-2.68	2.39
56	-3.23	3.61	-3.59	3.24	-3.75	3.08
57	-1.26	3.41	-1.62	3.05	-1.78	2.89
58	-1.56	3.08	-1.92	2.72	-2.08	2.56
59	-1.14	5.27	-1.50	4.91	-1.66	4.75
60	-2.49	2.74	-2.85	2.38	-3.01	2.22
61	-1.80	1.52	-2.16	1.16	-2.32	1.00
62	–	–	–	–	–	–
63	-1.46	-0.49	-1.83	-0.85	-1.99	-1.01
64	-2.94	2.67	-3.30	2.30	-3.46	2.14
65	–	1.09	–	0.73	–	0.57

Electron Transfer Potentials - MP2

Table S5: Summary of the computed electron transfer potentials at the MP2/Def2-TZVPP/SMD level of theory. The HCOOH/HCOO$^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.14	1.96	-2.45	1.65	-2.61	1.49
2	-2.98	2.48	-3.29	2.17	-3.45	2.01
3	-3.22	2.47	-3.53	2.16	-3.69	2.00
4	-2.00	2.30	-2.32	1.99	-2.48	1.83
5	-2.62	1.54	-2.93	1.23	-3.09	1.07
6	-2.85	1.97	-3.16	1.66	-3.32	1.50
7	-2.48	1.74	-2.79	1.43	-2.95	1.27
8	-2.22	2.35	-2.53	2.04	-2.69	1.88
9	-3.50	2.50	-3.82	2.18	-3.98	2.02
10	-3.29	2.43	-3.60	2.12	-3.76	1.96
11	-3.47	2.60	-3.79	2.29	-3.95	2.13
12	-3.27	2.42	-3.58	2.11	-3.74	1.95
13	-2.27	2.23	-2.59	1.92	-2.75	1.76
14	-2.80	1.70	-3.11	1.39	-3.27	1.23
15	-2.88	2.26	-3.19	1.95	-3.35	1.79
16	-2.30	2.62	-2.62	2.31	-2.78	2.15
17	-5.84	2.12	-6.15	1.81	-6.31	1.65
18	-2.96	2.12	-3.27	1.81	-3.43	1.65
19	-4.61	1.61	-4.92	1.30	-5.08	1.14
20	-2.96	1.41	-3.27	1.10	-3.43	0.94
21	-4.88	1.63	-5.19	1.32	-5.35	1.16
22	-3.04	1.21	-3.35	0.90	-3.51	0.74
23	-3.82	0.82	-4.13	0.50	-4.29	0.34
24	-3.10	1.21	-3.41	0.90	-3.57	0.74
25	-4.88	1.25	-5.19	0.93	-5.35	0.77
26	-3.23	1.00	-3.54	0.69	-3.70	0.53
27	-3.83	0.69	-4.14	0.38	-4.30	0.22
28	-2.99	1.26	-3.30	0.95	-3.46	0.79
29	-2.74	2.20	-3.05	1.89	-3.21	1.73
30	-3.25	2.12	-3.56	1.81	-3.72	1.65
31	-3.78	1.68	-4.09	1.37	-4.25	1.21
32	-3.32	2.24	-3.64	1.92	-3.80	1.76
33	-3.04	1.54	-3.36	1.23	-3.52	1.07
34	-2.52	2.47	-2.84	2.16	-3.00	2.00
35	-4.16	1.88	-4.47	1.56	-4.63	1.40
36	-3.56	2.82	-3.87	2.50	-4.03	2.34

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
37	-2.83	1.78	-3.14	1.47	-3.30	1.31
38	-2.65	2.24	-2.96	1.93	-3.12	1.77
39	-2.59	2.22	-2.90	1.91	-3.06	1.75
40	unstable	4.06	unstable	3.74	unstable	3.58
41	unstable	4.99	unstable	4.68	unstable	4.52
42	unstable	3.70	unstable	3.39	unstable	3.23
43	unstable	2.28	unstable	1.96	unstable	1.80
44	unstable	4.85	unstable	4.54	unstable	4.38
45	-2.77	3.54	-3.08	3.23	-3.24	3.07
46	-1.75	3.08	-2.06	2.77	-2.22	2.61
47	-2.77	3.65	-3.08	3.33	-3.24	3.17
48	-2.94	3.25	-3.25	2.94	-3.41	2.78
49	-3.01	3.28	-3.33	2.97	-3.49	2.81
50	-1.90	3.13	-2.22	2.82	-2.38	2.66
51	-2.97	1.42	-3.28	1.11	-3.44	0.95
52	-4.96	0.59	-5.27	0.27	-5.43	0.11
53	-5.33	1.26	-5.64	0.95	-5.80	0.79
54	-3.46	2.82	-3.77	2.51	-3.93	2.35
55	-2.06	3.08	-2.37	2.77	-2.53	2.61
56	-3.30	4.07	-3.61	3.76	-3.77	3.60
57	-1.13	3.58	-1.44	3.27	-1.60	3.11
58	-1.47	3.28	-1.78	2.97	-1.94	2.81
59	-1.15	5.04	-1.47	4.72	-1.63	4.56
60	-2.45	2.98	-2.77	2.67	-2.93	2.51
61	-1.53	1.41	-1.84	1.10	-2.00	0.94
62	–	–	–	–	–	–!
63	-1.37	-0.16	-1.68	-0.47	-1.84	-0.63
64	-2.91	2.80	-3.23	2.49	-3.39	2.33
65	–	1.24	–	0.93	–	0.77

Electron Transfer Potentials - B97D

Table S6: Summary of the computed electron transfer potentials at the B97D/6-311++G**/SMD level of theory. The $HCOOH/HCOO^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.30	1.34	-2.31	1.32	-2.47	1.16
2	-3.15	1.90	-3.17	1.89	-3.33	1.73
3	-3.21	1.52	-3.23	1.51	-3.39	1.35
4	-1.97	1.30	-1.98	1.28	-2.14	1.12
5	-2.64	0.72	-2.65	0.71	-2.81	0.55
6	-2.76	1.14	-2.78	1.12	-2.94	0.96
7	-2.59	1.01	-2.61	0.99	-2.77	0.83
8	-2.24	1.33	-2.26	1.32	-2.42	1.16
9	-4.19	1.60	-4.21	1.58	-4.37	1.42
10	-3.37	1.59	-3.39	1.57	-3.55	1.41
11	-3.43	1.75	-3.44	1.74	-3.60	1.58
12	-3.17	1.61	-3.19	1.60	-3.35	1.44
13	-2.37	1.28	-2.38	1.26	-2.54	1.10
14	-2.91	1.07	-2.93	1.06	-3.09	0.90
15	-3.00	1.59	-3.01	1.58	-3.17	1.42
16	-2.31	1.95	-2.32	1.94	-2.48	1.78
17	-4.20	1.66	-4.22	1.64	-4.38	1.48
18	-3.07	1.41	-3.08	1.40	-3.24	1.24
19	-3.97	0.86	-3.98	0.85	-4.14	0.69
20	-3.12	0.84	-3.13	0.82	-3.29	0.66
21	-4.00	0.86	-4.02	0.84	-4.18	0.68
22	-3.21	0.59	-3.22	0.58	-3.38	0.42
23	-3.67	0.09	-3.68	0.08	-3.84	-0.08
24	-3.26	0.57	-3.27	0.56	-3.43	0.40
25	-4.07	0.50	-4.08	0.49	-4.24	0.33
26	-3.34	0.34	-3.35	0.33	-3.51	0.17
27	-3.67	-0.02	-3.68	-0.04	-3.84	-0.20
28	-3.12	0.63	-3.14	0.62	-3.30	0.46
29	-2.74	1.52	-2.76	1.50	-2.92	1.34
30	-3.09	1.53	-3.10	1.51	-3.26	1.35
31	-4.08	1.14	-4.09	1.12	-4.25	0.96
32	-3.31	1.73	-3.33	1.72	-3.49	1.56
33	-3.07	0.71	-3.08	0.70	-3.24	0.54
34	-2.27	1.47	-2.29	1.45	-2.45	1.29
35	-3.13	1.15	-3.15	1.14	-3.31	0.98
36	-3.39	2.20	-3.41	2.19	-3.57	2.03

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
37	-2.93	1.03	-2.94	1.01	-3.10	0.85
38	-2.61	1.42	-2.63	1.41	-2.79	1.25
39	-2.72	1.49	-2.73	1.48	-2.89	1.32
40	unstable	3.59	unstable	3.58	unstable	3.42
41	unstable	4.27	unstable	4.26	unstable	4.10
42	unstable	2.91	unstable	2.89	unstable	2.73
43	unstable	1.86	unstable	1.85	unstable	1.69
44	unstable	3.45	unstable	3.43	unstable	3.27
45	-2.73	2.04	-2.75	2.02	-2.91	1.86
46	-1.75	2.33	-1.76	2.32	-1.92	2.16
47	-2.76	2.25	-2.77	2.24	-2.93	2.08
48	-2.87	1.91	-2.88	1.90	-3.04	1.74
49	-2.97	1.83	-2.99	1.81	-3.15	1.65
50	-1.92	2.14	-1.93	2.13	-2.09	1.97
51	-2.97	0.96	-2.98	0.95	-3.14	0.79
52	-4.16	0.23	-4.17	0.22	-4.33	0.06
53	-4.17	1.03	-4.19	1.02	-4.35	0.86
54	-3.37	2.04	-3.38	2.02	-3.54	1.86
55	-2.11	2.37	-2.13	2.35	-2.29	2.19
56	-3.17	2.92	-3.18	2.91	-3.34	2.75
57	-1.13	2.90	-1.14	2.88	-1.30	2.72
58	-1.39	2.67	-1.41	2.65	-1.57	2.49
59	-0.87	4.21	-0.89	4.20	-1.05	4.04
60	-2.58	2.17	-2.60	2.15	-2.76	1.99
61	-1.76	0.80	-1.78	0.79	-1.94	0.63
62	-1.71	0.72	-1.72	0.70	-1.88	0.54
63	-1.64	-0.33	-1.66	-0.34	-1.82	-0.50
64	-3.03	2.20	-3.05	2.18	-3.21	2.02
65	–	0.59	–	0.58	–	0.42

Electron Transfer Potentials - B3LYP-D3

Table S7: Summary of the computed electron transfer potentials at the B3LYP-D3/6-311++G**/SMD level of theory. The HCOOH/$HCOO^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.37	1.45	-2.34	1.49	-2.50	1.33
2	-3.13	1.88	-3.10	1.92	-3.26	1.76
3	-3.34	1.72	-3.30	1.75	-3.46	1.59
4	-2.09	1.47	-2.06	1.50	-2.22	1.34
5	-2.71	0.92	-2.67	0.95	-2.83	0.79
6	-2.82	1.27	-2.78	1.30	-2.94	1.14
7	-2.64	1.10	-2.60	1.14	-2.76	0.98
8	-2.33	1.44	-2.29	1.48	-2.45	1.32
9	-3.56	1.72	-3.52	1.75	-3.68	1.59
10	-3.41	1.72	-3.37	1.76	-3.53	1.60
11	-3.42	1.91	-3.38	1.94	-3.54	1.78
12	-3.18	1.64	-3.15	1.68	-3.31	1.52
13	-2.35	1.43	-2.32	1.47	-2.48	1.31
14	-2.93	1.20	-2.90	1.24	-3.06	1.08
15	-3.01	1.70	-2.98	1.73	-3.14	1.57
16	-2.34	2.09	-2.31	2.12	-2.47	1.96
17	-4.29	1.97	-4.26	2.00	-4.42	1.84
18	-3.16	1.59	-3.13	1.63	-3.29	1.47
19	-4.31	1.53	-4.28	1.56	-4.44	1.40
20	-3.12	0.92	-3.08	0.96	-3.24	0.80
21	-3.81	0.97	-3.78	1.00	-3.94	0.84
22	-3.22	0.68	-3.18	0.72	-3.34	0.56
23	-3.64	0.19	-3.61	0.22	-3.77	0.06
24	-3.28	0.64	-3.24	0.68	-3.40	0.52
25	-3.82	0.59	-3.78	0.62	-3.94	0.46
26	-3.34	0.45	-3.31	0.48	-3.47	0.32
27	-3.65	0.07	-3.61	0.10	-3.77	-0.06
28	-3.15	0.73	-3.11	0.76	-3.27	0.60
29	-2.78	1.65	-2.74	1.69	-2.90	1.53
30	-3.11	1.63	-3.07	1.66	-3.23	1.50
31	-3.72	1.25	-3.69	1.29	-3.85	1.13
32	-3.32	1.82	-3.28	1.85	-3.44	1.69
33	-3.15	0.85	-3.12	0.88	-3.28	0.72
34	-2.32	2.18	-2.29	2.22	-2.45	2.06
35	-3.45	1.27	-3.42	1.31	-3.58	1.15
36	-3.39	2.26	-3.36	2.30	-3.52	2.14

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
37	-2.98	1.13	-2.95	1.16	-3.11	1.00
38	-2.67	1.56	-2.63	1.60	-2.79	1.44
39	-2.75	1.61	-2.71	1.65	-2.87	1.49
40	unstable	3.74	unstable	3.77	unstable	3.61
41	unstable	4.70	unstable	4.73	unstable	4.57
42	unstable	3.32	unstable	3.35	unstable	3.19
43	unstable	2.03	unstable	2.06	unstable	1.90
44	unstable	4.15	unstable	4.18	unstable	4.02
45	-2.71	2.40	-2.68	2.44	-2.84	2.28
46	-1.78	2.52	-1.75	2.55	-1.91	2.39
47	-2.70	2.56	-2.66	2.59	-2.82	2.43
48	-2.86	2.21	-2.82	2.25	-2.98	2.09
49	-2.95	2.19	-2.91	2.23	-3.07	2.07
50	-1.98	2.40	-1.95	2.44	-2.11	2.28
51	-3.00	1.24	-2.96	1.28	-3.12	1.12
52	-3.88	0.42	-3.85	0.46	-4.01	0.30
53	-3.91	1.18	-3.87	1.21	-4.03	1.05
54	-3.34	2.18	-3.31	2.22	-3.47	2.06
55	-2.15	2.51	-2.11	2.55	-2.27	2.39
56	-3.14	3.17	-3.10	3.21	-3.26	3.05
57	-1.14	3.05	-1.11	3.09	-1.27	2.93
58	-1.44	2.75	-1.40	2.78	-1.56	2.62
59	-0.90	4.66	-0.86	4.70	-1.02	4.54
60	-2.59	2.35	-2.56	2.38	-2.72	2.22
61	-1.83	0.91	-1.79	0.94	-1.95	0.78
62	-1.77	0.88	-1.73	0.92	-1.89	0.76
63	-1.62	-0.30	-1.59	-0.27	-1.75	-0.43
64	-3.05	2.28	-3.01	2.32	-3.17	2.16
65	–	0.68	–	0.72	–	0.56

Electron Transfer Potentials - B3PW91-D3

Table S8: Summary of the computed electron transfer potentials at the B3PW91-D3/6-311++G**/SMD level of theory. The $HCOOH/HCOO^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.22	1.62	-2.27	1.56	-2.43	1.40
2	-3.00	2.09	-3.05	2.04	-3.21	1.88
3	-3.17	1.81	-3.22	1.76	-3.38	1.60
4	-1.92	1.63	-1.97	1.58	-2.13	1.42
5	-2.57	1.04	-2.62	0.98	-2.78	0.82
6	-2.70	1.40	-2.76	1.35	-2.92	1.19
7	-2.50	1.21	-2.56	1.16	-2.72	1.00
8	-2.18	1.64	-2.23	1.59	-2.39	1.43
9	-3.45	1.81	-3.51	1.76	-3.67	1.60
10	-3.30	1.82	-3.35	1.77	-3.51	1.61
11	-3.31	1.99	-3.36	1.94	-3.52	1.78
12	-3.12	1.72	-3.17	1.67	-3.33	1.51
13	-2.28	1.57	-2.33	1.52	-2.49	1.36
14	-2.84	1.31	-2.89	1.26	-3.05	1.10
15	-2.90	1.82	-2.96	1.77	-3.12	1.61
16	-2.22	2.22	-2.27	2.16	-2.43	2.00
17	-3.87	2.03	-3.92	1.98	-4.08	1.82
18	-2.97	1.68	-3.02	1.62	-3.18	1.46
19	-3.70	1.06	-3.75	1.01	-3.91	0.85
20	-3.02	1.04	-3.07	0.99	-3.23	0.83
21	-3.77	1.03	-3.82	0.98	-3.98	0.82
22	-3.08	0.81	-3.14	0.76	-3.30	0.60
23	-3.57	0.28	-3.63	0.23	-3.79	0.07
24	-3.10	0.73	-3.15	0.68	-3.31	0.52
25	-3.84	0.69	-3.89	0.63	-4.05	0.47
26	-3.24	0.56	-3.29	0.51	-3.45	0.35
27	-3.60	0.17	-3.65	0.12	-3.81	-0.04
28	-3.01	0.85	-3.06	0.80	-3.22	0.64
29	-2.67	1.79	-2.73	1.73	-2.89	1.57
30	-3.13	1.71	-3.18	1.66	-3.34	1.50
31	-3.56	1.31	-3.62	1.26	-3.78	1.10
32	-3.25	1.91	-3.30	1.86	-3.46	1.70
33	-3.04	0.99	-3.09	0.94	-3.25	0.78
34	-2.25	2.29	-2.31	2.24	-2.47	2.08
35	-3.44	1.35	-3.49	1.30	-3.65	1.14
36	-3.32	2.39	-3.37	2.34	-3.53	2.18

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
37	-2.85	1.27	-2.91	1.22	-3.07	1.06
38	-2.53	1.71	-2.58	1.66	-2.74	1.50
39	-2.64	1.75	-2.69	1.70	-2.85	1.54
40	unstable	3.82	unstable	3.77	unstable	3.61
41	unstable	4.80	unstable	4.74	unstable	4.58
42	unstable	3.39	unstable	3.34	unstable	3.18
43	unstable	2.15	unstable	2.09	unstable	1.93
44	unstable	4.24	unstable	4.19	unstable	4.03
45	-2.63	2.48	-2.68	2.42	-2.84	2.26
46	-1.66	2.66	-1.71	2.61	-1.87	2.45
47	-2.63	2.63	-2.68	2.58	-2.84	2.42
48	-2.78	2.28	-2.83	2.23	-2.99	2.07
49	-2.86	2.30	-2.92	2.25	-3.08	2.09
50	-1.85	2.52	-1.91	2.47	-2.07	2.31
51	-2.89	1.33	-2.94	1.27	-3.10	1.11
52	-3.89	0.55	-3.94	0.50	-4.10	0.34
53	-3.87	1.22	-3.93	1.17	-4.09	1.01
54	-3.30	2.26	-3.35	2.21	-3.51	2.05
55	-2.03	2.62	-2.08	2.57	-2.24	2.41
56	-3.10	3.25	-3.15	3.20	-3.31	3.04
57	-1.02	3.24	-1.08	3.19	-1.24	3.03
58	-1.36	2.89	-1.41	2.84	-1.57	2.68
59	-0.85	4.65	-0.90	4.60	-1.06	4.44
60	-2.48	2.43	-2.53	2.37	-2.69	2.21
61	-1.66	1.07	-1.71	1.02	-1.87	0.86
62	-1.63	1.07	-1.68	1.02	-1.84	0.86
63	-1.52	-0.17	-1.57	-0.22	-1.73	-0.38
64	-2.90	2.43	-2.95	2.38	-3.11	2.22
65	–	0.78	–	0.73	–	0.57

Electron Transfer Potentials - PBE0-D3

Table S9: Summary of the computed electron transfer potentials at the PBE0-D3/6-311++G**/SMD level of theory. The $HCOOH/HCOO^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.15	1.71	-2.32	1.55	-2.48	1.39
2	-2.92	2.14	-3.09	1.97	-3.25	1.81
3	-3.12	1.95	-3.29	1.78	-3.45	1.62
4	-1.86	1.74	-2.03	1.58	-2.19	1.42
5	-2.50	1.14	-2.67	0.97	-2.83	0.81
6	-2.64	1.50	-2.81	1.33	-2.97	1.17
7	-2.43	1.29	-2.59	1.12	-2.75	0.96
8	-2.10	1.74	-2.27	1.57	-2.43	1.41
9	-3.38	1.88	-3.54	1.71	-3.70	1.55
10	-3.22	1.90	-3.39	1.73	-3.55	1.57
11	-3.23	2.07	-3.40	1.90	-3.56	1.74
12	-3.04	1.78	-3.21	1.62	-3.37	1.46
13	-2.21	1.66	-2.38	1.49	-2.54	1.33
14	-2.76	1.39	-2.93	1.22	-3.09	1.06
15	-2.82	1.91	-2.99	1.74	-3.15	1.58
16	-2.15	2.30	-2.32	2.13	-2.48	1.97
17	-3.74	2.10	-3.91	1.93	-4.07	1.77
18	-2.89	1.77	-3.06	1.60	-3.22	1.44
19	-3.60	1.13	-3.77	0.96	-3.93	0.80
20	-2.93	1.12	-3.10	0.95	-3.26	0.79
21	-3.66	1.11	-3.83	0.94	-3.99	0.78
22	-3.00	0.90	-3.17	0.73	-3.33	0.57
23	-3.47	0.35	-3.64	0.18	-3.80	0.02
24	-3.07	0.85	-3.24	0.68	-3.40	0.52
25	-3.70	0.76	-3.87	0.59	-4.03	0.43
26	-3.16	0.65	-3.33	0.48	-3.49	0.32
27	-3.49	0.24	-3.66	0.07	-3.82	-0.09
28	-2.93	0.93	-3.10	0.76	-3.26	0.60
29	-2.61	1.88	-2.77	1.71	-2.93	1.55
30	-3.00	1.78	-3.17	1.61	-3.33	1.45
31	-3.52	1.39	-3.69	1.22	-3.85	1.06
32	-3.19	1.98	-3.36	1.81	-3.52	1.65
33	-2.98	1.09	-3.15	0.92	-3.31	0.76
34	-2.18	2.36	-2.35	2.19	-2.51	2.03
35	-3.36	1.42	-3.53	1.25	-3.69	1.09
36	-3.27	2.46	-3.43	2.29	-3.59	2.13

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
37	-2.78	1.36	-2.95	1.19	-3.11	1.03
38	-2.40	1.81	-2.57	1.64	-2.73	1.48
39	-2.57	1.84	-2.74	1.67	-2.90	1.51
40	unstable	3.92	unstable	3.75	unstable	3.59
41	unstable	4.93	unstable	4.76	unstable	4.60
42	unstable	3.54	unstable	3.37	unstable	3.21
43	unstable	2.22	unstable	2.06	unstable	1.90
44	unstable	4.38	unstable	4.21	unstable	4.05
45	-2.55	2.59	-2.72	2.42	-2.88	2.26
46	-1.59	2.97	-1.75	2.80	-1.91	2.64
47	-2.56	2.74	-2.73	2.57	-2.89	2.41
48	-2.70	2.39	-2.87	2.22	-3.03	2.06
49	-2.79	2.44	-2.96	2.27	-3.12	2.11
50	-1.78	2.65	-1.95	2.48	-2.11	2.32
51	-2.81	1.43	-2.98	1.26	-3.14	1.10
52	-3.76	1.21	-3.93	1.04	-4.09	0.88
53	-3.76	1.30	-3.93	1.14	-4.09	0.98
54	-3.22	2.34	-3.39	2.17	-3.55	2.01
55	-1.95	2.75	-2.12	2.58	-2.28	2.42
56	-3.02	3.34	-3.19	3.17	-3.35	3.01
57	-0.96	3.33	-1.13	3.17	-1.29	3.01
58	-1.29	2.96	-1.46	2.80	-1.62	2.64
59	-0.83	4.78	-1.00	4.61	-1.16	4.45
60	-2.40	2.50	-2.57	2.33	-2.73	2.17
61	-1.58	1.17	-1.75	1.00	-1.91	0.84
62	-1.52	1.19	-1.69	1.02	-1.85	0.86
63	-1.45	-0.14	-1.62	-0.31	-1.78	-0.47
64	-2.85	2.52	-3.02	2.35	-3.18	2.19
65	–	0.92	–	0.75	–	0.59

Electron Transfer Potentials - BHandH-D3

Table S10: Summary of the computed electron transfer potentials at the BHandH-D3/6-311++G**/SMD level of theory. The HCOOH/$HCOO^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.06	2.02	-2.63	1.44	-2.79	1.28
2	-2.80	2.45	-3.38	1.88	-3.54	1.72
3	-3.01	2.21	-3.59	1.63	-3.75	1.47
4	-1.81	2.11	-2.39	1.54	-2.55	1.38
5	-2.38	1.44	-2.96	0.86	-3.12	0.70
6	-2.57	1.78	-3.15	1.20	-3.31	1.04
7	-2.32	1.56	-2.89	0.98	-3.05	0.82
8	-1.99	2.08	-2.57	1.51	-2.73	1.35
9	-3.41	2.15	-3.99	1.57	-4.15	1.41
10	-3.11	2.20	-3.69	1.62	-3.85	1.46
11	-3.08	2.33	-3.66	1.75	-3.82	1.59
12	-3.02	1.99	-3.60	1.41	-3.76	1.25
13	-2.11	1.96	-2.69	1.39	-2.85	1.23
14	-2.61	1.69	-3.19	1.11	-3.35	0.95
15	-2.70	2.19	-3.27	1.61	-3.43	1.45
16	-2.05	2.61	-2.62	2.03	-2.78	1.87
17	-3.54	2.64	-4.12	2.07	-4.28	1.91
18	-2.76	2.08	-3.34	1.50	-3.50	1.34
19	-3.41	1.37	-3.99	0.79	-4.15	0.63
20	-2.80	1.36	-3.38	0.79	-3.54	0.63
21	-3.46	1.41	-4.04	0.83	-4.20	0.67
22	-2.87	1.17	-3.44	0.59	-3.60	0.43
23	-3.34	0.65	-3.92	0.07	-4.08	-0.09
24	-2.88	1.09	-3.46	0.52	-3.62	0.36
25	-3.47	1.09	-4.05	0.51	-4.21	0.35
26	-3.04	0.92	-3.61	0.34	-3.77	0.18
27	-3.37	0.52	-3.95	-0.06	-4.11	-0.22
28	-2.77	1.17	-3.35	0.59	-3.51	0.43
29	-2.51	2.18	-3.09	1.61	-3.25	1.45
30	-2.92	2.03	-3.50	1.45	-3.66	1.29
31	-3.45	1.63	-4.03	1.05	-4.19	0.89
32	-3.10	2.23	-3.68	1.65	-3.84	1.49
33	-2.92	1.41	-3.50	0.84	-3.66	0.68
34	-2.02	2.62	-2.60	2.04	-2.76	1.88
35	-3.20	1.70	-3.77	1.12	-3.93	0.96
36	-3.21	2.72	-3.78	2.15	-3.94	1.99

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
37	-2.68	1.64	-3.26	1.06	-3.42	0.90
38	-2.36	2.13	-2.93	1.55	-3.09	1.39
39	-2.49	2.13	-3.06	1.55	-3.22	1.39
40	unstable	4.62	unstable	4.05	unstable	3.89
41	unstable	5.42	unstable	4.84	unstable	4.68
42	unstable	4.04	unstable	3.47	unstable	3.31
43	unstable	2.60	unstable	2.03	unstable	1.87
44	unstable	5.07	unstable	4.49	unstable	4.33
45	-2.41	3.10	-2.99	2.52	-3.15	2.36
46	-1.46	3.31	-2.04	2.73	-2.20	2.57
47	-2.44	3.13	-3.02	2.55	-3.18	2.39
48	-2.58	2.83	-3.16	2.26	-3.32	2.10
49	-2.68	2.92	-3.25	2.34	-3.41	2.18
50	-1.66	3.16	-2.24	2.59	-2.40	2.43
51	-2.69	1.91	-3.27	1.33	-3.43	1.17
52	-3.59	1.68	-4.17	1.10	-4.33	0.94
53	-3.50	1.64	-4.08	1.06	-4.24	0.90
54	-3.12	2.67	-3.70	2.09	-3.86	1.93
55	-1.83	3.00	-2.41	2.42	-2.57	2.26
56	-2.94	3.90	-3.52	3.32	-3.68	3.16
57	-0.82	3.60	-1.40	3.02	-1.56	2.86
58	-1.15	3.19	-1.73	2.61	-1.89	2.45
59	-0.72	5.37	-1.29	4.79	-1.45	4.63
60	-2.27	2.76	-2.84	2.18	-3.00	2.02
61	-1.48	1.46	-2.05	0.88	-2.21	0.72
62	-1.38	1.42	-1.96	0.85	-2.12	0.69
63	-1.26	0.10	-1.84	-0.47	-2.00	-0.63
64	-2.79	2.79	-3.37	2.22	-3.53	2.06
65	–	1.16	–	0.58	–	0.42

Electron Transfer Potentials - M06-2X

Table S11: Summary of the computed electron transfer potentials at the M06-2X/6-311++G**/SMD level of theory. The HCOOH/$HCOO^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.24	1.90	-2.35	1.79	-2.51	1.63
2	-3.06	2.36	-3.17	2.24	-3.33	2.08
3	-3.22	2.11	-3.33	2.00	-3.49	1.84
4	-2.01	2.01	-2.13	1.90	-2.29	1.74
5	-2.59	1.40	-2.71	1.29	-2.87	1.13
6	-2.77	1.67	-2.88	1.55	-3.04	1.39
7	-2.55	1.47	-2.66	1.36	-2.82	1.20
8	-2.21	1.96	-2.32	1.85	-2.48	1.69
9	-3.52	2.03	-3.63	1.92	-3.79	1.76
10	-3.34	2.00	-3.46	1.89	-3.62	1.73
11	-3.37	2.15	-3.48	2.03	-3.64	1.87
12	-3.18	1.96	-3.29	1.85	-3.45	1.69
13	-2.32	1.87	-2.43	1.76	-2.59	1.60
14	-2.82	1.54	-2.93	1.43	-3.09	1.27
15	-2.89	2.04	-3.01	1.93	-3.17	1.77
16	-2.26	2.47	-2.37	2.36	-2.53	2.20
17	-4.00	2.34	-4.11	2.23	-4.27	2.07
18	-2.97	1.92	-3.08	1.80	-3.24	1.64
19	-3.75	1.31	-3.86	1.20	-4.02	1.04
20	-2.99	1.27	-3.10	1.16	-3.26	1.00
21	-3.80	1.32	-3.91	1.21	-4.07	1.05
22	-3.09	1.09	-3.20	0.98	-3.36	0.82
23	-3.54	0.52	-3.65	0.41	-3.81	0.25
24	-3.13	1.03	-3.24	0.92	-3.40	0.76
25	-3.82	0.93	-3.93	0.82	-4.09	0.66
26	-3.20	0.80	-3.31	0.68	-3.47	0.52
27	-3.52	0.39	-3.63	0.28	-3.79	0.12
28	-2.98	1.08	-3.09	0.97	-3.25	0.81
29	-2.73	2.05	-2.85	1.94	-3.01	1.78
30	-3.28	1.92	-3.39	1.81	-3.55	1.65
31	-3.57	1.50	-3.69	1.39	-3.85	1.23
32	-3.30	2.09	-3.41	1.98	-3.57	1.82
33	-3.07	1.27	-3.18	1.16	-3.34	1.00
34	-2.26	2.42	-2.37	2.31	-2.53	2.15
35	-3.54	1.57	-3.65	1.46	-3.81	1.30
36	-3.34	2.53	-3.45	2.42	-3.61	2.26

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
37	-2.87	1.52	-2.98	1.41	-3.14	1.25
38	-2.55	1.99	-2.66	1.88	-2.82	1.72
39	-2.68	2.01	-2.80	1.90	-2.96	1.74
40	unstable	4.12	unstable	4.01	unstable	3.85
41	unstable	5.19	unstable	5.08	unstable	4.92
42	unstable	3.32	unstable	3.20	unstable	3.04
43	unstable	2.17	unstable	2.06	unstable	1.90
44	unstable	4.83	unstable	4.72	unstable	4.56
45	-2.66	2.81	-2.77	2.70	-2.93	2.54
46	-1.70	3.20	-1.81	3.09	-1.97	2.93
47	-2.68	2.91	-2.79	2.80	-2.95	2.64
48	-2.83	2.56	-2.94	2.45	-3.10	2.29
49	-2.91	2.62	-3.02	2.51	-3.18	2.35
50	-1.90	2.88	-2.01	2.77	-2.17	2.61
51	-2.91	1.73	-3.02	1.61	-3.18	1.45
52	-3.90	1.44	-4.01	1.32	-4.17	1.16
53	-3.92	1.54	-4.03	1.43	-4.19	1.27
54	-3.29	2.52	-3.41	2.41	-3.57	2.25
55	-2.04	2.95	-2.16	2.84	-2.32	2.68
56	-3.14	3.56	-3.25	3.45	-3.41	3.29
57	-1.05	3.38	-1.16	3.27	-1.32	3.11
58	-1.40	3.10	-1.51	2.99	-1.67	2.83
59	-0.90	5.23	-1.01	5.12	-1.17	4.96
60	-2.49	2.69	-2.60	2.58	-2.76	2.42
61	-1.66	1.36	-1.77	1.25	-1.93	1.09
62	-1.59	1.36	-1.70	1.25	-1.86	1.09
63	-1.42	-0.19	-1.53	-0.30	-1.69	-0.46
64	-3.00	2.63	-3.11	2.52	-3.27	2.36
65	–	1.09	–	0.98	–	0.82

Electron Transfer Potentials - M06-HF

Table S12: Summary of the computed electron transfer potentials at the M06-HF/6-311++G**/SMD level of theory. The HCOOH/$HCOO^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.23	2.13	-2.26	2.10	-2.42	1.94
2	-2.96	2.49	-2.99	2.46	-3.15	2.30
3	-3.07	2.33	-3.11	2.30	-3.27	2.14
4	-2.05	2.32	-2.08	2.29	-2.24	2.13
5	-2.54	1.68	-2.58	1.64	-2.74	1.48
6	-2.78	1.87	-2.81	1.84	-2.97	1.68
7	-2.56	1.68	-2.59	1.65	-2.75	1.49
8	-2.28	2.23	-2.31	2.20	-2.47	2.04
9	-3.46	2.17	-3.49	2.14	-3.65	1.98
10	-3.38	2.06	-3.41	2.02	-3.57	1.86
11	-3.36	2.15	-3.39	2.12	-3.55	1.96
12	-3.19	2.15	-3.22	2.11	-3.38	1.95
13	-2.36	2.18	-2.39	2.15	-2.55	1.99
14	-2.74	1.75	-2.77	1.71	-2.93	1.55
15	-2.87	2.21	-2.90	2.18	-3.06	2.02
16	-2.23	2.71	-2.27	2.68	-2.43	2.52
17	-3.66	2.42	-3.69	2.38	-3.85	2.22
18	-2.93	2.07	-2.96	2.03	-3.12	1.87
19	-3.60	1.33	-3.63	1.30	-3.79	1.14
20	-2.96	1.39	-2.99	1.36	-3.15	1.20
21	-3.60	1.29	-3.64	1.26	-3.80	1.10
22	-3.04	1.20	-3.07	1.17	-3.23	1.01
23	-3.34	0.61	-3.38	0.58	-3.54	0.42
24	-2.99	1.10	-3.02	1.06	-3.18	0.90
25	-3.63	1.04	-3.66	1.00	-3.82	0.84
26	-3.09	0.92	-3.12	0.88	-3.28	0.72
27	-3.36	0.50	-3.39	0.46	-3.55	0.30
28	-2.39	1.24	-2.42	1.21	-2.58	1.05
29	-2.66	2.19	-2.69	2.15	-2.85	1.99
30	-3.14	2.07	-3.18	2.04	-3.34	1.88
31	-3.56	1.59	-3.59	1.56	-3.75	1.40
32	-3.34	2.22	-3.38	2.19	-3.54	2.03
33	-2.96	1.42	-2.99	1.39	-3.15	1.23
34	-2.18	2.38	-2.21	2.35	-2.37	2.19
35	-3.35	1.71	-3.38	1.68	-3.54	1.52
36	-3.36	2.60	-3.39	2.57	-3.55	2.41

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
37	-2.82	1.69	-2.85	1.66	-3.01	1.50
38	-2.54	2.21	-2.57	2.17	-2.73	2.01
39	-2.66	2.20	-2.69	2.17	-2.85	2.01
40	unstable	4.51	unstable	4.48	unstable	4.32
41	unstable	5.33	unstable	5.30	unstable	5.14
42	unstable	4.13	unstable	4.10	unstable	3.94
43	unstable	2.98	unstable	2.95	unstable	2.79
44	unstable	5.23	unstable	5.19	unstable	5.03
45	-2.65	2.90	-2.68	2.87	-2.84	2.71
46	-1.70	3.40	-1.73	3.37	-1.89	3.21
47	-2.63	3.04	-2.66	3.01	-2.82	2.85
48	-2.78	2.64	-2.81	2.60	-2.97	2.44
49	-2.87	2.67	-2.90	2.64	-3.06	2.48
50	-1.88	3.22	-1.92	3.19	-2.08	3.03
51	-2.80	2.53	-2.83	2.50	-2.99	2.34
52	-3.75	1.59	-3.79	1.56	-3.95	1.40
53	-3.66	1.69	-3.69	1.66	-3.85	1.50
54	-3.44	2.70	-3.47	2.67	-3.63	2.51
55	-2.02	3.13	-2.05	3.10	-2.21	2.94
56	-3.43	3.67	-3.46	3.64	-3.62	3.48
57	-0.99	3.56	-1.02	3.53	-1.18	3.37
58	-1.31	2.60	-1.34	2.57	-1.50	2.41
59	-0.72	5.68	-0.75	5.65	-0.91	5.49
60	-2.47	2.86	-2.51	2.83	-2.67	2.67
61	-1.66	1.63	-1.69	1.60	-1.85	1.44
62	-1.53	1.70	-1.56	1.67	-1.72	1.51
63	-1.21	-0.16	-1.24	-0.19	-1.40	-0.35
64	-2.97	2.74	-3.01	2.71	-3.17	2.55
65	–	1.23	–	1.20	–	1.04

Electron Transfer Potentials - ωB97X-D

Table S13: Summary of the computed electron transfer potentials at the ωB97X-D/6-311++G**/SMD level of theory. The HCOOH/$HCOO^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.32	1.69	-2.40	1.60	-2.56	1.44
2	-3.12	2.19	-3.21	2.10	-3.37	1.94
3	-3.32	1.93	-3.40	1.84	-3.56	1.68
4	-2.13	1.80	-2.22	1.71	-2.38	1.55
5	-2.63	1.15	-2.72	1.06	-2.88	0.90
6	-2.81	1.49	-2.90	1.40	-3.06	1.24
7	-2.60	1.28	-2.68	1.19	-2.84	1.03
8	-2.39	1.79	-2.47	1.70	-2.63	1.54
9	-4.06	1.87	-4.15	1.79	-4.31	1.63
10	-4.15	1.88	-4.24	1.79	-4.40	1.63
11	-3.41	2.04	-3.50	1.96	-3.66	1.80
12	-3.47	1.80	-3.56	1.72	-3.72	1.56
13	-2.41	1.68	-2.49	1.60	-2.65	1.44
14	-2.90	1.35	-2.99	1.26	-3.15	1.10
15	-2.97	1.85	-3.06	1.76	-3.22	1.60
16	-2.30	2.26	-2.39	2.17	-2.55	2.01
17	-4.18	2.17	-4.27	2.09	-4.43	1.93
18	-3.00	1.71	-3.08	1.62	-3.24	1.46
19	-4.19	1.14	-4.28	1.06	-4.44	0.90
20	-3.08	1.08	-3.17	0.99	-3.33	0.83
21	-4.19	1.13	-4.27	1.04	-4.43	0.88
22	-3.15	0.87	-3.24	0.79	-3.40	0.63
23	-3.91	0.34	-4.00	0.25	-4.16	0.09
24	-3.21	0.82	-3.29	0.73	-3.45	0.57
25	-4.20	0.73	-4.28	0.65	-4.44	0.49
26	-3.27	0.61	-3.35	0.53	-3.51	0.37
27	-3.99	0.21	-4.08	0.13	-4.24	-0.03
28	-3.06	0.89	-3.15	0.81	-3.31	0.65
29	-2.80	1.88	-2.89	1.79	-3.05	1.63
30	-3.42	1.74	-3.51	1.66	-3.67	1.50
31	-3.72	1.27	-3.80	1.19	-3.96	1.03
32	-4.17	1.92	-4.25	1.84	-4.41	1.68
33	-3.14	1.07	-3.23	0.98	-3.39	0.82
34	-2.28	1.88	-2.37	1.79	-2.53	1.63
35	-3.65	1.41	-3.73	1.32	-3.89	1.16
36	-3.70	2.39	-3.79	2.30	-3.95	2.14

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
37	-2.94	1.32	-3.02	1.24	-3.18	1.08
38	-2.62	1.80	-2.70	1.71	-2.86	1.55
39	-2.75	1.80	-2.84	1.72	-3.00	1.56
40	unstable	3.90	unstable	3.81	unstable	3.65
41	unstable	5.02	unstable	4.93	unstable	4.77
42	unstable	3.67	unstable	3.58	unstable	3.42
43	unstable	2.22	unstable	2.13	unstable	1.97
44	unstable	4.69	unstable	4.60	unstable	4.44
45	-2.70	2.70	-2.78	2.61	-2.94	2.45
46	-1.75	3.02	-1.84	2.94	-2.00	2.78
47	-2.73	2.79	-2.82	2.70	-2.98	2.54
48	-2.87	2.44	-2.96	2.36	-3.12	2.20
49	-2.95	2.51	-3.04	2.42	-3.20	2.26
50	-1.96	2.87	-2.05	2.79	-2.21	2.63
51	-2.96	1.48	-3.05	1.39	-3.21	1.23
52	-4.15	1.19	-4.23	1.10	-4.39	0.94
53	-4.11	1.37	-4.20	1.28	-4.36	1.12
54	-3.39	2.36	-3.47	2.27	-3.63	2.11
55	-2.13	2.63	-2.21	2.55	-2.37	2.39
56	-3.18	3.38	-3.27	3.30	-3.43	3.14
57	-1.12	3.21	-1.20	3.12	-1.36	2.96
58	-1.46	2.90	-1.54	2.82	-1.70	2.66
59	-1.05	4.92	-1.13	4.84	-1.29	4.68
60	-2.53	2.52	-2.62	2.43	-2.78	2.27
61	-1.77	1.16	-1.86	1.07	-2.02	0.91
62	-1.71	1.13	-1.79	1.05	-1.95	0.89
63	-1.51	-0.25	-1.59	-0.33	-1.75	-0.49
64	-3.01	2.45	-3.10	2.37	-3.26	2.21
65	–	0.91	–	0.82	–	0.66

Electron Transfer Potentials - HSE06

Table S14: Summary of the computed electron transfer potentials at the HSE06/6-311++G**/SMD level of theory. The HCOOH/$HCOO^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.16	1.68	-2.31	1.53	-2.47	1.37
2	-2.94	2.14	-3.09	1.99	-3.25	1.83
3	-3.12	1.89	-3.27	1.74	-3.43	1.58
4	-1.86	1.70	-2.01	1.55	-2.17	1.39
5	-2.51	1.10	-2.66	0.95	-2.82	0.79
6	-2.65	1.46	-2.80	1.31	-2.96	1.15
7	-2.44	1.26	-2.59	1.11	-2.75	0.95
8	-2.10	1.69	-2.25	1.54	-2.41	1.38
9	-3.42	1.85	-3.57	1.70	-3.73	1.54
10	-3.24	1.87	-3.39	1.72	-3.55	1.56
11	-3.20	2.01	-3.35	1.86	-3.51	1.70
12	-3.04	1.75	-3.20	1.60	-3.36	1.44
13	-2.22	1.62	-2.37	1.47	-2.53	1.31
14	-2.77	1.36	-2.92	1.21	-3.08	1.05
15	-2.84	1.88	-2.99	1.73	-3.15	1.57
16	-2.17	2.27	-2.32	2.12	-2.48	1.96
17	-3.73	2.11	-3.88	1.96	-4.04	1.80
18	-2.91	1.74	-3.07	1.59	-3.23	1.43
19	-3.54	1.10	-3.70	0.95	-3.86	0.79
20	-2.94	1.09	-3.09	0.94	-3.25	0.78
21	-3.66	1.07	-3.81	0.92	-3.97	0.76
22	-3.02	0.87	-3.17	0.72	-3.33	0.56
23	-3.47	0.36	-3.63	0.21	-3.79	0.05
24	-3.05	0.74	-3.20	0.59	-3.36	0.43
25	-3.69	0.72	-3.84	0.57	-4.00	0.41
26	-3.18	0.62	-3.33	0.47	-3.49	0.31
27	-3.49	0.22	-3.64	0.07	-3.80	-0.09
28	-2.90	0.90	-3.05	0.75	-3.21	0.59
29	-2.61	1.85	-2.76	1.70	-2.92	1.54
30	-3.00	1.76	-3.15	1.61	-3.31	1.45
31	-3.78	1.35	-3.93	1.20	-4.09	1.04
32	-3.20	1.95	-3.35	1.80	-3.51	1.64
33	-3.00	1.06	-3.15	0.91	-3.31	0.75
34	-2.20	2.34	-2.35	2.19	-2.51	2.03
35	-3.36	1.40	-3.51	1.25	-3.67	1.09
36	-3.48	2.43	-3.63	2.28	-3.79	2.12

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
37	-2.80	1.33	-2.95	1.18	-3.11	1.02
38	-2.47	1.72	-2.62	1.57	-2.78	1.41
39	-2.59	1.81	-2.74	1.66	-2.90	1.50
40	unstable	3.88	unstable	3.73	unstable	3.57
41	unstable	4.87	unstable	4.72	unstable	4.56
42	unstable	3.48	unstable	3.33	unstable	3.17
43	unstable	2.17	unstable	2.02	unstable	1.86
44	unstable	4.06	unstable	3.91	unstable	3.75
45	-2.56	2.56	-2.71	2.41	-2.87	2.25
46	-1.60	2.94	-1.75	2.79	-1.91	2.63
47	-2.55	2.71	-2.70	2.56	-2.86	2.40
48	-2.71	2.36	-2.86	2.21	-3.02	2.05
49	-2.80	2.42	-2.95	2.27	-3.11	2.11
50	-1.79	2.61	-1.94	2.46	-2.10	2.30
51	-2.82	1.40	-2.97	1.25	-3.13	1.09
52	-3.73	1.19	-3.88	1.04	-4.04	0.88
53	-3.78	1.30	-3.93	1.15	-4.09	0.99
54	-3.22	2.31	-3.37	2.16	-3.53	2.00
55	-1.97	2.72	-2.12	2.57	-2.28	2.41
56	-3.03	3.31	-3.18	3.16	-3.34	3.00
57	-0.97	3.25	-1.12	3.10	-1.28	2.94
58	-1.30	2.93	-1.45	2.78	-1.61	2.62
59	-0.83	4.75	-0.98	4.60	-1.14	4.44
60	-2.42	2.47	-2.57	2.32	-2.73	2.16
61	-1.60	1.13	-1.75	0.98	-1.91	0.82
62	-1.55	1.11	-1.70	0.96	-1.86	0.80
63	-1.47	-0.11	-1.62	-0.26	-1.78	-0.42
64	-2.83	2.49	-2.98	2.34	-3.14	2.18
65	–	0.91	–	0.76	–	0.60

Electron Transfer Potentials - M06-2X/PCM

HCOOH/HCOO$^-$ Reference

Table S15: Summary of the computed electron transfer potentials at the M06-2X/6-311++G**/PCM level of theory. The HCOOH/HCOO$^-$ acid-base couple was used to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

	Effective absolute potential		E_{abs}(nhe) = 4.28V		E_{abs}(nhe) = 4.44V	
Compound	Reduction	Oxidation	Reduction	Oxidation	Reduction	Oxidation
1	-2.10	2.30	-2.34	2.06	-2.50	1.90
2	-2.98	2.79	-3.22	2.54	-3.38	2.38
3	-3.05	2.46	-3.29	2.22	-3.45	2.06
4	-1.89	2.38	-2.13	2.14	-2.29	1.98
5	-2.41	1.71	-2.65	1.47	-2.81	1.31
6	-2.62	2.02	-2.86	1.78	-3.02	1.62
7	-2.46	1.92	-2.70	1.67	-2.86	1.51
8	-2.09	2.38	-2.33	2.13	-2.49	1.97
9	-3.41	2.54	-3.65	2.30	-3.81	2.14
10	-3.30	2.46	-3.54	2.22	-3.70	2.06
11	-3.22	2.65	-3.46	2.41	-3.62	2.25
12	-3.06	2.42	-3.30	2.18	-3.46	2.02
13	-2.09	2.21	-2.34	1.97	-2.50	1.81
14	-2.67	1.91	-2.91	1.67	-3.07	1.51
15	-2.80	2.43	-3.04	2.19	-3.20	2.03
16	-2.11	2.89	-2.35	2.64	-2.51	2.48
17	-3.71	2.84	-3.95	2.59	-4.11	2.43
18	-2.86	2.32	-3.10	2.08	-3.26	1.92
19	-3.28	1.77	-3.52	1.53	-3.68	1.37
20	-2.92	1.68	-3.16	1.44	-3.32	1.28
21	-3.32	1.81	-3.56	1.57	-3.72	1.41
22	-3.03	1.52	-3.27	1.27	-3.43	1.11
23	-3.25	0.95	-3.49	0.71	-3.65	0.55
24	-3.01	1.40	-3.25	1.16	-3.41	1.00
25	-3.39	1.47	-3.64	1.23	-3.80	1.07
26	-3.08	1.25	-3.32	1.01	-3.48	0.85
27	-3.33	0.79	-3.57	0.55	-3.73	0.39
28	-2.99	1.51	-3.23	1.27	-3.39	1.11
29	-2.56	2.35	-2.81	2.11	-2.97	1.95
30	-2.91	2.38	-3.16	2.14	-3.32	1.98
31	-3.34	1.89	-3.58	1.65	-3.74	1.49
32	-3.14	2.52	-3.39	2.28	-3.55	2.12
33	-2.93	1.63	-3.17	1.39	-3.33	1.23

Compound	Effective absolute potential Reduction	Oxidation	E_{abs}(nhe) = 4.28V Reduction	Oxidation	E_{abs}(nhe) = 4.44V Reduction	Oxidation
34	-1.93	2.65	-2.17	2.40	-2.33	2.24
35	-3.15	1.98	-3.39	1.74	-3.55	1.58
36	-3.21	2.99	-3.45	2.75	-3.61	2.59
37	-2.76	1.91	-3.00	1.67	-3.16	1.51
38	-2.41	2.31	-2.65	2.06	-2.81	1.90
39	-2.54	2.40	-2.78	2.16	-2.94	2.00
40	unstable	4.02	unstable	3.77	unstable	3.61
41	unstable	5.13	unstable	4.89	unstable	4.73
42	unstable	4.07	unstable	3.83	unstable	3.67
43	unstable	3.28	unstable	3.04	unstable	2.88
44	unstable	5.08	unstable	4.84	unstable	4.68
45	-2.35	3.32	-2.59	3.07	-2.75	2.91
46	-1.44	3.65	-1.68	3.41	-1.84	3.25
47	-2.35	3.45	-2.60	3.21	-2.76	3.05
48	-2.50	3.02	-2.74	2.78	-2.90	2.62
49	-2.61	3.09	-2.85	2.84	-3.01	2.68
50	-1.62	3.44	-1.87	3.19	-2.03	3.03
51	-2.75	2.12	-2.99	1.87	-3.15	1.71
52	-3.54	1.85	-3.78	1.61	-3.94	1.45
53	-3.58	1.96	-3.82	1.72	-3.98	1.56
54	-2.99	3.06	-3.23	2.82	-3.39	2.66
55	-1.81	3.35	-2.05	3.11	-2.21	2.95
56	-2.77	3.97	-3.02	3.73	-3.18	3.57
57	-0.73	3.96	-0.97	3.72	-1.13	3.56
58	-1.13	3.49	-1.37	3.25	-1.53	3.09
59	-0.70	5.39	-0.95	5.14	-1.11	4.98
60	-2.38	3.11	-2.62	2.87	-2.78	2.71
61	-1.49	1.75	-1.74	1.51	-1.90	1.35
62	-1.47	1.73	-1.71	1.49	-1.87	1.33
63	-1.15	0.15	-1.39	-0.10	-1.55	-0.26
64	-2.93	3.07	-3.17	2.82	-3.33	2.66
65	–	1.48	–	1.23	–	1.07

Pentafluorothiophenol Reference

Table S16: Summary of the computed electron transfer potentials at the M06-2X/6-311++G**/PCM level of theory obtained using the effective absolute potential method. Pentafluorothiophenol was used as reference to compute the effective absolute potential. All potentials are stated in [V] vs. nhe in water.

Compound	Reduction	Oxidation
1	-2.56	1.84
2	-3.44	2.32
3	-3.51	2.00
4	-2.35	1.92
5	-2.87	1.25
6	-3.08	1.56
7	-2.92	1.45
8	-2.55	1.91
9	-3.87	2.08
10	-3.76	2.00
11	-3.68	2.19
12	-3.52	1.96
13	-2.56	1.75
14	-3.13	1.45
15	-3.26	1.97
16	-2.57	2.42
17	-4.17	2.37
18	-3.32	1.86
19	-3.74	1.31
20	-3.38	1.22
21	-3.78	1.35
22	-3.49	1.05
23	-3.71	0.49
24	-3.47	0.94
25	-3.86	1.01
26	-3.54	0.79
27	-3.79	0.33
28	-3.45	1.05
29	-3.03	1.89
30	-3.38	1.92
31	-3.80	1.43
32	-3.61	2.06
33	-3.39	1.17
34	-2.39	2.18
35	-3.61	1.52
36	-3.67	2.53

Compound	Reduction	Oxidation
37	-3.22	1.45
38	-2.87	1.84
39	-3.00	1.94
40	unstable	3.55
41	unstable	4.67
42	unstable	3.61
43	unstable	2.82
44	unstable	4.62
45	-2.81	2.85
46	-1.90	3.19
47	-2.82	2.99
48	-2.96	2.56
49	-3.07	2.62
50	-2.09	2.97
51	-3.21	1.65
52	-4.00	1.39
53	-4.04	1.50
54	-3.45	2.60
55	-2.27	2.89
56	-3.24	3.51
57	-1.19	3.50
58	-1.59	3.03
59	-1.17	4.92
60	-2.84	2.65
61	-1.96	1.29
62	-1.93	1.27
63	-1.61	-0.32
64	-3.39	2.60
65	–	1.01

Summary of Gibbs Free Energies - B97D

Table S17: Summary of the Gibbs free energies obtained at the B97D/6-311++G**/SMD level of theory. All energies are stated in [Ha].

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
1	-385.660978	-385.588751	-385.382773
2	-271.385824	-271.344857	-271.118214
3	-349.932516	-349.893803	-349.681158
4	-539.132414	-539.047939	-538.843465
5	-537.196858	-537.137016	-536.953756
6	-669.588258	-669.533085	-669.334526
7	-233.28375	-233.222249	-233.028477
8	-540.344755	-540.270355	-540.064612
9	-195.154802	-195.152099	-194.936577
10	-272.513383	-272.480511	-272.265383
11	-235.657072	-235.626305	-235.405208
12	-271.596498	-271.556383	-271.340448
13	-2923.606437	-2923.536681	-2923.332979
14	-382.53014	-382.480464	-382.2842
15	-307.322253	-307.275682	-307.06043
16	-399.560722	-399.488809	-399.26019
17	-307.46836	-307.465988	-307.24832
18	-346.572081	-346.528148	-346.319451
19	-251.691111	-251.680205	-251.491808
20	-287.442375	-287.400248	-287.212661
21	-292.161301	-292.151613	-291.963323
22	-518.489712	-518.45083	-518.272388
23	-520.832819	-520.810932	-520.650673
24	-365.958258	-365.921188	-365.743457
25	-292.144353	-292.137172	-291.962045
26	-342.763838	-342.72979	-342.560502
27	-445.653718	-445.631814	-445.475942
28	-326.71593	-326.673872	-326.493891
29	-630.343929	-630.287981	-630.075497
30	-344.407307	-344.364031	-344.151075
31	-249.301921	-249.295055	-249.096549
32	-229.923291	-229.888256	-229.667728
33	-478.061226	-478.017122	-477.834276
34	-797.788504	-797.715232	-797.504596
35	-301.331052	-301.289366	-301.090144
36	-226.105551	-226.073482	-225.835764
37	-363.605925	-363.556739	-363.362187
38	-706.506702	-706.445902	-706.236849

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
39	-383.473574	-383.416669	-383.205145
40	unstable	-5190.184635	-5189.895919
41	unstable	-1879.027276	-1878.713499
42	unstable	-2882.377429	-2882.113848
43	unstable	-13886.222215	-13885.996951
44	unstable	-999.046765	-998.763252
45	-348.97962	-348.923222	-348.691605
46	-345.446879	-345.354393	-345.111978
47	-271.630406	-271.574945	-271.335392
48	-309.712972	-309.661519	-309.434413
49	-388.25351	-388.205935	-387.982059
50	-384.722113	-384.635822	-384.400296
51	-420.171764	-420.124053	-419.931988
52	-385.61841	-385.614431	-385.449016
53	-228.534731	-228.531363	-228.336772
54	-325.764006	-325.731103	-325.499472
55	-459.920882	-459.841738	-459.597967
56	-306.370292	-306.329985	-306.065791
57	-532.800788	-532.685496	-532.422324
58	-805.124737	-805.019113	-804.764332
59	-977.038823	-976.914097	-976.602524
60	-248.17674	-248.114818	-247.87845
61	-539.197003	-539.105015	-538.918873
62	-1000.928032	-1000.833938	-1000.650879
63	-381.504637	-381.408212	-381.263478
64	-232.112665	-232.067375	-231.829911
65	unstable	-2940.776581	-2940.598055
H2		-1.184552	
HCOOH		-189.715036	
$HCOO^-$		-189.271308	

Summary of Gibbs Free Energies - B3LYP-D3

Table S18: Summary of the Gibbs free energies obtained at the B3LYP-D3/6-311++G**/SMD level of theory. All energies are stated in [Ha].

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
1	-385.969006	-385.897532	-385.685501
2	-271.601095	-271.557651	-271.329918
3	-350.207927	-350.171939	-349.950339
4	-539.561102	-539.479344	-539.26689
5	-537.589789	-537.530799	-537.338513
6	-669.804415	-669.749382	-669.544247
7	-233.467714	-233.406079	-233.206989
8	-540.772723	-540.699721	-540.488116
9	-195.33353	-195.305734	-195.083956
10	-272.728854	-272.695587	-272.473769
11	-235.839819	-235.806905	-235.578244
12	-271.791894	-271.750307	-271.531301
13	-2922.588852	-2922.51676	-2922.305536
14	-382.801544	-382.750715	-382.54801
15	-307.551225	-307.5033	-307.282283
16	-399.85533	-399.782801	-399.547528
17	-307.677651	-307.676891	-307.445992
18	-346.830732	-346.788385	-346.571263
19	-251.889712	-251.889684	-251.67489
20	-287.665715	-287.621668	-287.429219
21	-292.38745	-292.368982	-292.174848
22	-518.879892	-518.839512	-518.655779
23	-521.222598	-521.197854	-521.032367
24	-366.240104	-366.201962	-366.019842
25	-292.371917	-292.353624	-292.173538
26	-343.023512	-342.987815	-342.812835
27	-445.999482	-445.975008	-445.814002
28	-326.968443	-326.925525	-326.740223
29	-630.532835	-630.476347	-630.25697
30	-344.647808	-344.603398	-344.385037
31	-249.509852	-249.488117	-249.283464
32	-230.090029	-230.053288	-229.827902
33	-478.41739	-478.374614	-478.184822
34	-798.087136	-798.013965	-797.775152
35	-301.529199	-301.497574	-301.292217
36	-226.27119	-226.237205	-225.995532
37	-363.889916	-363.840911	-363.640815
38	-706.756957	-706.696466	-706.48054

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
39	-383.764168	-383.7065	-383.488731
40	unstable	-5187.622299	-5187.326319
41	unstable	-1879.012145	-1878.680903
42	unstable	-2881.289522	-2881.009105
43	unstable	-13878.383762	-13878.150724
44	unstable	-999.087588	-998.776568
45	-349.237607	-349.178753	-348.93187
46	-345.704719	-345.611638	-345.360578
47	-271.827357	-271.767834	-271.515266
48	-309.941109	-309.88749	-309.647669
49	-388.542164	-388.49188	-388.252734
50	-385.009725	-384.923933	-384.67699
51	-420.47662	-420.428156	-420.223842
52	-385.898985	-385.883003	-385.708972
53	-228.69434	-228.679452	-228.477693
54	-325.999748	-325.964084	-325.725388
55	-460.254078	-460.174373	-459.923495
56	-306.581417	-306.538115	-306.262916
57	-533.17456	-533.057947	-532.787136
58	-805.369614	-805.263958	-805.004364
59	-977.574104	-977.44843	-977.118501
60	-248.36889	-248.305609	-248.060826
61	-539.628196	-539.536778	-539.344923
62	-1001.730177	-1001.63654	-1001.44552
63	-381.777307	-381.678389	-381.530992
64	-232.299068	-232.252412	-232.010008
65	unstable	-2939.761702	-2939.578118
H2		-1.181	
HCOOH		-189.828037	
$HCOO^-$		-189.387871	

Summary of Gibbs Free Energies - B3PW91-D3

Table S19: Summary of the Gibbs free energies obtained at the B3PW91-D3/6-311++G**/SMD level of theory. All energies are stated in [Ha].

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
1	-385.817157	-385.743263	-385.528477
2	-271.494646	-271.449457	-271.21726
3	-350.073653	-350.034813	-349.812946
4	-539.342325	-539.257542	-539.04219
5	-537.38015	-537.31922	-537.125763
6	-669.648519	-669.592513	-669.385587
7	-233.378209	-233.314834	-233.114898
8	-540.558562	-540.483142	-540.267382
9	-195.260889	-195.232458	-195.01067
10	-272.633491	-272.599249	-272.376982
11	-235.749878	-235.71617	-235.487752
12	-271.684609	-271.643798	-271.425306
13	-2922.433271	-2922.361549	-2922.148537
14	-382.649834	-382.598787	-382.395279
15	-307.428833	-307.380196	-307.157753
16	-399.691054	-399.617222	-399.380423
17	-307.570935	-307.557775	-307.327642
18	-346.69372	-346.647363	-346.430409
19	-251.797722	-251.778265	-251.583853
20	-287.552045	-287.507511	-287.313724
21	-292.276818	-292.260091	-292.066805
22	-518.682012	-518.63998	-518.454769
23	-521.029397	-521.00538	-520.83972
24	-366.098481	-366.057015	-365.874887
25	-292.258709	-292.244304	-292.063731
26	-342.890195	-342.853754	-342.677761
27	-445.837574	-445.8144	-445.652617
28	-326.842509	-326.79761	-326.610933
29	-630.389566	-630.332473	-630.111475
30	-344.507852	-344.467412	-344.249008
31	-249.412996	-249.38857	-249.185054
32	-229.997381	-229.961372	-229.73563
33	-478.232405	-478.188727	-477.997046
34	-797.878803	-797.806273	-797.566673
35	-301.40812	-301.379027	-301.173937
36	-226.182431	-226.148887	-225.905647
37	-363.750116	-363.699618	-363.49745
38	-706.587937	-706.52551	-706.307265

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
39	-383.613315	-383.554871	-383.335199
40	unstable	-5187.573921	-5187.277999
41	unstable	-1878.783277	-1878.451611
42	unstable	-2881.151241	-2880.871214
43	unstable	-13878.565381	-13878.331153
44	unstable	-998.949454	-998.638364
45	-349.106787	-349.047891	-348.80154
46	-345.56445	-345.469934	-345.216646
47	-271.720619	-271.661847	-271.409903
48	-309.823652	-309.77053	-309.531299
49	-388.397247	-388.347127	-388.107141
50	-384.855757	-384.768525	-384.520466
51	-420.305303	-420.256045	-420.051947
52	-385.744812	-385.732356	-385.556702
53	-228.597413	-228.584422	-228.384165
54	-325.874918	-325.840714	-325.602257
55	-460.069543	-459.988812	-459.737127
56	-306.460797	-306.419419	-306.144598
57	-532.961483	-532.84375	-532.5693
58	-805.175306	-805.069715	-804.808102
59	-977.193468	-977.069146	-976.742989
60	-248.268301	-248.203988	-247.959473
61	-539.417014	-539.322566	-539.127836
62	-1001.339507	-1001.243889	-1001.049296
63	-381.62113	-381.521666	-381.372537
64	-232.206697	-232.15794	-231.913152
65	unstable	-2939.602627	-2939.418416
H2		-1.180018	
HCOOH		-189.750319	
$HCOO^-$		-189.307468	

Summary of Gibbs Free Energies - PBE0-D3

Table S20: Summary of the Gibbs free energies obtained at the PBE0-D3/6-311++G**/SMD level of theory. All energies are stated in [Ha].

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
1	-385.493389	-385.421236	-385.207144
2	-271.257472	-271.213821	-270.984115
3	-349.763441	-349.727146	-349.504573
4	-538.892147	-538.809326	-538.594118
5	-536.955833	-536.896584	-536.703566
6	-669.307545	-669.253509	-669.047421
7	-233.170332	-233.108382	-232.90985
8	-540.101892	-540.02802	-539.813062
9	-195.082583	-195.055571	-194.835297
10	-272.391511	-272.358777	-272.137817
11	-235.525269	-235.492989	-235.265839
12	-271.450398	-271.410923	-271.194263
13	-2921.822735	-2921.752727	-2921.540622
14	-382.356944	-382.307194	-382.104991
15	-307.182232	-307.134957	-306.913814
16	-399.379396	-399.307431	-399.071683
17	-307.330438	-307.316893	-307.088662
18	-346.409577	-346.364849	-346.148805
19	-251.572421	-251.553547	-251.360917
20	-287.311325	-287.267988	-287.075738
21	-292.006161	-291.989626	-291.797745
22	-518.25667	-518.215736	-518.031595
23	-520.59003	-520.566571	-520.402638
24	-365.784114	-365.745955	-365.563606
25	-291.988598	-291.973438	-291.79444
26	-342.608767	-342.573722	-342.398833
27	-445.445264	-445.422578	-445.262663
28	-326.564935	-326.521412	-326.336194
29	-630.085525	-630.030189	-629.80996
30	-344.245634	-344.20478	-343.988199
31	-249.201061	-249.179373	-248.977373
32	-229.815678	-229.78182	-229.558049
33	-477.850392	-477.808916	-477.617796
34	-797.467631	-797.396704	-797.158751
35	-301.182704	-301.155149	-300.951849
36	-226.002435	-225.97137	-225.729773
37	-363.452167	-363.403298	-363.202188
38	-706.229187	-706.166446	-705.948754

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
39	-383.308968	-383.2525	-383.033878
40	unstable	-5188.914734	-5188.619704
41	unstable	-1878.307353	-1877.975165
42	unstable	-2880.601767	-2880.320551
43	unstable	-13877.479736	-13877.246892
44	unstable	-998.650458	-998.338553
45	-348.808104	-348.750705	-348.504361
46	-345.287036	-345.194209	-344.934011
47	-271.485876	-271.428856	-271.177097
48	-309.562031	-309.510275	-309.271308
49	-388.061956	-388.013374	-387.772576
50	-384.541973	-384.456312	-384.208007
51	-419.983768	-419.936069	-419.732536
52	-385.430661	-385.417724	-385.222142
53	-228.429717	-228.416703	-228.217654
54	-325.609413	-325.576592	-325.339631
55	-459.709161	-459.629903	-459.377801
56	-306.226013	-306.18596	-305.912134
57	-532.570596	-532.454758	-532.181135
58	-804.789537	-804.685857	-804.425833
59	-976.599276	-976.478754	-976.151901
60	-248.063291	-248.000523	-247.757496
61	-538.970121	-538.877254	-538.683266
62	-1000.512285	-1000.417168	-1000.222227
63	-381.331575	-381.233908	-381.088051
64	-232.005475	-231.959004	-231.715326
65	unstable	-2938.984968	-2938.800218
H2		-1.169607	
HCOOH		-189.617888	
$HCOO^-$		-189.175943	

Summary of Gibbs Free Energies - BHandH-D3

Table S21: Summary of the Gibbs free energies obtained at the BHandH-D3/6-311++G**/SMD level of theory. All energies are stated in [Ha].

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
1	-382.965022	-382.904521	-382.694266
2	-269.43969	-269.406572	-269.180327
3	-347.400945	-347.375494	-347.158156
4	-535.370484	-535.300957	-535.087194
5	-533.694026	-533.645427	-533.456573
6	-666.648309	-666.606849	-666.405352
7	-231.589846	-231.538918	-231.345445
8	-536.552278	-536.489291	-536.276678
9	-193.734184	-193.7236	-193.50851
10	-270.543819	-270.522039	-270.305185
11	-233.872554	-233.849701	-233.62818
12	-269.716559	-269.691568	-269.482282
13	-2917.272956	-2917.214617	-2917.006395
14	-380.11502	-380.07482	-379.876694
15	-305.288291	-305.251301	-305.034924
16	-396.965151	-396.904263	-396.672225
17	-305.535524	-305.529502	-305.296304
18	-344.243857	-344.209233	-343.996673
19	-249.893205	-249.882626	-249.69627
20	-285.457727	-285.424679	-285.238466
21	-290.016906	-290.008156	-289.820256
22	-515.008199	-514.977501	-514.798457
23	-517.275911	-517.262763	-517.102788
24	-363.389428	-363.359191	-363.182944
25	-290.00043	-289.991916	-289.815882
26	-340.447099	-340.422636	-340.252776
27	-442.478013	-442.465727	-442.31054
28	-324.439996	-324.405761	-324.226835
29	-627.702918	-627.659231	-627.442875
30	-342.236942	-342.208136	-341.997638
31	-247.582953	-247.573588	-247.37774
32	-228.42841	-228.406387	-228.188353
33	-474.90204	-474.873407	-474.685422
34	-794.229773	-794.168084	-793.93589
35	-299.453475	-299.434912	-299.236378
36	-224.615589	-224.597323	-224.361167
37	-361.125525	-361.087914	-360.891632
38	-703.371097	-703.321595	-703.107325

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
39	-380.940492	-380.895773	-380.681344
40	unstable	-5182.16238	-5181.856423
41	unstable	-1874.458372	-1874.123238
42	unstable	-2876.588238	-2876.303593
43	unstable	-13889.751553	-13889.519834
44	unstable	-996.296307	-995.974053
45	-346.573024	-346.52571	-346.275829
46	-343.150046	-343.067614	-342.809977
47	-269.753881	-269.707413	-269.456344
48	-307.598316	-307.5572	-307.317028
49	-385.555298	-385.517596	-385.274342
50	-382.134214	-382.059144	-381.806856
51	-417.507447	-417.470148	-417.264079
52	-383.09211	-383.088116	-382.890311
53	-227.175372	-227.167927	-226.971646
54	-323.609997	-323.588587	-323.354582
55	-456.954	-456.885297	-456.639024
56	-304.454843	-304.426852	-304.147496
57	-529.532902	-529.42715	-529.158861
58	-801.767714	-801.673954	-801.420672
59	-972.13815	-972.028437	-971.694974
60	-246.479225	-246.426442	-246.188974
61	-535.459881	-535.378059	-535.188409
62	-994.015912	-993.930548	-993.742138
63	-379.107157	-379.017378	-378.877535
64	-230.457355	-230.423805	-230.185084
65	unstable	-2934.379036	-2934.200267
H2		-1.126932	
HCOOH		-188.636207	
$HCOO^-$		-188.200567	

Summary of Gibbs Free Energies - M06-2X

Table S22: Summary of the Gibbs free energies obtained at the M06-2X/6-311++G**/SMD level of theory. All energies are stated in [Ha].

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
1	-385.78395	-385.712887	-385.489792
2	-271.45857	-271.417723	-271.177965
3	-350.01771	-349.982919	-349.752171
4	-539.304767	-539.225592	-538.998464
5	-537.346643	-537.288782	-537.084168
6	-669.62811	-669.576708	-669.362314
7	-233.339721	-233.280082	-233.072788
8	-540.511645	-540.439678	-540.214371
9	-195.218883	-195.194979	-194.96714
10	-272.584284	-272.553975	-272.327145
11	-235.688916	-235.659407	-235.427335
12	-271.637131	-271.600889	-271.375644
13	-2922.430067	-2922.362058	-2922.140126
14	-382.633148	-382.583605	-382.373833
15	-307.407649	-307.360828	-307.132569
16	-399.680308	-399.610133	-399.366164
17	-307.537697	-307.531603	-307.292321
18	-346.663818	-346.619771	-346.396164
19	-251.743858	-251.728402	-251.527163
20	-287.523613	-287.480322	-287.280534
21	-292.204339	-292.190884	-291.989123
22	-518.633495	-518.593715	-518.400364
23	-520.959535	-520.936476	-520.76426
24	-366.053187	-366.015004	-365.824044
25	-292.188884	-292.176167	-291.988831
26	-342.859449	-342.823742	-342.641319
27	-445.761689	-445.737877	-445.57044
28	-326.804212	-326.760539	-326.567624
29	-630.379323	-630.326623	-630.098038
30	-344.484636	-344.451898	-344.228032
31	-249.384057	-249.362214	-249.153754
32	-229.983209	-229.95122	-229.721252
33	-478.200523	-478.160111	-477.960058
34	-797.882603	-797.812357	-797.570343
35	-301.39588	-301.372752	-301.161696
36	-226.166837	-226.13631	-225.890127
37	-363.722368	-363.674585	-363.465376
38	-706.580651	-706.521031	-706.294597

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
39	-383.592332	-383.537784	-383.310811
40	unstable	-5187.639647	-5187.334856
41	unstable	-1878.882988	-1878.539163
42	unstable	-2881.164203	-2880.889158
43	unstable	-13878.383762	-13878.150724
44	unstable	-998.977742	-998.647018
45	-349.050212	-348.994721	-348.738183
46	-345.540387	-345.449666	-345.178801
47	-271.672031	-271.617197	-271.357045
48	-309.775449	-309.72618	-309.478739
49	-388.33064	-388.284303	-388.034858
50	-384.822796	-384.739266	-384.480128
51	-420.291354	-420.245003	-420.02839
52	-385.696888	-385.687043	-385.481089
53	-228.584835	-228.575657	-228.36583
54	-325.835195	-325.80306	-325.557161
55	-460.04321	-459.965128	-459.703638
56	-306.436738	-306.398885	-306.114889
57	-532.954852	-532.840126	-532.562532
58	-805.179487	-805.07762	-804.810438
59	-977.242725	-977.122727	-976.777192
60	-248.248895	-248.187292	-247.935229
61	-539.376725	-539.284491	-539.081143
62	-1001.270647	-1001.17577	-1000.972406
63	-381.610423	-381.509462	-381.363202
64	-232.177544	-232.134413	-231.884547
65	unstable	-2939.602475	-2939.40923
H2		-1.169696	
HCOOH		-189.748116	
$HCOO^-$		-189.308236	

Summary of Gibbs Free Energies - M06-HF

Table S23: Summary of the Gibbs free energies obtained at the M06-HF/6-311++G**/SMD level of theory. All energies are stated in [Ha].

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
1	-385.857983	-385.783788	-385.549316
2	-271.509524	-271.462162	-271.214626
3	-350.079991	-350.036876	-349.795234
4	-539.404513	-539.323682	-539.08234
5	-537.429872	-537.367252	-537.149566
6	-669.692671	-669.638557	-669.413572
7	-233.382396	-233.32034	-233.102581
8	-540.61256	-540.540173	-540.302062
9	-195.255568	-195.226569	-194.990706
10	-272.635711	-272.603848	-272.372201
11	-235.724191	-235.691606	-235.456382
12	-271.673029	-271.634146	-271.399148
13	-2922.718917	-2922.649581	-2922.413302
14	-382.690089	-382.634646	-382.414397
15	-307.457819	-307.40708	-307.169768
16	-399.742926	-399.668884	-399.413109
17	-307.592389	-307.570885	-307.325961
18	-346.721414	-346.673083	-346.441061
19	-251.790404	-251.766585	-251.561528
20	-287.576401	-287.528999	-287.321678
21	-292.252454	-292.228765	-292.025083
22	-518.724671	-518.680229	-518.479927
23	-521.052945	-521.01971	-520.841004
24	-366.121515	-366.075313	-365.878911
25	-292.237539	-292.214799	-292.020639
26	-342.921882	-342.879284	-342.689502
27	-445.845032	-445.812385	-445.638029
28	-326.882281	-326.813829	-326.612154
29	-630.440375	-630.382002	-630.145556
30	-344.538894	-344.498321	-344.266181
31	-249.436714	-249.411402	-249.196727
32	-230.021307	-229.988082	-229.750364
33	-478.284889	-478.237568	-478.02909
34	-797.962962	-797.88702	-797.643355
35	-301.445443	-301.412543	-301.193511
36	-226.205073	-226.172281	-225.920656
37	-363.795262	-363.74266	-363.524254
38	-706.657456	-706.594581	-706.35737

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
39	-383.659038	-383.600661	-383.363671
40	unstable	-5188.09733	-5187.775328
41	unstable	-1878.958083	-1878.606088
42	unstable	-2881.418785	-2881.11097
43	unstable	-13880.511971	-13880.246193
44	unstable	-999.024578	-998.676379
45	-349.09855	-349.039737	-348.776901
46	-345.592882	-345.499333	-345.218213
47	-271.704094	-271.644742	-271.376963
48	-309.817259	-309.763307	-309.510352
49	-388.383854	-388.33303	-388.078707
50	-384.880336	-384.793488	-384.518958
51	-420.355641	-420.3023	-420.053189
52	-385.746426	-385.728269	-385.513681
53	-228.612703	-228.591179	-228.372808
54	-325.873677	-325.843826	-325.588399
55	-460.10789	-460.025839	-459.754551
56	-306.459064	-306.428932	-306.137934
57	-533.017237	-532.897474	-532.610557
58	-805.244884	-805.136966	-804.885213
59	-977.304224	-977.174497	-976.809537
60	-248.294373	-248.229174	-247.967824
61	-539.478797	-539.383591	-539.16764
62	-1001.467208	-1001.367309	-1001.148701
63	-381.666256	-381.554532	-381.404389
64	-232.222826	-232.175997	-231.919006
65	unstable	-2939.890212	-2939.688847
H2		-1.169397	
HCOOH		-189.760127	
$HCOO^-$		-189.323312	

Summary of Gibbs Free Energies - HSE06

Table S24: Summary of the Gibbs free energies obtained at the HSE06/6-311++G**/SMD level of theory. All energies are stated in [Ha].

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
1	-385.519912	-385.447614	-385.234075
2	-271.275825	-271.232161	-271.0016
3	-349.78488	-349.747907	-349.526776
4	-538.931308	-538.847852	-538.633574
5	-536.992842	-536.933245	-536.741067
6	-669.341761	-669.287489	-669.081944
7	-233.185401	-233.123378	-232.925463
8	-540.136632	-540.062056	-539.84812
9	-195.093431	-195.067356	-194.847575
10	-272.405301	-272.372554	-272.151984
11	-235.538108	-235.504039	-235.278263
12	-271.468182	-271.428325	-271.212371
13	-2921.82364	-2921.75336	-2921.542037
14	-382.38538	-382.335422	-382.133528
15	-307.204988	-307.157513	-306.936737
16	-399.409796	-399.337707	-399.102372
17	-307.351794	-307.337218	-307.107844
18	-346.433676	-346.38904	-346.173465
19	-251.588029	-251.566539	-251.374322
20	-287.331856	-287.288223	-287.096337
21	-292.020907	-292.003552	-291.812493
22	-518.287508	-518.246669	-518.062931
23	-520.617945	-520.593888	-520.429049
24	-365.807062	-365.767333	-365.588376
25	-292.003491	-291.987321	-291.809042
26	-342.632146	-342.597075	-342.422466
27	-445.467454	-445.443903	-445.284175
28	-326.588388	-326.543091	-326.358255
29	-630.117977	-630.062277	-629.842588
30	-344.271395	-344.229876	-344.013602
31	-249.208134	-249.195164	-248.993743
32	-229.833617	-229.799465	-229.57604
33	-477.882433	-477.84103	-477.650435
34	-797.512515	-797.441442	-797.203741
35	-301.206505	-301.178274	-300.975211
36	-226.012567	-225.988583	-225.747377
37	-363.477247	-363.428284	-363.227677
38	-706.264368	-706.203521	-705.988464

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
39	-383.336737	-383.280031	-383.061914
40	unstable	-5188.874472	-5188.580251
41	unstable	-1878.380127	-1878.04922
42	unstable	-2880.600943	-2880.321328
43	unstable	-13877.239789	-13877.008244
44	unstable	-998.689429	-998.38851
45	-348.827217	-348.769468	-348.523511
46	-345.312708	-345.21969	-344.959874
47	-271.503067	-271.444997	-271.193763
48	-309.580575	-309.528359	-309.289728
49	-388.082226	-388.033313	-387.792495
50	-384.569178	-384.483061	-384.235341
51	-420.015923	-419.967952	-419.764603
52	-385.455666	-385.44092	-385.245506
53	-228.448951	-228.436135	-228.236723
54	-325.63028	-325.597016	-325.36027
55	-459.742274	-459.662794	-459.411233
56	-306.248048	-306.207701	-305.934142
57	-532.611268	-532.495232	-532.223952
58	-804.831978	-804.727993	-804.468535
59	-976.680555	-976.55942	-976.233157
60	-248.081993	-248.019231	-247.776591
61	-539.00625	-538.913169	-538.719904
62	-1000.570816	-1000.475884	-1000.28323
63	-381.361427	-381.26376	-381.115898
64	-232.023466	-231.975859	-231.73269
65	unstable	-2938.985623	-2938.800537
H2		-1.169752	
HCOOH		-189.634272	
$HCOO^-$		-189.192921	

Summary of Gibbs Free Energies - ωB97X-D

Table S25: Summary of the Gibbs free energies obtained at the ωB97X-D/6-311++G**/SMD level of theory. All energies are stated in [Ha].

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
1	-385.808899	-385.739965	-385.52373
2	-271.488959	-271.449656	-271.215067
3	-350.065069	-350.032802	-349.807784
4	-539.330365	-539.25459	-539.034371
5	-537.382028	-537.324597	-537.128331
6	-669.66889	-669.618053	-669.409157
7	-233.37162	-233.312946	-233.111958
8	-540.546576	-540.480179	-540.26024
9	-195.234821	-195.230035	-195.007021
10	-272.597751	-272.596265	-272.373206
11	-235.741442	-235.712789	-235.483571
12	-271.672071	-271.645439	-271.425039
13	-2922.466195	-2922.400543	-2922.184507
14	-382.654161	-382.606752	-382.403121
15	-307.428267	-307.383476	-307.161427
16	-399.693703	-399.624211	-399.38709
17	-307.565629	-307.565181	-307.331233
18	-346.693843	-346.649799	-346.432852
19	-251.777497	-251.77741	-251.581333
20	-287.547918	-287.507044	-287.313313
21	-292.258237	-292.257946	-292.062356
22	-518.68144	-518.643239	-518.457015
23	-521.018231	-521.00785	-520.841334
24	-366.093255	-366.057017	-365.872872
25	-292.242063	-292.24213	-292.061069
26	-342.888196	-342.854176	-342.677521
27	-445.81913	-445.811604	-445.649702
28	-326.837882	-326.7963	-326.609301
29	-630.411133	-630.359895	-630.136856
30	-344.50468	-344.476205	-344.258048
31	-249.407342	-249.389794	-249.188948
32	-229.96684	-229.965883	-229.741101
33	-478.230497	-478.191757	-477.998333
34	-797.911138	-797.840897	-797.617725
35	-301.408212	-301.388107	-301.18223
36	-226.170098	-226.151962	-225.910067
37	-363.744688	-363.698484	-363.495735
38	-706.609192	-706.551306	-706.331027

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
39	-383.610912	-383.557839	-383.337435
40	unstable	-5187.658741	-5187.361389
41	unstable	-1878.927021	-1878.588406
42	unstable	-2881.202369	-2880.91356
43	unstable	-13878.663616	-13878.427883
44	unstable	-999.018537	-998.692019
45	-349.106059	-349.050988	-348.797729
46	-345.563791	-345.474079	-345.208837
47	-271.71841	-271.664678	-271.407985
48	-309.82262	-309.774004	-309.530149
49	-388.395338	-388.349753	-388.103469
50	-384.854478	-384.772402	-384.512732
51	-420.311533	-420.266208	-420.057709
52	-385.741949	-385.740275	-385.542423
53	-228.597998	-228.595006	-228.390565
54	-325.876024	-325.846337	-325.605476
55	-460.073302	-459.997337	-459.746447
56	-306.466162	-306.42909	-306.150651
57	-532.97258	-532.859499	-532.587547
58	-805.20934	-805.108823	-804.848082
59	-977.267046	-977.151356	-976.816378
60	-248.266393	-248.205215	-247.95849
61	-539.405385	-539.316473	-539.11988
62	-1001.325433	-1001.234096	-1001.038381
63	-381.626794	-381.52805	-381.382988
64	-232.199966	-232.156654	-231.912408
65	unstable	-2939.645766	-2939.458196
H2		-1.177479	
HCOOH		-189.761613	
$HCOO^-$		-189.318753	

Summary of Gibbs Free Energies - M06-2X/PCM

Table S26: Summary of the Gibbs free energies obtained at the M06-2X/6-311++G**/PCM level of theory. All energies are stated in [Ha].

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
1	-385.774514	-385.703346	-385.470433
2	-271.450025	-271.410999	-271.160218
3	-350.008624	-349.972409	-349.733497
4	-539.292568	-539.213604	-538.977783
5	-537.338924	-537.278989	-537.06759
6	-669.622004	-669.569852	-669.347261
7	-233.331897	-233.273781	-233.054952
8	-540.49949	-540.427751	-540.192051
9	-195.213028	-195.189788	-194.948087
10	-272.574551	-272.54729	-272.308435
11	-235.684896	-235.654901	-235.409203
12	-271.632156	-271.596294	-271.359012
13	-2922.422089	-2922.350675	-2922.121123
14	-382.626825	-382.576642	-382.357897
15	-307.399788	-307.354243	-307.116634
16	-399.674688	-399.603736	-399.349324
17	-307.540215	-307.528252	-307.275646
18	-346.656979	-346.613722	-346.380075
19	-251.750202	-251.722276	-251.508677
20	-287.513504	-287.472391	-287.262232
21	-292.211463	-292.18518	-291.970361
22	-518.620584	-518.583558	-518.379452
23	-520.955295	-520.92631	-520.742927
24	-366.043246	-366.005346	-365.805602
25	-292.193769	-292.170098	-291.967774
26	-342.850035	-342.814702	-342.620439
27	-445.753787	-445.727827	-445.550443
28	-326.793382	-326.754789	-326.550859
29	-630.373981	-630.319857	-630.085021
30	-344.488601	-344.447318	-344.211556
31	-249.380859	-249.355188	-249.137384
32	-229.980874	-229.948035	-229.706983
33	-478.191478	-478.150664	-477.942397
34	-797.880048	-797.802425	-797.556793
35	-301.399493	-301.366776	-301.145496
36	-226.161662	-226.13113	-225.872928
37	-363.711711	-363.664757	-363.446179
38	-706.572838	-706.51302	-706.279898

Compound	G(Reduced) [Ha]	G(Neutral) [Ha]	G(Oxidized) [Ha]
39	-383.585862	-383.530813	-383.294231
40	unstable	-5187.635046	-5187.339099
41	unstable	-1878.879493	-1878.542482
42	unstable	-2881.158778	-2880.860834
43	unstable	-13879.131243	-13878.862296
44	unstable	-998.971626	-998.636578
45	-349.050429	-348.988335	-348.71806
46	-345.538753	-345.443208	-345.160556
47	-271.674778	-271.612897	-271.337797
48	-309.776452	-309.719841	-309.460443
49	-388.329592	-388.277044	-388.015278
50	-384.819735	-384.730985	-384.456314
51	-420.294888	-420.247522	-420.021393
52	-385.710406	-385.691977	-385.475508
53	-228.598608	-228.581758	-228.361341
54	-325.835718	-325.797273	-325.53634
55	-460.041176	-459.959198	-459.687703
56	-306.440856	-306.394369	-306.100135
57	-532.955008	-532.833456	-532.539614
58	-805.176397	-805.069402	-804.792596
59	-977.248107	-977.125581	-976.779215
60	-248.242836	-248.181744	-247.919042
61	-539.365095	-539.271632	-539.059024
62	-1001.250375	-1001.155968	-1000.944027
63	-381.61676	-381.510508	-381.356721
64	-232.169021	-232.128224	-231.867179
65	unstable	-2939.592191	-2939.389549
H2		-1.169696	
HCOOH		-189.744499	
$HCOO^-$		-189.299795	

Summary of Total Energies - CCSD(T)

Table S27: Summary of the total energies obtained at the CCSD(T)/Def2-TZVPP/SMD level of theory. All energies are stated in [Ha].

Compound	E(Reduced) [Ha]	E(Neutral) [Ha]	E(Oxidized) [Ha]
1	-385.23437797	-385.17890421	-384.95828867
2	-271.08969804	-271.06275685	-270.82393709
3	-349.5735306	-349.5512368	-349.3206971
4	-538.5262386	-538.46469026	-538.2387032
5	-536.6420241	-536.6004579	-536.4011504
6	-668.80673724	-668.7724906	-668.5572536
7	-233.03443494	-232.99088425	-232.77820989
8	-539.7614597	-539.7066779	-539.479827
9	-194.97658559	-194.96787489	-194.73091531
10	-272.25189102	-272.23489785	-272.00227788
11	-235.42646811	-235.41530401	-235.17519572
12	-271.3220746	-271.30459843	-271.07068351
13	-2920.4841778	-2920.433091	-2920.2102648
14	-382.12272147	-382.09083303	-381.88825028
15	-306.98524454	-306.95626445	-306.73179087
16	-399.11112695	-399.05955064	-398.82093063
17	-307.13902508	-307.19148868	-306.95301924
18	-346.20560288	-346.17779263	-345.95792507
19	-251.44130197	-251.46629365	-251.26652807
20	-287.12756851	-287.10138006	-286.9067717
21	-291.87767164	-291.91119948	-291.71104885
22	-517.9805277	-517.955845	-517.7715507
23	-520.3526038	-520.353053	-520.1831154
24	-365.5845378	-365.55965487	-365.37583115
25	-291.88191548	-291.89524899	-291.71075684
26	-342.40219659	-342.38313247	-342.2031515
27	-445.2420232	-445.2429896	-445.0777399
28	-326.37070457	-326.34451388	-326.15536425
29	-629.59248519	-629.5553223	-629.3313714
30	-344.04025975	-344.0216295	-343.79844295
31	-249.04433542	-249.04345278	-248.83992358
32	-229.66012235	-229.64656201	-229.41930971
33	-477.5561653	-477.5343639	-477.3397264
34	-796.8832825	-796.80921625	-796.575436
35	-300.96827467	-300.98104414	-300.77415153
36	-225.84602935	-225.83325857	-225.59246464
37	-363.20608057	-363.17440981	-362.97074712
38	-705.67625622	-705.63430227	-705.41198897

Compound	E(Reduced) [Ha]	E(Neutral) [Ha]	E(Oxidized) [Ha]
39	-383.05138122	-383.01355631	-382.789747
40	unstable	-5184.6514914	-5184.3547227
41	unstable	-1876.9178793	-1876.5853265
42	unstable	-2879.3422045	-2879.047378
43	unstable	-633.51143212	-633.27970189
44	unstable	-997.93944046	-997.61044725
45	-348.648355	-348.60797247	-348.3478895
46	-345.0600264	-344.98477955	-344.72732831
47	-271.36222955	-271.32249631	-271.05842009
48	-309.40964356	-309.37497936	-309.12523923
49	-387.8916653	-387.85959674	-387.609086
50	-384.3047506	-384.2354942	-383.977906
51	-419.69984005	-419.67163368	-419.46669839
52	-385.2103372	-385.24773075	-385.0703196
53	-228.23124023	-228.28079136	-228.08364451
54	-325.44319268	-325.42587826	-325.18137348
55	-459.437767	-459.3753033	-459.1183953
56	-306.05530159	-306.03406341	-305.75305639
57	-532.21903289	-532.12136699	-531.8451776
58	-804.21262107	-804.12717291	-803.884977
59	-976.0921349	-975.9932594	-975.6615291
60	-247.89463627	-247.84732064	-247.59778932
61	-538.6096906	-538.5332835	-538.3317159
62	–	–	–
63	-381.07098834	-380.9789585	-380.8519954
64	-231.845089	-231.81880603	-231.56871566
65	unstable	-2937.6707481	-2937.4851901
H2		-1.1723386695	
HCOOH		-189.515079	
$HCOO^-$		-189.0532935	

Summary of Total Energies - CCSD

Table S28: Summary of the total energies obtained at the CCSD/Def2-TZVPP/SMD level of theory. All energies are stated in [Ha].

Compound	E(Reduced) [Ha]	E(Neutral) [Ha]	E(Oxidized) [Ha]
1	-385.1411583	-385.08931679	-384.86931503
2	-271.02806129	-271.00311555	-270.76727507
3	-349.49553114	-349.47555463	-349.24809088
4	-538.39612495	-538.3395113	-538.11323434
5	-536.53341307	-536.49485241	-536.29612601
6	-668.732556	-668.70090174	-668.48720709
7	-232.98287049	-232.94213195	-232.73193264
8	-539.63209883	-539.58172744	-539.35589929
9	-194.93582608	-194.92893243	-194.6959352
10	-272.19289542	-272.17769054	-271.94873827
11	-235.37917927	-235.36956564	-235.13370346
12	-271.27214894	-271.25747619	-271.02762641
13	-2920.3920967	-2920.3440028	-2920.1229922
14	-382.05086603	-382.02012593	-381.81747362
15	-306.92250808	-306.89512247	-306.67300821
16	-399.02776195	-398.97861925	-398.74172646
17	-307.08668576	-307.14369916	-306.90026567
18	-346.13471553	-346.10866747	-345.89085329
19	-251.39251079	-251.41981978	-251.22208212
20	-287.06469083	-287.04013779	-286.84728194
21	-291.81977837	-291.85737663	-291.66004622
22	-517.87529001	-517.85255969	-517.66910639
23	-520.25150587	-520.25489915	-520.08761438
24	-365.5048868	-365.48185338	-365.29898824
25	-291.80394479	-291.84125707	-291.65983889
26	-342.32941018	-342.31196491	-342.13374835
27	-445.1501692	-445.15410688	-444.99150789
28	-326.29973946	-326.27520994	-326.08804245
29	-629.52764169	-629.49253675	-629.26930298
30	-343.97678181	-343.96087489	-343.74076198
31	-248.99029198	-248.99163551	-248.79139191
32	-229.61379431	-229.60260987	-229.37828549
33	-477.4545763	-477.43561339	-477.24138543
34	-796.77011623	-796.71573919	-796.4853904
35	-300.91273805	-300.92683988	-300.72194508
36	-225.7978722	-225.78678165	-225.54979202
37	-363.12230988	-363.09306658	-362.89117861
38	-705.58952222	-705.55050198	-705.32834824

Compound	E(Reduced) [Ha]	E(Neutral) [Ha]	E(Oxidized) [Ha]
39	-382.96731081	-382.93234711	-382.70997397
40	unstable	-5184.6235969	-5184.3250487
41	unstable	-1876.8696096	-1876.5331655
42	unstable	-2879.2823189	-2878.9807122
43	unstable	-633.48154742	-633.24790399
44	unstable	-997.90641649	-997.57133355
45	-348.58376473	-348.54475519	-348.28380871
46	-344.98707653	-344.91424293	-344.66012849
47	-271.31415062	-271.27573532	-271.01193108
48	-309.3528035	-309.31963275	-309.0699062
49	-387.8187417	-387.78837128	-387.53691767
50	-384.22352649	-384.15699916	-383.90116197
51	-419.61581809	-419.58937848	-419.38140413
52	-385.1384883	-385.18045724	-385.0060039
53	-228.19344089	-228.24581351	-228.04536489
54	-325.3847943	-325.36881982	-325.1258771
55	-459.34751984	-459.287396	-459.03355955
56	-306.00441758	-305.98449838	-305.70506034
57	-532.11503651	-532.0204382	-531.74730989
58	-804.12708271	-804.04430776	-803.78563498
59	-975.98567772	-975.88861733	-975.55019285
60	-247.8395592	-247.793694	-247.54568515
61	-538.47765076	-538.40502974	-538.20417837
62	–	–	–
63	-380.99393678	-380.9047725	-380.78072801
64	-231.79151875	-231.76698849	-231.52019664
65	unstable	-2937.5809856	-2937.3961274
H2		-1.1723386695	
HCOOH		-189.4897853	
$HCOO^-$		-189.02657786	

Summary of Total Energies - MP2

Table S29: Summary of the total energies obtained at the MP2/Def2-TZVPP/SMD level of theory. All energies are stated in [Ha].

Compound	E(Reduced) [Ha]	E(Neutral) [Ha]	E(Oxidized) [Ha]
1	-385.12496962789	-385.06408710684	-384.84479364299
2	-270.99802124722	-270.96961979039	-270.72697597677
3	-349.44765615786	-349.42437787136	-349.18622759676
4	-538.37537431859	-538.30839122242	-538.07714231344
5	-536.50007894077	-536.45601887706	-536.25463012149
6	-668.691309637	-668.65679892672	-668.43800674645
7	-232.9489045785	-232.89856205402	-232.68694834107
8	-539.5986341887	-539.53992575703	-539.30692306072
9	-194.89724326911	-194.88600443931	-194.64410551065
10	-272.14968039634	-272.13042667772	-271.89239394571
11	-235.31902371147	-235.30688514833	-235.0629063229
12	-271.22726785597	-271.20733046109	-270.96854425297
13	-2920.3599771057	-2920.3050006287	-2920.0768951777
14	-382.03501557895	-382.00266292846	-381.79526238634
15	-306.90363029387	-306.87379304188	-306.6443508818
16	-399.01931337345	-398.96551183476	-398.72216551724
17	-307.04900968466	-307.10363954064	-306.8784707145
18	-346.1053123466	-346.07650720003	-345.85164162247
19	-251.33859485903	-251.36504135854	-251.15819518073
20	-287.04118148633	-287.01423332645	-286.81632974186
21	-291.74828518114	-291.78386569069	-291.57652539003
22	-517.82459091682	-517.79901877534	-517.60983016196
23	-520.17401309019	-520.17309279095	-519.99767031781
24	-365.46336659455	-365.43741412306	-365.24767892772
25	-291.73165959989	-291.76734799814	-291.57563463628
26	-342.30571027802	-342.28607379592	-342.10301821582
27	-445.0723535216	-445.07185443813	-444.90116897511
28	-326.26755566142	-326.24086449992	-326.04823937927
29	-629.49706949358	-629.45850264468	-629.23160338049
30	-343.9587649414	-343.93896906234	-343.71251351386
31	-248.96777238218	-248.96582992026	-248.75697879591
32	-229.60379879105	-229.58741158436	-229.35814747012
33	-477.43396584738	-477.40990175853	-477.20781247561
34	-796.7436066454	-796.69534920604	-796.45824287917
35	-300.90224056411	-300.91447372918	-300.69973272781
36	-225.78577706373	-225.77810588502	-225.52635178252
37	-363.10897583524	-363.07490666185	-362.86288797015
38	-705.56680052792	-705.52519972179	-705.2959063493

Compound	E(Reduced) [Ha]	E(Neutral) [Ha]	E(Oxidized) [Ha]
39	-382.95540306775	-382.91537508912	-382.68455224877
40	unstable	-5184.6061076246	-5184.3105306531
41	unstable	-1876.8166827472	-1876.4857162911
42	unstable	-2879.2462617637	-2878.9613007187
43	unstable	-633.53098488522	-633.30094786401
44	unstable	-997.85559642401	-997.52984947088
45	-348.52494297902	-348.48482183201	-348.20462355747
46	-344.96959897974	-344.89196291421	-344.62904236136
47	-271.26468719496	-271.22524037562	-270.94139920461
48	-309.30297443789	-309.26913301386	-308.99989461532
49	-387.75001055994	-387.71889954207	-387.4494504561
50	-384.1977398585	-384.1252278077	-383.86217998676
51	-419.60853573541	-419.57813960044	-419.37770352056
52	-385.09449991856	-385.1330688783	-384.95523384902
53	-228.18490522282	-228.23589882022	-228.04376779178
54	-325.34165651178	-325.32665502407	-325.07291985886
55	-459.32360817406	-459.25806698453	-458.99602859384
56	-305.97589064186	-305.95668538044	-305.65826839795
57	-532.11792125083	-532.01675561429	-531.73569830036
58	-804.10506570694	-804.0172393492	-803.74947021812
59	-975.98971516424	-975.89150048519	-975.5597591928
60	-247.82430025549	-247.7752728907	-247.51640340168
61	-538.46444810337	-538.38004677341	-538.18124270249
62	–	–	–
63	-380.99279302937	-380.89843854651	-380.76043659838
64	-231.76957571233	-231.74214950809	-231.48855693807
65	unstable	-2937.5414910336	-2937.3494352568
H2		-1.1646181	
HCOOH		-189.4838122	
$HCOO^-$		-189.0262689	

Summary of Entropy and Zero-point Energy Corrections for Ab-initio Calculations

Table S30: Summary of entropy and zero-point energy corrections used in connection with the ab-initio computations. The data were extracted from PBE0-D3/6-311++G**/SMD calculations. All energies are stated in [Ha].

Compound	S+ZPE (Reduced) [Ha]	S+ZPE (Neutral) [Ha]	S+ZPE (Oxidized) [Ha]
1	0.109184	0.115553	0.114039
2	0.090062	0.098054	0.092564
3	0.140826	0.145019	0.143376
4	0.146146	0.151376	0.150382
5	0.133017	0.138428	0.139454
6	0.087236	0.093977	0.093313
7	0.088938	0.093208	0.091284
8	0.170302	0.175881	0.175091
9	0.082581	0.088429	0.084082
10	0.117423	0.123172	0.123402
11	0.126282	0.13231	0.129647
12	0.10265	0.108433	0.104493
13	0.10654	0.113819	0.113595
14	0.06723	0.077911	0.078817
15	0.064774	0.074996	0.074345
16	0.063967	0.071316	0.070122
17	0.108118	0.093946	0.092642
18	0.092847	0.101131	0.100157
19	0.126696	0.129619	0.127907
20	0.077363	0.08737	0.087061
21	0.168458	0.170714	0.168992
22	0.168845	0.177281	0.178512
23	0.217784	0.222195	0.22258
24	0.132227	0.138227	0.138877
25	0.168572	0.170648	0.17056
26	0.095422	0.102855	0.102322
27	0.213646	0.218326	0.218973
28	0.10352	0.112916	0.112548
29	0.061889	0.068558	0.068309
30	0.065255	0.071914	0.069349
31	0.075552	0.08054	0.079299
32	0.036588	0.043851	0.042587
33	0.117823	0.127695	0.128094
34	0.070283	0.075128	0.074553
35	0.041568	0.046767	0.046796

Compound	S+ZPE (Reduced) [Ha]	S+ZPE (Neutral) [Ha]	S+ZPE (Oxidized) [Ha]
36	0.03721	0.044671	0.042256
37	0.090877	0.09873	0.098115
38	0.075451	0.082421	0.081285
39	0.077875	0.08838	0.085014
40	unstable	-0.000572	-0.001271
41	unstable	-0.021352	-0.023006
42	unstable	0.073616	0.070492
43	unstable	-0.003285	-0.003827
44	unstable	0.029792	0.028256
45	0.142199	0.146138	0.141923
46	0.074778	0.078798	0.074853
47	0.10435	0.108953	0.104933
48	0.115681	0.119742	0.115841
49	0.167945	0.171916	0.168947
50	0.100288	0.103626	0.101562
51	0.06363	0.070048	0.067645
52	0.124834	0.126924	0.116436
53	0.019591	0.02071	0.020696
54	0.105695	0.10933	0.105014
55	0.103429	0.107943	0.105085
56	0.063923	0.069377	0.066467
57	0.066223	0.069476	0.065709
58	0.062582	0.066522	0.065012
59	0.005772	0.010963	0.010121
60	0.05432	0.060963	0.057535
61	0.153159	0.158291	0.157246
62	–	–	–
63	0.051093	0.052119	0.053973
64	0.061227	0.07254	0.067733
65	unstable	0.126168	0.125535
H2		-0.001429	
HCOOH		0.009214	
$HCOO^-$		-0.002905	