

On the Radical Scavenging Ability of Gallic Acid toward OH and OOH Radicals. Reaction Mechanism and Rate Constants from the Density Functional Theory

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Table S1. Gibbs free energies of reaction (ΔG , kcal/mol), reorganization energy (λ , kcal/mol), and Gibbs free energy of activation ($\Delta G^\ddagger$) for the SET reactions involving H₄GA.

	ΔG	λ	$\Delta G^\ddagger$
R1	2.29	16.77	5.41
R2	30.45	7.14	49.47
R3	28.79	7.15	45.16
R4	32.11	8.48	48.58
R5	29.09	6.43	49.06
R6	35.64	11.37	48.60
R7	34.67	10.79	47.89
R8	31.33	8.84	45.63
R9	39.33	11.50	56.15
R10	38.59	16.61	45.86
R11	27.45	17.71	28.79
R12	21.80	17.97	22.00
R13	16.11	18.17	16.17
R14	37.81	17.27	43.91
R15	30.80	15.92	34.28
R16	37.99	16.70	44.78
R17	-4.70	10.46	0.79
R18	20.01	17.93	20.07
R19	15.62	30.38	17.42
R20	16.65	4.38	25.26
R21	30.83	20.89	32.01

Table S2. Gibbs free energies of reaction (ΔG , kcal/mol), reorganization energy (λ , kcal/mol), and Gibbs free energy of activation ($\Delta G^\ddagger$) for the SET reactions involving H_3GA^- .

	ΔG	λ	$G^\ddagger$
R1	-17.07	29.91	1.38
R2	11.09	20.28	12.13
R3	9.43	20.29	10.88
R4	12.75	21.61	13.66
R5	9.73	19.57	10.97
R6	16.28	24.51	16.97
R7	15.31	23.93	16.09
R8	11.97	21.98	13.11
R9	19.97	24.64	20.19
R10	19.23	29.75	20.16
R11	8.09	30.85	12.29
R12	2.44	31.11	9.04
R13	-3.25	31.30	6.29
R14	18.45	30.41	19.62
R15	11.44	29.06	14.11
R16	18.63	29.84	19.69
R17	-24.06	23.60	0.00
R18	0.65	31.07	8.10
R19	-3.74	43.52	9.09
R20	-2.71	17.51	3.13
R21	11.47	34.02	15.20

Table S3. Gibbs free energies of reaction (ΔG , kcal/mol), reorganization energy (λ , kcal/mol), and Gibbs free energy of activation ($\Delta G^\ddagger$) for the SET reactions involving H_2GA^{2-} .

	ΔG	λ	$G^\ddagger$
R1	-28.91	18.64	1.42
R2	0.47	7.14	2.03
R3	-1.03	7.15	1.31
R4	2.61	8.47	3.62
R5	-1.10	4.32	0.60
R6	6.33	11.19	6.85
R7	5.23	10.69	5.93
R8	1.71	8.96	3.18
R9	9.98	11.33	10.02
R10	9.21	16.11	9.95
R11	-1.81	17.22	3.45
R12	-7.60	17.32	1.36
R13	-13.23	17.66	0.28
R14	8.51	16.74	9.52
R15	1.50	15.48	4.65
R16	8.41	16.44	9.39
R17	-34.90	4.60	49.84
R18	-10.29	17.47	0.74
R19	-15.41	29.44	1.67
R20	-15.92	6.92	2.92
R21	0.89	20.86	5.67