Supporting Information

Mechanisms of Hydride Abstractions by Quinones

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1). Kinetics of the Reactions of DDQ with 2

CH_2Cl_2 was freshly distilled over CaH_2 before use. Commercially available cyclohexane, *n*-Bu_2O and THF were further purified by distillation over DDQ to remove the impurities which may react with DDQ. Acetone and CH_3CN were purchased from Acros and used without further purification. Most rate constants were determined photometrically. The temperature of the solutions during all kinetic studies was kept constant (20.0 ± 0.1 °C) by using a circulating bath thermostat. For the evaluation of fast kinetics a stopped-flow spectrophotometer (Hi-Tech SF-61DX2) was used. The rates of slow reactions were determined by using a conventional UV/Vis diode array spectrophotometer (J&M TIDAS) connected to a Hellma 661.502-QX quartz Suprasil immersion probe (5 mm light path) via fiber optic cables. Rate constants k_{obs} (s^{-1}) were obtained by least-squares fitting of the absorbances to the monoexponential function $A_t = A_0 e^{-k_{obs}t} + C$ (for decreasing absorbance) or $A_t = A_0 (1- e^{-k_{obs}t}) + C$ (for increasing absorbance). Because of the poor solubility of DDQ in cyclohexane, in this case, ~1%(v/v) stock solution of DDQ in CH_2Cl_2 was used.

Table S1. Kinetics of the reaction of DDQ (**1a**) with penta-1,4-diene (**2a**) in CH_2Cl_2 (20 °C, Conventional UV/Vis, at 340 nm)

[DDQ] / mol L^{-1}	[**2a**] / mol L^{-1}	k_{obs} / s^{-1}
5.0×10^{-4}	0.19	8.0×10^{-5}
5.0×10^{-4}	0.28	1.3×10^{-4}
5.0×10^{-4}	0.37	1.8×10^{-4}
5.0×10^{-4}	0.46	2.2×10^{-4}

$k_2 = 5.2 \times 10^{-4}$ L mol^{-1} s^{-1}

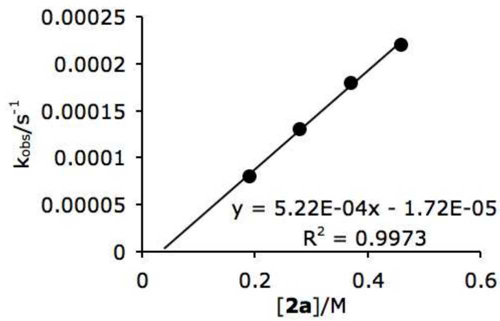


Table S2. Kinetics of the reaction of DDQ (**1a**) with 3-methylpenta-1,4-diene (**2b**) in CH_2Cl_2 (20 °C, Conventional UV/Vis, at 340 nm)

[DDQ] / mol L^{-1}	[**2b**] / mol L^{-1}	k_{obs} / s^{-1}
5.0×10^{-4}	0.082	1.3×10^{-4}
5.0×10^{-4}	0.16	3.2×10^{-4}
5.0×10^{-4}	0.24	4.6×10^{-4}
5.0×10^{-4}	0.31	6.4×10^{-4}

$k_2 = 2.2 \times 10^{-3}$ L mol^{-1} s^{-1}

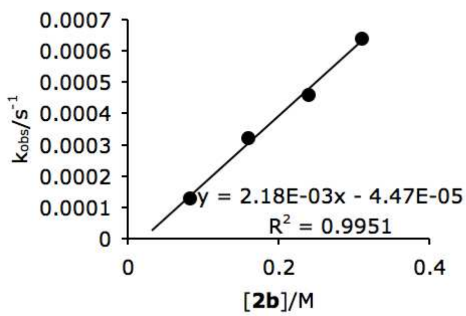


Table S3. Kinetics of the reaction of DDQ (**1a**) with 3-propylcyclopent-1-ene (**2c**) in CH_2Cl_2 (20 °C, Stopped-flow, at 390 nm)

[DDQ] / mol L^{-1}	[**2c**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-3}	0.50	3.7×10^{-3}
1.0×10^{-3}	1.0	7.3×10^{-3}
1.0×10^{-3}	1.5	1.1×10^{-2}
1.0×10^{-3}	2.0	1.5×10^{-2}

$k_2 = 7.5 \times 10^{-3}$ L mol^{-1} s^{-1}

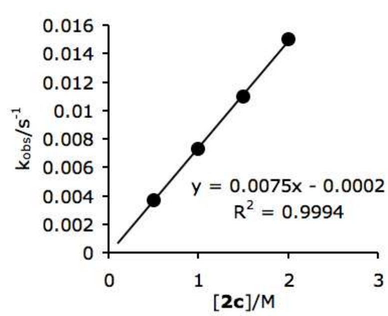


Table S4. Kinetics of the reaction of DDQ (**1a**) with cyclohepta-1,3,5-triene (**2d**) in CH_2Cl_2 (20 ^oC, Stopped-flow, at 350 nm)

[DDQ] / mol L^{-1}	[**2d**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-2}	2.2×10^{-2}
1.0×10^{-4}	2.0×10^{-2}	4.4×10^{-2}
1.0×10^{-4}	3.0×10^{-2}	6.6×10^{-2}
1.0×10^{-4}	4.0×10^{-2}	8.8×10^{-2}
1.0×10^{-4}	5.0×10^{-2}	1.1×10^{-1}

$k_2 = 2.2$ L mol^{-1} s^{-1}

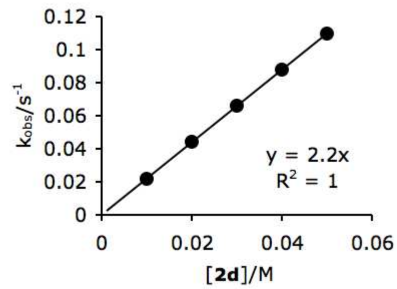


Table S5. Kinetics of the reaction of DDQ (**1a**) with cyclohexa-1,4-diene (**2e**) in CH_2Cl_2 (20 ^oC, Stopped-flow, at 390 nm)

[DDQ] / mol L^{-1}	[**2e**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-3}	2.5×10^{-2}	1.4×10^{-2}
1.0×10^{-3}	5.0×10^{-2}	2.8×10^{-2}
1.0×10^{-3}	1.0×10^{-1}	5.3×10^{-2}
1.0×10^{-3}	1.5×10^{-1}	7.9×10^{-2}
1.0×10^{-3}	2.0×10^{-1}	1.1×10^{-1}
1.0×10^{-3}	2.5×10^{-1}	1.2×10^{-1}

$k_2 = 0.49$ L mol^{-1} s^{-1}

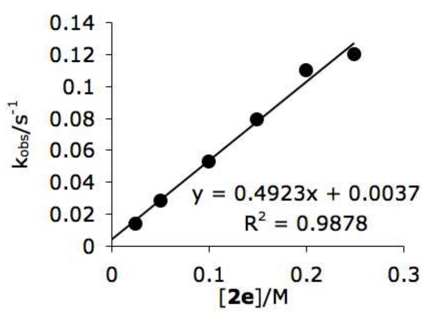


Table S6. Kinetics of the reaction of DDQ (**1a**) with cyclohexa-1,4-diene (**2e**) in CH_3CN (20 ^oC, Conventional UV/Vis, at 286 nm)

[DDQ] / mol L^{-1}	[**2e**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	3.9×10^{-3}	2.8×10^{-4}
1.0×10^{-4}	5.7×10^{-3}	3.8×10^{-4}
1.0×10^{-4}	7.5×10^{-3}	4.9×10^{-4}
1.0×10^{-4}	9.2×10^{-3}	6.1×10^{-4}

$k_2 = 6.2 \times 10^{-2}$ L mol^{-1} s^{-1}

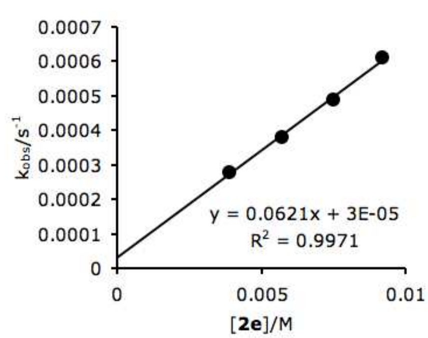


Table S7. Kinetics of the reaction of DDQ (**1a**) with cyclohexa-1,4-diene (**2e**) in cyclohexane (20 °C, Conventional UV/Vis, at 286 nm)

[DDQ] / mol L^{-1}	[**2e**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	2.0×10^{-3}	3.0×10^{-4}
1.0×10^{-4}	4.0×10^{-3}	4.5×10^{-4}
1.0×10^{-4}	8.0×10^{-3}	1.2×10^{-3}
1.0×10^{-4}	1.2×10^{-2}	1.6×10^{-3}

$k_2 = 0.14$ L mol^{-1} s^{-1}

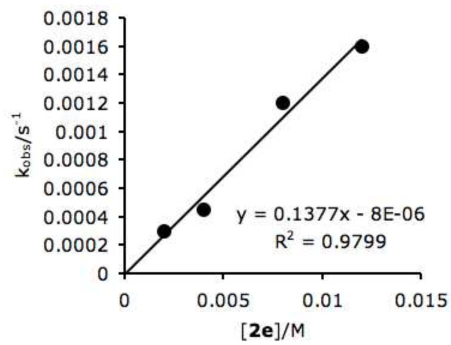


Table S8. Kinetics of the reaction of DDQ (**1a**) with cyclohexa-1,4-diene (**2e**) in acetone (20 °C, Stopped-flow, at 350 nm)

[DDQ] / mol L^{-1}	[**2e**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-1}	2.4×10^{-3}
1.0×10^{-4}	2.0×10^{-1}	3.7×10^{-3}
1.0×10^{-4}	3.0×10^{-1}	4.8×10^{-3}
1.0×10^{-4}	4.0×10^{-1}	5.9×10^{-3}

$k_2 = 1.2 \times 10^{-2}$ L mol^{-1} s^{-1}

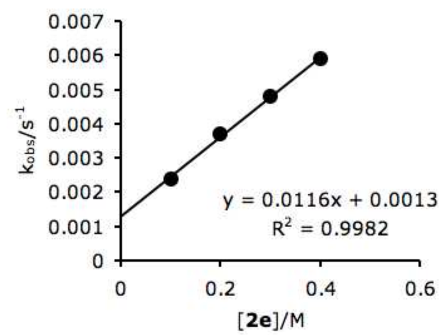


Table S9. Kinetics of the reaction of DDQ (**1a**) with cyclohexa-1,4-diene (**2e**) in THF (20 °C, Conventional UV/Vis, at 286 nm)

[DDQ] / mol L^{-1}	[**2e**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-2}	4.5×10^{-5}
1.0×10^{-4}	2.0×10^{-2}	1.0×10^{-4}
1.0×10^{-4}	3.9×10^{-2}	1.7×10^{-4}

$k_2 = 4.2 \times 10^{-3}$ L mol^{-1} s^{-1}

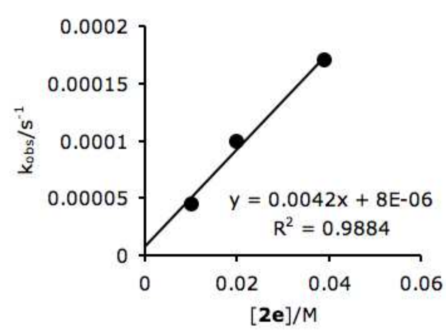


Table S10. Kinetics of the reaction of DDQ (**1a**) with cyclohexa-1,4-diene (**2e**) in *n*-Bu_2O (20 °C, Conventional UV/Vis, at 390 nm)

[DDQ] / mol L^{-1}	[**2e**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-3}	1.0×10^{-2}	5.3×10^{-4}
1.0×10^{-3}	2.0×10^{-2}	9.2×10^{-4}
1.0×10^{-3}	3.0×10^{-2}	1.4×10^{-3}
1.0×10^{-3}	4.0×10^{-2}	1.9×10^{-3}

$k_2 = 4.6 \times 10^{-2}$ L mol^{-1} s^{-1}

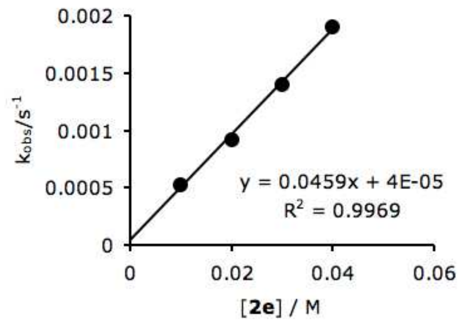


Table S11. Kinetics of the reaction of DDQ (**1a**) with **2e-D₈** in CH_2Cl_2 (20 °C, Conventional UV/Vis, at 286 nm)

[DDQ] / mol L^{-1}	[**2e-D$_8$**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	6.0×10^{-5}
1.0×10^{-4}	2.9×10^{-3}	1.5×10^{-4}
1.0×10^{-4}	3.8×10^{-3}	2.2×10^{-4}
1.0×10^{-4}	5.7×10^{-3}	3.8×10^{-4}

$k_2 = 6.8 \times 10^{-2}$ L mol^{-1} s^{-1}

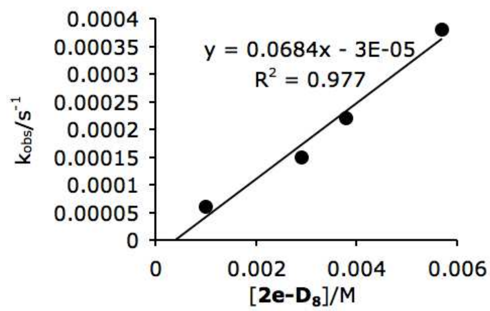


Table S12. Kinetics of the reaction of DDQ (**1a**) with **2e-D$_8$** in CH_3CN (20 °C, Conventional UV/Vis, at 390 nm)

[DDQ] / mol L^{-1}	[**2e-D$_8$**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-3}	1.0×10^{-2}	1.6×10^{-4}
1.0×10^{-3}	2.0×10^{-2}	2.7×10^{-4}
1.0×10^{-3}	3.0×10^{-2}	3.4×10^{-4}
1.0×10^{-3}	4.0×10^{-2}	4.6×10^{-4}

$k_2 = 9.7 \times 10^{-3}$ L mol^{-1} s^{-1}

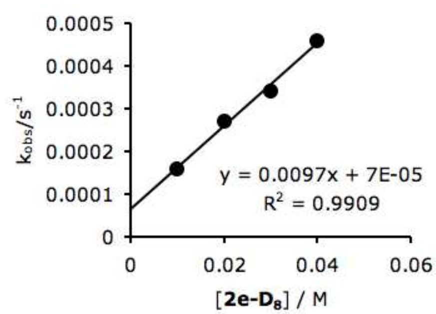


Table S13. Kinetics of the reaction of DDQ (**1a**) with **2e-D₈** in THF (20 °C, Conventional UV/Vis, at 390 nm)

[DDQ] / mol L^{-1}	[**2e-D$_8$**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-3}	2.0×10^{-2}	2.2×10^{-5}
1.0×10^{-3}	4.0×10^{-2}	3.3×10^{-5}
1.0×10^{-3}	6.0×10^{-2}	5.1×10^{-5}

$k_2 = 7.3 \times 10^{-4}$ L mol^{-1} s^{-1}

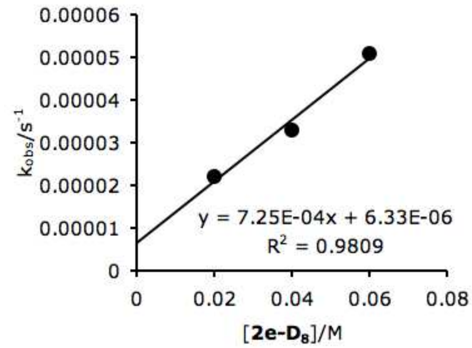


Table S14. Kinetics of the reaction of DDQ (**1a**) with **2e-D$_8$** in *n*-Bu_2O (20 °C, Conventional UV/Vis, at 390 nm)

[DDQ] / mol L^{-1}	[**2e-D$_8$**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-3}	1.0×10^{-2}	6.1×10^{-5}
1.0×10^{-3}	2.0×10^{-2}	1.1×10^{-4}
1.0×10^{-3}	3.0×10^{-2}	1.7×10^{-4}
1.0×10^{-3}	4.0×10^{-2}	2.1×10^{-4}

$k_2 = 5.1 \times 10^{-3}$ L mol^{-1} s^{-1}

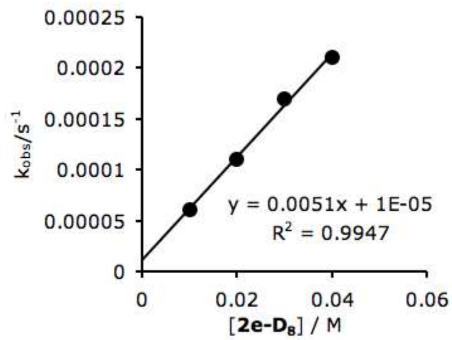


Table S15. Kinetics of the reaction of DDQ (**1a**) with 1,4-dimethylcyclohexa-1,4-diene (**2f**) in CH_2Cl_2 (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2f**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	0.10
1.0×10^{-4}	2.0×10^{-3}	0.21
1.0×10^{-4}	3.0×10^{-3}	0.31
1.0×10^{-4}	4.0×10^{-3}	0.42
1.0×10^{-4}	5.0×10^{-3}	0.53

$k_2 = 1.1 \times 10^{2}$ L mol^{-1} s^{-1}

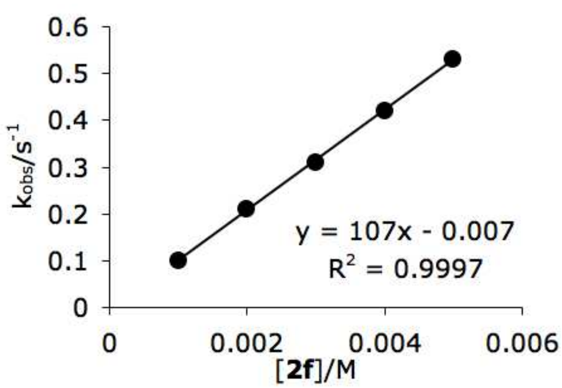


Table S16. Kinetics of the reaction of DDQ (**1a**) with1,3,5-trimethylcyclohexa-1,4-diene (**2g**) in CH_2Cl_2 (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2g**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	1.2
1.0×10^{-4}	2.0×10^{-3}	2.3
1.0×10^{-4}	3.0×10^{-3}	3.5
1.0×10^{-4}	4.0×10^{-3}	4.7
1.0×10^{-4}	5.0×10^{-3}	5.9

$k_2 = 1.2 \times 10^3$ L mol^{-1} s^{-1}

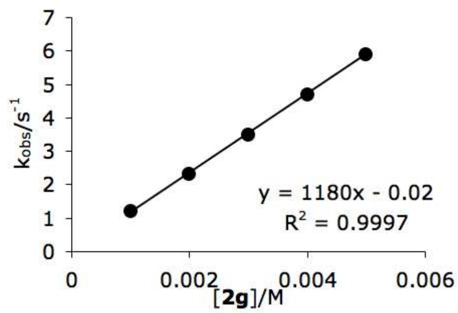


Table S17. Kinetics of the reaction of DDQ (**1a**) with 1,2,4,5-tetramethylcyclohexa-1,4-diene (**2h**) in CH_2Cl_2 (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2h**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	51
1.0×10^{-4}	2.0×10^{-3}	1.0×10^{2}
1.0×10^{-4}	3.0×10^{-3}	1.7×10^{2}
1.0×10^{-4}	4.0×10^{-3}	2.3×10^{2}
1.0×10^{-4}	5.0×10^{-3}	2.8×10^{2}

$k_2 = 5.9 \times 10^4$ L mol^{-1} s^{-1}

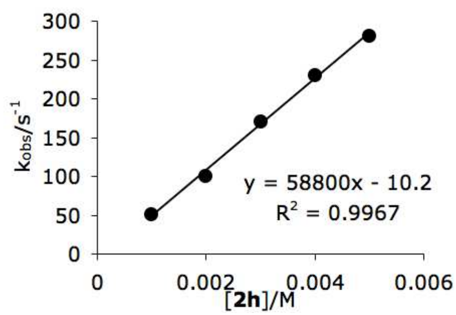


Table S18. Kinetics of the reaction of DDQ (**1a**) with bis(4-methoxyphenyl)methane (**2i**) in CH_2Cl_2 (20 °C, Conventional UV/Vis, at 350 nm)

[DDQ] / mol L^{-1}	[**2i**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	5.3×10^{-5}
1.0×10^{-4}	2.0×10^{-3}	9.0×10^{-5}
1.0×10^{-4}	2.9×10^{-3}	1.1×10^{-4}
1.0×10^{-4}	3.9×10^{-3}	1.6×10^{-4}
1.0×10^{-4}	4.8×10^{-3}	2.0×10^{-4}

$k_2 = 3.8 \times 10^{-2}$ L mol^{-1} s^{-1}

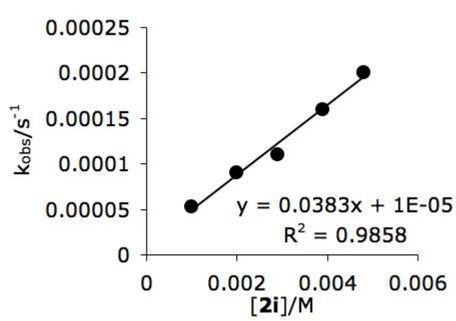


Table S19. Kinetics of the reaction of DDQ (**1a**) with 9H-xanthene (**2j**) in CH_2Cl_2 (20 ^oC, Conventional UV/Vis, at 390 nm)

[DDQ] / mol L^{-1}	[**2j**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-3}	1.0×10^{-2}	6.5×10^{-2}
1.0×10^{-3}	1.2×10^{-2}	7.8×10^{-2}
1.0×10^{-3}	1.4×10^{-2}	9.0×10^{-2}
1.0×10^{-3}	1.6×10^{-2}	1.0×10^{-1}
1.0×10^{-3}	1.8×10^{-2}	1.2×10^{-1}

$k_2 = 6.6$ L mol^{-1} s^{-1}

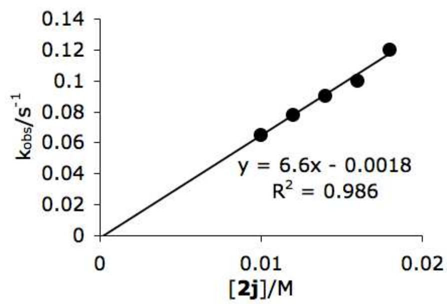


Table S20. Kinetics of the reaction of DDQ (**1a**) with tetrabutylstannane (**2m**) in CH_2Cl_2 (20 ^oC, Conventional UV/Vis, at 286 nm)

[DDQ] / mol L^{-1}	[**2m**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	2.0×10^{-3}	1.1×10^{-4}
1.0×10^{-4}	3.9×10^{-3}	1.8×10^{-4}
1.0×10^{-4}	5.7×10^{-3}	3.5×10^{-4}
1.0×10^{-4}	7.5×10^{-3}	4.3×10^{-4}

$k_2 = 6.2 \times 10^{-2}$ L mol^{-1} s^{-1}

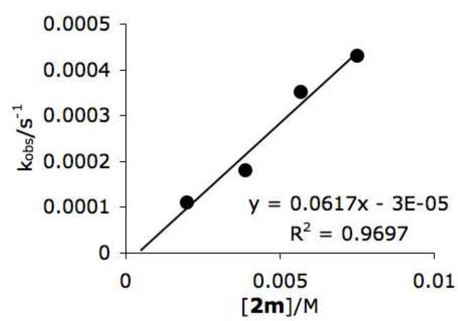


Table S21. Kinetics of the reaction of DDQ (**1a**) with Bu_3SnH (**2n**) in CH_2Cl_2 (20 ^oC, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2n**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	0.55
1.0×10^{-4}	2.0×10^{-3}	1.1
1.0×10^{-4}	3.0×10^{-3}	1.7
1.0×10^{-4}	4.0×10^{-3}	2.4
1.0×10^{-4}	5.0×10^{-3}	3.0

$k_2 = 6.2 \times 10^{2}$ L mol^{-1} s^{-1}

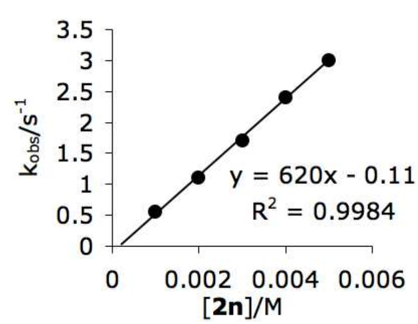
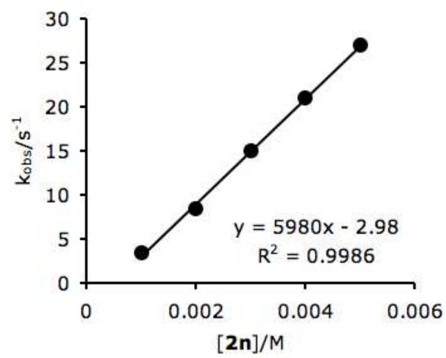


Table S22. Kinetics of the reaction of DDQ (**1a**) with Bu_3SnH (**2n**) in CH_3CN (20 °C, Stopped-flow, at 286 nm)

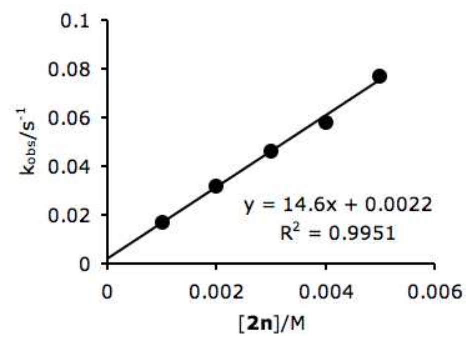
[DDQ] / mol L^{-1}	[**2n**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	3.4
1.0×10^{-4}	2.0×10^{-3}	8.4
1.0×10^{-4}	3.0×10^{-3}	15
1.0×10^{-4}	4.0×10^{-3}	21
1.0×10^{-4}	5.0×10^{-3}	27



$k_2 = 6.0 \times 10^3$ L mol^{-1} s^{-1}

Table S23. Kinetics of the reaction of DDQ (**1a**) with Bu_3SnH (**2n**) in cyclohexane (20 °C, Stopped-flow, at 286 nm)

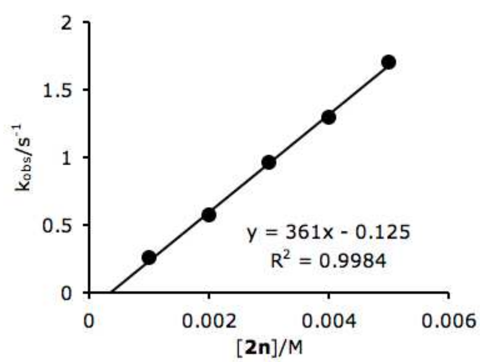
[DDQ] / mol L^{-1}	[**2n**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	1.7×10^{-2}
1.0×10^{-4}	2.0×10^{-3}	3.2×10^{-2}
1.0×10^{-4}	3.0×10^{-3}	4.6×10^{-2}
1.0×10^{-4}	4.0×10^{-3}	5.8×10^{-2}
1.0×10^{-4}	5.0×10^{-3}	7.7×10^{-2}



$k_2 = 15$ L mol^{-1} s^{-1}

Table S24. Kinetics of the reaction of DDQ (**1a**) with Bu_3SnH (**2n**) in acetone (20 °C, Stopped-flow, at 350 nm)

[DDQ] / mol L^{-1}	[**2n**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	0.26
1.0×10^{-4}	2.0×10^{-3}	0.57
1.0×10^{-4}	3.0×10^{-3}	0.96
1.0×10^{-4}	4.0×10^{-3}	1.3
1.0×10^{-4}	5.0×10^{-3}	1.7



$k_2 = 3.6 \times 10^2$ L mol^{-1} s^{-1}

Table S25. Kinetics of the reaction of DDQ (**1a**) with Bu_3SnH (**2n**) in THF (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2n**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	4.7×10^{-2}
1.0×10^{-4}	2.0×10^{-3}	9.2×10^{-2}
1.0×10^{-4}	3.0×10^{-3}	0.14
1.0×10^{-4}	4.0×10^{-3}	0.19
1.0×10^{-4}	5.0×10^{-3}	0.24

$k_2 = 4.8 \times 10^1$ L mol^{-1} s^{-1}

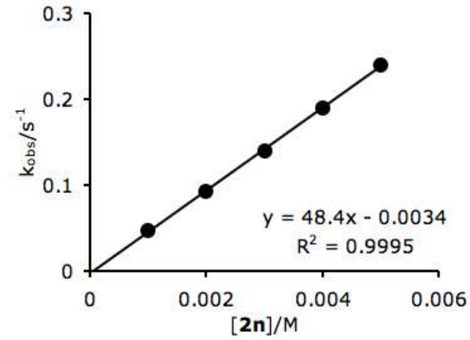


Table S26. Kinetics of the reaction of DDQ (**1a**) with Bu_3SnH (**2n**) in *n*-Bu_2O (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2n**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	2.2×10^{-2}
1.0×10^{-4}	2.0×10^{-3}	4.4×10^{-2}
1.0×10^{-4}	3.0×10^{-3}	6.8×10^{-2}
1.0×10^{-4}	4.0×10^{-3}	9.5×10^{-2}
1.0×10^{-4}	5.0×10^{-3}	1.2×10^{-1}

$k_2 = 2.5 \times 10^1$ L mol^{-1} s^{-1}

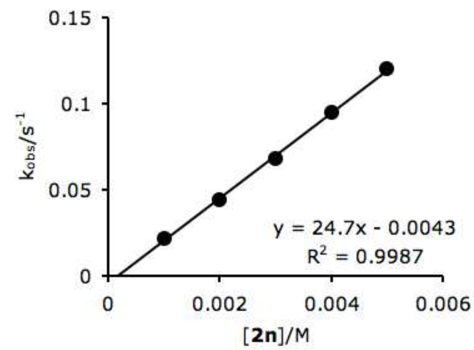


Table S27. Kinetics of the reaction of DDQ (**1a**) with **2n-D** in CH_2Cl_2 (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2n-D**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	0.34
1.0×10^{-4}	2.0×10^{-3}	0.67
1.0×10^{-4}	3.0×10^{-3}	1.0
1.0×10^{-4}	4.0×10^{-3}	1.4
1.0×10^{-4}	5.0×10^{-3}	1.8

$k_2 = 3.7 \times 10^2$ L mol^{-1} s^{-1}

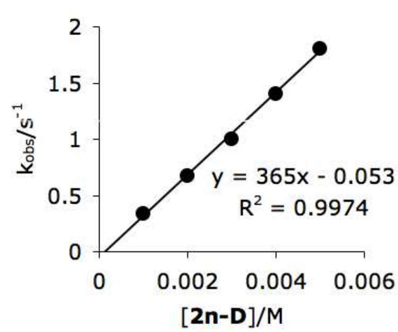


Table S28. Kinetics of the reaction of DDQ (**1a**) with **2n-D** in CH_3CN (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2n-D**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	2.3
1.0×10^{-4}	2.0×10^{-3}	4.3
1.0×10^{-4}	3.0×10^{-3}	6.8
1.0×10^{-4}	4.0×10^{-3}	9.6
1.0×10^{-4}	5.0×10^{-3}	13

$k_2 = 2.7 \times 10^3$ L mol^{-1} s^{-1}

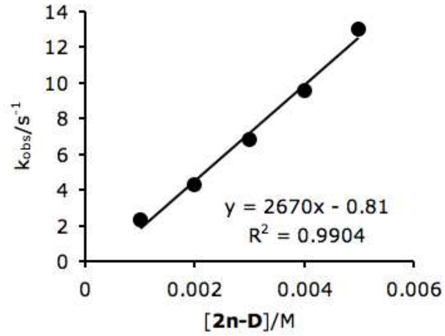


Table S29. Kinetics of the reaction of DDQ (**1a**) with **2n-D** in cyclohexane (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2n-D**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	1.8×10^{-2}
1.0×10^{-4}	2.0×10^{-3}	3.3×10^{-2}
1.0×10^{-4}	3.0×10^{-3}	5.0×10^{-2}
1.0×10^{-4}	4.0×10^{-3}	6.7×10^{-2}
1.0×10^{-4}	5.0×10^{-3}	8.2×10^{-2}

$k_2 = 1.6 \times 10^1$ L mol^{-1} s^{-1}

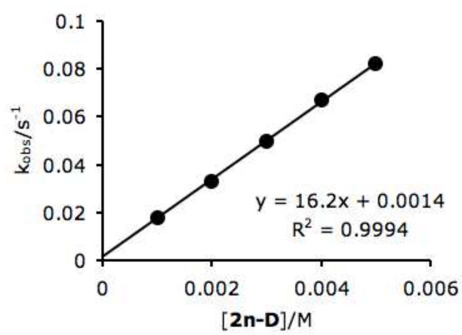


Table S30. Kinetics of the reaction of DDQ (**1a**) with **2n-D** in acetone (20 °C, Stopped-flow, at 350 nm)

[DDQ] / mol L^{-1}	[**2n-D**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	0.26
1.0×10^{-4}	2.0×10^{-3}	0.49
1.0×10^{-4}	3.0×10^{-3}	0.77
1.0×10^{-4}	4.0×10^{-3}	1.1
1.0×10^{-4}	5.0×10^{-3}	1.3

$k_2 = 2.7 \times 10^2$ L mol^{-1} s^{-1}

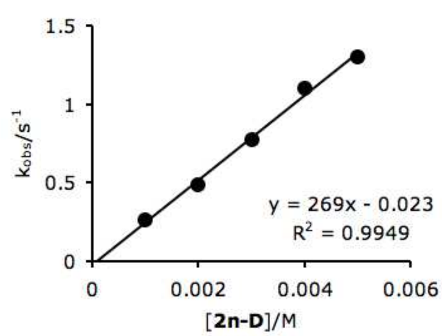


Table S31. Kinetics of the reaction of DDQ (**1a**) with **2n-D** in THF (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2n-D**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	3.6×10^{-2}
1.0×10^{-4}	2.0×10^{-3}	7.3×10^{-2}
1.0×10^{-4}	3.0×10^{-3}	0.11
1.0×10^{-4}	4.0×10^{-3}	0.15
1.0×10^{-4}	5.0×10^{-3}	0.18

$k_2 = 3.7 \times 10^1$ L mol^{-1} s^{-1}

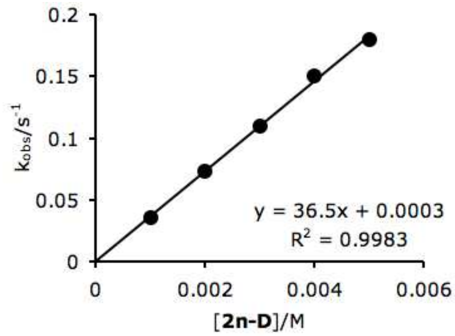


Table S32. Kinetics of the reaction of DDQ (**1a**) with **2n-D** in *n*-Bu_2O (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2n-D**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	1.4×10^{-2}
1.0×10^{-4}	2.0×10^{-3}	2.8×10^{-2}
1.0×10^{-4}	3.0×10^{-3}	4.3×10^{-2}
1.0×10^{-4}	4.0×10^{-3}	5.7×10^{-2}
1.0×10^{-4}	5.0×10^{-3}	7.1×10^{-2}

$k_2 = 1.4 \times 10^1$ L mol^{-1} s^{-1}

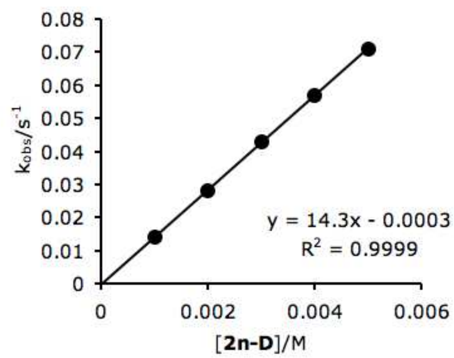


Table S33. Kinetics of the reaction of DDQ (**1a**) with Ph_3SnH (**2o**) in CH_2Cl_2 (20 °C, Stopped-flow, at 350 nm)

[DDQ] / mol L^{-1}	[**2o**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-2}	1.6×10^{-2}
1.0×10^{-4}	2.0×10^{-2}	3.4×10^{-2}
1.0×10^{-4}	3.0×10^{-2}	5.3×10^{-2}
1.0×10^{-4}	4.0×10^{-2}	7.7×10^{-2}
1.0×10^{-4}	5.0×10^{-2}	0.10

$k_2 = 2.1$ L mol^{-1} s^{-1}

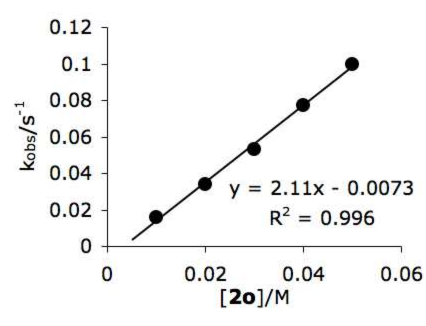


Table S34. Kinetics of the reaction of DDQ (**1a**) with $Me_3N\text{-}BH_3$ (**2p**) in CH_2Cl_2 (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2p**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-2}	2.7×10^{-2}
1.0×10^{-4}	2.0×10^{-2}	5.7×10^{-2}
1.0×10^{-4}	3.0×10^{-2}	8.5×10^{-2}
1.0×10^{-4}	4.0×10^{-2}	0.12
1.0×10^{-4}	5.0×10^{-2}	0.15

$k_2 = 3.1$ L mol^{-1} s^{-1}

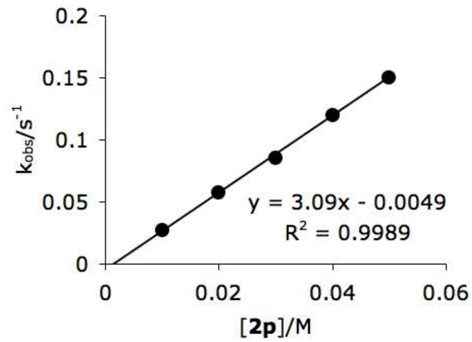


Table S35. Kinetics of the reaction of DDQ (**1a**) with $Et_3N\text{-}BH_3$ (**2q**) in CH_2Cl_2 (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2q**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	0.23
1.0×10^{-4}	1.5×10^{-3}	0.35
1.0×10^{-4}	2.0×10^{-3}	0.43
1.0×10^{-4}	2.5×10^{-3}	0.49
1.0×10^{-4}	3.0×10^{-3}	0.58

$k_2 = 1.7 \times 10^2$ L mol^{-1} s^{-1}

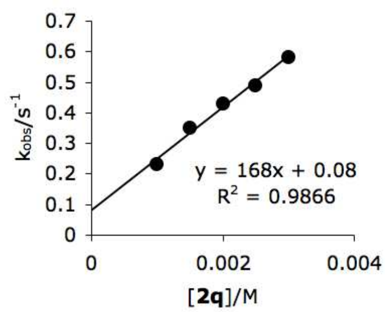


Table S36. Kinetics of the reaction of DDQ (**1a**) with $Py\text{-}BH_3$ (**2r**) in CH_2Cl_2 (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2r**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	7.3
1.0×10^{-4}	2.0×10^{-3}	13
1.0×10^{-4}	3.0×10^{-3}	17
1.0×10^{-4}	4.0×10^{-3}	23
1.0×10^{-4}	5.0×10^{-3}	28

$k_2 = 5.1 \times 10^3$ mol^{-1} L s^{-1}

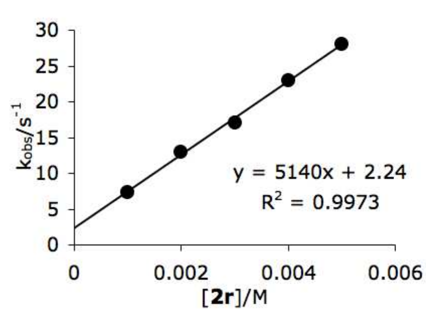


Table S37. Kinetics of the reaction of DDQ (**1a**) with Py-BH_3 (**2r**) in CH_3CN (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2r**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	2.0
1.0×10^{-4}	2.0×10^{-3}	4.0
1.0×10^{-4}	3.0×10^{-3}	6.1
1.0×10^{-4}	4.0×10^{-3}	8.3
1.0×10^{-4}	5.0×10^{-3}	11

$k_2 = 2.2 \times 10^3$ L mol^{-1} s^{-1}

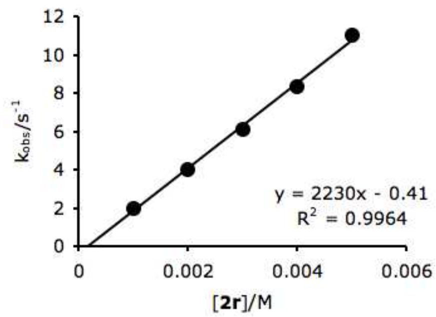


Table S38. Kinetics of the reaction of DDQ (**1a**) with Py-BH_3 (**2r**) in cyclohexane (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2r**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	34
1.0×10^{-4}	1.5×10^{-3}	48
1.0×10^{-4}	2.0×10^{-3}	64
1.0×10^{-4}	2.5×10^{-3}	78

$k_2 = 3.0 \times 10^4$ L mol^{-1} s^{-1}

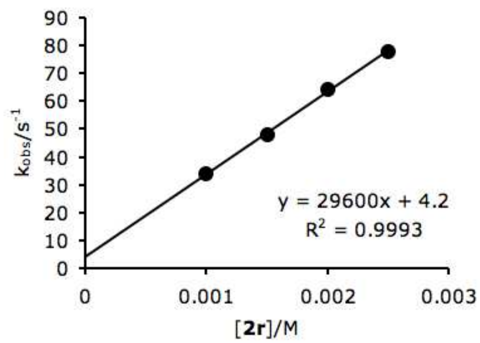


Table S39. Kinetics of the reaction of DDQ (**1a**) with Py-BH_3 (**2r**) in acetone (20 °C, Stopped-flow, at 350 nm)

[DDQ] / mol L^{-1}	[**2r**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	0.90
1.0×10^{-4}	2.0×10^{-3}	2.0
1.0×10^{-4}	3.0×10^{-3}	3.6
1.0×10^{-4}	4.0×10^{-3}	5.4
1.0×10^{-4}	5.0×10^{-3}	7.6

$k_2 = 1.7 \times 10^3$ L mol^{-1} s^{-1}

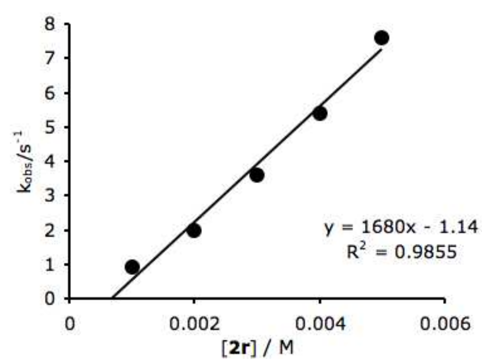


Table S40. Kinetics of the reaction of DDQ (**1a**) with Py-BH_3 (**2r**) in THF (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2r**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	0.47
1.0×10^{-4}	2.0×10^{-3}	0.98
1.0×10^{-4}	3.0×10^{-3}	1.5
1.0×10^{-4}	4.0×10^{-3}	2.1
1.0×10^{-4}	5.0×10^{-3}	2.6

$k_2 = 5.4 \times 10^2$ L mol^{-1} s^{-1}

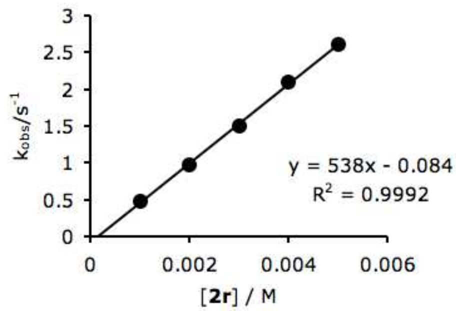


Table S41. Kinetics of the reaction of DDQ (**1a**) with Py-BH_3 (**2r**) in *n*-Bu_2O (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2r**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	7.0
1.0×10^{-4}	2.0×10^{-3}	14
1.0×10^{-4}	3.0×10^{-3}	21
1.0×10^{-4}	4.0×10^{-3}	26

$k_2 = 6.4 \times 10^3$ L mol^{-1} s^{-1}

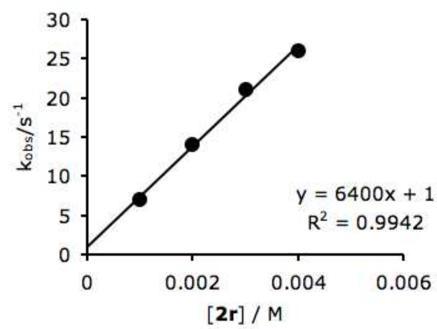


Table S42. Kinetics of the reaction of DDQ (**1a**) with **2r-D$_3$** in CH_2Cl_2 (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2r-D$_3$**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	2.8
1.0×10^{-4}	2.0×10^{-3}	5.8
1.0×10^{-4}	3.0×10^{-3}	8.7
1.0×10^{-4}	4.0×10^{-3}	11
1.0×10^{-4}	5.0×10^{-3}	14

$k_2 = 2.8 \times 10^3$ L mol^{-1} s^{-1}

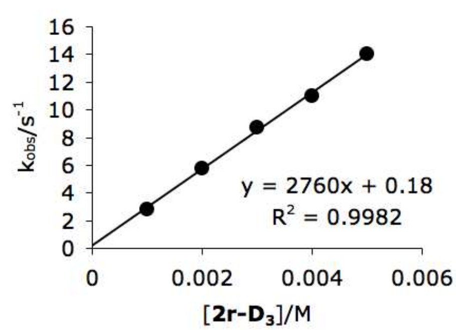


Table S43. Kinetics of the reaction of DDQ (**1a**) with **2r-D$_3$** in CH_3CN (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2r-D$_3$**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	0.80
1.0×10^{-4}	2.0×10^{-3}	1.7
1.0×10^{-4}	3.0×10^{-3}	2.7
1.0×10^{-4}	4.0×10^{-3}	3.7
1.0×10^{-4}	5.0×10^{-3}	4.8

$k_2 = 1.0 \times 10^3$ L mol^{-1} s^{-1}

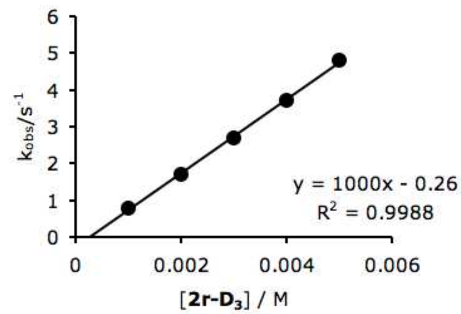


Table S44. Kinetics of the reaction of DDQ (**1a**) with **2r-D$_3$** in cyclohexane (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2r-D$_3$**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	18
1.0×10^{-4}	1.5×10^{-3}	27
1.0×10^{-4}	2.0×10^{-3}	32
1.0×10^{-4}	2.5×10^{-3}	38

$k_2 = 1.3 \times 10^4$ L mol^{-1} s^{-1}

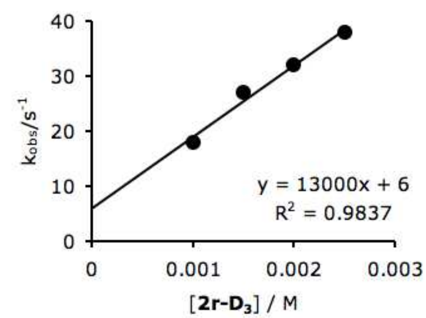


Table S45. Kinetics of the reaction of DDQ (**1a**) with **2r-D$_3$** in acetone (20 °C, Stopped-flow, at 350 nm)

[DDQ] / mol L^{-1}	[**2r-D$_3$**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	0.55
1.0×10^{-4}	2.0×10^{-3}	1.2
1.0×10^{-4}	3.0×10^{-3}	2.0
1.0×10^{-4}	4.0×10^{-3}	2.8
1.0×10^{-4}	5.0×10^{-3}	3.7

$k_2 = 7.9 \times 10^2$ L mol^{-1} s^{-1}

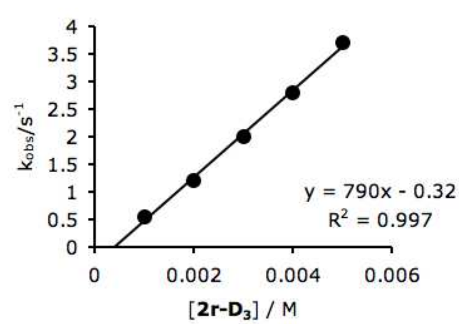


Table S46. Kinetics of the reaction of DDQ (**1a**) with **2r-D$_3$** in THF (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2r-D$_3$**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	0.20
1.0×10^{-4}	2.0×10^{-3}	0.41
1.0×10^{-4}	3.0×10^{-3}	0.62
1.0×10^{-4}	4.0×10^{-3}	0.84
1.0×10^{-4}	5.0×10^{-3}	1.1

$k_2 = 2.2 \times 10^2$ L mol^{-1} s^{-1}

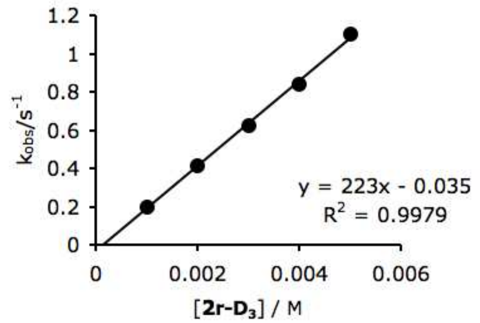


Table S47. Kinetics of the reaction of DDQ (**1a**) with **2r-D$_3$** in *n*-Bu_2O (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2r-D$_3$**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	4.4
1.0×10^{-4}	2.0×10^{-3}	8.4
1.0×10^{-4}	3.0×10^{-3}	13
1.0×10^{-4}	4.0×10^{-3}	17

$k_2 = 4.2 \times 10^3$ L mol^{-1} s^{-1}

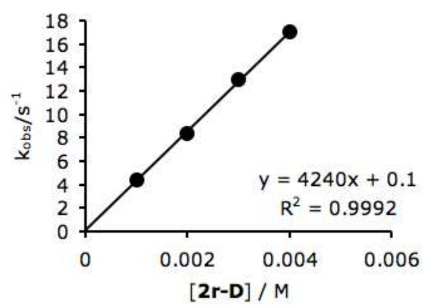


Table S48. Kinetics of the reaction of DDQ (**1a**) with 1,3-bis-(2,6-diisopropylphenyl) imidazolylidene borane complex (**2s**) in CH_2Cl_2 (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2s**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-3}	2.8
1.0×10^{-4}	1.5×10^{-3}	4.0
1.0×10^{-4}	2.0×10^{-3}	5.4
1.0×10^{-4}	2.5×10^{-3}	7.1

$k_2 = 2.9 \times 10^3$ L mol^{-1} s^{-1}

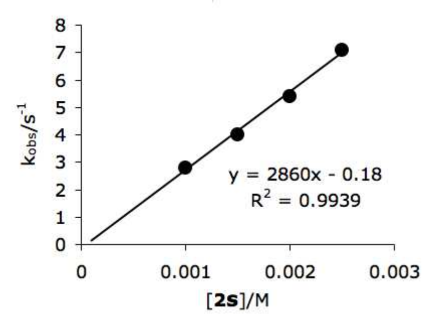
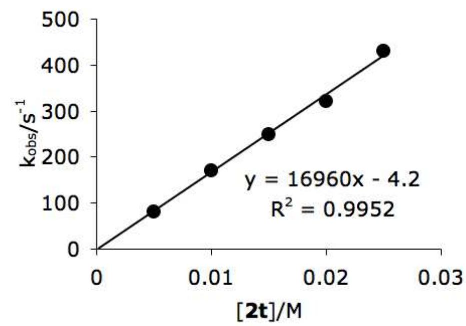


Table S49. Kinetics of the reaction of DDQ (**1a**) with 1,3-dimethylimidazolylidene borane complex (**2t**) in CH_2Cl_2 (20 °C, Stopped-flow, at 286 nm)

[DDQ] / mol L^{-1}	[**2t**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	5.0×10^{-3}	81
1.0×10^{-4}	1.0×10^{-2}	1.7×10^{2}
1.0×10^{-4}	1.5×10^{-2}	2.5×10^{2}
1.0×10^{-4}	2.0×10^{-2}	3.2×10^{2}
1.0×10^{-4}	2.5×10^{-2}	4.3×10^{2}

$k_2 = 1.7 \times 10^{4}$ L mol^{-1} s^{-1}



2). Kinetics of the Reactions of Bu_3SnH (2n) with Other Quinones

Table S50. Kinetics of the reaction of Bu_3SnH (**2n**) with p-benzoquinone (**1f**) in CD_3CN (20 °C, ^1H NMR, 4.58-4.69 ppm)

[**1f**] / mol L^{-1}	[**2n**] / mol L^{-1}	k_{obs} / s^{-1}
1.5×10^{-2}	1.0×10^{-1}	2.1×10^{-5}
2.0×10^{-2}	2.0×10^{-1}	2.8×10^{-5}
2.0×10^{-2}	3.0×10^{-1}	4.1×10^{-5}
2.0×10^{-2}	4.0×10^{-1}	4.8×10^{-5}

$k_2 = 9.4 \times 10^{-5}$ L mol^{-1} s^{-1}

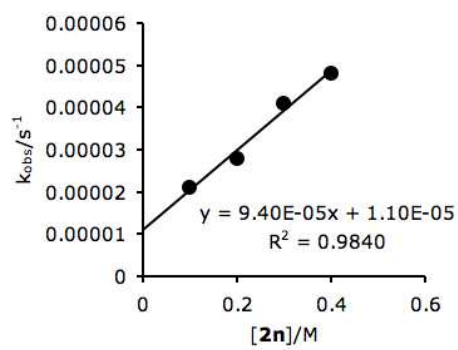


Table S51. Kinetics of the reaction of Bu_3SnH (**2n**) with 2,5-dichloro-benzoquinone (**1b**) in CH_3CN (20 °C, Conventional UV/Vis, at 270 nm)

[**1b**] / mol L^{-1}	[**2n**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.5×10^{-2}	4.5×10^{-4}
1.0×10^{-4}	2.9×10^{-2}	7.9×10^{-4}
1.0×10^{-4}	4.3×10^{-2}	1.1×10^{-3}
1.0×10^{-4}	5.7×10^{-2}	1.5×10^{-3}

$k_2 = 2.5 \times 10^{-2}$ L mol^{-1} s^{-1}

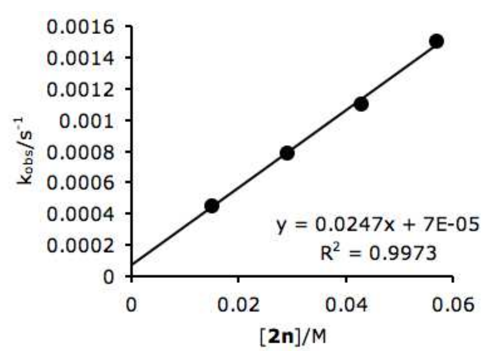


Table S52. Kinetics of the reaction of Bu_3SnH (**2n**) with p-chloranil (**1c**) in CH_3CN (20 °C, Conventional UV/Vis, at 287 nm)

[**1c**] / mol L^{-1}	[**2n**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	7.3×10^{-3}	4.7×10^{-3}
1.0×10^{-4}	1.5×10^{-2}	1.1×10^{-2}
1.0×10^{-4}	2.2×10^{-2}	1.7×10^{-2}
1.0×10^{-4}	2.9×10^{-2}	2.5×10^{-2}

$k_2 = 9.3 \times 10^{-1}$ L mol^{-1} s^{-1}

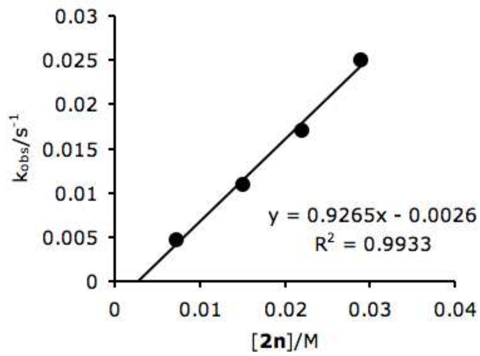


Table S53. Kinetics of the reaction of Bu_3SnH (**2n**) with p-fluoranil (**1d**) in CH_3CN (20 °C, Stopped-flow, at 256 nm)

[**1d**] / mol L^{-1}	[**2n**] / mol L^{-1}	k_{obs} / s^{-1}
5.0×10^{-5}	1.0×10^{-2}	1.4×10^{-2}
5.0×10^{-5}	2.0×10^{-2}	2.8×10^{-2}
5.0×10^{-5}	3.0×10^{-2}	4.6×10^{-2}
5.0×10^{-5}	4.0×10^{-2}	5.7×10^{-2}

$k_2 = 1.5$ L mol^{-1} s^{-1}

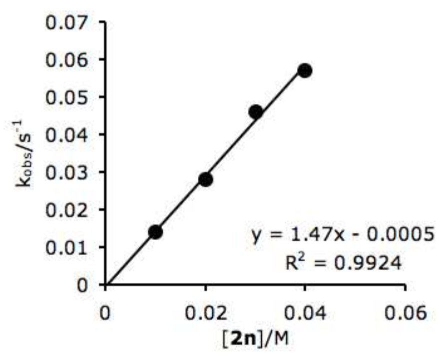
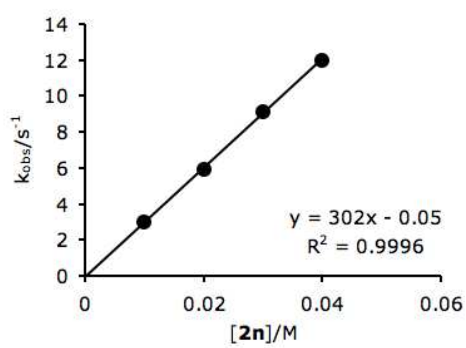


Table S54. Kinetics of the reaction of Bu_3SnH (**2n**) with o-chloranil (**1e**) in CH_3CN (20 °C, Stopped-flow, at 457 nm)

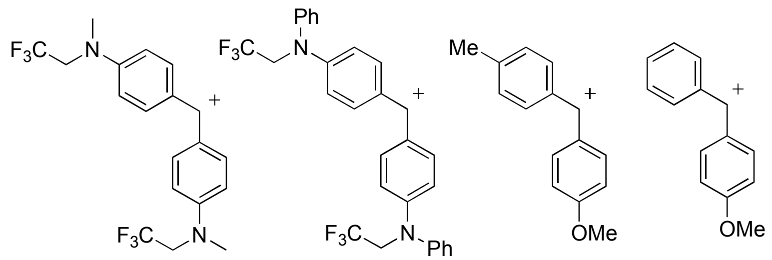
[**1e**] / mol L^{-1}	[**2n**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-4}	1.0×10^{-2}	3.0
1.0×10^{-4}	2.0×10^{-2}	5.9
1.0×10^{-4}	3.0×10^{-2}	9.1
1.0×10^{-4}	4.0×10^{-2}	12

$k_2 = 3.0 \times 10^{2}$ L mol^{-1} s^{-1}



3). Determination of the Nucleophilicity Parameters of 2f-i

In order to determine the nucleophilicity parameters N and s_N for the nucleophiles **2f-i** the rates of the reactions with the benzhydrylium ions Ar_2CH^+ have been determined photometrically in CH_2Cl_2 solution. The nucleophilicity parameters of **2f-i** in CH_2Cl_2 were determined according to the correlation log $k_2 = s_N$ ($N + E$) by plots of the second-order rate constants (log k_2) for the reactions of **2f-i** with the employed benzhydrylium ions Ar_2CH^+ versus the corresponding electrophilicity parameters *E*.



Ar_2CH^+	mfa_2CH^+	pfa_2CH^+	$ani(tol)CH^+$	$ani(Ph)CH^+$
E	-3.85	-3.14	1.48	2.11

Figure S1. Benzhydrylium ions Ar_2CH^+ and their electrophilicity parameters E[S5] used for the determination of the nucleophilicity parameters (N and s_N) for **2f-i** in CH_2Cl_2.

Table S55. Kinetics of the reaction of 1,4-dimethylcyclohexa-1,4-diene (**2f**) with mfa_2CH^+ in CH_2Cl_2 (20 °C, J&M, at 593 nm)

$[mfa_2CH^+]$ / mol L^{-1}	[**2f**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-5}	3.9×10^{-3}	4.5×10^{-5}
1.0×10^{-5}	4.8×10^{-3}	5.6×10^{-5}
1.0×10^{-5}	5.7×10^{-3}	6.9×10^{-5}
1.0×10^{-5}	7.4×10^{-3}	8.9×10^{-5}

$k_2 = 1.3 \times 10^{-2}$ L mol^{-1} s^{-1}

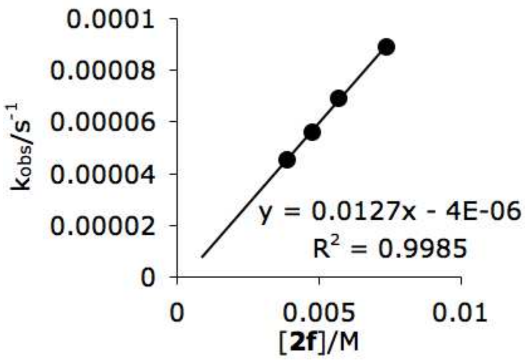


Table S56. Kinetics of the reaction of 1,4-dimethylcyclohexa-1,4-diene (**2f**) with pfa_2CH^+ in CH_2Cl_2 (20 °C, J&M, at 601 nm)

$[pfa_2CH^+]$ / mol L^{-1}	[**2f**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-5}	1.0×10^{-3}	6.1×10^{-5}
1.0×10^{-5}	2.0×10^{-3}	1.2×10^{-4}
1.0×10^{-5}	3.9×10^{-3}	2.5×10^{-4}
1.0×10^{-5}	4.8×10^{-3}	2.9×10^{-4}

$k_2 = 6.2 \times 10^{-2}$ L mol^{-1} s^{-1}

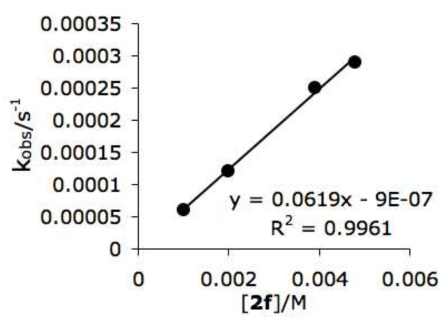


Table S57. Kinetics of the reaction of 1,3,5-trimethylcyclohexa-1,4-diene (**2g**) with mfa_2CH^+ in CH_2Cl_2 (20 °C, J&M, at 593 nm)

$[mfa_2CH^+]$ / mol L^{-1}	[**2g**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-5}	1.0×10^{-3}	6.8×10^{-3}
1.0×10^{-5}	2.0×10^{-3}	1.3×10^{-2}
1.0×10^{-5}	2.9×10^{-3}	2.1×10^{-2}
1.0×10^{-5}	3.9×10^{-3}	2.8×10^{-2}

$k_2 = 7.4$ L mol^{-1} s^{-1}

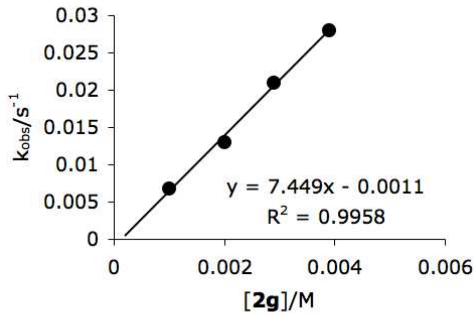


Table S58. Kinetics of the reaction of 1,3,5-trimethylcyclohexa-1,4-diene (**2g**) with pfa_2CH^+ in CH_2Cl_2 (20 °C, Stopped-flow, at 601 nm)

$[pfa_2CH^+]$ / mol L^{-1}	[**2g**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-5}	1.0×10^{-3}	2.6×10^{-2}
1.0×10^{-5}	1.2×10^{-3}	3.1×10^{-2}
1.0×10^{-5}	1.4×10^{-3}	3.6×10^{-2}
1.0×10^{-5}	1.6×10^{-3}	4.1×10^{-2}
1.0×10^{-5}	2.0×10^{-3}	5.3×10^{-2}

$k_2 = 27$ L mol^{-1} s^{-1}

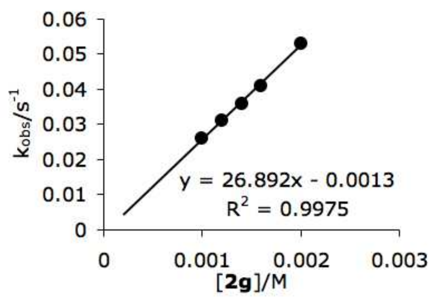


Table S59. Kinetics of the reaction of 1,2,4,5-tetramethylcyclohexa-1,4-diene (**2h**) with mfa_2CH^+ in CH_2Cl_2 (20 °C, Stopped-flow, at 593 nm)

$[mfa_2CH^+]$ / mol L^{-1}	[**2h**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-5}	1.0×10^{-3}	2.2×10^{-3}
1.0×10^{-5}	2.0×10^{-3}	4.4×10^{-3}
1.0×10^{-5}	2.9×10^{-3}	6.6×10^{-3}
1.0×10^{-5}	3.9×10^{-3}	8.8×10^{-3}

$k_2 = 2.3$ L mol^{-1} s^{-1}

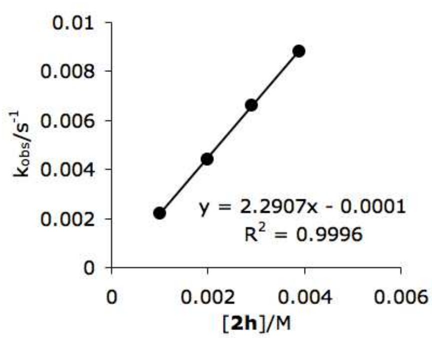


Table S60. Kinetics of the reaction of 1,2,4,5-tetramethylcyclohexa-1,4-diene (**2h**) with pfa_2CH^+ in CH_2Cl_2 (20 °C, J&M, at 601 nm)

$[pfa_2CH^+]$ / mol L^{-1}	[**2h**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-5}	1.0×10^{-4}	9.1×10^{-4}
1.0×10^{-5}	2.0×10^{-4}	1.7×10^{-3}
1.0×10^{-5}	2.9×10^{-4}	2.6×10^{-3}
1.0×10^{-5}	3.9×10^{-4}	3.5×10^{-3}
1.0×10^{-5}	4.8×10^{-4}	4.5×10^{-3}

$k_2 = 9.4$ L mol^{-1} s^{-1}

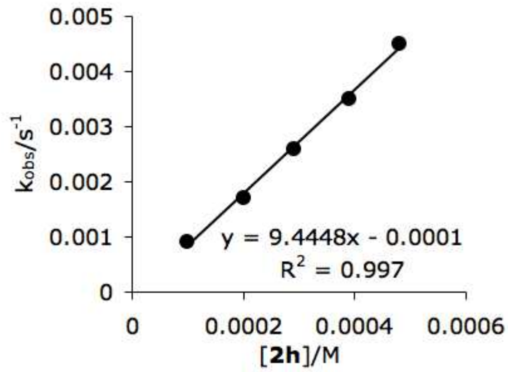


Table S61. Kinetics of the reaction of bis(4-methoxyphenyl)methane (**2i**) with (ani,Ph)CH^+ in CH_2Cl_2 (20 °C, J&M, at 513 nm)

[(ani,Ph)CH^+] / mol L^{-1}	[**2i**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-5}	1.9×10^{-3}	2.6×10^{-3}
1.0×10^{-5}	2.9×10^{-3}	3.4×10^{-3}
1.0×10^{-5}	4.0×10^{-3}	5.0×10^{-3}
1.0×10^{-5}	5.7×10^{-3}	6.4×10^{-3}

$k_2 = 1.0$ L mol^{-1} s^{-1}

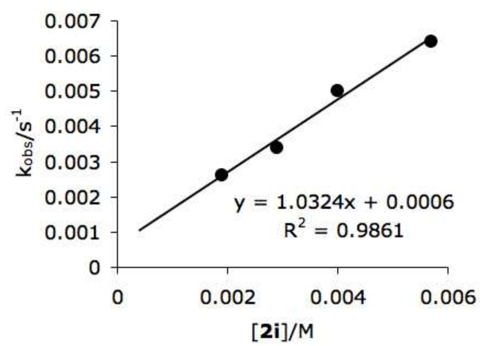


Table S62. Kinetics of the reaction of bis(4-methoxyphenyl)methane (**2i**) with (ani,tol)CH^+ in CH_2Cl_2 (20 °C, J&M, at 513 nm)

[(ani,tol)CH^+] / mol L^{-1}	[**2i**] / mol L^{-1}	k_{obs} / s^{-1}
1.0×10^{-5}	4.0×10^{-3}	1.2×10^{-3}
1.0×10^{-5}	8.1×10^{-3}	2.0×10^{-3}
1.0×10^{-5}	1.6×10^{-2}	3.8×10^{-3}
1.0×10^{-5}	2.0×10^{-2}	5.1×10^{-3}

$k_2 = 0.24$ L mol^{-1} s^{-1}

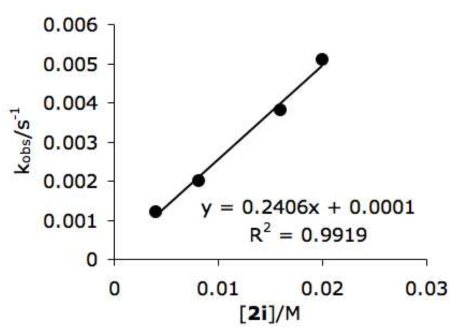


Table S63. Determination of the nucleophilicity parameters (N and s_N) of **2f-i**.

Nu	Electrophile	E	k_2/ L mol^{-1} s^{-1}	log k_2
2f	mfa_2CH^+	-3.85	1.3×10^{-2}	-1.89
	pfa_2CH^+	-3.14	6.2×10^{-2}	-1.21
	$N = 1.88$, $s_N = 0.96$			
2g	mfa_2CH^+	-3.85	7.4	0.87
	pfa_2CH^+	-3.14	27	1.43
	$N = 4.95$, $s_N = 0.79$			
2h	mfa_2CH^+	-3.85	2.3	0.36
	pfa_2CH^+	-3.14	9.4	0.97
	$N = 4.27$, $s_N = 0.86$			
2i	ani(tol)CH^+	1.48	0.24	-0.62
	ani(Ph)CH^+	2.11	1.0	0
	$N = –2.11$, $s_N = 0.98$			

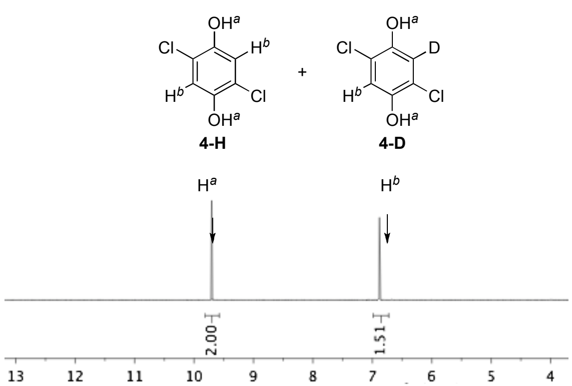
4). The Reaction of 2,5-Dichlorobenzoquinone (1b) with Deuterated Hydride Donors.

^{1}H NMR spectra were recorded on a 400 MHz spectrometer in d_6-DMSO solution. Mass spectra were determined with Finnigan MAT 95 (70 eV) or Agilent 6890N Gas Chromatograph equipped with Agilent 5973N MSD.

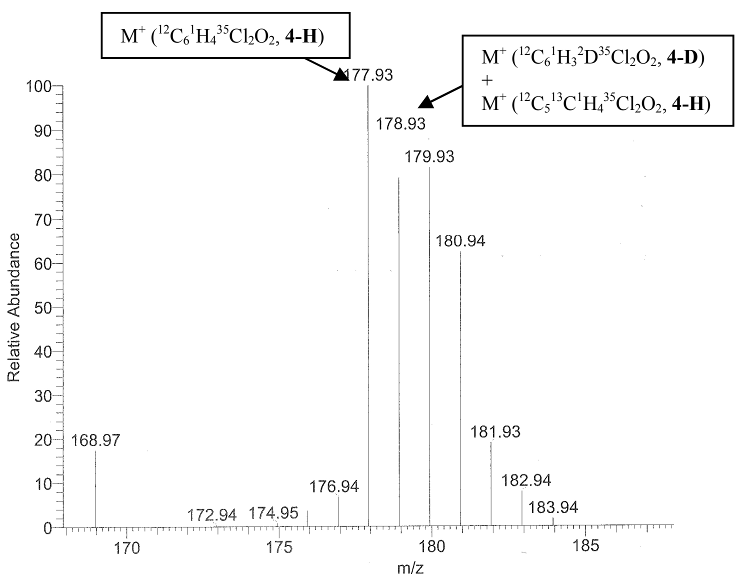
Procedure for the reaction of 2,5-dichlorobenzoquinone with Bu_3SnD

A solution of 2,5-dichlorobenzoquinone (89 mg, 0.50 mmol) and Bu_3SnD (293 mg, 1.00 mmol) in CH_2Cl_2 (1.0 mL) in a 5 mL round-bottom flask was stirred under nitrogen at 20 ºC for 6 h. The solvent was removed under reduced pressure. The crude material was purified by flash column chromatography (silica gel, eluent: MeOH/CH_2Cl_2 = 1/10) to afford a mixture of **4-H** and **4-D** (white solid, 72 mg, 80%). The ratio [**4-H/4-D**] was analyzed by ^{1}H NMR and EI-MS spectroscopies.

^{1}H NMR spectrum



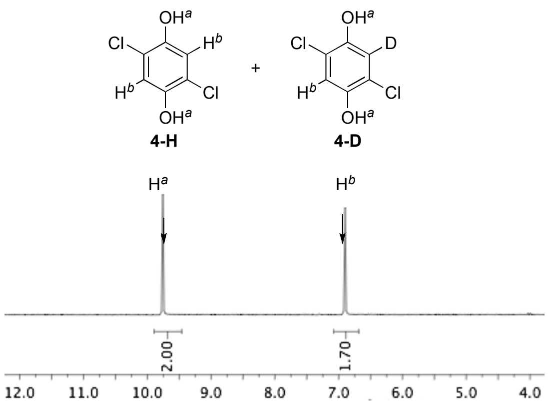
EI-MS spectrum



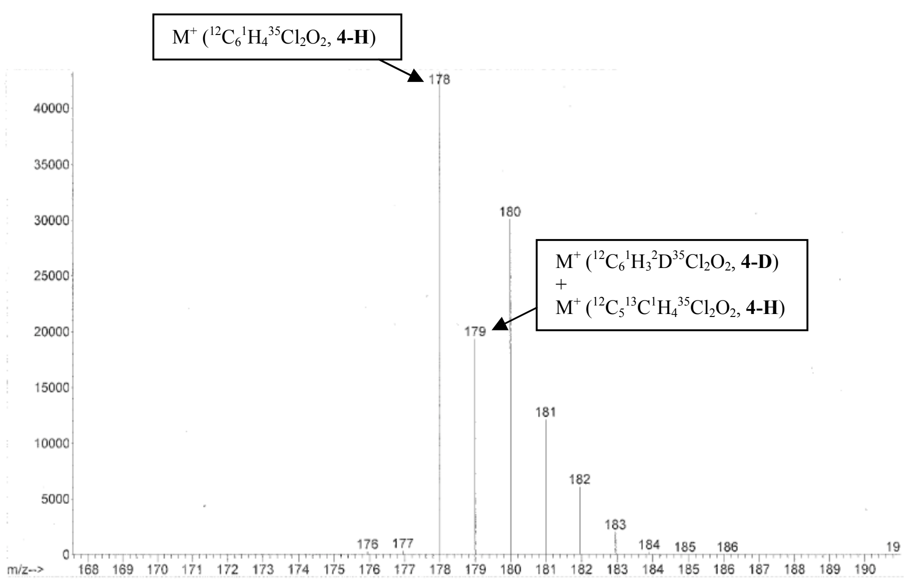
Procedure for the reaction of 2,5-dichlorobenzoquinone with $PyBD_3$

A solution of 2,5-dichlorobenzoquinone (89 mg, 0.50 mmol) and $PyBD_3$ (96 mg, 1.00 mmol) in CH_2Cl_2 (1.0 mL) in a 5 mL round-bottom flask was stirred under nitrogen at 20 ºC for 6 h. The solvent was removed under reduced pressure. The crude material was purified by flash column chromatography (silica gel, eluent: ethyl MeOH/CH_2Cl_2 = 1/10) to afford a mixture of **4-H** and **4-D** (white solid, 78 mg, 87%). The ratio [**4-H**/**4-D**] was analyzed by ^1H NMR and Mass spectroscopies.

^1H NMR spectrum



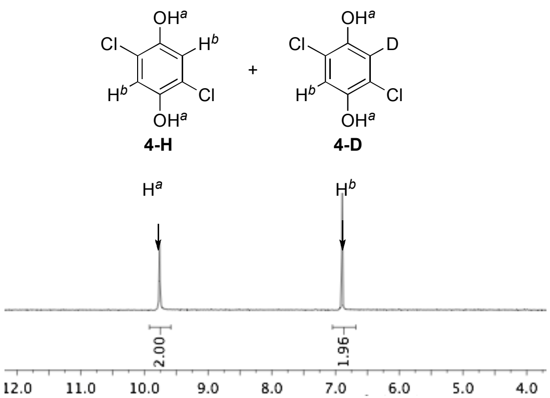
EI-MS spectrum



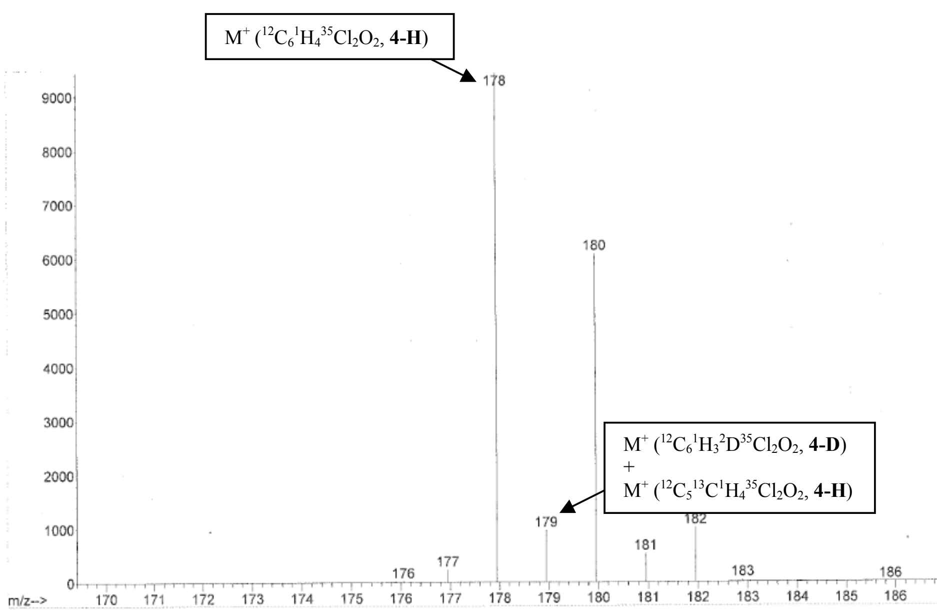
Procedure for the reaction of 2,5-dichlorobenzoquinone with cyclohexadiene-D_8

A solution of 2,5-dichlorobenzoquinone (89 mg, 0.50 mmol) and cyclohexadiene-D_8 (88 mg, 1.00 mmol) in CH_2Cl_2 (1.0 mL) in a 5 mL round-bottom flask was stirred under nitrogen at 20 ºC for 48 h. The solvent was removed under reduced pressure. The crude material was purified by flash column chromatography (silica gel, eluent: $MeOH/CH_2Cl_2$ = 1/10) to afford a mixture of **4-H** and **4-D** (white solid, 15 mg, 17%). The ratio [**4-H**/**4-D**] was analyzed by ^1H NMR and Mass spectroscopies.

^1H NMR spectrum



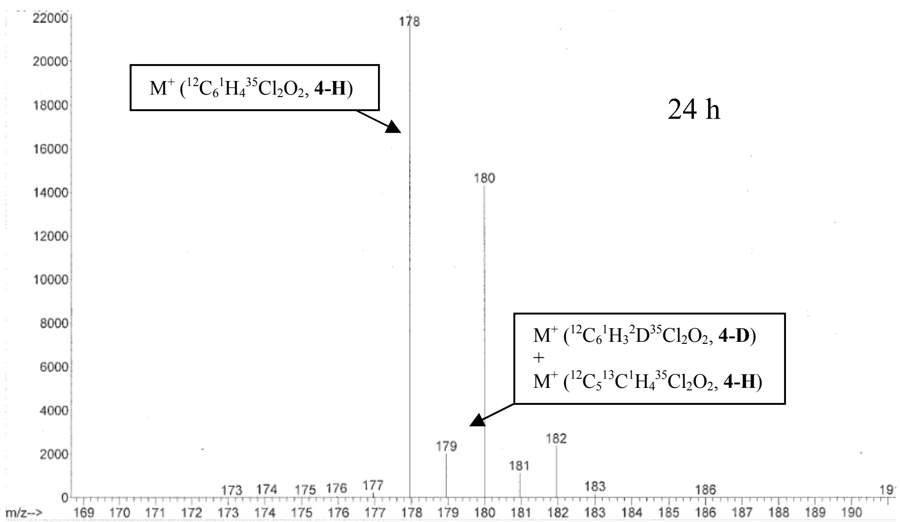
EI-MS spectrum

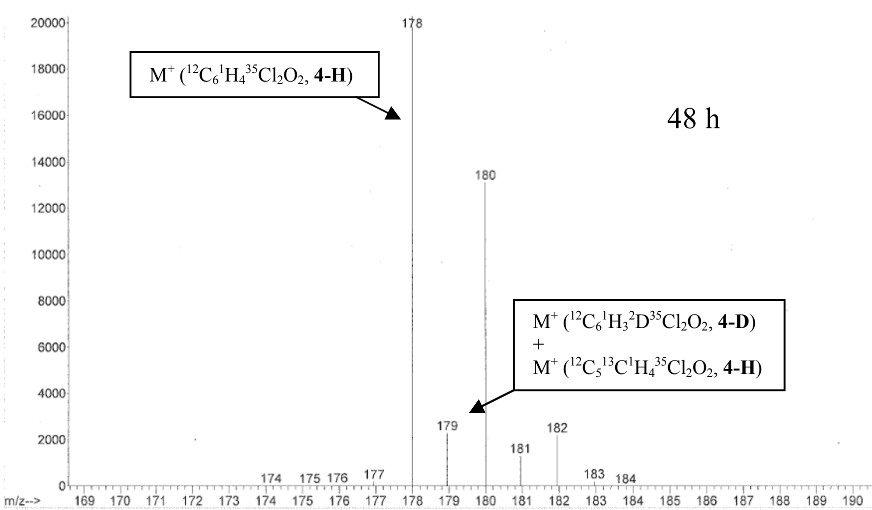


Procedure for the examination for deuterium exchange of *O*-deuterated 2,5-dichlorohydroquinone

O-deuterated 2,5-dichloro-hydroquinone was synthesized by deuterium exchange of 2,5-dichloro-hydroquinone (90 mg, 0.50 mmol) with heavy water (10 mL) in a 25 mL round-bottom flask at room temperature for 30 min and the remaining heavy water was removed under vacuum. The resulting *O*-deuterated 2,5-dichloro-hydroquinone was dissolved in dichloromethane (1.0 mL). The solution was stirred at 20 ºC under nitrogen. After 24 h, a portion of the solution was taken out and passing through a short column on silica gel (MeOH/CH_2Cl_2) then the solvent was evaporated. The resulting mixture was analyzed by Mass spectroscopy. After another 24 h, the remaining solution was treated using the same method and analyzed by Mass spectroscopy.

EI-MS spectra





5) Quantum chemical calculations.

DFT studies on the reactions of DDQ with hydride donors **2** were performed using Gaussian 09.[16] The B97D functional was used in combination with the 6-31+G(d,p) basis set (LANL2DZ ECP for Sn atom) for structure optimization and frequency calculations together with the PCM/UFF model for CH_2Cl_2. Geometries of the transition states were verified by vibrational frequency calculations. The nature of the most favorable transition states was further verified by IRC calculations (50 steps in each direction) and subsequent structure optimizations to the next local minimum energy structure. Thermal corrections were calculated from unscaled frequencies at 298.15 K and 1 atm. Refined electronic energies were obtained from single-point calculations on the B97D geometries using Truhlar's meta hybrid exchange–correlation functional M06-2X with the triple-ζ quality def2-TZVPP basis sets, again using the PCM/UFF model for CH_2Cl_2. All free energies in solution have been corrected to correspond to a standard state of 1 mol/L. The stabilities of the restricted wave functions (RB97D and RM06-2X) have been checked for all transition states. An ultrafine grid was used throughout this study for numerical integration of the density. Transition state distortion/interaction analysis was carried out at the same level of theory as the single-point calculations. Conformer search was carried out with Avogadro 1.1.0 software by using molecular mechanics with force field MMFF94. The conformer search for transition structures was achieved by rotating the reactants along the reaction axes (approaching directions) and, in each case, 3-6 initial structures were submitted to transition structure optimization.

5.1 Total energies and Gibbs free energies

Table S64. Energies for the optimized structures and transition states (the most favorable comformers are marked with yellow color)[a]

		RB97D/6-31+g(d,p)//PCM/UFF				RM06-2X/def2-TZVPP//PCM/UFF	
		E	ZPE	Hcorr	Gcorr	E	$\Delta G(^{\ddagger})$/kJ mol^{-1}
1a		-1484.766118	0.05981	0.073476	0.018762	-1485.122467	
2a	cfr1	-195.173741	0.110202	0.117309	0.080756	-195.27242	
	cfr2	-195.173147	0.110082	0.117221	0.080488	-195.2720099	
O-Attack-TS	cfr1	-1679.932904	0.166893	0.187109	0.117752	-1680.363476	122.3
	cfr2	-1679.936348	0.166947	0.187203	0.117933	-1680.36747	112.3
	cfr3	-1679.936385	0.166911	0.187195	0.117651	-1680.367174	112.3
	cfr4	-1679.939193	0.166761	0.187082	0.11757	-1680.369712	105.5
C-Attack-TS	cfr1	-1679.923522	0.167941	0.188085	0.119519	-1680.356284	145.8
	cfr2	-1679.927948	0.167872	0.188017	0.119657	-1680.361245	133.1
	cfr3	-1679.929779	0.167464	0.187862	0.117853	-1680.362888	124.1
	cfr4	-1679.932340	0.167377	0.187685	0.118655	-1680.364888	121.0
2b	cfr1	-234.463280	0.137695	0.146067	0.106599	-234.5813468	
	cfr2	-234.463503	0.137458	0.145961	0.106095	-234.5810496	
O-Attack-TS	cfr1	-1719.226650	0.194182	0.215921	0.143733	-1719.676046	113.6

	cfr2	-1719.228843	0.194148	0.215984	0.143201	-1719.679131	104.2
	cfr3	-1719.228701	0.194267	0.216058	0.143464	-1719.678978	105.2
	cfr4	-1719.230562	0.194624	0.216326	0.143992	-1719.680602	102.4
C-Attack-TS	cfr1	-1719.219459	0.194902	0.216632	0.144589	-1719.671635	127.5
	cfr2	-1719.222502	0.195014	0.216727	0.14502	-1719.675218	119.2
	cfr3	-1719.223182	0.194952	0.216773	0.1445	-1719.675283	117.7
	cfr4	-1719.225252	0.195173	0.216867	0.144818	-1719.677169	113.5
2c	cfr1	-313.063878	0.195498	0.205352	0.161754	-313.2258501	
	cfr2	-313.063439	0.195457	0.205348	0.161592	-313.2252479	
	cfr3	-313.063472	0.19574	0.205485	0.162112	-313.2252958	
	cfr4	-313.062943	0.195761	0.205528	0.161929	-313.224474	
	cfr5	-313.062599	0.195681	0.205518	0.161681	-313.224165	
O-Attack-TS	cfr1	-1797.831672	0.251468	0.27497	0.198134	-1798.323079	104.5
	cfr2	-1797.832477	0.251601	0.275033	0.198267	-1798.323544	103.6
	cfr3	-1797.833042	0.251397	0.274893	0.197748	-1798.323631	102.0
C-Attack-TS	cfr1	-1797.829793	0.252508	0.2758	0.200376	-1798.326011	102.7
	cfr2	-1797.826774	0.252215	0.275707	0.199274	-1798.323063	107.5
2d		-271.329763	0.124339	0.131167	0.09515	-271.4840192	
O-Attack-TS		-1756.112002	0.182632	0.202716	0.134585	-1756.595164	76.0
C-Attack-TS		-1756.102697	0.182223	0.202795	0.132234	-1756.587636	89.6
2e		-233.259748	0.118152	0.124569	0.089419	-233.3941041	
CT1		-1718.047713	0.179395	0.199743	0.130555	-1718.527669	21.7
O-Attack-TS (TS1)	cfr1	-1718.031716	0.174512	0.194183	0.125888	-1718.492719	101.1
	cfr2	-1718.037176	0.17513	0.19441	0.128345	-1718.502472	81.9
	cfr3	-1718.023396	0.173558	0.193736	0.121085	-1718.478955	124.6
IM1		-1718.063448	0.179252	0.199773	0.129232	-1718.540516	-15.5
P1	cfr1	-1486.019698	0.083289	0.097554	0.042530	-1486.385654	
	cfr2	-1486.021198	0.083518	0.097604	0.043317	-1486.387632	
	cfr3	-1486.022499	0.083641	0.097622	0.043777	-1486.3894	
P2		-232.087702	0.097705	0.103176	0.070163	-232.227419	-247.8 (P1+P2)
C-Attack-TS (TS2)		-1718.018233	0.174547	0.194585	0.124432	-1718.481867	125.7
IM2		-1718.027054	0.178390	0.199313	0.124171	-1718.502180	71.8
IM3	cfr1	-1485.988857	0.082943	0.097003	0.041524	-1486.346905	
	cfr2	1485.989159	0.083282	0.097257	0.041517	-1486.34703	-142.6 (IM3+P2)
C-Attack-TS (TS3)		-1718.028250	0.175135	0.194761	0.127167	-1718.495116	98.2
IM4		-1718.057531	0.183085	0.20227	0.136152	-1718.550563	-23.7
TS4		-1718.039706	0.180495	0.199949	0.132229	-1718.513878	62.2
C-Attack-TS (TS5)		-1718.027675	0.175005	0.194618	0.127353	-1718.495142	98.6
2f		-311.848828	0.172061	0.181576	0.139436	-312.0206302	
O-Attack-TS	cfr1	-1796.634053	0.2289	0.25158	0.178171	-1797.135797	63.6
	cfr2	-1796.634428	0.229338	0.251822	0.179451	-1797.135828	66.9
C-Attack-TS	cfr1	-1796.625896	0.229322	0.251935	0.179315	-1797.12999	81.8
	cfr2	-1796.625299	0.229199	0.252009	0.178023	-1797.128952	81.2
2g		-351.139454	0.199234	0.210275	0.164579	-351.3296487	
O-Attack-TS		-1835.929165	0.256852	0.281009	0.205086	-1836.449672	55.5

C-Attack-TS		-1835.923408	0.256496	0.280811	0.204002	-1836.445901	62.6
2h		-390.431685	0.225917	0.239038	0.18813	-390.6396432	
O-Attack-TS		-1875.226388	0.283408	0.309301	0.229524	-1875.76246	50.5
C-Attack-TS		-1875.215109	0.28306	0.309408	0.227346	-1875.753634	68.0
2j		-576.238250	0.18694	0.198115	0.15065	-576.6113409	
O-Attack-TS	cfr1	-2061.019419	0.243884	0.268409	0.189957	-2061.719902	82.4
	cfr2	-2061.017238	0.243775	0.268318	0.189347	-2061.717224	87.9
	cfr3	-2061.022678	0.244091	0.268503	0.190809	-2061.722994	76.6
C-Attack-TS		-2061.010640	0.244151	0.268835	0.19023	-2061.715243	95.4
2n′		-123.658235	0.111696	0.121505	0.077524	-334.5387658	
CT2		-1608.419486	0.172485	0.197165	0.113321	-1819.667015	21.6
O-Attack-TS (TS6)		-1608.403904	0.170303	0.194051	0.114374	-1819.637008	103.1
IM5		-1608.469780	0.178993	0.202635	0.124053	-1819.736515	-132.6
P3	cfr1	-1608.512121	0.178759	0.202428	0.123544	-1819.784676	-260.2
	cfr2	-1608.510506	0.178974	0.202599	0.123921	-1819.782806	-254.3
C-Attack-TS (TS7)		-1608.412640	0.171078	0.194956	0.114264	-1819.652753	61.5
IM6		-1608.418232	0.175845	0.199628	0.120282	-1819.668542	35.8
IM7		-1608.458118	0.178051	0.201638	0.122712	-1819.713487	-75.7
2p		-201.034070	0.151429	0.159299	0.122401	-201.1165711	
CT3		-1685.810516	0.212024	0.233724	0.161165	-1686.245804	26.8
O-Attack-TS (TS8)	cfr1	-1685.789104	0.208612	0.230203	0.157749	-1686.204633	125.8
	cfr2	-1685.790876	0.208725	0.230381	0.157103	-1686.207682	116.1
	cfr3	-1685.790248	0.208564	0.230314	0.156389	-1686.207148	115.7
IM8		-1685.851078	0.21858	0.239683	0.169514	-1686.307572	-113.3
P4	cfr1	-1685.896354	0.218253	0.239289	0.168929	-1686.361559	-256.5
	cfr2	-1685.897855	0.218058	0.239146	0.168595	-1686.363597	-262.7
C-Attack-TS (TS9)		-1685.800183	0.210798	0.232267	0.160666	-1686.229238	68.9
IM9		-1685.801615	0.212767	0.234611	0.162124	-1686.233796	60.8
IM10		-1685.842842	0.217312	0.238348	0.166878	-1686.288474	-70.1
2q	cfr1	-318.893241	0.235569	0.246841	0.20225	-319.0307575	
	cfr2	-318.897413	0.235513	0.247094	0.201295	-319.0340045	
	cfr3	-318.901595	0.2355	0.247132	0.200948	-319.038377	
	cfr4	-318.900944	0.235475	0.247063	0.201125	-319.0377888	
	cfr5	-318.895345	0.235372	0.246877	0.201395	-319.0330159	
O-Attack-TS	cfr1	-1803.657073	0.292953	0.318266	0.237282	-1804.126972	127.0
	cfr2	-1803.661370	0.292865	0.318256	0.236722	-1804.131649	113.3
C-Attack-TS	cfr1	-1803.668551	0.294338	0.319669	0.239422	-1804.150189	71.7
	cfr2	-1803.673175	0.294737	0.319975	0.240071	-1804.15456	62.0
2r		-274.773775	0.11846	0.12594	0.087839	-274.928951	
O-Attack-TS	cfr1	-1759.543913	0.17718	0.197727	0.127929	-1760.035228	90.5
	cfr2	-1759.542889	0.176337	0.197312	0.122862	-1760.024384	105.6
C-Attack-TS	cfr1	-1759.551594	0.178008	0.198619	0.128666	-1760.053935	43.4
	cfr2	-1759.545400	0.177686	0.198452	0.126972	-1760.045108	62.1
	cfr3	-1759.546186	0.177719	0.19847	0.126948	-1760.047138	56.7

2t	-331.295022	0.155119	0.165432	0.120381	-331.4772843	
O-Attack-TS	-1816.076119	0.215151	0.237892	0.164424	-1816.591269	80.6
C-Attack-TS	-1816.081974	0.215817	0.238734	0.164676	-1816.606929	40.2

a) The stability check shows that the restricted wave function RB97D is always stable for all examined structures. However, the RM06-2X wave function shows a RHF→UHF instability for O-attack transition state **TS6** and **TS8** (resulting in stabilization of 2.4 and 10 kJ/mol, respectively, when using UM06-2X).

5.2 Transition state distortion/interaction analysis

A transition state distortion/interaction analysis was carried out to rationalize the different barriers for O- and C-attack.

$$\Delta E^{\neq} = \Delta E_{\mathrm{d}}^{\neq} + \Delta E_{\mathrm{i}}^{\neq} \qquad \text{(S1)}$$

In eq. (S1) the distortion energy term $\Delta E_{\mathrm{d}}^{\neq}$ reflects the energy which is needed to distort the reactants into the transition structure while there is no interaction between the reactants. The interaction energy $\Delta E_{\mathrm{i}}^{\neq}$ between these distorted fragments is calculated as the difference between the activation energy ($\Delta E^{\neq}$) and distortion energy ($\Delta E_{\mathrm{d}}^{\neq}$).

Table S65. Transition state distortion and interaction energies in gas phase and CH_2Cl_2 solution

		$E_d^{\neq}$ /kJ mol^{-1} (distortion energy)		$E^{\neq}$ /kJ mol^{-1} (activation energy)		$E_i^{\neq}$ /kJ mol^{-1} (interaction energy)	
		gas	CH_2Cl_2	gas	CH_2Cl_2	gas	CH_2Cl_2
DDQ + **2e**	O-attack (**TS1**)	106.5	105.7	41.2	37.0	-65.3	-68.7
	frag1 (DDQ)	37.0	36.3				
	frag2 (**2e**)	69.5	69.4				
	C-attack (**TS3**)	178.1	178.6	68.2	56.3	-109.9	-122.3
	frag1 (DDQ)	59.7	60.4				
	frag2 (**2e**)	118.4	118.2				
DDQ + **2n'**	O-attack (**TS6**)	50.3	46.5	66.4	63.6	16.1	17.1
	frag1 (DDQ)	29.6	28.9				
	frag2 (**2n'**)	20.7	17.6				
	C-attack (**TS7**)	66.9	62.9	40.8	22.3	-26.1	-40.6
	frag1 (DDQ)	42.6	43.0				
	frag2 (**2n'**)	24.3	19.9				
DDQ + **2p**	O-attack (**TS8**)	76.2	71.8	83.6	83.7	7.4	11.9
	frag1 (DDQ)	38.7	37.8				
	frag2 (**2p**)	37.5	34.0				
	C-attack (**TS9**)	139.7	134.3	46.4	25.7	-93.3	-108.6
	frag1 (DDQ)	72.8	73.2				
	frag2 (**2p**)	66.9	61.1				

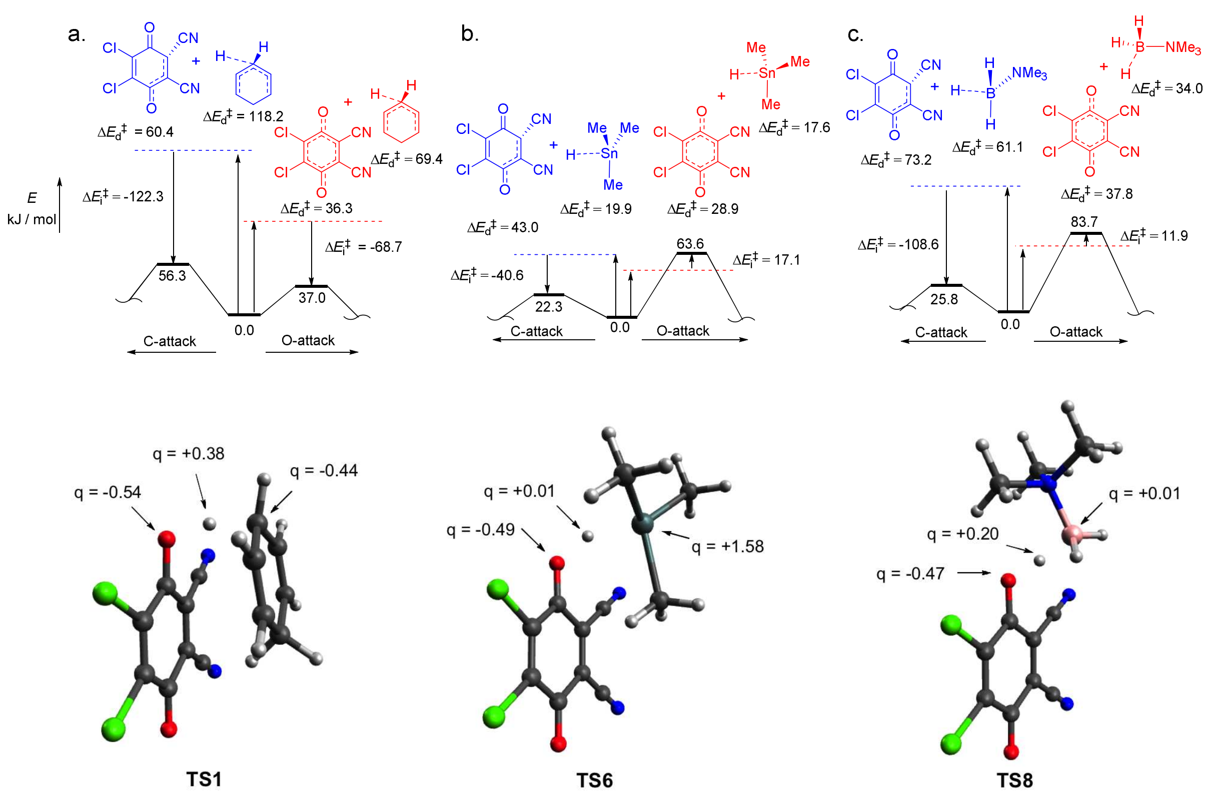


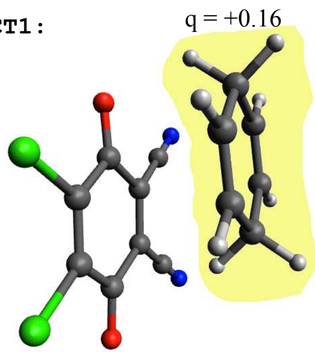
Figure S2. Transition state distortion/interaction analysis of the reactions of DDQ (**1a**) with a) cyclohexadiene (**2e**), b) Me_3SnH (**2n'**), and c) trimethylamine borane (**2p**); and charge distribution in O-attack transition states for **TS1**, **TS6**, and **TS8** calculated from natural population analysis [RM06-2X/def2-TZVPP//PCM/UFF] in CH_2Cl_2.

The results of the transition state distortion/interaction analyses for the reactions of DDQ (**1a**) with cyclohexadiene (**2e**), trimethylstannane (**2n'**), and trimethylamine borane (**2p**) are shown in Table S65 and illustrated in Fig. S2. In all three cases, the distortion energies $\Delta E_{\mathrm{d}}^{\neq}$ for DDQ (**1a**) as well as for the hydride donor are higher in the case of C-attack than in the case of O-attack. While all transition states for C-attack show large interaction energies, large differences were observed for O-attack. While the interaction energy $\Delta E_{\mathrm{i}}^{\neq}$ between DDQ (**1a**) and cyclohexadiene (**2e**) fragments of the O-attack transition state is stabilizing by 69 kJ/mol, the analogous interactions of the fragments of the O-attack are destabilizing by 17 kJ/mol for trimethylstannane **2n'** and by 12 kJ/mol for amine borane **2p**.

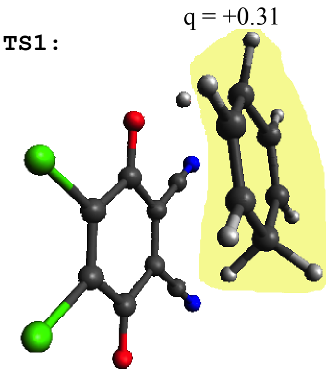
Different electrostatic interactions between the reaction centers and the migrating hydrogen, which can be derived from the charge distributions shown in the lower part of Figure 11, may be an important factor for the differences in $\Delta E_{\mathrm{i}}^{\neq}$. As expected from the higher electronegativity of C (**TS1**) compared to Sn (**TS6**) and B (**TS8**), the migrating hydrogen has a significantly higher positive charge in the transition state for the C-H hydride donor (**TS1**) than in that of Sn-H (**TS6**) and B-H (**TS8**) hydride donors (+0.38 compared with +0.01 and +0.20). As Figure S2 also shows large differences in distortion energies for the different transition states, detailed distortion/interaction analysis for reactions of other quinones with other hydride donors would be needed to arrive at a definite explanation for the origin of the different regioselectivities of C-H, Sn-H and B-H hydride donors.

5.3 Mulliken charge distribution in some key structures

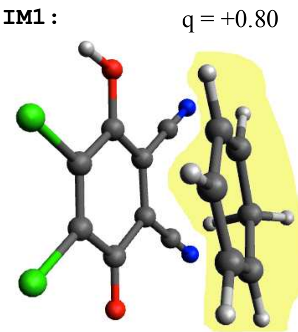
CT1:



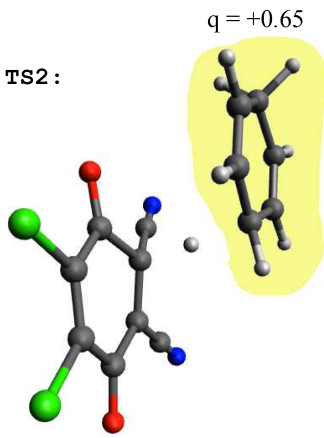
TS1:



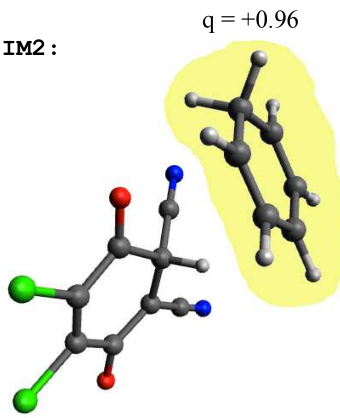
IM1:



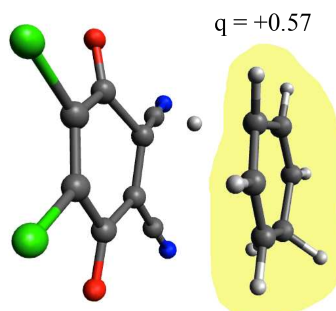
TS2:



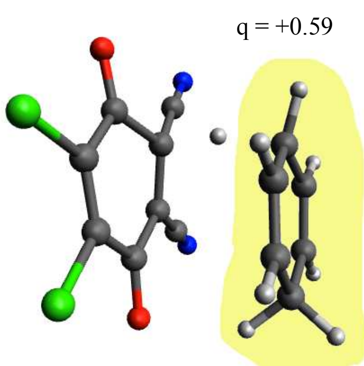
IM2:



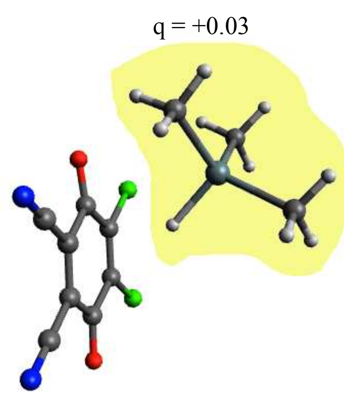
TS3:



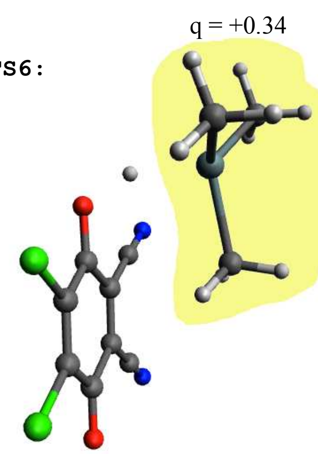
TS5:



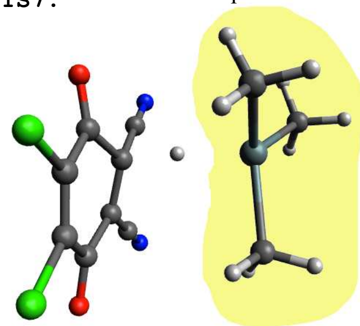
CT2:



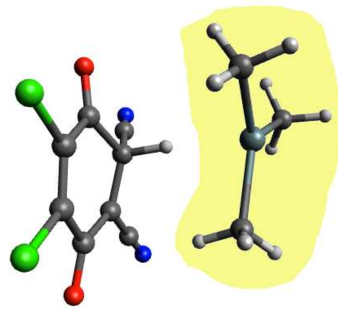
TS6:



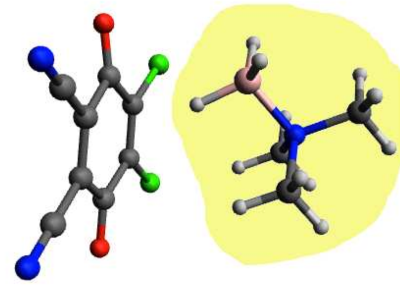
TS7: q = +0.69



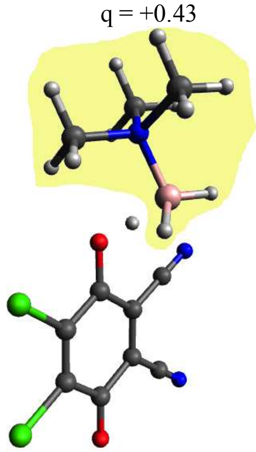
IM6: q = +0.85



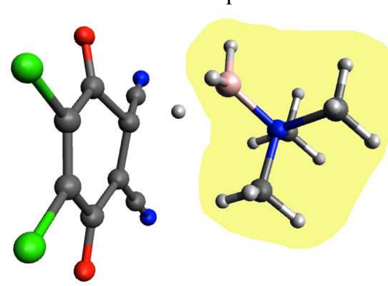
CT3: q = +0.05



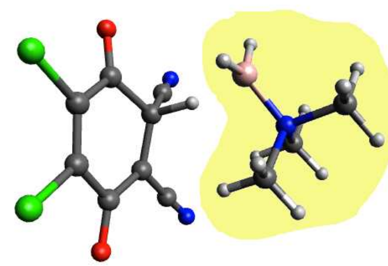
TS8: q = +0.43



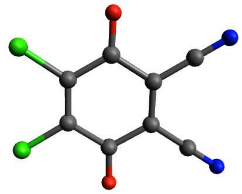
TS9: q = +0.71



IM9: q = +0.93

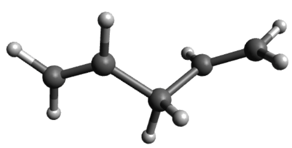


5.4 Geometries for the optimized structures and transition states (only the most favorable conformers are listed)



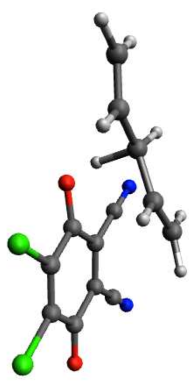
DDQ (**1a**)

C	1.41018	0.68519	-0.00011
C	0.11701	1.46908	0.00051
C	-1.16322	0.68597	-0.00026
C	-1.16331	-0.68593	-0.00040
C	0.11691	-1.46915	-0.00009
C	1.41006	-0.68531	0.00015
O	0.14303	2.69394	0.00169
Cl	-2.60640	1.62233	0.00011
Cl	-2.60649	-1.62222	-0.00043
O	0.14289	-2.69398	-0.00008
C	2.61848	-1.44904	0.00038
N	3.61026	-2.07493	0.00135
C	2.61857	1.44892	-0.00069
N	3.61027	2.07495	-0.00199



Penta-1,4-diene (**2a**)

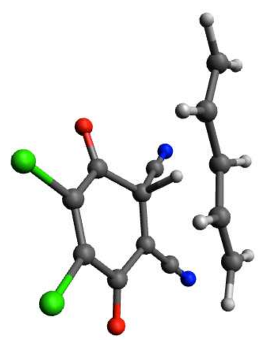
C	0.00000	0.68521	-0.00000
C	1.17071	-0.16801	0.44794
C	-1.17071	-0.16801	-0.44794
H	0.32793	1.33535	-0.82947
H	-0.32793	1.33535	0.82947
C	2.37332	-0.19431	-0.15331
H	0.98448	-0.81275	1.31360
H	2.58376	0.43356	-1.02387
H	3.17807	-0.83788	0.20797
C	-2.37332	-0.19431	0.15331
H	-0.98448	-0.81275	-1.31360
H	-2.58376	0.43357	1.02387
H	-3.17807	-0.83788	-0.20797



O-Attack-TS (DDQ **1a** + **2a**)

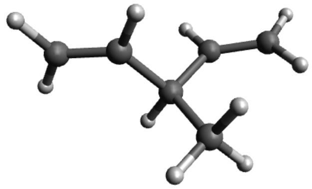
C	-3.12649	0.57664	0.66009
H	-2.36996	0.46813	-0.39002
C	0.68165	1.36252	-0.46110
C	2.00433	1.12500	-0.10450

C	-5.43246	0.30294	-0.22589
C	-0.24540	0.26108	-0.71853
Cl	-0.93047	-2.37118	-0.71378
Cl	2.11845	-2.95565	0.20012
C	2.92619	2.19678	0.09075
C	0.18668	2.69224	-0.65545
O	3.69090	-0.46136	0.44355
O	-1.39052	0.49544	-1.24765
N	3.68443	3.07849	0.25281
N	-0.22323	3.78257	-0.79268
C	1.52915	-1.35372	-0.08169
C	-4.31581	-0.22134	0.33573
C	2.51475	-0.25471	0.11253
C	0.22694	-1.10424	-0.46324
H	-4.26196	-1.29380	0.54213
C	-1.08254	0.83943	2.02725
C	-2.13834	0.08203	1.60677
H	-2.17303	-0.97891	1.86669
H	-3.26708	1.66645	0.64573
H	-0.30321	0.41783	2.66152
H	-1.02677	1.90335	1.79278
H	-5.50103	1.36805	-0.45822
H	-6.29601	-0.32277	-0.45277



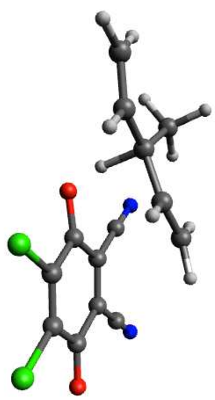
C-Attack-TS (DDQ **1a** + **2a**)

C	-1.57957	-0.92557	1.68097
H	-1.35026	-0.42603	0.37442
C	-1.10016	0.20839	-0.77584
C	-0.58642	1.51182	-0.42086
C	-2.37567	-3.23175	1.28018
C	-0.10527	-0.86551	-1.23692
Cl	2.27942	-2.12831	-0.81289
Cl	3.28810	0.65873	0.49560
C	-1.42707	2.65746	-0.44273
C	-2.39020	0.14385	-1.43908
O	1.34465	2.82377	0.04981
O	-0.46687	-1.81273	-1.92086
N	-2.13355	3.59746	-0.46061
N	-3.44618	0.08029	-1.94051
C	1.69995	0.45996	-0.14217
C	-1.37764	-2.37009	1.59202
C	0.84189	1.71311	-0.14691
C	1.27084	-0.72716	-0.67872
H	-0.36634	-2.74289	1.77181
C	-0.80807	1.29396	2.37348
C	-0.60428	-0.05747	2.29039
H	0.37360	-0.47767	2.53674
H	-2.62200	-0.58007	1.68890
H	-0.03107	1.96223	2.74235
H	-1.78266	1.72838	2.14961
H	-3.38834	-2.87468	1.08085
H	-2.19502	-4.30514	1.22267



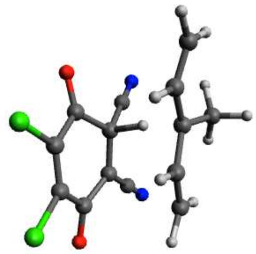
3-Methylpenta-1,4-diene (**2b**)

C	0.00000	0.31273	-0.23487
C	1.24251	-0.24687	0.43035
C	-1.24250	-0.24688	0.43036
C	2.18533	-0.97429	-0.19352
H	1.35192	-0.01628	1.49653
H	2.09844	-1.21798	-1.25610
H	3.06534	-1.34427	0.33657
C	-2.18533	-0.97429	-0.19352
H	-1.35190	-0.01631	1.49654
H	-2.09845	-1.21796	-1.25610
H	-3.06533	-1.34428	0.33657
C	-0.00001	1.86388	-0.15139
H	0.00000	0.01170	-1.29550
H	-0.89575	2.27394	-0.64172
H	0.89573	2.27395	-0.64172
H	-0.00001	2.19184	0.90043



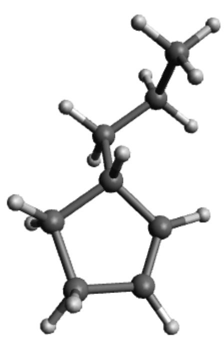
O-Attack-TS (DDQ **1a** + **2b**)

C	-3.00839	0.21562	0.55927
H	-2.22499	0.11107	-0.45205
C	0.71818	1.32866	-0.52443
C	2.04652	1.24914	-0.12308
C	-5.22015	-0.68019	-0.25816
C	-0.07379	0.12454	-0.77815
Cl	-0.46297	-2.56617	-0.71742
Cl	2.60687	-2.78564	0.28449
C	2.83613	2.42124	0.07541
C	0.08772	2.59035	-0.77226
O	3.87878	-0.12535	0.51955
O	-1.22836	0.21558	-1.32355
N	3.48521	3.38544	0.24143
N	-0.43118	3.62652	-0.95279
C	1.85066	-1.26713	-0.05307
C	-3.99541	-0.85627	0.29149
C	2.69960	-0.05962	0.14527
C	0.54077	-1.17339	-0.47497
H	-3.67336	-1.86969	0.54705
C	-0.99657	0.73589	1.97264
C	-1.96416	-0.11947	1.53518
H	-1.87868	-1.17446	1.80858
C	-3.47931	1.66790	0.44222
H	-0.19801	0.37928	2.62290
H	-1.01581	1.80073	1.74459
H	-5.59187	0.30372	-0.54594
H	-5.88111	-1.53255	-0.41739
H	-2.64120	2.37019	0.49793
H	-4.18500	1.89115	1.25705
H	-3.98854	1.83210	-0.51555



C-Attack-TS (DDQ **1a** + **2b**)

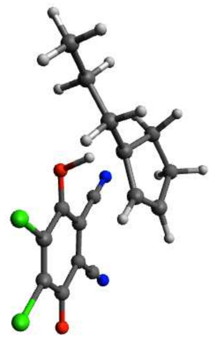
C	-1.74446	-0.75296	1.39549
H	-1.24946	-0.30628	0.16627
C	-0.81181	0.30679	-0.95841
C	-0.23881	1.56348	-0.54610
C	-2.53917	-3.08788	0.90883
C	0.13348	-0.85244	-1.30172
Cl	2.35807	-2.29211	-0.64152
Cl	3.44890	0.42184	0.74990
C	-0.99286	2.76576	-0.61321
C	-2.02067	0.34032	-1.76031
O	1.72429	2.72484	0.13525
O	-0.23484	-1.77872	-2.01088
N	-1.62757	3.75455	-0.66563
N	-3.01064	0.35868	-2.38506
C	1.91966	0.34059	-0.03887
C	-1.58194	-2.21628	1.30295
C	1.16265	1.65494	-0.12157
C	1.45353	-0.81519	-0.61152
H	-0.59359	-2.60196	1.56688
C	-0.67756	1.31710	2.29677
C	-0.71232	-0.03765	2.13442
H	0.16006	-0.62087	2.43887
C	-3.14544	-0.16201	1.28659
H	0.17705	1.79036	2.77895
H	-1.50826	1.96300	2.01867
H	-3.54033	-2.76558	0.62185
H	-2.32846	-4.15673	0.87451
H	-3.69818	-0.60338	0.44959
H	-3.12024	0.92372	1.14365
H	-3.69084	-0.37663	2.21802



3-Propylcyclopent-1-ene (**2c**)

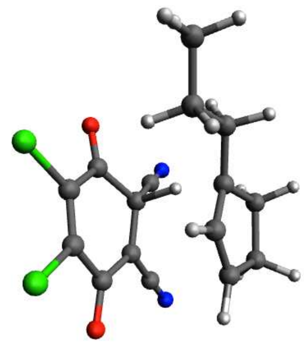
C	1.43649	1.23047	0.09843
C	0.33263	0.25543	0.47322
C	0.91120	-1.11023	-0.01477
C	2.45122	-0.90323	-0.12840
C	2.58161	0.60619	-0.23665
C	-1.04547	0.59923	-0.12584
C	-2.15072	-0.38489	0.29569
C	-3.52370	-0.01725	-0.29473
H	1.29563	2.31316	0.13645
H	0.22041	0.24368	1.57598
H	0.49992	-1.32305	-1.01543
H	0.63954	-1.94687	0.64376
H	2.88828	-1.43795	-0.98744
H	2.97688	-1.27072	0.77258
H	3.51361	1.10530	-0.51030

H	-0.96056	0.60625	-1.22748
H	-1.33329	1.62034	0.18067
H	-2.21068	-0.40433	1.39790
H	-1.87130	-1.40290	-0.02267
H	-3.83129	0.98950	0.03206
H	-4.30168	-0.73096	0.01851
H	-3.48511	-0.01576	-1.39625



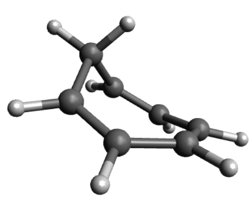
O-Attack-TS (DDQ **1a** + **2c**)

C	-2.44358	0.47209	0.74782
H	-1.77485	0.30223	-0.36684
C	1.19744	1.13001	-0.73682
C	2.52125	0.94312	-0.33243
C	-0.69437	1.39238	1.97304
C	0.26875	0.01730	-0.83162
Cl	-0.41483	-2.59603	-0.50784
Cl	2.61196	-3.04887	0.52791
C	3.44284	2.03083	-0.29189
C	0.72696	2.41383	-1.15658
O	4.18680	-0.54532	0.49201
O	-0.91981	0.19484	-1.30600
N	4.19972	2.92840	-0.25476
N	0.33771	3.47169	-1.48261
C	2.03418	-1.49469	0.02908
C	-1.32523	0.21691	1.63916
C	3.01959	-0.38235	0.09844
C	0.73760	-1.29819	-0.40846
H	-0.98706	-0.77877	1.92185
C	-1.44961	2.58681	1.47389
C	-2.70142	1.98546	0.77842
C	-3.59534	-0.50657	0.58177
H	0.20975	1.46273	2.57827
H	-3.61323	2.17176	1.37022
H	-2.87500	2.40639	-0.22073
H	-1.71054	3.25104	2.31629
H	-0.83872	3.20587	0.79635
H	-4.23818	-0.40945	1.47732
H	-3.20350	-1.53501	0.57553
C	-4.44347	-0.25627	-0.67956
H	-4.83414	0.77349	-0.65661
C	-5.60828	-1.25409	-0.79114
H	-3.79571	-0.33382	-1.56750
H	-6.27614	-1.17337	0.08146
H	-5.23173	-2.28852	-0.83508
H	-6.20408	-1.06765	-1.69712



C-Attack-TS (DDQ **1a** + **2c**)

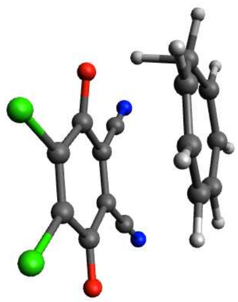
C	-1.04780	1.67366	-0.93543
H	-0.79338	0.86966	0.20095
C	-0.74860	-0.03747	1.18415
C	-1.16887	-1.28972	0.58904
C	-1.90541	-0.13444	-2.08908
C	0.74394	0.14582	1.50019
Cl	3.35377	-0.21546	0.77199
Cl	2.27114	-2.54074	-1.19763
C	-2.50403	-1.74170	0.71747
C	-1.62616	0.56689	2.17055
O	-0.52741	-3.21550	-0.65387
O	1.11797	0.94644	2.34745
N	-3.62503	-2.08550	0.82504
N	-2.35005	1.08174	2.93344
C	1.21898	-1.64939	-0.16398
C	-0.76417	0.60001	-1.85432
C	-0.22265	-2.13686	-0.12843
C	1.67655	-0.63731	0.64066
H	0.23309	0.33499	-2.19807
C	-3.12539	0.53501	-1.53480
C	-2.56870	1.80384	-0.83340
C	-0.15761	2.87406	-0.68874
H	-1.94066	-1.05047	-2.67824
H	-2.86733	2.72217	-1.36277
H	-2.91601	1.91200	0.20350
H	-3.81901	0.78305	-2.35670
H	-3.69419	-0.12796	-0.86300
H	-0.28346	3.21307	0.35258
H	-0.55755	3.69241	-1.31489
C	1.33106	2.66548	-1.00856
H	1.71000	1.79057	-0.46169
C	2.17123	3.89849	-0.63786
H	1.44401	2.44110	-2.08083
H	2.09318	4.11008	0.43995
H	1.82294	4.78770	-1.18667
H	3.23173	3.73782	-0.88097



Cyclohepta-1,3,5-triene (**2d**)

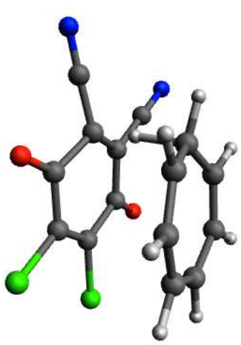
C	0.24922	-1.42743	0.69047
C	0.24922	-1.42743	-0.69047
C	-0.25059	-0.36246	-1.53642
C	-0.25059	0.96536	-1.21874
C	-0.25059	-0.36246	1.53642
C	-0.25059	0.96536	1.21874
C	0.48095	1.48775	0.00000
H	0.50889	-2.36687	1.18623
H	0.50889	-2.36687	-1.18623
H	-0.68295	-0.66562	-2.49474
H	-0.77460	1.67565	-1.86324
H	-0.68295	-0.66562	2.49474

H	-0.77460	1.67565	1.86324
H	1.51510	1.09709	0.00000
H	0.52003	2.58455	0.00000



O-Attack-TS (DDQ **1a** + **2d**)

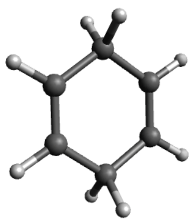
C	-0.89668	-2.89247	0.50094
H	-0.66422	-2.49925	-0.67350
C	-1.13423	0.43525	-1.07930
C	-0.89356	1.61740	-0.37086
C	0.85291	-1.61010	1.88500
C	-0.07679	-0.52872	-1.31150
Cl	2.54377	-1.27505	-1.34088
Cl	3.13465	1.45426	0.27718
C	-1.94728	2.53942	-0.09844
C	-2.44075	0.11995	-1.57432
O	0.67411	3.04241	0.72179
O	-0.35311	-1.70190	-1.76115
N	-2.82278	3.28475	0.14198
N	-3.51011	-0.11135	-1.99889
C	1.53759	1.01894	-0.23660
C	0.39051	-2.69410	1.16826
C	0.46023	1.98331	0.10786
C	1.28208	-0.15343	-0.92308
H	1.11206	-3.49569	1.00080
C	-2.20203	-0.92576	1.53404
C	-2.09023	-2.12730	0.86406
H	-3.02420	-2.54761	0.48658
H	-1.11303	-3.94853	0.28965
H	-3.21386	-0.52677	1.61941
C	-1.17923	-0.11386	2.12224
C	0.16734	-0.41240	2.26695
H	1.89393	-1.66616	2.20633
H	-1.51433	0.83239	2.54841
H	0.77331	0.33030	2.78698



C-Attack-TS (DDQ **1a** + **2d**)

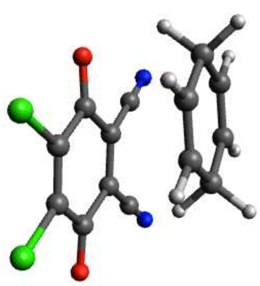
C	-1.09689	-1.90383	1.27111
H	-1.27729	-1.19006	0.13939
C	-1.49372	-0.20184	-0.83501
C	-1.59574	1.04272	-0.11326
C	1.27184	-2.82268	1.01872
C	-0.20259	-0.54552	-1.56580
Cl	2.49399	-0.27136	-1.87917
Cl	2.26139	2.33574	0.00393
C	-2.84499	1.46215	0.41315
C	-2.68875	-0.74011	-1.45105

O	-0.49168	2.95221	0.77347
O	-0.15051	-1.50243	-2.33434
N	-3.88537	1.79120	0.85527
N	-3.66267	-1.19219	-1.92036
C	0.88307	1.38527	-0.41336
C	-0.10485	-2.91206	0.94546
C	-0.43614	1.87980	0.14933
C	0.99021	0.26899	-1.20271
H	-0.51098	-3.83728	0.53388
C	0.33059	-0.20224	2.53064
C	-0.87191	-0.79731	2.19499
H	-1.77151	-0.35788	2.62636
H	-2.11773	-2.30075	1.31126
H	0.26274	0.67218	3.17975
C	1.65254	-0.58342	2.15263
C	2.06304	-1.73523	1.49532
H	1.82920	-3.68715	0.65575
H	2.44383	0.09581	2.47104
H	3.14001	-1.84884	1.36329



Cyclohexa-1,4-diene (**2e**)

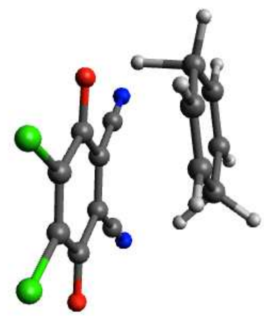
C	-0.67331	1.26395	-0.00040
C	0.67334	1.26395	-0.00040
C	1.50969	-0.00003	0.00067
C	0.67331	-1.26395	-0.00040
H	2.18677	-0.00003	0.87663
H	2.18911	-0.00003	-0.87344
C	-0.67334	-1.26396	-0.00040
C	-1.50969	0.00003	0.00067
H	-2.18677	0.00003	0.87664
H	-2.18911	0.00003	-0.87344
H	-1.21422	2.21444	-0.00122
H	1.21427	2.21443	-0.00122
H	1.21422	-2.21444	-0.00122
H	-1.21428	-2.21443	-0.00122



Charge transfer complex **CT1** (**1a** + **2e**)

C	-2.16004	-2.03485	0.85467
C	-1.06878	-3.02953	0.59630
C	0.24759	-2.66951	1.22270
C	0.42910	-1.55654	1.97008
C	-0.67601	-0.58166	2.26616
C	-1.98113	-0.92126	1.60861
O	-0.40340	-1.46185	-1.99929
C	-0.12054	-0.49214	-1.29377
C	-1.16866	0.51325	-0.91707
C	-0.83706	1.67367	-0.24588
C	0.57048	1.96930	0.17293
C	1.59381	0.92408	-0.13467
C	1.27410	-0.22413	-0.81613
C	-2.49139	0.28285	-1.41226
N	-3.57132	0.11908	-1.83943

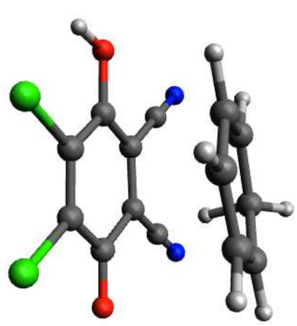
C	-1.82072	2.65683	0.08114
N	-2.63515	3.45434	0.35965
Cl	3.19516	1.26401	0.41444
O	0.85443	3.03666	0.72075
Cl	2.45479	-1.40028	-1.26583
H	-0.93492	-3.14253	-0.50173
H	1.08579	-3.34457	1.04361
H	1.41182	-1.33946	2.39281
H	-0.36641	0.44462	1.96370
H	-0.81448	-0.47181	3.35911
H	-2.81528	-0.23492	1.76569
H	-3.13325	-2.22997	0.40165
H	-1.38985	-4.03928	0.91880



O-attack **TS1** (**1a** + **2e**)

C	-1.63507	-2.74129	0.37551
H	-1.26447	-2.26953	-0.76585
C	-1.02007	0.74809	-0.85450
C	-0.46450	1.85428	-0.21051
C	0.08093	-1.77803	1.86166
C	-0.22403	-0.44029	-1.13364
Cl	2.13434	-1.80710	-1.21255
Cl	3.41766	0.70826	0.34959
C	-1.24576	3.01599	0.06673
C	-2.37183	0.77087	-1.33202
O	1.45282	2.88136	0.76087
O	-0.76340	-1.46202	-1.69367
N	-1.89474	3.96468	0.30706
N	-3.46968	0.82056	-1.74160
C	1.75145	0.67010	-0.11880
C	-0.34204	-2.79912	1.05899
C	0.96024	1.88657	0.20570
C	1.19313	-0.42037	-0.75808
H	0.31845	-3.63925	0.84691
H	1.07378	-1.81426	2.31148
C	-0.78510	-0.60657	2.19299
H	-0.27721	0.33973	1.88182
H	-0.85283	-0.47189	3.29037
C	-2.14931	-0.65681	1.58903
H	-2.84162	0.14855	1.83723
C	-2.55895	-1.68490	0.78375
H	-3.56512	-1.68444	0.36570
H	-2.07392	-3.69105	0.04592

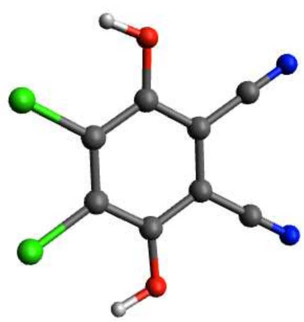
IM1



O-attack intermediate **IM1** (**1a** + **2e**)

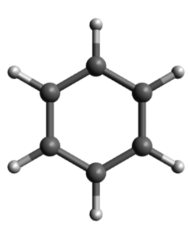
C	-2.42729	-0.20051	2.10706

H	-0.21641	3.32246	-0.20750
C	1.72534	0.79118	-0.30073
C	1.69202	-0.60600	-0.62888
C	-0.84119	-2.03237	2.03376
C	0.56517	1.57515	-0.41152
Cl	-2.04676	2.00358	-1.02718
Cl	-2.12149	-1.08203	-1.93617
C	2.87159	-1.39629	-0.51295
C	2.91573	1.38558	0.21642
O	0.47681	-2.45310	-1.55071
O	0.64003	2.88129	-0.05619
N	3.83908	-2.05549	-0.40011
N	3.89829	1.86217	0.64963
C	-0.67460	-0.36259	-1.30597
C	-2.14742	-1.58754	1.97792
C	0.50788	-1.24742	-1.21257
C	-0.63457	0.97271	-0.92598
H	-2.96795	-2.29222	1.85084
H	-0.60314	-3.09157	1.94218
C	0.27112	-1.07445	2.13986
H	0.79828	-1.10168	1.11905
H	1.10457	-1.42274	2.77316
C	-0.07909	0.34004	2.34834
H	0.72355	1.05445	2.52399
C	-1.40347	0.75142	2.30663
H	-1.65885	1.80272	2.43077
H	-3.46329	0.13648	2.06480



2,3-Dichloro-5,6-dicyanohydroquinone (**P1**)

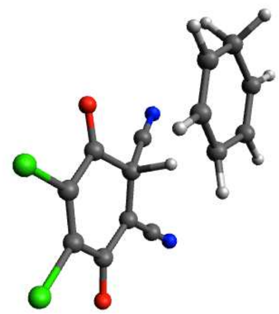
O	-0.20072	-2.78029	-0.00027
C	-2.57937	-1.43691	-0.00012
C	-1.34707	-0.71318	-0.00017
C	-1.34710	0.71319	-0.00011
C	-2.57958	1.43660	0.00014
C	-0.12915	1.42970	-0.00040
O	-0.20100	2.78033	-0.00075
C	1.09076	0.70408	0.00004
Cl	2.57981	1.60946	-0.00001
C	1.09081	-0.70400	0.00002
Cl	2.57980	-1.60937	0.00042
C	-0.12906	-1.42974	-0.00010
H	0.69114	3.17302	-0.00043
N	-3.59314	2.02839	0.00124
N	-3.59309	-2.02845	-0.00038
H	0.69146	-3.17288	-0.00018



Benzene (**P2**)

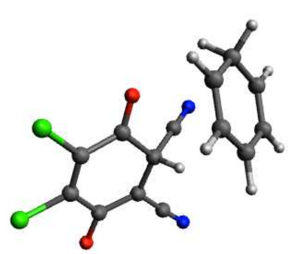
H	2.42190	0.61396	-0.00000
C	1.36409	0.34582	-0.00000
C	0.38255	1.35422	0.00000
H	0.67916	2.40441	0.00000

C	-0.98152	1.00839	0.00000
H	-1.74267	1.79039	0.00000
C	-1.36409	-0.34582	-0.00000
H	-2.42190	-0.61396	-0.00001
C	-0.38255	-1.35422	0.00000
H	-0.67918	-2.40440	0.00001
C	0.98152	-1.00839	0.00000
H	1.74268	-1.79038	0.00000



C-attack **TS2** (**1a** + **2e**)

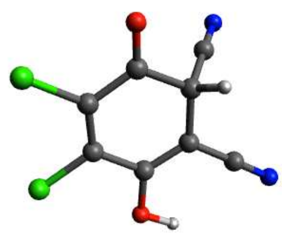
C	1.91339	-1.57346	-1.21488
C	1.82194	-0.14411	-1.47204
C	3.00666	0.68229	-1.29054
C	4.12349	0.16957	-0.69707
C	4.20598	-1.25992	-0.26625
C	3.02346	-2.10225	-0.62273
C	0.29108	0.77302	0.63471
C	-0.67832	1.76302	0.21778
C	-1.99331	1.37281	-0.25101
C	-2.33154	-0.10751	-0.15390
C	-1.50457	-1.03198	0.43626
C	-0.19674	-0.63422	1.01043
C	1.41230	1.22483	1.44096
N	2.34748	1.58465	2.04663
C	-0.31012	3.12789	0.12334
N	0.01055	4.25919	0.05192
O	0.52421	-1.38930	1.65464
Cl	-3.86546	-0.55211	-0.80524
O	-2.82907	2.17640	-0.69982
Cl	-1.92484	-2.70778	0.61576
H	0.97559	0.33910	-0.42081
H	2.96611	1.72733	-1.59605
H	4.99874	0.79922	-0.53509
H	4.36971	-1.30262	0.83110
H	5.13039	-1.72129	-0.66624
H	3.07688	-3.16981	-0.40755
H	1.06520	-2.20723	-1.47159
H	1.08303	0.18994	-2.21150



C-attack intermediate **IM2** (**1a** + **2e**)

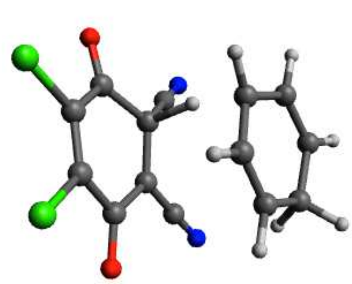
C	-2.66148	-1.29801	1.65980
C	-2.88519	0.09293	1.83019
C	-3.64656	0.86055	0.90629
C	-4.16693	0.25122	-0.21522
C	-3.93916	-1.18868	-0.47514
C	-3.16750	-1.93458	0.54398
C	-0.20744	0.83743	-0.29115

C	0.96527	1.75621	-0.02534
C	2.28635	1.27080	0.19961
C	2.45890	-0.24111	0.08920
C	1.45893	-1.12160	-0.26351
C	0.10788	-0.65372	-0.59925
C	-1.12647	1.35538	-1.31933
N	-1.85359	1.77815	-2.13302
C	0.70141	3.13064	0.13220
N	0.44086	4.27670	0.25833
O	-0.78258	-1.38501	-1.03593
Cl	4.05326	-0.81079	0.43160
O	3.27833	1.98505	0.48011
Cl	1.71537	-2.84422	-0.40815
H	-0.81476	0.75045	0.64292
H	-3.79714	1.92362	1.08585
H	-4.74104	0.81984	-0.94555
H	-3.40562	-1.29003	-1.44655
H	-4.89780	-1.70196	-0.69407
H	-2.99830	-2.99813	0.38134
H	-2.08106	-1.84542	2.40062
H	-2.47582	0.58771	2.71213



4,5-Dichloro-3-hydroxy-6-oxocyclohexa-2,4-diene-1,2-dicarbonitrile (**IM3**)

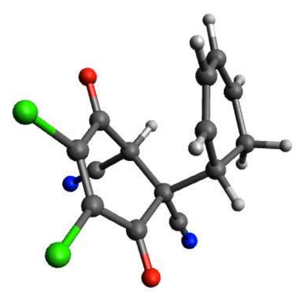
H	1.75260	-1.38503	-1.37379
C	1.31506	-1.04618	-0.41968
C	1.51725	0.45737	-0.28321
C	-0.16698	-1.54109	-0.45199
Cl	-2.83533	-1.15166	-0.07051
Cl	-2.15614	1.94396	0.39157
C	2.83311	0.97288	-0.39634
C	2.01088	-1.76064	0.66849
O	0.55740	2.64061	0.06331
O	-0.39720	-2.71561	-0.70537
N	3.91770	1.42170	-0.48797
N	2.56780	-2.31016	1.53850
C	-0.92243	0.78908	0.04207
C	0.45648	1.30596	-0.06091
C	-1.22033	-0.54439	-0.14782
H	1.48396	2.93732	-0.00525



C-attack **TS3** (**1a** + **2e**)

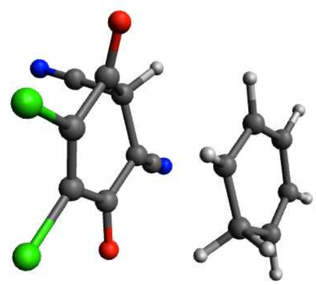
C	-1.32074	0.68704	-1.85590
H	-0.79743	0.97706	-0.58372
C	-0.40577	1.00847	0.71343
C	-0.48051	-0.35843	1.17690
C	-1.81090	-1.66129	-1.38570
C	0.97027	1.60335	0.41405

Cl	3.43647	1.27876	-0.71781
Cl	3.02791	-1.89240	-0.22067
C	-1.64042	-0.85687	1.80936
C	-1.36548	1.95388	1.24994
O	0.61050	-2.46759	1.33534
O	1.16031	2.81311	0.42479
N	-2.62323	-1.28499	2.29949
N	-2.17044	2.70674	1.64561
C	1.83722	-0.72868	0.23111
C	-0.94303	-0.71261	-1.86064
C	0.62465	-1.28989	0.95476
C	2.00737	0.61251	0.00135
H	0.06767	-0.98762	-2.16013
H	-1.49728	-2.70330	-1.31539
C	-3.22037	-1.33442	-1.02072
H	-3.39416	-1.59983	0.04948
H	-3.90937	-2.02446	-1.54583
C	-3.62059	0.08634	-1.25021
H	-4.66546	0.35080	-1.08545
C	-2.72741	1.03196	-1.65726
H	-3.03438	2.06732	-1.80032
H	-0.70036	1.38733	-2.42407



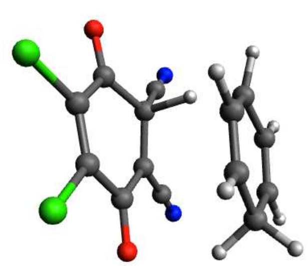
C-attack intermediate **IM4** (**1a** + **2e**)

C	1.24955	-2.30156	-1.21315
H	1.70869	-0.39011	1.37503
C	0.75428	0.12299	1.19506
C	0.86939	1.00312	-0.09723
C	1.59213	0.18035	-1.29776
C	-0.32802	-0.98572	1.08850
Cl	-2.83870	-1.78322	0.39953
Cl	-3.15116	1.02423	-1.14198
C	1.68088	2.19837	0.18063
C	0.42020	0.92209	2.38321
O	-0.62175	2.49576	-1.27529
O	-0.20447	-2.02084	1.72469
N	2.36348	3.12083	0.40807
N	0.13040	1.55027	3.32738
C	-1.67417	0.55086	-0.38338
C	0.82892	-1.08079	-1.64170
C	-0.51804	1.47044	-0.61296
C	-1.55687	-0.63413	0.31019
H	-0.08597	-0.98921	-2.22545
H	1.54639	0.88183	-2.14136
C	3.08706	-0.12967	-1.00339
H	3.57238	0.70929	-0.48623
H	3.58723	-0.20114	-1.98676
C	3.32601	-1.43070	-0.27320
H	4.24351	-1.53703	0.30713
C	2.45323	-2.46232	-0.39974
H	2.64065	-3.42153	0.08267
H	0.66003	-3.18638	-1.45732



Rearrangement **TS4** (**1a** + **2e**)

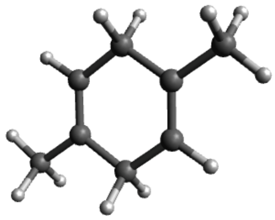
C	-3.74202	0.63498	-1.28229
H	-0.53802	2.29062	-0.39134
C	0.16727	1.65533	0.16249
C	-0.54625	0.42139	0.72484
C	-1.54721	-0.41480	-1.16654
C	1.32544	1.30503	-0.81695
Cl	3.57896	-0.13741	-1.36399
Cl	2.49260	-2.28208	0.78484
C	-1.69499	0.70461	1.52015
C	0.75066	2.46685	1.24967
O	-0.20496	-1.70078	1.72608
O	1.59060	2.05309	-1.74736
N	-2.65763	1.01175	2.12104
N	1.21877	3.09305	2.12162
C	1.60616	-0.85555	0.39694
C	-2.38346	0.67138	-1.55326
C	0.24080	-0.75193	1.05551
C	2.08988	0.06999	-0.49912
H	-1.94846	1.54602	-2.03545
H	-0.55753	-0.49430	-1.61572
C	-2.18368	-1.70338	-0.72883
H	-1.63953	-2.16778	0.11709
H	-2.02812	-2.43804	-1.54714
C	-3.64275	-1.63348	-0.41708
H	-4.10859	-2.52116	0.01128
C	-4.37450	-0.51216	-0.67955
H	-5.44039	-0.47471	-0.45798
H	-4.36101	1.48908	-1.55957



C-attack **TS5** (**1a** + **2e**)

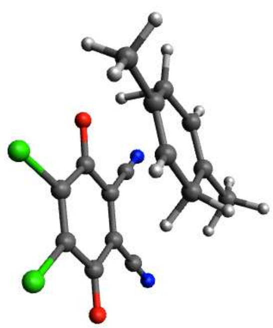
C	1.35292	0.11800	2.11057
H	0.92929	0.89255	1.02237
C	0.66461	1.38477	-0.22577
C	0.92328	0.26413	-1.09526
C	0.28947	-2.05343	1.66598
C	-0.78773	1.78011	0.06966
Cl	-3.38728	1.05393	0.47200
Cl	-2.58231	-1.78906	-0.83619
C	2.15605	0.13219	-1.79105
C	1.58176	2.50770	-0.27748
O	0.16767	-1.85920	-1.82690
O	-1.06092	2.90096	0.48566
N	3.15640	0.05473	-2.40568
N	2.34597	3.39479	-0.28961
C	-1.44635	-0.50241	-0.67053
C	0.23776	-0.81214	2.23575
C	-0.06833	-0.78387	-1.24487
C	-1.78829	0.69637	-0.09700
H	-0.65747	-0.48363	2.76321

H	-0.56051	-2.72999	1.75870
C	1.49015	-2.54593	0.93345
H	1.20198	-2.80764	-0.11357
H	1.81771	-3.52392	1.33858
C	2.63397	-1.59110	0.90781
H	3.54929	-1.91376	0.41104
C	2.58854	-0.37011	1.52509
H	3.45568	0.28958	1.50647
H	1.40951	0.94777	2.82315



1,4-Dimethylcyclohexa-1,4-diene (**2f**)

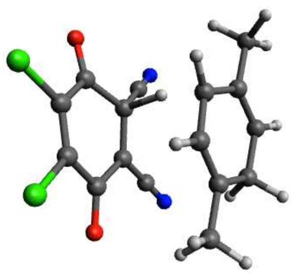
C	0.73940	-1.22066	-0.00001
C	1.45094	-0.07480	-0.00000
C	-0.77163	-1.28195	0.00002
C	-1.45094	0.07480	0.00000
C	-0.73940	1.22066	0.00001
C	0.77163	1.28195	0.00002
H	1.27155	-2.17721	-0.00003
C	2.96120	-0.05251	-0.00002
H	-1.12687	-1.86411	-0.87389
C	-2.96120	0.05251	-0.00001
H	-1.27155	2.17721	-0.00001
H	1.12685	1.86407	0.87396
H	1.12687	1.86411	-0.87389
H	-1.12684	-1.86407	0.87396
H	-3.34475	-0.48541	-0.88483
H	-3.38175	1.06914	-0.00001
H	-3.34477	-0.48541	0.88479
H	3.38175	-1.06914	-0.00007
H	3.34477	0.48536	0.88482
H	3.34475	0.48546	-0.88480



O-Attack-TS (DDQ **1a** + **2f**)

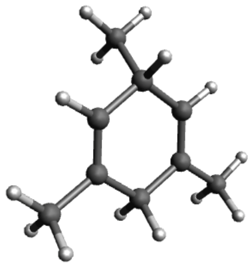
C	1.44219	-2.63351	0.01149
H	1.22621	-1.97718	-1.06403
C	-1.25869	-0.26454	-1.01729
C	-1.96743	0.70325	-0.30233
C	1.68227	-0.80570	1.62160
C	0.16979	-0.12766	-1.27329
Cl	2.50346	1.28380	-1.22479
Cl	0.93875	3.42774	0.60579
C	-3.38102	0.61113	-0.12345
C	-1.93221	-1.38479	-1.60520
O	-1.92675	2.75773	0.90443
O	0.79957	-1.03746	-1.92521
N	-4.54459	0.54350	0.02093
N	-2.50760	-2.28428	-2.09034
C	0.15720	2.01645	-0.02520
C	2.27785	-1.66419	0.73833
C	-1.29721	1.89950	0.26502
C	0.83906	1.07399	-0.77312

C	3.74683	-1.60896	0.41181
C	0.23779	-0.88075	1.99241
H	-0.26418	0.08755	1.75106
H	0.12423	-0.92743	3.09264
C	-0.53910	-1.99075	1.35379
C	-1.96606	-2.15884	1.77670
C	0.06912	-2.83364	0.45251
H	1.95530	-3.50975	-0.40602
H	2.28556	-0.04472	2.11956
H	-0.51037	-3.63301	-0.01002
H	-2.47886	-2.93439	1.19446
H	-2.50872	-1.20559	1.66728
H	-2.01768	-2.41912	2.84686
H	4.23291	-2.55871	0.68699
H	4.24400	-0.78763	0.94393
H	3.89447	-1.46887	-0.67027



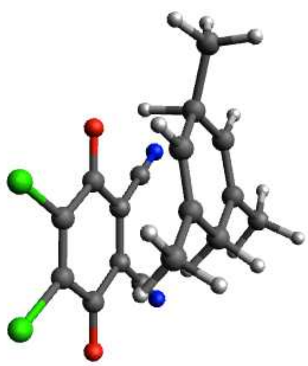
C-Attack-TS (DDQ **1a** + **2f**)

C	1.11563	0.35133	2.02198
H	0.55951	1.07434	0.97664
C	0.22039	1.56987	-0.26658
C	0.71428	0.55798	-1.16718
C	0.53863	-1.92312	1.35511
C	-1.28785	1.67555	-0.02646
Cl	-3.73734	0.48210	0.17208
Cl	-2.34440	-2.13011	-1.12302
C	1.96298	0.68397	-1.82736
C	0.91496	2.84211	-0.23482
O	0.39357	-1.62276	-2.03699
O	-1.78552	2.70832	0.41232
N	2.97473	0.78853	-2.42072
N	1.50728	3.85079	-0.17713
C	-1.47636	-0.66063	-0.86801
C	0.18731	-0.78228	2.02512
C	-0.05627	-0.65005	-1.40259
C	-2.06343	0.43522	-0.28613
C	-1.13252	-0.62120	2.73185
H	-0.15708	-2.76330	1.32690
C	1.86095	-2.11183	0.69365
H	1.69901	-2.35713	-0.38195
H	2.34830	-3.02850	1.07926
C	2.81039	-0.95860	0.80136
C	4.15805	-1.09725	0.16511
C	2.44808	0.17533	1.49409
H	3.15732	0.99835	1.58899
H	0.97032	1.11859	2.79130
H	-1.62230	0.32132	2.44407
H	-0.97433	-0.57417	3.82132
H	-1.81160	-1.45379	2.50936
H	4.85964	-0.33819	0.53505
H	4.05627	-0.95708	-0.92628
H	4.57475	-2.10231	0.32868



1,3,5-Trimethylcyclohexa-1,4-diene (**2g**)

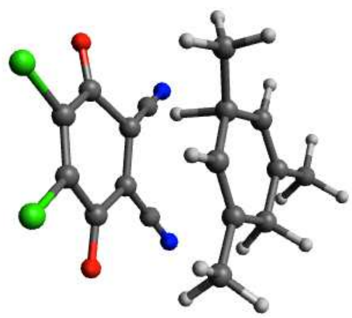
C	-0.16786	0.74034	1.25831
C	-0.16786	-0.60792	1.27885
C	-0.14123	1.58066	0.00000
C	-0.16786	0.74034	-1.25831
C	-0.16786	-0.60792	-1.27885
C	-0.16363	-1.42257	0.00000
C	-0.17502	-1.40612	2.56139
H	-1.03510	2.23690	0.00000
C	-0.17502	-1.40612	-2.56139
H	0.71478	-2.09885	0.00000
H	-1.03303	-2.11051	0.00000
H	-0.17937	-0.75195	3.44574
H	0.70925	-2.06510	2.61666
H	-1.06023	-2.06461	2.60722
H	-0.17937	-0.75195	-3.44574
H	-1.06023	-2.06461	-2.60722
H	0.70925	-2.06510	-2.61666
C	1.08801	2.53256	0.00000
H	-0.16694	1.28810	-2.20650
H	-0.16694	1.28810	2.20650
H	2.02019	1.94648	0.00000
H	1.07886	3.17680	0.89356
H	1.07886	3.17680	-0.89356



O-Attack-TS (DDQ **1a** + **2g**)

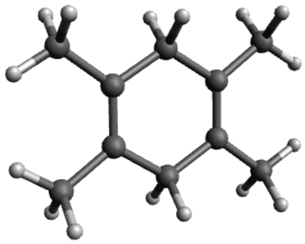
C	-2.57353	-1.39937	0.01336
H	-1.98726	-1.17921	-1.04420
C	-0.17582	1.29921	-1.01701
C	0.82957	1.94883	-0.30091
C	-0.66114	-1.51289	1.60896
C	-0.08160	-0.12331	-1.34053
Cl	1.25930	-2.49837	-1.40840
Cl	3.60983	-1.00458	0.22870
C	0.77003	3.35074	-0.03395
C	-1.29171	2.02602	-1.54582
O	2.94353	1.81982	0.78978
O	-1.01455	-0.69820	-1.99028
N	0.72975	4.50398	0.18376
N	-2.18022	2.64970	-1.98992
C	2.13661	-0.20255	-0.21511
C	-1.51553	-2.12354	0.73437
C	2.04739	1.23384	0.16345
C	1.12919	-0.84063	-0.91142
C	-0.83249	-0.06467	1.96681
H	0.10592	0.48665	1.72444
H	-0.89261	0.04649	3.06617
C	-1.98755	0.64239	1.32121

C	-2.21877	2.06839	1.72604
C	-2.80822	-0.01393	0.44200
C	-3.79704	-2.21046	-0.43989
C	0.45774	-2.24683	2.28874
H	-3.03134	2.53008	1.15150
H	-1.29924	2.65954	1.58732
H	-2.46104	2.12372	2.80031
H	0.52084	-3.29087	1.95653
H	0.32406	-2.22406	3.38290
H	1.41861	-1.74876	2.08110
H	-1.37343	-3.17753	0.49051
H	-3.63813	0.52285	-0.02015
H	-4.41083	-1.62523	-1.13794
H	-4.41209	-2.47062	0.43554
H	-3.48020	-3.13896	-0.93389



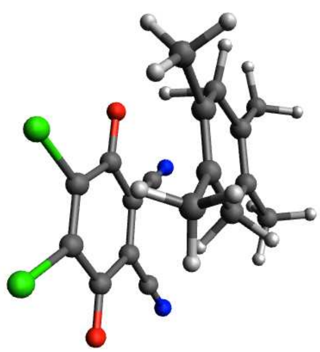
C-Attack-TS (DDQ **1a** + **2g**)

C	1.02830	-0.80571	-1.59256
H	0.49530	-1.06748	-0.40185
C	0.06101	-1.13640	0.96228
C	0.19874	0.21268	1.43322
C	1.32767	1.62264	-1.20694
C	-1.31052	-1.65734	0.57161
Cl	-3.70616	-1.18547	-0.65651
Cl	-3.15308	1.95125	-0.09256
C	1.36430	0.64810	2.10711
C	0.97920	-2.13448	1.46190
O	-0.76548	2.38330	1.55685
O	-1.55755	-2.85917	0.53450
N	2.33604	1.04311	2.64291
N	1.75242	-2.93288	1.83221
C	-2.04571	0.71972	0.39361
C	0.57084	0.57349	-1.67180
C	-0.83652	1.20662	1.17005
C	-2.27606	-0.60778	0.13603
C	0.81447	3.02829	-1.19512
C	2.73767	1.39520	-0.74138
H	2.85609	1.77654	0.29343
H	3.41115	2.04956	-1.32780
C	3.24336	-0.01995	-0.80299
C	2.43949	-1.02761	-1.24369
C	0.34108	-1.84693	-2.47101
C	4.65774	-0.24652	-0.35408
H	-0.13997	3.11827	-1.72941
H	1.55131	3.72054	-1.63072
H	0.65052	3.34547	-0.14921
H	4.95683	-1.29661	-0.46889
H	4.75558	0.03721	0.70802
H	5.35490	0.39396	-0.91858
H	-0.43494	0.76055	-2.05051
H	2.81208	-2.05220	-1.27777
H	0.73752	-1.76824	-3.49550
H	-0.74412	-1.68195	-2.50718
H	0.53950	-2.86258	-2.10387



1,2,4,5-Tetramethylcyclohexa-1,4-diene (**2h**)

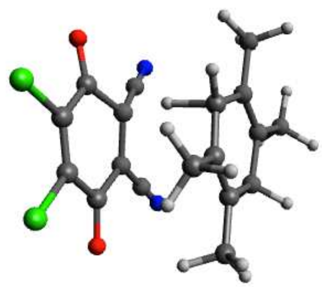
C	1.29553	0.67664	-0.00002
C	1.29553	-0.67664	-0.00002
C	0.00000	1.46547	-0.00015
C	-1.29553	0.67664	-0.00005
C	-1.29553	-0.67664	-0.00001
C	0.00000	-1.46547	-0.00009
C	2.52332	1.56163	0.00007
C	2.52332	-1.56163	0.00007
H	-0.00001	2.15183	0.87191
C	-2.52332	1.56163	0.00003
C	-2.52332	-1.56163	0.00011
H	-0.00001	-2.15162	-0.87232
H	0.00001	-2.15177	0.87203
H	-2.51471	2.22407	0.88374
H	-3.47015	1.00861	-0.00004
H	-2.51469	2.22425	-0.88355
H	3.47015	-1.00861	-0.00034
H	2.51452	-2.22448	-0.88333
H	2.51489	-2.22384	0.88396
H	0.00001	2.15155	-0.87245
H	3.47015	1.00861	0.00047
H	2.51447	2.22437	0.88356
H	2.51494	2.22395	-0.88374
H	-3.47015	-1.00861	0.00001
H	-2.51472	-2.22402	0.88386
H	-2.51469	-2.22430	-0.88343



O-Attack-TS (DDQ **1a** + **2h**)

C	-1.42520	-2.43354	-0.10037
H	-1.03038	-1.88417	-1.16650
C	-0.74479	1.12780	-1.00108
C	-0.21658	2.16331	-0.21990
C	0.24313	-1.57205	1.48526
C	0.05551	-0.03096	-1.36614
Cl	2.43100	-1.36045	-1.51892
Cl	3.67005	1.01508	0.27552
C	-1.00150	3.30530	0.12126
C	-2.06264	1.22380	-1.54835
O	1.65848	3.08065	0.93233
O	-0.45876	-0.98999	-2.04605
N	-1.64610	4.24497	0.40637
N	-3.13386	1.34826	-2.01152
C	1.99777	0.98734	-0.18889
C	-0.14522	-2.55892	0.60564
C	1.18850	2.15274	0.25066
C	1.46129	-0.03818	-0.94486
C	0.69707	-3.76449	0.27385
C	-0.69213	-0.46174	1.84653

H	-0.19397	0.51712	1.64530
H	-0.80204	-0.42251	2.94939
C	-2.04627	-0.45500	1.21834
C	-3.00382	0.61147	1.67191
C	-2.41980	-1.45151	0.33407
H	-1.83461	-3.36923	-0.50489
C	1.57204	-1.57925	2.19584
C	-3.81139	-1.52896	-0.23802
H	-3.61559	0.98456	0.83876
H	-2.47227	1.45281	2.13600
H	-3.70021	0.19996	2.42328
H	0.67156	-3.96700	-0.80696
H	0.28335	-4.65143	0.78272
H	1.74109	-3.64864	0.58489
H	2.39968	-1.76006	1.49514
H	1.60527	-2.38250	2.95057
H	1.74899	-0.62483	2.70885
H	-3.89975	-2.35235	-0.95825
H	-4.09011	-0.59019	-0.73946
H	-4.54279	-1.69112	0.57031

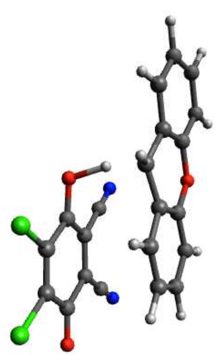


C-Attack-TS (DDQ **1a** + **2h**)

C	-1.20589	0.50402	-1.54764
H	-0.54706	0.92388	-0.43338
C	-0.00870	1.11391	0.86459
C	0.08035	-0.22065	1.40704
C	-1.42365	-1.83775	-0.90617
C	1.25040	1.80714	0.37943
Cl	3.71243	1.65022	-0.79797
Cl	3.69344	-1.47587	0.00464
C	-0.96334	-0.76612	2.18764
C	-1.00749	1.99682	1.42657
O	1.31985	-2.24580	1.52679
O	1.29369	3.02409	0.22029
N	-1.83936	-1.23053	2.82495
N	-1.84359	2.69018	1.86547
C	2.37674	-0.42357	0.38229
C	-0.70283	-0.85542	-1.56569
C	1.23636	-1.06573	1.14456
C	2.38410	0.90082	0.02785
C	-0.92628	-3.24758	-0.78269
C	-2.78424	-1.53734	-0.36141
H	-2.80577	-1.79218	0.72154
H	-3.48995	-2.27673	-0.78930
C	-3.33832	-0.15734	-0.55424
C	-2.58427	0.81861	-1.15481
C	-3.06848	2.23373	-1.40004
H	-0.74237	1.19871	-2.25936
C	0.59925	-1.14519	-2.27577
C	-4.74389	0.04751	-0.05981
H	-2.22120	2.90597	-1.59198
H	-3.62660	2.62764	-0.54157
H	-3.72956	2.26851	-2.28145
H	-0.07772	-3.28270	-0.07504
H	-0.55328	-3.62631	-1.74624
H	-1.71033	-3.91861	-0.40942
H	1.19270	-0.23171	-2.41060
H	0.38785	-1.55429	-3.27793
H	1.20635	-1.88742	-1.74282
H	-5.13621	1.04244	-0.29701
H	-4.77606	-0.09059	1.03461
H	-5.41725	-0.70979	-0.49314

9*H*-Xanthene (**2j**)

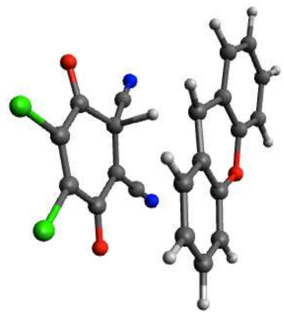
C	-0.81628	-0.18427	3.59371
C	0.58826	-0.22842	3.68039
C	1.35948	-0.09029	2.51509
C	0.75852	0.09702	1.25616
C	-0.64811	0.12159	1.19545
C	-1.43937	-0.01450	2.34873
O	-1.33816	0.28421	0.00000
C	-0.64811	0.12159	-1.19545
C	0.75852	0.09702	-1.25616
C	1.58120	0.31076	0.00000
H	-1.42746	-0.28972	4.49083
H	1.07641	-0.36832	4.64532
H	2.44959	-0.11853	2.57373
H	-2.52513	0.00947	2.25490
C	-1.43937	-0.01450	-2.34873
C	1.35948	-0.09029	-2.51509
H	1.98487	1.34032	0.00000
H	2.45629	-0.35796	0.00000
C	-0.81628	-0.18427	-3.59371
C	0.58826	-0.22842	-3.68039
H	-2.52513	0.00947	-2.25490
H	2.44959	-0.11853	-2.57373
H	-1.42746	-0.28972	-4.49083
H	1.07641	-0.36832	-4.64532



O-Attack-TS (DDQ **1a** + **2j**)

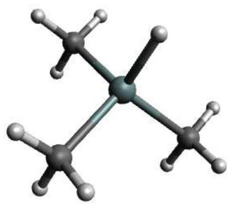
C	-1.78505	-1.30566	0.78564
H	-1.14757	-1.47638	-0.33495
C	0.73902	0.65213	-1.21984
C	1.84184	1.42834	-0.85127
C	-1.42966	1.12579	1.15502
C	0.74334	-0.78826	-1.05919
Cl	1.92644	-3.14623	-0.38628
Cl	4.53561	-1.39328	0.36147
C	1.82731	2.84674	-1.00063
C	-0.43013	1.24802	-1.79055
O	4.07400	1.50291	-0.02154
O	-0.31194	-1.48027	-1.33022
N	1.80884	4.01520	-1.11839
N	-1.38177	1.73831	-2.27120
C	3.07665	-0.66846	-0.22881
C	-0.98384	-0.22152	1.33733
C	3.08582	0.81628	-0.33122
C	1.96629	-1.41742	-0.56154
C	0.28776	-0.42571	1.93027
C	-0.63080	2.22108	1.51103
O	-2.65944	1.40237	0.63072
C	-3.53250	0.38936	0.29027
C	-4.80806	0.78253	-0.13986

C	-3.15523	-0.97540	0.38623
C	-4.11180	-1.95539	0.03011
H	-1.62890	-2.29886	1.22418
C	1.09136	0.65724	2.27946
H	0.62989	-1.44790	2.08833
C	0.63592	1.97953	2.05123
H	-0.99838	3.23156	1.34271
H	1.27508	2.82301	2.30935
H	2.07192	0.49062	2.72238
C	-5.38646	-1.57952	-0.39606
C	-5.73163	-0.20938	-0.48485
H	-5.05287	1.84187	-0.19822
H	-6.72613	0.08001	-0.82356
H	-6.11746	-2.34155	-0.66446
H	-3.83190	-3.00727	0.09483



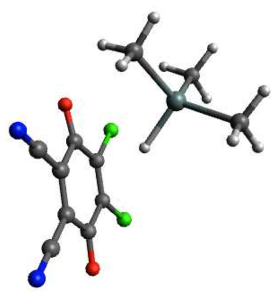
C-Attack-TS (DDQ **1a** + **2j**)

C	1.06887	-0.31135	-1.44121
H	0.45865	-0.89961	-0.31926
C	-0.07576	-1.21692	0.88658
C	-0.43135	0.04704	1.49472
C	1.13582	1.97445	-0.51425
C	-1.18214	-2.10543	0.31702
Cl	-3.58306	-2.33365	-0.96518
Cl	-4.14345	0.70702	-0.03968
C	0.48071	0.72270	2.34363
C	1.03144	-1.95223	1.46813
O	-2.02464	1.80102	1.64662
O	-0.99224	-3.29994	0.11103
N	1.24922	1.26643	3.05046
N	1.95097	-2.52382	1.91429
C	-2.67836	-0.11236	0.35568
C	0.46114	0.99233	-1.29881
C	-1.70599	0.68284	1.21245
C	-2.43968	-1.40058	-0.05024
C	-0.82536	1.31120	-1.81477
C	0.54565	3.21410	-0.22422
O	2.40020	1.76478	-0.03608
C	3.08952	0.61663	-0.36196
C	4.42442	0.54223	0.06030
C	2.47833	-0.43118	-1.10095
C	3.25458	-1.57528	-1.41186
H	0.67011	-0.98294	-2.20812
C	-1.40089	2.54898	-1.55553
H	-1.34403	0.56532	-2.41668
C	-0.72225	3.48936	-0.73908
H	1.08167	3.93076	0.39504
H	-1.19255	4.44556	-0.51341
H	-2.38478	2.78854	-1.95466
C	4.58618	-1.65443	-1.00802
C	5.16635	-0.59762	-0.26613
H	4.85513	1.36528	0.62814
H	6.20456	-0.66834	0.05727
H	5.17885	-2.53491	-1.25303
H	2.78783	-2.38904	-1.96736



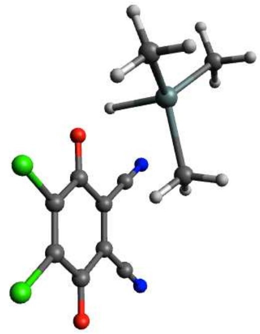
Trimethylstannane (**2n'**)

Sn	0.00009	-0.00004	-0.23693
C	-1.05397	-1.76086	0.46864
C	2.05202	-0.03191	0.46879
C	-0.99853	1.79300	0.46852
H	-1.06835	-1.78217	1.56999
H	-0.56258	-2.67976	0.11173
H	-2.09521	-1.76306	0.10945
H	-1.01282	1.81448	1.56987
H	-2.03904	1.82811	0.10880
H	-0.47838	2.69610	0.11206
H	0.00038	-0.00039	-1.96291
H	2.07748	-0.03149	1.57014
H	2.60245	0.85220	0.11015
H	2.57433	-0.93344	0.11149



Charge transfer complex **CT2** (**1a** + **2n'**)

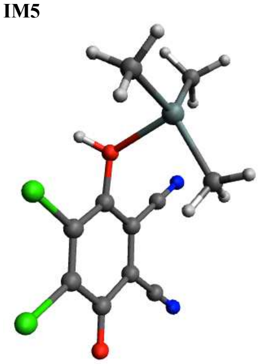
O	0.10790	-0.02098	2.41450
C	0.84057	0.07031	1.43626
C	1.48040	-1.12241	0.78728
Cl	0.99903	-2.65123	1.40940
C	2.41036	-0.98019	-0.21103
Cl	3.19010	-2.32075	-0.95892
C	2.81161	0.37039	-0.72278
O	3.65663	0.52112	-1.59990
C	2.11716	1.56871	-0.12584
C	2.47743	2.84670	-0.65492
C	1.16712	1.42640	0.85300
C	0.47565	2.54472	1.41332
N	2.77226	3.89622	-1.08842
N	-0.09722	3.46296	1.86547
H	-0.68607	0.21538	-0.59335
Sn	-2.38541	-0.10452	-0.48041
C	-3.19223	1.19244	1.05379
C	-2.62910	-2.18772	0.06074
C	-3.25952	0.31446	-2.41799
H	-3.09641	1.36652	-2.69893
H	-4.34442	0.12581	-2.39288
H	-2.81322	-0.32692	-3.19376
H	-2.20196	-2.38216	1.05598
H	-2.12691	-2.84299	-0.66757
H	-3.69919	-2.44815	0.08369
H	-2.69623	1.00614	2.01836
H	-4.27122	1.00729	1.17535
H	-3.04734	2.25069	0.78807



O-attack **TS6** (**1a** + **2n’**)

O	-4.21253	0.05645	-1.11511
C	-3.16665	0.07092	-0.45331
C	-2.46142	-1.17174	-0.03246
Cl	-3.18052	-2.65818	-0.54069
C	-1.30039	-1.12700	0.71259
Cl	-0.43290	-2.55285	1.17617
C	-0.73028	0.14655	1.15824
O	0.32053	0.19683	1.88354
C	-1.35975	1.38133	0.69924
C	-0.72193	2.61284	1.05550
C	-2.53685	1.35758	-0.03713
C	-3.19151	2.55977	-0.44181
N	-0.18768	3.62100	1.32877
N	-3.72884	3.54885	-0.77618
H	1.56599	0.08726	1.20843
Sn	2.65593	0.02167	-0.30906
C	1.03501	0.26630	-1.73812
C	3.59581	-1.92438	-0.39818
C	4.03706	1.68439	-0.27181
H	3.48929	2.63240	-0.16864
H	4.60815	1.70220	-1.21420
H	4.74168	1.58339	0.56658
H	2.83326	-2.71620	-0.36848
H	4.28714	-2.05913	0.44656
H	4.16478	-2.00997	-1.33815
H	0.32398	-0.57022	-1.68831
H	1.47647	0.28793	-2.74844
H	0.49760	1.21180	-1.57795

IM5

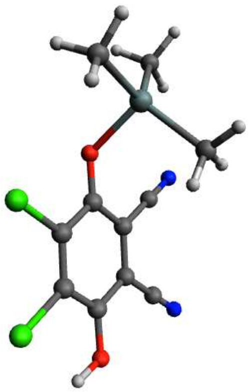


O-attack intermediate **IM5** (**1a** + **2n’**)

O	4.37901	0.45553	0.66285
C	3.20568	0.33117	0.23254
C	2.58368	-0.98431	-0.02603
Cl	3.57041	-2.38118	0.29264
C	1.27478	-1.12046	-0.49565
Cl	0.53169	-2.68268	-0.78020
C	0.49895	0.03105	-0.77019
O	-0.85912	-0.08047	-1.15526
C	1.01035	1.31488	-0.54928
C	0.17001	2.44527	-0.80025
C	2.33707	1.47559	-0.05686
C	2.86273	2.77760	0.16747
N	-0.53557	3.36409	-0.99298
N	3.29871	3.85520	0.35482
H	-0.95811	-0.58388	-1.98517
Sn	-2.53134	-0.05962	0.35821
C	-1.24938	0.51129	1.97237

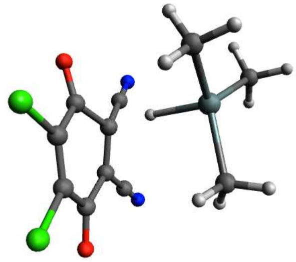
C	-3.14597	-2.10857	0.22279
C	-3.72320	1.42969	-0.61132
H	-3.09815	2.30616	-0.83258
H	-4.54783	1.73312	0.05156
H	-4.14671	1.02978	-1.54373
H	-2.44672	-2.75044	0.77558
H	-3.17611	-2.42526	-0.83039
H	-4.15446	-2.21665	0.65024
H	-0.36965	-0.14703	2.00548
H	-1.79700	0.41261	2.92186
H	-0.92320	1.55375	1.85785

P3



O-Trimethylstannyl-2,3-dichloro-5,6-dicyanohydroquinone (**P3**)

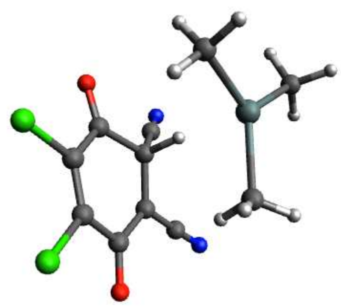
O	-0.87393	-0.20737	-0.97722
Sn	-2.53107	-0.07673	0.22705
C	0.04839	2.39214	-0.60619
C	0.92433	1.27973	-0.42678
C	2.29278	1.47965	-0.06881
C	2.81221	2.79861	0.10683
C	3.14605	0.37022	0.11594
O	4.43651	0.62082	0.44623
C	2.61432	-0.93758	-0.04897
Cl	3.69646	-2.28647	0.20353
C	1.26429	-1.13260	-0.39533
Cl	0.60067	-2.72785	-0.57096
C	0.38615	-0.02324	-0.60701
N	3.23010	3.88683	0.25143
N	-0.69097	3.29471	-0.74417
C	-3.79173	1.24982	-0.89473
C	-1.67623	0.68377	2.05097
C	-3.20521	-2.11715	0.31118
H	-1.43468	1.75178	1.95269
H	-0.75641	0.13074	2.29592
H	-2.38688	0.55887	2.88222
H	-3.31032	2.23391	-0.98517
H	-4.76412	1.36972	-0.39255
H	-3.96520	0.84037	-1.90140
H	-3.26985	-2.53135	-0.70634
H	-4.20174	-2.17083	0.77640
H	-2.50521	-2.72858	0.89903
H	4.93021	-0.21327	0.54766



C-attack **TS7** (**1a** + **2n'**)

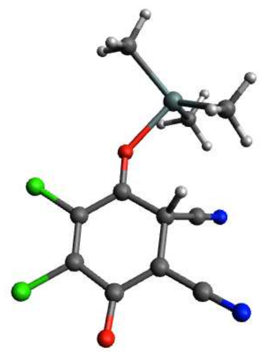
Sn	2.05811	-0.62803	-0.52738
H	0.79120	0.40104	0.39953
C	-0.29479	1.26253	1.04304

C	0.56550	2.03114	1.91984
N	1.27153	2.65094	2.61857
C	-1.05085	1.94568	0.05944
C	-0.70692	3.26397	-0.34676
N	-0.41617	4.35451	-0.67825
C	-2.08479	1.24400	-0.70668
O	-2.71197	1.77729	-1.62934
C	-2.35613	-0.20036	-0.32097
Cl	-3.45255	-1.04516	-1.34540
C	-1.80446	-0.78141	0.79245
Cl	-2.17467	-2.38863	1.31505
C	-0.88427	-0.00886	1.67529
O	-0.56253	-0.36217	2.79989
C	1.92569	-2.59356	0.35379
C	3.89435	0.43993	-0.15178
C	1.22156	-0.41753	-2.50822
H	0.97516	-3.07433	0.08177
H	2.75958	-3.21150	-0.01508
H	1.99460	-2.52573	1.44935
H	3.82157	1.46895	-0.53170
H	4.72332	-0.07333	-0.66446
H	4.10547	0.46683	0.92697
H	1.93484	-0.81459	-3.24790
H	0.27775	-0.97633	-2.58495
H	1.03279	0.64273	-2.73183



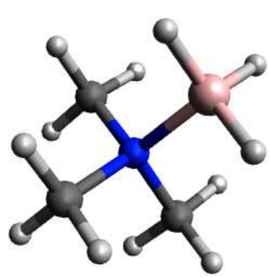
C-attack intermediate **IM6** (**1a** + **2n’**)

Sn	2.21232	-0.70902	-0.60315
H	0.71312	0.45613	0.58058
C	-0.17158	1.02136	1.09057
C	0.46957	1.74395	2.19647
N	0.98386	2.33184	3.06731
C	-0.86174	1.89128	0.10123
C	-0.31757	3.16123	-0.19193
N	0.16154	4.21461	-0.42555
C	-1.95852	1.41038	-0.68471
O	-2.53555	2.06487	-1.57864
C	-2.42786	-0.01378	-0.37948
Cl	-3.63389	-0.62692	-1.44826
C	-1.97731	-0.75906	0.68461
Cl	-2.59749	-2.33736	1.08077
C	-0.96695	-0.21800	1.61837
O	-0.67488	-0.73211	2.69029
C	1.68760	-2.67123	0.08795
C	3.95660	0.26260	0.18155
C	1.18039	0.13578	-2.27745
H	0.71737	-2.97159	-0.32961
H	2.46373	-3.38193	-0.23663
H	1.64041	-2.67933	1.18648
H	3.89147	1.34485	0.00460
H	4.84693	-0.13622	-0.33036
H	4.04273	0.06123	1.25843
H	1.89201	0.67356	-2.91997
H	0.67037	-0.65452	-2.84519
H	0.42944	0.85705	-1.91212



C-attack intermediate **IM7** (**1a** + **2n'**)

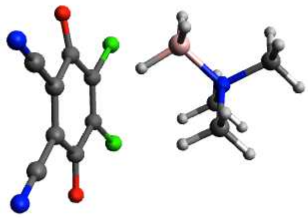
Sn	2.71754	-0.07600	-0.13632
H	-0.15331	1.47702	-1.00862
C	-0.72010	1.15322	-0.11601
C	-0.07558	1.78284	1.05682
N	0.42515	2.29558	1.98265
C	-2.16144	1.61452	-0.23815
C	-2.37625	2.99198	-0.43896
N	-2.52535	4.15123	-0.61196
C	-3.27248	0.72808	-0.16247
O	-4.47981	1.05420	-0.23876
C	-2.89552	-0.73933	-0.00807
Cl	-4.22460	-1.81309	0.07607
C	-1.59210	-1.24101	0.04365
Cl	-1.23932	-2.94512	0.16991
C	-0.47427	-0.35380	-0.01449
O	0.71920	-0.80046	0.02557
C	3.45883	-1.76607	-1.22326
C	3.22094	0.05477	1.94174
C	2.51266	1.74554	-1.25985
H	2.91420	-1.87220	-2.17290
H	4.52942	-1.63410	-1.44206
H	3.32870	-2.68093	-0.62713
H	2.70708	0.90840	2.40340
H	4.30863	0.18249	2.04998
H	2.92102	-0.87277	2.45091
H	3.51717	2.08564	-1.55624
H	1.92957	1.57465	-2.17714
H	2.04562	2.53933	-0.66096



Trimethylamine borane complex (**2p**)

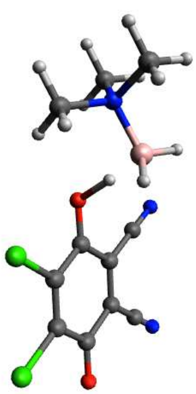
H	1.99948	0.99220	0.64696
B	1.66640	0.00299	0.00345
N	0.01270	0.00006	-0.00003
C	-0.49967	-0.07784	1.40505
C	-0.49286	-1.18031	-0.77068
C	-0.49776	1.25547	-0.63744
H	-1.59292	-1.18277	-0.77224
H	-0.11070	-2.09051	-0.29530
H	-0.11060	-1.11161	-1.79525
H	-1.59974	-0.08042	1.40226
H	-0.12218	0.78993	1.95731
H	-0.11778	-0.99859	1.86003
H	-1.59779	1.25363	-0.63899
H	-0.11546	1.30052	-1.66326
H	-0.11932	2.11002	-0.06552
H	2.00299	-1.04758	0.53880

H	2.00481	0.06588	-1.17351



Charge transfer complex **CT3** (**1a** + **2p**)

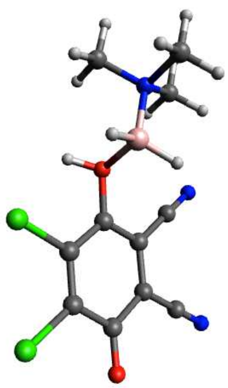
C	-1.95198	-0.59319	-0.51786
C	-1.59974	-0.84928	0.78334
C	-0.85797	0.17692	1.61107
C	-0.32730	1.37718	0.87741
C	-0.65573	1.61518	-0.43204
C	-1.50730	0.66431	-1.21538
C	-1.97229	-2.05633	1.45128
N	-2.27080	-3.05104	1.99592
O	-0.75761	0.04325	2.82317
Cl	0.65250	2.44034	1.80694
Cl	-0.11274	3.01021	-1.29134
O	-1.82080	0.86794	-2.38558
C	-2.70774	-1.52405	-1.29619
N	-3.32640	-2.28866	-1.93531
B	1.97986	-1.46030	0.91075
N	2.85388	-1.32096	-0.46988
C	4.26106	-1.77407	-0.22106
C	2.87168	0.10664	-0.92460
C	2.24468	-2.16873	-1.54610
H	4.23385	-2.82006	0.10344
H	4.68826	-1.15070	0.57238
H	4.84983	-1.67468	-1.14440
H	1.83902	0.42176	-1.10544
H	3.46133	0.19597	-1.84792
H	3.30953	0.71860	-0.12881
H	1.21989	-1.82076	-1.71961
H	2.22823	-3.20749	-1.19851
H	2.83771	-2.08157	-2.46763
H	2.46249	-0.69295	1.72759
H	2.00328	-2.63727	1.23663
H	0.83755	-1.12108	0.59818



O-attack **TS8** (**1a** + **2p**)

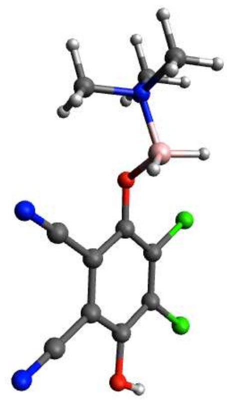
C	2.41254	1.26498	0.06083
C	3.03665	-0.07401	0.22726
C	2.13296	-1.23805	0.03483
C	0.79931	-1.07876	-0.29002
C	0.22269	0.24575	-0.49727
C	1.06296	1.40416	-0.25580
O	4.23915	-0.19484	0.50983
Cl	2.85640	-2.79991	0.23684
Cl	-0.27437	-2.42828	-0.49632
O	-1.00351	0.40617	-0.85696
C	0.45336	2.69475	-0.37902
N	-0.04516	3.75270	-0.47051

C	3.25650	2.40143	0.24128
N	3.95116	3.33647	0.39060
B	-2.88337	0.46113	1.12676
N	-4.21171	0.09413	0.31867
C	-4.09443	-1.27400	-0.29863
C	-4.46201	1.10947	-0.76505
C	-5.36548	0.10698	1.28885
H	-1.89919	0.45417	0.15726
H	-5.43980	1.10796	1.72782
H	-5.17176	-0.63626	2.07010
H	-6.28819	-0.14115	0.74627
H	-3.24099	-1.26847	-0.98432
H	-5.02221	-1.50763	-0.83715
H	-3.92280	-1.99944	0.50348
H	-3.61113	1.09464	-1.45414
H	-4.54849	2.09667	-0.29914
H	-5.38844	0.85041	-1.29410
H	-2.53286	-0.44100	1.85239
H	-2.88707	1.61380	1.49092



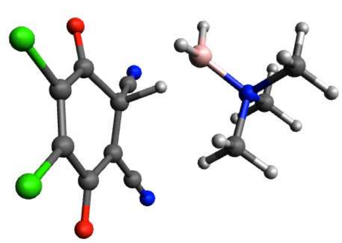
O-attack intermediate **IM8** (**1a** + **2p**)

B	-2.24738	-0.46212	0.77251
N	-1.23998	3.18187	-0.63614
C	-0.47663	2.30564	-0.47178
C	0.47044	1.25158	-0.27868
C	0.06347	-0.08136	-0.37640
C	0.97860	-1.14565	-0.20808
C	2.32164	-0.87277	0.06057
C	2.84063	0.50175	0.20992
C	1.83361	1.54819	0.01304
N	-3.75063	-0.17279	0.30049
C	-4.59307	-0.31453	1.54602
O	-1.32708	-0.34287	-0.59432
Cl	0.37191	-2.78289	-0.39654
Cl	3.47651	-2.16115	0.23746
O	4.04309	0.75004	0.47184
C	2.26180	2.90046	0.11457
N	2.62048	4.01829	0.19954
C	-4.22270	-1.17429	-0.72044
C	-3.92143	1.22063	-0.24904
H	-1.41474	-1.13134	-1.16936
H	-4.24393	0.41219	2.28762
H	-4.48314	-1.33398	1.93107
H	-5.63943	-0.11673	1.28251
H	-3.65492	-1.03259	-1.64705
H	-5.28754	-1.00553	-0.92257
H	-4.06442	-2.18168	-0.32060
H	-3.30452	1.32265	-1.14592
H	-3.58815	1.93401	0.51001
H	-4.97958	1.37771	-0.49200
H	-2.15228	-1.59835	1.15085
H	-1.84882	0.42595	1.47175



O-attack product **P4** (**1a** + **2p**)

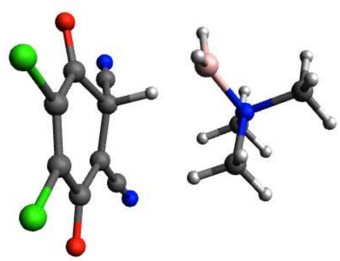
C	0.06860	-0.06335	-0.22960
C	-0.45070	1.25381	-0.15602
C	-1.84874	1.49147	0.01341
C	-2.74619	0.40477	0.10645
C	-2.23391	-0.91627	0.02162
C	-0.85412	-1.14777	-0.14028
C	0.45004	2.35614	-0.28620
N	1.16897	3.27531	-0.41339
C	-2.35807	2.82414	0.08539
N	-2.76936	3.92244	0.14460
O	-4.06043	0.69193	0.26642
Cl	-3.37741	-2.23421	0.12931
Cl	-0.22464	-2.76329	-0.25163
O	1.36880	-0.28456	-0.41937
B	2.27631	-0.23338	0.79775
N	3.78861	-0.14366	0.18896
C	3.96286	1.09122	-0.64892
C	4.09966	-1.35533	-0.64294
C	4.73867	-0.08778	1.34834
H	5.13076	-1.28465	-1.01560
H	3.39283	-1.39192	-1.47792
H	3.97914	-2.24371	-0.01317
H	4.99778	1.13675	-1.01430
H	3.73147	1.96324	-0.02908
H	3.26150	1.04131	-1.48698
H	-4.58424	-0.12870	0.31694
H	5.76828	-0.03616	0.96954
H	4.60037	-0.98987	1.95472
H	4.50695	0.80195	1.94419
H	2.22463	-1.26670	1.44605
H	2.09070	0.77899	1.45145



C-attack **TS9** (**1a** + **2p**)

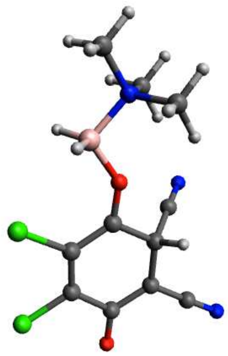
O	-1.34316	2.08733	-1.91464
C	-1.06693	1.40220	-0.91653
C	-1.94291	0.20742	-0.55110
Cl	-3.16862	-0.18568	-1.69817
C	-1.80805	-0.48301	0.62518
Cl	-2.86257	-1.77381	1.10625
C	-0.75754	-0.11106	1.60726
O	-0.72070	-0.52010	2.75756
C	0.38301	0.77801	1.04524
C	1.25254	1.30960	2.08816
C	0.05866	1.67013	-0.04421
C	0.92265	2.74329	-0.38060
N	1.95877	1.74212	2.91444

N	1.65093	3.62795	-0.65341
H	1.12654	-0.26701	0.63907
B	1.73280	-1.58731	0.51287
N	2.64913	-1.46657	-0.77337
C	1.86986	-0.88875	-1.92844
C	3.07907	-2.87528	-1.12233
C	3.88248	-0.63590	-0.51916
H	3.73514	-2.82774	-2.00157
H	2.18657	-3.46984	-1.34265
H	3.62071	-3.29762	-0.26837
H	2.50504	-0.88705	-2.82261
H	1.57686	0.13600	-1.67734
H	0.98006	-1.50679	-2.08764
H	4.49475	-0.62536	-1.42915
H	4.43405	-1.08758	0.31139
H	3.58333	0.38296	-0.25754
H	0.74420	-2.23773	0.30995
H	2.34098	-1.62644	1.54686



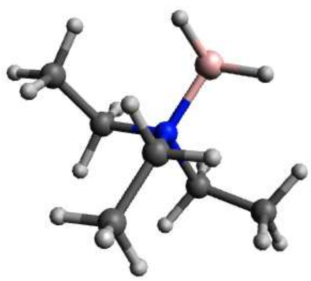
C-attack intermediate **IM9** (**1a** + **2p**)

C	0.15467	1.44503	0.53023
C	-0.96746	1.63649	-0.34636
C	-1.96173	0.47757	-0.43609
C	-1.90568	-0.63572	0.36521
C	-0.84088	-0.78958	1.38181
C	0.38807	0.15846	1.20718
O	-1.16982	2.66954	-1.01398
Cl	-3.21830	0.68215	-1.59942
Cl	-3.09310	-1.90600	0.32522
O	-0.84190	-1.64467	2.25537
C	1.18663	0.23596	2.43300
N	1.83446	0.31543	3.40345
C	1.13893	2.45738	0.60278
N	1.98434	3.27767	0.66845
B	1.83672	-1.80096	-0.14874
N	2.69187	-1.01910	-1.20121
C	3.65942	-0.05750	-0.55034
C	1.81429	-0.27088	-2.17853
C	3.47429	-2.08698	-1.94448
H	1.04277	-0.59327	0.51038
H	4.08822	-1.58642	-2.70423
H	2.76694	-2.77422	-2.42122
H	4.11319	-2.61856	-1.23023
H	2.45395	0.20453	-2.93127
H	1.25538	0.49275	-1.62779
H	1.12902	-0.98474	-2.64607
H	4.28280	0.39340	-1.33137
H	4.27404	-0.61351	0.16421
H	3.08876	0.72213	-0.03661
H	0.87308	-2.34740	-0.59681
H	2.41765	-2.12273	0.84379



C-attack intermediate **IM10** (**1a** + **2p**)

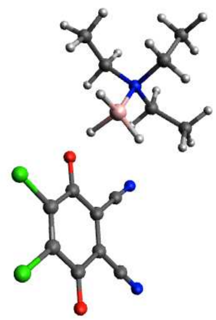
C	-2.05775	1.44834	-0.25792
C	-2.90034	0.32207	-0.04719
C	-2.15778	-1.00188	0.03924
C	-0.77007	-1.17960	-0.05595
C	0.07935	-0.04376	-0.19308
C	-0.54553	1.34934	-0.32092
O	-4.15029	0.34307	0.03261
Cl	-3.17194	-2.36512	0.24596
Cl	-0.05112	-2.76993	-0.01221
O	1.35512	-0.02434	-0.24251
C	0.08135	2.22411	0.69463
N	0.56039	2.92668	1.49856
C	-2.62976	2.72109	-0.44869
N	-3.08409	3.79860	-0.61520
B	2.55026	-0.98578	-0.09421
N	3.83144	0.01964	-0.09400
C	3.79378	0.95640	1.08345
C	3.90955	0.82018	-1.36516
C	5.05453	-0.84881	0.01257
H	-0.19938	1.70964	-1.30897
H	5.94564	-0.20834	0.03044
H	5.08444	-1.51914	-0.85337
H	4.98799	-1.43235	0.93742
H	4.81759	1.43664	-1.34654
H	3.02181	1.45736	-1.43172
H	3.93683	0.12319	-2.21003
H	4.69455	1.58376	1.07178
H	3.75765	0.35529	1.99853
H	2.89726	1.57941	1.00966
H	2.63849	-1.69174	-1.07178
H	2.52087	-1.53801	0.97969



Triethylamine borane complex (**2q**)

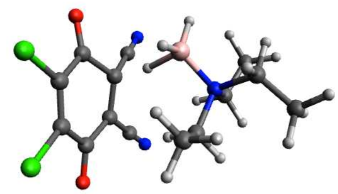
B	0.00013	-1.66985	1.08807
H	-1.00775	-1.58665	1.77456
N	0.00002	-0.36721	0.06111
H	0.00021	-2.66049	0.36304
H	1.00801	-1.58648	1.77455
C	-1.21307	-0.42792	-0.85577
C	1.21310	-0.42776	-0.85579
C	-0.00004	0.89896	0.88888
C	-2.56751	-0.23123	-0.17360
H	-1.16324	-1.41675	-1.32863
H	-1.07844	0.33392	-1.63797
C	2.56753	-0.23107	-0.17361
H	1.07842	0.33415	-1.63792

H	1.16332	-1.41655	-1.32875
H	-2.71782	-0.95696	0.63381
H	-3.35043	-0.37666	-0.93208
H	-2.67708	0.78400	0.23233
H	2.67702	0.78410	0.23249
H	3.35045	-0.37630	-0.93213
H	2.71791	-0.95693	0.63367
H	-0.88107	0.83482	1.53655
C	-0.00015	2.20422	0.08818
H	0.88102	0.83494	1.53651
H	-0.89244	2.29525	-0.54673
H	0.89216	2.29541	-0.54669
H	-0.00024	3.04578	0.79550



O-Attack-TS (DDQ **1a** + **2q**)

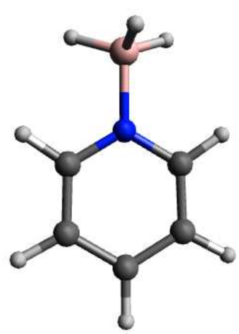
C	2.58610	1.52259	-0.11741
C	3.54388	0.48440	0.34640
C	3.07864	-0.92240	0.23446
C	1.83650	-1.24011	-0.28003
C	0.92609	-0.20407	-0.76477
C	1.32823	1.18351	-0.61087
O	4.65896	0.79115	0.79638
Cl	4.19017	-2.13277	0.78409
Cl	1.26947	-2.87576	-0.39766
O	-0.21014	-0.49162	-1.28997
C	0.39997	2.19083	-1.02826
N	-0.35739	3.02254	-1.36085
C	3.00979	2.88240	-0.02943
N	3.35683	4.00191	0.04443
H	-1.22015	-0.74777	-0.37733
H	-4.78290	-0.14394	-1.40112
H	-4.64092	-2.55084	-1.96551
H	-2.38920	1.38055	-0.81160
H	-5.21907	-2.35612	-0.29814
C	-4.35162	-2.22032	-0.95790
C	-3.93588	-0.75357	-1.06005
C	-3.19989	1.36207	-0.07530
H	-3.11696	-0.63063	-1.77964
H	-4.11323	1.72929	-0.56161
B	-2.06719	-0.82100	0.69590
H	-2.64062	3.24947	0.73941
N	-3.42645	-0.11881	0.23742
H	-1.97547	1.88341	1.66295
C	-2.85970	2.24424	1.12432
H	-3.53015	-2.85564	-0.60701
H	-2.20399	-2.00386	0.88532
H	-1.42389	-0.15496	1.47627
H	-3.70030	2.32436	1.82650
C	-4.42464	-0.30061	1.37609
H	-6.29774	-0.14502	0.24946
H	-4.49994	-1.37986	1.54615
C	-5.80299	0.31238	1.11649
H	-5.74725	1.39806	0.96237
H	-3.95764	0.14416	2.26219
H	-6.42680	0.12549	2.00166



C-Attack-TS (DDQ **1a** + **2q**)

O	1.81923	0.43517	2.75407
C	1.60258	0.55055	1.53946
C	2.35466	-0.31925	0.54107
Cl	3.35558	-1.53932	1.23390
C	2.27379	-0.13047	-0.81403
Cl	3.18413	-1.05134	-1.96444
C	1.42703	0.95467	-1.38073
O	1.49684	1.34140	-2.53694
C	0.36688	1.52724	-0.41636
C	-0.33697	2.68749	-0.93600
C	0.63775	1.49187	0.98722
C	-0.14632	2.25224	1.89476
N	-0.91221	3.62251	-1.34091
N	-0.81147	2.87922	2.63623
H	-0.57315	0.51938	-0.80398
B	-1.42912	-0.38373	-1.42664
H	-0.67343	-1.23967	-1.79918
H	-1.97100	0.32876	-2.22736
H	-3.81082	-2.99445	1.01403
H	-4.94540	-3.19244	-0.33930
H	-3.72181	1.32876	-1.51560
C	-4.31489	-2.46735	0.19338
H	-4.57842	1.86168	-0.05104
H	-4.96910	-1.69303	0.61482
H	-2.37069	1.07326	0.64406
C	-4.16807	0.98711	-0.57476
C	-3.13805	0.34649	0.35295
C	-3.31790	-1.88972	-0.81350
H	-4.99972	0.30505	-0.79528
H	-2.68189	-2.67694	-1.23275
H	-3.62409	-0.00910	1.27007
N	-2.36951	-0.84466	-0.23060
H	-3.83658	-1.39895	-1.64472
C	-1.53836	-1.42170	0.92031
H	-0.06792	-2.56992	-0.22999
H	-1.43579	-3.54075	0.38559
C	-0.76453	-2.70045	0.60593
H	-2.22912	-1.59218	1.75541
H	-0.85805	-0.61482	1.21690
H	-0.18421	-2.95924	1.50245

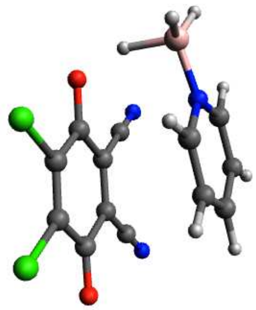
2r



Pyridine borane complex (**2r**)

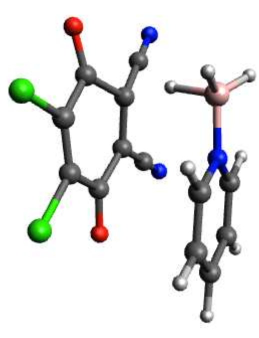
H	2.84075	-0.02310	1.21013
B	2.52934	0.00025	0.02030
N	0.90595	0.00054	-0.02150
C	0.21735	-1.16939	-0.01558
C	0.21652	1.16998	-0.01565
C	-1.17876	-1.20771	0.00419
C	-1.17965	1.20718	0.00408
H	2.89708	-1.01171	-0.56366
H	2.89652	1.03349	-0.52506
C	-1.89496	-0.00051	0.01380

H	0.82585	2.07059	-0.02841
H	-1.68628	-2.17061	0.00730
H	0.82715	-2.06975	-0.02912
H	-2.98448	-0.00086	0.02534
H	-1.68801	2.16965	0.00750



O-Attack-TS (DDQ **1a** + **2r**)

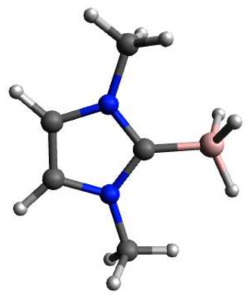
O	1.35639	2.87632	0.41209
C	1.00890	1.79561	-0.08318
C	1.90002	0.60668	-0.13348
Cl	3.47854	0.81892	0.54484
C	1.47908	-0.59466	-0.66361
Cl	2.48500	-2.00456	-0.68090
C	0.13899	-0.74707	-1.25322
O	-0.25677	-1.84592	-1.76286
C	-0.74772	0.41156	-1.23128
C	-2.04613	0.25613	-1.81527
C	-0.34791	1.62004	-0.67385
C	-1.21313	2.75557	-0.65667
N	-3.11202	0.13841	-2.29036
N	-1.93114	3.68392	-0.63116
H	-0.93871	-2.77850	-0.84687
B	-1.54107	-3.20170	0.29162
N	-1.55813	-1.87059	1.08371
C	-0.43577	-1.45277	1.74385
C	-2.64899	-1.04462	1.03409
C	-0.36784	-0.20352	2.35459
C	-2.64128	0.21049	1.63271
H	-0.73144	-3.98481	0.73339
H	-2.64534	-3.54173	-0.06133
C	-1.47913	0.65203	2.29058
H	-3.50576	-1.43501	0.49221
H	0.54844	0.09094	2.86166
H	0.38838	-2.16081	1.75941
H	-1.44542	1.63834	2.75099
H	-3.52737	0.83771	1.56475



C-Attack-TS (DDQ **1a** + **2r**)

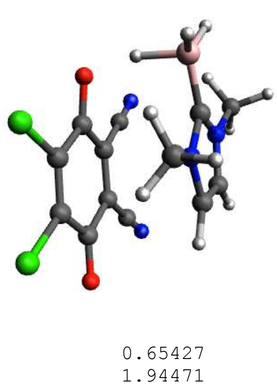
O	0.95723	-1.04463	-2.03888
C	0.24229	-0.31430	-1.34100
C	-1.08486	-0.81873	-0.80256
Cl	-1.44751	-2.46604	-1.16236
C	-1.95789	-0.01619	-0.11506
Cl	-3.50196	-0.55485	0.45048
C	-1.65031	1.42512	0.11687
O	-2.47879	2.24158	0.49211
C	-0.18774	1.82412	-0.10658
C	0.08489	3.23881	0.02891

C	0.61455	1.05632	-0.98857
C	1.84516	1.56109	-1.49487
N	0.31726	4.38056	0.14247
N	2.85725	1.98604	-1.91584
H	0.09989	1.43571	1.35877
B	0.57272	0.81595	2.46937
N	1.32708	-0.35386	1.79604
C	0.77384	-1.60340	1.74073
C	2.50748	-0.11304	1.14975
C	1.39273	-2.64142	1.05339
C	3.16655	-1.11202	0.43798
H	-0.40492	0.46118	3.07642
H	1.31095	1.67540	2.88759
C	2.60194	-2.39477	0.37997
H	2.89389	0.89837	1.23767
H	0.92278	-3.62176	1.03512
H	-0.16701	-1.72277	2.27091
H	3.09386	-3.18958	-0.17826
H	4.09760	-0.87530	-0.07142



1,3-dimethylimidazolylidene borane complex (**2t**)

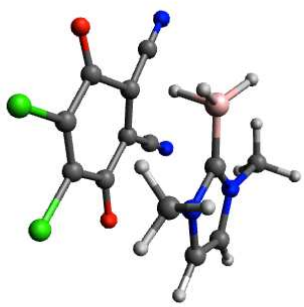
C	-0.77506	-1.52926	0.00510
C	0.59075	-1.60108	-0.00389
N	1.05577	-0.29302	-0.01367
C	0.02053	0.59907	-0.00517
N	-1.10376	-0.17745	0.00472
B	0.18969	2.20476	-0.00087
C	-2.48582	0.31302	0.00105
H	-1.53246	-2.30290	0.00727
H	-2.46180	1.40526	0.03714
H	-3.01470	-0.08163	0.87870
H	-2.99150	-0.02090	-0.91505
H	1.26339	-2.44945	-0.00743
C	2.46615	0.10283	0.00798
H	3.07738	-0.76553	-0.26184
H	2.73998	0.45928	1.01024
H	2.61612	0.91466	-0.71313
H	0.82722	2.51509	1.01380
H	-0.89847	2.77204	-0.02087
H	0.86294	2.51606	-0.99225



O-Attack-TS (DDQ **1a** + **2t**)

C	0.65427	0.02412	-2.19457
C	1.94471	0.35615	-1.82621
N	2.41924	-0.67207	-1.05722
C	1.47460	-1.67131	-0.93858
N	0.38886	-1.20518	-1.64666
C	-0.83415	-1.97744	-1.91501
H	-0.06151	0.55344	-2.81055
H	-0.96026	-2.72312	-1.12791

H	-0.73724	-2.47547	-2.88817
H	-1.68691	-1.29163	-1.92903
H	2.53875	1.23230	-2.05271
C	3.79189	-0.76125	-0.53262
H	4.20834	0.24954	-0.48927
H	4.39067	-1.39318	-1.20032
H	3.76334	-1.19785	0.46838
C	0.30025	1.72599	0.49046
C	-1.04644	1.84443	-0.12959
C	-1.97138	0.70465	0.11645
C	-1.58618	-0.40494	0.84035
C	-0.23688	-0.52050	1.41372
C	0.65866	0.61387	1.25044
O	-1.37371	2.84653	-0.78229
Cl	-3.56070	0.86588	-0.55869
Cl	-2.65697	-1.73658	1.13520
O	0.17130	-1.58485	1.98224
C	1.93420	0.53599	1.89199
N	2.97692	0.48994	2.42784
C	1.19012	2.82984	0.32265
N	1.92925	3.73060	0.17762
H	0.93472	-2.48151	1.02809
B	1.56130	-2.96938	-0.07389
H	2.66966	-3.25243	0.32343
H	0.81154	-3.86545	-0.40065



C-Attack-TS (DDQ **1a** + **2t**)

O	-0.43010	-1.08962	2.20967
C	-0.01384	-0.18608	1.46764
C	1.39811	-0.22403	0.92382
Cl	2.35131	-1.56536	1.44938
C	1.90501	0.74762	0.09961
Cl	3.53921	0.74432	-0.47857
C	1.08580	1.93242	-0.28777
O	1.54876	2.91552	-0.85316
C	-0.39768	1.83240	0.04485
C	-1.16609	3.02400	-0.23172
C	-0.83302	0.95341	1.06892
C	-2.12875	1.06167	1.63965
N	-1.80432	3.97934	-0.45937
N	-3.19654	1.15537	2.12419
H	-0.60747	1.09772	-1.34089
B	-0.83280	0.22223	-2.35946
H	0.20361	0.20528	-2.97947
H	-1.79461	0.75767	-2.86577
C	-0.81817	-2.95328	-0.30693
C	-2.09263	-2.49691	-0.04915
N	-2.25686	-1.33966	-0.77115
C	-1.12049	-1.04912	-1.48549
N	-0.23980	-2.05689	-1.17138
C	1.08144	-2.23079	-1.79519
H	-0.29006	-3.82408	0.05899
H	0.95358	-2.60710	-2.81750
H	1.65050	-2.94823	-1.19727
H	1.59747	-1.26777	-1.82288
H	-2.87333	-2.89542	0.58549
C	-3.52912	-0.60451	-0.85508
H	-3.89606	-0.40989	0.15787
H	-4.25260	-1.21377	-1.41149
H	-3.35602	0.33719	-1.38072