



TS	Reaction	k = A T ⁿ exp(-E _a /RT)		
		A	n	E _a
H-abs	p-benzoquinone + H → p-C ₆ H ₃ O ₂ + H ₂	1.01×10 ⁸	2.06	13156
	p-benzoquinone + CH ₃ → p-C ₆ H ₃ O ₂ + CH ₄	3.76×10 ¹	3.44	10314
	p-benzoquinone e + O → p-C ₆ H ₃ O ₂ + OH	3.56×10 ⁵	2.74	9384
	p-benzoquinone + OH → p-C ₆ H ₃ O ₂ + H ₂ O	4.73×10 ¹	3.47	-2005
TS ₁₋₁	p-C ₆ H ₃ O ₂ +C ₂ H ₂ → p-C ₆ H ₃ O ₂ CHCH	7.15×10 ⁴	2.31	1590
TS ₁₋₂	p-C ₆ H ₃ O ₂ CHCH → p-C ₆ H ₂ O ₂ CHCH ₂	4.24×10 ³	2.51	26260
TS ₁₋₃	p-C ₆ H ₂ O ₂ CHCH ₂ +C ₂ H ₂ → p-C ₆ H ₂ O ₂ C ₄ H ₅	2.11×10 ⁴	2.31	3050
TS ₁₋₄	p-C ₆ H ₂ O ₂ C ₄ H ₅ → p-NPhQ-H	3.94×10 ¹¹	0.06	1050
TS ₁₋₅	p-NPhQ-H → p-naphthoquinone +H	1.75×10 ¹¹	0.88	33140

Figure S3. Top panel: PES of the growth from p-benzoquinone to p-naphthoquinone via C₂H₂ addition. Barrier heights (in kcal/mol) at 0K calculated at the CBS-Q/CAM-B3LYP/6-311+G(2d,p) level of theory, including ZPE. **Bottom panel:** The corresponding rate constants (k) for a temperatures range of 500 to 2000 K computed at CBS-Q/CAM-B3LYP/6-311+G(2d,p) level of theory. Units are in cm, mol, s and cal.