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Oxidation of Mono-Phenols to *para*-Benzoquinones: a Comparative Study

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General procedure for the oxidations with H_2O_2 and Br_2

A solution of the phenol (1 mmol) and Br_2 (0.5 mmol) was added to a solution of H_2O_2 (30%, 0.2 mL, 4 mmol,) and concentrated H_2SO_4 (0.1 mL) in methanol (3 mL). The resulting mixture was refluxed for 2 hours, the total volume then reduced to eliminate excess of methanol, extracted with ether, and dried over anhydrous $MgSO_4$. The solvent was evaporated, and the *para*-benzoquinone product was isolated by flash chromatography on silica gel using as eluent a mixture of 9:1 hexane: ethyl acetate.

General procedure for the oxidations with IBX

The phenol (0.3 mol) was dissolved in 5.7 mL of anhydrous CH_2Cl_2 or anhydrous DMF, IBX (0.3 mol) was added, and the mixture stirred for 24 hours. The reaction mixture was diluted with EtOAc (20 mL), washed with water (10 mL), and this aqueous phase extracted with EtOAc (2 × 10 mL).The organic phase was washed with brine, dried over anhydrous $MgSO_4$ and concentrated.

Table S1. NMR spectral data and melting points of the *para*-benzoquinone products

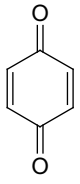
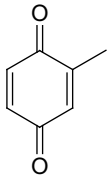
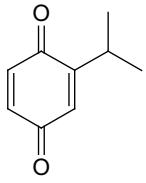
Product	^{1}H NMR ($CDCl_3$/TMS) δ, J(Hz)	^{13}C NMR ($CDCl_3$/TMS) δ	mp / °C	Lit. mp / °C
 **12**	6.79 (4H, s)	136.6, 187.2	110-114	113-115[16]
 **13**	1.90 (CH_3,s), 6.62 (CH, s), 6.75 (CH, d), 6.77 (CH, d)	15.8, 133.3, 136.4, 136.5, 145.9, 187.5, 187.7	65-68	67-70[26]
 **14**	1.14 ($2CH_3$, d, J 6.8 Hz), 3.05 (CH, dhept, J 6.8; 1.1 Hz), 6.55 (CH, m, J 1.1 Hz), 6.73 (CH, d, J 2.5 Hz), 6.74 (CH, d, J 2.5 Hz)	16.5, 26.2, 130.3, 135.9, 137.0, 154.9, 187.1, 188.1	57-60	54-58[16]

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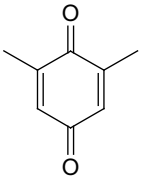
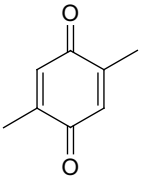
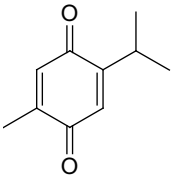
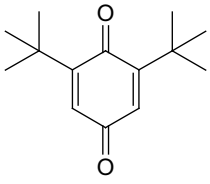
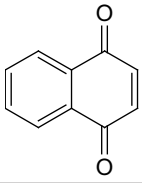
Table S1. (cont.)

Product	^{1}H NMR ($CDCl_3$/TMS) δ, J(Hz)	^{13}C NMR ($CDCl_3$/TMS) δ	mp / °C	Lit. mp / °C
 **15**	2.10 (6H, m), 6.56 (2H, m)	15.9, 133.3, 145.7, 187.1	69-72	71-73[27]
 **16**	2.04 (6H, d, *J* 1.6 Hz), 6.60 (2H, q, *J* 1.6 Hz)	15.6, 133.3, 145.7, 188.7	121-123	124-125[22]
 **17**	1.13 (6H, d, *J* 6.8 Hz), 2.04 (3H, d, *J* 1.6 Hz), 3.03 (1H, d hept, *J* 1.2 e 6.8 Hz), 6.52 (1H, d, *J* 1.2 Hz), 6.59 (1H, q, *J* 1.6 Hz).	15.3, 21.4, 26.5, 130.3, 133.8, 145.1, 154.9, 187.4, 188.5	47-48	45-47[20]
 **18**	1.28 (CH_3, s), 6.51 (CH, s)	29.3, 35.5, 130.1, 157.9, 188.7, 189.0	64-66	65-68[34]
 **19**	8.09 (2CH, aa′bb′), 7.77 (2CH, aa′bb′), 6.98 (2CH, s)	126.4, 133.9, 134.1, 138.7, 185.3	118-120	120-122[27]