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Supporting Information

For

Reactions of Primary and Secondary Amines with Substituted Hydroquinones: Nuclear Amination, Side-chain Amination and Indolequinone Formation

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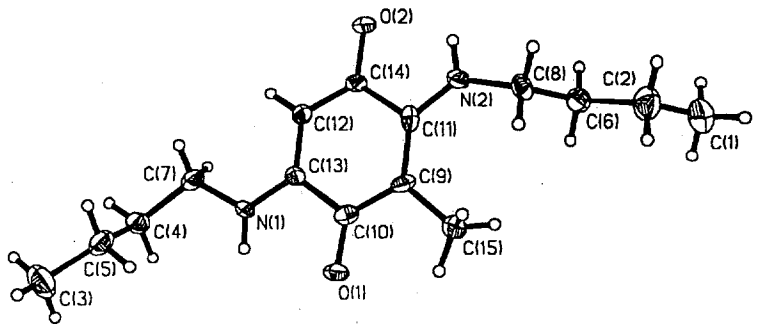
X-ray crystallographic data for



3,6-Bis(*n*-butylamino)toluquinone (7)

Table 1. Crystal data and structure refinement for C_{15} H_{24} N_2 O_2.

Formula weight	264.36
Temperature	293 K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	Pbca
Unit cell dimensions	a = 7.615(10) Å
	b = 16.04(3) Å
	c = 24.09(3) Å
Volume	2943(7) $Å^3$
Z	8
Density (calculated)	1.193 Mg/m^3
Absorption coefficient	0.079 mm^{-1}
F(000)	1152
Theta range for data collection	2.54 to 22.49°.
Index ranges	$-1 \le h \le 9$, $-1 \le k \le 19$, $-1 \le l \le 28$
Reflections collected	2571
Independent reflections	1921 [R_{int} = 0.1403]
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1913 / 0 / 172
Goodness-of-fit on F^2	1.020
Final R indices [$I>2\sigma(I)$]	R1 = 0.0890, wR2 = 0.1531
R indices (all data)	R1 = 0.2275, wR2 = 0.2152
Largest diff. peak and hole	0.243 and -0.260 $e.Å^{-3}$

Table 2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for C_{15} H_{24} N_2 O_2. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
O(1)	832(6)	1436(3)	4816(2)	27(1)
O(2)	-5741(6)	674(3)	5440(2)	28(2)
N(1)	-5440(8)	1626(4)	4590(2)	25(2)
N(2)	428(7)	510(4)	5704(2)	24(2)
C(1)	-742(10)	1289(5)	4935(3)	22(2)
C(2)	-1055(9)	735(5)	5439(3)	19(2)
C(3)	-2713(9)	536(5)	5600(3)	21(2)
C(4)	-4177(10)	832(5)	5306(3)	17(2)
C(5)	-3884(10)	1404(5)	4802(3)	22(2)
C(6)	-2197(10)	1592(5)	4636(3)	22(2)
C(7)	-5896(11)	2193(5)	4143(3)	28(2)
C(8)	-6240(10)	1784(5)	3589(3)	31(2)
C(9)	-6862(11)	2392(6)	3153(3)	45(3)
C(10)	-7206(12)	1990(6)	2596(3)	57(3)
C(11)	362(9)	10(5)	6214(3)	31(2)
C(12)	2147(9)	-48(5)	6501(3)	26(2)
C(13)	2807(10)	760(5)	6733(3)	33(2)
C(14)	4512(10)	666(6)	7061(3)	51(3)
C(15)	-1747(9)	2161(5)	4150(3)	32(2)

Table 3. Bond lengths [Å] and angles [°] for C_{15} H_{24} N_2 O_2.

O(1)-C(1)	1.255(8)	C(4)-C(5)	1.539(10)
O(2)-C(4)	1.260(8)	C(5)-C(6)	1.379(10)
N(1)-C(5)	1.339(9)	C(6)-C(15)	1.524(10)
N(1)-C(7)	1.452(8)	C(7)-C(8)	1.510(9)
N(2)-C(2)	1.346(8)	C(8)-C(9)	1.509(10)
N(2)-C(11)	1.468(8)	C(9)-C(10)	1.512(10)
C(1)-C(6)	1.407(10)	C(11)-C(12)	1.528(9)
C(1)-C(2)	1.525(10)	C(12)-C(13)	1.498(10)
C(2)-C(3)	1.359(9)	C(13)-C(14)	1.528(10)
C(3)-C(4)	1.402(9)		

C(5)-N(1)-C(7)	131.5(7)	N(1)-C(5)-C(6)	131.0(7)
C(2)-N(2)-C(11)	120.9(6)	N(1)-C(5)-C(4)	109.4(7)
O(1)-C(1)-C(6)	124.8(7)	C(6)-C(5)-C(4)	119.6(7)
O(1)-C(1)-C(2)	116.1(7)	C(5)-C(6)-C(1)	120.7(7)
C(6)-C(1)-C(2)	119.1(7)	C(5)-C(6)-C(15)	124.2(7)
N(2)-C(2)-C(3)	125.6(7)	C(1)-C(6)-C(15)	115.0(7)
N(2)-C(2)-C(1)	113.8(6)	N(1)-C(7)-C(8)	115.1(6)
C(3)-C(2)-C(1)	120.6(7)	C(7)-C(8)-C(9)	112.8(7)
C(2)-C(3)-C(4)	121.1(7)	C(10)-C(9)-C(8)	113.3(8)
O(2)-C(4)-C(3)	123.7(7)	N(2)-C(11)-C(12)	112.4(6)
O(2)-C(4)-C(5)	117.3(7)	C(13)-C(12)-C(11)	114.5(7)
C(3)-C(4)-C(5)	119.0(7)	C(12)-C(13)-C(14)	113.2(7)

Table 4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for $C_{15}\ H_{24}\ N_2\ O_2$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}\ U^{11} + \ldots + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
O(1)	16(3)	35(3)	28(3)	6(3)	4(3)	-2(3)
O(2)	17(3)	41(4)	25(3)	5(3)	6(3)	-3(3)
N(1)	18(4)	32(4)	25(4)	7(4)	2(3)	4(4)
N(2)	12(3)	38(4)	21(4)	6(4)	-1(3)	2(3)
C(1)	19(5)	23(5)	23(5)	-3(4)	7(4)	3(4)
C(2)	15(4)	25(5)	17(4)	-7(4)	3(4)	7(4)
C(3)	22(5)	28(5)	14(4)	6(4)	0(4)	-7(5)
C(4)	17(4)	19(5)	16(4)	-1(4)	0(4)	-10(4)
C(5)	26(5)	23(5)	17(4)	-5(4)	-6(4)	3(5)
C(6)	21(5)	25(5)	21(5)	3(4)	11(4)	2(4)
C(7)	27(5)	28(5)	28(5)	8(4)	-6(5)	7(5)
C(8)	27(5)	39(5)	26(5)	-6(4)	2(4)	4(5)
C(9)	50(6)	59(7)	27(5)	-3(5)	-8(5)	-2(6)
C(10)	44(7)	91(9)	36(6)	8(6)	-10(5)	4(6)
C(11)	29(5)	39(5)	24(5)	10(5)	8(4)	-1(5)
C(12)	21(4)	31(5)	25(5)	2(5)	1(4)	3(5)
C(13)	38(5)	36(6)	24(5)	3(5)	1(4)	-10(5)
C(14)	41(6)	58(7)	52(6)	1(6)	-16(5)	-18(6)
C(15)	23(5)	37(6)	37(5)	10(5)	-3(4)	-5(5)

Table 5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10 ^{3}) for C_{15} H_{24} N_2 O_2.

	x	y	z	U(eq)
H(1)	-6327(8)	1392(4)	4746(2)	30
H(2)	1428(7)	660(4)	5572(2)	28
H(3)	-2881(9)	199(5)	5909(3)	26
H(7A)	-4949(11)	2591(5)	4098(3)	33
H(7B)	-6937(11)	2502(5)	4250(3)	33
H(8A)	-7120(10)	1352(5)	3636(3)	37
H(8B)	-5169(10)	1519(5)	3461(3)	37
H(9A)	-7934(11)	2655(6)	3282(3)	54
H(9B)	-5983(11)	2824(6)	3108(3)	54
H(10A)	-7595(12)	2406(6)	2337(3)	86
H(10B)	-8096(12)	1570(6)	2635(3)	86
H(10C)	-6144(12)	1738(6)	2461(3)	86
H(11A)	-42(9)	-548(5)	6124(3)	37
H(11B)	-480(9)	256(5)	6467(3)	37
H(12A)	2065(9)	-450(5)	6800(3)	31
H(12B)	3000(9)	-257(5)	6236(3)	31
H(13A)	1914(10)	995(5)	6973(3)	39
H(13B)	2999(10)	1147(5)	6430(3)	39
H(14A)	4870(10)	1201(6)	7200(3)	76
H(14B)	5411(10)	446(6)	6824(3)	76
H(14C)	4326(10)	293(6)	7367(3)	76
H(15A)	-495(9)	2200(5)	4113(3)	48
H(15B)	-2226(9)	2706(5)	4216(3)	48
H(15C)	-2238(9)	1936(5)	3815(3)	48