

Supporting Material for

Modulating Spin Delocalization in Phenoxy Radicals Conjugated with Heterocycles,

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Experimental Details.

4-(2-Pyridyl)-2,6-di-*t*-butylphenol (5): 3,5-Di-*t*-butyl-4-(trimethylsilyloxy) phenylboronic acid[Satoh, Y., Shi, C. *Synthesis* **1994**, 1146] (352 mg, 1.1 mmol), palladium acetate (4.5 mg, 0.02 mmol), and potassium carbonate (414 mg, 3.0 mmol) were placed into a r.b. flask and subjected to three-fold freeze-pump-thaw purging under nitrogen. 2-Bromopyridine (158 mg, 1.0 mmol) was added by syringe, then 2.0 mL of reagent grade acetone and 2.0 mL of water, resulting in a yellow suspension. The suspension was heated at reflux for 8 h, cooled to room temperature, extracted with 3 × 10 mL of ethyl acetate, washed with brine, and dried over magnesium sulfate. The red solution was concentrated and purified by chromatography on silica gel, first with hexane to get rid of a colored impurity, then with 1:1 hexane-ethyl acetate. Combination of the UV-fluorescent fractions and removal of solvent gave 202 mg (71%) of white solid with mp 126-127 °C (lit¹ mp 126-127 °C). ¹H NMR (200 MHz, CDCl₃): δ 1.51 (s, 18 H), 5.39(s, 1 H), 7.12-7.18 (m, 1 H), 7.61-7.74 (m, 2 H), 7.80 (s, 2 H), 8.63-8.67 (m, 1 H). IR (KBr, cm⁻¹): 3632 (sharp, -OH), 2955 (s, C-H str), 1588, 1426.

4-(2-Pyridyl)-2,6-di-*t*-butylphenoxy (1): Phenol **5** (2.8 mg, 10 micromoles) was dissolved into 2 mL of dry benzene in a Schlenk tube under nitrogen. Lead dioxide (9.6 mg, 40 micromoles) was added afterward. The reaction turned red immediately, then turned into purple after stirring with lead dioxide for longer period. The color of the solution faded after overnight under nitrogen. UV-vis (PhH, ambient temp): 339 (strong), 496 nm. ESR (9.791 GHz, PhH): 1.83 (2 H), 1.41 (N), 0.52 (H), 0.63 (H), 1.94 (H), 2.08 (H), g = 2.0042 vs solid DPPH (g = 2.0037).

4-(5-Pyrimidyl)-2,6-di-*t*-butylphenol (6): 3,5-Di-*t*-butyl-4-(trimethylsilyloxy) phenylboronic acid (1.0 g, 3.14 mmol), 5-bromopyrimidine (0.46 g, 2.89 mmol), and potassium carbonate (1.34 g, 9.7 mmol) were placed into a r.b. flask. The reaction was purged with nitrogen, then 7.0 mL of acetone and 7.5 mL of water were added by syringe, resulting in a white suspension. The reaction mixture was subjected to threefold freeze-pump-thaw purging under nitrogen, then palladium acetate (13.5 mg, 0.06 mmol) in 0.5 mL of reagent grade acetone was added by syringe. The resulting yellow suspension was heated at reflux for 5 h, cooled to room temperature, extracted with 3 × 30 mL of ethyl acetate, washed with brine, and dried over magnesium sulfate. The organic solution was concentrated under vacuum without heating and purified by chromatography (silica gel, dichloromethane). Combination of the major product fractions and removal of solvent gave 0.50 g (61%) of white solid with mp 175-177 °C (lit¹ mp 181 °C). ¹H NMR (200 MHz, CDCl₃): δ 1.50 (s, 18H), 5.46 (s, 1H), 7.37 (s, 2H), 8.90 (s, 2H), 9.15 (s, 1H). IR (KBr, cm⁻¹): 3200-3600 (broad, -OH with H-bonding), 2959 (s, C-H str), 1560, 1408.

4-(5-Pyrimidyl)-2,6-di-*t*-butylphenoxy (2): Phenol **6** (2.8 mg, 10 micromoles) was dissolved into 2 mL of dry benzene in a Schlenk tube under nitrogen. Lead dioxide (12 mg, 50 micromoles) was added afterward and the mixture agitated. The reaction turned green immediately. The color of the solution faded after three days under nitrogen. UV-vis (PhH, ambient temp): 321 (strong), 428, 614 nm. ESR (9.791 GHz, PhH): 1.78 (2 H), 1.62 (2 H), 0.52 (2 N), 1.87 (2 H), g = 2.0041 vs solid DPPH (g = 2.0037).

3-(3',5'-Di-*t*-butyl-4'-hydroxyphenyl)furan (7): 3,5-Di-*t*-butyl-4-(trimethylsilyloxy)phenylboronic acid (352 mg, 1.1 mmol), 3-bromofuran (147 mg, 1.0 mmol), potassium carbonate (414 mg, 3.0 mmol), tetrakis(triphenylphosphine) palladium (60 mg, 0.05 mmol), 4 mL of dimethoxyethane and 2 mL of water were heated at reflux under argon overnight, then cooled to room temperature. The reaction was extracted with 3 × 30 mL of dichloromethane. The combined organic layers were washed with brine, dried over magnesium sulfate, evaporated to dryness, and purified by chromatography on silica gel using hexane as eluent. The product was obtained as 180 mg (66%) of white crystals with mp 102-103 °C. The product oxidized slowly in the air and turned yellow over several days. Analysis calculated for C₁₈H₂₄O₂: C 79.37, H 8.88. Found C 79.47 H 8.96. ¹H NMR (200 MHz, CDCl₃): δ 1.47 (s, 18 H), 5.22(s, 1 H), 6.50(m, 1 H), 7.29 (s, 2 H.), 7.45 (t, J = 2 Hz, 1 H), 7.63 (m, 1 H). IR (film on NaCl, cm⁻¹): 3622 (sharp, -OH), 2957 (s, C-H str), 879 (3-subst furan).

3-(3',5'-Di-*t*-butyl-4'-oxyphenyl)furan (3): Phenol **7** (2.7 mg, 10 micromoles) was dissolved into 2 mL of dry benzene in air. Lead dioxide (9.6 mg, 40 micromoles) was added afterward. The reaction turned yellow immediately, then turned red after stirring for a longer period. The solution was still red after four days in air. UV-vis (PhH, ambient temp): 398, 420 nm (strong). ESR (9.800 GHz, PhH): 1.62 (2H), 4.20 (H), 0.58 (H), 0.16 (H), $g = 2.0040$ vs solid DPPH ($g = 2.0037$).

3-(3',5'-Di-*t*-butyl-4'-hydroxyphenyl)thiophene (8): 3-Thiopheneboronic acid (Aldrich, 128 mg, 1.1 mmol), 4-bromo-2,6-di-*t*-butylphenol trimethylsilyl ether (357 mg, 1 mmol potassium carbonate (414 mg, 3 mmol), tetrakis(triphenylphosphine) palladium (60 mg, 0.05 mmol), 6 mL of dimethoxyethane, and 3 mL of water were heated at reflux under argon overnight, cooled to room temperature, and extracted with 3×30 mL of dichloromethane. The organic phase was washed with brine, dried over magnesium sulfate. Evaporated to dryness and purified by chromatography (silica gel) using petroleum ether (30-60 °C) as eluent. Got 126 mg white solid (44%), mp 107-108 °C. The product is oxidized slowly in the air. The product spot on TLC turned black red when standing in air for several hours. Analysis calculated for C₁₈H₂₄OS: C: 74.95 H 8.39 S 11.11. Found: C 74.67 H 8.20 S 10.92. ¹H NMR (200 MHz, CDCl₃): δ 1.48 (s, 18 H), 5.24(s, 1 H), 7.29-7.38 (m, 3 H), 7.39 (s, 2 H). IR (KBr, cm⁻¹): 3638 (sharp, -OH), 2956 (s, C-H str), 778 (3-subst thiophene).

3-(3',5'-Di-*t*-butyl-4'-oxyphenyl)thiophene (4): Phenol **8** (3.0 mg, 10 micromole) was dissolved in 2 mL of dry benzene in air. Lead dioxide (12 mg, 50 micromole) was added afterward and the mixture agitated. The reaction turned red immediately. The mixture was still red after one day in air. UV-vis (PhH, ambient temp): 359 (strong), 513, 555, 698 nm. ESR (9.798 GHz, PhH): 1.62 (2H), 3.3 (H), 0.83 (H), 0.27 (H), $g = 2.0043$ vs solid DPPH ($g = 2.0037$).

4-(5-Pyrimidyl)-2,6-di-*t*-butylphenol-CuCl₂ 1:1 complex: 4-(5-Pyrimidyl)-2,6-di-*t*-butylphenol (28.4 mg, 0.1 mmol) in 1.0 mL of ethanol was added into a solution of 17 mg (0.1 mmol) of copper(II) chloride dihydrate in 1.0 mL of ethanol at room temperature. In five minutes, a precipitate formed. After one hour the green solid was collected by vacuum filtration, washed with ethanol, and dried in vacuum to give 37.4 mg (90%) of green solid complex. Analysis calculated for C₁₈H₂₄CuCl₂N₂O : C: 51.62 H 5.78 N 6.69 Cu 15.17. Found: C 51.47 H 5.72 N 6.62 Cu 14.9, ¹H NMR (200 MHz, DMSO-d₆): δ 1.44 (s, 18 H), 7.36 (s, 2 H). IR (KBr, cm⁻¹): 3625 (sharp, -OH), 2958 (s, C-H str) 1593, 1415.

Gaussian Computational Archives for 1-4.

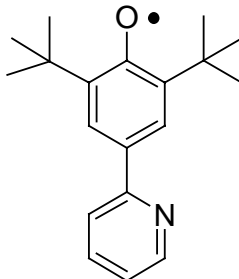
Radical 1:

Total atomic spin densities:

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2 C -0.043226
3 C 0.330084
4 C 0.225548
5 C 0.234887
6 C -0.094196
7 C -0.093944
8 H -0.010225
9 H -0.010662
10 H 0.002696
11 H 0.002483
12 C -0.055642
13 C 0.094748
14 N 0.057214
15 C 0.086787
16 C -0.031599
17 C -0.024176
18 H -0.004457
19 H -0.003864
20 H 0.001037
21 H 0.000774

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Sum of Mulliken spin densities= 1.00000

Atom	Isotropic Fermi Contact Couplings			
	a.u.	MegaHertz	Gauss	10(-4) cm-1
1 O(17)	0.03354	-20.33460	-7.25589	-6.78289
2 C(13)	-0.01494	-16.79363	-5.99239	-5.60175
3 C(13)	0.03216	36.15726	12.90181	12.06076
4 C(13)	0.01868	21.00353	7.49458	7.00602
5 C(13)	0.01949	21.91255	7.81895	7.30924
6 C(13)	-0.01470	-16.52343	-5.89597	-5.51162
7 C(13)	-0.01438	-16.16882	-5.76944	-5.39334
8 H	-0.00323	-14.45325	-5.15728	-4.82108
9 H	-0.00336	-15.01873	-5.35906	-5.00971
10 H	0.00078	3.49406	1.24677	1.16549
11 H	0.00084	3.73331	1.33214	1.24530
12 C(13)	-0.01156	-12.99055	-4.63535	-4.33318
13 C(13)	0.00872	9.80566	3.49890	3.27082
14 N(14)	0.00666	2.15067	0.76741	0.71739
15 C(13)	0.00810	9.10537	3.24902	3.03723
16 C(13)	-0.00495	-5.56750	-1.98662	-1.85712
17 C(13)	-0.00426	-4.79224	-1.70999	-1.59852
18 H	-0.00138	-6.17345	-2.20284	-2.05924
19 H	-0.00124	-5.52767	-1.97241	-1.84383
20 H	0.00031	1.38325	0.49358	0.46140
21 H	0.00021	0.92652	0.33060	0.30905

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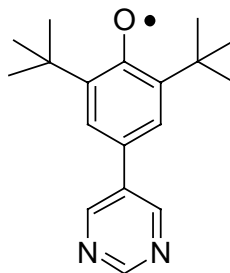
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Radical 2:

Total atomic spin densities:

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3	C	0.320559
4	C	0.240008
5	C	0.240008
6	C	-0.093576
7	C	-0.093576
8	H	-0.010843
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10	H	0.002701
11	H	0.002701
12	C	-0.047498
13	C	0.059379
14	C	0.060112
15	C	0.060112
16	N	-0.014473
17	N	-0.014473
18	H	-0.003355
19	H	-0.002217
20	H	-0.002217



Sum of Mulliken spin densities= 1.00000

Isotropic Fermi Contact Couplings

Atom	a.u.	MegaHertz	Gauss	10(-4) cm-1
1 O(17)	0.03534	-21.42217	-7.64396	-7.14567
2 C(13)	-0.01595	-17.92737	-6.39693	-5.97993
3 C(13)	0.03136	35.24903	12.57773	11.75781
4 C(13)	0.01994	22.41498	7.99823	7.47683
5 C(13)	0.01994	22.41498	7.99823	7.47683
6 C(13)	-0.01480	-16.64308	-5.93867	-5.55153
7 C(13)	-0.01480	-16.64308	-5.93867	-5.55153
8 H	-0.00345	-15.43095	-5.50615	-5.14721
9 H	-0.00345	-15.43095	-5.50615	-5.14721
10 H	0.00082	3.65704	1.30492	1.21986
11 H	0.00082	3.65704	1.30492	1.21986
12 C(13)	-0.01043	-11.72122	-4.18242	-3.90978
13 C(13)	0.00603	6.78264	2.42021	2.26244
14 C(13)	0.00875	9.84021	3.51123	3.28234
15 C(13)	0.00875	9.84021	3.51123	3.28234
16 N(14)	-0.00204	-0.65878	-0.23507	-0.21975
17 N(14)	-0.00204	-0.65878	-0.23507	-0.21975
18 H	-0.00107	-4.79080	-1.70948	-1.59804
19 H	-0.00087	-3.87730	-1.38352	-1.29333
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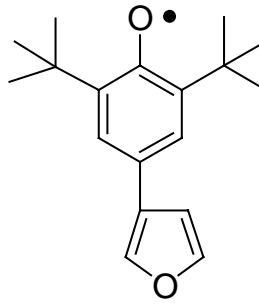
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Radical 3:

Total atomic spin densities:

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1	O	0.321985
2	C	-0.036287
3	C	0.313419
4	C	0.203974
5	C	0.229914
6	C	-0.085792
7	C	-0.081268
8	H	-0.009420
9	H	-0.010525
10	H	0.002358
11	H	0.002236
12	C	-0.048274
13	C	0.173537
14	C	0.017570
15	C	-0.003604
16	H	-0.008207
17	O	0.019507
18	H	-0.000865
19	H	-0.000258



Sum of Mulliken spin densities= 1.00000

Atom	Isotropic a.u.	Fermi Contact MegaHertz	Couplings Gauss	10(-4) cm-1
1 O(17)	0.03232	-19.59099	-6.99055	-6.53485
2 C(13)	-0.01391	-15.63943	-5.58054	-5.21675
3 C(13)	0.03013	33.86832	12.08506	11.29726
4 C(13)	0.01668	18.75234	6.69130	6.25511
5 C(13)	0.01907	21.43858	7.64982	7.15114
6 C(13)	-0.01385	-15.56676	-5.55461	-5.19251
7 C(13)	-0.01310	-14.73194	-5.25672	-4.91405
8 H	-0.00296	-13.24642	-4.72665	-4.41853
9 H	-0.00331	-14.81419	-5.28607	-4.94148
10 H	0.00067	3.01386	1.07542	1.00532
11 H	0.00064	2.87379	1.02544	0.95859
12 C(13)	-0.01098	-12.34728	-4.40582	-4.11861
13 C(13)	0.01585	17.82104	6.35899	5.94446
14 C(13)	0.00171	1.92495	0.68687	0.64210
15 C(13)	-0.00056	-0.63220	-0.22559	-0.21088
16 H	-0.00277	-12.37955	-4.41733	-4.12937
17 O(17)	0.00475	-2.88106	-1.02803	-0.96102
18 H	-0.00029	-1.29640	-0.46259	-0.43243
19 H	-0.00012	-0.51712	-0.18452	-0.17249

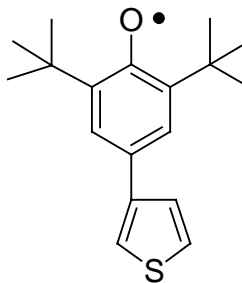
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Radical 4:

Total atomic spin densities:

Atom	Spin Density
1 O	0.327546
2 C	-0.037613
3 C	0.311753
4 C	0.228363
5 C	0.211055
6 C	-0.082239
7 C	-0.085254
8 H	-0.010398
9 H	-0.009680
10 H	0.002303
11 H	0.002305
12 C	-0.044737
13 C	0.142711
14 C	0.025491
15 C	-0.011123
16 H	-0.006614
17 S	0.037018
18 H	-0.001196
19 H	0.000309



Sum of Mulliken spin densities= 1.00000

Atom	Isotropic a.u.	Fermi Contact MegaHertz	Couplings Gauss	10 ⁽⁻⁴⁾ cm ⁻¹
1 O(17)	0.03300	-20.00346	-7.13773	-6.67244
2 C(13)	-0.01415	-15.90637	-5.67579	-5.30579
3 C(13)	0.03021	33.96666	12.12015	11.33006
4 C(13)	0.01875	21.08340	7.52308	7.03267
5 C(13)	0.01719	19.32620	6.89607	6.44652
6 C(13)	-0.01320	-14.84119	-5.29571	-4.95049
7 C(13)	-0.01371	-15.41142	-5.49918	-5.14070
8 H	-0.00327	-14.61460	-5.21485	-4.87490
9 H	-0.00304	-13.60766	-4.85555	-4.53903
10 H	0.00066	2.94110	1.04946	0.98104
11 H	0.00067	2.97667	1.06215	0.99291
12 C(13)	-0.01029	-11.56419	-4.12639	-3.85740
13 C(13)	0.01440	16.19148	5.77752	5.40089
14 C(13)	0.00347	3.90438	1.39318	1.30236
15 C(13)	-0.00155	-1.74524	-0.62274	-0.58215
16 H	-0.00212	-9.47397	-3.38055	-3.16018
17 S(33)	0.00323	1.11100	0.39643	0.37059
18 H	-0.00040	-1.80177	-0.64292	-0.60101
19 H	0.00008	0.34932	0.12465	0.11652

Test job not archived.

```

1\1\GINC-GROND\SP\UBLYP\6-31G(d)\C10H7O1S1(2)\LAHTI\02-Apr-2000\0\#P
DIRECT 6-31G(D) GFINPUT IOP(6/7=3) TEST UBLYP\3(4-phenoxy)-thiophene\
\0,2\O,0,-0.21986,0.121314,4.54634\C,0,-0.147547,0.099023,3.296633\C,0
,0.017923,0.048402,0.426447\C,0,0.206776,1.280053,2.524502\C,0,-0.4109
57,-1.110791,2.531071\C,0,-0.329431,-1.12193,1.163573\C,0,0.284981,1.2
42561,1.155469\H,0,0.399052,2.192877,3.080196\H,0,-0.664338,-2.004443,
3.093398\H,0,-0.505353,-2.049408,0.626332\H,0,0.529726,2.149989,0.6117
48\C,0,0.092476,0.027834,-1.031607\C,0,-0.48777,-0.940987,-1.833686\C,
0,0.773373,1.015956,-1.834091\C,0,0.69581,0.776123,-3.171774\H,0,-1.09
107,-1.7829,-1.524667\S,0,-0.221263,-0.660812,-3.51352\H,0,1.325372,1.
851529,-1.420601\H,0,1.131895,1.347376,-3.980023\Version=SGI-G98RevA.
3\HF=-858.4507103\S2=0.760483\S2-1=0.\S2A=0.750086\RMSD=2.121e-05\Dipo
le=0.1697932,0.0597847,-1.946228\PG=C01 [X(C10H7O1S1)]\ \@

```

Table S1. Crystal data and structure refinement for 2,6-di-*t*-butyl-4-(5-pyrimidyl)phenol, (**6**).

Identification code	2,6-di- <i>t</i> -butyl-4-(5-pyrimidyl)phenol, umass11z.	
Empirical formula	C ₁₈ H ₂₄ N ₂ O	
Formula weight	284.39	
Temperature	293(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	Pna2(1)	
Unit cell dimensions	$a = 12.118(1)$ Å	$\alpha = 90^\circ$.
	$b = 7.514(1)$ Å	$\beta = 90^\circ$.
	$c = 18.799(2)$ Å	$\gamma = 90^\circ$.
Volume	1711.8(2) Å ³	
Z	4	
Density (calculated)	1.104 Mg/m ³	
Absorption coefficient	0.534 mm ⁻¹	
F(000)	616	
Crystal size	0.25 x 0.46 x 0.29 mm ³	
Theta range for data collection	4.70 to 58.00°.	
Index ranges	0 ≤ h ≤ 13, -8 ≤ k ≤ 0, -1 ≤ l ≤ 20	
Reflections collected	1375	
Independent reflections	1324 [R(int) = 0.0075]	
Completeness to theta = 58.00°	100.0 %	
Absorption correction	Integration	
Max. and min. transmission	0.9044 and 0.8591	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	1324 / 1 / 194	
Goodness-of-fit on F ²	1.066	
Final R indices [I > 2σ(I)]	R1 = 0.0354, wR2 = 0.0915	
R indices (all data)	R1 = 0.0367, wR2 = 0.0928	
Absolute structure parameter	-0.2(4)	
Extinction coefficient	0.0069(7)	
Largest diff. peak and hole	0.161 and -0.146 e.Å ⁻³	

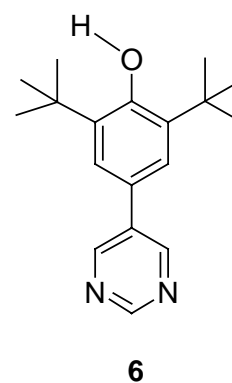


Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for *umass11z*. $U(\text{eq})$ is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	7868(2)	-390(3)	6368(1)	36(1)
O(1)	8410(2)	-1252(3)	6906(1)	54(1)
C(2)	7099(2)	985(4)	6490(1)	37(1)
C(2A)	6761(2)	1569(4)	7242(2)	48(1)
C(2B)	7769(3)	2241(5)	7667(2)	64(1)
C(2C)	6174(3)	44(5)	7632(2)	61(1)
C(2D)	5942(3)	3122(5)	7220(2)	80(1)
C(3)	6628(2)	1772(4)	5896(1)	36(1)
C(4)	6899(2)	1267(3)	5204(1)	33(1)
C(1')	6371(2)	2100(3)	4577(1)	33(1)
C(2')	5277(2)	2647(4)	4567(2)	40(1)
N(3')	4779(2)	3291(3)	3990(1)	46(1)
C(4')	5405(2)	3416(4)	3416(2)	45(1)
N(5')	6472(2)	3032(4)	3364(1)	50(1)
C(6')	6938(2)	2370(4)	3949(2)	44(1)
C(5)	7664(2)	-96(3)	5110(1)	35(1)
C(6)	8157(2)	-956(3)	5677(1)	33(1)
C(6A)	8977(2)	-2499(4)	5555(2)	42(1)
C(6B)	8562(3)	-4203(4)	5908(2)	63(1)
C(6C)	10127(2)	-2005(4)	5843(2)	58(1)
C(6D)	9117(3)	-2891(4)	4756(2)	64(1)

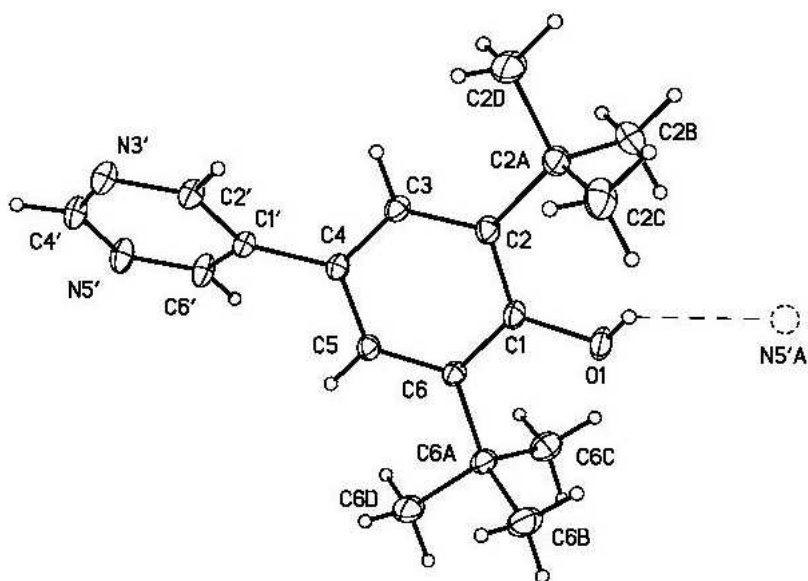
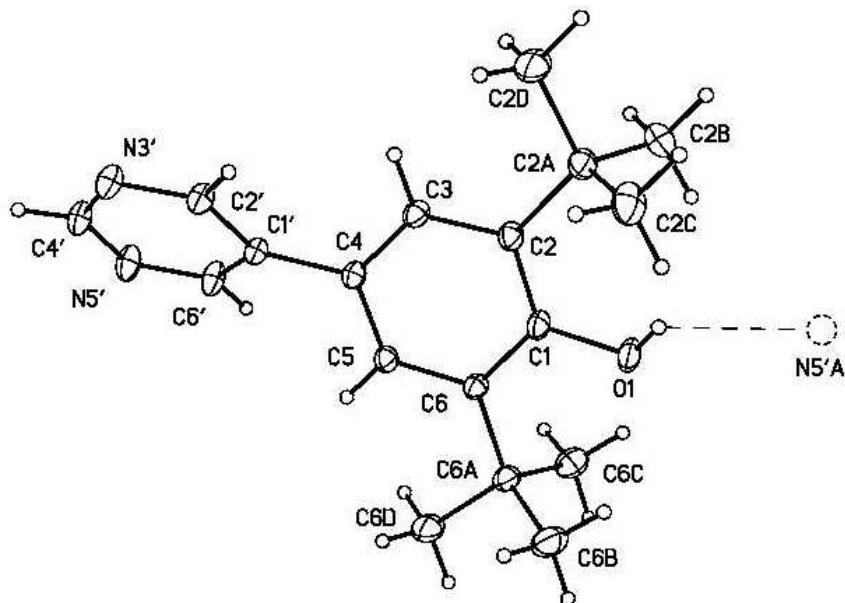


Table S3. Bond lengths [Å] and angles [°] for umass11z.

C(1)-O(1)	1.367(3)
C(1)-C(2)	1.410(4)
C(1)-C(6)	1.411(4)
C(2)-C(3)	1.387(4)
C(2)-C(2A)	1.535(4)
C(2A)-C(2D)	1.533(4)
C(2A)-C(2C)	1.535(5)
C(2A)-C(2B)	1.544(5)
C(3)-C(4)	1.394(4)
C(4)-C(5)	1.392(4)
C(4)-C(1')	1.480(4)
C(1')-C(6)	1.381(4)
C(1')-C(2')	1.388(4)
C(2')-N(3')	1.332(3)
N(3')-C(4')	1.321(4)
C(4')-N(5')	1.330(4)
N(5')-C(6')	1.333(4)
C(5)-C(6)	1.383(4)
C(6)-C(6A)	1.544(4)
C(6A)-C(6B)	1.527(4)
C(6A)-C(6C)	1.540(4)
C(6A)-C(6D)	1.541(5)



O(1)-C(1)-C(2)	122.9(2)
O(1)-C(1)-C(6)	114.7(2)
C(2)-C(1)-C(6)	122.3(2)
C(3)-C(2)-C(1)	117.0(2)
C(3)-C(2)-C(2A)	120.6(2)
C(1)-C(2)-C(2A)	122.4(2)
C(2D)-C(2A)-C(2C)	106.3(3)
C(2D)-C(2A)-C(2)	111.5(2)
C(2C)-C(2A)-C(2)	110.5(3)
C(2D)-C(2A)-C(2B)	106.1(3)
C(2C)-C(2A)-C(2B)	111.3(3)
C(2)-C(2A)-C(2B)	111.0(2)
C(2)-C(3)-C(4)	122.5(2)
C(5)-C(4)-C(3)	118.4(2)
C(5)-C(4)-C(1')	119.8(2)
C(3)-C(4)-C(1')	121.7(2)
C(6')-C(1')-C(2')	114.8(2)
C(6')-C(1')-C(4)	121.8(2)
C(2')-C(1')-C(4)	123.3(2)
N(3')-C(2')-C(1')	123.5(2)
C(4')-N(3')-C(2')	115.5(2)
N(3')-C(4')-N(5')	127.1(3)
C(4')-N(5')-C(6')	115.6(2)
N(5')-C(6')-C(1')	123.4(2)
C(6)-C(5)-C(4)	122.3(2)

C(5)-C(6)-C(1)	117.5(2)
C(5)-C(6)-C(6A)	121.0(2)
C(1)-C(6)-C(6A)	121.5(2)
C(6B)-C(6A)-C(6C)	110.4(3)
C(6B)-C(6A)-C(6D)	107.4(3)
C(6C)-C(6A)-C(6D)	106.8(3)
C(6B)-C(6A)-C(6)	110.7(2)
C(6C)-C(6A)-C(6)	110.4(2)
C(6D)-C(6A)-C(6)	111.1(2)

Symmetry transformations used to generate equivalent atoms:

Table S4. Anisotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for umass11z. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12}]$

	U ¹¹	U ²²	U ³³	U ²³	U ¹³	U ¹²
C(1)	39(1)	41(1)	28(1)	9(1)	-1(1)	4(1)
O(1)	62(1)	71(1)	30(1)	10(1)	-1(1)	31(1)
C(2)	38(1)	44(2)	30(1)	4(1)	3(1)	5(1)
C(2A)	52(2)	59(2)	33(2)	2(2)	6(1)	18(1)
C(2B)	85(2)	66(2)	40(2)	-8(2)	-3(2)	6(2)
C(2C)	55(2)	87(2)	42(2)	11(2)	12(2)	8(2)
C(2D)	96(3)	93(3)	49(2)	3(2)	17(2)	55(2)
C(3)	33(1)	39(1)	36(2)	5(1)	4(1)	9(1)
C(4)	32(1)	37(1)	31(1)	7(1)	0(1)	1(1)
C(1')	30(1)	36(1)	32(1)	6(1)	-2(1)	3(1)
C(2')	35(1)	47(1)	38(2)	9(1)	2(1)	6(1)
N(3')	34(1)	56(2)	46(1)	12(1)	-3(1)	6(1)
C(4')	41(2)	57(2)	38(2)	15(1)	-6(1)	4(1)
N(5')	40(1)	72(2)	38(1)	19(1)	0(1)	4(1)
C(6')	28(1)	65(2)	38(1)	18(1)	1(1)	5(1)
C(5)	39(1)	40(1)	26(1)	2(1)	2(1)	6(1)
C(6)	34(1)	34(1)	32(1)	4(1)	2(1)	4(1)
C(6A)	48(2)	37(1)	39(2)	2(1)	3(1)	12(1)
C(6B)	78(2)	40(2)	70(2)	8(2)	5(2)	6(2)
C(6C)	44(2)	59(2)	70(2)	0(2)	0(2)	17(1)
C(6D)	87(3)	56(2)	48(2)	-4(2)	10(2)	29(2)

Table S5. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($\text{\AA}^2 \times 10^3$) for umass11z.

	x	y	z	U(eq)
H(1A)	7980(30)	-1180(60)	7270(20)	81
H(2BA)	8311	1312	7697	95
H(2BB)	7540	2574	8137	95
H(2BC)	8083	3255	7431	95
H(2CA)	6657	-967	7658	92
H(2CB)	5516	-275	7378	92
H(2CC)	5983	421	8104	92
H(2DA)	5745	3453	7697	119
H(2DB)	5291	2767	6966	119
H(2DC)	6276	4119	6985	119
H(3A)	6111	2672	5962	43
H(2')	4870	2558	4985	48
H(4')	5060	3817	3004	55
H(6')	7683	2075	3934	52
H(5A)	7848	-439	4650	42
H(6BA)	9081	-5146	5826	94
H(6BB)	7860	-4523	5709	94
H(6BC)	8483	-4010	6410	94
H(6CA)	10626	-2977	5764	87
H(6CB)	10078	-1764	6343	87
H(6CC)	10393	-966	5600	87
H(6DA)	9628	-3855	4694	96
H(6DB)	9395	-1850	4520	96
H(6DC)	8416	-3213	4555	96

Table S6. Torsion angles [$^\circ$] for umass11z.

O(1)-C(1)-C(2)-C(3)	178.6(3)
C(6)-C(1)-C(2)-C(3)	0.1(4)
O(1)-C(1)-C(2)-C(2A)	-3.1(4)
C(6)-C(1)-C(2)-C(2A)	178.4(3)
C(3)-C(2)-C(2A)-C(2D)	-3.5(4)
C(1)-C(2)-C(2A)-C(2D)	178.3(3)
C(3)-C(2)-C(2A)-C(2C)	114.5(3)
C(1)-C(2)-C(2A)-C(2C)	-63.7(3)
C(3)-C(2)-C(2A)-C(2B)	-121.5(3)
C(1)-C(2)-C(2A)-C(2B)	60.3(4)
C(1)-C(2)-C(3)-C(4)	-0.8(4)
C(2A)-C(2)-C(3)-C(4)	-179.1(3)
C(2)-C(3)-C(4)-C(5)	0.8(4)
C(2)-C(3)-C(4)-C(1')	178.8(2)

C(5)-C(4)-C(1')-C(6)	-36.3(4)
C(3)-C(4)-C(1')-C(6)	145.8(3)
C(5)-C(4)-C(1')-C(2)	142.9(3)
C(3)-C(4)-C(1')-C(2)	-35.1(4)
C(6')-C(1')-C(2')-N(3)	3.7(4)
C(4)-C(1')-C(2')-N(3)	-175.6(2)
C(1')-C(2')-N(3')-C(4)	-1.2(4)
C(2')-N(3')-C(4')-N(5)	-2.6(5)
N(3')-C(4')-N(5')-C(6)	3.4(5)
C(4')-N(5')-C(6')-C(1)	-0.5(5)
C(2')-C(1')-C(6')-N(5)	-2.8(4)
C(4)-C(1')-C(6')-N(5)	176.5(3)
C(3)-C(4)-C(5)-C(6)	0.0(4)
C(1')-C(4)-C(5)-C(6)	-178.0(2)
C(4)-C(5)-C(6)-C(1)	-0.7(4)
C(4)-C(5)-C(6)-C(6A)	178.2(2)
O(1)-C(1)-C(6)-C(5)	-178.0(2)
C(2)-C(1)-C(6)-C(5)	0.6(4)
O(1)-C(1)-C(6)-C(6A)	3.1(4)
C(2)-C(1)-C(6)-C(6A)	-178.3(2)
C(5)-C(6)-C(6A)-C(6B)	-120.1(3)
C(1)-C(6)-C(6A)-C(6B)	58.8(4)
C(5)-C(6)-C(6A)-C(6C)	117.4(3)
C(1)-C(6)-C(6A)-C(6C)	-63.7(3)
C(5)-C(6)-C(6A)-C(6D)	-0.9(4)
C(1)-C(6)-C(6A)-C(6D)	178.0(3)

Symmetry transformations used to generate equivalent atoms:

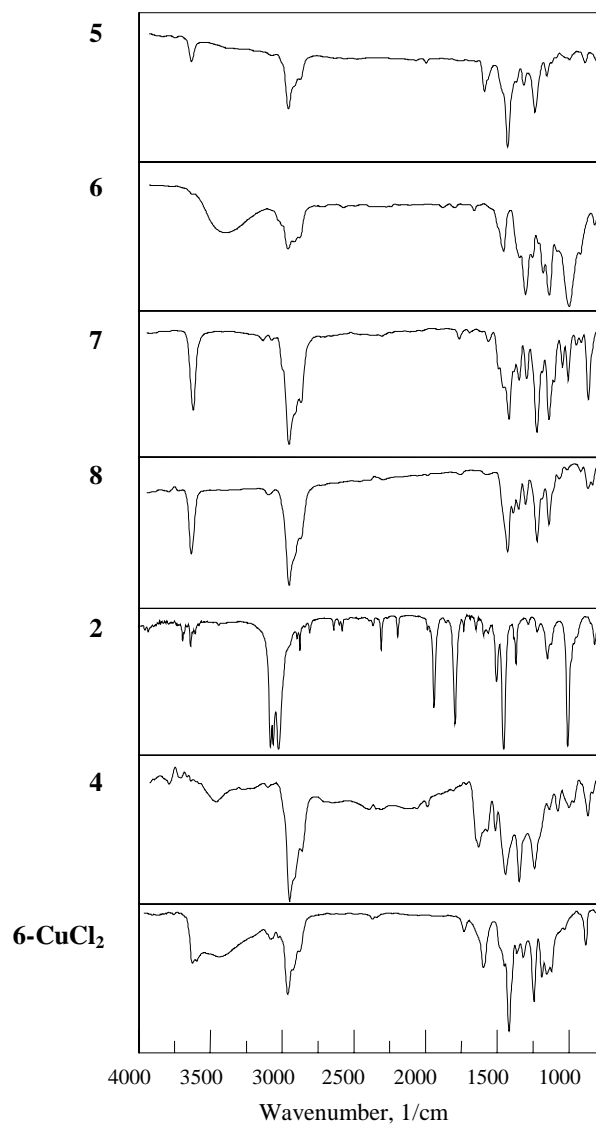
Table S7. Hydrogen bonds for umass11z [\AA and $^\circ$].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
O(1)-H(1A)...N(5')#1	0.85(4)	2.24(4)	2.797(3)	123(3)

Symmetry transformations used to generate equivalent atoms:

#1 -x+3/2,y-1/2,z+1/2

Figure S1. FTIR spectra for **5-8, 2, 4, 6-CuCl₂**.



All spectra are KBr pellets. The 3620 cm⁻¹ peak in the spectrum of **6-CuCl₂** is the sharp, -OH bond of 2,6-di-*t*-butylated phenols, superimposed on a residual hydrogen bonded -OH band.