Supporting Information

X-ray powder diffraction data. The powder patterns of 3- and 4-hydroxybenzoic acid were indexed as monoclinic using Checkcell.[1] The indexation of the lines is shown in Tables S1 and S2, where θ represents the diffraction angle, $\Delta 2\theta$ is the difference between the predicted and observed diffraction angle, and I/I^{o} is the normalized intensity.

Comparison between calculated and experimental bond distances and bond angles in 2-OHBA, 3-OHBA, and 4-OHBA. The experimental bond distances and angles found in the solid state[2-6] for 2-OHBA, 3-OHBA, and 4-OHBA, are compared in Table S3 with those computed for the most stable conformers (Figure 2) using the B3PW91/aug-cc-pVDZ and MPW1PW91/aug-cc-pVDZ models. Table S4 summarizes the structural data predicted by the same models for the corresponding carboxyphenoxyl radicals.

Combustion calorimetry. Detailed results of the combustion calorimetric experiments are shown in Tables S5 and S6, where m(3-OHBA) and m(4-OHBA) are the masses of 3- and 4-hydroxybenzoic acids, respectively; m(fuse) represents the mass of the cotton thread fuse; $n(HNO_3)$ is the amount of substance of nitric acid formed in the bomb process; $\Delta m(H_2O)$ represents the difference between the mass of water inside the calorimeter proper in each experiment and the average mass of water used in the calibration experiments (3751.99 g); ε^{i} and ε^{f} are the energy equivalents of the bomb contents in the initial and final states of the bomb process, respectively; T_i, and T_f represent the initial and final temperatures of the experiment; ΔT_c is the contribution to the observed temperature rise of the calorimeter proper due to the heat exchanged with the surroundings, the heat of stirring, and the heat dissipated by the temperature sensor; ΔU_{ign} is the electrical energy supplied for ignition of the sample; ΔU_{IBP} is the internal energy change associated with the bomb process under isothermal conditions, at 298.15 K; ΔU_{Σ} represents the sum of all corrections necessary to reduce ΔU_{IBP} to the standard state

(Washburn corrections);[7,8] $\Delta U(HNO_3)$ is the energy change associated with the formation of nitric acid; ΔU(fuse), ΔU(3-OHBA), and ΔU(4-OHBA), are the contributions of the cotton thread fuse and 3- and 4-hydroxybenzoic acids, respectively, to the energy of the isothermal bomb process; finally, $\Delta_c u^o$(3-OHBA) and $\Delta_c u^o$(4-OHBA) are the standard specific energies of combustion of 3- and 4-hydroxybenzoic acids.

The values of T_i, T_f , and ΔT_c were calculated by using a computer program[9] based on the Regnault-Pfaundler method,[10-12] and ΔU_{IBP} was derived from:[7]

$$\Delta U_{IBP} = [\varepsilon^o + \Delta m(H_2O)\, C^o_{p,m}(H_2O, l)](T_i - T_f + \Delta T_c) + \varepsilon^i(T_i - 298.15) + \varepsilon^f(298.15 - T_f + \Delta T_c) + \Delta U_{ign} \quad \text{(S1)}$$

The energy equivalent of the calorimeter was determined using the combustion of benzoic acid (NIST SRM 39j). The bomb contained 1.0 cm^3 of water and was charged with oxygen at a pressure p = 3.04 MPa. The standard massic energy of combustion of the benzoic acid sample under certificate conditions, –(26434±3) $J \cdot g^{-1}$, was corrected to the actual experimental conditions in each run as recommended in the certificate of analysis.[13] The value of ΔU_{ign} was calculated from:

$$\Delta U_{ign} = (V_i^2 - V_f^2) \cdot C / 2 \quad \text{(S2)}$$

where V_i and V_f stand for the potential of a condenser of capacitance C = 2990 μF, before and after its discharge through the platinum ignition wire, respectively.

The standard specific energies of combustion in Tables S5 and S6 refer to reaction:

$$C_7H_6O_3 \text{ (cr, monoclinic)} + 7O_2 \text{ (g)} = 7CO_2 \text{ (g)} + 3H_2O \text{ (l)} \quad \text{(S3)}$$

and were obtained from:

$$\Delta_c u^\circ = [\Delta U_{IBP} + \Delta U_\Sigma - \Delta U(HNO_3) - \Delta U(\text{fuse})]/m \quad \text{(S4)}$$

The standard state corrections, ΔU_Σ, were derived as recommended in the literature[7] by using the following heat capacity, density, and $-(\partial u/\partial p)_T$ data: for 3-OHBA, $C^\circ_{p,m}(\text{cr})$ = 1.17 J·K^{-1}·g^{-1},[14] ρ = 1.48 g·cm^{-3},[2] and $-(\partial u/\partial p)_T$ = 0.13 J·MPa^{-1}·g^{-1};[15] for 4-OHBA, $C^\circ_{p,m}(\text{cr})$ = 1.18 J·K^{-1}·g^{-1},[14] ρ = 1.50 g·cm^{-3},[16] and $-(\partial u/\partial p)_T$ = 0.13 J·MPa^{-1}·g^{-1}.[15] The values of $\Delta U(HNO_3)$ were based on –59.7 kJ·mol^{-1} for the molar internal energy of formation of HNO_3(aq) of concentration 0.1 mol·dm^{-3} from 5/4O_2 (g), 1/2N_2 (g), and 1/2H_2O.[17] The contribution from the cotton thread fuse of empirical formula $CH_{1.887}O_{0.902}$, ΔU(fuse), was calculated by using and $\Delta_c u^\circ$ = –(16565.9±8.6) J·g^{-1}.[18]

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TABLE S1: Powder Pattern Indexation for 3-OHBA; $P2_1/b$, with a = 550.3(2) pm, b = 2392.9(5) pm, c = 496.0(1) pm, β = 105.67°.

h k l	2θ / °	10^2 (I/I^o)	$\Delta 2\theta$ / °
0 0 2	7.670	0.115	0.002
0 0 4	15.380	0.029	0.010
-1 0 2	16.390	0.510	-0.014
1 0 0	16.725	0.847	0.007
0 1 1	18.305	0.023	0.024
-1 0 4	19.445	0.464	0.002
1 0 2	20.230	0.128	-0.004
0 1 3	21.315	0.039	0.008
0 1 4	23.670	0.757	0.018
-1 1 1	24.130	0.113	-0.015
-1 0 6	24.635	0.232	-0.030
-1 1 3	25.155	0.062	-0.003
-1 1 4	26.535	1	0.010
1 1 2	27.150	0.061	0.030
-1 1 5	28.390	0.381	0.017
1 1 3	29.100	0.047	-0.017
0 1 6	29.415	0.052	0.024
-1 1 6	30.650	0.163	0.027
0 0 8	31.025	0.093	-0.001
1 1 4	31.490	0.045	-0.001
1 0 6	32.250	0.017	0.002
0 1 7	32.610	0.015	-0.014

TABLE S2: Powder Pattern Indexation for 4-OHBA; $P2_1/a$, with a = 1845.6(1) pm, b = 523.2(4) pm, c = 634.4(8) pm, β = 93.45º.

h k l	2θ / º	10^2 (I/I^o)	$\Delta 2\theta$ / º
2 0 0	9.675	0.017	0.075
0 0 1	13.965	0.012	0.003
-2 0 1	16.550	0.009	0.066
2 0 1	17.475	0.622	0.030
1 1 0	17.665	0.890	0.027
4 0 0	19.355	0.162	0.086
2 1 0	19.545	0.287	0.018
0 1 1	22.030	0.087	-0.006
3 1 0	22.310	0.127	-0.025
-4 0 1	23.175	0.014	0.004
-2 1 1	23.760	0.038	0.021
4 0 1	24.550	1	-0.008
-3 1 1	26.015	0.053	0.056
3 1 1	26.870	0.383	-0.034
-2 0 2	29.205	0.049	-0.019
4 1 1	29.970	0.599	-0.029
-6 0 1	31.515	0.018	-0.082
-5 1 1	32.210	0.013	-0.060

TABLE S3: Calculated and Experimental Bond Distances (in pm) and Bond Angles (in degrees) for 2-, 3-, and 4-OHBA.

	B3PW91/ aug-cc-pVDZ	MPW1PW91/ aug-cc-pVDZ	Experimental (solid)[a]
		2-OHBA	
C1–C2	141.9	141.5	140.3±0.8
C2–C3	140.4	140.2	140.4±0.9
C3–C4	138.7	138.5	137.7±1.0
C4–C5	140.4	140.2	140.8±1.1
C5–C6	138.5	138.3	136.4±0.9
C6–C1	140.8	140.6	140.8±0.8
C1–C7	146.2	146.0	146.8
C7–O2	123.1	122.8	123.1
C7–O1	134.6	134.2	130.0
C2–O3	133.9	133.6	136.0
O1–H1	96.9	96.7	98.6
O3–H2	98.8	98.5	95.4
O2---H2	170.4	170.3	176.6
O2---O3	259.3	258.9	260.8
C1–C2–C3	119.2	119.2	119.5
C2–C3–C4	120.1	120.1	120.3
C3–C4–C5	121.1	121.2	120.5
C4–C5–C6	119.3	119.2	119.5

C5–C6–C1	120.8	120.8	121.2
C6–C1–C2	119.5	119.6	119.1
H–C3–C2	118.3	118.3	116.1
H–C4-C3	119.2	119.2	119.1
H–C5–C4	120.4	120.4	121.2
H–C6–C5	120.5	120.5	122.1
C7–C1–C2	118.5	118.5	119.7
O2–C7–C1	124.3	124.3	123.0
O1–C7–C1	115.1	115.1	116.0
H1–O1–C7	106.3	106.4	112.4
O1–C7–O2	120.7	120.7	121.0
H2–O3–C2	106.8	107	107.6
O3–C2–C3	118.3	118.3	117.7
O2---H2–O3	147.8	147.6	145.4

3-OHBA

C1–C2	140.0	139.8	139.8±0.3
C2–C3	139.4	139.1	137.8±0.3
C3–C4	140.0	139.8	138.5±0.3
C4–C5	139.3	139.1	138.6±0.3
C5–C6	139.5	139.3	138.5±0.4
C6–C1	139.9	139.7	138.4±0.3
C1–C7	148.6	148.3	148.9±0.3
C7–O2	121.4	121.1	126.9±0.3
C7–O1	135.4	135.0	126.1±0.2
C3–O3	136.4	136.1	138.9±0.2
O1–H1	96.9	96.7	115.0±4.0

O3–H2	96.4	96.2	84.2±4.0
C1–C2–C3	119.8	119.7	118.8±0.2
C2–C3–C4	120.1	120	121.1±0.2
C3–C4–C5	119.7	119.7	119.5±0.2
C4–C5–C6	120.9	120.8	120.6±0.2
C5–C6–C1	119.1	119	119.2±0.2
C6–C1–C2	120.5	120.6	120.9±0.2
H–C2–C3	121.5	121.5	123±2
H–C4–C3	121.3	119	119±2
H–C5–C4	119.3	119.3	120±2
H–C6–C5	120.8	120.8	121±2
C7–C1–C2	117.3	117.2	118.8±0.2
O2–C7–C1	124.8	124.8	118.2±0.2
O1–C7–C1	113.3	113.3	118.2±0.2
H1–O1–C7	105.9	106	115±2
O1–C7–O2	121.9	121.9	123.6±0.2
H2–O3–C3	109.4	109.5	105±2
O3–C3–C2	122.7	122.7	121.4±0.2
		4-OHBA	
C1–C2	140.1	139.9	138.6±0.2
C2–C3	138.9	138.7	138.3±0.2
C3–C4	140.1	139.9	138.0±0.2
C4–C5	140.0	139.8	138.0±0.2
C5–C6	138.9	138.7	138.2±0.2
C6–C1	140.4	140.1	138.6±0.2

C1–C7	147.8	147.6	148.0±0.2
C7–O2	121.5	121.2	126.6±0.2
C7–O1	135.7	135.3	126.6±0.2
C4–O3	135.9	135.6	137.7±0.2
O1–H1	96.9	96.7	83.1
O3–H2	96.4	96.2	87.4
C1–C2–C3	120.6	120.6	120.7±0.2
C2–C3–C4	119.7	119.7	119.2±0.2
C3–C4–C5	120.3	120.3	121.4±0.1
C4–C5–C6	119.6	119.6	119.2±0.2
C5–C6–C1	120.7	120.6	120.8±0.2
C6–C1–C2	119.2	119.2	119.1±0.1
H–C2–C3	120.7	120.7	121.3
H–C3–C4	120.1	120.3	119.0
H–C5–C4	119.1	119	118.3
H–C6–C5	119.7	119.8	120.2
C7–C1–C2	118.3	118.3	120.1±0.1
O2–C7–C1	125.1	125	118.2±0.1
O1–C7–C1	113.2	113.2	118.6±0.2
H1–O1–C7	105.7	105.8	113.6
O1–C7–O2	121.7	121.7	123.2±0.2
H2–O3–C4	109.6	109.7	108.4
O3–C4–C3	122.5	122.4	121.4±0.1

[a]2-OHBA, neutron diffraction, References 4-6; 3-OHBA, X-ray diffraction, References 2, 5, 6; 4-OHBA, X-ray diffraction, References 2, 5, 6.

TABLE S4: Calculated Bond Distances (in pm) and Bond Angles (in degrees) in the Carboxyphenoxyl Radicals.

	B3PW91/ aug-cc-pVDZ	MPW1PW91/ aug-cc-pVDZ
	2-HOOCPhO•	
C1–C2	146.1	145.8
C2–C3	145.0	144.8
C3–C4	137.5	137.3
C4–C5	141.2	141.0
C5–C6	140.7	140.5
C6–C1	138.1	137.9
C1–C7	150.7	150.5
C7–O1	133.2	132.8
C7–O2	121.1	120.9
C2–O3	126.0	125.7
O1–H1	99.2	98.9
O1---O3	260.1	259.9
C1–C2–C3	118.1	118.2
C2–C3–C4	120.8	120.7
C3–C4–C5	119.9	119.9
C4–C5–C6	120.9	120.9
C5–C6–C1	121.0	120.9
C6–C1–C2	119.3	119.3
H–C3–C2	116.9	116.8

H–C4-C3	120.4	120.4
H–C5–C4	119.6	119.6
H–C6–C5	120.9	120.9
C7–C1–C2	122.5	122.3
O2–C7–C1	121.3	121.2
O1–C7–C1	116.2	116.3
H1–O1–C7	108.1	108.2
O1–C7–O2	122.5	122.5
O3–C2–C3	120.2	120.2
O1-H1-O3	152.2	152.0

3-HOOCPhO$^{\bullet}$

C1–C2	138.4	138.2
C2–C3	144.9	144.6
C3–C4	145.1	144.8
C4–C5	137.9	137.7
C5–C6	140.8	140.6
C6–C1	141.3	141.0
C1–C7	149.1	148.9
C7=O2	121.0	120.8
C7–O1	135.3	134.9
C3–O3	125.5	125.3
O1–H1	96.9	96.7
C1–C2–C3	120.8	120.8
C2–C3–C4	117.3	117.3
C3–C4–C5	120.8	120.8

C4–C5–C6	120.5	120.4
C5–C6–C1	120.6	120.5
C6–C1–C2	120.1	120.2
H–C2–C3	118.4	118.5
H–C4–C3	117.2	117.2
H–C5–C4	120.3	120.3
H–C6–C5	120.0	120.1
C7–C1–C2	118.2	118.2
O2–C7–C1	124.7	124.6
O1–C7–C1	112.8	112.8
H1–O1–C7	106.2	106.3
O1–C7–O2	122.6	122.6
O3–C3–C2	121.2	121.2

4-HOOCPhO$^{\bullet}$

C1–C2	141.6	141.4
C2–C3	137.3	137.2
C3–C4	145.5	145.2
C4–C5	145.5	145.2
C5–C6	137.5	137.3
C6–C1	141.6	141.4
C1–C7	148.5	148.3
C7–O2	121.3	121.0
C7–O1	135.2	134.9
C4–O3	125.1	124.9
O1–H1	96.9	96.7

C1–C2–C3	120.3	120.2
C2–C3–C4	120.8	120.8
C3–C4–C5	117.2	117.3
C4–C5–C6	121.0	120.9
C5–C6–C1	120.1	120.0
C6–C1–C2	120.6	120.7
H–C2–C3	121.5	121.6
H–C3–C4	117.2	117.2
H–C5–C4	117.2	117.1
H–C6–C5	120.7	120.7
C7–C1–C2	117.6	117.6
O2–C7–C1	124.3	124.3
O1–C7–C1	113.1	113.2
H1–O1–C7	106.3	106.4
O1–C7–O2	122.5	122.5
O3–C4–C3	121.5	121.4

TABLE S5: Results of the Combustion Experiments on Monoclinic 3-Hydroxybenzoic acid (3-OHBA).[a]

Exp. Nr.	1	2	3	4	5	6
m(3-OHBA)/g	0.97327	1.08931	1.03899	0.99402	0.88144	0.95671
m(fuse)/mg	1.7791	2.1504	1.7681	1.9414	2.3111	1.6682
$n(HNO_3)\cdot 10^5$/mol	2.3	1.5	0.7	1.3	0.7	1.3
$\Delta m\ (H_2O)$/g	+ 1.69	- 0.10	+ 0.44	- 1.42	- 0.73	- 1.35
ε^{i}/J·K^{-1}	15.58	15.71	15.65	15.60	15.47	15.56
ε^{f}/J·K^{-1}	16.44	16.69	16.58	16.49	16.26	16.41
T_i/K	298.0455	298.0124	297.9731	298.0171	298.0711	298.0268
T_f/K	299.2446	299.3516	299.2537	299.2399	299.1681	299.2110
$\Delta T_c\cdot 10^2$/K	5.23	5.51	5.57	5.04	5.74	5.54
ΔU_{ign}/J	0.63	0.64	0.58	0.51	0.52	0.57
$-\Delta U_{IBP}$/J	21315.63	23857.77	22758.90	21775.37	19311.10	20954.67
ΔU_{Σ}/J	18.50	21.01	19.91	18.95	16.57	18.15
$\Delta U(HNO_3)$/J	1.37	0.90	0.42	0.78	0.42	0.78
$-\Delta U_{fuse}$/J	29.47	35.62	29.29	32.16	38.29	27.64
ΔU(3-OHBA)/J	21266.29	23800.24	22709.28	21723.48	19255.82	20908.10
$-\Delta_c u^{o}$(3-OHBA)/J·g^{-1}	21850.35	21848.91	21857.07	21854.17	21845.85	21854.17

[a] Average: $\Delta_c u^{o}$(3-OHBA) = -(21851.75 ± 1.68) J·g^{-1}

TABLE S6: Results of the Combustion Experiments on Monoclinic 4-Hydroxybenzoic acid (4-OHBA).[a]

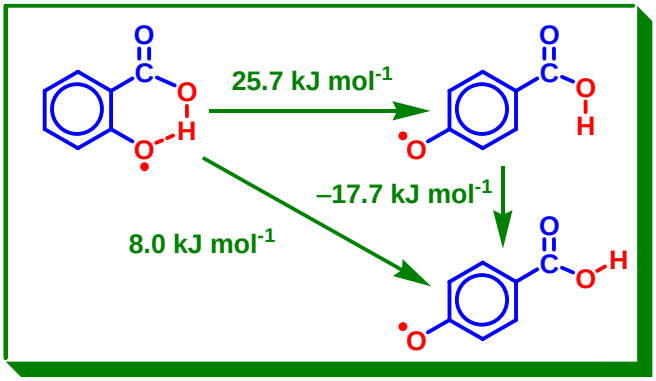
Exp. Nr.	1	2	3	4	5	6
m(4-OHBA)/g	1.13426	1.00069	0.88068	1.29768	1.15069	1.18417
m(fuse)/mg	2.17	2.14	1.97	2.22	1.67	1.98
$n(HNO_3)\cdot 10^5$/mol	2.2	1.9	1.3	1.9	1.7	2.1
$\Delta m\ (H_2O)$/g	- 0.33	+ 0.36	+ 0.73	- 0.86	+ 3.67	- 0.15
ε^{i}/J·K^{-1}	15.76	15.60	15.46	15.95	15.77	15.81
ε^{f}/J·K^{-1}	16.78	16.50	16.25	17.12	16.81	16.88
T_i/K	297.8486	298.0539	297.9978	298.0298	298.0625	298.0187
T_f/K	299.3984	299.2857	299.0930	299.5999	299.4151	299.4645
$\Delta T_c\cdot 10^2$/K	4.29	5.33	5.77	4.20	5.90	5.17
ΔU_{ign}/J	0.58	0.57	0.63	0.58	0.59	0.61
$-\Delta U_{IBP}$/J	24814.88	21895.98	19278.14	28387.38	25170.08	25900.72
ΔU_{Σ}/J	22.00	19.10	16.55	25.67	22.36	23.11
$\Delta U(HNO_3)$/J	1.31	1.13	0.78	1.10	1.01	1.25
$-\Delta U_{fuse}$/J	35.95	35.48	32.59	36.81	27.59	32.72
ΔU(4-OHBA)/J	24755.62	21840.27	19228.22	28323.80	25119.12	25843.64
$-\Delta_c u^{o}$(4-OHBA)/J·g^{-1}	21826.50	21825.21	21833.38	21826.49	21829.62	21824.27

[a] Average: $\Delta_c u^{o}$(4-OHBA) = -(21827.58 ± 1.37) J·g^{-1}

TABLE S7: Total Energies at 298.15 K, thermal corrections ($ZPE+E_v+E_{rot}+E_t$) and ZPE from the Calculations. Data in hartree.[a,b]

	B3PW91/aug-cc-pVDZ	MPW1PW91/aug-cc-pVDZ	MPW1PW91/aug-cc-pVTZ// MPW1PW91/aug-cc-pVDZ	CBS-QMPW1[c]
C_6H_6	-232.079655	-232.110632	-232.163817	-231.783871
	0.104652	0.105209		
	0.100223	0.100752		
C_6H_5OH	-307.283393	-307.324608	-307.394924	-306.931559
	0.110069	0.110744		
	0.104546	0.105244		
C_6H_5COOH	-420.597749	-420.655584	-420.750256	-420.146613
	0.122658	0.123362		
	0.115533	0.116261		
2-OHBA	-495.812339	-495.880459	-495.992165	-495.303844
	0.128498	0.129344		
	0.120745	0.121632		
3-OHBA	-495.801718	-495.869688	-495.981556	-495.295664
	0.128113	0.128974		
	0.119833	0.120757		
4-OHBA	-495.803612	-495.871614	-495.983494	-495.296165
	0.128215	0.129042		
	0.119970	0.120844		
$C_6H_5O^{\bullet}$	-306.649382	-306.691662	-306.7598663	-306.297144
	0.096566	0.097084		
	0.091237	0.091780		
2-HOOCPhO$^{\bullet}$, **1**	-495.168696	-495.237588	-495.347478	-494.661100
	0.114773	0.115495		
	0.107041	0.107802		
3-HOOCPhO$^{\bullet}$	-495.164127	-495.233236	-495.343006	-494.656357
	0.114486	0.115162		
	0.106392	0.107113		
4-HOOCPhO$^{\bullet}$, **3**	-495.165537	-495.234556	-495.344322	-494.658857
	0.114543	0.115215		
	0.106442	0.107158		
2		-495.227812		

[a] 1 hartree = 2625.5000 kJ·mol^{-1}. [b] For each species the values of the thermal corrections ($ZPE+E_v+E_{rot}+E_t$) and of ZPE are given in the second and third lines, respectively. [c] In the CBS-QMPW1 procedure geometries and frequencies are based on MPW1PW91/aug-cc-pVDZ calculations (see main text).



Graphic TOC