Supporting Information

TABLE 1S: B3LYP/6-311++G(3df,2pd) calculated OH bond lengths and bond length differences relative to the shortest OH bond for the resorcinol rotamers.

Bond	r/Å	Δr/ Å	Δr/fm
IA	0.96169675	2.7586×10^{-4}	27.586
IB	0.96161586	1.9497×10^{-4}	19.497
II	0.96156752	1.4663×10^{-4}	14.663
III	0.96142089	0	0

TABLE 2S: Observed and calculated OH-stretching local mode parameters (cm^{-1}) for the resorcinol rotamers.

Parameter[a]	IA		IB		II		III
	obsd	calcd	obsd	calcd	obsd	calcd	calcd
$\tilde{\omega}$	3821.5±2.7	3823.9	3819.9±1.3	3825.9	3819.6±1.4	3826.5	3827.0
$\tilde{\omega}x$	83.71±0.65	83.96	83.10±0.32	84.38	83.00±0.33	84.66	84.14

[a]Scaling factors of 0.995771 and 0.8600 were applied to $\tilde{\omega}$ and $\tilde{\omega}x$, respectively. The local mode parameters were calculated at the B3LYP/6-311++G(3df,2pd) level of theory.

TABLE 3S: Observed and calculated OH-stretching local mode parameters (cm^{-1}) for the hydroquinone rotamers.

Parameter[a]		*cis*	*trans*
	obsd	calcd	calcd
$\tilde{\omega}$	3829.2±0.3	3832.3	3831.9
$\tilde{\omega}x$	84.02±0.30	86.09	86.02

[a]Scaling factors of 0.995771 and 0.8600 were applied to $\tilde{\omega}$ and $\tilde{\omega}x$, respectively. The local mode parameters were calculated at the B3LYP/6-311++G(3df,2pd) level of theory.

TABLE 4S: Calculated OH-stretching transition wavenumbers (cm^{-1}) and oscillator strengths for the resorcinol rotamers.[a]

Δv_{OH}	IA		IB		II		III	
	freq.	*f*	freq.	*f*	freq.	*f*	freq.	*f*
1	3655	8.2×10^{-6}	3658	8.8×10^{-6}	3658	1.7×10^{-5}	3658	1.5×10^{-5}
2	7143	7.1×10^{-7}	7147	7.1×10^{-7}	7148	1.4×10^{-6}	7148	1.4×10^{-6}
3	10461	3.5×10^{-8}	10467	3.7×10^{-8}	10469	7.5×10^{-8}	10470	7.4×10^{-8}
4	13611	2.6×10^{-9}	13619	2.4×10^{-9}	13622	4.9×10^{-9}	13623	4.5×10^{-9}
5	16592	2.5×10^{-10}	16603	2.2×10^{-10}	16606	4.2×10^{-10}	16607	3.6×10^{-10}

[a]Calculated with the scaled local mode parameters from Table 2S. Intensities for rotamer II and III include both OH bonds for each.

TABLE 5S: Calculated OH-stretching transition wavenumbers (cm^{-1}) and total oscillator strengths for the hydroquinone rotamers.

	trans		*cis*	
Δv_{OH}	freq.	*f*	freq.	*f*
1	3659.9	$1.6x10^{-5}$	3660.1	$1.6x10^{-5}$
2	7147.7	$1.4x10^{-6}$	7148.1	$1.4x10^{-6}$
3	10463.5	$7.6x10^{-8}$	10463.8	$7.6x10^{-8}$
4	13607.2	$5.1x10^{-9}$	13607.4	$5.2x10^{-9}$
5	16578.9	$4.5x10^{-10}$	16578.8	$4.6x10^{-10}$

[a]Calculated with the scaled local mode parameters from Table 3S. Intensities for the *cis* and *trans* rotamers include both OH bonds for each.