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Supporting Information

for

OH radicals reactivity towards phenol-related pollutants in water: temperature dependence of the rate constants and novel insights into the [OH–phenol]$^{\bullet}$ adduct formation

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Table S1. Light absorption shares in the H_2O_2-KSCN-phenol system at λ = 308 nm used for correcting the measured rate constants for the internal absorption.

Compound	Light absorption (%)			$A_{total,\ 308nm}$ (%)	$\Delta[OH]_0$ (%)
	H_2O_2	KSCN	studied phenol		
Phenol (mol L^{-1})					
0	100.00	0.00	0.00	4.644	0.000
$5.0 \cdot 10^{-5}$	99.95	0.00	0.05	4.646	0.001
$1.0 \cdot 10^{-4}$	99.91	0.00	0.09	4.648	0.002
$1.5 \cdot 10^{-4}$	99.86	0.00	0.14	4.650	0.003
$2.0 \cdot 10^{-4}$	99.82	0.00	0.18	4.652	0.004
Phloroglucinol (mol L^{-1})					
0	100.00	0.00	0.00	8.483	0.00
$2.00 \cdot 10^{-5}$	100.00	0.00	0.00	8.483	0.00
$4.00 \cdot 10^{-5}$	100.00	0.00	0.00	8.483	0.00
$6.00 \cdot 10^{-5}$	100.00	0.00	0.00	8.483	0.00
$8.00 \cdot 10^{-5}$	100.00	0.00	0.00	8.483	0.00
Catechol (mol L^{-1})					
0	100.00	0.00	0.00	4.644	0.000
$5.02 \cdot 10^{-5}$	98.84	0.00	1.16	4.697	0.027
$1.00 \cdot 10^{-4}$	97.71	0.00	2.29	4.750	0.055
$1.51 \cdot 10^{-4}$	96.60	0.00	3.40	4.803	0.082
$2.01 \cdot 10^{-4}$	95.52	0.00	4.48	4.856	0.110
Pyrogallol (mol L^{-1})					
0	100.00	0.00	0.00	9.072	0.000
$2.00 \cdot 10^{-5}$	82.31	0.00	17.69	10.911	0.989
$4.00 \cdot 10^{-5}$	69.94	0.00	30.06	12.713	1.964
$6.00 \cdot 10^{-5}$	60.80	0.00	39.20	14.479	2.927
$8.00 \cdot 10^{-5}$	53.77	0.00	46.23	16.209	3.877
3-Methylcatechol (mol L^{-1})					
0	100.00	0.00	0.00	4.644	0.000
$2.44 \cdot 10^{-5}$	72.16	0.00	27.84	6.377	0.895
$4.87 \cdot 10^{-5}$	56.44	0.00	43.56	8.079	1.780
$7.31 \cdot 10^{-5}$	46.35	0.00	53.65	9.750	2.654
$9.74 \cdot 10^{-5}$	39.32	0.00	60.68	11.391	3.518

ε_{308nm} (H_2O_2) = 0.59 ± 0.01 L mol^{-1} cm^{-1} (He et al.[1]) and ε_{308nm} (KSCN) = 0 L mol^{-1} cm^{-1}

Table S2. A comparison of not yet corrected and corrected kinetic rate constants, k_{uncorr} and k_{corr}, at different temperatures, T.

	Phe*	Phlo*	Cat		Pyr		3-MeC	
$\varepsilon_{308\mathrm{nm}}$ = /L mol^{-1} cm^{-1}	0.05	0.00	1.38		63.40		93.47	
T /K	k_{uncorr} /L mol^{-1} s^{-1}	k_{uncorr} /L mol^{-1} s^{-1}	k_{corr} /L mol^{-1} s^{-1}	k_{uncorr} /L mol^{-1} s^{-1}	k_{corr} /L mol^{-1} s^{-1}	k_{uncorr} /L mol^{-1} s^{-1}	k_{corr} /L mol^{-1} s^{-1}	k_{uncorr} /L mol^{-1} s^{-1}
278.15	$(9.9 \pm 0.7) \cdot 10^{9}$	$(6.4 \pm 0.7) \cdot 10^{9}$	$(7.9 \pm 0.2) \cdot 10^{9}$	$(8.0 \pm 0.2) \cdot 10^{9}$	$(8.5 \pm 0.9) \cdot 10^{9}$	$(9.2 \pm 1.0) \cdot 10^{9}$	$(9.0 \pm 0.3) \cdot 10^{9}$	$(9.6 \pm 0.4) \cdot 10^{9}$
288.15	$(1.3 \pm 0.1) \cdot 10^{10}$	$(1.0 \pm 0.1) \cdot 10^{10}$	$(1.1 \pm 0.1) \cdot 10^{10}$	$(1.1 \pm 0.1) \cdot 10^{10}$	$(1.1 \pm 0.1) \cdot 10^{10}$	$(1.2 \pm 0.1) \cdot 10^{10}$	$(9.3 \pm 0.8) \cdot 10^{9}$	$(1.0 \pm 0.1) \cdot 10^{10}$
298.15	$(1.6 \pm 0.1) \cdot 10^{10}$	$(1.1 \pm 0.1) \cdot 10^{10}$	$(1.4 \pm 0.1) \cdot 10^{10}$	$(1.4 \pm 0.1) \cdot 10^{10}$	$(1.2 \pm 0.1) \cdot 10^{10}$	$(1.3 \pm 0.1) \cdot 10^{10}$	$(1.4 \pm 0.1) \cdot 10^{10}$	$(1.5 \pm 0.1) \cdot 10^{10}$
308.15	$(2.1 \pm 0.2) \cdot 10^{10}$	$(1.3 \pm 0.1) \cdot 10^{10}$	$(1.7 \pm 0.1) \cdot 10^{10}$	$(1.7 \pm 0.1) \cdot 10^{10}$	$(1.5 \pm 0.1) \cdot 10^{10}$	$(1.6 \pm 0.1) \cdot 10^{10}$	$(1.9 \pm 0.1) \cdot 10^{10}$	$(2.0 \pm 0.1) \cdot 10^{10}$
318.15	$(2.7 \pm 0.2) \cdot 10^{10}$	$(2.1 \pm 0.3) \cdot 10^{10}$	$(2.0 \pm 0.1) \cdot 10^{10}$	$(2.0 \pm 0.1) \cdot 10^{10}$	$(2.0 \pm 0.1) \cdot 10^{10}$	$(2.2 \pm 0.2) \cdot 10^{10}$	$(2.6 \pm 0.3) \cdot 10^{10}$	$(2.7 \pm 0.4) \cdot 10^{10}$

*no correction needed

Table S3: OH radical rate constants, k, of the reaction with studied substituted phenols at different temperatures, T. Estimated diffusion-limited rate constants, k_{diff}, are added for comparison.

	Phe		Phlo		Cat		Pyr		3-MeC	
T /K	k /L mol^{-1} s^{-1}	k_{diff} /L mol^{-1} s^{-1}	k /L mol^{-1} s^{-1}	k_{diff} /L mol^{-1} s^{-1}	k /L mol^{-1} s^{-1}	k_{diff} /L mol^{-1} s^{-1}	k /L mol^{-1} s^{-1}	k_{diff} /L mol^{-1} s^{-1}	k /L mol^{-1} s^{-1}	k_{diff} /L mol^{-1} s^{-1}
278.15	$(9.9 \pm 0.7) \cdot 10^{9}$	$7.4 \cdot 10^{9}$	$(6.4 \pm 0.7) \cdot 10^{9}$	$7.5 \cdot 10^{9}$	$(7.9 \pm 0.2) \cdot 10^{9}$	$7.4 \cdot 10^{9}$	$(8.5 \pm 0.9) \cdot 10^{9}$	$7.5 \cdot 10^{9}$	$(9.0 \pm 0.3) \cdot 10^{9}$	$7.4 \cdot 10^{9}$
288.15	$(1.3 \pm 0.1) \cdot 10^{10}$	$1.2 \cdot 10^{10}$	$(1.0 \pm 0.1) \cdot 10^{10}$	$1.0 \cdot 10^{10}$	$(1.1 \pm 0.1) \cdot 10^{10}$	$1.0 \cdot 10^{10}$	$(1.1 \pm 0.1) \cdot 10^{10}$	$1.0 \cdot 10^{10}$	$(9.3 \pm 0.8) \cdot 10^{9}$	$1.0 \cdot 10^{10}$
298.15	$(1.6 \pm 0.1) \cdot 10^{10}$	$1.4 \cdot 10^{10}$	$(1.1 \pm 0.1) \cdot 10^{10}$	$1.4 \cdot 10^{10}$	$(1.4 \pm 0.1) \cdot 10^{10}$	$1.4 \cdot 10^{10}$	$(1.2 \pm 0.1) \cdot 10^{10}$	$1.4 \cdot 10^{10}$	$(1.4 \pm 0.1) \cdot 10^{10}$	$1.4 \cdot 10^{10}$
308.15	$(2.1 \pm 0.2) \cdot 10^{10}$	$1.7 \cdot 10^{10}$	$(1.3 \pm 0.1) \cdot 10^{10}$	$1.8 \cdot 10^{10}$	$(1.7 \pm 0.1) \cdot 10^{10}$	$1.7 \cdot 10^{10}$	$(1.5 \pm 0.1) \cdot 10^{10}$	$1.8 \cdot 10^{10}$	$(1.9 \pm 0.1) \cdot 10^{10}$	$1.7 \cdot 10^{10}$
318.15	$(2.7 \pm 0.2) \cdot 10^{10}$	$2.2 \cdot 10^{10}$	$(2.1 \pm 0.3) \cdot 10^{10}$	$2.2 \cdot 10^{10}$	$(2.0 \pm 0.1) \cdot 10^{10}$	$2.2 \cdot 10^{10}$	$(2.0 \pm 0.1) \cdot 10^{10}$	$2.2 \cdot 10^{10}$	$(2.6 \pm 0.3) \cdot 10^{10}$	$2.2 \cdot 10^{10}$

Diffusion limit calculation

Diffusion rate constants between $OH^{\bullet}$ and the reacting phenol species, k_{diff} /L mol^{-1} s^{-1}, were calculated using the Smoluchowski equation[2] (Eq. S1),

$$k_{diff} = 4\pi \cdot N_A(r_{OH} + r_{RH})(D_{OH} + D_{RH})/1000\ /L\,mol^{-1}s^{-1} \tag{S1}$$

the Avogadro's number, N_A, the radii of $OH^{\bullet}$ and the reactant, r /cm, and the diffusion coefficient, D /cm^2 s^{-1}. Diffusion coefficients were obtained according to the Stokes–Einstein relationship modified by Wilke and Chang (Eq. S2),[3]

$$D = 7.4 \cdot 10^{-8} \cdot \frac{(X \cdot M)^{0.5} \cdot T}{V_m^{0.6} \cdot \eta}\ /cm^2s^{-1} \tag{S2}$$

where X is the association parameter of the solvent recommended by Hayduk and Laudie[4] (X = 2.26 for water was used), the molar mass of the solvent, M /g mol^{-1}, the temperature, T /K, the molar volume, V_{m} /cm^3 mol^{-1}, and the temperature-dependent dynamic viscosity of water, η /10^{-9} kg m^{-1} s^{-1}.[5] Used values of the latter are gathered in Table S4.

Table S4: Used values for the dynamic viscosity of water, η, taken from Kestin et al.[5]

T /K	η /10^{-9} kg m^{-1} s^{-1}
273.15	1.5193
278.15	1.1383
288.15	1.002
293.15	0.8902
298.15	0.7191
308.15	0.5961

V_{m} was estimated using the Joback group contribution method for the determination of critical volume, V_{c}, which is temperature independent.[6] V_{c} was then converted into the molar volume (Eq. S3) according to the method adopted from Tyn and Calus.[7] V_{m} is the molar volume and V_{c} is the critical volume at the boiling point (Table S5).

$$V_m = 0.285 \cdot V_c^{1.048}\ /cm^3 \tag{S3}$$

The diffusion coefficient of D_{OH}(298 K) = 2.2 · 10^{-5} cm^2 s^{-1} was calculated thereof, which is in the range of the reported values, D_{OH} = (1.0–2.3) · 10^{-5} cm^2 s^{-1}.[8, 9] The radius of $OH^{\bullet}$ (r_{OH} =

$2.2 \cdot 10^{-8}$ cm) was adopted from Buxton et al.[9] and was taken to be invariant with temperature, yielding the molar volume of 26.9 cm^3 mol^{-1}.

The radii of the reactants were calculated using the following equation (Eq. S4).[10]

$$r = \sqrt[3]{\frac{3 \cdot V_m}{4\pi \cdot N_A}} / cm \tag{S4}$$

Table S5: Calculated critical and molar volumes, V_c and V_m, using groups and group contributions according to the Joback method[6] for phenol and the related compounds.

compound	Phe	Phlo	Cat	Pyr	3-MeC
	=CH- (ring) **41**	=CH- (ring) **41**	=CH- (ring) **41**	=CH- (ring) **41**	=CH- (ring) **41**
	=CH- (ring) **41**	=CH- (ring) **41**	=CH- (ring) **41**	=CH- (ring) **41**	=CH- (ring) **41**
	=CH- (ring) **41**	=CH- (ring) **41**	=CH- (ring) **41**	=CH- (ring) **41**	=CH- (ring) **41**
	=CH- (ring) **41**	=C< (ring) **32**	=CH- (ring) **41**	=C< (ring) **32**	=C< (ring) **32**
	=CH- (ring) **41**	=C< (ring) **32**	=C< (ring) **32**	=C< (ring) **32**	=C< (ring) **32**
	=C< (ring) **32**	=C< (ring) **32**	=C< (ring) **32**	=C< (ring) **32**	=C< (ring) **32**
	-OH (phe) **−25**	-OH (phe) **−25**	-OH (phe) **−25**	-OH (phe) **−25**	-OH (phe) **−25**
	/	-OH (phe) **−25**	-OH (phe) **−25**	-OH (phe) **−25**	-OH (phe) **−25**
	/	-OH (phe) **−25**	/	-OH (phe) **−25**	-CH_3 **65**
V_c /cm^3 mol^{-1}	**229.5**	**161.5**	**195.5**	**161.5**	**251.5**
V_m /cm^3 mol^{-1}	**84.91**	**58.75**	**71.77**	**58.75**	**93.46**
	73.311*	84.468*	78.163*	87.587*	99.562*

*calculated by DFT

Some derived D of the studied compounds are gathered in Table S6 for comparison with the published data**.** The calculated values are slightly higher than the measured D from the literature, which could arise from the used X or V_m values in Eq. S2. The effect of V_m on the calculated D and k_{diff} at 298.15 K was further investigated in Figure S1. It is shown, however, that a wide range of estimated V_m values (i.e., V_m = 30–300 cm^3 mol^{-1}) results in a narrow range of the calculated rate constants, k_{diff} (298.15 K) = $(1.3–1.5) \cdot 10^{10}$ L mol^{-1} s^{-1}, from which we estimate that the precision of calculated k_{diff} at 298.15 K be $0.1 \cdot 10^{10}$ L mol^{-1} s^{-1}. We additionally calculated V_m of all the studied compounds with DFT and confirmed that they all fall within the range with only a small influence on the determined k_{diff} (i.e. V_m(DFT) = 73.311–99.562 cm^3 mol^{-1}, see Table S5).

Table S6: Derived diffusion coefficients, D /cm^2 s^{-1}, of phenol and the related compounds.

compound	calculated	literature values	disagreement
Phe	$6.02 \cdot 10^{-6}$ (278.15 K)	$5.43 \cdot 10^{-6}$ (277.2 K)[a]	10%
	$9.62 \cdot 10^{-6}$ (293.15 K)	$8.9 \cdot 10^{-6}$ (293.2 K)[b]	7 %
	$1.10 \cdot 10^{-5}$ (298.15 K)	$9.98 \cdot 10^{-6}$ (298.2 K)[a]	9%
	$1.94 \cdot 10^{-5}$ (323.15 K)	$1.79 \cdot 10^{-5}$ (323.2 K)[a]	19 %
Phlo	$1.37 \cdot 10^{-5}$ (298.15 K)		
Cat	$1.22 \cdot 10^{-5}$ (298.15 K)	$7.8 \cdot 10^{-6}$ (298.15 K)[c]	36%
Pyr	$1.37 \cdot 10^{-5}$ (298.15 K)		
3-MeC	$1.04 \cdot 10^{-5}$ (298.15 K)		

[a]Niesner and Heintz[11], [b]Lide[12], [c]Codling et al.[13]

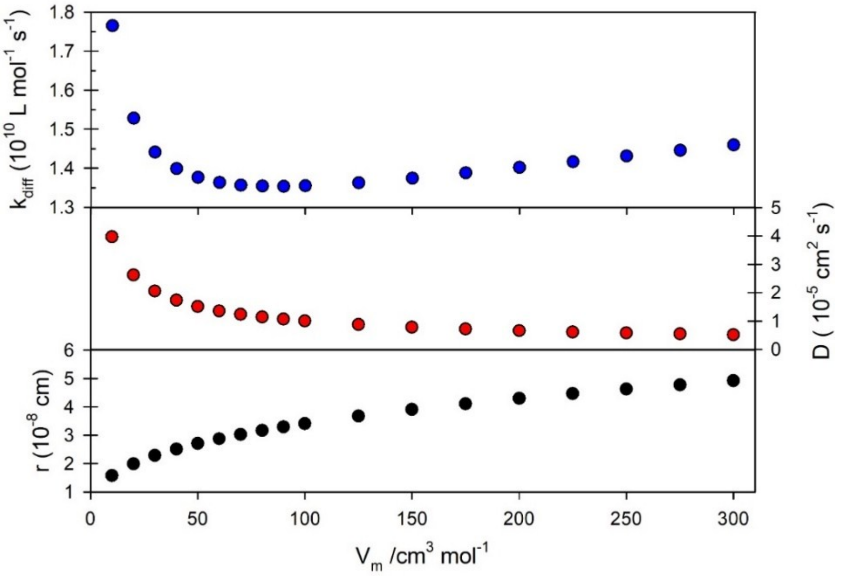

Figure S1: The derived radii, *r* (black), diffusion coefficients, *D* (red) and the resulting diffusion-limited rate constants, k_{diff} (blue), at 298.15 K in respect to the estimated molar volume, V_m.

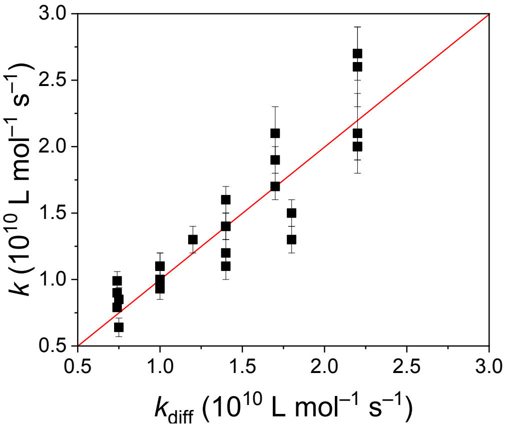

Figure S2: A correlation between the measured and the calculated diffusion-limited rate constants.

Hammett Relationships

In the 1930s, Hammett observed the relationship between the structure, i.e. meta and para substituents on a benzene ring, and the reaction rate, and described it by a simple empirical formula (Eq. 6).[14]

$$\log k = \log k_0 + \rho\sigma \qquad \text{(S5)}$$

k and k_0 are the rate constants of substituted and unsubstituted aromatic compounds, σ is the substituent constant and ρ is the constant typical of the investigated reaction. Initially, σ was exclusively determined for the meta and para substituents, which are believed to only exert inductive and mesomeric effects, hence ortho substituents often causing steric hindrance effects (and others, such as the effect of intramolecular hydrogen bonding) were avoided. Nevertheless, attempts have later been made to determine also σ-ortho values. In this paper, the values of σ constants for meta and para substituents were taken from Hansch et al.,[15] whereas σ constant values predicted by means of DFT were used for the ortho substituents.[16] For the disubstituted phenols, σ was calculated as a sum of the contributions of both substituents. Where more than one OH group is present, the numbering with more activating groups (ortho and para) was given the advantage and the so derived σ was used in the linear regression in Figure S3. However, the alternative option is always given for comparison by a dark blue symbol on the Hammett plot, cf. Table S7.

Table S7. Hammett constants (σ) used in Figure S3. The values of σ were taken from Hansch et al.[15] (unless otherwise specified).

	o-OH	*m*-OH	*p*-OH	*o*-OCH$_3$	*m*-OCH$_3$	*p*-OCH$_3$	*o*-CH$_3$	*m*-CH$_3$	*p*-CH$_3$	$\Sigma\sigma$
σ	−0.05[a]	0.12	−0.37	−0.39[a]	0.12	−0.26	−0.17[a]	−0.07	−0.17	
Phe										0
Gua				x						−0.39
3-MeOP					x					0.12
Res		x								0.12
Cat	x									−0.05
Phlo		xx								0.24
Pyr	xx									−0.10
	x	x								0.07
3-MeOC	x			x						−0.44
	x				x					0.07
Syr				xx						−0.78
Creo				x					x	−0.56
3-MeC	x						x			−0.22
	x							x		−0.12

[a] Takahata et al.[16]

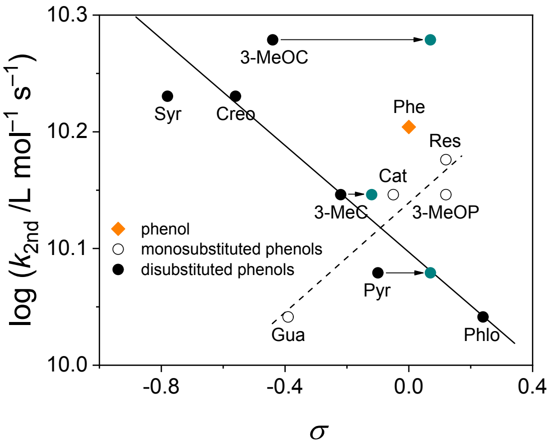

Figure S3. Hammett plot (OH radical rate constants at 298.15 K). The dashed line represents the linear relationship for monosubstituted phenols (open symbols) and the solid line represents the relationship for disubstituted phenols (solid symbols). Phenol (orange) was not considered in any of the regression analyses. Cyan symbols are shown as examples of different parametrization (see text for details) and were not considered in the fits.

Table S8. Activation parameters of the $OH^{\bullet}$ reaction with studied substituted phenols in aqueous solution at 298.15 K. The Arrhenius pre-exponential factor, A, and activation energy, E_A; the Gibbs free energy, $\Delta G^{\ddagger}$, enthalpy, $\Delta H^{\ddagger}$, and entropy, $\Delta S^{\ddagger}$, of activation. Data are gathered from this work and Ref.[1]

Reactant	A /L mol^{-1} s^{-1}	E_A /kJ mol^{-1}	$\Delta H^{\ddagger}$ /kJ mol^{-1}	$\Delta S^{\ddagger}$ /J K^{-1} mol^{-1}	$\Delta G^{\ddagger}$ /kJ mol^{-1}
Phe	$(2.4 \pm 0.1) \cdot 10^{13}$	18 ± 1	16 ± 1	3 ± 0.1	15 ± 1
Res[1]	$(2.6 \pm 0.1) \cdot 10^{13}$	19 ± 1	16.0 ± 0.9	3.6 ± 0.1	15 ± 1
Phlo	$(2.6 \pm 0.1) \cdot 10^{13}$	19 ± 3	17 ± 3	4 ± 0.2	16 ± 4
3-MeOP[1]	$(5.2 \pm 0.3) \cdot 10^{13}$	20 ± 4	18 ± 4	9.3 ± 0.5	15 ± 4
Cat	$(1.2 \pm 0.1) \cdot 10^{13}$	17 ± 1	14 ± 1	−(3 ± 0.1)	15 ± 1
Pyr	$(4.6 \pm 0.1) \cdot 10^{12}$	15 ± 2	12 ± 2	−(11 ± 0.4)	15 ± 3
Gua[1]	$(1.2 \pm 0.1) \cdot 10^{13}$	17 ± 1	14.8 ± 0.8	−2.9 ± 0.1	16 ± 2
3-MeOC[1]	$(4.5 \pm 0.1) \cdot 10^{12}$	13 ± 2	11 ± 1	−11.1 ± 0.2	14 ± 2
Creo[1]	$(9.1 \pm 0.1) \cdot 10^{12}$	15.5 ± 0.5	13.0 ± 0.4	−5.2 ± 0.1	14.6 ± 0.6
Syr[1]	$(1.9 \pm 0.1) \cdot 10^{13}$	17.4 ± 0.8	14.9 ± 0.7	0.8 ± 0.1	14.6 ± 0.8
3-MeC	$(5.4 \pm 0.2) \cdot 10^{13}$	20 ± 3	18 ± 3	10 ± 0.5	15 ± 3

The errors determined with 95% confidence during the data analysis do not always account for all preceding errors (e.g., precision of solution preparation). The error of $\Delta S^{\ddagger}$ may be underestimated.

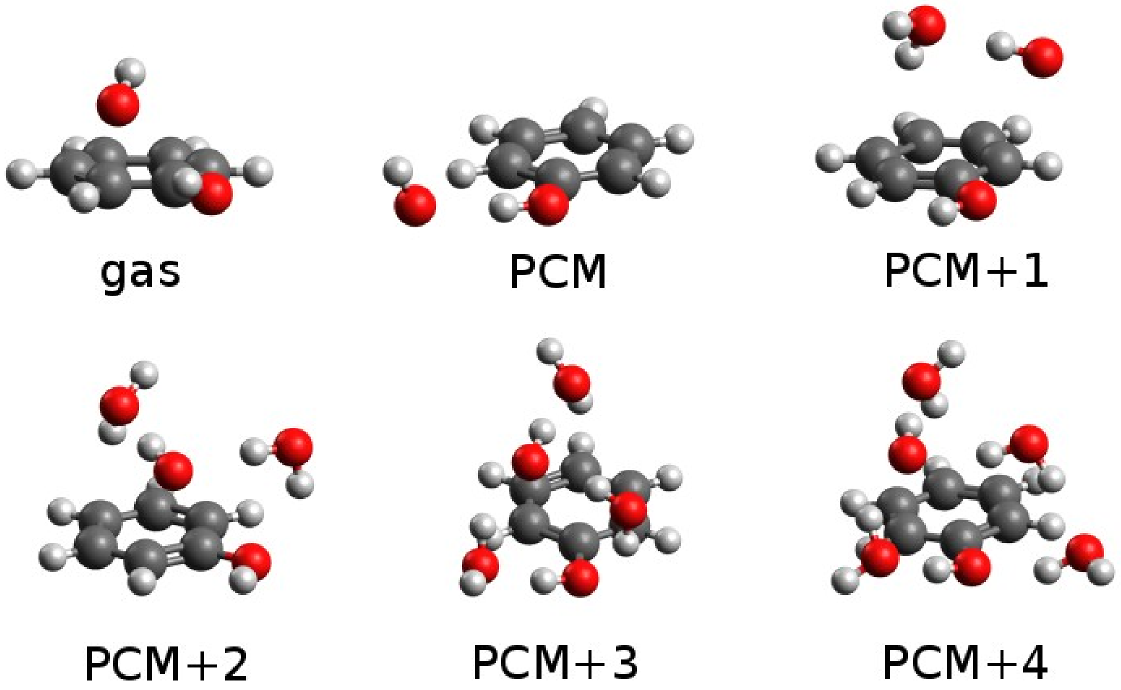

Figure S4: Pre-reaction complexes of the OH radical and phenol.

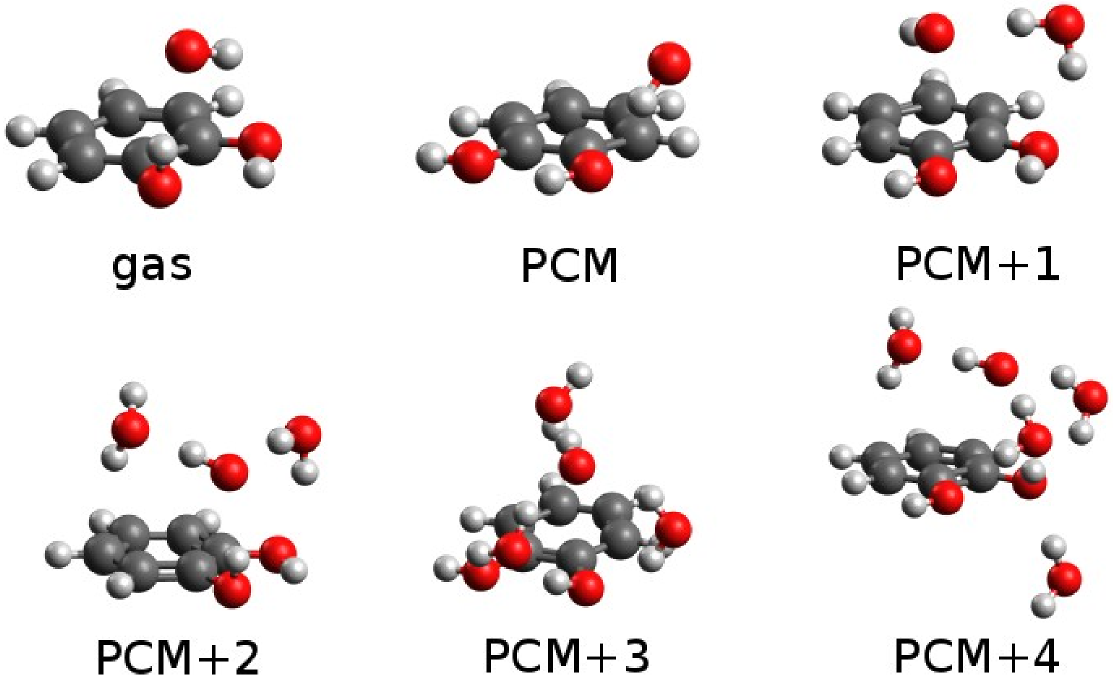

Figure S5: Pre-reaction complexes of the OH radical and catechol.

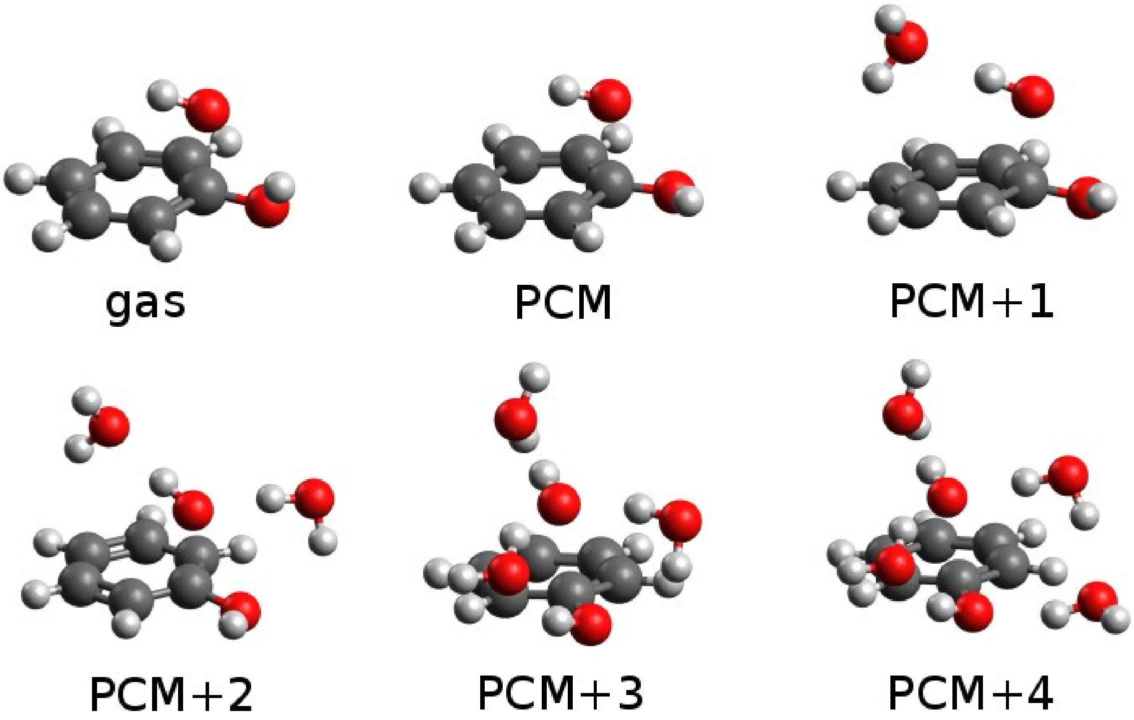

Figure S6: Transition states of the OH radical and phenol.

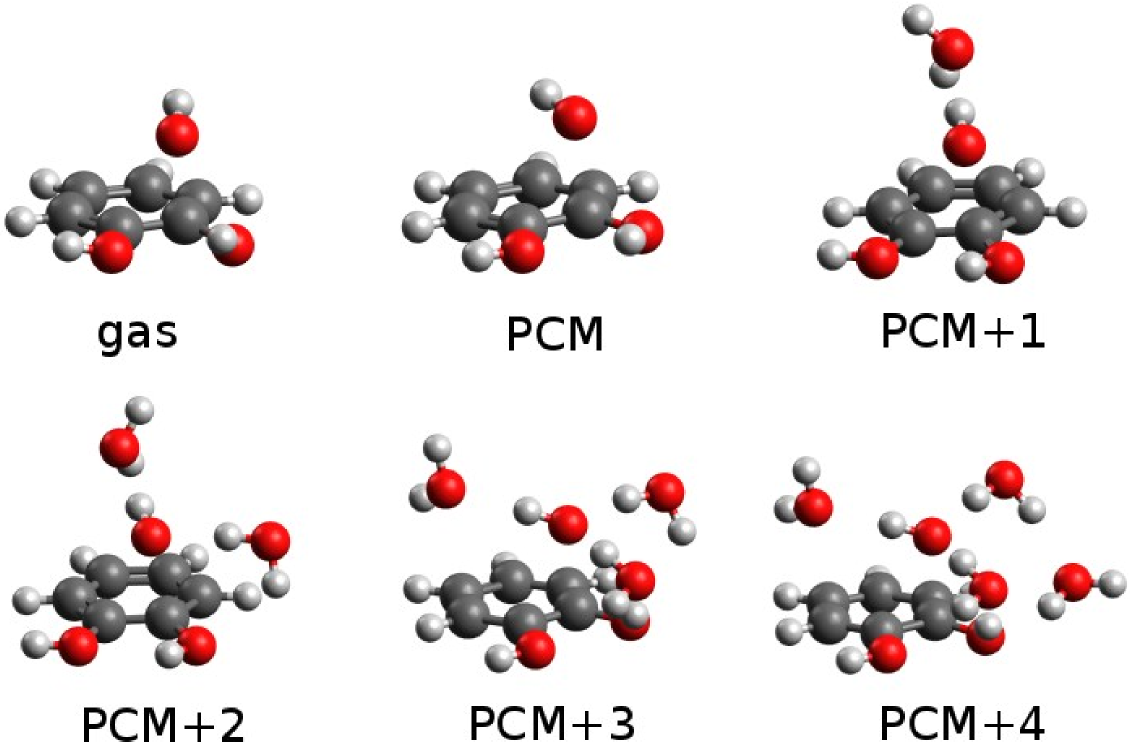

Figure S7: Transition states of the OH radical and catechol.

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