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Thermodynamic Parameters Including Acid Dissociation Constants for

Bromochlorophenols (BCPs)

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22

23   **Abstract**

24

25   This contribution reports standard gas-phase enthalpies of formation ($\Delta_f H°_{298}$), entropies

26   ($S°_{298}$) and heat capacities ($C_p°(T)$) for all plausible 64 bromochlorophenols (BCPs) at the

27   M062X meta hybrid level using a polarised basis set of 6-311+G(d,p). Isodesmic work

28   reactions served to calculate the standard enthalpies of formation for all bromochlorophenol

29   molecules and several bromochlorophenoxy radicals. Standard entropies and heat capacities

30   comprise correction terms due to the treatment of O-H bonds as hindered rotors. Values of

31   the bond dissociation enthalpies (BDHs) of O-H bonds, calculated for a selected series of

32   bromochlorophenols, vary slightly with the change in the pattern and degree of halogenation

33   of the phenyl ring. A thermodynamic cycle facilitated the estimation of pK_a values, based on

34   the calculated solvation and gas-phase deprotonation energies. We estimated the solvation

35   energies of 19 out of 64 BCPs and their respective anions based on the integral equation

36   formalism polarisable continuum model using optimised structures in the aqueous phase.

37   Values of pK_a decrease significantly from around 9 for monohalogenated to around 3 for

38   pentahalogenated phenols.

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41   **Key Words**

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43   Halogenated phenols, Structure optimisation, Enthalpy, Entropy and Gibbs energy of

44   formation, Heat capacity, Bond dissociation enthalpy (BDH), pK_a

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1. Introduction

Phenols and their halogenated derivatives, such as chlorophenols (CPs), bromophenols (BPs) and bromochlorophenols (BCPs) find frequent use in industrial and agricultural applications. BCPs function as feedstocks and intermediates for many chemical products, most notably, herbicides, fungicides, wood preservatives and flame retardants.[1-4] Once utilised, these compounds can undergo long-range environmental transport via air and water bodies. Because of their diverse applications, BCPs have been detected in marine ecosystems[5-7] and in industrial effluents.[8-11] BCPs have properties typical of persistent organic pollutants (POPs). Furthermore, typical combustion processes and accidental fires generate complete homologue profiles of BCPs.[12-13] BCPs affect the thyroid hormone system.[14-15] Environmental as well as health impacts of BCPs depend primarily on their physical and chemical properties.

Previous studies have focused on elucidating reaction pathways,[16-17] molecular structures and thermodynamic parameters[18-20] of halogenated homologue profiles of CPs and BPs. In comparison ~~to~~ with CPs and BPs, the corresponding data on BCPs are rather scarce. By analogy with the well-established role of CPs and BPs as precursors for the formation of polychlorinated dibenzo-*p*-dioxins and dibenzofurans (PCDD/Fs) and polybrominated dibenzo-*p*-dioxins and dibenzofurans (PBDD/Fs), BCPs act as building blocks in the generation of mixed halogenated dibenzo-*p*-dioxins and dibenzofurans (PXDD/Fs, X=Br, Cl). PXDD/Fs appear to be common environmental pollutants, with known carcinogenicity and typical POP-like properties.[21-25] Mixed halogenation at the lateral position of 2,3,7,8- induces PXDD/Fs to exhibit enhanced toxicity effects, if compared with their analogous PCDD/F and PBDD/F congeners.[26-27] PXDD/Fs have been identified in several

71 environmental matrices such as air,[28] soil and sediments,[28-29] and in tissues of aquatic

72 animals.[30]

73

74 Consensus in the literature points to the formation of PXDD/Fs from CPs and BPs in thermal

75 systems. Recent experimental studies have reported that, PXDD/Fs could also arise from the

76 municipal waste incineration and industrial processes containing trace sources of brominated

77 and chlorinated compounds.[25, 31-34] For example, Schwind et al.[35] detected formation of

78 appreciable concentrations of PXDD/Fs in the fly ash of a typical municipal waste

79 incinerator. Evans et al.[36-37] identified various congeners of PXDD/Fs during the course of

80 high temperature oxidation and pyrolysis of a mixture of CPs and BPs.

81

82 Overall, PXDD/Fs share similar chemical properties and formation mechanisms with their

83 chlorinated and brominated analogues.[38] The yield and degree of halogenation of the

84 PXDD/Fs depend strongly on available chlorine and bromine content and operational

85 conditions, especially the ability of catalytic surfaces to induce halogenation and

86 dehalogenation reactions.[39-42] Even trace quantities of bromine exert significant effects on the

87 emission of products of incomplete combustion, such as PBDD/Fs and PXDD/Fs.[41-43] BPs

88 are more active precursors for the formation of PBDD/Fs[44-47] than CPs for the generation of

89 PCDD/Fs.[47-49]

90

91 This article develops accurate thermochemical and structural parameters of the complete

92 series of BCPs and acid dissociation constants for selected species. Precise and detailed

93 knowledge of physical and chemical properties of BCPs are a prerequisite for gaining a better

94 understanding of the environmental fate and transformation chemistry of BCPs, including

95 formation pathways of PXDD/Fs from BCPs. Along the same line of inquiry, calculated

96   thermochemical properties may shed light on the effects of thermodynamic stability on the

97   distribution of congeners in thermal or environmental reservoirs. To this end, the present

98   contribution reports theoretically-derived thermochemical and structural properties of BCP

99   congeners.

100

101

102   **2.   Computational Details**

103

104   The Guassian09 program[50] provided a means to optimise chemical structures and to compute

105   energies, at the M062X/6-311+G(d,p)[51] level of theory. M062X is a relatively new meta-

106   hybrid density functional theory parameterised to yield accurate thermochemistry for general

107   applications in organic compounds. The extended basis set of 6-311+G(3df,2p) facilitated

108   the computation of single point energies. The ChemRate[52] code aided the calculation of some

109   thermochemical parameters, such as standard entropies, heat capacities and NASA

110   polynomials. Finally, computation of acid/base behaviour of halogenated phenols demanded

111   the estimation of solvation energies ($\Delta_{\mathrm{solv}}G^{*}$). We evaluated solvation energies of neutral and

112   anionic species based on the integral equation formalism polarisable continuum model

113   (IEFPCM) developed by Tomasi and co-workers. [53,54] Section 3.6 presents the adopted

114   computational approach for obtaining the acid dissociation constants (pK_{a}) for selected BCP

115   congeners.

116

117

118   **3.   Results and Discussion**

119

120   **3.1   Optimised Geometries**

By analogy with the 2-chlorophenol molecule,[55-56] the presence of the H atom in the OH group pointing toward a C(halogen) atom (*syn*) rather than toward a C(H) site (*anti*) is expected to produce slightly more stable isomers. Accordingly, in all optimised geometries of BCPs, we consider *syn* conformers in optimising all BCPs isomers. Figure 1 depicts optimised structures and geometrical features of the selected congeners of BCPs. Overall, variation in the degree and pattern of halogenation induces rather minor changes in the geometries of BCP congeners. For instance, calculated lengths of O-H and C-O bonds of all BCPs vary in ranges of 0.961-0.966 Å and 1.340-1.41 Å, respectively. Calculated geometries of BCPs accord with theoretical predictions of corresponding BPs[57] and CPs.[58] For example, calculated bond distances in O-H and C-O in pentachlorophenol ~~amount to~~ are 0.968 Å and 1.329 Å, respectively; i.e., they are in excellent agreement with relevant distances in BCP congeners.

3.2 Heat Capacities and Standard Entropies

Table 1 lists values of standard heat capacities ($C_p°(T)$) and standard entropies ($S°_{298}$) of all 64 possible BCP congeners, at selected temperatures; i.e., for BCPs in a physical state of an ideal gas. Accurate determination of $C_p°(T)$ and $S°_{298}$ calls for ~~the~~ treatment of the internal rotation of the H atom in the hydroxyl group around the C-O bond, as hindered rotors (HR). The literature describes well the need and the procedure for such a treatment.[59] This treatment basically eliminates the vibrational frequency corresponding to the internal rotation and replaces it with the overall barrier of the rotor, its moment of inertia and its symmetry number, i.e., 2 in the considered BCP systems. Figure 2 shows rotor potentials and Table 2 provides estimates of the HR corrections for $C_p°(300\ K)$, $C_p°(1000\ K)$ and $S°_{298}$.

3.3 Standard Enthalpy of Formation of BCPs and Their Radicals

Standard enthalpies of formation ($\Delta_f H°_{298}$) for all BCP congeners ~~of BCP~~ are computed using two isodesmic reactions R1 and R2. Isodesmic reaction R1 employs the *para*-bromophenol and *ortho*-chlorophenol as resultant products. Taking into account the remaining isomers of chlorophenols and bromophenols in casting the isodesmic reactions, the calculated standard enthalpy of formation of BCP congeners may change within 4.7 kJ mol^{-1}.
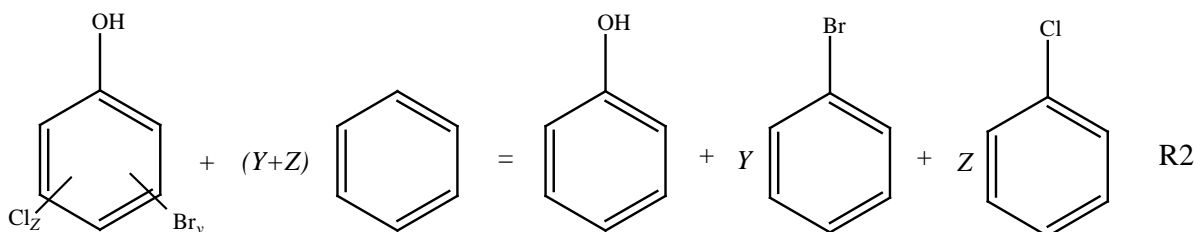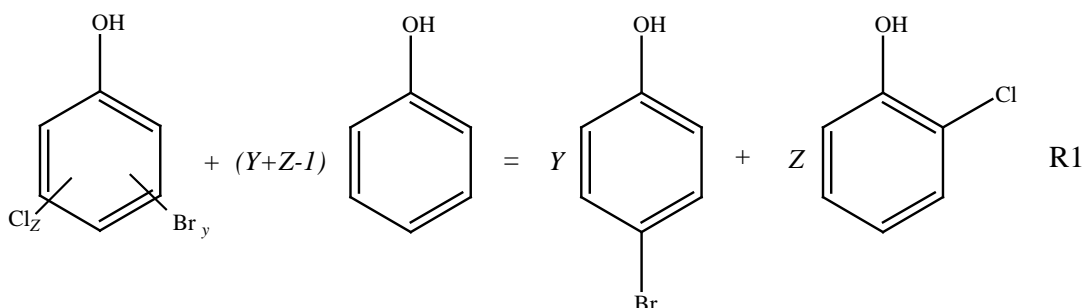
Scheme 1: Isodesmic reactions for obtaining the standard enthalpy of formation of BCP

These isodesmic reactions utilise experimental values of $\Delta_f H°_{298}$ for phenol (-96.3 ± 0.59 kJ mol^{-1}),[60] *o*-chlorophenol (-131 kJ mol^{-1}),[61] *o*-bromophenol (-78 ± 1.9 kJ mol^{-1}),[62] *p*-chlorophenol (-145.5 ± 8.4 kJ mol^{-1}),[63] *p*-bromophenol (-69.3 ± 2.1 kJ mol^{-1}),[64] benzene (82.9 ± 0.9 kJ mol^{-1}),[64] bromobenzene (105.4 ± 4.20 kJ mol^{-1})[65] and chlorobenzene (52.4 ± 0.42 kJ mol^{-1}).[66] Table 3 provides calculated reaction enthalpies for R1 ($\Delta_{R1} H°_{298}$) and R2 ($\Delta_{R2} H°_{298}$) and $\Delta_f H°_{298}$ of the target species.

165   The two isodesmic reactions yield similar estimates of $\Delta_f H°_{298}$, with the recommended value

166   corresponding to their average. The uncertainty limit of the two isodesmic reactions (u_j)

167   follows from the orthogonal addition of the uncertainty associated with each $\Delta_f H°_{298}$ of the

168   reference species; i.e., as $(\Sigma u_i{}^2)^{1/2}$. The overall uncertainty in enthalpy of formation is thus

169   estimated as $1/[\Sigma(1/u_j{}^2)]^{1/2}$.[67] Table 4 presents typical overall uncertainties for three BCP

170   congeners.

171

172   Values of $\Delta_f H°_{298}$ for selected bromochlorophenoxy radicals are calculated ~~based on~~ via

173   Reaction R3:

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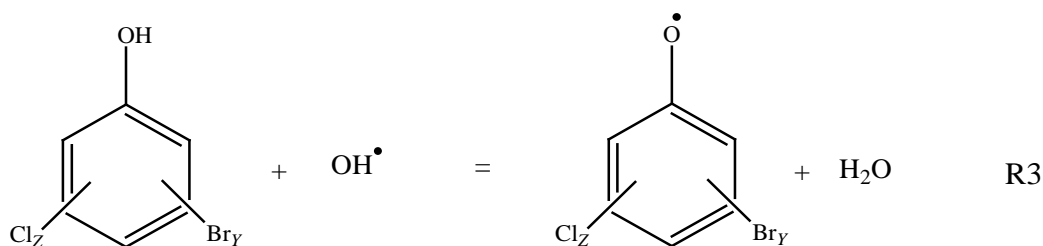
176   Scheme 2: An isodesmic reaction for obtaining the standard enthalpy of formation of BCP

177   radicals

178

179   Reaction R3 deploys experimental values of $\Delta_f H°_{298}$ for H_2O (-241.8 ± 0.040 kJ mol^{-1})[68] and

180   OH$^\bullet$ (37.3 ± 0.13 kJ mol^{-1})[68] with calculated values of $\Delta_f H°_{298}$ for BCPs listed in Table 3.

181   Table 5 presents calculated $\Delta_f H°_{298}$ values for a selected series of ~~selected~~ 19

182   bromochlorophenoxy radicals. While we have considered isomers of all plausible BCP

183   molecules, we elect to choose representative isomers of radicals of BCPs in each homologue

184   group. As demonstrated in the upcoming discussion, the degree of halogenation has a

185   minimal effect on the properties among the isomers in each homologue.
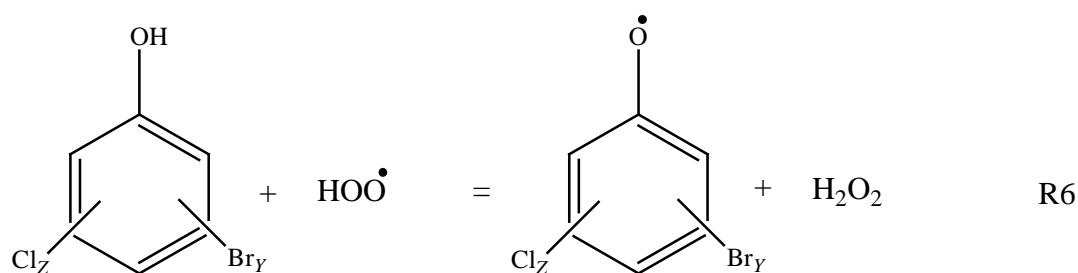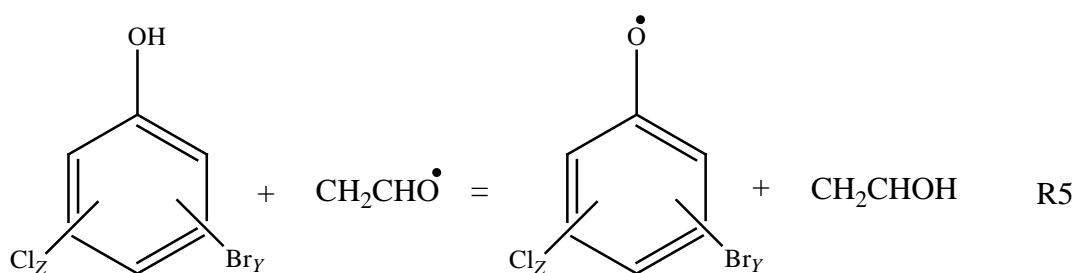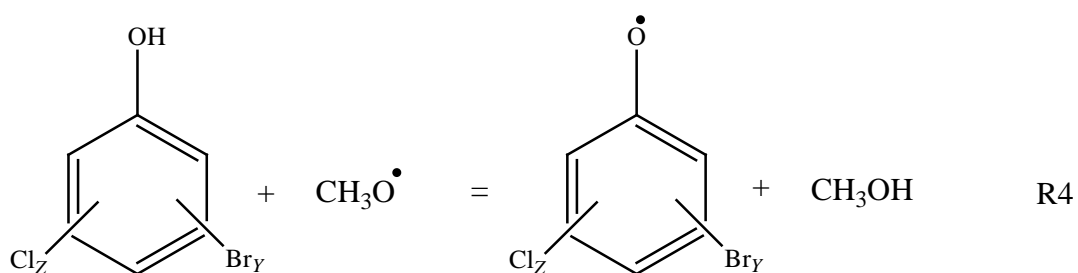
3.4 Bond Dissociation Enthalpies

We estimate the bond dissociation enthalpies (BDH) of the O-H bond in 19 BCP congeners based on values of $\Delta_f H^{\circ}{}_{298}$ of BCPs (Table 3) and bromochlorophenoxy radicals (Table 5) using three isodesmic reactions:

Scheme 3: Isodesmic reaction for estimating of O-H bond dissociation enthalpies (see text for explanation)
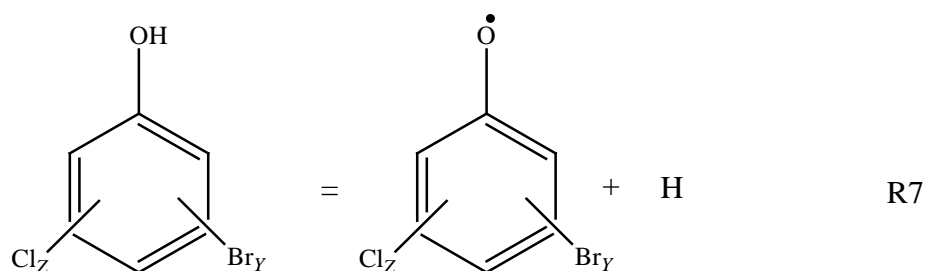
Reaction R7 signifies a direct fission of the O-H bond. In principle, values of BDHs of O-H bonds follow directly from R7. However, in order to improve the accuracy of calculated results, we applied the isodesmic reactions R4-R6 to compute the BDH of the O-H bonds by

200 applying equation (E1).[69] This is because R4-R6 maintain the same number and type of

201 bonds on both sides of the reactions, which results in the cancellation of systematic errors in

202 the calculation of reaction enthalpies.

203

Scheme 4: Direct fission of the O-H bond in halogenated phenols

208 Prior to taking averages, the BDHs for O-H bonds in BCPs were calculated separately from

209 each isodesmic reaction (R4 – R6). For example, Equation E1 presents a formula for

210 obtaining the BDHs for Reaction R4:

211

212 $\quad$ $BDH(BCP) = \Delta_{R4}H°_{298} + \Delta_{f}H°_{298}(H) - \Delta_{f}H°_{298}(CH_3OH) + \Delta_{f}H°_{298}(CH_3O·)$ $\qquad$ E1

213

214 Reactions R4-R6 deploy the experimental values of $\Delta_{f}H°_{298}$ of $CH_3O·$ (18.57 ± 2.9 kJ mol$^-$

215 ^{1}),[70] CH_3OH (-200.93 ± 0.21 kJ mol^{-1}),[71] $CH_2CHO·$ (12.87 ± 2.1 kJ mol^{-1}),[72] CH_2CHOH (-

216 125.0 ± 8.4 kJ mol^{-1}),[73] $HOO·$ (13.37 ± 2.09 kJ mol^{-1})[74] and H_2O_2 (-135.98 ± 0.21 kJ mol^{-1}).[75]

217 The final BDHs correspond to averages based on Reactions R4-R6; see the right-most

218 column in Table 5 for numerical values of BDHs, for selected BCP congeners.

219

220 Our calculated BDH values of O-H bonds in BCP congeners fall in the range of 379.0 to

221 392.4 kJ mol^{-1}. These values are in agreement with the analogue estimates of BDH reported

222 in the literature for O-H in phenol (370.0 to 374.4 kJ mol^{-1})[69] and substituted phenols (356.1

223 to 383.6 kJ mol^{-1}).[76] We remark that patterns and degrees of halogenation induce a fairly

224 slight variation in O-H BDHs.

225

226

227 **3.5 Gibbs Energies of Formation of BCPs and Their Anions in Gaseous and Aqueous**

228 **Phases**

229

230 Table 6 lists the standard Gibbs energy of formation ($\Delta_f G°_{298}$) for selected BCP congeners,

231 based on the computed values of $\Delta_f H°_{298}$ and $S°_{298}$ of BCP molecules as presented in

232 Equation E2:

233

234 $\qquad \Delta_f G°_{298(gas)} = \Delta_f H°_{298} - TS°_{298}$ (BCP congeners)

235 $\qquad\qquad\qquad\qquad\qquad + T\sum S°_{298}$ (elements in their standard state) $\qquad$ E2

236

237 We extracted the values of $S°_{298}$ for elements from reference 75. Gibbs energies of solvation

238 ($\Delta_{solv} G^*$) are estimated using an integral equation formalism polarisable continuum model

239 based on the HF/6-31+G(d) optimised aqueous-phase geometries,[52-53] whereas the

240 calculations of Gibbs ~~free~~ energy of formation in aqueous phase ($\Delta_f G^{aq}_{298}$) follow Equation

241 E3:

242

243 $\qquad \Delta_f G^{aq}_{298} = \Delta_{solv} G^* + \Delta_f G°_{298}$

244 $\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad$ E3

245

246 Table 6 presents values of $\Delta_{solv}G^*$ and $\Delta_f G^{aq}_{298}$. Calculated estimates of $\Delta_{solv}G^*$ indicate that

247 it is unaffected by the pattern and degree of halogenation on the phenol ring. This seems to

248 be in contrast to results of previous theoretical predictions for chlorinated isomers of aniline

249 and benzoic acid where $\Delta_{solv}G^*$ decreases with degree of chlorination.[76-77]

250

251

252 **3.6 Acid Dissociation Constants (pK_a)**

253

254 Biochemical and environmental applications require knowledge of the pH dependence of

255 deprotonation of substituted phenolic compounds. Theoretical determination of pK_a typically

256 involves constructing a thermodynamic cycle that deploys values of gas-phase deprotonation

257 energies, gas-phase Gibbs energies of formation, as well as solvation energies of BCPs and

258 their corresponding anions. Computations of pK_a also include experimentally-based values

259 of the solvation and gas-phase energies for H^+.[78] In calculations of Scheme 5, we employed

260 the value of $G_{gas}(H^+) = -26.3$ kJ mol^{-1} derived from the Sackur-Tetrode equation[79] and the

261 experimentally-based result of $\Delta_{solv}G^{*III} = 1107.1$ kJ mol^{-1}.[80]

262

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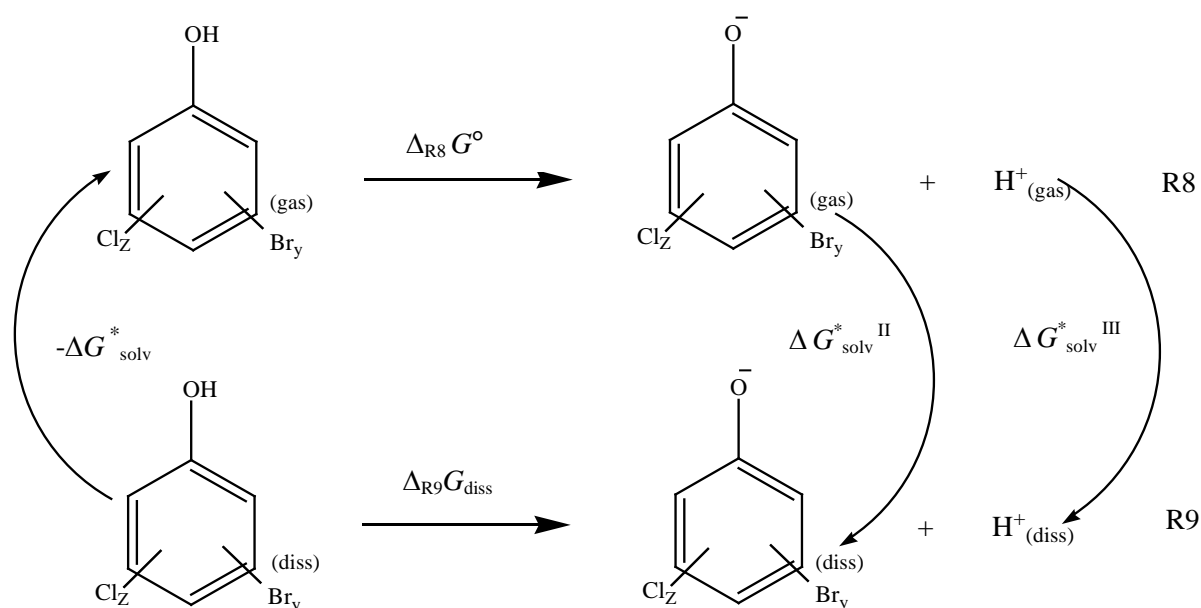
263   Scheme 5: Thermodynamic cycle for calculating pK_a

264

265   Liptak et al.,[81] applied the analogous thermodynamic cycle to derive accurate predictions of

266   the absolute pK_a values for substituted phenols. In their cycle, they computed the gas-phase

267   deprotonation energies ($\Delta_{R8}G°$) using the CBS-QB3 composite method where R8 represents

268   dissociation of halogenated phenols into their analogous phenolate anions and H$^+$ cations.

269   Solvation energies were estimated based on the conductor-like polarisable continuum model

270   (CPCM) and HF/6-31+G(d) optimised geometries for the aqueous-phase species. In the

271   present study, we calculate $\Delta_{R8}G°$ at the M06/6-311+(3df,2p)//M062X/6-311+g(d,p) level of

272   theory and the solvation energies; i.e., $\Delta_{solv}G^*$ and $\Delta_{solv}G^{*II}$, at the (UHF)IEFPCM/HF/6-

273   31+G(d) level, based on optimised solvated-phase geometries. The correction term RT

274   ln(24.46) is added to the values of $\Delta_{R8}G°$ to switch the reference state from the gas phase of 1

275   atm to the aqueous phase of 1 M; i.e., $\Delta_{R8}G^*$. Table 7 summarises the calculated values of

276   pK_a based on Equation E5.

277

278      $\Delta_{R8}G° = \Delta_f G°$(halogenated phenolate) $+ \Delta_f G°$(H$^+$) $- \Delta_f G°$(halogenated phenol)   E4

279      $$pK_a = \frac{\Delta_{R8}G^* - \Delta G^*_{solv} + \Delta G^*_{solv}{}^{II} + \Delta G^*_{solv}{}^{III}}{2.303\ RT}$$ E5

280   where $\Delta_{R8}G^* = \Delta_{R8}G° + RT\ln(24.46)$ E6

281

282   To set a further bench mark for the accuracy of the calculated Gibbs ~~free~~ energies of

283   solvation, we compute the gas-phase and aqueous-phase acidities for *m*- and *p* –

284   chlorophenols with respect to phenol according to the general reaction $C_6H_5O^- + AH \rightarrow$

285      $C_6H_5OH + A^-$ in which A signifies *m*-/*p*–chlorophenol. Values in the aqueous phase are

286   based on optimised geometries in the aqueous medium. Contrasting values with analogous

287   experimental estimates yield a satisfactory agreement. For example, our calculated gas and

288   aqueous phase acidities for *m*-chlorophenol are -25.5 kJ mol^{-1} and -3.3 kJ mol^{-1}, respectively.

289   These two values are in a reasonable agreement with analogous literature values of -29.7[82]/-

290   33.1[83] and -3.3 kJ mol^{-1} [82-83], in that order. While deploying a thermodynamic cycle to

291   predict pK_a values produces accurate results for carboxylic acids and phenol, some serious

292   drawbacks have been documented for certain classes of organic acids.[84] Substantial errors in

293   predicting pK_a values may originate from the fundamental shortcoming of quantum chemical

294   methods in evaluating solvation energies for ionic species that can induce a discrepancy of 7

295   or more units in the estimated pK_a in comparison with experimental values.[85] Other

296   contributing factors include the significant difference in the experimental and/or theoretical

297   values of proton solvation energies in the range between -1083.6 and -1114.6 kJ mol^{-1}.[80,85]

298   Nevertheless, the present method yields relatively accurate pK_a values for a wide variety of

299   organic systems.[86-88]

300

301   In the case of mixed halogenated phenols, we find that pK_a values depend strongly on the

302   degree of bromination and chlorination on the phenol ring. From the results of the

303   calculations, we deduce that, the substitution of a large number of bromine and chlorine

304   atoms on the phenol ring induces stronger acidity, with such compounds expected to

305   dissociate more easily in aqueous media in comparison with less halogenated BCP congeners

306   as depicted in figure 3. Analogously, Li et al.,[89] measured the pK_a values of polychlorinated

307   congeners of phenols experimentally and point out to a decreasing trend for pK_a values as the

308   number of chlorine atoms attached to the aromatic ring increases. To demonstrate the

309   accuracy and reliability of our predictions of pK_a values, in Table 7, we compare the

310   calculated values of pK_a for phenol, *o*-chlorophenol, *m*-chlorophenol, *p*-chlorophenol, and *o*-

311   bromophenol with the measurements available in literature.[80, 90-94] as well as with estimates

312   from the Marvin software[95] which deploys a neural network algorithm. For example, our

313   calculated pK_a value for phenol is 9.83; in good agreement with another theoretical estimate

314   of 9.88 offered by Liptak et al.[81] While obtaining values of $\Delta_{R8}G°$ based on the CBS-QB3 -

315   as in the study by Liptak et al.[81] - might be computationally unfeasible for high-molecular-

316   weight halogenated phenols, we have shown in this study a more computationally affordable

317   approach for estimating pK_a.

318

319

320   **4. Conclusions**

321

322   The present study provides standard gas-phase enthalpies of formation, entropies and heat

323   capacities for the complete series of bromochlorophenols, as well as standard aqueous-phase

324   Gibbs energies of formation and pK_a for 19 selected congeners of bromochlorophenols.

325   Overall, optimised structures exhibit minor changes in geometrical features. Although the

326   calculated Gibbs energies of solvation of bromochlorophenols in water are highly exergonic,

327   with the Gibbs energy of solvation increasing with the degree of substitution, the Gibbs

328   energy change of the dissociation (Reaction R9) displays an opposite trend, mirrored by pK_a.

329   This is because Reaction R9 includes other contributions, especially the gas-phase

330   deprotonation energies that decrease with the increase in the degree of halogen substitution.

331   Thus, we conclude that bromochlorophenols characterised by high degrees of halogenation

332   display stronger acidity and dissociate more easily in aqueous media (i.e., they are stronger

333   acids than lower substituted phenols).

334

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345 **Supporting Information**

346

347 Cartesian coordinates for optimised structures and NASA polynomials for selected

348 congeners. This material is available free of charge via the Internet at http://pubs.acs.org.

349 The authors declare no competing financial interest.

350

351

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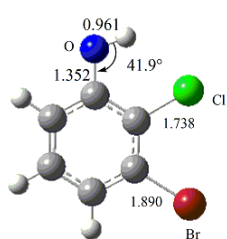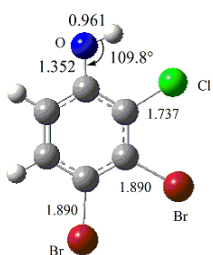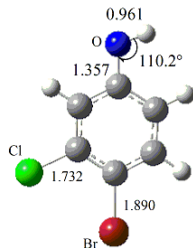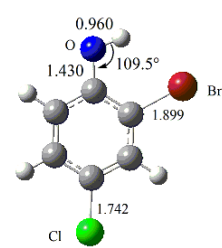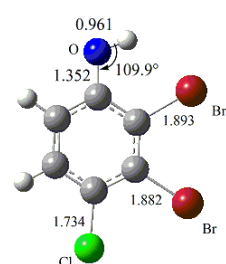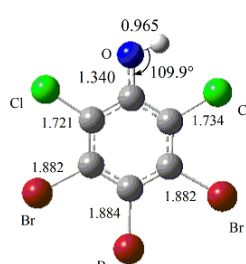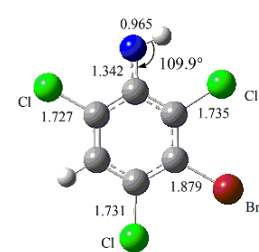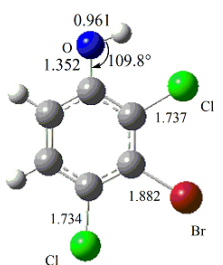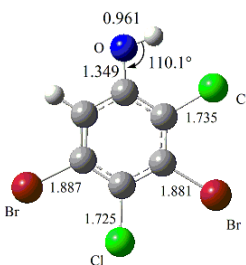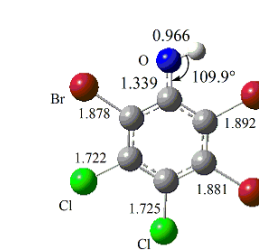
Figure 1. Optimised geometries of selected bromochlorophenol congeners with distances measured in Å and angles are in degrees.

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Figure 2. Potential energy profiles for internal rotations of H around C-O bond in BCP congeners. (P) denotes chlorophenol.
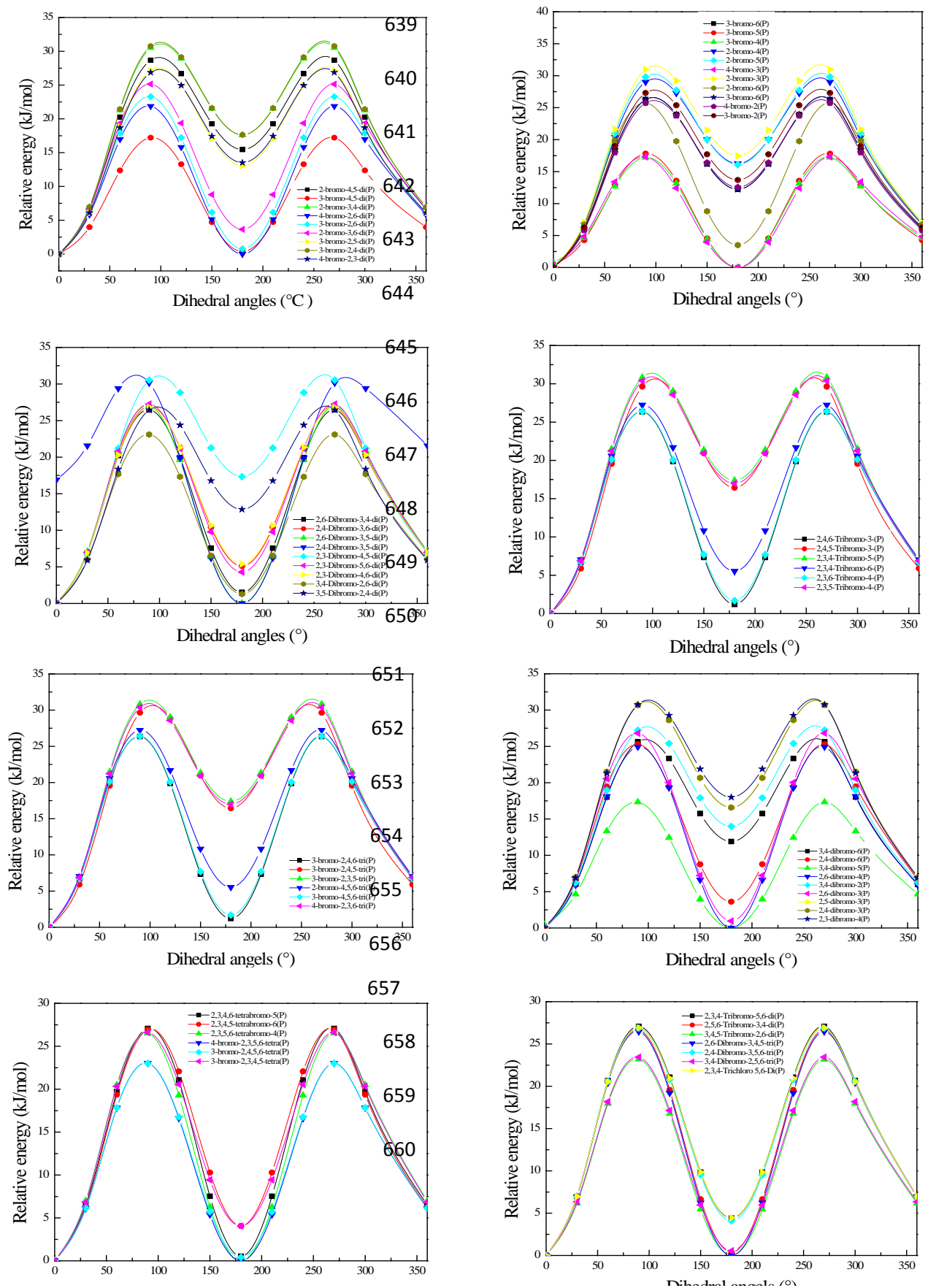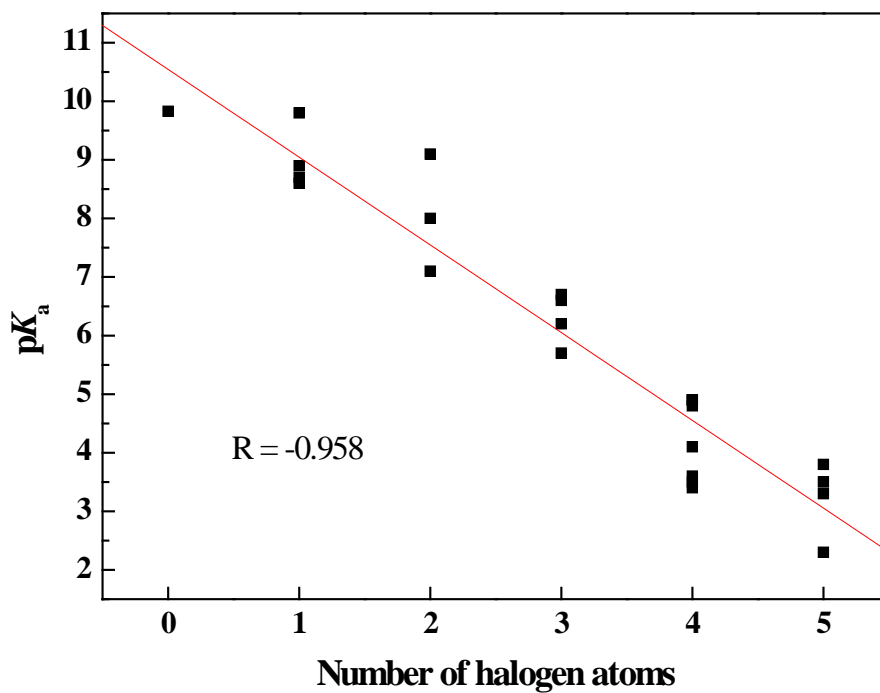
Figure 3. Correlation between the calculated acid dissociation constant (pK_a) and the number of halogen atoms attached to the aromatic ring.

Table 1. $S°_{298}$ and $C_p°(T)$; both in J mol^{-1} K^{-1}.

Compound Name	$S°_{298}$	$C_p•(T)$				
		300 K	500 K	800 K	1000 K	1500 K
3-bromo-2-chlorophenol	391.9	138.2	191.6	235.6	252.2	274.8
3-bromo-5-chlorophenol	396.4	139.7	192.5	234.7	250.5	273.1
3-bromo-4-chlorophenol	393.3	138.7	191.8	236.0	252.5	279.3
2-bromo-4-chlorophenol	392.9	138.2	191.5	235.6	252.1	274.8
2-bromo-5-chlorophenol	393.8	138.5	191.9	235.7	252.1	274.6
4-bromo-3-chlorophenol	395.2	139.5	192.2	234.3	250.3	272.9
2-bromo-3-chlorophenol	391.0	137.9	191.3	235.6	252.3	275.0
2-bromo-6-chlorophenol	392.4	137.8	191.2	235.2	251.6	274.2
3-bromo-6-chlorophenol	393.5	138.4	191.7	235.5	251.8	274.3
4-bromo-2-chlorophenol	393.6	138.4	191.6	235.4	251.7	272.3
3-bromo-2-chlorophenol	391.5	138.1	191.4	235.5	251.9	274.5
2-bromo-4,5-dichlorophenol	422.1	153.8	204.8	245.6	260.3	279.8
3-bromo-4,5-dichlorophenol	424.2	155.1	205.5	244.4	258.5	278.0
2-bromo-3,4-dichlorophenol	419.0	153.4	204.6	245.7	260.5	280.1
4-bromo-2,6-dichlorophenol	424.2	154.1	182.6	244.9	259.2	278.7
3-bromo-2,6-dichlorophenol	421.8	153.7	204.8	245.0	259.5	278.8
2-bromo-3,6-dichlorophenol	423.3	153.8	204.9	245.3	259.8	279.2
3-bromo-2,5-dichlorophenol	422.8	154.2	205.2	245.7	260.3	279.6
3-bromo-2,4-dichlorophenol	420.2	153.9	204.8	245.7	260.6	280.1
4-bromo-2,3-dichlorophenol	420.9	153.9	204.9	245.5	260.2	279.5
3-bromo-2,4,6-trichlorophenol	451.2	169.6	218.3	255.1	267.7	283.9
3-bromo-2,4,5-trichlorophenol	450.1	169.7	218.6	255.7	268.5	284.6

4-bromo-2,3,5-trichlorophenol	450.4	170.0	218.6	255.7	268.5	284.6
2-bromo-4,5,6-trichlorophenol	450.7	169.2	218.0	255.3	268.0	284.2
3-bromo-4,5,6-trichlorophenol	450.0	169.5	218.3	255.6	268.4	286.4
4-bromo-2,3,6-trichlorophenol	440.1	162.5	213.5	252.6	266.6	285.1
4-bromo-2,3,5,6-tetrachlorophenol	479.2	185.3	231.7	265.3	276.1	289.0
3-bromo-2,4,5,6-tetrachlorophenol	480.0	185.7	231.9	265.3	276.1	289.1
2-bromo-3,4,5,6-tetrachlorophenol	478.0	184.9	231.4	265.6	276.6	289.6
3,4-dibromo-6-chlorophenol	434.0	155.9	206.1	246.0	260.4	279.5
2,4-dibromo-6-chlorophenol	431.2	155.7	206.0	246.0	260.4	279.6
3,4-dibromo-5-chlorophenol	433.2	157.3	206.8	245.1	259.0	278.2
2,6-dibromo-4-chlorophenol	433.8	155.5	205.8	245.7	260.1	279.3
3,4-dibromo-2-chlorophenol	432.7	156.0	206.1	246.2	260.6	279.8
2,6-dibromo-3-chlorophenol	432.6	155.3	205.6	245.8	260.4	279.6
2,5-dibromo-3-chlorophenol	442.5	156.5	206.2	246.4	261.0	280.3
2,4-dibromo-3-chlorophenol	432.0	155.6	205.8	246.2	261.0	280.3
2,3-dibromo-4-chlorophenol	431.4	155.7	205.9	246.3	261.0	280.3
2,3-dibromo-5,6-dichlorophenol	461.5	170.9	219.0	256.0	268.7	284.8
2,3-dibromo-4,5-dichlorophenol	462.6	169.9	218.0	255.0	268.2	285.9
2,4-dibromo-3,6-dichlorophenol	462.6	171.1	217.5	256.0	268.7	284.7
2,6-dibromo-3,5-dichlorophenol	461.7	171.1	219.1	256.0	268.7	284.8
2,4-dibromo-3,5-dichlorophenol	460.9	171.5	219.4	256.4	269.2	285.7
2,6-dibromo-3,4-dichlorophenol	461.6	171.0	219.0	255.9	268.6	284.7
3,4-dibromo-2,6-dichlorophenol	462.3	171.3	219.2	255.6	268.1	284.1
2,3-dibromo-4,6-dichlorophenol	461.7	171.3	219.2	256.1	268.7	284.7
3,5-dibromo-4,6-dichlorophenol	461.2	171.5	219.6	256.2	268.8	284.7

2,6-dibromo-3,4,5-trichlorophenol	489.1	186.5	232.4	266.0	276.9	289.8
3,4-dibromo-2,5,6-trichlorophenol	489.6	187.2	232.9	265.9	276.6	289.3
2,4-dibromo-3,5,6-trichlorophenol	489.3	186.7	232.5	266.1	277.1	289.8
2,3-dibromo-4,5,6-trichlorophenol	489.0	186.7	232.5	266.1	277.0	289.8
2,3,4-tribromo-6-chlorophenol	470.9	173.0	220.1	256.5	269.1	284.9
2,3,4-tribromo-5-chlorophenol	471.8	173.4	220.5	257.0	269.7	285.6
2,3,6-tribromo-4-chlorophenol	472.8	172.9	220.0	256.7	269.5	285.5
2,3,5-tribromo-4-chlorophenol	471.6	173.1	220.4	256.9	269.7	285.6
2,4,6-tribromo-3-chlorophenol	473.6	172.8	220.0	256.4	268.9	284.8
2,4,5-tribromo-3-chlorophenol	465.2	170.9	218.9	256.1	269.0	285.1
2,3,4-tribromo-5,6-dichlorophenol	500.6	188.9	233.8	266.9	277.5	290.1
2,3,5-tribromo-4,6-dichlorophenol	499.7	190.5	234.8	267.4	277.9	290.3
2,5,6-tribromo-3,4-dichlorophenol	500.3	188.9	233.8	266.8	277.5	290.1
3,4,5-tribromo-2,6-dichlorophenol	500.9	189.2	234.1	266.5	277.0	289.5
2,3,4,5-tetrabromo-6-chlorophenol	511.2	190.9	235.0	267.4	277.9	290.3
2,3,4,6-tetrabromo-5-chlorophenol	493.3	190.5	234.7	267.3	277.9	290.3
2,3,5,6-tetrabromo-4-chlorophenol	510.6	190.5	234.8	267.4	277.9	290.3

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671 **Table 2.** Contribution from treatment of internal rotors as hindered rotors to the values of

672 S^{o}_{298}, $C_p{}^{o}$(300 K), and $C_p{}^{o}$(1000 K); <mark>all</mark> in J mol^{-1} K^{-1}.

Compound Name	S^{o}_{298}	$C_p{}^{\bullet}(T)$	
		300 K	1000 K
3-bromo-2-chlorophenol	8.14	-2.30	-3.97
3-bromo-5-chlorophenol	-1.20	1.88	-0.84
3-bromo-4-chlorophenol	-2.58	1.30	1.21
2-bromo-4-chlorophenol	-1.72	1.71	1.09
2-bromo-5-chlorophenol	-2.17	33.0	16.9
4-bromo-3-chlorophenol	-0.89	1.96	-0.96
2-bromo-3-chlorophenol	-2.42	1.38	1.25
2-bromo-6-chlorophenol	-1.58	1.67	0.71
3-bromo-6-chlorophenol	-1.42	1.76	0.79
4-bromo-2-chlorophenol	-1.60	1.66	0.71
3-bromo-2-chlorophenol	-1.63	1.67	0.92
2-bromo-4,5-dichlorophenol	-2.10	1.50	1.00
3-bromo-4,5-dichlorophenol	-0.66	2.04	-1.00
2-bromo-3,4-dichlorophenol	-3.11	1.09	1.17
4-bromo-2,6-dichlorophenol	-0.69	2.01	0.08
3-bromo-2,6-dichlorophenol	-1.01	1.88	0.33
2-bromo-3,6-dichlorophenol	-1.38	1.71	0.63
3-bromo-2,5-dichlorophenol	-1.70	1.67	0.88
3-bromo-2,4-dichlorophenol	-2.20	1.46	1.21
4-bromo-2,3-dichlorophenol	-1.82	1.59	0.84

3-bromo-2,4,6-trichlorophenol	-0.74	2.01	0.29
3-bromo-2,4,5-trichlorophenol	-2.06	1.46	0.79
4-bromo-2,3,5-trichlorophenol	-1.40	1.76	0.84
2-bromo-4,5,6-trichlorophenol	-1.09	1.92	0.63
3-bromo-4,5,6-trichlorophenol	-1.84	1.55	0.75
4-bromo-2,3,6-trichlorophenol	-11.7	-4.85	-0.71
4-bromo-2,3,5,6-tetrachlorophenol	-0.63	2.09	0.33
3-bromo-2,4,5,6-tetrachlorophenol	12.4	2.47	0.33
2-bromo-3,4,5,6-tetrachlorophenol	-1.63	1.67	0.84
3,4-dibromo-6-chlorophenol	-1.98	1.50	0.66
2,4-dibromo-6-chlorophenol	-36.0	1.67	0.67
3,4-dibromo-5-chlorophenol	-1.75	1.76	-0.96
2,6-dibromo-4-chlorophenol	-1.16	1.88	0.63
3,4-dibromo-2-chlorophenol	-1.43	1.80	0.92
2,6-dibromo-3-chlorophenol	-1.11	1.92	0.88
2,5-dibromo-3-chlorophenol	6.74	2.13	1.30
2,4-dibromo-3-chlorophenol	-2.15	1.30	1.21
2,3-dibromo-4-chlorophenol	-2.30	1.42	1.25
2,3-dibromo-5,6-dichlorophenol	-1.16	1.88	0.92
2,3-dibromo-4,5-dichlorophenol	-4.94	17.1	8.57
2,4-dibromo-3,6-dichlorophenol	-1.55	1.71	0.88
2,6-dibromo-3,5-dichlorophenol	-1.17	1.92	0.92
2,4-dibromo-3,5-dichlorophenol	-1.79	1.67	1.21
2,6-dibromo-3,4-dichlorophenol	-1.31	1.84	0.79

3,4-dibromo-2,6-dichlorophenol	-1.48	1.67	0.29
2,3-dibromo-4,6-dichlorophenol	-1.30	1.84	0.88
3,5-dibromo-4,6-dichlorophenol	-1.81	1.55	0.79
2,6-dibromo-3,4,5-trichlorophenol	-1.15	1.88	0.79
3,4-dibromo-2,5,6-trichlorophenol	-0.99	1.88	0.38
2,4-dibromo-3,5,6-trichlorophenol	-1.68	1.67	0.88
2,3-dibromo-4,5,6-trichlorophenol	-1.22	1.88	0.88
2,3,4-tribromo-6-chlorophenol	-37.5	1.84	0.92
2,3,4-tribromo-5-chlorophenol	-2.50	1.34	1.25
2,3,6-tribromo-4-chlorophenol	-2.22	1.50	1.25
2,3,5-tribromo-4-chlorophenol	-2.46	1.38	1.21
2,4,6-tribromo-3-chlorophenol	-1.54	1.71	0.88
2,4,5-tribromo-3-chlorophenol	-1.99	1.55	17.9
2,3,4-tribromo-5,6-dichlorophenol	-1.57	1.67	0.88
2,3,5-tribromo-4,6-dichlorophenol	-2.24	3.51	1.30
2,5,6-tribromo-3,4-dichlorophenol	-1.47	1.71	0.84
3,4,5-tribromo-2,6-dichlorophenol	-0.69	2.05	0.33
2,3,4,5-tetrabromo-6-chlorophenol	-1.26	1.84	0.88
2,3,4,6-tetrabromo-5-chlorophenol	-38.8	1.84	0.92
2,3,5,6-tetrabromo-4-chlorophenol	-1.21	1.88	0.88

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Table 3. $\Delta_f H^\circ_{298}$ (kJ mol^{-1}) and $\Delta_R H^\circ_{298}$ (kJ mol^{-1}) for all mixed brominated and chlorinated

676 congeners of phenol.

Compound Name	$\Delta_{R1} H^\circ_{298}$	$\Delta_{R2} H^\circ_{298}$	$\Delta_{f1} H^\circ_{298}$	$\Delta_{f2} H^\circ_{298}$	$\Delta_{favg} H^\circ_{298}$
3-bromo-2-chlorophenol	-9.78	-1.1	-102.9	-102.9	-102.9
3-bromo-5-chlorophenol	-15.1	-6.5	-97.6	-97.6	-97.6
3-bromo-4-chlorophenol	-24.5	-15.9	-88.2	-88.2	-88.2
2-bromo-4-chlorophenol	-10.4	-1.8	-102.3	-102.3	-102.3
2-bromo-5-chlorophenol	-7.77	0.9	-104.9	-105.0	-104.9
4-bromo-3-chlorophenol	-23.7	-15.1	-89.0	-89.0	-89.0
2-bromo-3-chlorophenol	-15.4	-6.8	-97.3	-97.3	-97.3
2-bromo-6-chlorophenol	-15.7	-7.0	-97.0	-97.1	-97.1
3-bromo-6-chlorophenol	-9.79	-1.1	-102.9	-102.9	-102.9
4-bromo-2-chlorophenol	-11.5	-2.9	-101.2	-101.2	-101.2
3-bromo-2-chlorophenol	-17.3	-8.7	-95.4	-95.4	-95.4
2-bromo-4,5-dichlorophenol	-28.6	-16.4	-118.8	-95.5	-107.2
3-bromo-4,5-dichlorophenol	-43.5	-31.3	-103.9	-103.2	-103.6
2-bromo-3,4-dichlorophenol	-35.8	-23.6	-111.6	-110.8	-111.2
4-bromo-2,6-dichlorophenol	-30.3	-18.1	-117.1	-116.3	-116.7
3-bromo-2,6-dichlorophenol	-30.7	-18.5	-116.7	-115.9	-116.3
2-bromo-3,6-dichlorophenol	-29.2	-17.0	-118.2	-117.4	-117.8
3-bromo-2,5-dichlorophenol	-28.3	-16.1	-119.1	-118.3	-118.7
3-bromo-2,4-dichlorophenol	-37.9	-25.7	-109.5	-108.8	-109.1
4-bromo-2,3-dichlorophenol	-37.1	-24.9	-110.3	-109.6	-109.9
3-bromo-2,4,6-trichlorophenol	-58.3	-42.6	-123.8	-122.3	-123.0

3-bromo-2,4,5-trichlorophenol	-59.3	-43.6	-122.8	-121.3	-122.0
4-bromo-2,3,5-trichlorophenol	-58.8	-43.0	-123.3	-121.8	-122.6
2-bromo-4,5,6-trichlorophenol	-56.6	-40.8	-125.6	-124.0	-124.8
3-bromo-4,5,6-trichlorophenol	-59.1	-43.4	-123.0	-121.4	-122.2
4-bromo-2,3,6-trichlorophenol	-57.8	-42.0	-124.3	-122.8	-123.6
4-bromo-2,3,5,6-tetrachlorophenol	-89.1	-69.9	-127.7	-125.4	-126.5
3-bromo-2,4,5,6-tetrachlorophenol	-87.0	-67.7	-129.8	-127.5	-128.6
2-bromo-3,4,5,6-tetrachlorophenol	-87.0	-67.7	-129.8	-127.5	-128.6
3,4-dibromo-6-chlorophenol	-32.4	-18.7	-62.0	-62.8	-62.4
2,4-dibromo-6-chlorophenol	-30.2	-16.5	-64.2	-65.0	-64.6
3,4-dibromo-5-chlorophenol	-46.0	-32.3	-48.4	-49.2	-48.8
2,6-dibromo-4-chlorophenol	-29.7	-15.9	-64.7	-65.6	-65.1
3,4-dibromo-2-chlorophenol	-40.2	-26.4	-54.2	-55.1	-54.6
2,6-dibromo-3-chlorophenol	-33.8	-20.0	-60.6	-61.5	-61.0
2,5-dibromo-3-chlorophenol	-28.1	-14.4	-66.3	-67.1	-66.7
2,4-dibromo-3-chlorophenol	-37.3	-23.6	-57.1	-57.9	-57.5
2,3-dibromo-4-chlorophenol	-38.9	-25.2	-55.5	-56.3	-55.9
2,3-dibromo-5,6-dichlorophenol	-56.3	-39.0	-72.8	-72.9	-72.8
2,3-dibromo-4,5-dichlorophenol	-60.4	-43.1	-68.7	-68.7	-68.7
2,4-dibromo-3,6-dichlorophenol	-57.8	-40.5	-71.3	-71.3	-71.3
2,6-dibromo-3,5-dichlorophenol	-54.3	-37.0	-74.8	-74.9	-74.8
2,4-dibromo-3,5-dichlorophenol	-58.9	-41.6	-70.2	-70.2	-70.2
2,6-dibromo-3,4-dichlorophenol	-56.8	-39.5	-72.3	-72.4	-72.4
3,4-dibromo-2,6-dichlorophenol	-60.4	-43.1	-68.7	-68.7	-68.7

2,3-dibromo-4,6-dichlorophenol	-59.3	-42.0	-69.8	-69.9	-69.8
3,5-dibromo-4,6-dichlorophenol	-61.4	-44.1	-67.7	-67.8	-67.8
2,6-dibromo-3,4,5-trichlorophenol	-88.2	-67.4	-75.6	-74.9	-75.2
3,4-dibromo-2,5,6-trichlorophenol	-92.3	-71.5	-71.5	-70.8	-71.1
2,4-dibromo-3,5,6-trichlorophenol	-89.3	-68.4	-74.5	-73.8	-74.2
2,3-dibromo-4,5,6-trichlorophenol	-90.6	-69.7	-73.2	-72.5	-72.9
2,3,4-tribromo-6-chlorophenol	-61.7	-42.8	-14.4	-16.1	-15.2
2,3,4-tribromo-5-chlorophenol	-63.2	-44.4	-12.9	-14.5	-13.7
2,3,6-tribromo-4-chlorophenol	-59.6	-40.8	-16.5	-18.1	-17.3
2,3,5-tribromo-4-chlorophenol	-62.6	-43.7	-13.5	-15.2	-14.3
2,4,6-tribromo-3-chlorophenol	-58.1	-39.2	-18.0	-19.7	-18.9
2,4,5-tribromo-3-chlorophenol	-61.9	-43.1	20.5	-15.8	2.3
2,3,4-tribromo-5,6-dichlorophenol	-93.5	-71.1	-17.3	-18.2	-17.8
2,3,5-tribromo-4,6-dichlorophenol	-93.1	-70.7	-17.7	-18.5	-18.1
2,5,6-tribromo-3,4-dichlorophenol	-91.1	-68.7	-19.7	-20.6	-20.1
3,4,5-tribromo-2,6-dichlorophenol	-96.2	-73.8	-14.6	-15.5	-15.1
2,3,4,5-tetrabromo-6-chlorophenol	-97.4	-73.4	39.6	37.1	38.3
2,3,4,6-tetrabromo-5-chlorophenol	-94.6	-70.7	36.9	34.4	35.7
2,3,5,6-tetrabromo-4-chlorophenol	-95.3	-71.3	37.5	35.0	36.3

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679 **Table 4.** Calculated uncertainty in $\Delta_fH°_{298}$ of three congeners of bromochlorophenol in kJ

680 mol^{-1}.

Compound Name	Reaction 1 u_j	Reaction 2 u_j	Overall uncertainty
3-bromo-2-chlorophenol	2.2	2.7	1.7
3,4-dibrmo-2-chlorophenol	4.4	4.7	3.2
2,4,5-tribromo-3-chlorophenol	6.5	6.7	4.6

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Table 5. $\Delta_{R3}H°_{298}$ for R3 (kJ), $\Delta_fH°_{298}$ (kJ mol^{-1}) of selected bromochlorophenoxy radicals and BDH of the O-H bond in selected BCP molecules (kJ mol^{-1}).

Compound Name	$\Delta_{R3}H°_{298}$	$\Delta_fH°_{298}$	BDH
3-bromo-2-chlorophenoxy radical	-106.6	77.1	390.4
4-bromo-3-chlorophenoxy radical	-115.0	75.2	382.0
2-bromo-4-chlorophenoxy radical	-112.6	64.5	384.4
3-bromo-2,4-dichlorophenoxy radical	-111.1	59.0	385.9
4-bromo-2,3,6-trichlorophenoxy radical	-116.4	38.7	380.6
3-bromo-4,5,6-trichloro-phenoxy radical	-107.6	48.5	389.4
2-bromo-3,4,5,6-tetrachlorophenoxy radical	-111.9	38.2	385.1
3,4-dibromo-2-chlorophenoxy radical	-109.9	115.0	387.0
2,6-dibromo-4-chlorophenoxy radical	-117.9	96.5	379.0
2,3-dibromo-4-chlorophenoxy radical	-109.7	114.3	387.3
3,5-dibromo-2,4-dichlorophenoxy radical	-107.4	104.0	389.6
2,3-dibromo-6,4-dichlorophenoxy radical	-116.0	93.3	381.0
2,3-dibromo-4,5,6-trichloro-phenoxy radical	-113.9	92.0	383.0
2,4,5-tribromo-3-chlorophenoxy radical	-104.7	194.9	392.2
2,3,5-tribromo-4-chlorophenoxy radical	-106.2	159.4	390.8
2,3,6-tribromo-4-chlorophenoxy radical	-115.3	147.3	381.7
3,4,5-tribromo-2,6-dichlorophenoxy radical	-113.9	150.6	383.1
2,5,6-tribromo-3,4-dichlorophenoxy radical	-113.0	146.4	384.0
2,3,5,6-tetrabromo-4-chlorophenoxy radical	-113.7	202.9	383.3

Table 6. Standard Gibbs energies of formation in the gas phase $\Delta_f G^\circ_{298}$, Gibbs ~~free~~ energies of solvation $\Delta_{solv} G^*$, and standard Gibbs energies in the aqueous phase $\Delta_f G^{aq}_{298}$ for selected mixed halogenated congeners of phenol. Note that, $\Delta_f G^\circ_{298}$ for the remaining BCPs can be obtained directly from Equation E2. All values are in kJ mol^{-1}.

Compound Name	$\Delta_f G^\circ_{298}$	ΔG^*_{solv}	$\Delta_f G^{aq}_{298}$
Phenol	308.6	-26.9	281.7
o-chlorophenol	272.3	-20.1	252.2
m-chlorophenol	291.8	-27.7	264.2
p-chlorophenol	299.4	-28.0	271.4
o-bromophenol	367.2	-20.0	347.2
3-bromo-2-chlorophenol	356.7	-21.1	335.6
4-bromo-3-chlorophenol	362.1	-29.3	332.7
2-bromo-4-chlorophenol	349.7	-20.3	329.3
3-bromo-2,4-dichlorophenol	349.5	-22.3	327.2
4-bromo-2,3,6-trichlorophenol	343.6	-23.5	320.1
3-bromo-4,5,6-trichlorophenol	341.7	-21.8	319.8
3,4-dibromo-2-chlorophenol	403.6	-22.6	380.9
2,6-dibromo-4-chlorophenol	392.7	-28.3	364.4
2,3-dibromo-4-chlorophenol	403.1	-21.9	381.2
3,5-dibromo-4,6-dichlorophenol	396.6	-22.4	374.2
2,3-dibromo-4,6-dichlorophenol	394.3	-23.3	371.0
2,6-dibromo-3,5-dichlorophenol	389.3	-29.4	359.9
2,3-dibromo-4,5,6-trichlorophenol	397.8	-24.1	373.7
2,4,5-tribromo-3-chlorophenol	486.5	-22.1	464.4

2,3,5-tribromo-4-chlorophenol	450.6	-22.1	428.5
2,3,6-tribromo-4-chlorophenol	447.8	-23.5	423.8
3,4,5-tribromo-2,6-dichlorophenol	455.8	-31.7	424.1
2,5,6-tribromo-3,4-dichlorophenol	450.6	-30.9	419.9
2,3,5,6-tetrabromo-4-chlorophenol	507.9	-31.8	476.2

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Table 7. Calculated pK_a values of phenol and selected halogenated phenols.

Compound Name	$\Delta_{R8}G^{\bullet}_g$	$\Delta G^{*}_{solv}{}^{II}_s$	$\Delta_{R9}G_{dis}$	calc pK_a	exptl pK_a	p$K_a{}^{81}$	Marvin pK_a
Phenol	1398.1	-268.7	56.1	9.83	9.98 [94]	9.88	10.02
o-chlorophenol	1385.3	-254.3	50.8	8.9	8.56 [92]	7.66	8.0
m-chlorophenol	1375.4	-246.9	50.0	9.8	9.12 [92]	9.29	8.8
p-chlorophenol	1369.0	-248.5	49.3	8.6	9.3 [92]	9.84	8.9
o-bromophenol	1380.4	-250.3	49.9	8.7	8.5 [93]		8.2
3-bromo-2-chlorophenol	1356.9	-237.6	40.3	7.1			7.3
4-bromo-3-chlorophenol	1349.8	-226.9	52.1	9.1			
2-bromo-4-chlorophenol	1355.0	-229.4	45.7	8.0			
3-bromo-2,4-dichlorophenol	1338.9	-222.5	38.5	6.7			
4-bromo-2,3,6-trichlorophenol	1306.7	-210.1	19.9	3.4			
3-bromo-4,5,6-trichlorophenol	1314.8	-208.3	28.1	4.9			
3,4-dibromo-2-chlorophenol	1335.4	-220.0	37.8	6.6			
2,6-dibromo-4-chlorophenol	1320.8	-215.9	33.0	5.7			
2,3-dibromo-4-chlorophenol	1336.8	-223.0	35.6	6.2			
3,5-dibromo-4,6-dichlorophenol	1313.9	-208.0	28.2	4.9			
2,3-dibromo-4,6-dichlorophenol	1307.4	-210.1	20.5	3.6			
2,6-dibromo-3,5-dichlorophenol	1301.4	-206.9	23.9	4.1			
2,3-dibromo-4,5,6-trichlorophenol	1291.2	-201.8	13.4	2.3			
2,4,5-tribromo-3-chlorophenol	1310.9	-205.0	27.8	4.8			
2,3,5-tribromo-4-chlorophenol	1312.3	-206.1	28.2	4.9			

2,3,6-tribromo-4-chlorophenol	1304.4	-207.6	20.2	3.5
3,4,5-tribromo-2,6-dichlorophenol	1289.8	-202.4	19.1	3.3
2,5,6-tribromo-3,4-dichlorophenol	1289.7	-200.3	20.2	3.5
2,3,5,6-tetrabromo-4-chlorophenol	1290.7	-200.3	22.0	3.8

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