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Supplementary information for

Mechanism and thermal rate constants for complete series reactions of bromochlorophenols with H

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Keywords

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Table S1. Comparision of the bond lengths of C–O and O–H bonds (in Å) of the selected BCPs, the O–H bond dissociation enthalpies BDH (in kcal/mol, 298.15 K) for bromochlorophenols (BCPs) and the standard enthalpies of the formation $\Delta_R H^{\circ}_{298}$ for reactions of BCPs + OH → BCPRs + H_2O (in kcal/mol, 298.15 K) at MPWB1K/6-311+G(3df,2p)//MPWB1K/6-31+G(d,p) level involving in this study and those at M062X/6-311+G(3df,2p)//M062X/6-311+G(d,p) level by Saeed. [68] (Reproduced with permission from A. Saeed.[68] Copyright 2015, American Chemical Society).

Table S2. Imaginary frequencies v (in cm^{-1}), zero point energies and total energies of the transition states involved in this study and the O-H bond dissociation energies D_0(O–H) (in kcal/mol, 0 K, including ZPE correction) of the reactions of bromochlorophenols (BCPs) with H. For comparison, the D_0(O–H) of the reactions of bromophenols (BPs)[a] and chlorophenols (CPs)[b] with H are also provided ([a] Reproduced with permission from R. Gao et al.[53] Copyright 2013, Elsevier. [b] Reproduced with permission from Q. Z. Zhang et al.[52] Copyright 2009, American Chemical Society).

Table S3. Potential barrier ΔE_0 (in kcal/mol, 0 K, including ZPE correction) and reaction heat ΔH_0 (in kcal/mol, 0 K, including ZPE correction) for reactions of anti-BCPs with H. For comparison, ΔE_0 and ΔH_0 of reactions of anti-BPs[a] and anti-CPs[b] with H are also calculated. ([a]Reproduced with permission from R. Gao et al.[29]

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Table S4. Arrhenius formulas for reaction of the anti-BCPs with H over the temperature range 600–1200 K (cm^3 $molecule^{-1}$ s^{-1})

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Figure S2. MPWB1K/6-31+G(d,p) optimized geometries for 96 congeners of bromochlorophenols (BCPs). Distance are in angstroms. gray sphere, C; white sphere, H; red sphere, O; blue sphere, Br; green sphere, Cl;

Figure S3. MPWB1K/6-31+G(d,p) optimized geometries for transition states of 96 congeners of bromochlorophenols with H. Distance are in angstroms. Gray sphere, C; white sphere, H; red sphere, O; blue sphere, Br; green sphere, Cl;

Figure S4. MPWB1K/6-31+G(d,p) optimized geometries for 96 congeners of bromochlorophenoxy radicals (BCPRs). Distance are in angstroms. Gray sphere, C; white sphere, H; red sphere, O; green sphere, Cl; blue sphere, Br.

Table S1. Comparision of the bond lengths of C–O and O–H bonds (in Å) of the selected BCPs, the O–H bond dissociation enthalpies BDH (in kcal/mol, 298.15 K) for bromochlorophenols (BCPs) and the standard enthalpies of the formation $\Delta_R H^{\circ}_{298}$ for reactions of BCPs + OH → BCPRs + H_2O (in kcal/mol, 298.15 K) at MPWB1K/6-311+G(3df,2p)//MPWB1K/6-31+G(d,p) level involving in this study and those at M062X/6-311+G(3df,2p)//M062X/6-311+G(d,p) level by Saeed. [68] (Reproduced with permission from A. Saeed.[68] Copyright 2015, American Chemical Society).

BCP	C–O		O–H		BDH		$\Delta_R H^{\circ}_{298}$	
	MPWB1K	M062X	MPWB1K	M062X	MPWB1K	M062	MPWB1K	M062X
3B-2CP	1.338	1.352	0.958	0.961	94.35	93.27	-26.01	-25.47
4B-3CP	1.346	1.357	0.954	0.961	91.68	91.26	-28.68	-27.47
2B-4CP	1.339	1.430	0.959	0.960	92.64	91.83	-27.72	-26.90
3B-2,4DCP	1.337	1.352	0.959	0.961	92.95	92.19	-25.08	-26.54
4B-2,3,6TCP	1.331	-	0.959	-	91.88	90.93	-28.48	-27.81
3B-4,5,6TCP	1.335	1.349	0.959	0.961	93.71	93.03	-26.65	-25.71
2B-3,4,5,6TeCP	1.329	1.339	0.960	0.966	92.26	92.00	-28.10	-26.73
3,4DB-2CP	1.336	1.352	0.958	0.961	93.25	92.45	-27.11	-26.26
2,6DB-4CP	1.332	1.342	0.960	0.965	91.25	90.54	-29.11	-28.17
2,3DB-4CP	1.337	1.352	0.960	0.961	93.19	92.53	-27.17	-26.21
3,5DB-2,4DCP	1.335	1.349	0.959	0.961	93.85	93.08	-26.51	-25.66
2,3DB-4,6DCP	1.330	1.340	0.960	0.965	91.66	91.02	-28.70	-27.71
2,3DB-4,5,6TCP	1.329	1.339	0.961	0.966	92.25	91.50	-28.11	-27.21
2,4,5TB-3CP	1.334	1.349	0.960	0.961	94.53	93.70	-25.83	-25.01
2,3,5TB-4CP	1.335	1.349	0.961	0.961	94.58	93.36	-25.78	-25.37
2,3,6TB-4CP	1.331	1.342	0.961	0.966	91.74	91.19	-28.62	-27.55
3,4,5TB-2,6DCP	1.330	1.340	0.960	0.965	92.16	91.52	-28.20	-27.21
2,3,6TB-4,5DCP	1.330	1.339	0.961	0.966	92.21	91.74	-28.20	-27.00
2,3,5,6TeB-4CP	1.331	1.430	0.961	0.960	92.14	91.57	-28.22	-27.16

Table S2. Imaginary frequencies v (in cm^{-1}), zero point energies and total energies of the transition states involved in this study and the O-H bond dissociation energies D_0(O–H) (in kcal/mol, 0 K, including ZPE correction) of the reactions of bromochlorophenols (BCPs) with H. For comparison, the D_0(O–H) of the reactions of bromophenols (BPs)[a] and chlorophenols (CPs)[b] with H are also provided ([a] Reproduced with permission from R. Gao et al.[53] Copyright 2013, Elsevier. [b] Reproduced with permission from Q. Z. Zhang et al.[52] Copyright 2009, American Chemical Society).

BCP	*v*	ZPE	Total energy	D_0(O-H)	BP	D_0(O-H)[a]	CP	D_0(O-H)[b]
2B-3CP	-2214i	0.08526	-3341.45531	86.82	2,3-DBP	86.71	2,3-DCP	86.71
3B-2CP	-2223i	0.08530	-3341.45485	86.62				
2B-4CP	-2228i	0.08499	-3341.45836	84.89	2,4-DBP	84.11	2,4-DCP	85.58
4B-2CP	-2232i	0.08521	-3341.45821	84.94				
2B-5CP	-2212i	0.08523	-3341.45792	86.89	2,5-DBP	86.92	2,5-DCP	86.77
3B-6CP	-2219i	0.08504	-3341.45762	86.78				
2B-6CP	-2235i	0.08475	-3341.45634	84.83	2,6-DBP	84.94	2,6-DCP	84.66
3B-4CP	-2200i	0.08485	-3341.45501	83.76	3,4-DBP	84.04	3,4-DCP	83.89
4B-3CP	-2202i	0.08509	-3341.45499	84.02				
3B-5CP	-2202i	0.08441	-3341.45683	86.08	3,5-DBP	86.03	3,5-DCP	86.17
2B-3,4DCP	-2232i	0.07562	-3801.13313	85.55	2,3,4-TBP	85.71	2,3,4-TCP	85.37
3B-2,4DCP	-2233i	0.07598	-3801.13249	85.23				
4B-2,3DCP	-2236i	0.07580	-3801.13282	85.67				
2,3DB-4CP	-2235i	0.07630	-5915.33243	85.43				
2,4DB-3CP	-2236i	0.07606	-5915.33282	85.82				
3,4DB-2CP	-2231i	0.07619	-5915.33194	85.54				
2B-3,5DCP	-2209i	0.07573	-3801.13515	87.71	2,3,5-TBP	87.49	2,3,5-TCP	87.50
3B-2,5DCP	-2218i	0.07548	-3801.13481	87.41				
3B-5,6DCP	-2211i	0.07543	-3801.13501	87.36				
2,3DB-5CP	-2211i	0.07607	-5915.33478	87.59				
2,5DB-3CP	-2209i	0.07553	-5915.33512	87.59				
3,5DB-2CP	-2209i	0.07548	-5915.33486	87.37				
2B-3,6DCP	-2232i	0.07545	-3801.13387	85.32	2,3,6-TBP	85.30	2,3,6-TCP	85.11
2B-5,6DCP	-2231i	0.07517	-3801.13398	85.26				
3B-2,6DCP	-2239i	0.07555	-3801.13362	85.08				
2,3DB-6CP	-2227i	0.07593	-5915.33360	85.14				
2,5DB-6CP	-2239i	0.07545	-5915.33380	85.14				
2,6DB-3CP	-2215i	0.07548	-5915.33402	85.49				

Table S2. *Cont*.

BCP	*v*	ZPE	Total energy	D_0(O-H)	BP	D_0(O-H)[a]	CP	D_0(O-H)[b]
2B-4,5DCP	-2235i	0.07514	-3801.13594	85.56	2,4,5-TBP	85.86	2,4,5-TCP	85.37
3B-4,6DCP	-2232i	0.07556	-3801.13533	85.30				
4B-2,5DCP	-2235i	0.07575	-3801.13543	85.71				
2,4DB-5CP	-2230i	0.07582	-5915.33578	85.84				
2,5DB-4CP	-2232i	0.07546	-5915.33564	85.60				
3,4DB-6CP	-2229i	0.07595	-5915.33489	85.65				
2B-4,6DCP	-2236i	0.07513	-3801.13669	83.42	2,4,6-TBP	83.76	2,4,6-TCP	83.29
4B-2,6DCP	-2239i	0.07522	-3801.13633	83.53				
2,4DB-6CP	-2240i	0.07504	-5915.33669	83.68				
2,6DB-4CP	-2196i	0.07492	-5915.33673	83.48				
3B-4,5DCP	-2210i	0.07539	-3801.13188	84.66	3,4,5-TBP	85.11	3,4,5-TCP	84.79
4B-3,5DCP	-2207i	0.07535	-3801.13159	85.11				
3,4DB-5CP	-2210i	0.07606	-5915.33117	85.07				
3,5DB-4CP	-2207i	0.07571	-5915.33164	84.71				
2B-3,4,5TCP	-2232i	0.06564	-4260.80952	86.32	2,3,4,5-TeBP	87.37	2,3,4,5-TeCP	86.14
3B-2,4,5TCP	-2234i	0.06618	-4260.80884	86.16				
3B-4,5,6TCP	-2226i	0.06581	-4260.80911	85.97				
4B-2,3,5TCP	-2230i	0.06616	-4260.80883	86.48				
2,3DB-4,5DCP	-2231i	0.06637	-6375.00873	86.43				
2,4DB-3,5DCP	-2227i	0.06647	-6375.00899	86.79				
2,5DB-3,4DCP	-2224i	0.06607	-6375.00931	87.03				
3,4DB-2,5DCP	-2227i	0.06721	-6375.00800	86.47				
3,4DB-5,6DCP	-2232i	0.06614	-6375.00834	86.41				
3,5DB-2,4DCP	-2233i	0.06635	-6375.00872	86.14				
2,3,4TB-5CP	-2230i	0.06677	-8489.20776	87.03				
2,3,5TB-4CP	-2230i	0.06632	-8489.20847	86.84				
2,4,5TB-3CP	-2227i	0.06691	-8489.20848	86.80				
3,4,5TB-2CP	-2230i	0.06759	-8489.20752	86.50				
2B-3,4,6TCP	-2237i	0.06573	-4260.81093	83.99	2,3,4,6-TeBP	84.35	2,3,4,6-TeCP	83.93
2B-4,5,6TCP	-2237i	0.06532	-4260.81102	83.85				
3B-2,4,6TCP	-2241i	0.06588	-4260.81044	83.87				
4B-2,3,6TCP	-2239i	0.06602	-4260.81056	84.19				
2,3DB-4,6DCP	-2234i	0.06656	-6375.01033	83.90				
2,4DB-3,6DCP	-2241i	0.06604	-6375.01087	84.38				
2,4DB-5,6DCP	-2240i	0.06612	-6375.01085	84.04				
2,5DB-4,6DCP	-2238i	0.06581	-6375.01062	83.75				
2,6DB-3,4DCP	-2209i	0.06586	-6375.01088	84.06				

Table S2. *Cont*.

BCP	*v*	ZPE	Total energy	D_0(O-H)	BP	D_0(O-H)[a]	CP	D_0(O-H)[b]
3,4DB-2,6DCP	-2243i	0.06644	-6375.00997	84.17				
2,3,4TB-6CP	-2235i	0.06687	-8489.20975	84.26				
2,3,6TB-4CP	-2208i	0.06652	-8489.21024	83.97				
2,4,5TB-6CP	-2239i	0.06663	-8489.21022	83.94				
2,4,6TB-3CP	-2210i	0.06608	-8489.21068	84.50				
2B-3,5,6TCP	-2236i	0.06568	-4260.81075	85.83	2,3,5,6-TeBP	85.93	2,3,5,6-TeCP	85.61
3B-2,5,6TCP	-2243i	0.06567	-4260.81055	85.54				
2,3DB-5,6DCP	-2234i	0.06579	-6375.01046	85.71				
2,5DB-3,6DCP	-2232i	0.06589	-6375.01068	85.66				
2,6DB-3,5DCP	-2206i	0.06604	-6375.01047	85.76				
3,5DB-2,6DCP	-2238i	0.06591	-6375.01040	85.58				
2,3,5TB-6CP	-2239i	0.06601	-8489.21029	85.89				
2,3,6TB-5CP	-2210i	0.06571	-8489.21013	86.04				
2B-3,4,5,6TeCP	-2239i	0.05555	-4720.48414	84.52	PBP	84.76	PCP	84.38
3B-2,4,5,6TeCP	-2246i	0.05550	-4720.48350	84.40				
4B-2,3,5,6TeCP	-2248i	0.05576	-4720.48341	84.71				
2,3DB-4,5,6TCP	-2240i	0.05583	-6834.68335	84.50				
2,4DB-3,5,6TCP	-2247i	0.05666	-6834.68351	84.81				
2,5DB-3,4,6TCP	-2245i	0.05686	-6834.68361	84.43				
2,6DB-3,4,5TCP	-2213i	0.05534	-6834.68389	84.56				
3,4DB-2,5,6TCP	-2246i	0.05694	-6834.68256	84.51				
3,5DB-2,4,6TCP	-2245i	0.05653	-6834.68307	84.31				
2,3,4TB-5,6DCP	-2243i	0.05714	-8948.88242	84.79				
2,3,5TB-4,6DCP	-2243i	0.05692	-8948.88290	84.42				
2,3,6TB-4,5DCP	-2213i	0.05743	-8948.88308	84.45				
2,4,5TB-3,6DCP	-2242i	0.05705	-8948.88263	84.63				
2,4,6TB-3,5DCP	-2214i	0.05659	-8948.88321	84.97				
3,4,5TB-2,6DCP	-2241i	0.05766	-8948.88169	84.47				
2,3,4,5TeB-6CP	-2239i	0.05736	-11063.08142	84.71				
2,3,4,6TeB-5CP	-2215i	0.05718	-11063.08203	84.86				
2,3,5,6TeB-4CP	-2211i	0.05742	-11063.08221	84.39				

Table S3. Potential barrier ΔE_0 (in kcal/mol, 0 K, including ZPE correction) and reaction heat ΔH_0 (in kcal/mol, 0 K, including ZPE correction) for reactions of anti-BCPs with H. For comparison, ΔE_0 and ΔH_0 of reactions of anti-BPs[a] and anti-CPs[b] with H are also calculated. ([a]Reproduced with permission from R. Gao et al.[29] Copyright 2013, Elsevier. [b]Reproduced with permission from Q. Z. Zhang et al.[28] Copyright 2009, American Chemical Society).

BCP^{anti}	**ΔE_0**	**ΔH_0**	**BP^{anti}**	**$\Delta E_0{}^a$**	**$\Delta H_0{}^a$**	**CP^{anti}**	**$\Delta E_0{}^b$**	**$\Delta H_0{}^b$**
2B-3CP^{anti}	10.55	-14.74	2,3-DBP^{anti}	10.79	-14.92	2,3-DCP^{anti}	10.83	-14.64
3B-2CP^{anti}	10.88	-14.79						
2B-4CP^{anti}	10.12	-16.46	2,4-DBP^{anti}	10.17	-16.76	2,4-DCP^{anti}	10.48	-16.04
4B-2CP^{anti}	10.44	-16.26						
2B-5CP^{anti}	11.10	-14.42	2,5-DBP^{anti}	11.08	-14.52	2,5-DCP^{anti}	11.13	-14.32
3B-6CP^{anti}	11.10	-14.40						
2B-3,4DCP^{anti}	10.21	-16.15	2,3,4-TBP^{anti}	10.37	-16.36	2,3,4-TCP^{anti}	10.37	-15.73
3B-2,4DCP^{anti}	10.57	-16.19						
4B-2,3DCP^{anti}	10.49	-15.80						
2,3DB-4CP^{anti}	10.01	-16.29						
2,4DB-3CP^{anti}	10.31	-15.83						
3,4DB-2CP^{anti}	10.39	-15.92						
2B-3,5DCP^{anti}	11.20	-13.87	2,3,5-TBP^{anti}	11.27	-14.08	2,3,5-TCP^{anti}	11.16	-13.87
3B-2,5DCP^{anti}	11.45	-13.99						
3B-5,6DCP^{anti}	11.49	-13.95						
2,3DB-5CP^{anti}	11.08	-14.02						
2,5DB-3CP^{anti}	11.17	-13.94						
3,5DB-2CP^{anti}	11.32	-13.96						
2B-4,5DCP^{anti}	10.43	-15.75	2,4,5-TBP^{anti}	10.63	-15.89	2,4,5-TCP^{anti}	10.76	-15.19
3B-4,6DCP^{anti}	10.62	-15.75						
4B-2,5DCP^{anti}	10.84	-15.37						
2,4DB-5CP^{anti}	10.72	-15.38						
2,5DB-4CP^{anti}	10.45	-15.65						
3,4DB-6CP^{anti}	10.77	-15.38						
2B-3,4,5TCP^{anti}	10.62	-15.39	2,3,4,5-TeBP^{anti}	10.46	-15.54	2,3,4,5-TeCP^{anti}	10.85	-13.94
3B-2,4,5TCP^{anti}	10.88	-15.20						
3B-4,5,6TCP^{anti}	11.28	-15.12						
4B-2,3,5TCP^{anti}	11.04	-14.81						
2,3DB-4,5DCP^{anti}	10.63	-15.25						
2,4DB-3,5DCP^{anti}	10.81	-14.77						
2,5DB-3,4DCP^{anti}	10.57	-14.69						
3,4DB-2,5DCP^{anti}	11.66	-14.16						
3,4DB-5,6DCP^{anti}	10.81	-14.97						
3,5DB-2,4DCP^{anti}	10.77	-15.22						
2,3,4TB-5CP^{anti}	10.67	-14.56						
2,3,5TB-4CP^{anti}	10.63	-14.75						
2,4,5TB-3CP^{anti}	10.74	-14.74						
3,4,5TB-2CP^{anti}	10.98	-14.87						

ΔE_0, potential barrier (in kcal mol^{-1}, 0 K, including ZPE correction), the relative energy of the transition state with respect to the total energy of the separated reactants. Calculated at the MPWB1K/6-311+G(3df,2p)//MPWB1K/6-31+G(d,p) level of theory. ΔH_0, reaction heat (in kcal mol^{-1}, 0 K, including ZPE correction), the relative energy of total energy of the separated products with respect to the total energy of the separated reactants. Calculated at the MPWB1K/6-311+G(3df,2p)//MPWB1K/6-31+G(d,p) level of theory.

Table S4. Arrhenius formulas for reaction of the anti-BCPs with H over the temperature range 600–1200 K (cm^3 $molecule^{-1}$ s^{-1})

Reactions	Arrhenius formulas
2B-3CP^{anti} + H → 2B-3CPR + H_2	k (T) = (9.7×10^{-12}) exp (-2966.0/T)
3B-2CP^{anti} + H → 3B-2CPR + H_2	k (T) = (3.2×10^{-12}) exp (-3197.4/T)
2B-4CP^{anti} + H → 2B-4CPR + H_2	k (T) = (7.9×10^{-12}) exp (-2951.6/T)
4B-2CP^{anti} + H → 4B-2CPR + H_2	k (T) = (2.8×10^{-12}) exp (-3070.8/T)
2B-5CP^{anti} + H → 2B-5CPR + H_2	k (T) = (7.6×10^{-12}) exp (-3450.2/T)
3B-6CP^{anti} + H → 3B-6CPR + H_2	k (T) = (2.2×10^{-13}) exp (-4125.9/T)
2B-3,4DCP^{anti} + H → 2B-3,4DCPR + H_2	k (T) = (1.0×10^{-11}) exp (-2996.7/T)
3B-2,4DCP^{anti} + H → 3B-2,4DCPR + H_2	k (T) = (4.5×10^{-12}) exp (-2895.0/T)
4B-2,3DCP^{anti} + H → 4B-2,3DCPR + H_2	k (T) = (8.1×10^{-12}) exp (-2686.1/T)
2,3DB-4CP^{anti} + H → 2,3DB-4CPR + H_2	k (T) = (8.2×10^{-12}) exp (-2799.0T)
2,4DB-3CP^{anti} + H → 2,4DB-3CPR + H_2	k (T) = (1.0×10^{-11}) exp (-3041.5/T)
3,4DB-2CP^{anti} + H → 3,4DB-2CPR + H_2	k (T) = (1.0×10^{-11}) exp (-2863.2/T)
2B-3,5DCP^{anti} + H → 2B-3,5DCPR + H_2	k (T) = (6.9×10^{-12}) exp (-3373.4/T)
3B-2,5DCP^{anti} + H → 3B-2,5DCPR + H_2	k (T) = (5.1×10^{-12}) exp (-3467.6/T)
3B-5,6DCP^{anti} + H → 3B-5,6DCPR + H_2	k (T) = (5.9×10^{-12}) exp (-3185.5/T)
2,3DB-5CP^{anti} + H → 2,3DB-5CPR + H_2	k (T) = (1.6×10^{-12}) exp (-2898.1/T)
2,5DB-3CP^{anti} + H → 2,5DB-3CPR + H_2	k (T) = (8.0×10^{-12}) exp (-3139.8/T)
3,5DB-2CP^{anti} + H → 3,5DB-2CPR + H_2	k (T) = (4.6×10^{-12}) exp (-3083.3/T)
2B-4,5DCP^{anti} + H → 2B-4,5DCPR + H_2	k (T) = (4.0×10^{-12}) exp (-2929.7/T)
3B-4,6DCP^{anti} + H → 3B-4,6DCPR + H_2	k (T) = (7.8×10^{-12}) exp (-3032.2/T)
4B-2,5DCP^{anti} + H → 4B-2,5DCPR + H_2	k (T) = (6.9×10^{-12}) exp (-2925.5/T)
2,4DB-5CP^{anti} + H → 2,4DB-5CPR + H_2	k (T) = (1.1×10^{-13}) exp (-2606.5/T)
2,5DB-4CP^{anti} + H → 2,5DB-4CPR + H_2	k (T) = (1.9×10^{-13}) exp (-2766.3/T)
3,4DB-6CP^{anti} + H → 3,4DB-6CPR + H_2	k (T) = (1.0×10^{-11}) exp (-3252.7/T)
2B-3,4,5TCP^{anti} + H → 2B-3,4,5TCPR + H_2	k (T) = (1.1×10^{-11}) exp (-3127.1/T)
3B-2,4,5TCP^{anti} + H → 3B-2,4,5TCPR + H_2	k (T) = (7.1×10^{-12}) exp (-2744.0/T)
3B-4,5,6TCP^{anti} + H → 3B-4,5,6TCPR + H_2	k (T) = (4.8×10^{-12}) exp (-3056.3/T)
4B-2,3,5TCP^{anti} + H → 4B-2,3,5TCPR + H_2	k (T) = (8.1×10^{-12}) exp (-3122.5/T)
2,3DB-4,5DCP^{anti} + H → 2,3DB-4,5DCPR + H_2	k (T) = (9.4×10^{-12}) exp (-2987.4/T)
2,4DB-3,5DCP^{anti} + H → 2,4DB-3,5DCPR + H_2	k (T) = (9.0×10^{-12}) exp (-3029.0/T)
2,5DB-3,4DCP^{anti} + H → 2,5DB-3,4DCPR + H_2	k (T) = (1.0×10^{-11}) exp (-3024.2/T)
3,4DB-2,5DCP^{anti} + H → 3,4DB-2,5DCPR + H_2	k (T) = (6.1×10^{-12}) exp (-3496.0/T)
3,4DB-5,6DCP^{anti} + H → 3,4DB-5,6DCPR + H_2	k (T) = (7.8×10^{-12}) exp (-4221.8/T)
3,5DB-2,4DCP^{anti} + H → 3,5DB-2,4DCPR + H_2	k (T) = (1.6×10^{-12}) exp (-2708.2/T)
2,3,4TB-5CP^{anti} + H → 2,3,4TB-5CPR + H_2	k (T) = (1.7×10^{-11}) exp (-3567.3/T)
2,3,5TB-4CP^{anti} + H → 2,3,5TB-4CPR + H_2	k (T) = (4.9×10^{-12}) exp (-3206.5/T)
2,4,5TB-3CP^{anti} + H → 2,4,5TB-3CPR + H_2	k (T) = (9.0×10^{-12}) exp (-2777.5/T)
3,4,5TB-2CP^{anti} + H → 3,4,5TB-2CPR + H_2	k (T) = (7.3×10^{-12}) exp (-3370.3/T)

Table S5. CVT/SCT rate constants for the reactions of the bromochlorophenols (BCPs) with H over the temperature range of 600−1200 K (cm^3 $molecule^{-1}$ s^{-1}).

T(K)	CVT/SCT Rate Constants			
	2B-3CP + H	3B-2CP + H	2B-4CP + H	4B-2CP + H
600	2.2×10^{-16}	8.5×10^{-17}	3.8×10^{-16}	1.4×10^{-16}
700	1.2×10^{-15}	4.5×10^{-16}	1.8×10^{-15}	7.0×10^{-16}
800	4.4×10^{-15}	1.7×10^{-15}	6.1×10^{-15}	2.5×10^{-15}
900	1.3×10^{-14}	4.9×10^{-15}	1.7×10^{-14}	6.9×10^{-15}
1000	3.2×10^{-14}	1.2×10^{-14}	3.8×10^{-14}	1.6×10^{-14}
1100	6.9×10^{-14}	2.5×10^{-14}	7.7×10^{-14}	3.3×10^{-14}
1200	1.3×10^{-13}	4.7×10^{-14}	1.4×10^{-13}	6.0×10^{-14}
	2B-5CP + H	3B-6CP + H	2B-6CP + H	3B-4CP + H
600	1.1×10^{-16}	2.0×10^{-17}	2.3×10^{-16}	8.2×10^{-16}
700	6.9×10^{-16}	9.9×10^{-17}	9.7×10^{-16}	3.5×10^{-15}
800	2.8×10^{-15}	3.4×10^{-16}	3.1×10^{-15}	1.1×10^{-14}
900	8.4×10^{-15}	9.3×10^{-16}	8.2×10^{-15}	2.7×10^{-14}
1000	2.1×10^{-14}	2.1×10^{-15}	1.8×10^{-14}	5.7×10^{-14}
1100	4.6×10^{-14}	4.3×10^{-15}	3.6×10^{-14}	2.6×10^{-13}
1200	8.8×10^{-14}	7.9×10^{-15}	6.4×10^{-14}	4.5×10^{-13}
	4B-3CP + H	3B-5CP + H	2B-3,4DCP + H	3B-2,4DCP + H
600	2.4×10^{-15}	7.3×10^{-16}	3.2×10^{-16}	2.7×10^{-16}
700	9.4×10^{-15}	2.4×10^{-15}	1.6×10^{-15}	1.3×10^{-15}
800	2.8×10^{-14}	7.0×10^{-15}	5.8×10^{-15}	4.3×10^{-15}
900	6.6×10^{-14}	1.8×10^{-14}	1.6×10^{-14}	1.2×10^{-14}
1000	1.4×10^{-13}	3.8×10^{-14}	3.8×10^{-14}	2.7×10^{-14}
1100	2.6×10^{-13}	7.4×10^{-14}	7.8×10^{-14}	5.4×10^{-14}
1200	4.6×10^{-13}	1.3×10^{-13}	1.5×10^{-13}	9.8×10^{-14}
	4B-2,3DCP + H	2,3DB-4CP + H	2,4DB-3CP + H	3,4DB-2CP + H
600	7.2×10^{-16}	4.1×10^{-16}	3.4×10^{-16}	6.0×10^{-16}
700	3.1×10^{-15}	1.9×10^{-15}	1.7×10^{-15}	2.8×10^{-15}
800	10.0×10^{-15}	6.3×10^{-15}	6.2×10^{-15}	9.4×10^{-15}
900	2.6×10^{-14}	1.7×10^{-14}	1.8×10^{-14}	2.5×10^{-14}
1000	5.7×10^{-14}	3.8×10^{-14}	4.1×10^{-14}	5.8×10^{-14}
1100	1.1×10^{-13}	7.7×10^{-14}	8.5×10^{-14}	1.2×10^{-13}
1200	2.0×10^{-13}	1.4×10^{-13}	1.6×10^{-13}	2.2×10^{-13}

Table S5 *Cont*.

T(K)	CVT/SCT Rate Constants			
	2B-3,5DCP + H	3B-2,5DCP + H	3B-5,6DCP + H	2,3DB-5CP + H
600	9.5×10^{-17}	7.8×10^{-17}	1.7×10^{-16}	7.2×10^{-17}
700	5.8×10^{-16}	4.9×10^{-16}	8.8×10^{-16}	3.4×10^{-16}
800	2.4×10^{-15}	2.0×10^{-15}	3.2×10^{-15}	1.2×10^{-15}
900	7.4×10^{-15}	6.3×10^{-15}	9.2×10^{-15}	3.1×10^{-15}
1000	1.9×10^{-14}	1.6×10^{-14}	2.2×10^{-14}	7.3×10^{-15}
1100	4.1×10^{-14}	3.5×10^{-14}	4.6×10^{-14}	1.5×10^{-14}
1200	8.1×10^{-14}	6.9×10^{-14}	8.7×10^{-14}	2.7×10^{-14}
	2,5DB-3CP + H	3,5DB-2CP + H	2B-3,6DCP + H	2B-5,6DCP + H
600	2.2×10^{-16}	8.6×10^{-17}	4.9×10^{-16}	4.6×10^{-16}
700	1.1×10^{-15}	5.2×10^{-16}	2.2×10^{-15}	2.2×10^{-15}
800	4.1×10^{-15}	2.1×10^{-15}	7.5×10^{-15}	7.7×10^{-15}
900	1.2×10^{-14}	6.5×10^{-15}	2.0×10^{-14}	2.1×10^{-14}
1000	2.9×10^{-14}	1.7×10^{-14}	4.6×10^{-14}	4.8×10^{-14}
1100	6.0×10^{-14}	3.6×10^{-14}	9.3×10^{-14}	9.9×10^{-14}
1200	1.1×10^{-13}	7.2×10^{-14}	1.7×10^{-13}	1.8×10^{-13}
	3B-2,6DCP + H	2,3DB-6CP + H	2,5DB-6CP + H	2,6DB-3CP + H
600	6.0×10^{-16}	6.1×10^{-16}	7.4×10^{-16}	4.6×10^{-16}
700	2.9×10^{-15}	2.9×10^{-15}	3.5×10^{-15}	2.2×10^{-15}
800	9.7×10^{-15}	9.9×10^{-15}	1.2×10^{-14}	7.5×10^{-15}
900	2.6×10^{-14}	2.7×10^{-14}	3.3×10^{-14}	2.0×10^{-14}
1000	5.9×10^{-14}	6.2×10^{-14}	7.4×10^{-14}	4.7×10^{-14}
1100	1.2×10^{-13}	1.3×10^{-13}	1.5×10^{-13}	9.5×10^{-14}
1200	2.2×10^{-13}	2.3×10^{-13}	2.8×10^{-13}	1.8×10^{-13}
	2B-4,5DCP + H	3B-4,6DCP + H	4B-2,5DCP + H	2,4DB-5CP + H
600	2.1×10^{-16}	4.1×10^{-16}	4.7×10^{-16}	1.4×10^{-16}
700	9.8×10^{-16}	1.9×10^{-15}	2.2×10^{-15}	5.4×10^{-16}
800	3.3×10^{-15}	6.5×10^{-15}	7.1×10^{-15}	1.6×10^{-15}
900	8.9×10^{-15}	1.8×10^{-14}	1.9×10^{-14}	4.0×10^{-15}
1000	2.0×10^{-14}	4.0×10^{-14}	4.3×10^{-14}	8.5×10^{-15}
1100	4.1×10^{-14}	8.1×10^{-14}	8.5×10^{-14}	1.6×10^{-14}
1200	7.4×10^{-14}	1.5×10^{-13}	1.5×10^{-13}	2.9×10^{-14}
	2,5DB-4CP + H	3,4DB-6CP + H	2B-4,6DCP + H	4B-2,6DCP + H
600	1.3×10^{-17}	3.4×10^{-16}	7.9×10^{-16}	8.6×10^{-16}
700	6.2×10^{-17}	1.8×10^{-15}	3.4×10^{-15}	3.7×10^{-15}
800	2.2×10^{-16}	6.6×10^{-15}	1.1×10^{-14}	1.2×10^{-14}
900	5.9×10^{-16}	1.9×10^{-14}	2.7×10^{-14}	3.0×10^{-14}
1000	1.4×10^{-15}	4.4×10^{-14}	5.8×10^{-14}	6.4×10^{-14}
1100	2.8×10^{-15}	9.2×10^{-14}	1.1×10^{-13}	1.3×10^{-13}
1200	5.1×10^{-15}	1.7×10^{-13}	2.0×10^{-13}	2.2×10^{-13}

Table S5 *Cont*.

T(K)	CVT/SCT Rate Constants			
	2,4DB-6CP + H	2,6DB-4CP + H	3B-4,5DCP + H	4B-3,5DCP + H
600	4.1×10^{-17}	3.4×10^{-17}	1.4×10^{-15}	1.7×10^{-15}
700	1.7×10^{-16}	1.7×10^{-16}	6.1×10^{-15}	6.9×10^{-15}
800	5.5×10^{-16}	5.7×10^{-16}	2.0×10^{-14}	2.1×10^{-14}
900	1.4×10^{-15}	1.6×10^{-15}	5.2×10^{-14}	5.3×10^{-14}
1000	3.1×10^{-15}	3.6×10^{-15}	1.2×10^{-13}	1.2×10^{-13}
1100	6.0×10^{-15}	7.3×10^{-15}	2.3×10^{-13}	2.2×10^{-13}
1200	1.1×10^{-14}	1.4×10^{-14}	4.1×10^{-13}	4.0×10^{-13}
	3,4DB-5CP + H	3,5DB-4CP + H	2B-3,4,5TCP + H	3B-2,4,5TCP + H
600	1.2×10^{-15}	1.2×10^{-15}	2.4×10^{-16}	5.9×10^{-16}
700	5.4×10^{-15}	4.8×10^{-15}	1.3×10^{-15}	2.6×10^{-15}
800	1.8×10^{-14}	1.5×10^{-14}	4.8×10^{-15}	8.2×10^{-15}
900	4.7×10^{-14}	3.8×10^{-14}	1.4×10^{-14}	2.1×10^{-14}
1000	1.1×10^{-13}	8.2×10^{-14}	3.3×10^{-14}	4.7×10^{-14}
1100	2.1×10^{-13}	1.6×10^{-13}	7.0×10^{-14}	9.4×10^{-14}
1200	3.8×10^{-13}	2.8×10^{-13}	1.3×10^{-13}	1.7×10^{-13}
	3B-4,5,6TCTP + H	4B-2,3,5TCP + H	2,3DB-4,5DCP + H	2,4DB-3,5DCP + H
600	2.5×10^{-16}	3.0×10^{-16}	3.2×10^{-16}	3.1×10^{-16}
700	1.2×10^{-15}	1.6×10^{-15}	1.6×10^{-15}	1.6×10^{-15}
800	4.3×10^{-15}	5.6×10^{-15}	5.7×10^{-15}	5.6×10^{-15}
900	1.2×10^{-14}	1.6×10^{-14}	1.6×10^{-14}	1.6×10^{-14}
1000	2.7×10^{-14}	3.7×10^{-14}	3.7×10^{-14}	3.7×10^{-14}
1100	5.6×10^{-14}	7.6×10^{-14}	7.7×10^{-14}	7.7×10^{-14}
1200	1.0×10^{-13}	1.4×10^{-13}	1.4×10^{-13}	1.4×10^{-13}
	2,5DB-3,4DCP + H	3,4DB-2,5DCP + H	3,4DB-5,6DCP + H	3,5DB-2,4DCP + H
600	3.0×10^{-16}	1.6×10^{-16}	2.9×10^{-16}	1.4×10^{-16}
700	1.6×10^{-15}	9.2×10^{-16}	1.5×10^{-15}	5.9×10^{-16}
800	5.6×10^{-15}	3.6×10^{-15}	5.6×10^{-15}	1.9×10^{-15}
900	1.6×10^{-14}	1.1×10^{-14}	1.6×10^{-14}	4.7×10^{-15}
1000	3.7×10^{-14}	2.7×10^{-14}	3.9×10^{-14}	1.0×10^{-14}
1100	7.6×10^{-14}	5.8×10^{-14}	8.0×10^{-14}	2.0×10^{-14}
1200	1.4×10^{-13}	1.1×10^{-13}	1.5×10^{-13}	3.7×10^{-14}
	2,3,4TB-5CP + H	2,3,5TB-4CP + H	2,4,5TB-3CP + H	3,4,5TB-2CP + H
600	1.7×10^{-16}	1.5×10^{-16}	5.5×10^{-16}	1.3×10^{-16}
700	9.9×10^{-16}	8.5×10^{-16}	2.5×10^{-15}	7.6×10^{-16}
800	4.0×10^{-15}	3.3×10^{-15}	8.2×10^{-15}	3.0×10^{-15}
900	1.2×10^{-14}	9.7×10^{-15}	2.2×10^{-14}	8.9×10^{-15}
1000	3.0×10^{-14}	2.4×10^{-14}	4.8×10^{-14}	2.2×10^{-14}
1100	6.5×10^{-14}	5.0×10^{-14}	9.6×10^{-14}	4.7×10^{-14}
1200	1.3×10^{-13}	9.6×10^{-14}	1.7×10^{-13}	9.0×10^{-14}

Table S5 *Cont.*

T(K)	CVT/SCT Rate Constants			
	2B-3,4,6TCP + H	2B-4,5,6TCP + H	3B-2,4,6TCP + H	4B-2,3,6TCP + H
600	7.5×10^{-16}	4.6×10^{-16}	9.0×10^{-16}	6.7×10^{-16}
700	3.6×10^{-15}	2.4×10^{-15}	4.0×10^{-15}	3.1×10^{-15}
800	1.2×10^{-14}	8.6×10^{-15}	1.3×10^{-14}	1.0×10^{-14}
900	3.3×10^{-14}	2.4×10^{-14}	3.3×10^{-14}	2.7×10^{-14}
1000	7.5×10^{-13}	5.7×10^{-14}	7.3×10^{-14}	6.2×10^{-14}
1100	1.5×10^{-13}	1.2×10^{-13}	1.4×10^{-13}	1.2×10^{-13}
1200	2.8×10^{-13}	2.2×10^{-13}	2.6×10^{-13}	2.3×10^{-13}
	2,3DB-4,6DCP + H	2,4DB-3,6DCP + H	2,4DB-5,6DCP + H	2,5DB-4,6DCP + H
600	9.0×10^{-16}	7.7×10^{-16}	6.4×10^{-17}	1.6×10^{-16}
700	4.0×10^{-15}	2.9×10^{-15}	2.9×10^{-16}	7.9×10^{-16}
800	1.3×10^{-14}	8.3×10^{-15}	9.7×10^{-16}	2.7×10^{-15}
900	3.4×10^{-14}	2.0×10^{-14}	2.5×10^{-15}	7.4×10^{-15}
1000	7.7×10^{-14}	4.1×10^{-14}	5.7×10^{-15}	1.7×10^{-14}
1100	1.5×10^{-13}	7.8×10^{-14}	1.1×10^{-14}	3.5×10^{-14}
1200	2.8×10^{-13}	1.4×10^{-13}	2.0×10^{-14}	6.3×10^{-14}
	2,6DB-3,4DCP + H	3,4DB-2,6DCP + H	2,3,4TB-6CP + H	2,3,6TB-4CP + H
600	7.5×10^{-16}	7.0×10^{-16}	5.1×10^{-16}	9.1×10^{-17}
700	4.0×10^{-15}	3.2×10^{-15}	2.6×10^{-15}	4.4×10^{-16}
800	1.4×10^{-14}	1.1×10^{-14}	9.4×10^{-15}	1.5×10^{-15}
900	4.0×10^{-14}	2.8×10^{-14}	2.6×10^{-14}	4.1×10^{-15}
1000	9.5×10^{-14}	6.4×10^{-14}	6.2×10^{-14}	9.6×10^{-15}
1100	2.0×10^{-13}	1.3×10^{-13}	1.3×10^{-13}	2.0×10^{-14}
1200	3.7×10^{-13}	2.3×10^{-13}	2.4×10^{-13}	3.6×10^{-14}
	2,4,5TB-6CP + H	2,4,6TB-3CP + H	2B-3,5,6TCP + H	3B-2,5,6TCP + H
600	7.9×10^{-16}	4.0×10^{-16}	3.0×10^{-16}	4.0×10^{-17}
700	3.5×10^{-15}	2.1×10^{-15}	1.6×10^{-15}	2.0×10^{-16}
800	1.2×10^{-14}	7.9×10^{-15}	5.8×10^{-15}	7.0×10^{-16}
900	3.0×10^{-14}	2.3×10^{-14}	1.7×10^{-14}	2.0×10^{-15}
1000	6.8×10^{-14}	5.4×10^{-14}	4.0×10^{-14}	4.6×10^{-15}
1100	1.4×10^{-13}	1.1×10^{-13}	8.4×10^{-14}	9.3×10^{-15}
1200	2.5×10^{-13}	2.1×10^{-13}	1.6×10^{-13}	1.7×10^{-14}
	2,3DB-5,6DCP + H	2,5DB-3,6DCP + H	2,6DB-3,5DCP + H	3,5DB-2,6DCP + H
600	4.4×10^{-16}	3.1×10^{-16}	8.7×10^{-16}	3.8×10^{-16}
700	2.2×10^{-15}	1.6×10^{-15}	4.9×10^{-15}	1.9×10^{-15}
800	8.0×10^{-15}	6.0×10^{-15}	1.9×10^{-14}	6.4×10^{-15}
900	2.2×10^{-14}	1.7×10^{-14}	5.7×10^{-14}	1.8×10^{-14}
1000	5.3×10^{-14}	4.2×10^{-14}	1.4×10^{-13}	4.1×10^{-14}
1100	1.1×10^{-13}	8.7×10^{-14}	3.0×10^{-13}	8.3×10^{-14}
1200	2.0×10^{-13}	1.6×10^{-13}	5.8×10^{-13}	1.5×10^{-13}

Table S5 *Cont*.

T(K)	CVT/SCT Rate Constants			
	2,3,5TB-6CP + H	2,3,6TB-5CP + H	2B-3,4,5,6TeCP + H	3B-2,4,5,6TeCP + H
600	6.2×10^{-17}	9.1×10^{-16}	4.6×10^{-17}	2.5×10^{-17}
700	3.4×10^{-16}	4.6×10^{-15}	2.3×10^{-16}	1.5×10^{-16}
800	1.2×10^{-15}	1.7×10^{-14}	7.9×10^{-16}	5.7×10^{-16}
900	3.6×10^{-15}	4.7×10^{-14}	2.2×10^{-15}	1.7×10^{-15}
1000	8.5×10^{-15}	1.1×10^{-13}	5.1×10^{-15}	4.3×10^{-15}
1100	1.8×10^{-14}	2.3×10^{-13}	1.0×10^{-14}	9.4×10^{-15}
1200	3.3×10^{-14}	4.3×10^{-13}	1.9×10^{-14}	1.8×10^{-14}
	4B-2,3,5,6TeCP + H	2,3DB-4,5,6TCP + H	2,4DB-3,5,6TCP + H	2,5DB-3,4,6TCP + H
600	4.8×10^{-16}	8.4×10^{-16}	6.1×10^{-16}	1.1×10^{-16}
700	2.2×10^{-15}	3.8×10^{-15}	2.9×10^{-15}	5.5×10^{-16}
800	7.5×10^{-15}	1.3×10^{-14}	1.0×10^{-14}	1.9×10^{-15}
900	2.0×10^{-14}	3.3×10^{-14}	2.7×10^{-14}	5.0×10^{-15}
1000	4.6×10^{-14}	7.5×10^{-14}	6.3×10^{-14}	1.1×10^{-14}
1100	9.2×10^{-14}	1.5×10^{-13}	1.3×10^{-13}	2.3×10^{-14}
1200	1.7×10^{-13}	2.7×10^{-13}	2.4×10^{-13}	4.1×10^{-14}
	2,6DB-3,4,5TCP + H	3,4DB-2,5,6TCP + H	3,5DB-2,4,6TCP + H	2,3,4TB-5,6DCP + H
600	8.7×10^{-16}	8.5×10^{-17}	5.0×10^{-16}	5.9×10^{-16}
700	4.7×10^{-15}	4.5×10^{-16}	2.3×10^{-15}	2.7×10^{-15}
800	1.7×10^{-14}	1.7×10^{-15}	7.7×10^{-15}	8.9×10^{-15}
900	5.0×10^{-14}	4.9×10^{-15}	2.0×10^{-14}	2.4×10^{-14}
1000	1.2×10^{-13}	1.2×10^{-14}	4.6×10^{-14}	5.5×10^{-14}
1100	2.5×10^{-13}	2.5×10^{-14}	9.2×10^{-14}	1.1×10^{-13}
1200	4.8×10^{-13}	4.7×10^{-14}	1.7×10^{-13}	2.1×10^{-13}
	2,3,5TB-4,6DCP + H	2,3,6TB-4,5DCP + H	2,4,5TB-3,6DCP + H	2,4,6TB-3,5DCP + H
600	4.8×10^{-16}	8.6×10^{-17}	4.8×10^{-16}	6.5×10^{-17}
700	2.2×10^{-15}	4.8×10^{-16}	2.3×10^{-15}	3.7×10^{-16}
800	7.4×10^{-15}	1.8×10^{-15}	7.9×10^{-15}	1.4×10^{-15}
900	2.0×10^{-14}	5.3×10^{-15}	2.1×10^{-14}	4.3×10^{-15}
1000	4.5×10^{-14}	1.3×10^{-14}	4.9×10^{-14}	1.1×10^{-14}
1100	9.1×10^{-14}	2.8×10^{-14}	9.9×10^{-14}	2.3×10^{-14}
1200	1.7×10^{-13}	5.2×10^{-14}	1.8×10^{-13}	4.5×10^{-14}
	3,4,5TB-2,6DCP + H	2,3,4,5TeB-6CP + H	2,3,4,6TeB-5CP + H	2,3,5,6TeB-4CP + H
600	4.5×10^{-16}	1.5×10^{-16}	4.8×10^{-16}	7.7×10^{-16}
700	2.2×10^{-15}	8.1×10^{-16}	2.4×10^{-15}	4.2×10^{-15}
800	7.6×10^{-15}	3.0×10^{-15}	8.7×10^{-15}	1.6×10^{-14}
900	2.1×10^{-14}	8.4×10^{-15}	2.4×10^{-14}	4.7×10^{-14}
1000	4.9×10^{-14}	2.0×10^{-14}	5.7×10^{-14}	1.1×10^{-13}
1100	9.9×10^{-14}	4.1×10^{-14}	1.2×10^{-13}	2.4×10^{-13}
1200	1.8×10^{-13}	7.6×10^{-14}	2.2×10^{-13}	4.6×10^{-13}

Table S6. CVT/SCT rate constants for the reactions of the anti-BCPs with H over the temperature range of 600−1200 K (cm^3 $molecule^{-1}$ s^{-1}).

T(K)	CVT/SCT Rate Constants			
	2B-3CP^{anti} + H	3B-2CP^{anti} + H	2B-4CP^{anti} + H	4B-2CP^{anti} + H
600	7.4×10^{-15}	1.4×10^{-15}	6.1×10^{-15}	1.6×10^{-15}
700	2.3×10^{-14}	4.7×10^{-15}	1.9×10^{-14}	5.2×10^{-15}
800	5.6×10^{-14}	1.3×10^{-14}	4.7×10^{-14}	1.4×10^{-14}
900	1.2×10^{-13}	2.9×10^{-14}	9.9×10^{-14}	3.0×10^{-14}
1000	2.3×10^{-13}	5.6×10^{-14}	1.9×10^{-13}	5.7×10^{-14}
1100	3.9×10^{-13}	1.0×10^{-13}	3.2×10^{-13}	9.8×10^{-14}
1200	6.4×10^{-13}	1.7×10^{-13}	5.2×10^{-13}	1.6×10^{-13}
	2B-5CP^{anti} + H	3B-6CP^{anti} + H	2B-3,4DCP^{anti} + H	3B-2,4DCP^{anti} + H
600	1.7×10^{-15}	9.2×10^{-18}	6.9×10^{-15}	4.0×10^{-15}
700	6.8×10^{-15}	5.0×10^{-17}	2.2×10^{-14}	1.2×10^{-14}
800	2.0×10^{-14}	1.8×10^{-16}	5.6×10^{-14}	3.0×10^{-14}
900	4.7×10^{-14}	5.2×10^{-16}	1.2×10^{-13}	6.2×10^{-14}
1000	9.7×10^{-14}	1.2×10^{-15}	2.3×10^{-13}	1.2×10^{-13}
1100	1.8×10^{-13}	2.5×10^{-15}	3.9×10^{-13}	2.0×10^{-13}
1200	3.0×10^{-13}	4.5×10^{-15}	6.2×10^{-13}	3.1×10^{-13}
	4B-2,3DCP^{anti} + H	2,3DB-4CP^{anti} + H	2,4DB-3CP^{anti} + H	3,4DB-2CP^{anti} + H
600	1.2×10^{-14}	9.2×10^{-15}	6.4×10^{-15}	1.0×10^{-14}
700	3.4×10^{-14}	2.7×10^{-14}	2.1×10^{-14}	3.0×10^{-14}
800	7.6×10^{-14}	6.3×10^{-14}	5.3×10^{-14}	7.2×10^{-14}
900	1.5×10^{-13}	1.3×10^{-13}	1.2×10^{-13}	1.5×10^{-13}
1000	2.7×10^{-13}	2.3×10^{-13}	2.2×10^{-13}	2.8×10^{-13}
1100	4.4×10^{-13}	3.9×10^{-13}	3.8×10^{-13}	4.7×10^{-13}
1200	6.9×10^{-13}	6.2×10^{-13}	6.2×10^{-13}	7.4×10^{-13}
	2B-3,5DCP^{anti} + H	3B-2,5DCP^{anti} + H	3B-5,6DCP^{anti} + H	2,3DB-5CP^{anti} + H
600	1.9×10^{-15}	1.1×10^{-15}	2.6×10^{-15}	1.5×10^{-15}
700	7.1×10^{-15}	4.4×10^{-15}	8.9×10^{-15}	4.4×10^{-15}
800	2.0×10^{-14}	1.3×10^{-14}	2.4×10^{-14}	1.1×10^{-14}
900	4.7×10^{-14}	3.1×10^{-14}	5.3×10^{-14}	2.2×10^{-14}
1000	1.9×10^{-14}	6.4×10^{-14}	1.1×10^{-13}	4.2×10^{-14}
1100	1.8×10^{-13}	1.2×10^{-13}	1.9×10^{-13}	7.1×10^{-14}
1200	2.9×10^{-13}	2.0×10^{-13}	3.1×10^{-13}	1.1×10^{-13}
	2,5DB-3CP^{anti} + H	3,5DB-2CP^{anti} + H	2B-4,5DCP^{anti} + H	3B-4,6DCP^{anti} + H
600	3.9×10^{-15}	2.6×10^{-15}	3.3×10^{-15}	5.0×10^{-15}
700	1.3×10^{-14}	8.5×10^{-15}	1.0×10^{-14}	1.6×10^{-14}
800	3.5×10^{-14}	2.2×10^{-14}	2.5×10^{-14}	4.1×10^{-14}
900	7.7×10^{-14}	4.8×10^{-14}	5.2×10^{-14}	8.8×10^{-14}
1000	1.5×10^{-13}	9.3×10^{-14}	9.7×10^{-14}	1.7×10^{-13}
1100	2.7×10^{-13}	1.6×10^{-13}	1.7×10^{-13}	2.9×10^{-13}
1200	4.4×10^{-13}	2.7×10^{-13}	2.7×10^{-13}	4.8×10^{-13}

Table S6 *Cont.*

T(K)	CVT/SCT Rate Constants			
	4B-2,5DCP^{anti} + H	2,4DB-5CP^{anti} + H	2,5DB-4CP^{anti} + H	3,4DB-6CP^{anti} + H
600	5.7×10^{-15}	2.1×10^{-15}	2.2×10^{-16}	3.8×10^{-15}
700	1.8×10^{-14}	5.5×10^{-15}	6.6×10^{-16}	1.4×10^{-14}
800	4.3×10^{-14}	1.2×10^{-14}	1.5×10^{-15}	3.8×10^{-14}
900	9.1×10^{-14}	2.4×10^{-14}	3.1×10^{-15}	8.6×10^{-14}
1000	1.7×10^{-13}	4.1×10^{-14}	5.6×10^{-15}	1.7×10^{-13}
1100	2.9×10^{-13}	6.8×10^{-14}	9.2×10^{-15}	3.0×10^{-13}
1200	4.7×10^{-13}	1.1×10^{-13}	1.4×10^{-14}	5.0×10^{-13}
	2B-3,4,5TCP^{anti} + H	3B-2,4,5TCP^{anti} + H	3B-4,5,6TCTP^{anti} + H	4B-2,3,5TCP^{anti} + H
600	5.5×10^{-15}	9.2×10^{-15}	2.9×10^{-15}	4.1×10^{-15}
700	1.9×10^{-14}	2.6×10^{-14}	9.4×10^{-15}	1.4×10^{-14}
800	4.9×10^{-14}	6.0×10^{-14}	2.4×10^{-14}	3.6×10^{-14}
900	1.1×10^{-13}	1.2×10^{-13}	5.2×10^{-14}	8.0×10^{-14}
1000	2.1×10^{-13}	2.2×10^{-13}	1.0×10^{-13}	1.6×10^{-13}
1100	3.7×10^{-13}	3.6×10^{-13}	1.8×10^{-13}	2.7×10^{-13}
1200	6.1×10^{-13}	5.7×10^{-13}	2.8×10^{-13}	4.5×10^{-13}
	2,3DB-4,5DCP^{anti} + H	2,4DB-3,5DCP^{anti} + H	2,5DB-3,4DCP^{anti} + H	3,4DB-2,5DCP^{anti} + H
600	6.7×10^{-15}	5.8×10^{-15}	6.7×10^{-15}	1.2×10^{-15}
700	2.1×10^{-14}	1.9×10^{-14}	2.2×10^{-14}	5.0×10^{-15}
800	5.3×10^{-14}	4.7×10^{-14}	5.5×10^{-14}	1.5×10^{-14}
900	1.1×10^{-13}	1.0×10^{-13}	1.2×10^{-13}	3.6×10^{-14}
1000	2.1×10^{-13}	1.9×10^{-13}	2.3×10^{-13}	7.4×10^{-14}
1100	3.7×10^{-13}	3.4×10^{-13}	3.9×10^{-13}	1.4×10^{-13}
1200	5.9×10^{-13}	5.5×10^{-13}	6.3×10^{-13}	2.3×10^{-13}
	3,4DB-5,6DCP^{anti} + H	3,5DB-2,4DCP^{anti} + H	2,3,4TB-5CP ^{anti}+ H	2,3,5TB-4CP^{anti} + H
600	2.0×10^{-16}	2.3×10^{-15}	2.8×10^{-15}	2.0×10^{-15}
700	2.1×10^{-15}	6.3×10^{-15}	1.2×10^{-14}	7.1×10^{-15}
800	6.0×10^{-15}	1.4×10^{-14}	3.5×10^{-14}	1.9×10^{-14}
900	1.8×10^{-14}	2.9×10^{-14}	8.6×10^{-14}	4.3×10^{-14}
1000	2.5×10^{-14}	5.2×10^{-14}	1.8×10^{-13}	8.5×10^{-14}
1100	7.7×10^{-14}	8.6×10^{-14}	3.4×10^{-13}	1.5×10^{-13}
1200	1.6×10^{-13}	1.4×10^{-13}	5.9×10^{-13}	2.5×10^{-13}
	2,4,5TB-3CP^{anti} + H	3,4,5TB-2CP^{anti} + H		
600	1.1×10^{-14}	2.0×10^{-15}		
700	3.1×10^{-14}	7.6×10^{-15}		
800	7.2×10^{-14}	2.2×10^{-14}		
900	1.5×10^{-13}	5.1×10^{-14}		
1000	2.7×10^{-13}	1.0×10^{-13}		
1100	4.4×10^{-13}	1.9×10^{-13}		
1200	7.0×10^{-13}	3.2×10^{-13}		

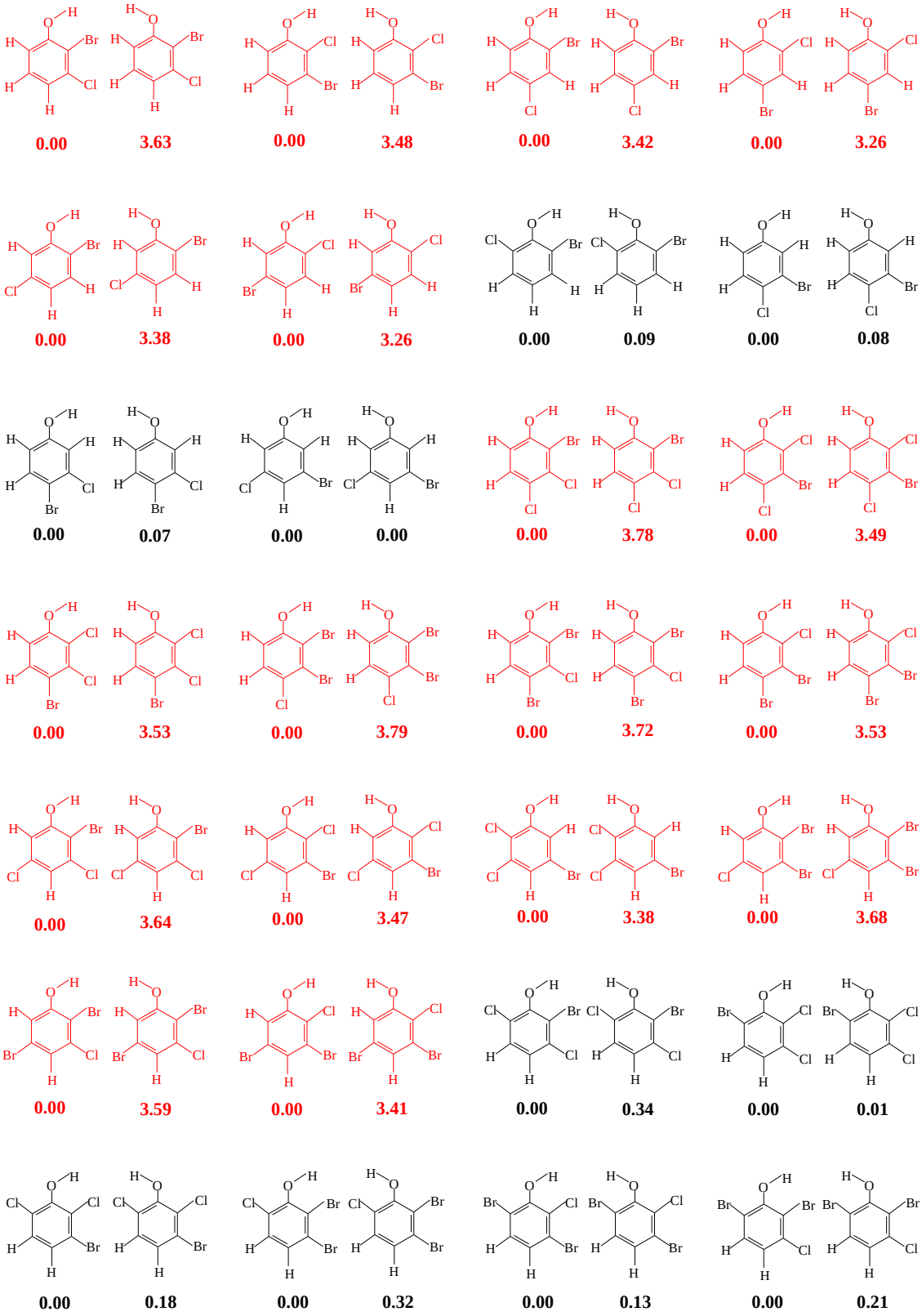
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Figure S1

Figure S1 *Cont*.

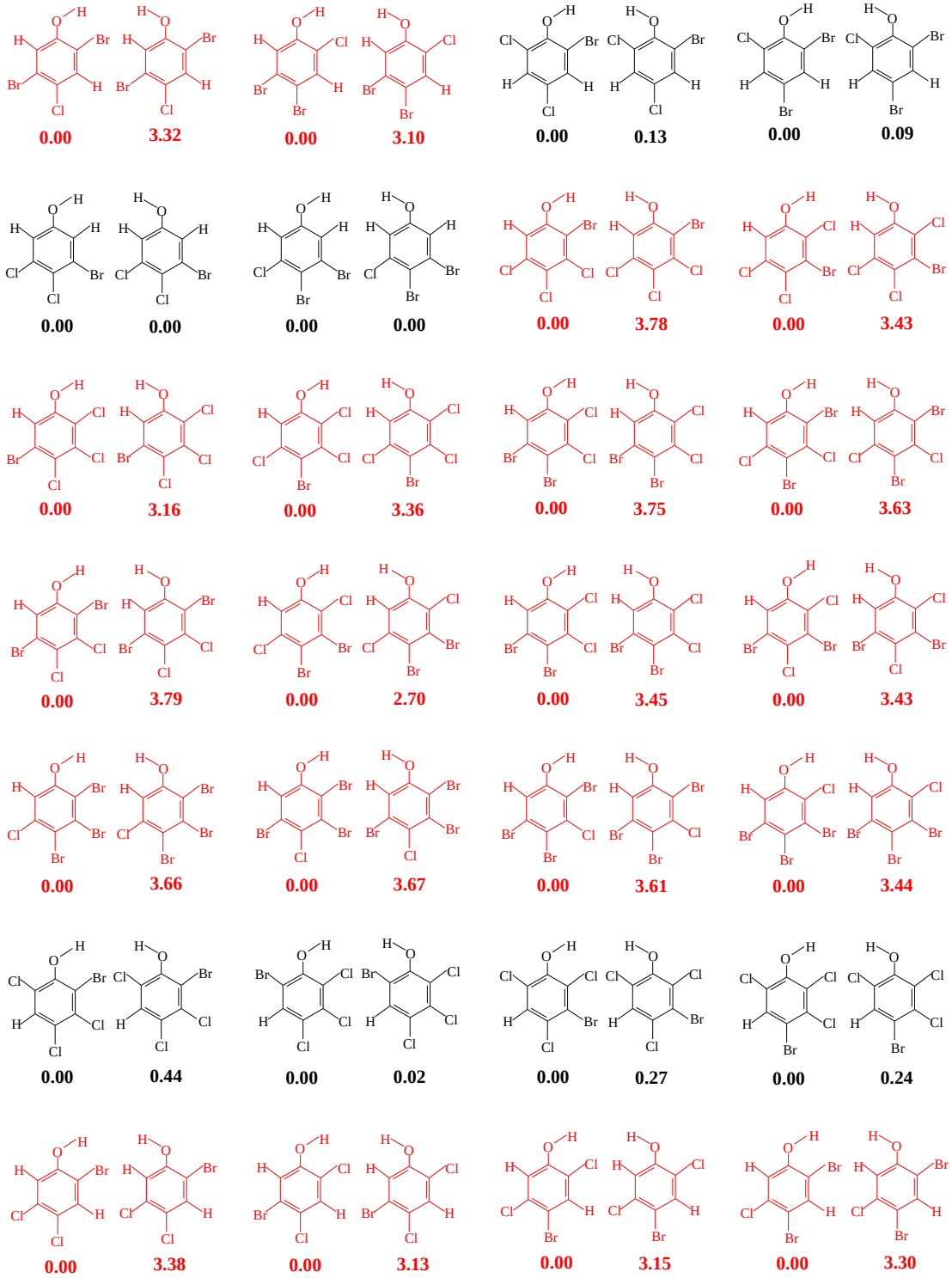


Figure S1 *Cont*.

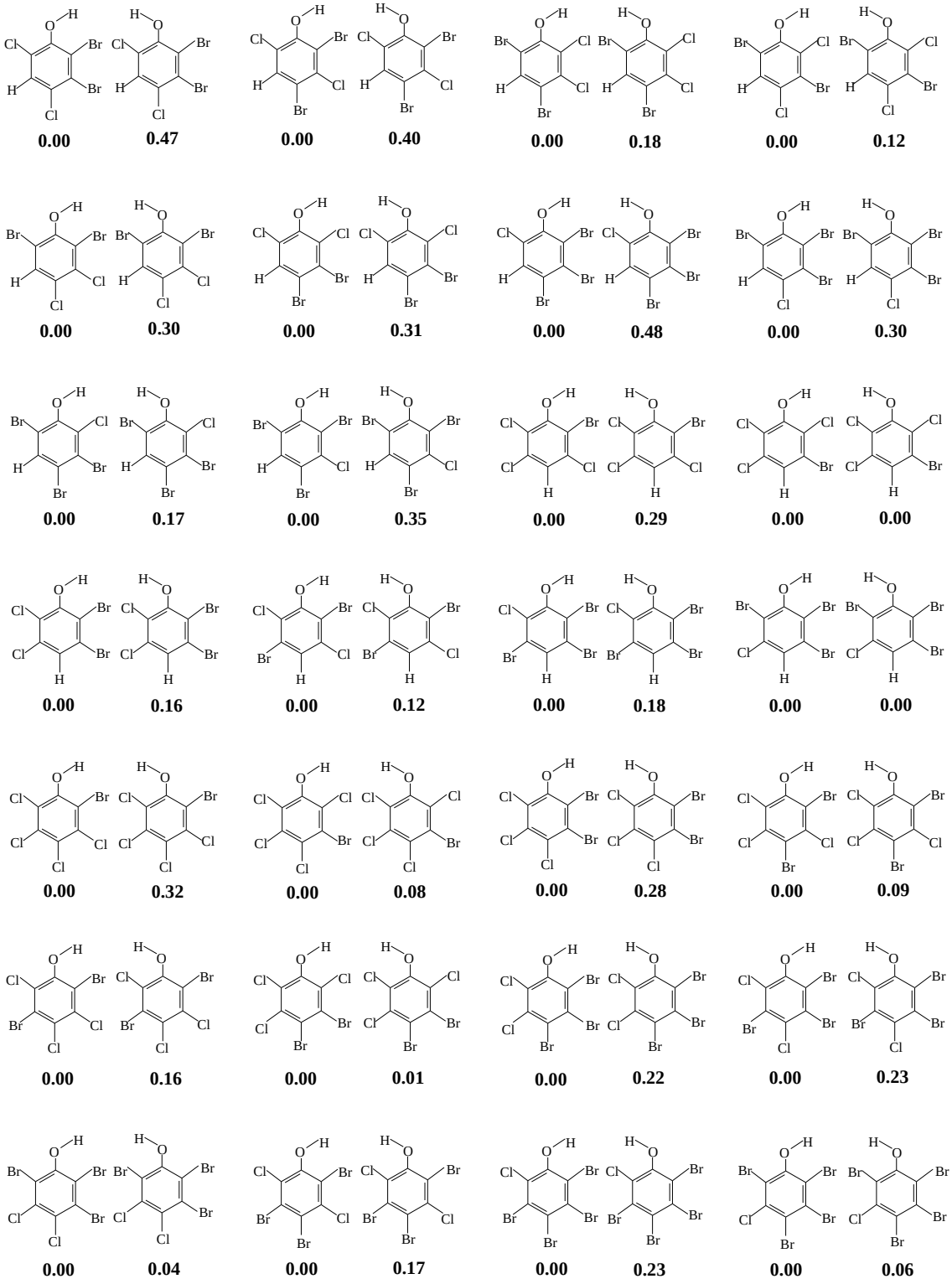
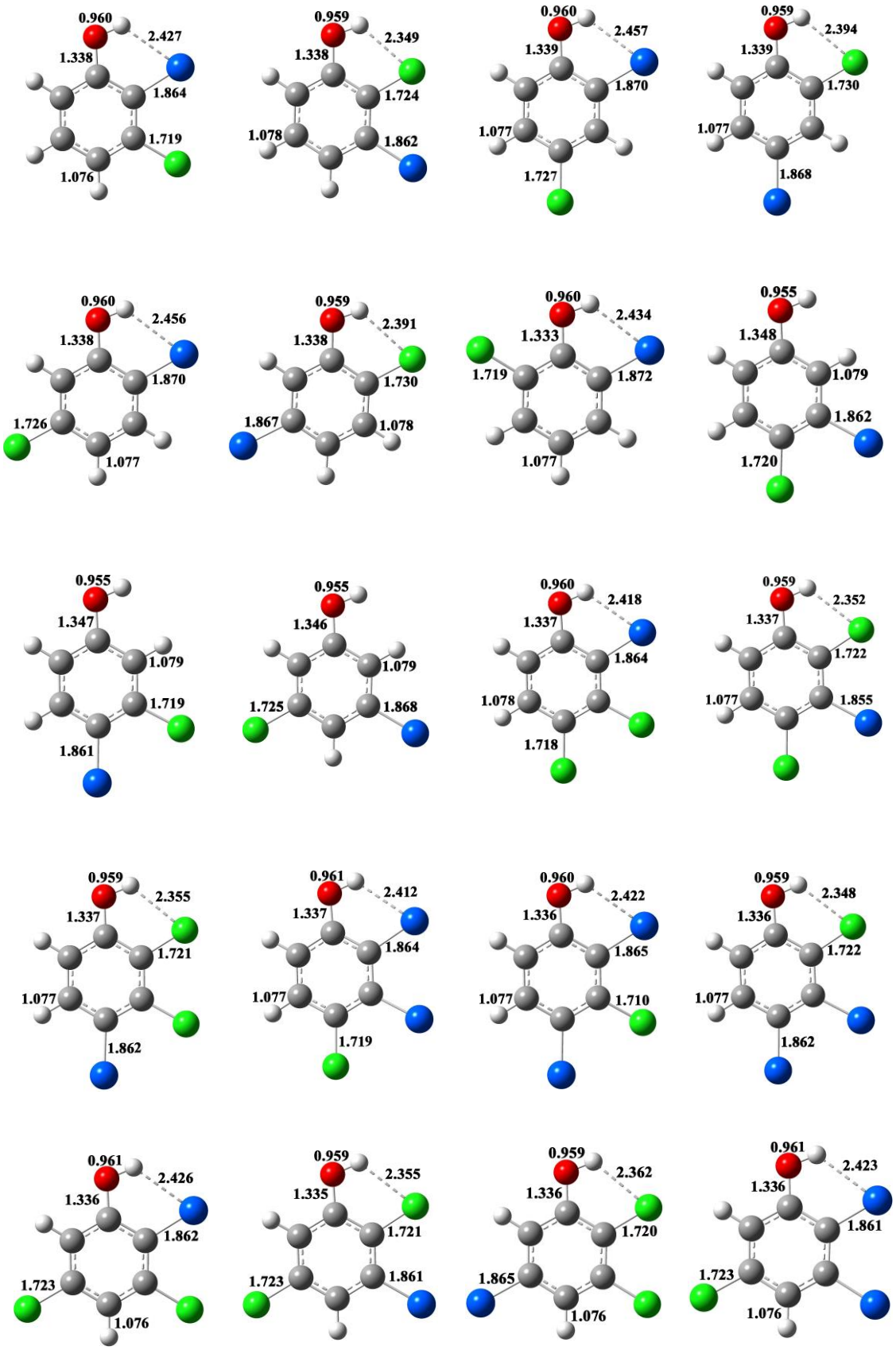


Figure S1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1.337
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1.077
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0.959
2.355
1.337
1.721
1.077
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1.337
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1.077
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Figure S2

Figure S2 *Cont*.

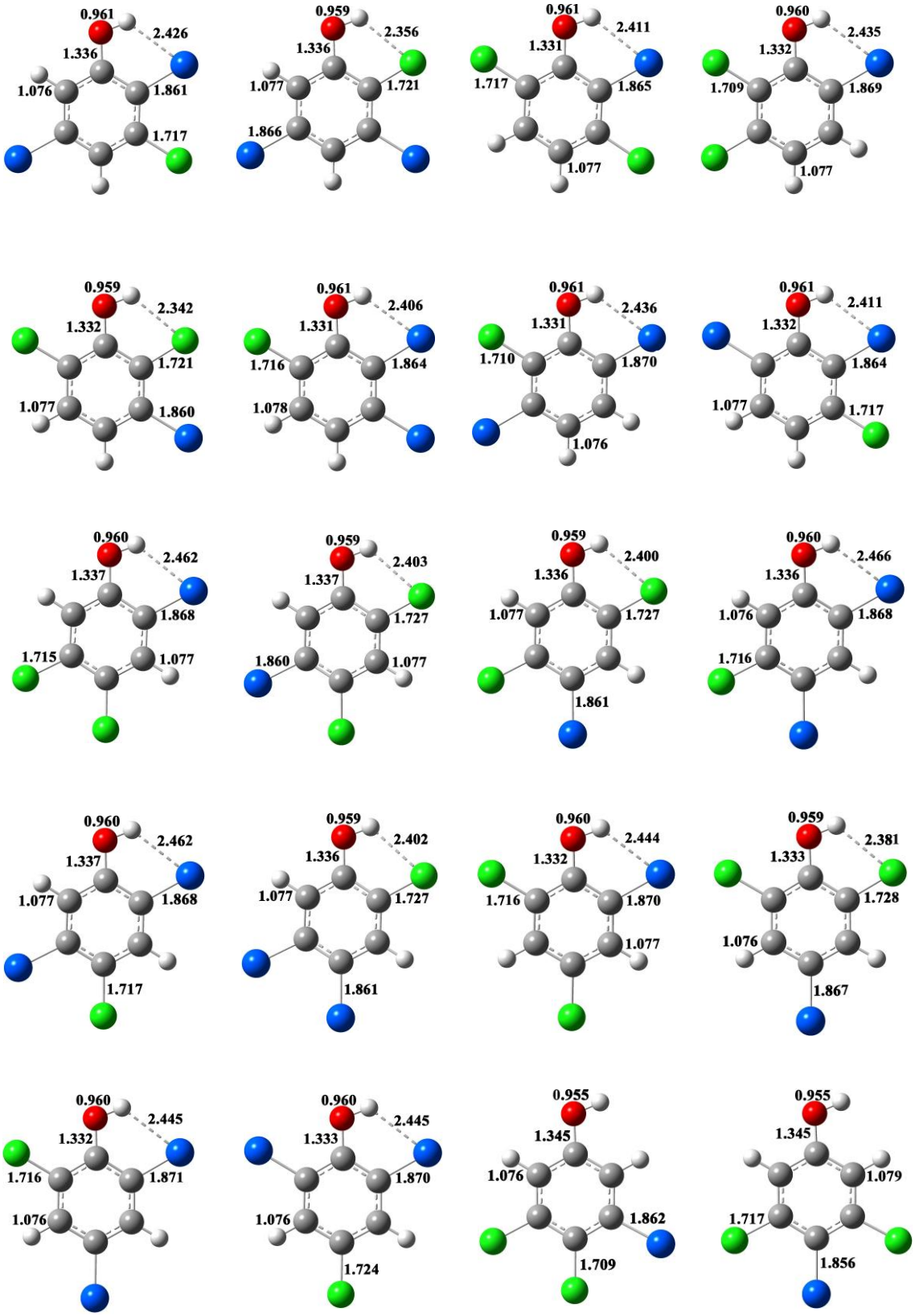


Figure S2 *Cont*.

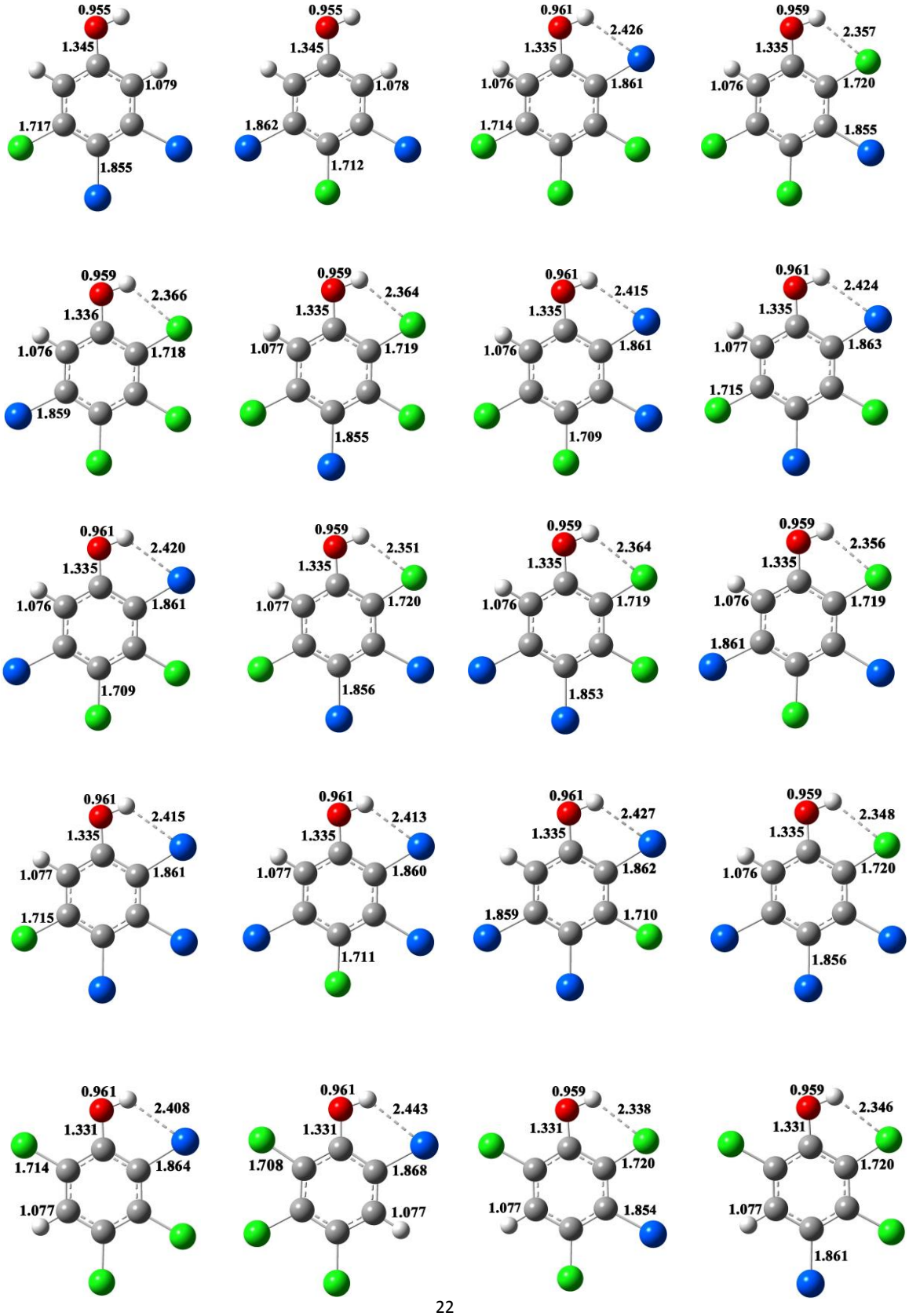


Figure S2 *Cont*.

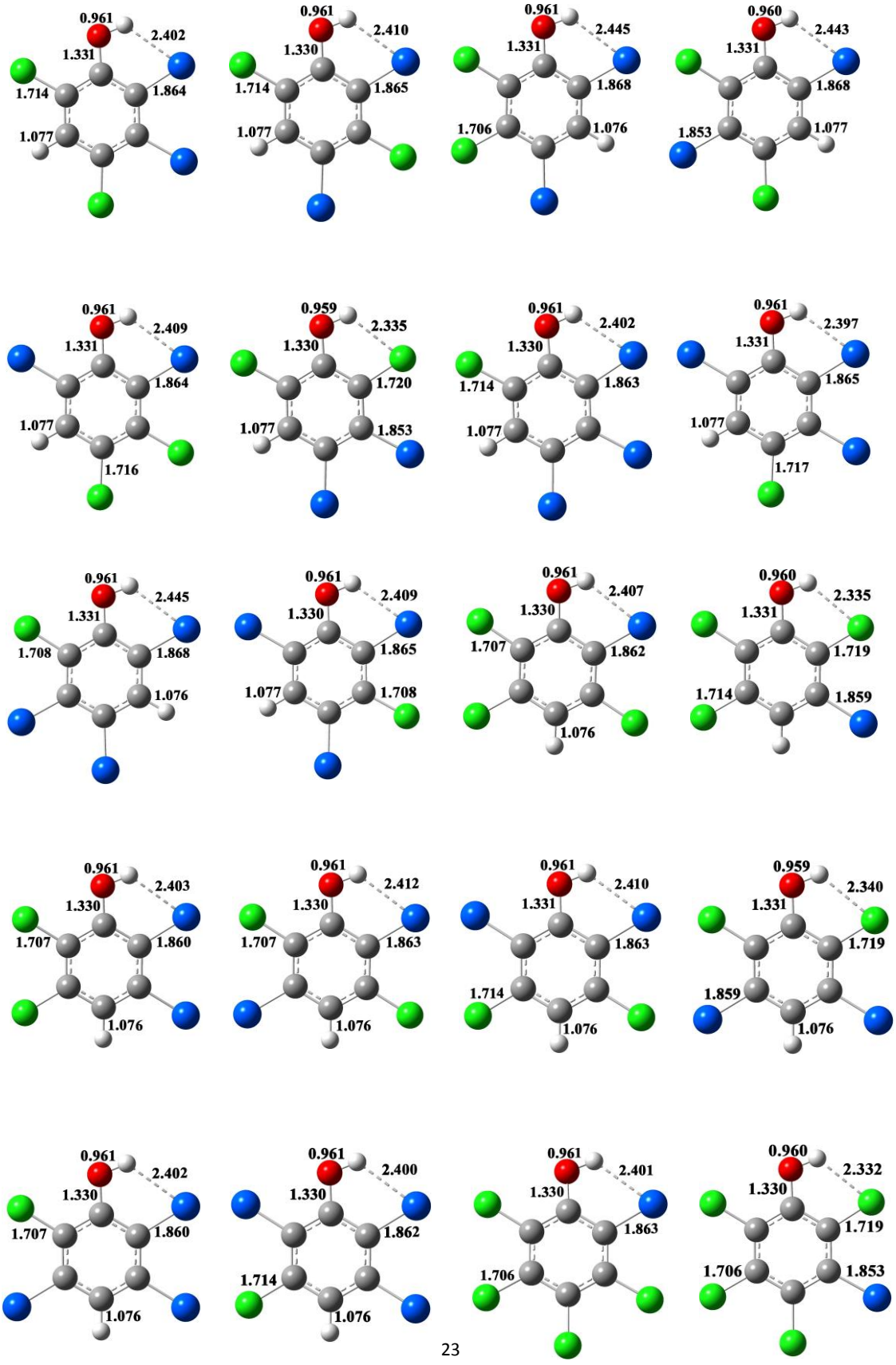


Figure S2 *Cont*.

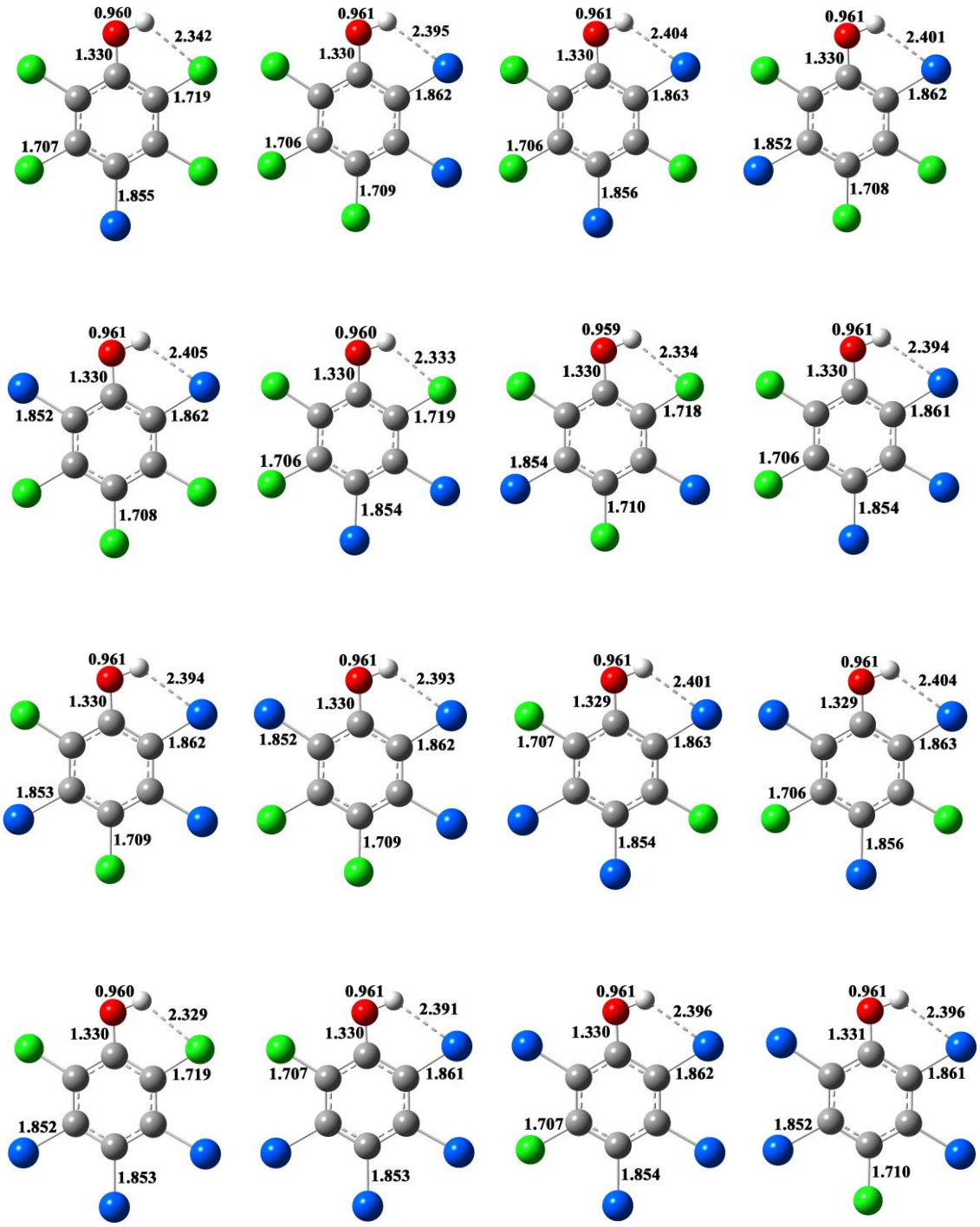
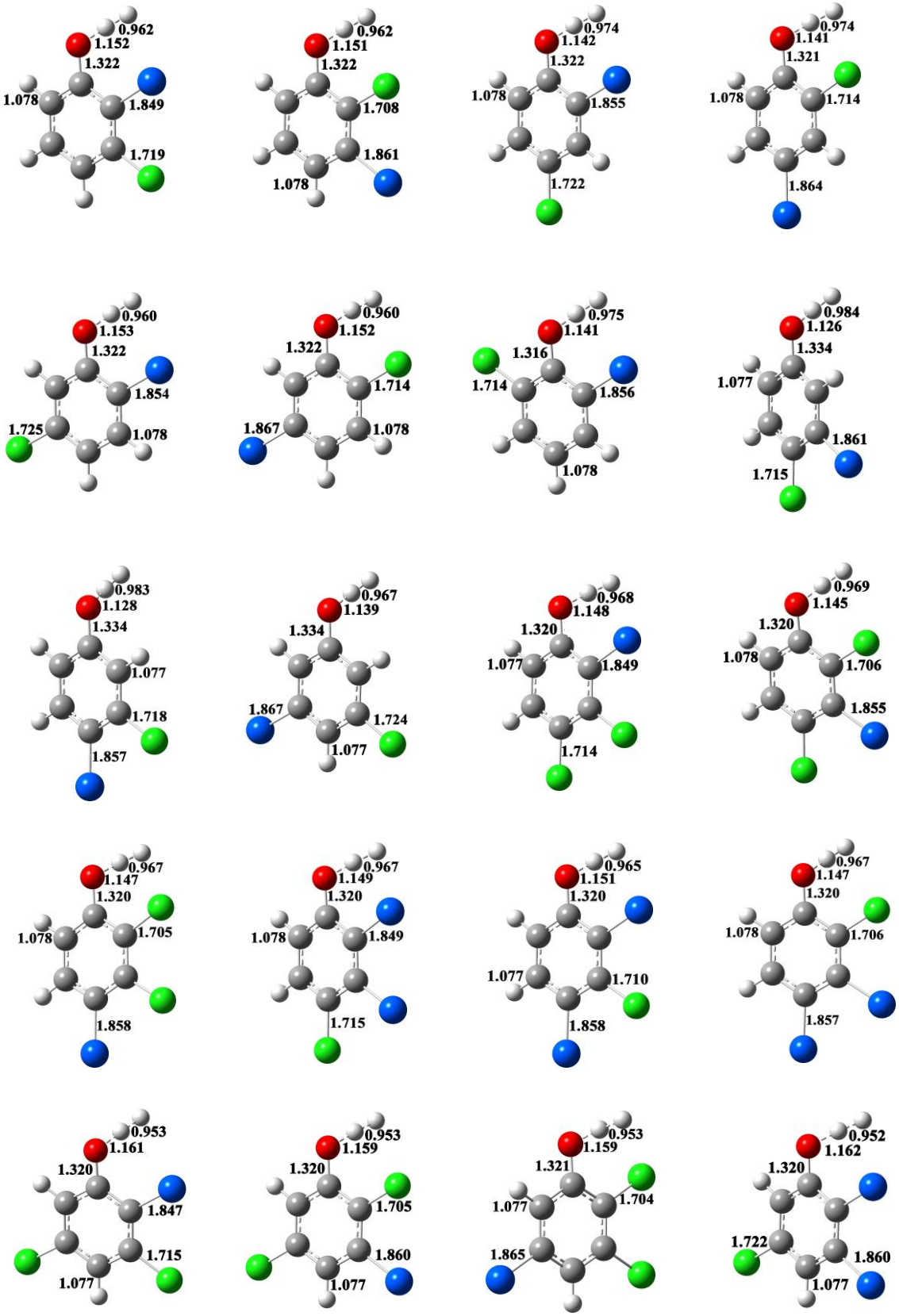


Figure S2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1.077

Figure S3

Figure S3 *Cont*.

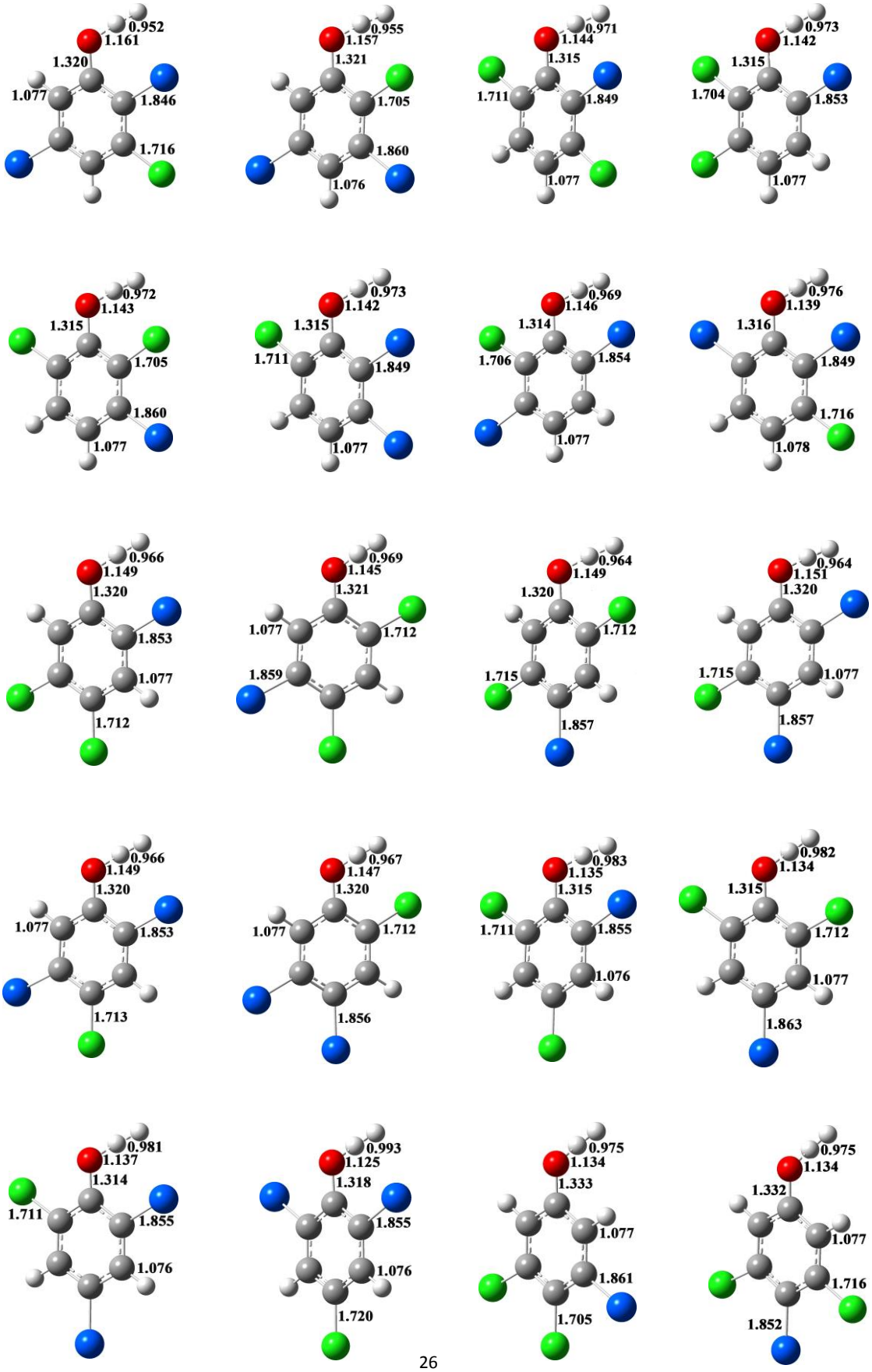


Figure S3 *Cont*.

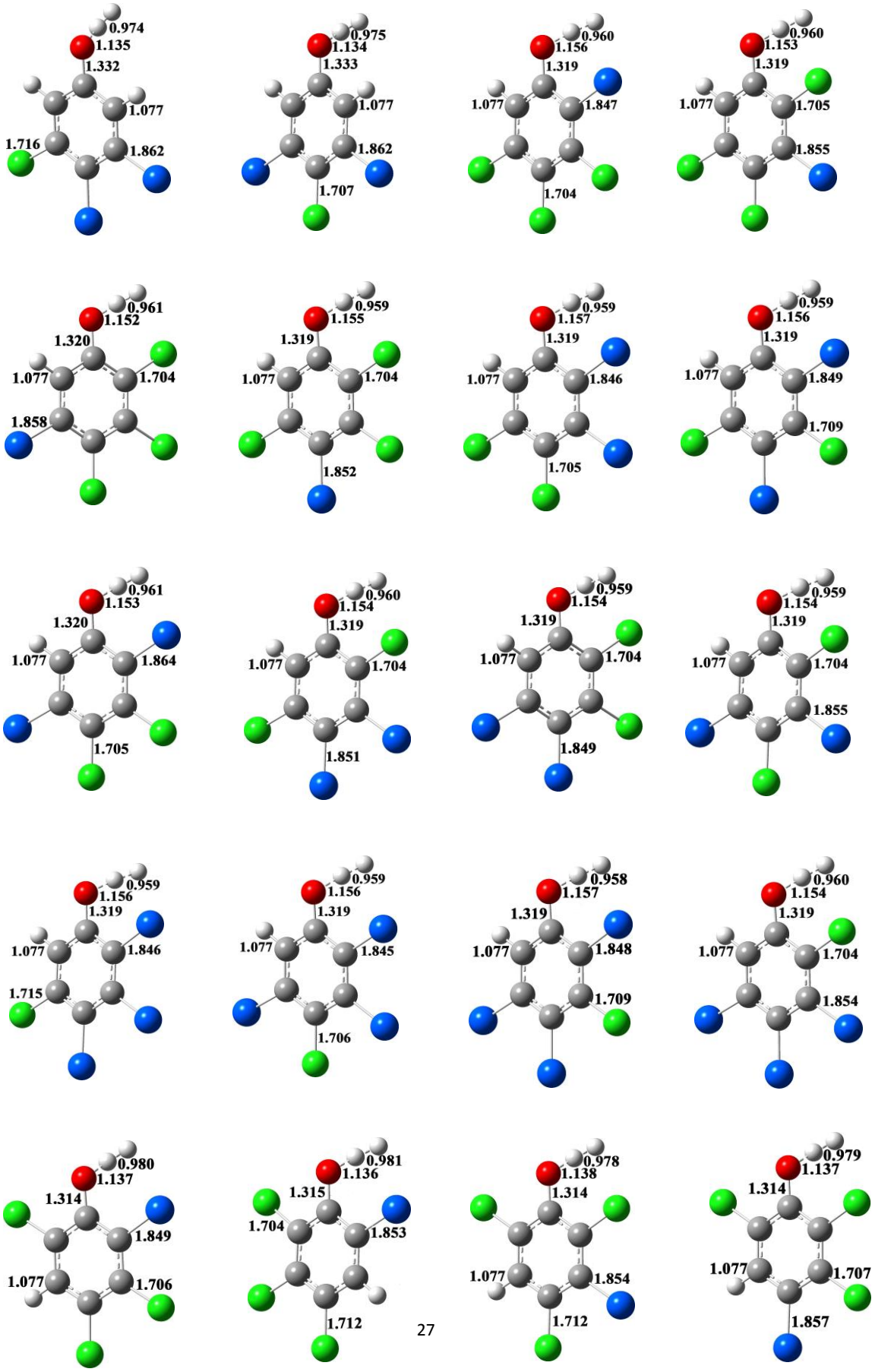
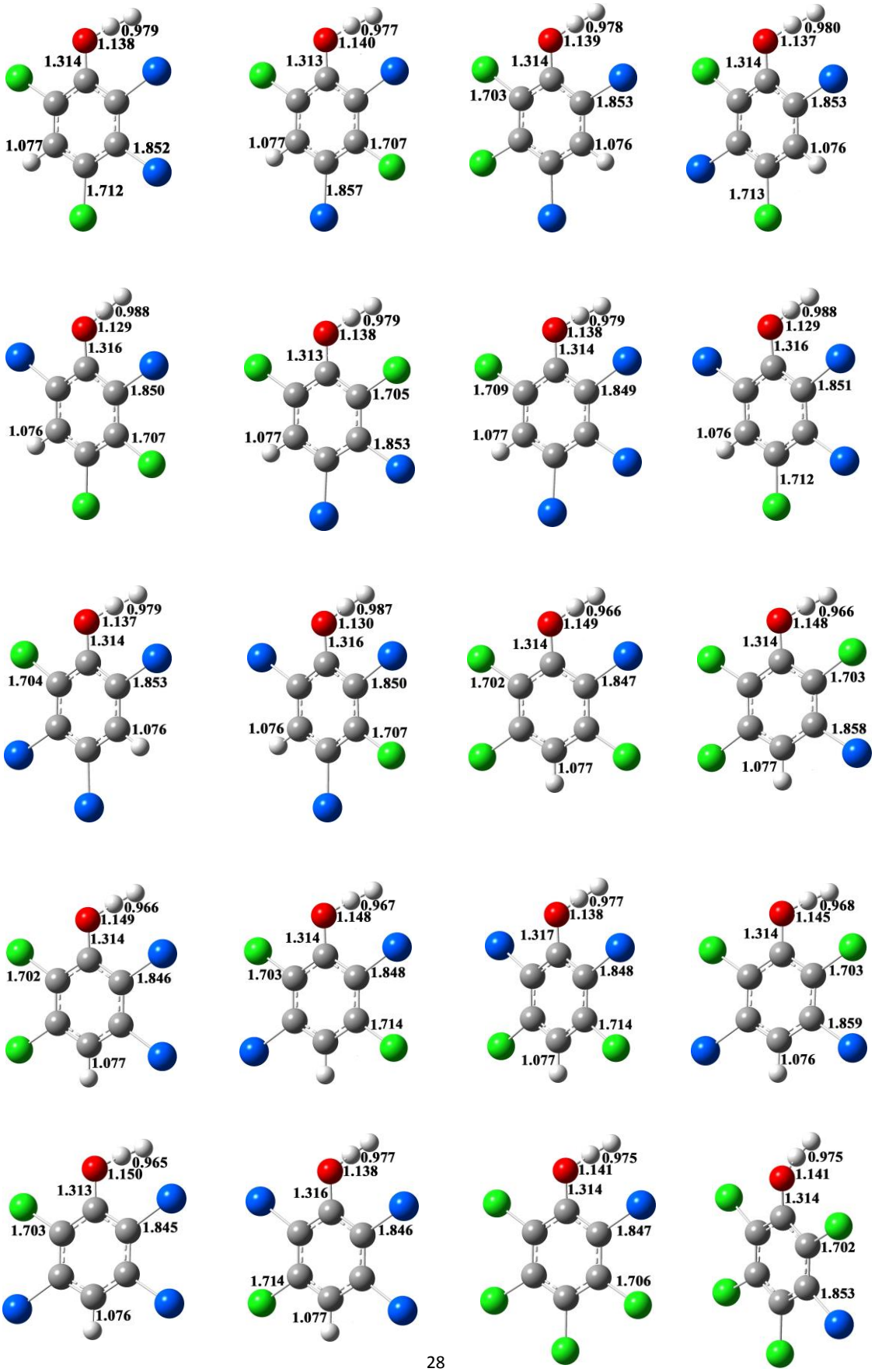


Figure S3 *Cont*.



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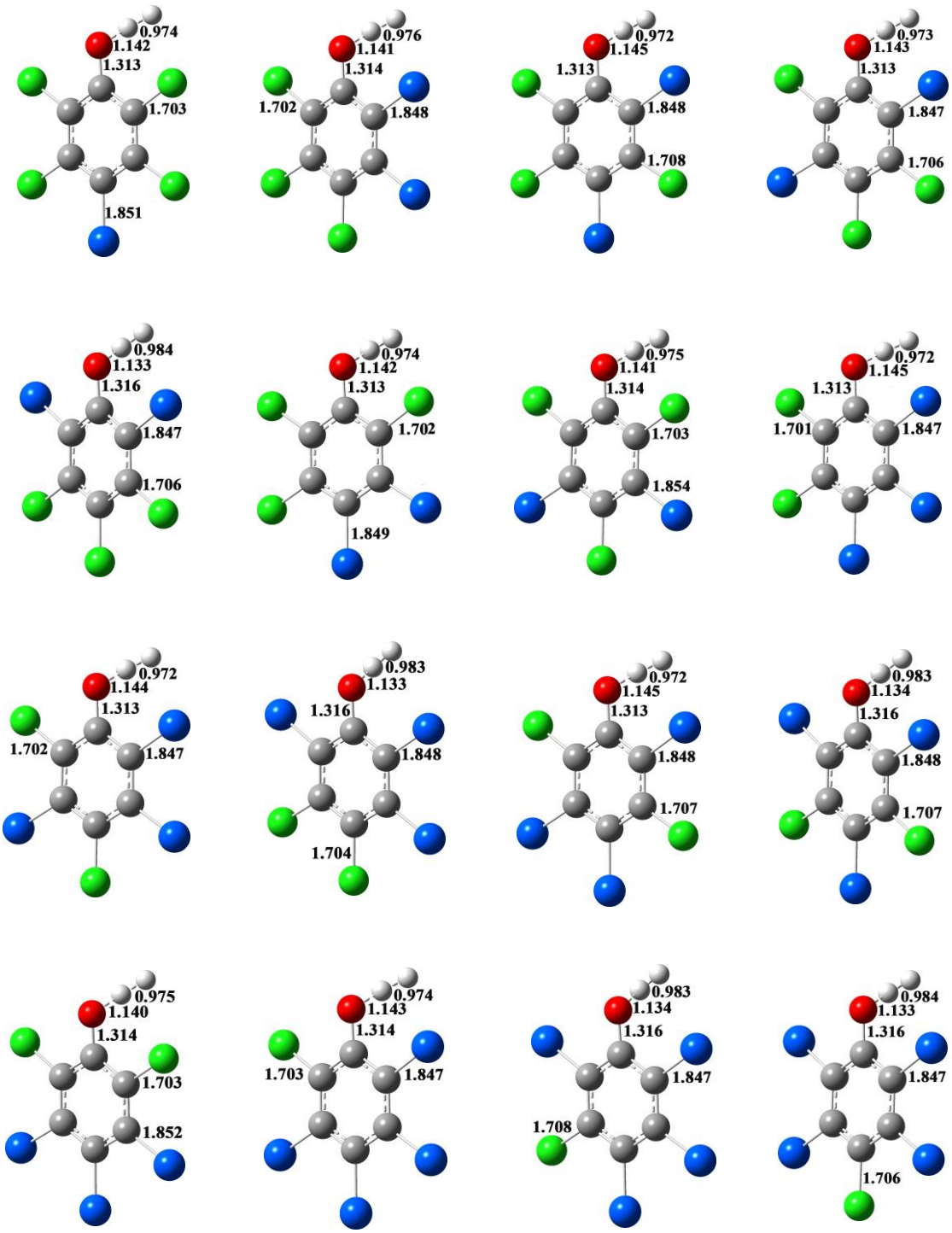
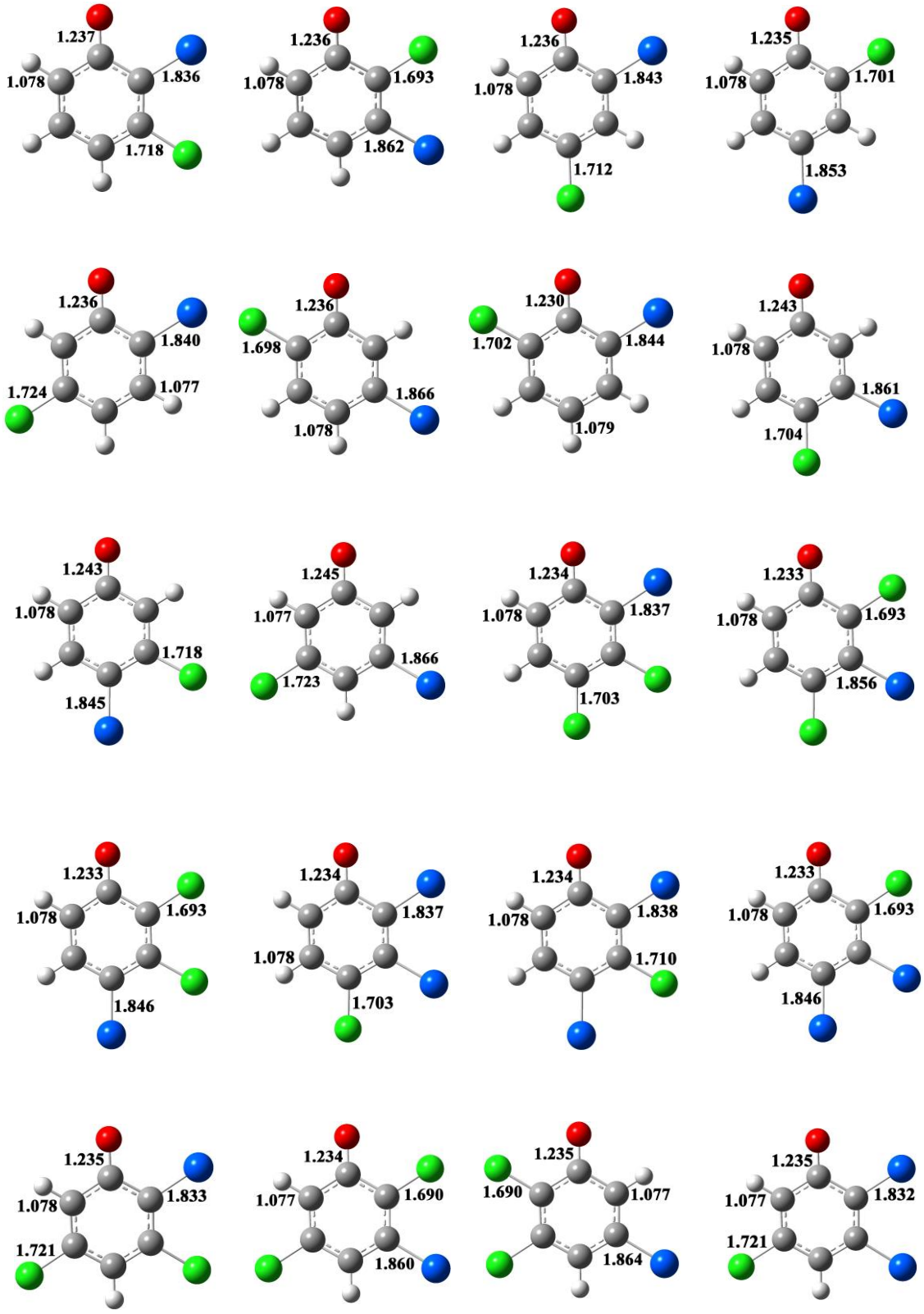


Figure S3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1.230
1.702
1.844
1.079
1.243
1.078
1.861
1.704
1.243
1.078
1.718
1.845
1.245
1.077
1.866
1.723
1.234
1.078
1.837
1.703
1.233
1.078
1.693
1.856
1.233
1.078
1.693
1.846
1.234
1.078
1.837
1.703
1.234
1.078
1.838
1.710
1.233
1.078
1.693
1.846
1.235
1.078
1.833
1.721
1.234
1.077
1.690
1.860
1.235
1.690
1.077
1.864
1.235
1.077
1.832
1.721

Figure S4

Figure S4 *Cont*.

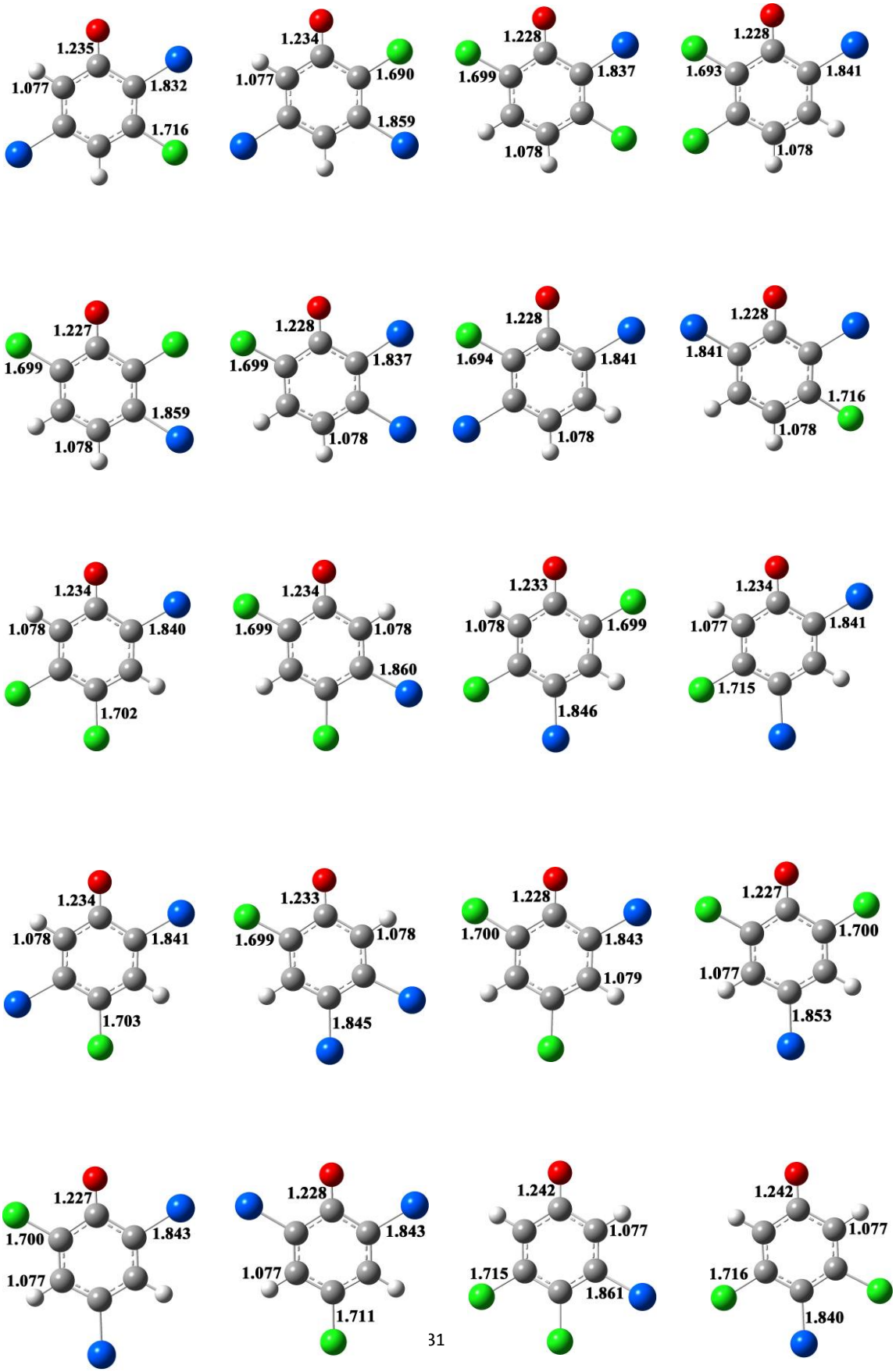

Figure S4 *Cont*.

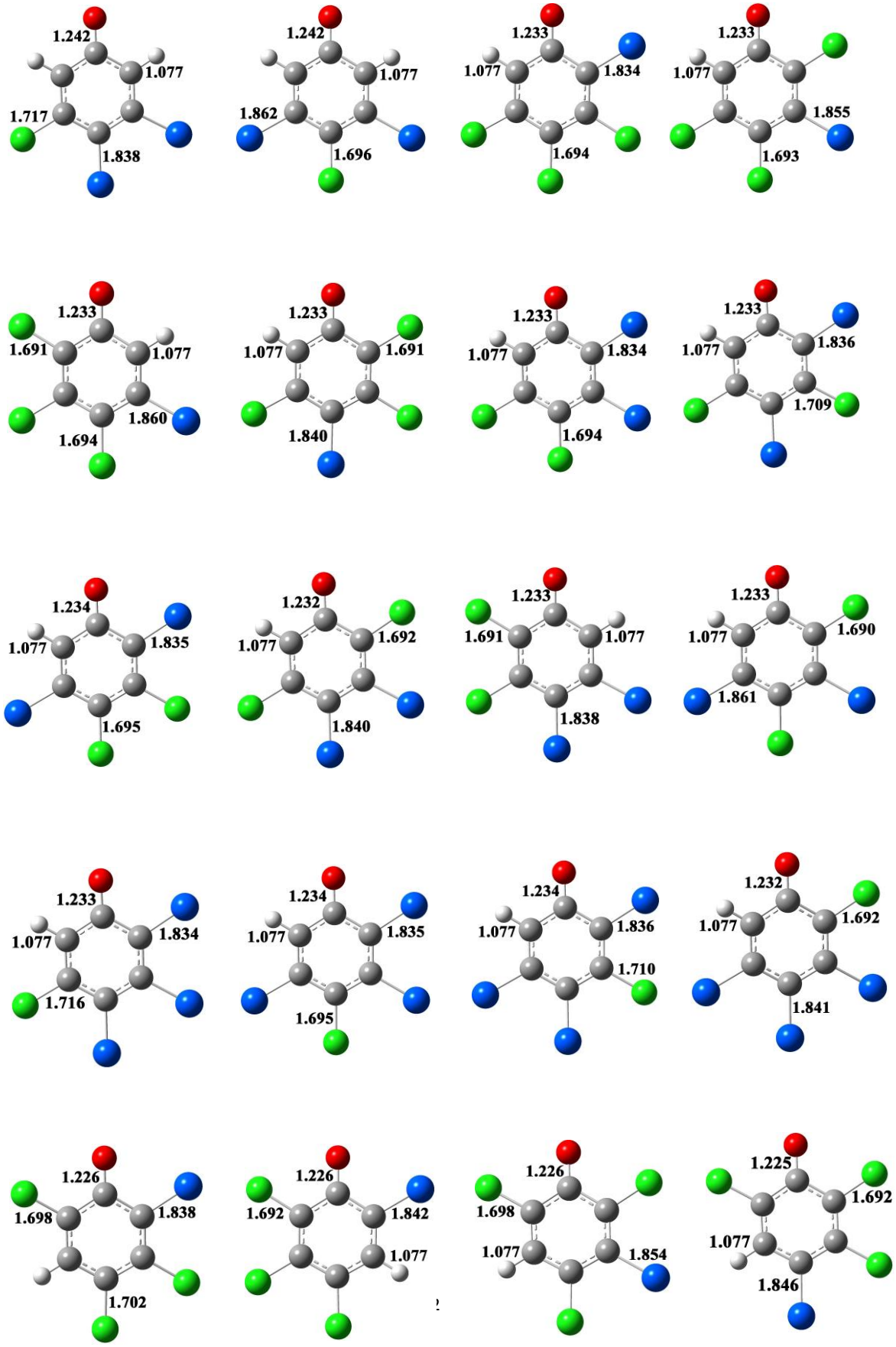

Figure S4 *Cont.*

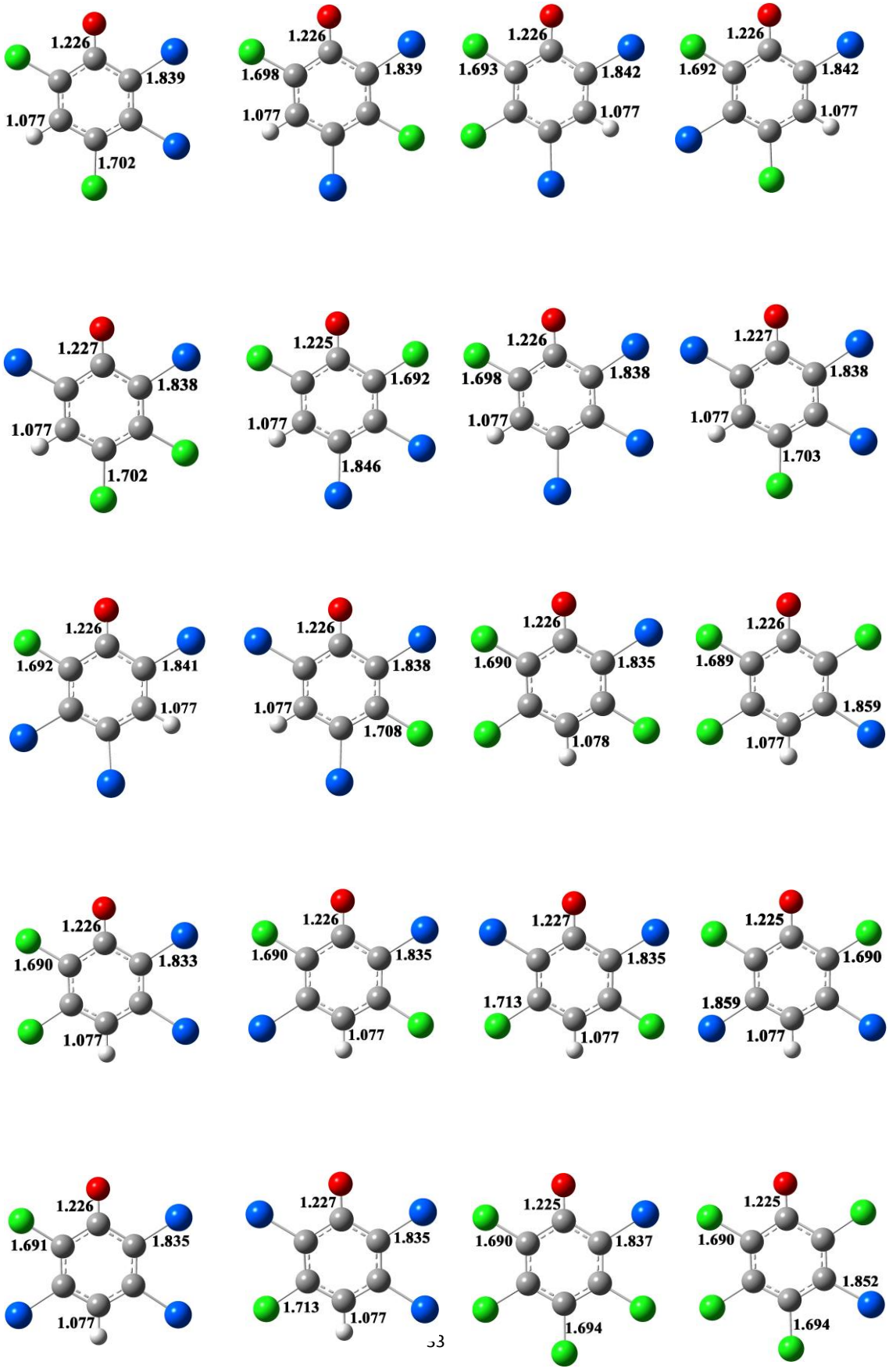

Figure S4. *Cont.*

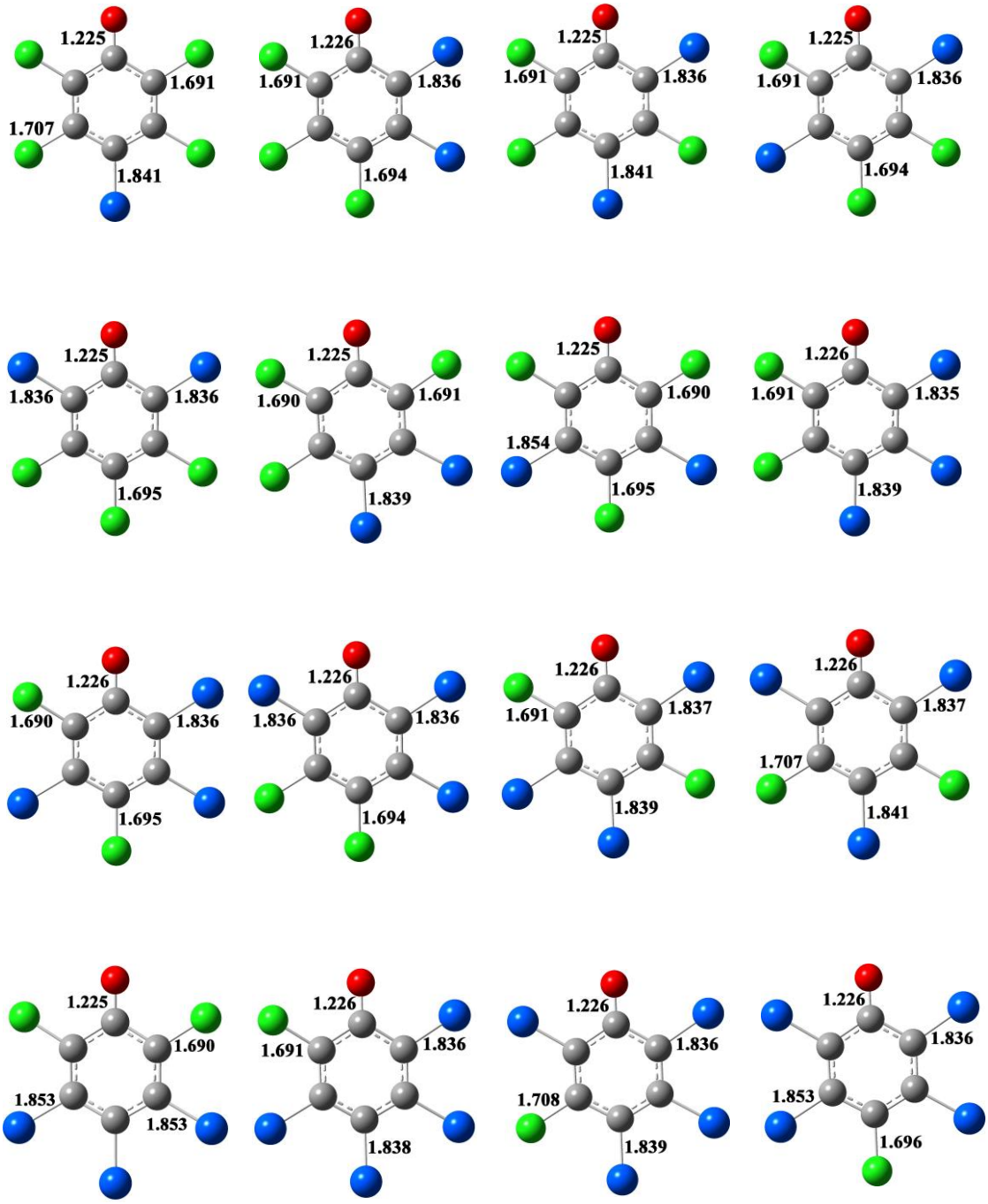

Figure S4