

## Supporting Document

### Computational Insights into Chlorine-dioxide Mediated Advance Oxidation Process of Halogenated Phenols

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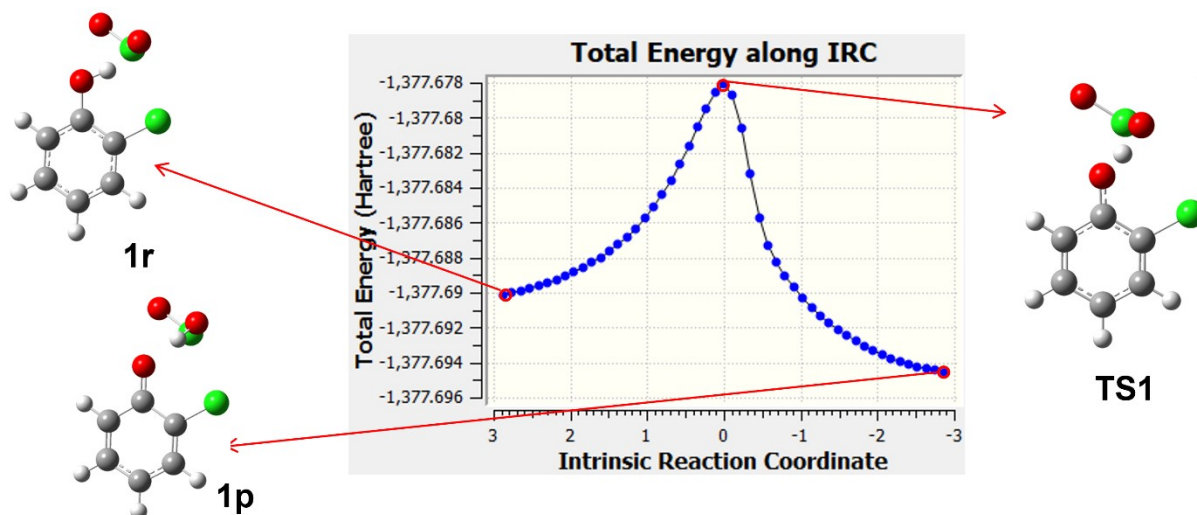


Figure S1: Step 1 IRC graph of ortho-chlorophenol computed at wB97XD /6-311g+(d,p) level of theory with IEFPCM solvent model (solvent=water)

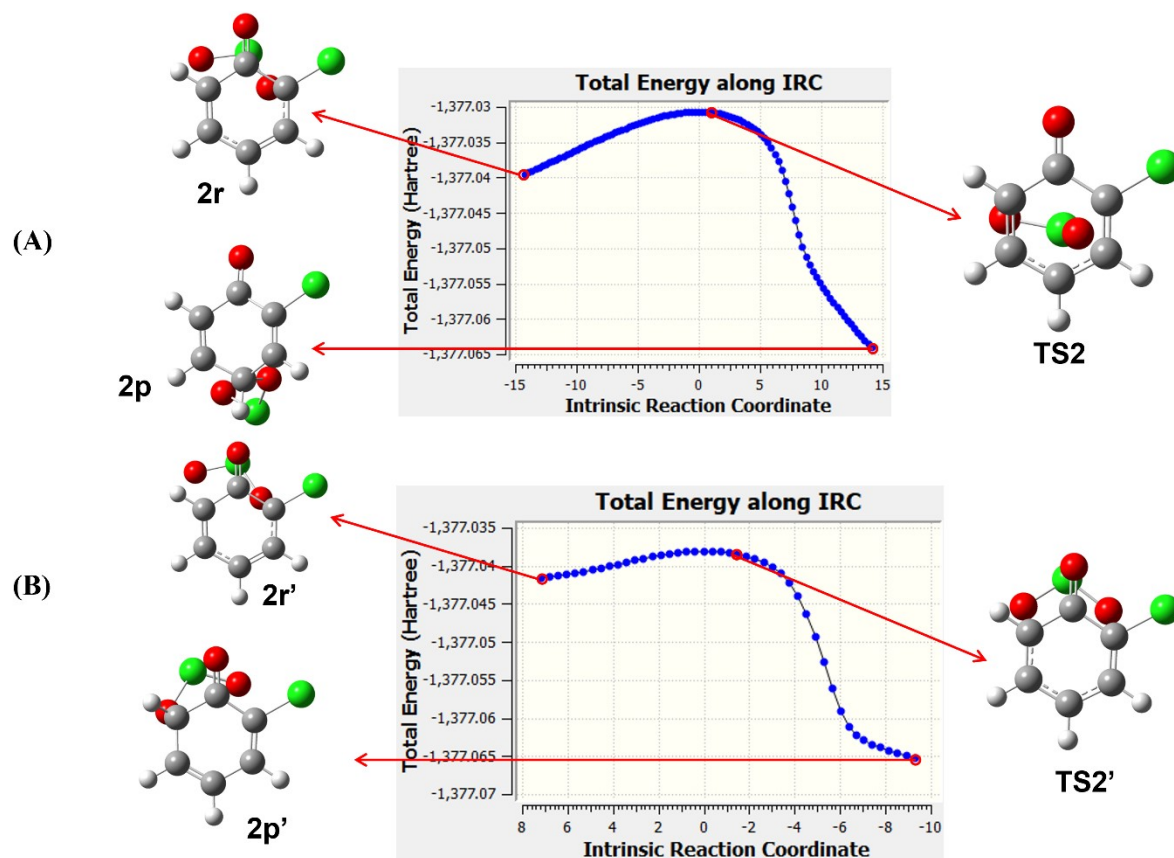
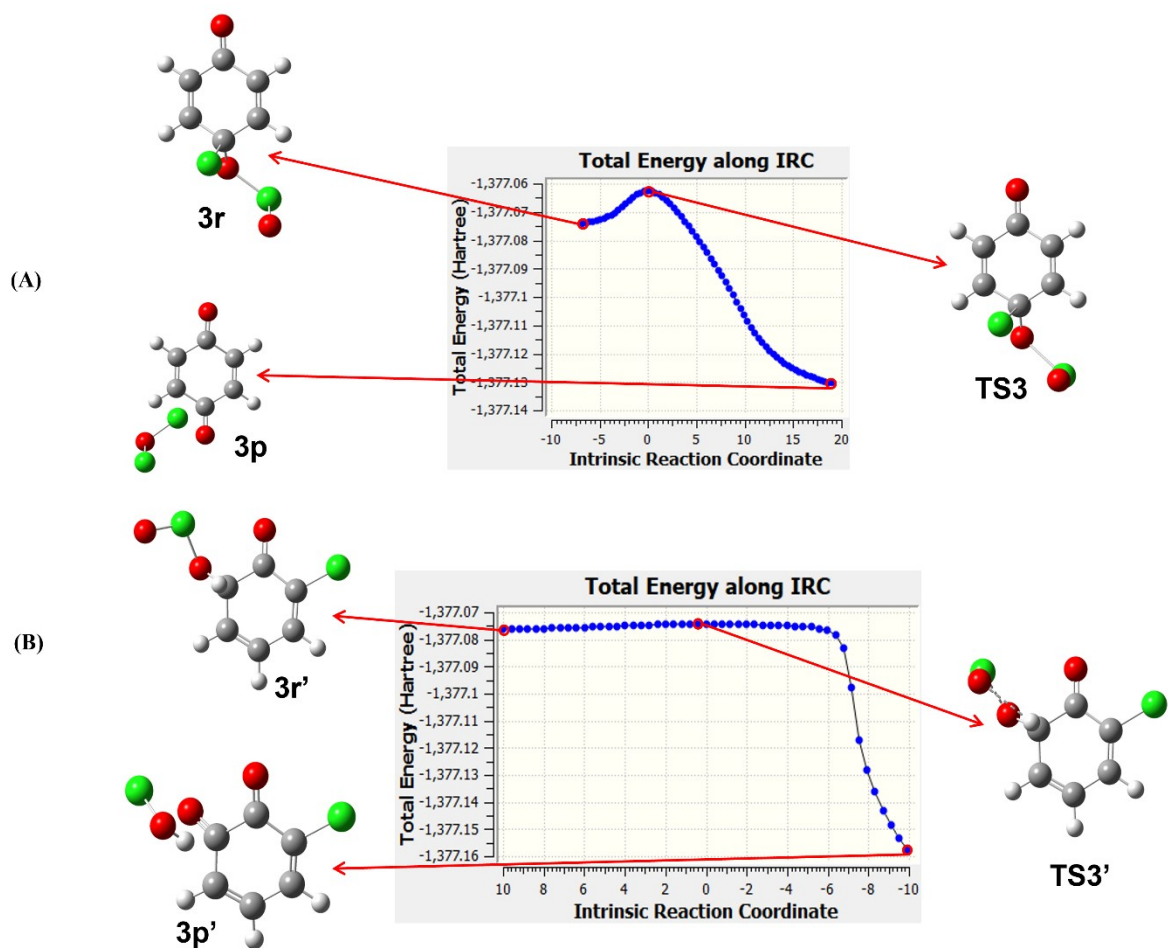
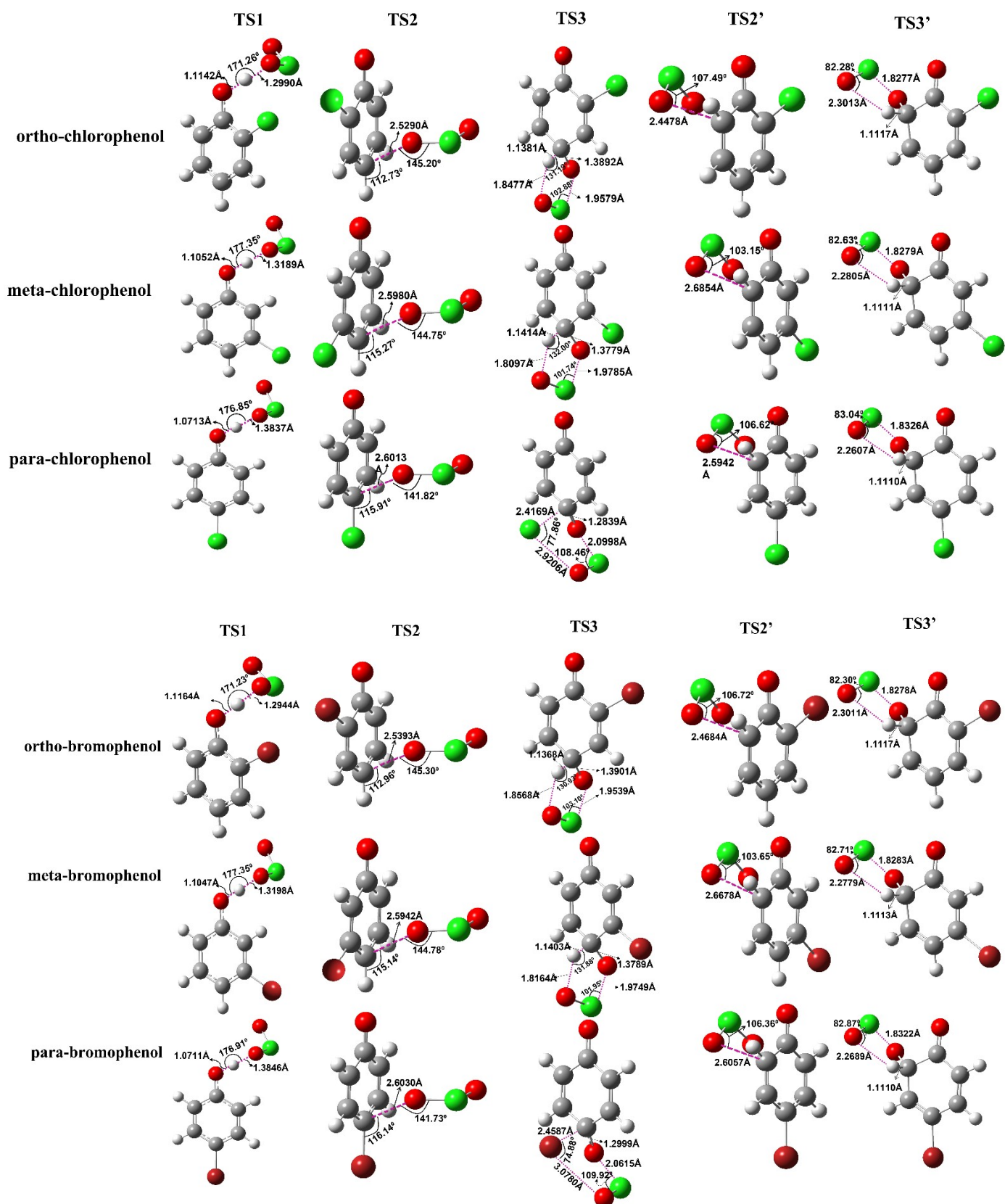


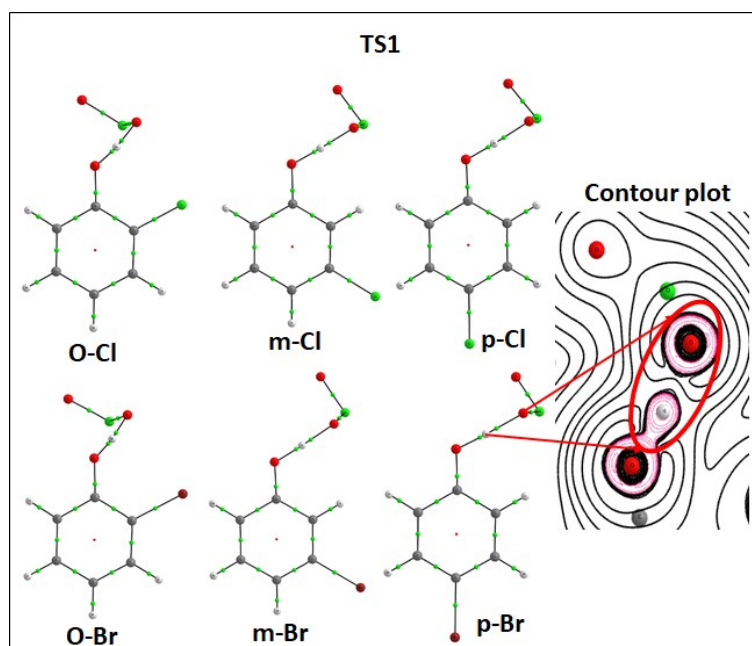
Figure S2: (A) P1 IRC of step 2 for ortho-chlorophenol (B) P2 IRC of step 2 for ortho-chlorophenol computed at wB97XD /6-311g+(d,p) level of theory with IEFPCM solvent model (solvent=water)



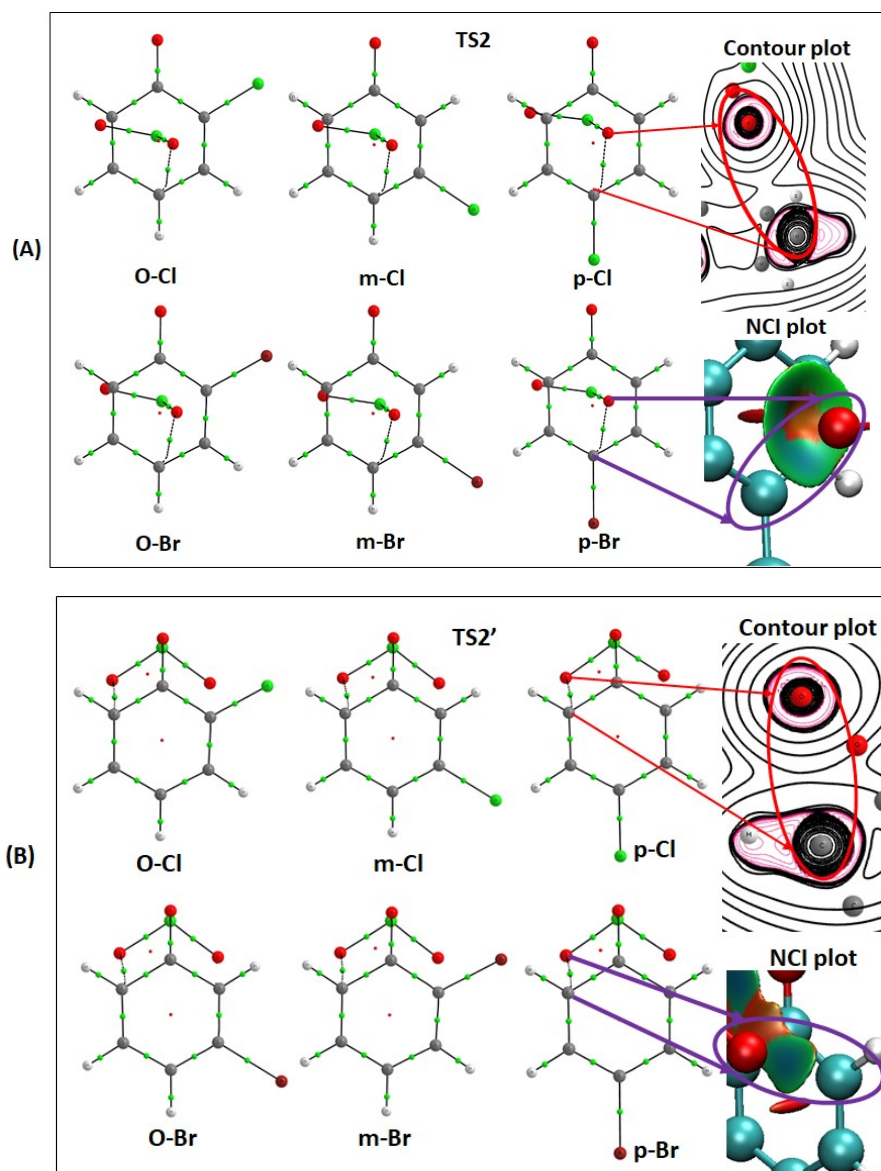
**Figure S3:** (A) P1 IRC of step2 for ortho-chlorophenol (B) P2 IRC of step 2 for ortho-chlorophenol computed at wB97XD6-311g+(d,p) level of theory with IEFPCM solvent model (solvent=water)



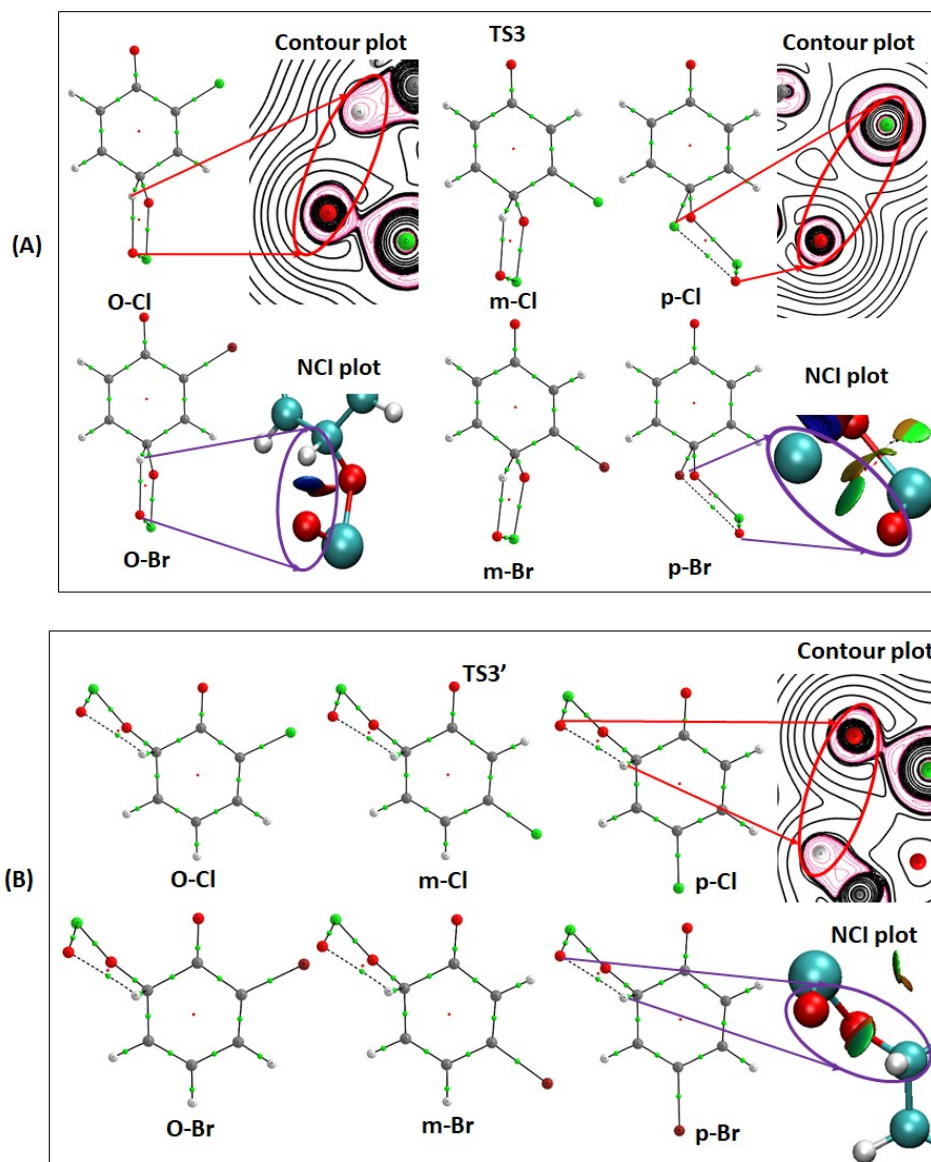
**Figure S4: Optimized structures of all the TS with selective bond lengths and bond angles, computed at *wB97XD/6-311g+(d,p)* level of theory with IEFPCM solvent model, solvent=water**



*Figure S5: Bader's analysis - molecular graph and contour plot of TS1 geometries*



*Figure S6: Bader's analysis - molecular graph, contour plot and NCI plot of (A) TS2 and (B) TS2' geometries*



**Figure S7: Bader's analysis - molecular graph, contour plot and NCI plot of (A) TS3 and (B) TS3' geometries**

**Table S1: Total energies of reaction species of para-chlorophenol in (i) solvent=PCM, water B3LYP/6-322+G(d,p) and (ii) solvent=IEFPCM, water B3LYP/6-322+G(d,p), M06/6-322+G(d,p) and wB97XD/6-322+G(d,p)**

compounds	Reported Values [6] at SCRF=PCM, B3LYP/6-311+G(d,p)	SCRF=PCM, B3LYP/6-311+G(d,p)	SCRF=IEFPCM, B3LYP/6-311+G(d,p)	SCRF=IEFPCM, M06/6-311+G(d,p)	SCRF=IEFPCM, wB97XD/6-311+G(d,p)
R	-767.08591	-767.09298	-767.09347	-766.837509	-766.96486
TS1	- 1377.59255	- 1377.58784	-1377.58850	-1377.22304	-1377.37828
int1	-766.46907	-766.46325	-766.46316	-766.20793	-766.33068
TS2	- 1376.95330	- 1376.94456	-1376.944564	-1376.58555	-1376.72966
int2	- 1376.99527	- 1376.98713	-1376.98795	-1376.63505	-1376.78653
TS3	- 1376.98363	- 1376.97415	-1376.97415	-1376.61443	-1376.75767
P	-381.49366	-381.48701	-381.48698	-381.23349	-381.34584

Where, R=reactant (para chlorophenol), TS1=transition state 1, int1=first intermediate (phenoxide radical), TS2=transition state 2, int2=second intermediate (cyclohexadienone analogue), TS3=transition state 3, P=product (para benzoquinone)

**Table S2: Electronic energies with Gibbs free energy (EE + G) and enthalpy (EE + H) corrections for ClO<sub>2</sub> and relevant reaction by-products calculated at the wB97XD/6-311+G(d,p) level of theory (in Hartree)**

	EE+G	EE+H
ClO <sub>2</sub>	-610.4465	-610.4167
HClO <sub>2</sub>	-611.0758	-611.0454
Cl <sub>2</sub> O	-995.5157	-995.4854
BrOCl	-3109.4995	-3109.4672
HOCl	-535.9759	-535.9491

**Table S3:**  
**Electronic**  
**energies**  
**with Gibbs**  
**free energy**  
**(EE + G)**  
**and enthalpy**  
**(EE + H)**  
**corrections**  
**for all the**  
**reacting**  
**species**  
**calculated at**  
**the**  
**wB97XD/6-**  
**311+G(d,p)**  
**level of**  
**theory (in**  
**Hartree)**

EE+G												
P1												
	R	TS1	int1	TS2	int2	TS3	P	TS2	int2	TS3	P	
<b>o-Cl</b>	-766.9950	-1377.4112	-766.3615	-1376.7648	-1376.8246	-1376.8206	-840.9923	-1376.7742	-1376.8229	-1376.8202	-840.9846	
<b>o-Br</b>	-2880.9621	-3491.3778	-2880.3283	-3490.7315	-3490.7916	-3490.7878	-2954.9592	-3490.7406	-3490.7901	-3490.78753	-2954.95	
<b>m-Cl</b>	-766.9964	-1377.4156	-766.3602	-1376.7606	-1376.8262	-1376.8221	-840.9923	-1376.7732	-1376.8256	-1376.82282	-840.9863	
<b>m-Br</b>	-2880.9629	-3491.3821	-2880.3269	-3490.7274	-3490.7926	-3490.7887	-2954.9591	-3490.74	-3490.7917	-3490.78905	-2954.953	
<b>p-Cl</b>	-766.9961	-1377.4188	-766.3625	-1376.7668	-1376.8242	-1376.7962	-381.3766	-1376.7778	-1376.8231	-1376.82035	-840.9863	
<b>p-Br</b>	-2880.9628	-3491.3853	-2880.3289	-3490.7328	-3490.7909	-3490.7697	-381.3766	-3490.7438	-3490.7898	-3490.78718	-2954.953	
EE+H												
P1												
	R	TS1	int1	TS2	int2	TS3	P	TS2	int2	TS3	P	
<b>o-Cl</b>	-766.9564	-1377.3608	-766.3224	-1376.7159	-1376.775	-1376.773	-840.951019	-1376.7269	-1376.7736	-1376.77277	-840.9425	
<b>o-Br</b>	-2880.922	-3491.3255	-2880.288	-3490.6812	-3490.741	-3490.739	-2954.9165	-3490.692	-3490.7395	-3490.73865	-2954.909	
<b>m-Cl</b>	-766.9576	-1377.3659	-766.321	-1376.7118	-1376.776	-1376.775	-840.950981	-1376.7257	-1376.7763	-1376.77529	-840.9443	
<b>m-Br</b>	-2880.923	-3491.3311	-2880.286	-3490.6773	-3490.742	-3490.74	-2954.91647	-3490.6913	-3490.7412	-3490.74018	-2954.909	
<b>p-Cl</b>	-766.9573	-1377.3667	-766.3233	-1376.7185	-1376.775	-1376.746	-381.338568	-1376.7303	-1376.7738	-1376.7727	-840.9443	
<b>p-Br</b>	-2880.923	-3491.3319	-2880.288	-3490.6832	-3490.741	-3490.718	-381.338568	-3490.695	-3490.7392	-3490.7382	-2954.909	

**Table S4: Topological parameters at the BCP for TS1, TS2 and TS3 computed at the same level of theory**

TS1								
	BCP	atoms	$\rho$	$\nabla^2\rho$	G	K	V	-(G/V)
o-Cl	12	O11 - H12	0.2185	-0.8048	0.0892	0.2904	-0.3797	0.2350
	15	H12 - O15	0.1307	0.0253	0.0848	0.0784	-0.1632	0.5194
m-Cl	11	O10 - H11	0.2284	-0.9663	0.0868	0.3283	-0.4151	0.2090
	14	H11 - O14	0.1236	0.0593	0.0844	0.0696	-0.1539	0.5482
p-Cl	12	O10 - H11	0.2531	-1.3327	0.0808	0.4140	-0.4949	0.1634
	15	H11 - O14	0.1033	0.1229	0.0762	0.0454	-0.1216	0.6264
o-Br	12	O11 - H12	0.2168	-0.7719	0.0899	0.2829	-0.3728	0.2412
	15	H12 - O15	0.1327	0.0165	0.0852	0.0810	-0.1662	0.5124
m-Br	12	O10 - H11	0.2287	-0.9709	0.0867	0.3294	-0.4161	0.2083
	15	H11 - O14	0.1233	0.0605	0.0843	0.0692	-0.1534	0.5493
p-Br	10	O9 - H10	0.2532	-1.3355	0.0808	0.4147	-0.4954	0.1630
	13	H10 - O13	0.1031	0.1233	0.0760	0.0452	-0.1213	0.6271
TS2								
	BCP	atoms	$\rho$	$\nabla^2\rho$	G	K	V	-(G/V)
o-Cl	12	C6 - O12	0.0225	0.0814	0.0177	-0.0026	-0.0151	1.1723
m-Cl	9	C6 - O11	0.0200	0.0772	0.0164	-0.0029	-0.0135	1.2146
p-Cl	10	C6 - O10	0.0202	0.0727	0.0157	-0.0025	-0.0132	1.1879
o-Br	12	C6 - O12	0.0220	0.0799	0.0174	-0.0026	-0.0148	1.1756
m-Br	11	C6 - O11	0.0201	0.0764	0.0163	-0.0028	-0.0135	1.2081
p-Br	10	C6 - O10	0.0201	0.0721	0.0156	-0.0025	-0.0131	1.1885
TS3								
	BCP	atoms	$\rho$	$\nabla^2\rho$	G	K	V	-(G/V)
o-Cl	13	C6 - O11	0.2706	-0.3940	0.2730	0.3715	-0.6445	0.4236
	14	O11 - Cl12	0.1142	0.2004	0.0753	0.0252	-0.1004	0.7494
	16	O13 - H14	0.0385	0.1183	0.0283	-0.0013	-0.0271	1.0464
	12	C6 - H14	0.2490	-0.7655	0.0347	0.2261	-0.2609	0.1332
	2	RCP2			5.0000	0.0226	0.1238	
m-Cl	11	C6 - O10	0.2782	-0.3955	0.2893	0.3882	-0.6775	0.4270
	12	O10 - Cl11	0.1091	0.2034	0.0725	0.0216	-0.0941	0.7703
	14	O12 - H13	0.0419	0.1251	0.0308	-0.0005	-0.0303	1.0160
	10	C6 - H13	0.2472	-0.7541	0.0345	0.2230	-0.2575	0.1339
	2	RCP2			5.0000	0.0232	0.1280	
p-Cl	13	C6 - O12	0.3458	-0.3239	0.4593	0.5402	-0.9995	0.4595
	14	O12 - Cl13	0.0812	0.2085	0.0589	0.0068	-0.0656	0.8970
	16	O14 - Cl15	0.0155	0.0487	0.0105	-0.0017	-0.0088	1.1911
	12	C6 - Cl15	0.0467	0.0677	0.0228	0.0059	-0.0287	0.7952
	2	RCP2			5.0000	0.0078	0.0349	
o-Br	13	C6 - O11	0.2699	-0.3939	0.2715	0.3700	-0.6416	0.4233
	14	O11 - Cl12	0.1152	0.1997	0.0758	0.0259	-0.1017	0.7454
	16	O13 - H14	0.0378	0.1167	0.0278	-0.0014	-0.0263	1.0539
	12	C6 - H14	0.2499	-0.7712	0.0347	0.2275	-0.2622	0.1324
	2	RCP2			5.0000	0.0225	0.1228	
m-Br	11	C6 - O10	0.2775	-0.3961	0.2876	0.3867	-0.6743	0.4266
	12	O10 - Cl11	0.1100	0.2030	0.0729	0.0222	-0.0951	0.7667
	14	O12 - H13	0.0412	0.1240	0.0303	-0.0007	-0.0297	1.0220
	10	C6 - H13	0.2480	-0.7590	0.0345	0.2242	-0.2587	0.1332
	2	RCP2			5.0000	0.0231	0.1274	
p-Br	13	O12 - Cl13	0.0886	0.2134	0.0635	0.0102	-0.0737	0.8620

	15	C6 - Br15	0.0525	0.0479	0.0213	0.0093	-0.0306	0.6960
	16	O14 - Br15	0.0140	0.0394	0.0087	-0.0011	-0.0076	1.1447
	12	C6 - O12	0.3338	-0.3693	0.4206	0.5129	-0.9335	0.4505
	2	RCP2			5.0000	0.0075	0.0331	

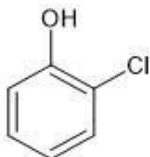
**Table S5: Topological parameters at the BCP for TS2' and TS3' computed at the same level of theory**

TS2'							
	BCP	atoms	$\rho$	$\nabla^2\rho$	G	K	V
o-Cl	10	C6 - O10	0.0279	0.0770	0.0182	-0.0010	-0.0172
m-Cl	10	C6 - O10	0.0182	0.0509	0.0114	-0.0013	-0.0102
p-Cl	9	C6 - O9	0.0213	0.0604	0.0138	-0.0013	-0.0124
o-Br	9	C6 - O9	0.0268	0.0744	0.0175	-0.0011	-0.0164
m-Br	9	C6 - O9	0.0188	0.0526	0.0118	-0.0013	-0.0105
p-Br	9	C6 - O9	0.0209	0.0592	0.0135	-0.0013	-0.0121
TS3'							
	BCP	atoms	$\rho$	$\nabla^2\rho$	G	K	V
o-Cl	10	C6 - H9	0.2681	-0.8818	0.0352	0.2556	-0.2908
	14	H9 - O12	0.0159	0.0523	0.0115	-0.0016	-0.0099
	12	O10 - Cl11	0.1531	0.1452	0.0971	0.0608	-0.1580
	11	C6 - O10	0.2532	-0.4112	0.2287	0.3315	-0.5601
m-Cl	10	C6 - H9	0.2684	-0.8837	0.0352	0.2561	-0.2913
	14	H9 - O12	0.0165	0.0540	0.0119	-0.0016	-0.0102
	12	O10 - Cl11	0.1531	0.1450	0.0970	0.0607	-0.1577
	11	C6 - O10	0.2522	-0.4052	0.2282	0.3295	-0.5577
p-Cl	10	C6 - H8	0.2689	-0.8871	0.0350	0.2568	-0.2917
	14	H8 - O11	0.0171	0.0558	0.0122	-0.0017	-0.0105
	12	O9 - Cl10	0.1514	0.1485	0.0960	0.0589	-0.1549
	11	C6 - O9	0.2522	-0.4115	0.2262	0.3290	-0.5552
o-Br	10	C6 - H9	0.2681	-0.8818	0.0352	0.2556	-0.2908
	14	H9 - O12	0.0159	0.0523	0.0115	-0.0016	-0.0099
	12	O10 - Cl11	0.1531	0.1453	0.0971	0.0608	-0.1579
	11	C6 - O10	0.2534	-0.4107	0.2294	0.3320	-0.5614
m-Br	11	C6 - H9	0.2683	-0.8828	0.0352	0.2559	-0.2911
	15	H9 - O12	0.0166	0.0542	0.0119	-0.0017	-0.0103
	13	O10 - Cl11	0.1529	0.1453	0.0969	0.0606	-0.1574
	12	C6 - O10	0.2522	-0.4051	0.2284	0.3296	-0.5580
p-Br	10	C6 - H8	0.2688	-0.8862	0.0350	0.2566	-0.2916
	14	H8 - O11	0.0168	0.0550	0.0121	-0.0017	-0.0104
	12	O9 - Cl10	0.1515	0.1484	0.0962	0.0590	-0.1552
	11	C6 - O9	0.2526	-0.4113	0.2271	0.3300	-0.5571

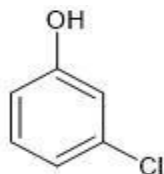
**Table S6: Coordinates of all the structures included in this study computed at wB97XD/6-311g+(d,p) level of theory with IEFPCM solvent model (solvent=water).**

ClO<sub>2</sub> Radical

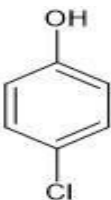
Cl	0.000000000	0.046848000	0.360361000
O	0.000000000	-1.230983000	-0.425222000
O	0.000000000	1.308404000	-0.451317000



C	-1.826050000	-1.281618000	0.012955000
C	-2.350224000	0.007886000	-0.021693000
C	-1.510159000	1.111235000	-0.017461000
C	-0.127246000	0.943692000	0.021589000
C	0.385951000	-0.354474000	0.056786000
C	-0.450182000	-1.461913000	0.052470000
H	-3.422962000	0.158092000	-0.053183000
H	-1.907661000	2.118942000	-0.044709000
O	0.650288000	2.049264000	0.023795000
H	1.580649000	1.800123000	0.048382000
H	-2.481471000	-2.143709000	0.009441000
H	-0.019174000	-2.455058000	0.080520000
Cl	2.125460000	-0.568288000	0.108175000

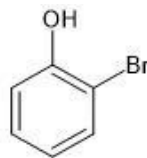


C	-1.838169000	-1.286047000	0.012579000
C	-2.349193000	0.008109000	-0.021669000
C	-1.510105000	1.112575000	-0.017259000
C	-0.130118000	0.925792000	0.022043000
C	0.407443000	-0.359761000	0.057788000
C	-0.460983000	-1.441849000	0.051964000
H	-3.422530000	0.154724000	-0.053369000
H	-1.909941000	2.118796000	-0.044615000
O	0.652320000	2.034255000	0.023991000
H	1.581402000	1.791520000	0.047997000
H	-2.492790000	-2.147504000	0.008798000
Cl	0.215339000	-3.059165000	0.096666000
H	1.479801000	-0.513768000	0.090386000

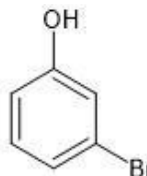


C	-1.821917000	-1.265785000	0.012813000
C	-2.359904000	0.013318000	-0.021940000
C	-1.510882000	1.111205000	-0.017254000
C	-0.131186000	0.926309000	0.021951000

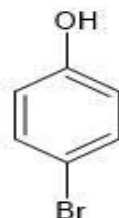
C	0.398265000	-0.361849000	0.057575000
C	-0.449641000	-1.462237000	0.052714000
H	-3.432764000	0.157406000	-0.053545000
H	-1.914850000	2.115989000	-0.044732000
O	0.649375000	2.038017000	0.023726000
H	1.577906000	1.793466000	0.047751000
H	1.472062000	-0.512687000	0.090121000
H	-0.038451000	-2.463707000	0.080403000
Cl	-2.893773000	-2.656626000	0.006236000



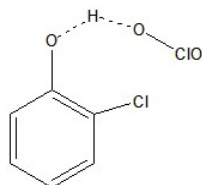
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C	-0.448630000	-1.459268000	0.052737000
H	-3.422163000	0.159561000	-0.053853000
H	-1.907445000	2.120208000	-0.045780000
O	0.644085000	2.056954000	0.023843000
H	1.576373000	1.812010000	0.051380000
H	-2.479253000	-2.142374000	0.010753000
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H	-0.022560000	-2.454430000	0.081069000



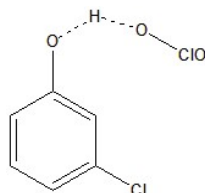
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C	-0.459539000	-1.442493000	0.051912000
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H	-1.909314000	2.119293000	-0.044458000
O	0.653270000	2.034926000	0.023987000
H	1.582279000	1.791890000	0.048159000
H	1.481351000	-0.507752000	0.090115000
H	-2.496431000	-2.144158000	0.008579000
Br	0.275692000	-3.199547000	0.100909000



C	-1.82302000	-1.267631000	0.012816000
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C	-0.131347000	0.926161000	0.021934000
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H	-3.432326000	0.161617000	-0.053564000
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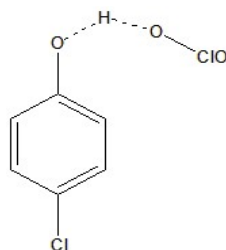


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H	-1.736916000	-2.055720000	0.766349000
H	-3.756097000	-0.806218000	1.520550000
H	-4.147568000	1.509404000	0.699628000
O	0.007861000	-1.179097000	-0.884221000
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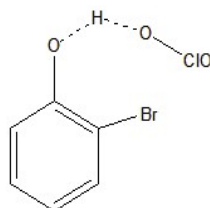


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C	-3.291507000	-0.480197000	0.628876000
C	-3.346727000	0.885639000	0.314076000
H	-2.086904000	-2.268034000	0.593658000
H	-4.146708000	-0.949556000	1.098061000
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O	-0.007793000	-1.321314000	-0.567800000
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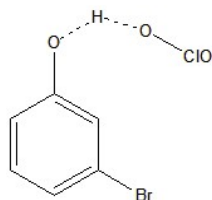
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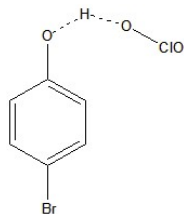
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H	-2.219161000	2.608596000	-0.460191000
H	-2.151121000	-2.265393000	0.560725000
H	-4.175148000	-0.913083000	1.084030000
O	-0.032951000	-1.353353000	-0.562285000
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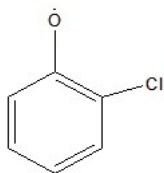
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H	-3.065713000	-0.194616000	-1.356622000
H	-0.205298000	2.919702000	1.261769000
H	-2.121746000	3.802022000	-0.063053000
H	-3.530841000	2.231322000	-1.381868000
O	0.448909000	0.457292000	1.454842000
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H	-4.233624000	1.463295000	0.540492000
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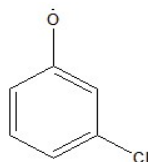


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H	-4.172170000	-0.914781000	1.095262000
O	-0.033312000	-1.355099000	-0.552163000
H	0.873049000	-0.825311000	-0.764723000
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O	2.082528000	-0.197247000	-1.009292000
H	-0.207666000	1.260295000	-1.002064000
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Br	-4.833924000	1.951782000	0.751448000

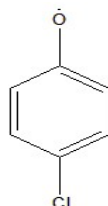


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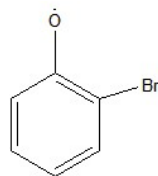
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H	-2.787903000	1.884305000	-0.051065000
H	-3.942683000	-0.318092000	-0.073565000
H	-2.610952000	-2.407795000	0.005950000
O	-0.212905000	2.156630000	0.050832000
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C	-0.716150000	-1.399053000	0.072721000
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O	-0.199219000	2.132572000	0.052067000
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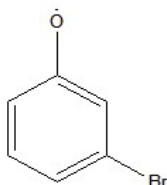


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H	-2.797399000	1.878451000	-0.051801000
H	-3.956175000	-0.320968000	-0.074123000
O	-0.204690000	2.135074000	0.051145000
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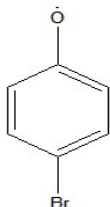


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C	-2.862746000	-0.258936000	-0.029153000
C	-2.106186000	-1.446811000	0.016143000
H	-2.788557000	1.885627000	-0.051966000
H	-3.943470000	-0.317133000	-0.074218000
O	-0.219709000	2.163158000	0.052617000
H	-2.609332000	-2.406038000	0.006970000
H	-0.147778000	-2.339439000	0.107273000
Br	1.822416000	-0.134035000	0.160599000



C	-0.714914000	-1.400311000	0.072836000
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C	-2.120714000	-1.454073000	0.015278000
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O	-0.197736000	2.133000000	0.052266000
H	1.035244000	-0.152604000	0.131159000
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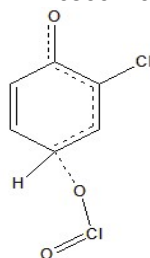


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H	1.023745000	-0.163887000	0.130838000
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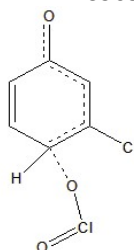
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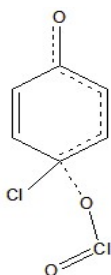
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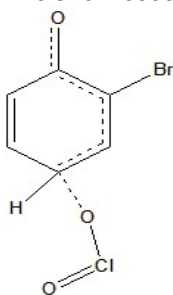
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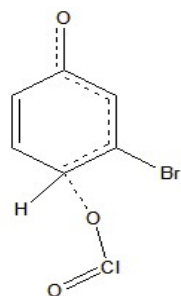
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H	0.942041000	1.313571000	1.973642000
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O	-0.818707000	-0.453859000	-0.752342000
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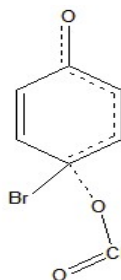
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O	1.629631000	2.169388000	-0.403605000
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H	2.099732000	0.253945000	-2.107767000
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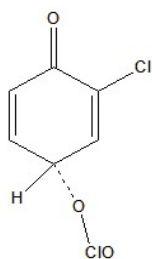
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C	0.881961000	-0.757007000	1.475236000
C	0.983600000	-1.695564000	0.399906000
H	1.010987000	1.308886000	2.004861000
H	0.578842000	-1.111365000	2.451764000
O	1.594232000	2.198415000	-0.367324000
O	-0.799805000	-0.471547000	-0.690765000
Cl	-2.256353000	0.009549000	-0.325515000
O	-2.322026000	0.621272000	1.100885000
H	0.730247000	-2.732278000	0.589596000
H	1.704370000	-2.136002000	-1.587488000
Br	2.272355000	0.509780000	-2.826099000



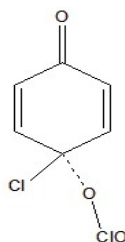
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C	1.453394000	0.992804000	-0.134431000
C	1.055478000	0.548573000	1.216753000
C	0.846336000	-0.762832000	1.463447000
C	0.961654000	-1.707597000	0.409146000
H	0.947957000	1.311527000	1.977068000
H	0.523101000	-1.110234000	2.435766000
O	1.607825000	2.171682000	-0.403029000
O	-0.818326000	-0.452473000	-0.749305000
Cl	-2.219125000	0.063891000	-0.266027000
O	-2.162380000	0.561983000	1.198188000
H	2.038409000	0.280846000	-2.128412000
Br	1.839384000	-2.721958000	-2.112710000
H	0.711164000	-2.744025000	0.602734000



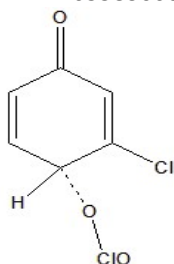
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C	1.471868000	0.991732000	-0.138336000
C	1.051968000	0.554285000	1.209867000
C	0.828182000	-0.747932000	1.471056000
C	0.962007000	-1.697159000	0.410957000
H	0.937571000	1.319344000	1.967413000
H	0.496603000	-1.084267000	2.444165000
O	1.637566000	2.169953000	-0.403044000
O	-0.824187000	-0.416355000	-0.756705000
Cl	-2.251787000	0.019965000	-0.255141000
O	-2.214992000	0.502040000	1.223133000
H	2.104613000	0.252732000	-2.106585000
H	1.723232000	-2.150968000	-1.572257000
Br	0.543343000	-3.467447000	0.764790000



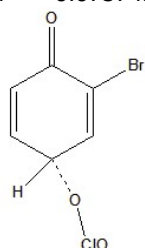
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C	0.496715000	2.551147000	-0.061100000
C	-0.794212000	2.273418000	0.105107000
C	-1.276085000	0.897701000	0.427831000
H	0.843918000	3.560194000	-0.249176000
H	-1.552781000	3.045854000	0.053065000
O	2.718329000	1.774718000	-0.133658000
O	-2.345969000	0.632416000	-0.510416000
Cl	-3.515575000	-0.480745000	0.065711000
O	-3.064710000	-1.933376000	-0.158394000
H	-0.568507000	-1.195942000	0.498652000
H	-1.698087000	0.913814000	1.441859000
Cl	2.265583000	-1.132820000	0.174961000



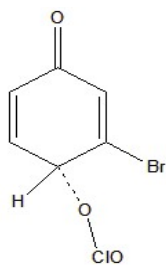
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C	0.471669000	2.516251000	-0.147385000
C	-0.802290000	2.324060000	0.181108000
C	-1.323043000	0.980472000	0.594780000
H	0.838288000	3.494266000	-0.435564000
H	-1.531845000	3.125038000	0.168699000
O	2.617338000	1.590262000	-0.440270000
O	-2.415604000	0.769927000	-0.276185000
Cl	-3.289937000	-0.728672000	-0.077052000
O	-2.637689000	-1.855886000	-0.880511000
H	1.673997000	-0.737007000	0.249478000
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H	-0.673749000	-1.115759000	0.868215000



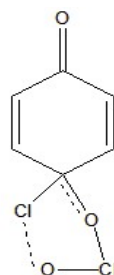
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C	0.355227000	2.509894000	-0.015138000
C	-0.877728000	2.020952000	0.081510000
C	-1.168060000	0.567171000	0.298213000
H	0.541550000	3.566124000	-0.168156000
H	-1.745651000	2.668194000	0.013130000
O	2.671769000	2.066891000	-0.018875000
O	-1.996055000	0.069974000	-0.774001000
Cl	-3.679472000	0.149045000	-0.431737000
O	-4.068720000	-0.925151000	0.592235000
H	-1.694302000	0.432390000	1.252223000
Cl	-0.238334000	-1.992271000	0.557685000
H	2.165610000	-0.459774000	0.305101000



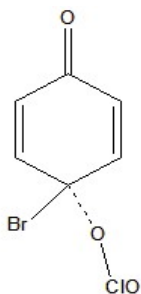
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C	1.543461000	1.513002000	-0.005102000
C	0.496322000	2.552840000	-0.063169000
C	-0.794651000	2.274824000	0.100872000
C	-1.274441000	0.898978000	0.423870000
H	0.843187000	3.562011000	-0.251474000
H	-1.553643000	3.046750000	0.047291000
O	2.719172000	1.785861000	-0.128911000
O	-2.344293000	0.630906000	-0.513057000
Cl	-3.513840000	-0.481116000	0.065968000
O	-3.062254000	-1.934037000	-0.154217000
H	-1.694503000	0.913137000	1.438835000
H	-0.569722000	-1.192440000	0.490799000
Br	2.374086000	-1.245332000	0.173626000



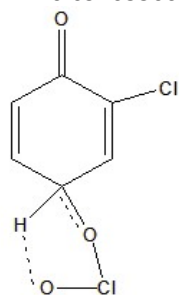
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C	0.344187000	2.504575000	-0.026483000
C	-0.884157000	2.004681000	0.072815000
C	-1.163030000	0.549595000	0.299492000
H	0.521126000	3.561456000	-0.185944000
H	-1.757461000	2.644580000	0.001079000
O	2.663959000	2.077965000	-0.028382000
O	-1.988223000	0.038470000	-0.769186000
Cl	-3.672338000	0.176823000	-0.455272000
O	-4.104622000	-0.844915000	0.605190000
H	2.181079000	-0.443317000	0.315222000
Br	-0.228731000	-2.155480000	0.602716000
H	-1.690818000	0.420041000	1.253259000



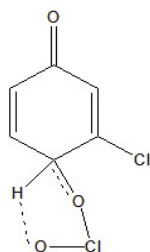
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C	-2.403942000	0.332339000	1.013682000
C	-1.132534000	0.392137000	1.411877000
C	-0.079876000	-0.251138000	0.608462000
H	0.377404000	-1.258282000	-1.296643000
H	-1.982009000	-1.373411000	-2.013896000
H	-3.203673000	0.776253000	1.594133000
H	-0.818891000	0.861041000	2.334854000
O	-3.943354000	-0.388858000	-0.615068000
O	0.971512000	-0.542547000	1.243937000
Cl	2.681148000	-0.927287000	0.138207000
O	2.848330000	0.205561000	-0.845200000
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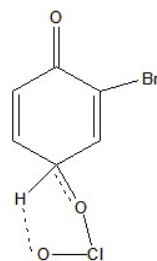
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C	0.472942000	2.516400000	-0.142934000
C	-0.809763000	2.315320000	0.148445000
C	-1.325885000	0.974382000	0.565105000
H	0.838349000	3.495390000	-0.429267000
H	-1.545034000	3.109761000	0.102417000
O	2.638800000	1.611854000	-0.340878000
O	-2.437678000	0.763075000	-0.275702000
Cl	-3.306536000	-0.737928000	-0.066651000
O	-2.660728000	-1.863388000	-0.877144000
H	1.678886000	-0.731366000	0.269207000
H	-0.683482000	-1.127592000	0.809743000
Br	-1.937277000	1.161867000	2.462948000



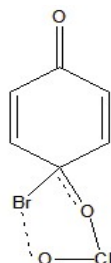
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C	2.082632000	1.096546000	0.219829000
C	0.777060000	1.305166000	0.049037000
C	-0.187858000	0.171410000	-0.055879000
H	-0.265943000	-2.016986000	-0.324271000
H	2.782060000	1.917895000	0.323183000
H	0.354861000	2.302789000	0.005234000
H	-0.721508000	0.171941000	0.982071000
O	3.855741000	-0.435173000	0.456118000
O	-1.163942000	0.379198000	-0.975223000
Cl	-2.853268000	0.489677000	0.033652000
O	-2.299698000	0.322720000	1.470153000
Cl	2.416527000	-2.976142000	-0.029265000



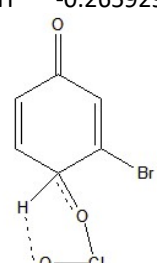
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C	2.087211000	1.096712000	0.214414000
C	0.780185000	1.302699000	0.061514000
C	-0.203052000	0.178730000	-0.050674000
H	2.785589000	1.920085000	0.307987000
H	0.352921000	2.298436000	0.024590000
H	-0.747641000	0.177781000	0.982625000
O	3.848121000	-0.458141000	0.421045000
O	-1.158086000	0.406337000	-0.976512000
Cl	-2.868441000	0.509414000	0.020075000
O	-2.319765000	0.308999000	1.453996000
Cl	-0.678702000	-2.503215000	-0.379928000
H	2.159222000	-2.386063000	0.012363000



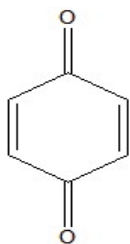
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C	2.669869000	-0.252634000	0.265832000
C	2.081855000	1.098569000	0.218952000
C	0.776539000	1.306782000	0.047151000
C	-0.186655000	0.171937000	-0.056008000
H	2.781134000	1.920266000	0.321011000
H	0.354096000	2.304218000	0.001290000
H	-0.718609000	0.168782000	0.982545000
O	3.857050000	-0.425945000	0.465589000
O	-1.164512000	0.376148000	-0.974275000
Cl	-2.851453000	0.491559000	0.036860000
O	-2.296861000	0.322174000	1.472624000
Br	2.477522000	-3.118548000	-0.038688000
H	-0.265929000	-2.012452000	-0.328305000



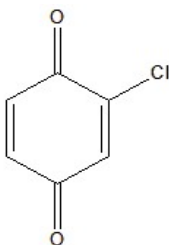
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C	-2.791455000	-0.348560000	-0.245240000
C	-2.396964000	0.327956000	1.010064000
C	-1.118771000	0.422188000	1.381250000
C	-0.062621000	-0.205478000	0.563323000
H	0.364793000	-1.236218000	-1.336553000
H	-2.005773000	-1.391280000	-2.008538000
H	-3.192197000	0.756211000	1.608255000
H	-0.799908000	0.899946000	2.298024000
O	-3.958538000	-0.434224000	-0.578669000
O	0.949660000	-0.593894000	1.234724000
Cl	2.677273000	-0.965493000	0.170958000
O	2.877989000	0.200106000	-0.775783000
Br	0.700914000	2.029568000	-0.463524000



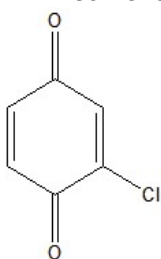
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C	2.084770000	1.096663000	0.214813000
C	0.777273000	1.298284000	0.060328000
C	-0.204852000	0.172402000	-0.051430000
H	2.780667000	1.922098000	0.308771000
H	0.347358000	2.292980000	0.023121000
H	-0.747138000	0.173841000	0.982544000
O	3.847218000	-0.456490000	0.422905000
O	-1.161081000	0.405392000	-0.975516000
Cl	-2.866142000	0.532039000	0.024564000
O	-2.318161000	0.327514000	1.458036000
H	2.167795000	-2.383224000	0.012201000
Br	-0.764985000	-2.637821000	-0.406074000



C	0.727357000	-1.070821000	0.090875000
C	-0.158623000	-0.073971000	0.106570000
C	0.279152000	1.343381000	0.051597000
C	1.737053000	1.612334000	-0.021689000
C	2.623033000	0.615515000	-0.037386000
C	2.185268000	-0.801873000	0.017302000
H	2.034560000	2.654012000	-0.062323000
H	3.691723000	0.788923000	-0.092140000
O	-0.528486000	2.252330000	0.065580000
O	2.992923000	-1.710789000	0.003661000
H	0.429853000	-2.112456000	0.131673000
H	-1.227280000	-0.247339000	0.161478000

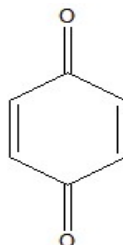


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C	1.735087000	1.609673000	-0.021597000
C	2.618002000	0.612237000	-0.037276000
C	2.176138000	-0.802578000	0.018817000
H	0.418856000	-2.112995000	0.132096000
H	2.033007000	2.650742000	-0.062685000
H	3.686531000	0.783829000	-0.092707000
O	-0.521276000	2.273695000	0.065815000
O	2.976589000	-1.715912000	0.004579000
Cl	-1.861197000	-0.354043000	0.191430000

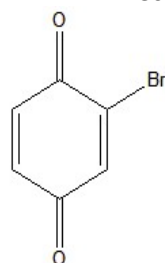


C	0.723161000	-1.070303000	0.091415000
C	-0.165324000	-0.075797000	0.107548000
C	0.278179000	1.337817000	0.051963000
C	1.734734000	1.607518000	-0.021911000
C	2.619101000	0.611367000	-0.037014000
C	2.200577000	-0.809779000	0.018268000

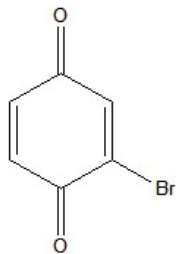
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H	3.687761000	0.782074000	-0.092335000
O	-0.532285000	2.242331000	0.066777000
O	3.007886000	-1.709457000	0.004104000
Cl	0.241775000	-2.727003000	0.153582000
H	-1.232832000	-0.250597000	0.162095000



C	0.727357000	-1.070821000	0.090875000
C	-0.158623000	-0.073971000	0.106570000
C	0.279152000	1.343381000	0.051597000
C	1.737053000	1.612334000	-0.021689000
C	2.623033000	0.615515000	-0.037386000
C	2.185268000	-0.801873000	0.017302000
H	2.034560000	2.654012000	-0.062323000
H	3.691723000	0.788923000	-0.092140000
O	-0.528486000	2.252330000	0.065580000
O	2.992923000	-1.710789000	0.003661000
H	0.429853000	-2.112456000	0.131673000
H	-1.227280000	-0.247339000	0.161478000



C	0.718570000	-1.068951000	0.091751000
C	-0.163436000	-0.068429000	0.106784000
C	0.275142000	1.366644000	0.051894000
C	1.736793000	1.609657000	-0.021878000
C	2.620157000	0.612752000	-0.037678000
C	2.176357000	-0.800411000	0.017941000
H	2.034805000	2.650775000	-0.062915000
H	3.688641000	0.784538000	-0.093085000
O	-0.514338000	2.282285000	0.066331000
O	2.973491000	-1.716522000	0.005711000
Br	-2.016454000	-0.381386000	0.198539000
H	0.422441000	-2.110032000	0.132241000



C	0.724242000	-1.073601000	0.091178000
C	-0.162869000	-0.077504000	0.107893000
C	0.279205000	1.338427000	0.052793000
C	1.734510000	1.609140000	-0.022770000
C	2.617762000	0.612131000	-0.037643000
C	2.200701000	-0.810518000	0.019504000
H	2.033604000	2.649804000	-0.065708000
H	3.686520000	0.782384000	-0.093883000
O	-0.533729000	2.240553000	0.068920000
O	3.014112000	-1.704957000	0.007832000
H	-1.231397000	-0.246309000	0.162126000
Br	0.191925000	-2.877041000	0.156205000

#### HOCl

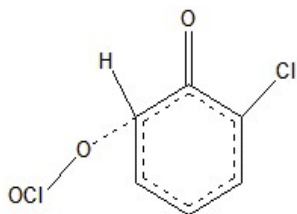
O	0.033363000	1.111412000	0.000000000
H	-0.902325000	1.348070000	0.000000000
Cl	0.034762000	-0.592693000	0.000000000

#### Cl<sub>2</sub>O

O	0.000000000	0.000000000	0.769009000
Cl	0.000000000	1.454880000	-0.180836000
Cl	0.000000000	-1.454880000	-0.180836000

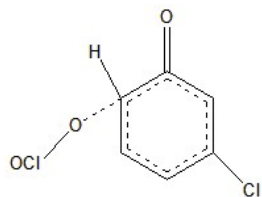
#### BrOCl

O	0.002662000	0.996516000	0.000000000
Cl	1.708495000	0.930470000	0.000000000
Br	-0.820082000	-0.669932000	0.000000000

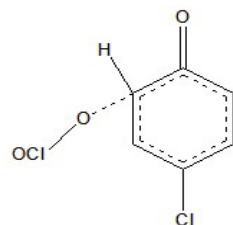


C	1.493945000	-1.209447000	-0.839547000
C	1.853939000	0.131439000	-0.961682000
C	1.581898000	1.100769000	0.019896000
C	0.898786000	0.740222000	1.145004000
C	0.501440000	-0.681181000	1.368769000
C	0.803872000	-1.630859000	0.271815000
H	1.766237000	-1.914131000	-1.613887000
H	2.403099000	0.445704000	-1.842348000
H	0.632011000	-2.675334000	0.489940000
O	-1.415897000	-1.701455000	-0.383122000
Cl	-2.170486000	-0.610810000	0.426628000

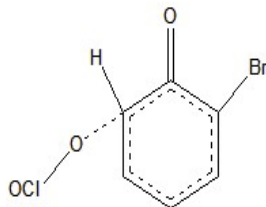
O	-1.384336000	0.714436000	0.236096000
O	-0.082299000	-1.046199000	2.371881000
H	1.904596000	2.123184000	-0.124115000
Cl	0.647844000	1.843912000	2.432164000



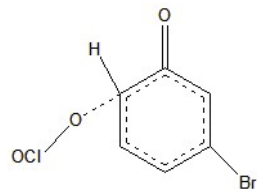
C	1.588172000	-1.261147000	-0.820625000
C	1.892876000	0.098433000	-0.973046000
C	1.516570000	1.053229000	-0.025343000
C	0.809903000	0.696402000	1.093210000
C	0.527776000	-0.733822000	1.333049000
C	0.886379000	-1.692053000	0.272511000
H	1.904312000	-1.959802000	-1.583712000
H	2.453893000	0.419006000	-1.843364000
H	0.688183000	-2.737189000	0.465771000
O	-1.412143000	-1.482202000	-0.397851000
Cl	-2.141965000	-0.468604000	0.514175000
O	-1.399129000	0.887284000	0.397554000
O	-0.070640000	-1.085863000	2.340417000
Cl	1.926802000	2.727784000	-0.294979000
H	0.581847000	1.390317000	1.889884000



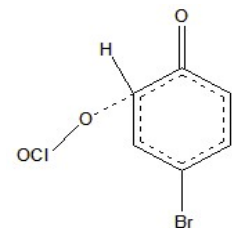
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C	1.886168000	0.096528000	-0.964164000
C	1.526164000	1.076680000	-0.026205000
C	0.819596000	0.702345000	1.082105000
C	0.527337000	-0.724053000	1.331920000
C	0.880491000	-1.683524000	0.265861000
H	1.900182000	-1.967792000	-1.590611000
H	0.683986000	-2.729053000	0.458785000
O	-1.394173000	-1.498538000	-0.403871000
Cl	-2.168156000	-0.504133000	0.507081000
O	-1.450061000	0.872086000	0.411916000
O	-0.045041000	-1.086256000	2.348686000
H	0.580223000	1.400165000	1.872452000
H	1.794488000	2.110392000	-0.196765000
Cl	2.775895000	0.591941000	-2.351084000



C	1.492868000	-1.207708000	-0.839227000
C	1.854408000	0.132729000	-0.960012000
C	1.585020000	1.099882000	0.025157000
C	0.901368000	0.740572000	1.151210000
C	0.498715000	-0.679188000	1.369335000
C	0.804930000	-1.628626000	0.273117000
H	1.763496000	-1.912242000	-1.614372000
H	0.629210000	-2.672885000	0.489130000
O	-1.431607000	-1.715445000	-0.382974000
Cl	-2.174689000	-0.620379000	0.427948000
O	-1.388120000	0.701971000	0.229157000
O	-0.094397000	-1.050209000	2.365782000
H	2.403633000	0.448226000	-1.840243000
H	1.913017000	2.120219000	-0.121216000
Br	0.638223000	1.947305000	2.554171000

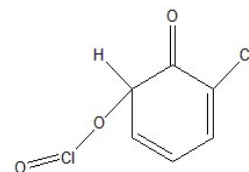


C	1.587243000	-1.262719000	-0.819389000
C	1.893930000	0.096270000	-0.971239000
C	1.519584000	1.053796000	-0.023324000
C	0.811557000	0.695983000	1.094203000
C	0.527037000	-0.734886000	1.334283000
C	0.883081000	-1.693070000	0.272891000
H	1.902668000	-1.961678000	-1.582602000
H	0.683779000	-2.738123000	0.465752000
O	-1.404650000	-1.475914000	-0.400677000
Cl	-2.141529000	-0.466741000	0.511972000
O	-1.401462000	0.891334000	0.401840000
O	-0.070354000	-1.086309000	2.342153000
H	0.580855000	1.385710000	1.893796000
Br	1.960680000	2.875280000	-0.318820000
H	2.455834000	0.411011000	-1.843052000

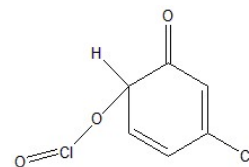


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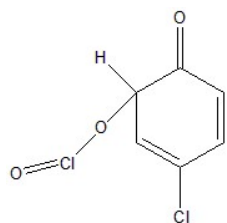
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C	0.527458000	-0.723877000	1.331767000
C	0.881921000	-1.682997000	0.267033000
H	1.898416000	-1.972161000	-1.587096000
H	0.685146000	-2.728654000	0.459516000
O	-1.396998000	-1.498536000	-0.404554000
Cl	-2.167294000	-0.504667000	0.508428000
O	-1.452108000	0.871788000	0.410370000
O	-0.050056000	-1.085353000	2.346552000
H	0.582056000	1.399638000	1.872834000
H	1.793002000	2.111521000	-0.191824000
Br	2.854106000	0.637135000	-2.478697000



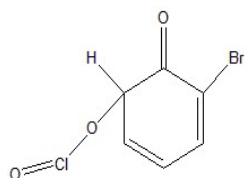
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C	1.273345000	0.246730000	-0.048587000
C	1.450568000	1.669910000	0.202230000
C	0.410183000	2.517151000	0.292145000
C	-0.967328000	2.042849000	0.085893000
C	-1.149066000	0.524583000	0.181419000
O	-2.220000000	0.091053000	-0.647753000
Cl	-3.777651000	0.345979000	0.045969000
O	-4.228747000	-0.918443000	0.789381000
H	-0.099405000	-1.356720000	-0.297065000
H	-1.390162000	0.341825000	1.242955000
O	-1.917857000	2.762388000	-0.116824000
H	2.162162000	-0.356610000	-0.181185000
H	2.460336000	2.055637000	0.281023000
Cl	0.636743000	4.228559000	0.476845000



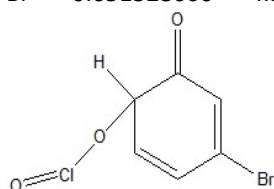
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C	0.408922000	2.530444000	0.287601000
C	-0.950078000	2.037193000	0.085446000
C	-1.145281000	0.522143000	0.191183000
O	-2.217756000	0.082037000	-0.635028000
Cl	-3.771054000	0.354230000	0.056226000
O	-4.233855000	-0.903927000	0.804976000
H	-0.091696000	-1.353595000	-0.309920000
H	-1.381201000	0.335389000	1.252412000
O	-1.901466000	2.760968000	-0.126213000
H	2.170161000	-0.357576000	-0.219078000
Cl	3.067039000	2.244166000	0.332569000
H	0.555349000	3.596927000	0.397587000



C	0.052027000	-0.313034000	-0.111463000
C	1.260320000	0.244988000	-0.056304000
C	1.455983000	1.670307000	0.199260000
C	0.419991000	2.518057000	0.297080000
C	-0.948339000	2.034687000	0.098961000
C	-1.149550000	0.519340000	0.198684000
O	-2.214198000	0.088157000	-0.644539000
Cl	-3.774593000	0.349208000	0.035329000
O	-4.237578000	-0.913801000	0.775511000
H	-0.102435000	-1.369082000	-0.290867000
H	-1.402243000	0.328460000	1.255088000
O	-1.894953000	2.761269000	-0.116021000
H	0.567336000	3.584319000	0.414751000
H	2.473112000	2.036724000	0.274962000
Cl	2.700503000	-0.708274000	-0.294471000

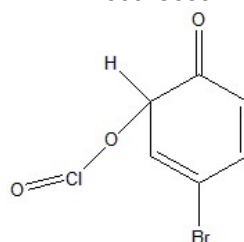


C	0.057369000	-0.300617000	-0.121140000
C	1.271660000	0.248552000	-0.050758000
C	1.445200000	1.671755000	0.206089000
C	0.403735000	2.519146000	0.296415000
C	-0.971019000	2.041648000	0.078478000
C	-1.149910000	0.522718000	0.179887000
O	-2.222515000	0.083516000	-0.644116000
Cl	-3.778228000	0.347594000	0.049774000
O	-4.231745000	-0.911746000	0.801384000
H	-0.098610000	-1.356463000	-0.304229000
H	-1.387269000	0.343462000	1.242896000
O	-1.923804000	2.754209000	-0.136794000
H	2.161938000	-0.352384000	-0.185005000
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Br	0.651328000	4.380888000	0.501195000

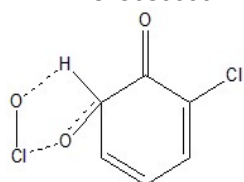


C	0.061644000	-0.297270000	-0.124099000
C	1.280756000	0.240941000	-0.070295000
C	1.437671000	1.669181000	0.194654000
C	0.408175000	2.529880000	0.286428000
C	-0.951864000	2.035654000	0.079865000

C	-1.146327000	0.521647000	0.189336000
O	-2.220885000	0.078335000	-0.632633000
Cl	-3.772444000	0.354377000	0.060745000
O	-4.231643000	-0.897610000	0.821978000
H	-0.091708000	-1.352035000	-0.316226000
H	-1.378802000	0.336868000	1.251753000
O	-1.901035000	2.760093000	-0.137729000
H	0.546712000	3.597023000	0.400108000
Br	3.210210000	2.302238000	0.353306000
H	2.166615000	-0.360148000	-0.227053000

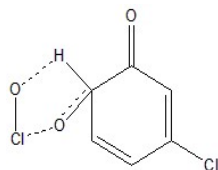


C	0.053611000	-0.311970000	-0.115523000
C	1.263173000	0.243922000	-0.054955000
C	1.455528000	1.669754000	0.205203000
C	0.418024000	2.517064000	0.297998000
C	-0.949153000	2.034690000	0.092618000
C	-1.149311000	0.520112000	0.195013000
O	-2.215373000	0.084735000	-0.643231000
Cl	-3.774556000	0.348351000	0.039125000
O	-4.234869000	-0.910949000	0.787081000
H	-0.107071000	-1.366179000	-0.300699000
H	-1.396724000	0.330676000	1.253094000
O	-1.894922000	2.760838000	-0.128073000
H	0.565068000	3.583272000	0.417362000
H	2.470052000	2.041474000	0.288508000
Br	2.825686000	-0.796816000	-0.317477000

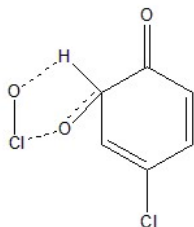


C	-0.146115000	1.963492000	-0.162140000
C	1.121104000	2.244761000	-0.478958000
C	2.158193000	1.233219000	-0.386857000
C	1.917999000	-0.014872000	0.057207000
C	0.583029000	-0.437902000	0.507787000
C	-0.535311000	0.575001000	0.219514000
H	-0.938578000	2.700904000	-0.205156000
H	-0.937852000	0.124691000	-0.774326000
O	-1.538887000	0.505752000	1.122125000
Cl	-3.049889000	-0.326906000	0.216957000
O	-2.431486000	-0.556006000	-1.183999000
O	0.340089000	-1.501876000	1.026463000
H	3.168848000	1.509399000	-0.665415000

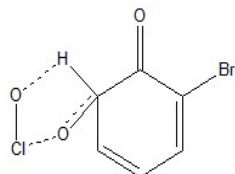
H	1.408265000	3.239598000	-0.794985000
Cl	3.201602000	-1.176231000	0.230265000



C	-0.144048000	1.953596000	-0.158218000
C	1.119759000	2.257589000	-0.462459000
C	2.148673000	1.232742000	-0.367291000
C	1.933316000	-0.023193000	0.067280000
C	0.600875000	-0.435755000	0.497196000
C	-0.533315000	0.561218000	0.212419000
H	-0.936260000	2.691671000	-0.197774000
H	-0.936414000	0.112492000	-0.780699000
O	-1.534917000	0.491154000	1.116543000
Cl	-3.065788000	-0.296338000	0.195208000
O	-2.443301000	-0.530679000	-1.203592000
O	0.368844000	-1.508947000	1.012131000
H	2.737458000	-0.739890000	0.174499000
H	1.406431000	3.257967000	-0.759222000
Cl	3.754217000	1.719201000	-0.821260000

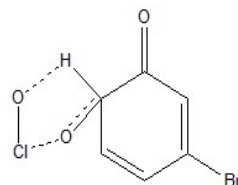


C	-0.160969000	1.954178000	-0.157804000
C	1.106913000	2.238183000	-0.454677000
C	2.165978000	1.242378000	-0.366771000
C	1.936026000	-0.008388000	0.067179000
C	0.604095000	-0.437845000	0.497413000
C	-0.536035000	0.553840000	0.210416000
H	-0.955539000	2.688468000	-0.200992000
H	-0.936250000	0.099005000	-0.778594000
O	-1.534137000	0.477554000	1.118246000
Cl	-3.080762000	-0.267962000	0.191947000
O	-2.464832000	-0.518152000	-1.206342000
O	0.377661000	-1.510089000	1.012951000
H	2.742374000	-0.724041000	0.172729000
Cl	1.580021000	3.848684000	-0.939736000
H	3.169828000	1.544384000	-0.642879000

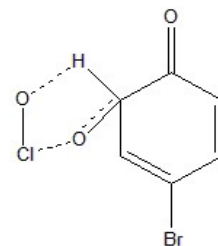


C	-0.147277000	1.964513000	-0.157994000
C	1.119856000	2.245490000	-0.475046000
C	2.155520000	1.231569000	-0.386825000

C	1.916246000	-0.018473000	0.055016000
C	0.582250000	-0.437872000	0.511576000
C	-0.536479000	0.575628000	0.220858000
H	-0.939354000	2.702557000	-0.198167000
H	-0.934998000	0.125388000	-0.774439000
O	-1.542887000	0.505903000	1.120058000
Cl	-3.049257000	-0.331077000	0.211250000
O	-2.427095000	-0.558785000	-1.188244000
O	0.334191000	-1.497968000	1.035685000
H	1.408236000	3.240792000	-0.788657000
H	3.163925000	1.511917000	-0.669333000
Br	3.315003000	-1.280248000	0.237849000

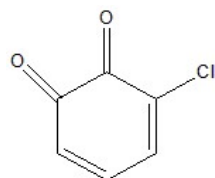


C	-0.144959000	1.953811000	-0.154661000
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C	2.148928000	1.232851000	-0.369200000
C	1.931861000	-0.022399000	0.066332000
C	0.598596000	-0.433722000	0.501678000
C	-0.535267000	0.561498000	0.214506000
H	-0.936801000	2.692525000	-0.192315000
H	-0.934440000	0.112733000	-0.780215000
O	-1.540124000	0.490283000	1.115124000
Cl	-3.066317000	-0.299412000	0.188978000
O	-2.439586000	-0.532870000	-1.208031000
O	0.369534000	-1.505203000	1.020881000
H	2.730552000	-0.745268000	0.173233000
Br	3.896650000	1.755772000	-0.870861000
H	1.400048000	3.260575000	-0.755182000

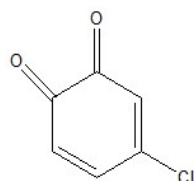


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C	1.934406000	-0.008960000	0.066792000
C	0.603580000	-0.437488000	0.500074000
C	-0.535505000	0.554117000	0.212373000
H	-0.957702000	2.685824000	-0.193278000
H	-0.933219000	0.102588000	-0.779102000
O	-1.536468000	0.478495000	1.117109000
Cl	-3.078727000	-0.270636000	0.188183000
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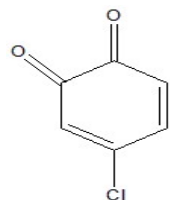
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H	3.170879000	1.537043000	-0.646087000
Br	1.615218000	3.992574000	-0.983247000



C	-1.706734000	0.152483000	0.000292000
C	-0.244237000	0.139001000	0.001310000
C	0.474310000	1.269908000	0.001135000
C	-0.192348000	2.589538000	0.000302000
C	-1.757833000	2.579581000	-0.003557000
C	-2.430491000	1.280583000	-0.001875000
H	-2.202447000	-0.810965000	0.001174000
H	0.254306000	-0.822608000	0.002318000
H	-3.513375000	1.274445000	-0.003016000
O	0.392163000	3.641161000	0.002346000
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Cl	2.206453000	1.262715000	0.002439000

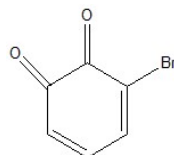


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C	-1.751529000	2.579190000	-0.004000000
C	-2.426336000	1.274130000	-0.001698000
H	-2.204901000	-0.824440000	0.001771000
H	-3.509365000	1.268221000	-0.002522000
O	0.398229000	3.633244000	0.003403000
O	-2.342306000	3.632443000	-0.009414000
Cl	0.523626000	-1.393237000	0.002243000
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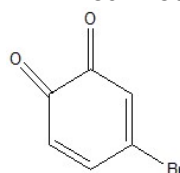


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C	-0.200322000	2.578238000	0.000555000
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C	-2.439713000	1.285382000	-0.001864000
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O	0.392854000	3.630195000	0.003905000

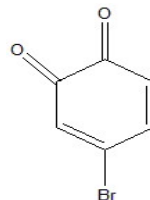
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Cl	-2.484282000	-1.388994000	0.002566000



C	-1.705712000	0.154373000	0.000540000
C	-0.242364000	0.142822000	0.001195000
C	0.478598000	1.273030000	0.000981000
C	-0.189604000	2.592465000	0.000924000
C	-1.756422000	2.581397000	-0.003852000
C	-2.429590000	1.281920000	-0.001699000
H	-3.512549000	1.277011000	-0.002806000
O	0.389464000	3.647146000	0.003695000
O	-2.333493000	3.641994000	-0.009591000
H	-2.199719000	-0.809978000	0.001618000
H	0.251158000	-0.821330000	0.001917000
Br	2.364279000	1.258596000	0.001916000



C	-1.713609000	0.142228000	0.000562000
C	-0.245299000	0.156410000	0.001130000
C	0.485183000	1.280664000	0.001000000
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C	-1.751626000	2.580870000	-0.004079000
C	-2.424946000	1.275837000	-0.001680000
H	-3.508090000	1.269214000	-0.002504000
O	0.399179000	3.633196000	0.003603000
O	-2.342371000	3.634371000	-0.009636000
H	1.567539000	1.279475000	0.001867000
Br	0.597122000	-1.531346000	0.002280000
H	-2.209254000	-0.820550000	0.001891000



C	-1.711290000	0.157803000	0.000390000
C	-0.242981000	0.140425000	0.000911000
C	0.470788000	1.272481000	0.000899000
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C	-1.757755000	2.580877000	-0.004079000
C	-2.439285000	1.283687000	-0.001839000
H	-3.521679000	1.284790000	-0.002765000
O	0.393452000	3.631116000	0.003910000

O	-2.348135000	3.636050000	-0.009500000
H	1.553889000	1.263711000	0.001591000
H	0.250532000	-0.823463000	0.001438000
Br	-2.557423000	-1.528058000	0.002800000