Oxidative removal of quinclorac by permanganate through a rate-limiting [3+2] cycloaddition reaction

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Fig. S1. The representative kinetics of QCR oxidation by permanganate in aqueous solution by using a 200 mL glass beaker in a water bath ($[QCR]_0$ = 0.1 mM, $[MnO_4^-]$ = 0.02 M, pH = 8.0, T = 25 °C).

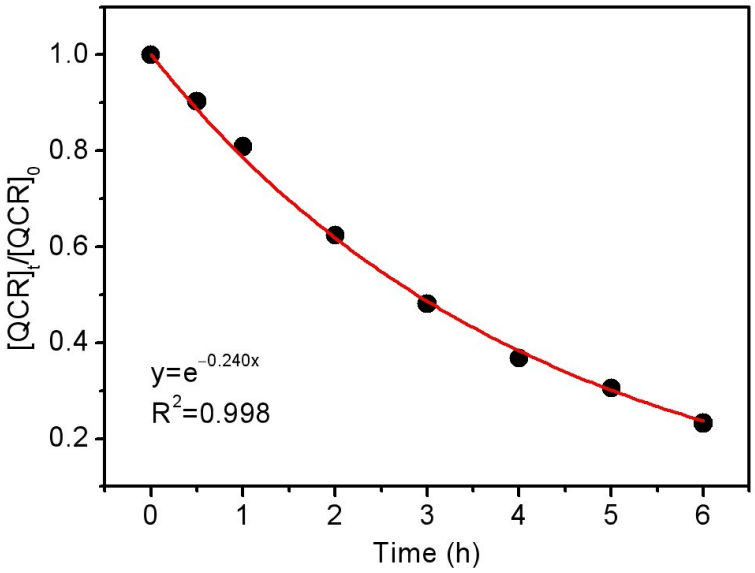

Fig. S2. The plot of log(k_p) as a function of log([MnO_4^-]) (pH = 8.0, T = 25 °C).

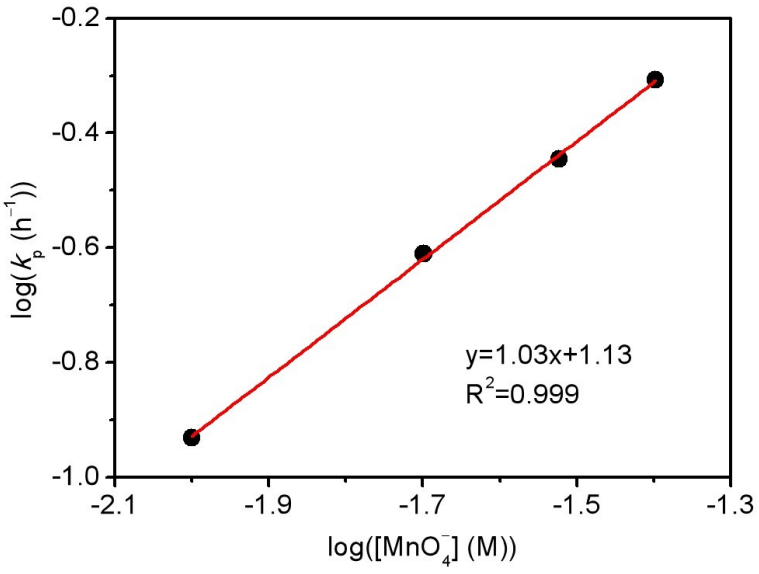

Fig. S3. The change of total organic carbon (TOC) in the QCR oxidation by permanganate in aqueous solution ($[QCR]_0$ = 0.1 mM, $[MnO_4^-]$ = 0.02 M, pH = 8.0, T = 25 °C).

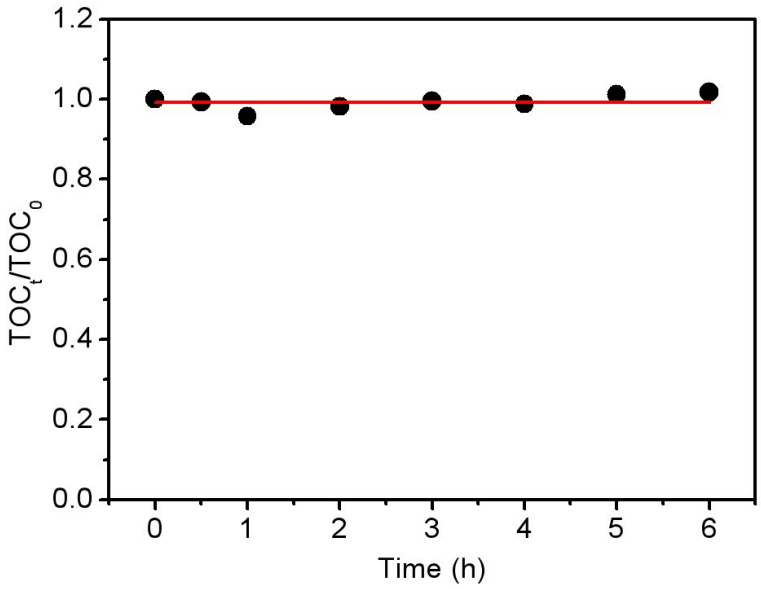

Fig. S4. Proposed degradation pathway of QCR during MnO_4^- oxidation process.

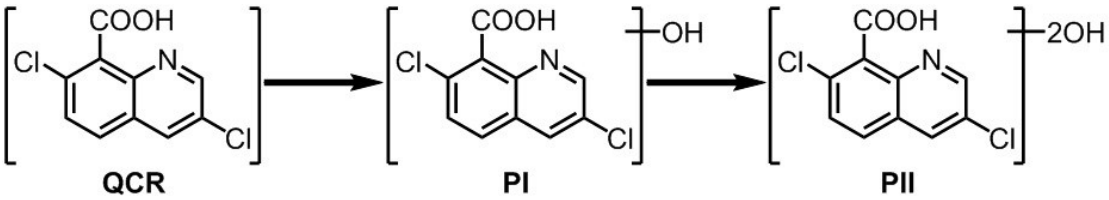

Fig. S5. Relationship between the computational L(C–O) (Å) and the experimental pK_a data of the hydroxyl group for the training set phenolates in water.

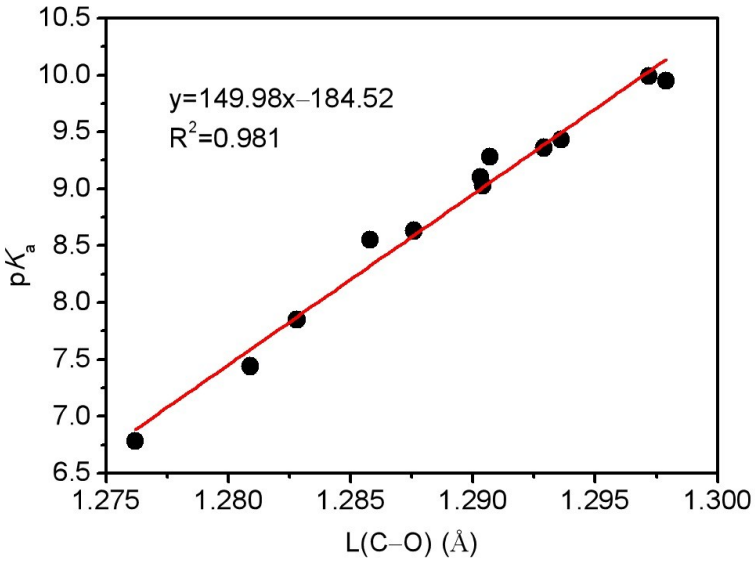

Table S1 – The computational L(C–C) (Å) for the anionic form PI and PII in water and the corresponding pK_a value of carboxylic group calculated by the established model (pK_a = 209.25 – 134.91 × L(C–C)) in our previous study.

Compound	L(C–C) (Å)	pK_a
$PI1_A$	1.5345	2.23
$PI2_A$	1.5332	2.41
$PI3_A$	1.5331	2.42
PII_A	1.5349	2.18

Table S2 – The computational L(C–O) (Å) and the corresponding pK_a value of hydroxyl group for the studied phenolates in water.

	Compound	L(C–O) (Å)	pK_a
Training set [a]	Phenolate	1.2972	9.99
	3-Fluoro-phenolate	1.2907	9.28
	4-Fluoro-phenolate	1.2979	9.95
	3-Bromo-phenolate	1.2904	9.03
	4-Bromo-phenolate	1.2929	9.36
	2-Chloro-phenolate	1.2858	8.55
	3-Chloro-phenolate	1.2903	9.10
	4-Chloro-phenolate	1.2936	9.43
	2,3-Dichloro-phenolate	1.2809	7.44
	2,4-Dichloro-phenolate	1.2828	7.85
	2,6-Dichloro-phenolate	1.2762	6.78
	3,4-Dichloro-phenolate	1.2876	8.63
Testing Set [b]	PI_D	1.2826	7.84
	PII_D	1.2913	9.15
	PII_T	1.3001 [c]	10.47

a pK_a values were taken from the references S1 and S2.

b pK_a values were calculated by the regression equation in Fig. S5.

c The value was the (C_5–O) bond length.

(S1) Gross, K. C.; Seybold, P. G. Substituent effects on the physical properties and pK_a of phenol. *Int. J. Quantum Chem.* **2001**, *85*, 569-579.

(S2) Du, J. S.; Sun, B.; Zhang, J.; Guan, X. H. Parabola-like shaped pH-rate profile for phenols oxidation by aqueous permanganate. *Environ. Sci. Technol.* **2012**, *46*, 8860-8867.

Table S3 – The predicted 96h *Fathead Minnow* 50% lethal concentration (LC50-96h, mg L^{-1}) and 48h *Daphnia Magna* 50% lethal concentration (LC50-48h, mg L^{-1}) of QCR, PI, and PII.

Compound	*Fathead Minnow* (LC50-96h, mg L^{-1})	*Daphnia Magna* (LC50-48h, mg L^{-1})
QCR	4.43	11.52
PI	6.43	10.41
PII	5.19	11.32

The following section gives the Cartesian coordinates of optimized structures, including MnO_4^-, QCR_A, TS11, TS12, TS13, TS14, P12, P13, P14, $PI1_A$, $PI2_A$, $PI3_A$, $PI1_D$, $PI2_D$, $PI3_D$, TS211, TS212, TS213, TS221, TS222, TS223, TS231, TS232, TS233, TS241, TS242, TS243, TS251, TS252, TS253, TS261, TS262, TS263, PII_A, PII_D, PII_T, 2-chloro-benzoate, phenolate, 3-fluoro-phenolate, 4-fluoro-phenolate, 3-bromo-phenolate, 4-bromo-phenolate, 2-chloro-phenolate, 3-chloro-phenolate, 4-chloro-phenolate, 2,3-dichloro-phenolate, 2,4-dichloro-phenolate, 2,6-dichloro-phenolate, 3,4-dichloro-phenolate.

MnO_4^-	Cartesian coordinates		
Atom	x	y	z
Mn	0	0	0
O	0.921033	0.921033	0.921033
O	-0.921033	-0.921033	0.921033
O	-0.921033	0.921033	-0.921033
O	0.921033	-0.921033	-0.921033

QCR_A	Cartesian coordinates		
Atom	x	y	z
Cl	-4.654002	-0.055162	0.000099
C	-2.897904	-0.035147	-0.000159
C	-2.199855	-1.269759	-0.000518
N	-0.884889	-1.345492	-0.000566
C	-0.153741	-0.189837	-0.000267
C	-0.783107	1.096505	0.000029
C	-2.200848	1.147446	0.00012
C	0.018737	2.268443	0.000221
C	1.39046	2.164321	0.000132
C	1.995697	0.884412	-0.000108
C	1.2739	-0.292388	-0.000306
C	1.939962	-1.672607	0.000299
O	2.183742	-2.167344	-1.131558
O	2.182807	-2.16608	1.132945
Cl	3.764301	0.836366	-0.000347
H	-2.757834	-2.203212	-0.00081
H	-2.711496	2.105175	0.000393
H	-0.45801	3.243714	0.000506
H	2.014275	3.051342	0.000341

TS11	Cartesian coordinates		
Atom	x	y	z
Cl	-5.388794	-1.316688	-0.122915
C	-3.786888	-0.606758	-0.020364
C	-3.485871	0.518428	-0.852584
N	-2.322667	1.114864	-0.849991
C	-1.322442	0.644383	-0.016142
C	-1.555415	-0.485424	0.861826
C	-2.840075	-1.101546	0.832804
C	-0.548876	-0.895621	1.748535
C	0.709281	-0.312199	1.709883
C	0.993976	0.756108	0.757441
C	-0.100986	1.324096	-0.000483
C	0.060437	2.625423	-0.788372
O	-0.302666	3.667341	-0.176652
O	0.527956	2.546678	-1.953919
Cl	2.182735	1.958291	1.425013
H	-4.252878	0.904592	-1.521216
H	-3.047522	-1.948325	1.47965
H	-0.756107	-1.674293	2.476374
H	1.425258	-0.501146	2.496677
Mn	2.611935	-1.436814	-0.553824
O	4.196279	-1.427417	-0.360849
O	2.098207	-2.180722	-1.864595
O	1.895835	-2.029741	0.781291
O	2.003852	0.127223	-0.508634

TS12	Cartesian coordinates		
Atom	x	y	z
Cl	4.76367	-1.900606	-0.122274
C	3.349355	-0.859062	-0.10749
C	3.382455	0.337991	0.630847
N	2.355921	1.177295	0.670075
C	1.225704	0.872345	-0.016577
C	1.102642	-0.334746	-0.758964
C	2.206744	-1.204857	-0.804883
C	-0.141878	-0.655751	-1.423749
C	-1.184511	0.308341	-1.432111
C	-0.971078	1.552394	-0.747058
C	0.146016	1.843022	-0.017337
C	0.330402	3.157716	0.747186
O	0.847332	4.108492	0.102409
O	-0.056579	3.155214	1.94616
Cl	-2.278078	2.736041	-0.881353
H	4.272565	0.608759	1.193447
H	2.151875	-2.129589	-1.369926
H	-0.113397	-1.385722	-2.223384
H	-1.922916	0.276289	-2.221781
Mn	-2.24314	-1.929584	0.461305
O	-3.23158	-3.081343	-0.035562
O	-2.129757	-1.777756	2.045812
O	-0.750889	-2.119998	-0.203645
O	-2.644933	-0.494352	-0.225053

TS13	Cartesian coordinates		
Atom	x	y	z
Cl	2.876763	2.370443	-1.054067
C	1.499372	1.423468	-0.497687
C	0.628122	2.030347	0.476611
N	-0.589522	1.633444	0.706065
C	-1.127504	0.62511	-0.086078
C	-0.389291	0.021132	-1.13746
C	1.001382	0.393073	-1.331831
C	-1.014307	-0.924018	-1.973677
C	-2.333105	-1.288538	-1.755296
C	-3.040064	-0.700727	-0.692743
C	-2.480157	0.252612	0.148936
C	-3.271546	0.903217	1.28891
O	-3.924199	1.939048	0.990768
O	-3.200319	0.329654	2.408445
Cl	-4.718053	-1.213917	-0.452676
H	1.019807	2.852232	1.073014
H	1.428476	0.267052	-2.318954
H	-0.452725	-1.376941	-2.78516
H	-2.818886	-2.021153	-2.39049
Mn	2.774112	-1.188521	0.612967
O	2.108647	-2.141404	1.700882
O	4.317619	-1.466655	0.330538
O	1.915467	-1.2298	-0.795294
O	2.540499	0.379497	1.006095

TS14	Cartesian coordinates		
Atom	x	y	z
Cl	2.927405	2.252882	1.146038
C	1.510995	1.377092	0.572183
C	1.063448	0.234994	1.372523
N	-0.260585	-0.145892	1.321713
C	-1.063197	0.378527	0.400406
C	-0.665279	1.489999	-0.453354
C	0.610933	2.022765	-0.279302
C	-1.602606	2.039673	-1.383371
C	-2.867799	1.529235	-1.47542
C	-3.252279	0.44595	-0.623974
C	-2.419353	-0.130848	0.297496
C	-2.854022	-1.280396	1.21117
O	-3.3656	-0.946534	2.313646
O	-2.664871	-2.445255	0.76925
Cl	-4.912241	-0.140485	-0.810782
H	1.497882	0.170469	2.367714
H	0.916285	2.914432	-0.817659
H	-1.294353	2.865772	-2.017529
H	-3.586287	1.933622	-2.179649
Mn	2.76043	-1.171855	-0.64588
O	2.057615	-2.139276	-1.693084
O	4.308879	-1.447531	-0.396949
O	2.520472	0.388962	-1.051042
O	1.92563	-1.175289	0.809758

P12	Cartesian coordinates		
Atom	x	y	z
Cl	4.952301	-1.925341	-0.026942
C	3.520355	-0.909033	-0.034987
C	3.608863	0.420616	0.376923
N	2.551618	1.238826	0.37464
C	1.357681	0.766129	-0.031867
C	1.185266	-0.572085	-0.444724
C	2.29025	-1.419074	-0.448017
C	-0.189094	-1.096259	-0.783853
C	-1.186944	-0.031995	-1.264388
C	-0.939484	1.31314	-0.608233
C	0.222214	1.710723	-0.05914
C	0.449964	3.115559	0.515768
O	0.829072	3.997526	-0.299725
O	0.2367	3.245047	1.751162
Cl	-2.296959	2.438935	-0.731947
H	4.556263	0.834146	0.712805
H	2.193685	-2.453762	-0.76222
H	-0.106232	-1.867039	-1.563712
H	-1.109641	0.107247	-2.35478
Mn	-2.547583	-1.673121	0.423151
O	-3.107905	-3.08767	-0.023071
O	-3.077959	-0.917399	1.711375
O	-0.739586	-1.693927	0.396021
O	-2.485454	-0.541297	-0.990403

P13	Cartesian coordinates		
Atom	x	y	z
Cl	2.762765	2.34819	-1.082298
C	1.572711	1.137634	-0.072436
C	0.49026	2.070178	0.428041
N	-0.758358	1.795564	0.406921
C	-1.202483	0.556661	-0.119722
C	-0.333117	-0.344861	-0.763692
C	1.108236	0.058062	-1.052961
C	-0.822972	-1.569622	-1.216951
C	-2.166962	-1.90347	-1.038061
C	-3.016635	-0.989958	-0.414585
C	-2.570111	0.249004	0.054373
C	-3.513529	1.246748	0.736212
O	-4.088873	2.068055	-0.027012
O	-3.629952	1.137621	1.98563
Cl	-4.718253	-1.442093	-0.22242
H	0.81928	3.002597	0.88528
H	1.145113	0.438134	-2.081921
H	-0.152247	-2.267564	-1.706788
H	-2.549497	-2.857808	-1.383841
Mn	2.974444	-1.072849	0.56889
O	2.389525	-2.145479	1.566811
O	4.51386	-0.940644	0.251769
O	2.006889	-1.035422	-0.957196
O	2.265511	0.599746	0.949429

P14	Cartesian coordinates		
Atom	x	y	z
Cl	2.677978	2.327125	1.169946
C	1.556362	1.075638	0.067067
C	1.115175	-0.03236	1.039111
N	-0.227584	-0.545998	0.816849
C	-1.121964	0.205043	0.257338
C	-0.828529	1.548599	-0.330695
C	0.460835	1.954396	-0.42805
C	-1.924713	2.336702	-0.864449
C	-3.184573	1.843043	-0.882106
C	-3.448633	0.512003	-0.368564
C	-2.504174	-0.298949	0.171248
C	-2.80568	-1.694345	0.725835
O	-3.139036	-1.748137	1.93917
O	-2.694519	-2.647125	-0.090538
Cl	-5.129678	-0.021622	-0.477618
H	1.11905	0.343612	2.071774
H	0.736775	2.864375	-0.951502
H	-1.708977	3.32565	-1.257182
H	-4.010065	2.421776	-1.281447
Mn	3.089841	-1.047158	-0.538814
O	2.6	-2.12766	-1.577958
O	4.605721	-0.850031	-0.152125
O	2.322276	0.598151	-0.927285
O	2.056125	-1.081029	0.943832

$PI1_A$	Cartesian coordinates		
Atom	x	y	z
Cl	-4.795884	0.175272	-0.000249
C	-3.04459	0.033296	-0.00019
C	-2.465868	-1.261971	-0.000254
N	-1.162705	-1.454207	-0.000197
C	-0.332423	-0.370349	-0.000075
C	-0.835139	0.97073	-0.000023
C	-2.244714	1.148356	-0.00008
C	0.06137	2.064941	0.000084
C	1.422653	1.842349	0.00014
C	1.911683	0.502189	0.000101
C	1.079677	-0.596113	0
C	1.622287	-2.03144	0.00007
O	1.819903	-2.542535	-1.132633
O	1.819489	-2.542551	1.132837
Cl	3.667795	0.2961	0.000198
H	-3.106764	-2.14015	-0.000357
H	-2.667502	2.147616	-0.000035
H	-0.31195	3.083726	0.000127
O	2.25699	2.915564	0.000244
H	3.182007	2.619179	0.000303

$PI2_A$	Cartesian coordinates		
Atom	x	y	z
Cl	-4.608138	-0.405867	-0.000264
C	-2.853331	-0.337511	-0.000171
C	-2.119819	-1.549327	-0.000157
N	-0.802783	-1.5861	-0.000085
C	-0.10052	-0.413003	-0.000021
C	-0.774735	0.850032	-0.000036
C	-2.190213	0.865421	-0.000113
C	-0.00164	2.048531	0.00003
C	1.374709	1.982197	0.000113
C	2.008296	0.716731	0.000127
C	1.327697	-0.481828	0.000063
C	2.031504	-1.84392	0.000088
O	2.289387	-2.33419	-1.131531
O	2.289195	-2.334243	1.131727
Cl	3.776772	0.727948	0.000238
H	-2.648655	-2.499651	-0.000206
H	-2.724507	1.807957	-0.000124
H	1.974058	2.88664	0.000169
O	-0.699276	3.222243	0.000006
H	-0.094334	3.977967	0.000034

$PI3_A$	Cartesian coordinates		
Atom	x	y	z
Cl	-4.445811	-0.535963	0.000124
C	-2.694986	-0.405729	-0.00027
C	-1.898204	-1.571094	-0.000458
N	-0.580738	-1.552938	-0.000392
C	0.050231	-0.337935	-0.000129
C	-0.667885	0.898127	-0.000075
C	-2.093468	0.840821	0.000246
C	0.035723	2.128796	-0.00031
C	1.412553	2.131072	-0.000337
C	2.112636	0.902954	-0.000081
C	1.481395	-0.32522	-0.000027
C	2.252795	-1.650105	0.000182
O	2.535081	-2.123642	-1.131955
O	2.534723	-2.12348	1.132479
Cl	3.880244	0.9882	0.000098
H	-2.388547	-2.541997	-0.000799
H	-0.513924	3.0626	-0.00064
H	1.964394	3.064506	-0.000556
O	-2.769701	2.007528	0.000514
H	-3.727659	1.844063	0.000219

$PI1_D$	Cartesian coordinates		
Atom	x	y	z
Cl	-4.784065	0.13399	-0.000278
C	-3.021138	0.009575	-0.000186
C	-2.433647	-1.278133	-0.000205
N	-1.120788	-1.442314	-0.000134
C	-0.308161	-0.351971	-0.000037
C	-0.820893	0.994379	-0.000023
C	-2.239853	1.138411	-0.0001
C	0.055235	2.093763	0.000065
C	1.466847	1.953878	0.000146
C	1.926805	0.560106	0.000141
C	1.113289	-0.547959	0.000054
C	1.665202	-1.977501	0.000035
O	1.867424	-2.499917	-1.130651
O	1.867031	-2.500108	1.130701
Cl	3.689653	0.333352	0.000262
H	-3.059086	-2.167125	-0.000277
H	-2.683817	2.129138	-0.000089
H	-0.351147	3.102502	0.000071
O	2.280851	2.939971	0.00022

$PI2_D$	Cartesian coordinates		
Atom	x	y	z
Cl	-4.624269	-0.371077	-0.00027
C	-2.858434	-0.3144	-0.000178
C	-2.131824	-1.523872	-0.000197
N	-0.811637	-1.563704	-0.000128
C	-0.100733	-0.389135	-0.000032
C	-0.775589	0.879867	-0.000016
C	-2.182353	0.886421	-0.000091
C	-0.036686	2.149731	0.00008
C	1.375835	2.017346	0.000161
C	1.986202	0.754518	0.000146
C	1.32262	-0.462131	0.000053
C	2.034714	-1.815719	0.000035
O	2.303016	-2.31953	-1.128525
O	2.302736	-2.319708	1.128582
Cl	3.775847	0.750801	0.000273
H	-2.661106	-2.47485	-0.00027
H	-2.699615	1.839909	-0.000075
H	1.983571	2.916194	0.000236
O	-0.645842	3.27844	0.000091

$PI3_D$	Cartesian coordinates		
Atom	x	y	z
Cl	-4.495532	-0.505454	-0.000284
C	-2.729049	-0.345988	-0.000171
C	-1.954564	-1.50744	-0.000198
N	-0.623285	-1.536079	-0.000127
C	0.015776	-0.323478	-0.000024
C	-0.684265	0.921777	0.000006
C	-2.154565	0.958202	-0.000051
C	0.043697	2.132987	0.000096
C	1.424218	2.133028	0.00016
C	2.101381	0.894948	0.000143
C	1.451237	-0.323716	0.000058
C	2.210705	-1.652919	0.000061
O	2.494968	-2.135592	-1.13063
O	2.494799	-2.135669	1.130761
Cl	3.880009	0.951586	0.000245
H	-2.460746	-2.47238	-0.000281
H	-0.508501	3.066794	0.00011
H	1.98707	3.060403	0.000223
O	-2.807063	2.044896	-0.000005

TS211	Cartesian coordinates		
Atom	x	y	z
Cl	4.902744	-1.627054	-0.285665
C	3.438361	-0.662563	-0.190856
C	3.439298	0.517241	0.577015
N	2.372991	1.298988	0.676311
C	1.233733	0.949632	0.027623
C	1.141029	-0.246372	-0.737446
C	2.289512	-1.0526	-0.85215
C	-0.102793	-0.623129	-1.365975
C	-1.200118	0.279179	-1.291414
C	-1.0251	1.534081	-0.594825
C	0.106993	1.861007	0.090328
C	0.241222	3.162023	0.891246
O	0.669042	4.161112	0.25568
O	-0.095544	3.09719	2.102733
Cl	-2.407819	2.630696	-0.629891
H	4.33583	0.82142	1.111431
H	2.260855	-1.965122	-1.43809
H	-0.065057	-1.268804	-2.234862
O	-2.152964	0.125872	-2.246851
H	-2.900873	0.716927	-2.061309
Mn	-1.908823	-2.107703	0.65599
O	-3.05701	-3.11223	0.17927
O	-1.487969	-2.23652	2.191493
O	-0.587218	-2.233866	-0.319595
O	-2.326795	-0.561268	0.303781

TS212	Cartesian coordinates		
Atom	x	y	z
Cl	3.093005	1.884006	-1.72439
C	1.686563	1.243452	-0.877519
C	0.896792	2.171773	-0.107989
N	-0.327302	1.937051	0.265514
C	-0.949477	0.772771	-0.164888
C	-0.29972	-0.165106	-1.01047
C	1.097108	0.047608	-1.353992
C	-1.000997	-1.276803	-1.503354
C	-2.32582	-1.484812	-1.143196
C	-2.95483	-0.55967	-0.278049
C	-2.302716	0.562249	0.212458
C	-3.011452	1.562369	1.134581
O	-3.62552	2.501445	0.563234
O	-2.917007	1.333349	2.369315
Cl	-4.638819	-0.883539	0.157659
H	1.358542	3.107354	0.201337
H	1.467962	-0.388219	-2.273269
H	-0.512819	-1.99485	-2.154267
O	-2.963543	-2.581243	-1.63782
H	-3.875489	-2.611783	-1.305455
Mn	2.856269	-1.014568	0.925938
O	4.370899	-1.464524	0.715755
O	2.170386	-1.562582	2.25453
O	2.727641	0.611933	0.84451
O	1.951185	-1.408203	-0.39533

TS213	Cartesian coordinates		
Atom	x	y	z
Cl	3.095178	2.115985	1.379511
C	1.62906	1.311039	0.83927
C	1.327652	0.00458	1.432807
N	0.030993	-0.470745	1.352811
C	-0.863113	0.164176	0.602043
C	-0.614915	1.460626	-0.01089
C	0.642888	2.042453	0.195297
C	-1.641712	2.114142	-0.743768
C	-2.875665	1.529968	-0.885338
C	-3.121287	0.249077	-0.276268
C	-2.17986	-0.429205	0.448622
C	-2.469396	-1.790384	1.0909
O	-2.939327	-1.759127	2.258577
O	-2.21807	-2.799162	0.380716
Cl	-4.737244	-0.431849	-0.508132
H	1.787018	-0.168631	2.405412
H	0.854085	3.041893	-0.171248
H	-1.453991	3.080534	-1.200908
O	-3.836416	2.178174	-1.597334
H	-4.652077	1.651066	-1.612367
Mn	2.909437	-0.981274	-0.888821
O	4.498502	-1.104199	-0.878062
O	2.16073	-1.949521	-1.904879
O	2.285154	-1.17783	0.666259
O	2.477589	0.568298	-1.13022

TS221	Cartesian coordinates		
Atom	x	y	z
Cl	-4.882568	-1.715648	-0.114303
C	-3.432889	-0.726951	-0.053562
C	-3.418467	0.515908	-0.711322
N	-2.360444	1.316531	-0.694555
C	-1.246659	0.929732	-0.02474
C	-1.179609	-0.326209	0.638133
C	-2.308067	-1.162192	0.623199
C	0.05753	-0.725175	1.277066
C	1.120468	0.213696	1.406087
C	0.962531	1.488197	0.766726
C	-0.12927	1.853477	0.032089
C	-0.247679	3.206574	-0.676945
O	-0.731999	4.151111	0.000806
O	0.155718	3.23621	-1.870103
Cl	2.296559	2.623641	1.000451
H	-4.295034	0.85643	-1.256817
H	-2.285545	-2.122591	1.124271
H	1.760879	0.149376	2.276754
O	-0.040048	-1.773253	2.142763
H	0.842457	-2.0505	2.430069
Mn	2.287067	-1.749889	-0.682964
O	2.946016	-3.154702	-0.301551
O	2.580528	-1.238634	-2.165855
O	0.669963	-1.788379	-0.397122
O	2.697134	-0.599782	0.420659

TS222	Cartesian coordinates		
Atom	x	y	z
Cl	2.886198	1.777766	-1.892493
C	1.51716	1.16476	-0.967564
C	0.659753	2.132203	-0.332436
N	-0.554138	1.87626	0.058544
C	-1.112068	0.636607	-0.233664
C	-0.385127	-0.352045	-0.948387
C	1.003631	-0.116539	-1.288004
C	-1.043753	-1.544292	-1.329761
C	-2.365758	-1.763094	-0.964945
C	-3.042226	-0.779551	-0.226566
C	-2.46371	0.424238	0.149273
C	-3.229723	1.501766	0.92564
O	-3.882251	2.328833	0.232984
O	-3.142551	1.449565	2.182269
Cl	-4.719318	-1.129282	0.215736
H	1.060626	3.125789	-0.140909
H	1.41998	-0.654381	-2.128965
H	-2.871485	-2.682242	-1.242562
O	-0.32639	-2.450304	-2.059
H	-0.882863	-3.2038	-2.302359
Mn	2.800139	-0.71297	1.138247
O	4.344232	-1.082229	0.994326
O	2.143744	-1.104541	2.535247
O	2.564715	0.872563	0.817368
O	1.933904	-1.356822	-0.109174

TS223	Cartesian coordinates		
Atom	x	y	z
Cl	2.972372	1.850881	1.650266
C	1.550414	1.101675	0.932431
C	1.151357	-0.206085	1.451836
N	-0.158837	-0.611014	1.320828
C	-1.001066	0.087495	0.563667
C	-0.651432	1.391097	0.013941
C	0.609126	1.910385	0.287488
C	-1.632292	2.124956	-0.737278
C	-2.883422	1.605439	-0.939193
C	-3.201453	0.327968	-0.383825
C	-2.335361	-0.436805	0.349075
C	-2.713746	-1.800772	0.934636
O	-3.232108	-1.78783	2.084387
O	-2.479975	-2.806222	0.210236
Cl	-4.842956	-0.251717	-0.702379
H	1.603841	-0.487182	2.400361
H	0.872949	2.915061	-0.020777
H	-3.630071	2.145346	-1.511629
O	-1.229157	3.336489	-1.221691
H	-1.953579	3.766904	-1.698421
Mn	2.806873	-1.047893	-0.887307
O	4.377912	-1.288682	-0.792104
O	2.076483	-1.801137	-2.081346
O	2.067261	-1.412869	0.573429
O	2.481343	0.5498	-0.920834

TS231	Cartesian coordinates		
Atom	x	y	z
Cl	4.899647	-1.09902	0.13732
C	3.350876	-0.272867	0.095009
C	3.166591	0.928413	0.792486
N	2.028197	1.608985	0.775713
C	0.987864	1.108455	0.058305
C	1.06207	-0.124679	-0.640664
C	2.294992	-0.819325	-0.633496
C	-0.095329	-0.65362	-1.322833
C	-1.261108	0.154623	-1.421887
C	-1.249993	1.444074	-0.792173
C	-0.219678	1.911796	-0.027992
C	-0.260911	3.26634	0.686874
O	0.150145	4.258596	0.02857
O	-0.709282	3.251827	1.864438
Cl	-2.694118	2.434725	-1.041217
H	3.988913	1.339503	1.373317
H	0.063674	-1.414289	-2.074901
H	-1.94338	-0.010794	-2.244576
O	2.389272	-1.969607	-1.331317
H	3.288027	-2.332153	-1.262349
Mn	-2.104444	-2.098334	0.544624
O	-2.880363	-3.413054	0.074043
O	-2.120681	-1.832603	2.118651
O	-0.560316	-2.108505	-0.02132
O	-2.659994	-0.780786	-0.262142

TS232	Cartesian coordinates		
Atom	x	y	z
Cl	-2.799357	2.541625	0.315674
C	-1.480455	1.414247	-0.000618
C	-0.59724	1.722935	-1.097329
N	0.625944	1.296144	-1.200082
C	1.179007	0.582104	-0.142295
C	0.455275	0.306854	1.045668
C	-0.951341	0.680733	1.112759
C	1.092233	-0.330324	2.125609
C	2.419233	-0.717701	2.018993
C	3.115932	-0.464842	0.826877
C	2.537173	0.18051	-0.25985
C	3.319398	0.477185	-1.544669
O	3.954834	1.564983	-1.565298
O	3.260322	-0.402099	-2.444777
Cl	4.802107	-0.997326	0.74099
H	-0.995994	2.335197	-1.903903
H	0.538759	-0.530554	3.03566
H	2.916309	-1.218533	2.842609
O	-1.458476	0.819373	2.36184
H	-2.387585	1.096655	2.319034
Mn	-2.681981	-1.383564	-0.498017
O	-4.153561	-1.697747	0.032959
O	-2.089897	-2.448644	-1.523475
O	-2.608043	0.1321	-1.117265
O	-1.65338	-1.159209	0.766448

TS233	Cartesian coordinates		
Atom	x	y	z
Cl	2.88918	1.89095	1.456877
C	1.51549	1.046825	0.705232
C	0.944742	-0.05242	1.473842
N	-0.354931	-0.393404	1.379485
C	-1.129604	0.234365	0.479516
C	-0.692765	1.395324	-0.268623
C	0.609953	1.853808	-0.058317
C	-1.596383	2.064839	-1.152785
C	-2.873956	1.602425	-1.308504
C	-3.29469	0.455012	-0.572488
C	-2.486786	-0.227408	0.303636
C	-2.96699	-1.453425	1.08728
O	-3.520842	-1.220836	2.195229
O	-2.77026	-2.571986	0.541835
Cl	-4.959066	-0.079478	-0.8421
H	1.447715	-0.317241	2.396586
H	-1.254062	2.932871	-1.704616
H	-3.568472	2.090289	-1.983049
O	1.008468	2.997529	-0.63651
H	1.937062	3.183002	-0.416508
Mn	2.721568	-1.289255	-0.732819
O	4.278309	-1.566926	-0.536623
O	2.039305	-2.021708	-1.969245
O	1.901703	-1.613666	0.66163
O	2.42545	0.345739	-0.782849

TS241	Cartesian coordinates		
Atom	x	y	z
Cl	-4.928008	-1.183902	0.304425
C	-3.387857	-0.332904	0.214432
C	-3.287102	0.82241	-0.581043
N	-2.158027	1.515224	-0.676429
C	-1.059694	1.09729	0.001112
C	-1.071379	-0.081643	0.806237
C	-2.28606	-0.790655	0.911645
C	0.118276	-0.533054	1.481542
C	1.314837	0.301336	1.471118
C	1.245437	1.495645	0.610979
C	0.141093	1.906262	-0.076402
C	0.116432	3.178143	-0.930019
O	-0.226905	4.241348	-0.343273
O	0.441682	3.044663	-2.14144
Cl	2.714629	2.480208	0.568817
H	-4.147458	1.182745	-1.139682
H	-2.342119	-1.685737	1.522575
H	-0.018209	-1.105918	2.392184
O	2.278713	0.082085	2.251602
Mn	1.562585	-2.367112	-0.635834
O	0.766884	-2.806956	-1.966527
O	2.038512	-0.798621	-0.755704
O	0.512222	-2.254805	0.642854
O	2.828007	-3.286968	-0.243382

TS242	Cartesian coordinates		
Atom	x	y	z
Cl	3.07618	1.99399	-1.594629
C	1.632465	1.328837	-0.821715
C	0.822302	2.218514	-0.052685
N	-0.40767	1.931344	0.301661
C	-0.989709	0.770308	-0.147202
C	-0.314625	-0.138447	-1.018594
C	1.084573	0.126232	-1.340231
C	-0.981971	-1.240391	-1.551756
C	-2.343762	-1.552025	-1.242109
C	-2.966829	-0.613779	-0.320511
C	-2.349837	0.504995	0.204128
C	-3.079739	1.470713	1.143095
O	-3.711924	2.416816	0.596828
O	-2.986693	1.229424	2.378701
Cl	-4.653525	-0.964817	0.125408
H	1.248614	3.160918	0.284105
H	1.462532	-0.244685	-2.28547
H	-0.457603	-1.917344	-2.221738
O	-2.952212	-2.56441	-1.729356
Mn	2.863468	-1.052385	0.879376
O	2.163349	-1.744523	2.138657
O	1.990975	-1.337795	-0.495575
O	2.690127	0.569495	0.946438
O	4.400265	-1.438302	0.662969

TS243	Cartesian coordinates		
Atom	x	y	z
Cl	3.30977	2.391676	1.099262
C	1.758161	1.621417	0.784834
C	1.466475	0.379727	1.504024
N	0.164119	-0.080683	1.500509
C	-0.701891	0.40052	0.613421
C	-0.407048	1.528541	-0.258716
C	0.87468	2.156711	-0.090912
C	-1.357305	1.997417	-1.153483
C	-2.663563	1.41936	-1.274553
C	-2.932193	0.307511	-0.348648
C	-2.032333	-0.184298	0.555665
C	-2.373163	-1.32117	1.523649
O	-2.845778	-0.968909	2.638714
O	-2.156608	-2.493408	1.116168
Cl	-4.552691	-0.398616	-0.448068
H	1.952368	0.283346	2.473281
H	1.106243	3.057053	-0.651612
H	-1.129255	2.841482	-1.799474
O	-3.525168	1.837164	-2.100954
Mn	2.383166	-1.351591	-0.83594
O	1.032945	-2.203795	-1.026866
O	2.441921	-0.019134	-1.745701
O	2.441549	-0.823272	0.77541
O	3.696314	-2.271615	-1.135426

TS251	Cartesian coordinates		
Atom	x	y	z
Cl	-4.945484	-1.530887	-0.148315
C	-3.452257	-0.59734	-0.063752
C	-3.354001	0.607888	-0.778641
N	-2.261297	1.362806	-0.746315
C	-1.195171	0.9591	-0.006976
C	-1.212514	-0.266907	0.717748
C	-2.382507	-1.038214	0.694637
C	-0.058545	-0.695093	1.533973
C	1.119137	0.164871	1.495575
C	1.025018	1.414932	0.804767
C	-0.03375	1.823911	0.040173
C	-0.060264	3.15618	-0.712502
O	-0.523661	4.148929	-0.085862
O	0.387409	3.141201	-1.892467
Cl	2.430524	2.493614	0.992387
H	-4.18824	0.959048	-1.381446
H	-2.420413	-1.964238	1.25775
H	1.754123	0.120016	2.371752
O	-0.136963	-1.670179	2.331036
Mn	2.197318	-1.840362	-0.674948
O	2.577444	-3.364992	-0.313251
O	0.561165	-1.676356	-0.704293
O	2.563772	-0.838621	0.594826
O	2.837599	-1.26345	-2.036164

TS252	Cartesian coordinates		
Atom	x	y	z
Cl	2.810299	1.765458	-1.938322
C	1.499332	1.113965	-0.922151
C	0.631212	2.093661	-0.298361
N	-0.583946	1.839554	0.08035
C	-1.154313	0.602777	-0.223887
C	-0.433033	-0.373242	-0.975615
C	0.925952	-0.125144	-1.313166
C	-1.083018	-1.59168	-1.445746
C	-2.436897	-1.769638	-1.00976
C	-3.075388	-0.809562	-0.236082
C	-2.495286	0.398051	0.170478
C	-3.258363	1.459452	0.965067
O	-3.927991	2.297892	0.296561
O	-3.165338	1.403059	2.224436
Cl	-4.759823	-1.155467	0.245735
H	1.039377	3.081914	-0.092471
H	1.376486	-0.71303	-2.100129
H	-2.955746	-2.676656	-1.302388
O	-0.490824	-2.445285	-2.190762
Mn	2.905779	-0.707374	1.112564
O	4.466677	-1.016672	0.928706
O	2.306771	-1.027174	2.560983
O	2.575406	0.856406	0.684061
O	2.035771	-1.474033	-0.050517

TS253	Cartesian coordinates		
Atom	x	y	z
Cl	2.783608	1.90103	1.74658
C	1.485304	1.035929	0.852687
C	0.965098	-0.136651	1.538482
N	-0.271914	-0.570326	1.379844
C	-1.128929	0.095607	0.544019
C	-0.746958	1.373638	-0.037887
C	0.517497	1.85828	0.195969
C	-1.708753	2.17284	-0.843946
C	-2.99026	1.578796	-1.032671
C	-3.285593	0.341922	-0.466825
C	-2.418841	-0.429411	0.321554
C	-2.832548	-1.773383	0.925228
O	-3.411352	-1.73886	2.048294
O	-2.569009	-2.805724	0.24515
Cl	-4.918687	-0.293019	-0.785971
H	1.559664	-0.584326	2.324811
H	0.801926	2.832518	-0.186539
H	-3.726384	2.10482	-1.630249
O	-1.38227	3.297177	-1.330758
Mn	3.039825	-0.980933	-0.85276
O	4.636843	-1.006602	-0.71153
O	2.456171	-1.581796	-2.216392
O	2.358453	-1.72553	0.440076
O	2.465267	0.576464	-0.619585

TS261	Cartesian coordinates		
Atom	x	y	z
Cl	4.934545	-1.258084	0.14541
C	3.379647	-0.414133	0.074608
C	3.230298	0.772507	0.779648
N	2.114124	1.513031	0.78162
C	1.064539	1.0385	0.058762
C	1.096362	-0.187688	-0.649481
C	2.320224	-0.982438	-0.71114
C	-0.080142	-0.660597	-1.320128
C	-1.232245	0.176297	-1.420992
C	-1.168832	1.464277	-0.791676
C	-0.121376	1.88567	-0.025566
C	-0.121119	3.236863	0.69249
O	0.318202	4.223341	0.040936
O	-0.573251	3.237953	1.870668
Cl	-2.577048	2.518052	-1.041628
H	4.065748	1.150728	1.367251
H	0.051039	-1.446484	-2.052055
H	-1.900318	0.047116	-2.262491
O	2.424403	-2.049013	-1.387459
Mn	-2.218145	-2.018236	0.537532
O	-3.0547	-3.306314	0.078416
O	-2.244718	-1.70781	2.108136
O	-0.667677	-2.120805	-0.000717
O	-2.682673	-0.687563	-0.315702

TS262	Cartesian coordinates		
Atom	x	y	z
Cl	-2.679828	2.745682	-0.293564
C	-1.510916	1.393687	-0.262463
C	-0.674938	1.307631	-1.43331
N	0.550063	0.856925	-1.459655
C	1.158105	0.52376	-0.25624
C	0.484901	0.631092	0.98891
C	-0.913683	1.107353	1.050287
C	1.177128	0.339531	2.176967
C	2.49649	-0.087583	2.141158
C	3.139681	-0.209389	0.899085
C	2.511955	0.089239	-0.304468
C	3.235045	-0.028182	-1.649448
O	3.861095	0.995491	-2.038826
O	3.149014	-1.142486	-2.23411
Cl	4.826845	-0.764174	0.905276
H	-1.113989	1.618149	-2.381054
H	0.657523	0.439341	3.123945
H	3.029712	-0.327652	3.055094
O	-1.483082	1.378282	2.133142
Mn	-2.733294	-1.480067	-0.131434
O	-3.920622	-1.802311	0.90716
O	-2.58959	-2.501105	-1.363157
O	-2.855002	0.077856	-0.685823
O	-1.313468	-1.357617	0.682053

TS263	Cartesian coordinates		
Atom	x	y	z
Cl	2.963888	1.886227	1.334133
C	1.487085	1.128056	0.706308
C	0.873157	0.166033	1.591386
N	-0.381883	-0.232086	1.487083
C	-1.161366	0.324536	0.497131
C	-0.734682	1.432499	-0.293817
C	0.604282	1.993261	-0.100173
C	-1.612581	2.014508	-1.231613
C	-2.885891	1.508261	-1.417659
C	-3.293068	0.410016	-0.633874
C	-2.483263	-0.19071	0.316728
C	-2.964167	-1.371748	1.164522
O	-3.557945	-1.082889	2.239754
O	-2.735684	-2.523304	0.702457
Cl	-4.936382	-0.204168	-0.90647
H	1.437664	-0.164959	2.454382
H	-1.265267	2.860561	-1.815866
H	-3.561709	1.936451	-2.14965
O	0.981884	3.066474	-0.611424
Mn	2.748733	-1.295913	-0.715376
O	4.349858	-1.298421	-0.857909
O	1.950878	-2.255343	-1.724715
O	2.330659	-1.632297	0.843473
O	2.167791	0.264168	-0.826378

PII_A	Cartesian coordinates		
Atom	x	y	z
Cl	-4.773507	-0.113853	0.000007
C	-3.020024	-0.221848	-0.000022
C	-2.415223	-1.505022	-0.000073
N	-1.109267	-1.673702	-0.000081
C	-0.292604	-0.578097	-0.000042
C	-0.832033	0.750616	-0.000007
C	-2.24179	0.908376	0.000008
C	0.048716	1.859144	0.000012
C	1.41769	1.655464	-0.000007
C	1.927585	0.331761	-0.000031
C	1.119324	-0.785873	-0.000044
C	1.690993	-2.210339	0.000054
O	1.901001	-2.720133	-1.131916
O	1.900777	-2.720031	1.132112
Cl	3.686868	0.175083	-0.000042
H	-3.038839	-2.395714	-0.000112
H	-2.678945	1.899802	0.000042
O	-0.480003	3.120283	0.000049
H	0.243084	3.767322	0.00008
O	2.197943	2.77511	0.000018
H	3.138893	2.536662	-0.000027

PII_D	Cartesian coordinates		
Atom	x	y	z
Cl	-4.765253	-0.153944	0.000065
C	-3.001019	-0.239792	-0.000017
C	-2.385748	-1.51863	0.000004
N	-1.07358	-1.664544	-0.00002
C	-0.269567	-0.563127	-0.000058
C	-0.822975	0.773121	-0.000117
C	-2.242716	0.902226	-0.000077
C	0.04604	1.868683	-0.000089
C	1.457631	1.743411	-0.000084
C	1.946044	0.386861	-0.000082
C	1.145686	-0.741817	-0.000033
C	1.728952	-2.158754	0.000008
O	1.945902	-2.678237	-1.130006
O	1.945824	-2.6782	1.13005
Cl	3.711931	0.204781	0.000054
H	-2.9974	-2.417518	0.000045
H	-2.698473	1.885914	-0.00011
O	-0.435817	3.159085	0.000015
H	0.388103	3.694357	0.00035
O	2.183507	2.811318	0.00008

PII_T	Cartesian coordinates		
Atom	x	y	z
Cl	-4.770093	-0.150819	0.000013
C	-2.994192	-0.237008	-0.000007
C	-2.377276	-1.516291	-0.000022
N	-1.065848	-1.659572	-0.000033
C	-0.255171	-0.550565	-0.000033
C	-0.812469	0.794304	-0.000015
C	-2.228448	0.901304	-0.000002
C	-0.002617	1.983206	0.000001
C	1.451793	1.80959	-0.000007
C	1.912931	0.45047	-0.000019
C	1.144684	-0.717916	-0.000033
C	1.761159	-2.115728	0.000021
O	1.995415	-2.645245	-1.127076
O	1.995409	-2.645143	1.127168
Cl	3.701344	0.252641	-0.000014
H	-2.987302	-2.41769	-0.000024
H	-2.670151	1.892369	0.000016
O	-0.53836	3.167824	0.000022
O	2.25813	2.82296	0.000003

2-Chloro-benzoate	Cartesian coordinates		
Atom	x	y	z
C	-2.678858	-0.079128	0.001161
C	-2.197202	-1.392379	0.002507
C	-0.821817	-1.630986	0.002238
C	0.105343	-0.574863	0.001268
C	-0.408244	0.726013	-0.000357
C	-1.779595	0.989492	-0.000668
H	-3.74653	0.117596	0.001009
H	-2.890965	-2.227861	0.003595
H	-0.451197	-2.652498	0.002737
H	-2.135366	2.014356	-0.00244
C	1.604526	-0.88151	0.001341
O	2.144247	-1.019134	-1.130389
O	2.150526	-0.991645	1.132923
Cl	0.701232	2.111459	-0.004124

Phenolate	Cartesian coordinates		
Atom	x	y	z
C	1.8276	-0.000004	0
C	1.104416	1.203731	0
C	-0.290525	1.211594	0
C	-1.063394	-0.000034	0
C	-0.290546	-1.211608	0
C	1.104397	-1.203713	0
H	2.913906	-0.000006	0
H	1.639535	2.152514	0
H	-0.829889	2.157595	0
H	1.639512	-2.152502	0.000001
O	-2.360618	0.000024	0
H	-0.829805	-2.157589	0

3-Fluoro-phenolate	Cartesian coordinates		
Atom	x	y	z
C	1.187515	1.104639	0
C	-0.059098	1.756741	0.000001
C	-1.258436	1.050655	0.000001
C	-1.299475	-0.388822	0
C	-0.015295	-1.039022	-0.000001
C	1.144795	-0.286438	-0.000001
H	2.130237	1.639615	0.000001
H	-0.081974	2.844568	0.000002
H	-2.206376	1.584231	0.000002
O	-2.40537	-1.054391	0
H	0.037458	-2.123987	-0.000002
F	2.351509	-0.966203	-0.000002

4-Fluoro-phenolate	Cartesian coordinates		
Atom	x	y	z
C	1.337006	0	0
C	0.659749	1.213506	0
C	-0.737404	1.211725	0
C	-1.509164	0	0
C	-0.737404	-1.211726	0
C	0.659749	-1.213506	0
H	1.21829	2.146032	0
H	-1.272685	2.158779	0
O	-2.807024	0	0
H	-1.272685	-2.158779	0
H	1.21829	-2.146032	0
F	2.725532	0	0

3-Bromo-phenolate	Cartesian coordinates		
Atom	x	y	z
C	-0.237871	1.518856	0.000001
C	-1.623104	1.756186	0.000002
C	-2.551372	0.72067	0.000002
C	-2.144705	-0.657798	0.000001
C	-0.72147	-0.884919	0
C	0.164359	0.181597	0
H	0.478873	2.331029	0.000001
H	-1.974204	2.786468	0.000003
H	-3.617113	0.938182	0.000002
O	-2.987933	-1.634625	0
H	-0.362906	-1.909267	-0.000001
Br	2.058966	-0.196485	-0.000001

4-Bromo-phenolate	Cartesian coordinates		
Atom	x	y	z
C	0.268395	0	0
C	-0.429704	1.210803	0
C	-1.822872	1.210512	0
C	-2.596497	0	0
C	-1.822872	-1.210512	0
C	-0.429704	-1.210802	0
H	0.110697	2.153619	0
H	-2.356761	2.158569	0
O	-3.889358	0	0
H	-2.35676	-2.15857	0
H	0.110698	-2.153618	0
Br	2.188757	0	0

2-Chloro-phenolate	Cartesian coordinates		
Atom	x	y	z
C	1.764137	-1.3464	0
C	2.343658	-0.067756	0
C	1.554263	1.078538	0
C	0.115745	1.046203	0
C	-0.41589	-0.291741	0
C	0.366726	-1.442987	0
H	2.375439	-2.24346	0
H	3.427248	0.033591	0
H	2.019403	2.06232	0
H	-0.116393	-2.416279	0
O	-0.60721	2.10955	0
Cl	-2.189403	-0.480454	0

3-Chloro-phenolate	Cartesian coordinates		
Atom	x	y	z
C	0.490722	1.424419	0.000001
C	-0.870174	1.776564	0.000001
C	-1.879745	0.819342	0.000001
C	-1.593654	-0.590148	0
C	-0.194091	-0.932963	-0.000001
C	0.777511	0.057218	0
H	1.276587	2.17046	0.000001
H	-1.136557	2.831755	0.000002
H	-2.923198	1.126582	0.000002
O	-2.51593	-1.492477	0
H	0.083407	-1.982661	-0.000001
Cl	2.496693	-0.443112	-0.000001

4-Chloro-phenolate	Cartesian coordinates		
Atom	x	y	z
C	-0.90922	0	0
C	-0.213889	-1.212185	0
C	1.180174	-1.211383	0
C	1.954079	0	0
C	1.180174	1.211383	0
C	-0.213889	1.212185	0
H	-0.758241	-2.152863	0
H	1.714119	-2.159339	0
O	3.247676	0	0
H	1.714119	2.159339	0
H	-0.758242	2.152863	0
Cl	-2.691631	0	0

2,3-Dichloro-phenolate	Cartesian coordinates		
Atom	x	y	z
C	0.192603	1.974958	0
C	-1.197413	2.16127	0
C	-2.075	1.085422	0
C	-1.631401	-0.280765	0.000001
C	-0.191161	-0.435914	0
C	0.671363	0.662083	0
H	-1.591903	3.174711	0
H	-3.149372	1.251722	0.000001
O	-2.438488	-1.27546	0.000001
Cl	0.437312	-2.084131	0
H	0.882142	2.810505	-0.000001
Cl	2.430516	0.434979	-0.000001

2,4-Dichloro-phenolate	Cartesian coordinates		
Atom	x	y	z
C	-1.425232	0.042157	0
C	-1.209977	1.423181	0.000001
C	0.090723	1.916388	0.000001
C	1.261578	1.080648	0
C	0.948597	-0.325602	0
C	-0.34491	-0.840679	0
H	-2.053069	2.107871	0.000001
H	0.255466	2.991042	0.000001
O	2.454857	1.551309	0
H	-0.505403	-1.913507	-0.000001
Cl	-3.080603	-0.602211	0
Cl	2.300573	-1.47852	-0.000001

2,6-Dichloro-phenolate	Cartesian coordinates		
Atom	x	y	z
C	0	-2.280383	0
C	1.205063	-1.567699	0
C	1.191941	-0.177957	0.000001
C	0	0.634135	0
C	-1.191941	-0.177957	-0.000001
C	-1.205063	-1.567699	0
H	2.155077	-2.09362	0.000002
O	0	1.910338	0
Cl	-2.748986	0.679268	-0.000002
H	0	-3.365222	0
H	-2.155076	-2.09362	0
Cl	2.748986	0.679268	0.000001

3,4-Dichloro-phenolate	Cartesian coordinates		
Atom	x	y	z
C	-0.544088	-0.714417	0
C	0.470902	-1.68118	0
C	1.811941	-1.319654	0
C	2.234701	0.054362	0
C	1.166611	1.018059	0
C	-0.169561	0.635841	0
H	0.19278	-2.731468	0
O	3.473519	0.405379	0
H	2.576244	-2.092782	0
H	1.421724	2.07307	0
Cl	-1.401163	1.911278	0
Cl	-2.234245	-1.231861	0