For being published in New Journal of Chemistry

The Conformational Preferences of Polychlorocyclohexanes

Shida Gong,[a, b] Yuan Chen,[a] Qiong Luo,[a]* Henry F. Schaefer[c]*

[a] MOE Key Laboratory of Theoretical Chemistry of Environment, Center for Computational Quantum Chemistry, South China Normal University, Guangzhou 510631, P. R. China

[b] School of Chemistry and Chemical Engineering, Qingdao University, Qingdao 266071, P. R. China

[c] Center for Computational Chemistry, University of Georgia, Athens, GA 30602, USA

Table S1-S10 Dipole moments of polychlorocyclohexane conformers in Debye at the MP2/cc-pVTZ level of theory, using the geometries optimized at MP2/DZP level of theory.

Table S11-S102 Optimized cartesian coordinates and total energies of cyclohexane and polychlorocyclohexane.

Table S1 Dipole moments of chlorocyclohexane conformers in Debye at the MP2/cc-pVTZ level of theory, using the geometries optimized at MP2/DZP level of theory.

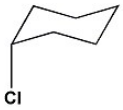
Species	Structure	Dipole Moment
Chlorocyclohexane		2.60
		2.25

Table 2 Dipole moments of dichlorocyclohexane conformers in Debye at the MP2/cc-pVTZ level of theory, using the geometries optimized at the MP2/DZP level of theory.

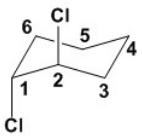
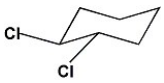
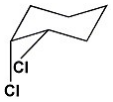
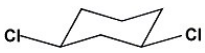
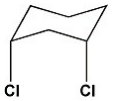
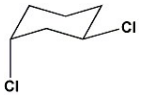
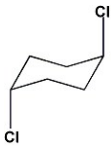
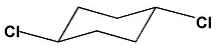
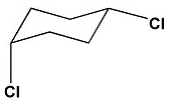
Species	Structure	Dipole Moment
trans-1, 2		1.07
		3.86
cis-1, 2		3.48
cis-1, 3		2.69
		4.03
trans-1, 3		2.67
trans-1, 4		0.00
		0.00
cis-1, 4		3.21

Table S3 Dipole moments of 1, 2, 3-trichlorocyclohexane in Debye at the MP2/cc-pVTZ level of theory, using the geometries optimized at the MP2/DZP level of theory.

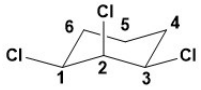
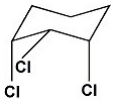
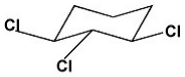
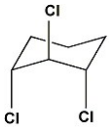
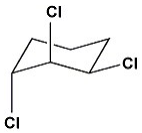
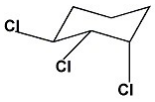
Species	Structure	Dipole Moment
r-1, *c*-2, *c*-3		3.59
		4.72
r-1, *t*-2, *c*-3		4.13
		2.26
r-1, *t*-2, *t*-3		2.45
		3.98

Table S4 Dipole moments of 1, 2, 4-trichlorocyclohexane in Debye at the MP2/cc-pVTZ level of theory, using the geometries optimized at the MP2/DZP level of theory.

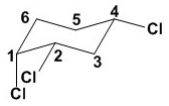
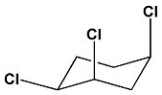
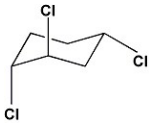
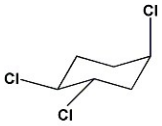
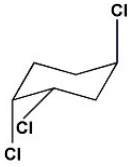
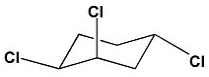
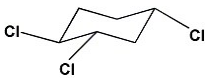
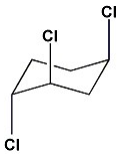
Species	Structure	Dipole Moment
r-1, *c*-2, *c*-4		3.46
		4.39
r-1, *t*-2, *c*-4		1.72
		3.81
r-1, *c*-2, *t*-4		2.19
		1.66
r-1, *t*-2, *t*-4		2.12
		1.90

Table S5 Dipole moments of 1, 3, 5-trichlorocyclohexane in Debye at the MP2/cc-pVTZ level of theory, using the geometries optimized at the MP2/DZP level of theory.

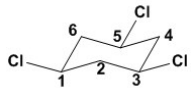
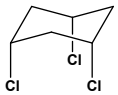
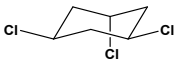
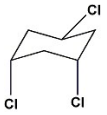
Species	Strucure	Dipole Moment
r-1, *c*-3, *c*-5		1.61
		5.59
r-1, *c*-3, *t*-5		1.94
		3.80

Table S6 Dipole moments of 1, 2, 3, 4-tetrachlorocyclohexane in Debye at the MP2/cc-pVTZ level of theory, using the geometries optimized at the MP2/DZP level of theory.

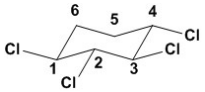
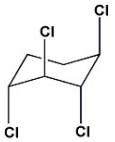
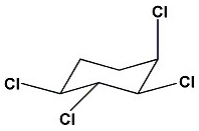
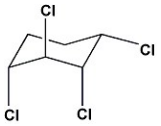
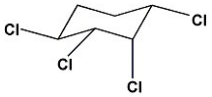
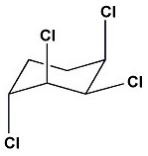
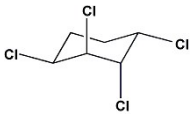
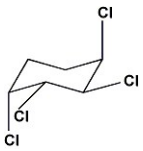
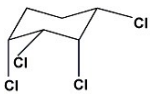
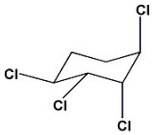
Species	Structure	Dipole Moment
r-1, *t*-2, *c*-3, *t*-4		3.25
		1.04
r-1, *t*-2, *c*-3, *c*-4		4.25
		2.67
r-1, *t*-2, *t*-3, *t*-4		2.74
		2.95
r-1, *c*-2, *t*-3, *t*-4		0.88
		3.37
r-1, *c*-2, *c*-3, *c*-4		4.51
r-1, *t*-2, *t*-3, *c*-4		3.17

Table S7 Dipole moments of 1, 2, 3, 5-tetrachlorocyclohexane in Debye at the MP2/cc-pVTZ level of theory, using the geometries optimized at the MP2/DZP level of theory.

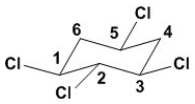
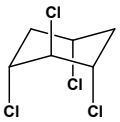
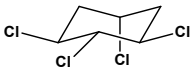
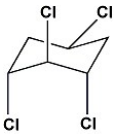
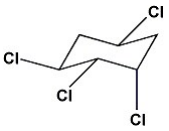
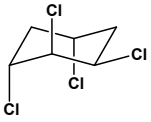
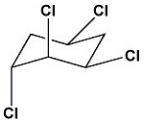
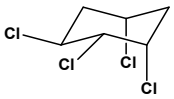
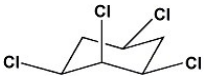
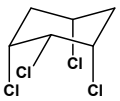
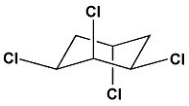
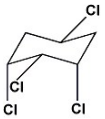
Species	Structure	Dipole Moment
r-1, *t*-2, *c*-3, *c*-5		1.94
		3.50
r-1, *t*-2, *c*-3, *t*-5		3.70
		1.74
r-1, *t*-2, *t*-3, *c*-5		1.92
		2.48
r-1, *t*-2, *t*-3, *t*-5		1.66
		4.47
r-1, *c*-2, *c*-3, *c*-5		2.90
		5.71
r-1, *c*-2, *c*-3, *t*-5		1.96
		3.27

Table S8 Dipole moments of 1, 2, 4, 5-tetrachlorocyclohexane in Debye at the MP2/cc-pVTZ level of theory, using the geometries optimized at the MP2/DZP level of theory.

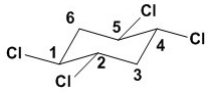
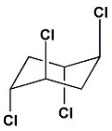
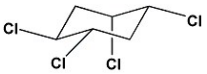
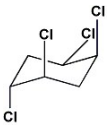
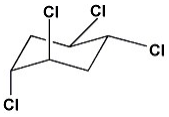
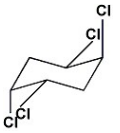
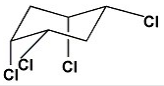
Species	Structure	Dipole Moment
r-1, *t*-2, *t*-4, *c*-5		0.00
		0.00
r-1, *t*-2, *t*-4, *t*-5		2.63
		2.53
r-1, *t*-2, *c*-4, *t*-5		2.72
r-1, *c*-2, *t*-4, *t*-5		0.00
r-1, *c*-2, *c*-4, c-5		4.32

Table S9 Dipole moments of 1, 2, 3, 4, 5-pentachlorocyclohexane in Debye at the MP2/cc-pVTZ level of theory, using the geometries optimized at the MP2/DZP level of theory.

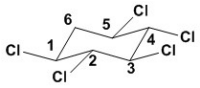
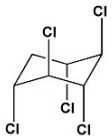
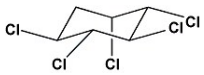
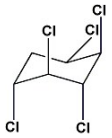
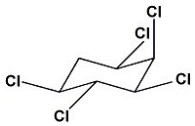
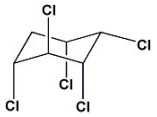
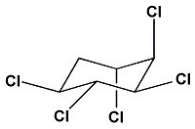
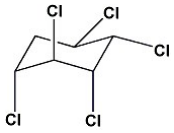
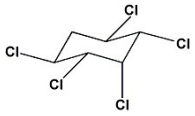
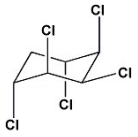
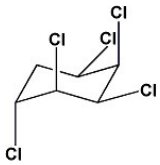
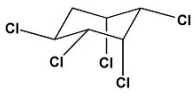
Species	Structure	Dipole Moment
r-1, *t*-2, *c*-3, *t*-4, *c*-5		1.66
		1.73
r-1, *t*-2, *c*-3, *t*-4, *t*-5		3.17
		1.29
r-1, *t*-2, *c*-3, *c*-4, *c*-5		2.67
		3.76
r-1, *t*-2, *c*-3, *c*-4, *t*-5		3.10
		2.82
r-1, *t*-2, *t*-3, *t*-4, *c*-5		1.05
		1.96
r-1, *t*-2, *t*-3, *t*-4, *t*-5		2.56
		3.65

Table S9, continued

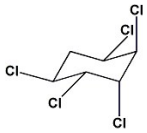
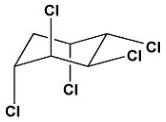
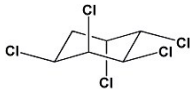
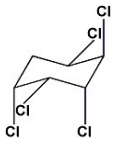
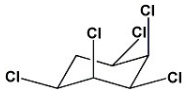
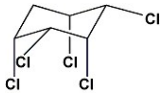
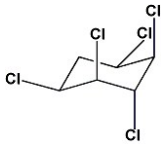
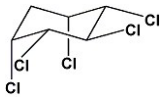
r-1, *t*-2, *t*-3, *c*-4, *c*-5		1.40
		3.36
r-1, *c*-2, *c*-3, *t*-4, *t*-5		1.72
		1.66
r-1, *c*-2, *c*-3, *c*-4, *c*-5		3.93
		5.52
r-1, *c*-2, *t*-3, *c*-4, *c*-5		2.30
		4.67

Table S10 Dipole moments of 1, 2, 3, 4, 5, 6-hexachlorocyclohexane in Debye at the

MP2/cc-pVTZ level of theory, using the geometries optimized at the MP2/DZP level of theory.

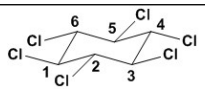
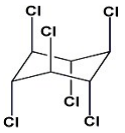
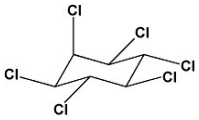
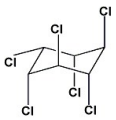
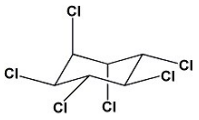
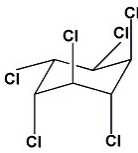
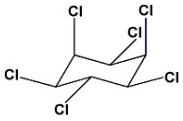
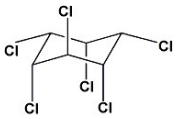
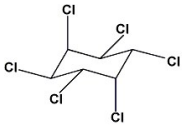
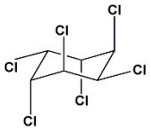
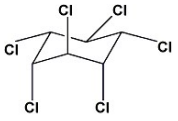
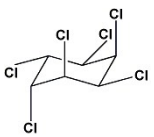
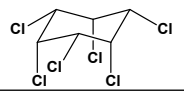
Species	Structure	Dipole Moment
r-1, *t*-2, *c*-3, *t*-4, *c*-5, *t*-6		0.00
		0.00
r-1, *t*-2, *c*-3, *t*-4, *c*-5, *c*-6		2.09
		2.03
r-1, *t*-2, *c*-3, *t*-4, *t*-5, *c*-6		2.38
		2.27
r-1, *t*-2, *c*-3, *c*-4, *c*-5, *c*-6		3.55
		3.50
r-1, *t*-2, *t*-3, *t*-4, *c*-5, *c*-6		0.00
		0.00
r-1, *t*-2, *c*-3, *c*-4, *t*-5, *c*-6		3.01
r-1, *t*-2, *t*-3, *t*-4, *t*-5, *c*-6		2.18
r-1, *c*-2, *c*-3, *c*- 4, *c*-5, *c*-6		5.02

Table S11 Optimized cartesian coordinates and total energies of chair-cyclohexane.

chair-cyclohexane			
E(MP2/cc-pVTZ) = -235.1019231 a.u.			
Atom	X	Y	Z
C	-1.264091	0.729824	0.236334
C	0.000000	1.459647	-0.236334
C	1.264091	0.729824	0.236334
C	1.264091	-0.729824	-0.236334
C	0.000000	-1.459647	0.236334
C	-1.264091	-0.729824	-0.236334
H	2.160223	1.247206	-0.126951
H	0.000000	1.501759	-1.333880
H	0.000000	2.494411	0.126951
H	1.300561	-0.750879	-1.333880
H	2.160223	-1.247206	0.126951
H	0.000000	-2.494411	-0.126951
H	0.000000	-1.501759	1.333880
H	-1.300561	-0.750879	-1.333880
H	-2.160223	-1.247206	0.126951
H	1.300561	0.750879	1.333880
H	-2.160223	1.247206	-0.126951
H	-1.300561	0.750879	1.333880

Table S12 Optimized cartesian coordinates and total energies of axial-chlorocyclohexane.

axial-chlorocyclohexane			
E(MP2/cc-pVTZ) = -694.4514077 a.u.			
Atom	X	Y	Z
C	0.031857	-1.085146	0.000000
C	-0.607631	-0.510291	1.265550
C	-0.607631	1.022572	1.265792
C	-1.281527	1.567624	0.000000
C	-0.607631	1.022572	-1.265792
C	-0.607631	-0.510291	-1.265550
H	-1.128822	1.387179	2.158213
H	-1.645538	-0.870139	1.293777
H	-0.096301	-0.904203	2.150355
H	-2.338918	1.269040	0.000000
H	-1.255567	2.663639	0.000000
H	-1.128822	1.387179	-2.158213
H	0.423818	1.388174	-1.318603
H	-1.645538	-0.870139	-1.293777
H	-0.096301	-0.904203	-2.150355
H	0.423818	1.388174	1.318603
Cl	1.801437	-0.752976	0.000000
H	-0.055091	-2.176358	0.000000

Table S13 Optimized cartesian coordinates and total energies of equatorial-chlorocyclohexane.

equatorial-chlorocyclohexane			
E(MP2/cc-pVTZ) = -694.4518085 a.u.			
Atom	X	Y	Z
C	-0.506770	0.514161	0.000000
C	0.171625	-0.013422	1.262086
C	0.171625	-1.548763	1.261276
C	0.848338	-2.098566	0.000000
C	0.171625	-1.548763	-1.261276
C	0.171625	-0.013422	-1.262086
H	0.677899	-1.916985	2.160916
H	1.203589	0.358104	1.286040
H	-0.340095	0.374010	2.149721
H	-1.559669	0.207994	0.000000
H	1.905427	-1.801800	0.000000
H	0.818168	-3.194297	0.000000
H	0.677899	-1.916985	-2.160916
H	-0.863794	-1.912154	-1.302779
H	1.203589	0.358104	-1.286040
H	-0.340095	0.374010	-2.149721
H	-0.863794	-1.912154	1.302779
Cl	-0.511032	2.307930	0.000000

Table S14 Optimized cartesian coordinates and total energies of *trans*-1ax, 2ax -dichlorocyclohexane.

trans-1ax, 2ax			
E(MP2/cc-pVTZ) = -1153.5720327 a.u.			
atom	X	Y	Z
C	-0.727470	0.243910	-0.678784
C	0.727470	-0.243910	-0.678784
C	1.473807	0.141086	0.598531
C	0.712778	-0.283078	1.859569
C	-0.712778	0.283078	1.859569
C	-1.473807	-0.141086	0.598531
H	2.472238	-0.307279	0.575829
H	1.241842	0.150565	-1.559730
H	-1.241842	-0.150565	-1.559730
H	0.673374	-1.376817	1.914004
H	1.255613	0.067069	2.744499
H	-1.255613	-0.067069	2.744499
H	-0.673374	1.376817	1.914004
H	-1.597603	-1.230221	0.594310
H	-2.472238	0.307279	0.575829
H	1.597603	1.230221	0.594310
Cl	-0.712778	2.030393	-0.879106
Cl	0.712778	-2.030393	-0.879106

Table S15 Optimized cartesian coordinates and total energies of *cis*-1ax, 2eq -

dichlorocyclohexane.

cis-1ax, 2eq			
E(MP2/cc-pVTZ) = -1153.5698586 a.u.			
atom	X	Y	Z
C	0.058634	0.685719	0.739139
C	-0.579569	-0.669597	0.425106
C	0.114516	-1.382466	-0.731195
C	1.605005	-1.565403	-0.407615
C	2.282141	-0.229408	-0.078251
C	1.545318	0.490200	1.056995
H	-0.361611	-2.355211	-0.890672
H	-0.457611	1.142104	1.589320
H	1.704255	-2.241233	0.452521
H	2.107071	-2.047714	-1.253884
H	3.323697	-0.400580	0.215049
H	2.294174	0.407972	-0.968583
H	1.612413	-0.110619	1.974263
H	1.998759	1.464495	1.266372
H	-0.011262	-0.794548	-1.645893
Cl	-0.128190	1.834023	-0.621424
Cl	-2.336440	-0.526074	0.145098
H	-0.467451	-1.274068	1.333980

Table S16 Optimized cartesian coordinates and total energies of *trans*-1eq, 2eq - dichlorocyclohexane.

trans-1eq, 2eq			
E(MP2/cc-pVTZ) = -1153.5701824 a.u.			
atom	X	Y	Z
C	-0.006527	0.764389	-0.171600
C	0.006527	-0.764389	-0.171600
C	0.675629	-1.302225	1.096161
C	-0.006527	-0.765365	2.358568
C	0.006527	0.765365	2.358568
C	-0.675629	1.302225	1.096161
H	0.649862	-2.396588	1.071178
H	-1.044700	-1.119974	2.396593
H	0.503189	-1.157366	3.245711
H	-0.503189	1.157366	3.245711
H	1.044700	1.119974	2.396593
H	-1.730386	1.000700	1.089193
H	-0.649862	2.396588	1.071178
H	1.730386	-1.000700	1.089193
Cl	0.862655	-1.405965	-1.603907
H	-1.027403	-1.122882	-0.235031
H	1.027403	1.122882	-0.235031
Cl	-0.862655	1.405965	-1.603907

Table S17 Optimized cartesian coordinates and total energies of *cis*-1ax, 3ax -

dichlorocyclohexane.

cis-1ax, 3ax			
E(MP2/cc-pVTZ) = -1153.5665204 a.u.			
atom	X	Y	Z
C	0.426493	0.571625	1.299612
C	1.185558	0.864758	0.000000
C	0.426493	0.571625	-1.299612
C	-1.008791	1.099563	-1.253372
C	-1.751297	0.629108	0.000000
C	-1.008791	1.099563	1.253372
H	0.966277	1.050057	-2.122605
H	1.383452	1.946395	0.000000
H	2.152819	0.353198	0.000000
H	0.966277	1.050057	2.122605
H	-0.955773	2.197518	-1.244114
H	-1.537235	0.800942	-2.164260
H	-2.767065	1.038692	0.000000
H	-1.834482	-0.462267	0.000000
H	-0.955773	2.197518	1.244114
H	-1.537235	0.800942	2.164260
Cl	0.426493	-1.176191	1.708528
Cl	0.426493	-1.176191	-1.708528

Table S18 Optimized cartesian coordinates and total energies of *trans*-1ax, 3eq - dichlorocyclohexane.

trans-1ax, 3eq			
E(MP2/cc-pVTZ) = -1153.5728699 a.u.			
atom	X	Y	Z
C	-1.288980	-0.278882	0.813803
C	0.186452	-0.675375	0.907330
C	0.994357	-0.102383	-0.255618
C	0.844382	1.414442	-0.340457
C	-0.634900	1.799461	-0.482225
C	-1.459551	1.234698	0.678668
H	0.586462	-0.268397	1.845028
H	0.283576	-1.764706	0.942612
H	-1.818912	-0.639604	1.700666
H	1.258059	1.858711	0.573804
H	1.425604	1.797697	-1.185874
H	-0.728191	2.890542	-0.504303
H	-1.028027	1.420824	-1.431965
H	-1.115062	1.685105	1.619567
H	-2.520538	1.478145	0.562023
Cl	-2.063622	-1.115082	-0.578627
Cl	2.718960	-0.546753	-0.060000
H	0.665735	-0.558888	-1.193913

Table S19 Optimized cartesian coordinates and total energies of *cis*-1eq, 3eq -

dichlorocyclohexane.

cis-1eq, 3eq			
E(MP2/cc-pVTZ) = -1153.5723147 a.u.			
atom	X	Y	Z
C	-0.329756	-0.192132	1.250907
C	0.358664	-0.739568	0.000000
C	-0.329756	-0.192132	-1.250907
C	-0.329756	1.334062	-1.266308
C	-1.010595	1.870299	0.000000
C	-0.329756	1.334062	1.266308
H	1.409722	-0.428476	0.000000
H	0.329716	-1.833714	0.000000
H	0.708324	1.685318	-1.309027
H	-0.841390	1.697157	-2.163782
H	-0.983674	2.965355	0.000000
H	-2.068122	1.575488	0.000000
H	0.708324	1.685318	1.309027
H	-0.841390	1.697157	2.163782
H	-1.363880	-0.555083	1.286949
Cl	0.474470	-0.835911	2.715842
Cl	0.474470	-0.835911	-2.715842
H	-1.363880	-0.555083	-1.286949

Table S20 Optimized cartesian coordinates and total energies of *trans*-1ax, 4ax - dichlorocyclohexane.

trans-1ax, 4ax			
E(MP2/cc-pVTZ) = -1153.5741937 a.u.			
atom	X	Y	Z
C	-0.223436	1.464684	0.000000
C	0.223436	0.732312	1.265951
C	-0.223436	-0.732312	1.265951
C	0.223436	-1.464684	0.000000
C	-0.223436	-0.732312	-1.265951
C	0.223436	0.732312	-1.265951
H	0.169052	-1.247588	2.148090
H	1.317813	0.782571	1.307870
H	-0.169052	1.247588	2.148090
H	0.171906	2.485124	0.000000
H	-0.171906	-2.485124	0.000000
H	0.169052	-1.247588	-2.148090
H	-1.317813	-0.782571	-1.307870
H	1.317813	0.782571	-1.307870
H	-0.169052	1.247588	-2.148090
H	-1.317813	-0.782571	1.307870
Cl	-2.015639	1.650044	0.000000
Cl	2.015639	-1.650044	0.000000

Table S21 Optimized cartesian coordinates and total energies of *cis*-1ax, 4eq -

dichlorocyclohexane.

cis-1ax, 4eq			
E(MP2/cc-pVTZ) = -1153.5730337 a.u.			
atom	X	Y	Z
C	0.297878	-1.761583	0.000000
C	-0.346115	-1.187288	1.262772
C	-0.346115	0.346669	1.263366
C	-1.025690	0.869817	0.000000
C	-0.346115	0.346669	-1.263366
C	-0.346115	-1.187288	-1.262772
H	-0.872666	0.718480	2.148277
H	-1.381561	-1.553013	1.296038
H	0.167286	-1.568840	2.151206
H	0.211430	-2.852643	0.000000
H	-0.872666	0.718480	-2.148277
H	0.680143	0.725531	-1.301600
H	-1.381561	-1.553013	-1.296038
H	0.167286	-1.568840	-2.151206
H	0.680143	0.725531	1.301600
Cl	2.062958	-1.420528	0.000000
Cl	-1.042191	2.661071	0.000000
H	-2.077245	0.557122	0.000000

Table S22 Optimized cartesian coordinates and total energies of *trans*-1eq, 4eq - dichlorocyclohexane.

trans-1eq, 4eq			
E(MP2/cc-pVTZ) = -1153.5730031 a.u.			
atom	X	Y	Z
C	-0.240162	1.446004	0.000000
C	0.240162	0.729206	1.259685
C	-0.240162	-0.729206	1.259685
C	0.240162	-1.446004	0.000000
C	-0.240162	-0.729206	-1.259685
C	0.240162	0.729206	-1.259685
H	0.128511	-1.247187	2.150977
H	1.336157	0.765035	1.288372
H	-0.128511	1.247187	2.150977
H	0.128511	-1.247187	-2.150977
H	-1.336157	-0.765035	-1.288372
H	1.336157	0.765035	-1.288372
H	-0.128511	1.247187	-2.150977
H	-1.336157	-0.765035	1.288372
Cl	-0.320399	-3.146510	0.000000
H	1.335871	-1.483481	0.000000
Cl	0.320399	3.146510	0.000000
H	-1.335871	1.483481	0.000000

Table S23 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3-1ax, 2ax, 3ax -

trichlorocyclohexane.

r-1, *t*-2, *c*-3-1ax, 2ax, 3ax			
E(MP2/cc-pVTZ) = -1612.6851258 a.u.			
atom	X	Y	Z
C	0.145783	0.136832	1.303639
C	0.919674	0.401369	0.000000
C	0.145783	0.136832	-1.303639
C	-1.285416	0.672214	-1.254888
C	-2.027714	0.206099	0.000000
C	-1.285416	0.672214	1.254888
H	0.698077	0.611598	-2.118642
H	1.856536	-0.162151	0.000000
H	0.698077	0.611598	2.118642
H	-1.235703	1.767833	-1.259578
H	-1.809964	0.358694	-2.162564
H	-3.040037	0.623553	0.000000
H	-2.121051	-0.884503	0.000000
H	-1.235703	1.767833	1.259578
H	-1.809964	0.358694	2.162564
Cl	0.145783	-1.612671	1.693342
Cl	1.374528	2.142606	0.000000
Cl	0.145783	-1.612671	-1.693342

Table S24 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-3-1ax, 2ax, 3eq - trichlorocyclohexane.

r-1, *t*-2, *t*-3-1ax, 2ax, 3eq			
E(MP2/cc-pVTZ) = -1612.6894115 a.u.			
atom	X	Y	Z
C	1.338124	0.663237	-0.204065
C	-0.144821	0.558069	-0.595545
C	-0.736308	-0.775141	-0.129829
C	-0.556298	-0.994008	1.368628
C	0.935308	-0.930921	1.729773
C	1.566231	0.391905	1.282973
H	-0.250369	0.654864	-1.679878
H	1.702122	1.658294	-0.474276
H	-1.118007	-0.231479	1.917895
H	-0.969022	-1.971379	1.637931
H	1.052956	-1.042709	2.812885
H	1.461998	-1.768416	1.258864
H	1.120733	1.220515	1.844573
H	2.642192	0.394156	1.483169
Cl	2.279155	-0.491992	-1.208298
Cl	-1.000147	1.953618	0.124382
Cl	-2.446946	-0.922415	-0.612453
H	-0.201073	-1.559267	-0.674509

Table S25 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3-1ax, 2eq, 3ax -

trichlorocyclohexane.

r-1, *c*-2, *c*-3-1ax, 2eq, 3ax			
E(MP2/cc-pVTZ) = -1612.6809700 a.u.			
atom	X	Y	Z
C	-0.448377	-0.220946	1.301599
C	-1.037743	0.336477	0.000000
C	-0.448377	-0.220946	-1.301599
C	-0.448377	-1.753294	-1.254521
C	0.246900	-2.288175	0.000000
C	-0.448377	-1.753294	1.254521
H	-1.083872	0.124392	2.122752
H	-1.494517	-2.089769	-1.257720
H	0.023740	-2.135709	-2.164728
H	0.208873	-3.382534	0.000000
H	1.300887	-1.993743	0.000000
H	-1.494517	-2.089769	1.257720
H	0.023740	-2.135709	2.164728
Cl	1.186298	0.385566	1.682277
H	-1.083872	0.124392	-2.122752
Cl	-1.126435	2.110807	0.000000
Cl	1.186298	0.385566	-1.682277
H	-2.079093	-0.013461	0.000000

Table S26 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3-1eq, 2ax, 3eq - trichlorocyclohexane.

r-1, *c*-2, *c*-3-1eq, 2ax, 3eq			
E(MP2/cc-pVTZ) = -1612.6866656 a.u.			
atom	X	Y	Z
C	-0.553842	0.355198	1.239910
C	-0.412996	-0.537858	0.000000
C	-0.553842	0.355198	-1.239910
C	0.504717	1.453259	-1.275781
C	0.414922	2.303313	0.000000
C	0.504717	1.453259	1.275781
H	1.495171	0.997706	-1.368591
H	0.340635	2.080534	-2.157425
H	1.214937	3.051447	0.000000
H	-0.535889	2.852510	0.000000
H	1.495171	0.997706	1.368591
H	0.340635	2.080534	2.157425
H	-1.547441	0.816708	-1.179299
Cl	-0.553842	-0.608072	-2.739777
Cl	-0.553842	-0.608072	2.739777
H	-1.547441	0.816708	1.179299
H	-1.199720	-1.298417	0.000000
Cl	1.138383	-1.412659	0.000000

Table S27 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-3-1eq, 2eq, 3ax -

trichlorocyclohexane.

r-1, *t*-2, *t*-3-1eq, 2eq, 3ax			
E(MP2/cc-pVTZ) = -1612.6870259 a.u.			
atom	X	Y	Z
C	-0.844590	0.546415	-0.368998
C	-0.217522	-0.429664	0.628003
C	1.312218	-0.309633	0.646224
C	1.733859	1.125232	0.968317
C	1.127074	2.118058	-0.025663
C	-0.398622	1.979067	-0.057809
H	1.381576	1.359180	1.981989
H	2.826755	1.185717	0.973174
H	1.389039	3.140693	0.265532
H	1.543723	1.945866	-1.022997
H	-0.814972	2.262009	0.917153
H	-0.834075	2.652066	-0.803619
Cl	-2.627956	0.470269	-0.294806
H	-0.557446	0.259214	-1.384656
Cl	2.028343	-0.815286	-0.915462
H	1.704861	-1.003641	1.395463
H	-0.569944	-0.165451	1.632892
Cl	-0.714742	-2.114542	0.345835

Table S28 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3-1eq, 2eq, 3eq - trichlorocyclohexane.

r-1, *t*-2, *c*-3-1eq, 2eq, 3eq			
E(MP2/cc-pVTZ) = -1612.6865852 a.u.			
atom	X	Y	Z
C	0.366878	0.221196	-1.263773
C	-0.278577	-0.363599	0.000000
C	0.366878	0.221196	1.263773
C	0.366878	1.749178	1.251990
C	1.067847	2.277970	0.000000
C	0.366878	1.749178	-1.251990
H	-0.670040	2.105612	1.275976
H	0.858650	2.107654	2.161901
H	1.056243	3.373056	0.000000
H	2.119755	1.964535	0.000000
H	-0.670040	2.105612	-1.275976
H	0.858650	2.107654	-2.161901
Cl	-0.118658	-2.140167	0.000000
H	-1.349966	-0.132430	0.000000
H	1.395458	-0.151609	1.332505
Cl	-0.485814	-0.355187	2.724108
Cl	-0.485814	-0.355187	-2.724108
H	1.395458	-0.151609	-1.332505

Table S29 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-4-1ax, 2ax, 4ax -

trichlorocyclohexane.

r-1, *t*-2, *t*-4-1ax, 2ax, 4ax			
E(MP2/cc-pVTZ) = -1612.6874155 a.u.			
atom	X	Y	Z
C	-1.305190	0.343406	-0.557140
C	-0.448222	1.010504	0.526037
C	0.294943	-0.006638	1.397428
C	0.977780	-1.156703	0.648289
C	0.066452	-1.773678	-0.413555
C	-0.529571	-0.713101	-1.340664
H	1.017461	0.512782	2.033379
H	-1.094084	1.616318	1.167286
H	-1.700553	1.111126	-1.227448
H	1.251917	-1.921230	1.381309
H	0.630808	-2.509891	-0.993216
H	-0.742146	-2.303934	0.102459
H	0.269541	-0.205603	-1.891727
H	-1.198467	-1.181100	-2.069247
H	-0.456685	-0.464783	2.052712
Cl	-2.737170	-0.396980	0.241006
Cl	0.654420	2.176174	-0.272478
Cl	2.534812	-0.654279	-0.093108

Table S30 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-4-1ax, 2ax, 4eq - trichlorocyclohexane.

r-1, *t*-2, *c*-4-1ax, 2ax, 4eq			
E(MP2/cc-pVTZ) = -1612.6925128 a.u.			
atom	X	Y	Z
C	1.542416	-0.293705	0.319180
C	0.930318	0.720966	-0.654522
C	-0.514363	0.380485	-1.023545
C	-1.372661	0.165501	0.221809
C	-0.783638	-0.913311	1.127136
C	0.648323	-0.542650	1.533195
H	-0.930830	1.183036	-1.639261
H	1.544845	0.776741	-1.557316
H	2.529943	0.055738	0.633376
H	-1.404649	-1.022579	2.021976
H	-0.792481	-1.870940	0.596583
H	0.638862	0.372423	2.136255
H	1.085564	-1.338235	2.144243
H	-0.512541	-0.539382	-1.618112
Cl	1.819252	-1.824689	-0.576855
Cl	1.016249	2.347654	0.104002
Cl	-3.035554	-0.277383	-0.270321
H	-1.460191	1.104587	0.776700

Table S31 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-4-1ax, 2eq, 4ax -

trichlorocyclohexane.

r-1, *c*-2, *t*-4-1ax, 2eq, 4ax			
E(MP2/cc-pVTZ) = -1612.6913901 a.u.			
atom	X	Y	Z
C	-0.858172	-0.612855	-0.789794
C	-0.467627	0.783638	-0.302537
C	0.336159	0.735145	0.993663
C	1.580177	-0.143694	0.835003
C	1.238934	-1.533578	0.297345
C	0.403765	-1.460003	-0.984120
H	0.630664	1.747213	1.284857
H	-1.409913	-0.528107	-1.730910
H	2.161782	-2.092293	0.114976
H	0.674518	-2.062266	1.073814
H	0.995884	-1.008220	-1.788517
H	0.114103	-2.464689	-1.306477
H	-0.288145	0.316575	1.790638
Cl	-1.966958	-1.426522	0.358215
H	2.089106	-0.229626	1.799711
H	0.148358	1.224366	-1.093430
Cl	-1.884867	1.849985	-0.126383
Cl	2.762662	0.663897	-0.257833

Table S32 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-4-1ax, 2eq, 4eq - trichlorocyclohexane.

r-1, *c*-2, *c*-4-1ax, 2eq, 4eq			
E(MP2/cc-pVTZ) = -1612.6895405 a.u.			
atom	X	Y	Z
C	-1.163835	0.821319	0.599089
C	-0.852761	-0.676842	0.621778
C	0.417793	-1.014496	-0.156307
C	1.591091	-0.223987	0.426121
C	1.329230	1.280004	0.414617
C	0.030637	1.593807	1.168119
H	0.618269	-2.087288	-0.080397
H	-2.061739	1.014990	1.193761
H	2.167469	1.802427	0.886251
H	1.259471	1.626023	-0.621089
H	0.138272	1.315257	2.225135
H	-0.181627	2.666756	1.130818
H	0.285945	-0.764978	-1.213265
Cl	-1.529565	1.393983	-1.054618
H	-0.708870	-0.940913	1.677215
Cl	-2.228896	-1.656349	0.054112
Cl	3.087997	-0.605833	-0.475787
H	1.767762	-0.551730	1.458057

Table S33 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-4-1eq, 2ax, 4ax -

trichlorocyclohexane.

r-1, *c*-2, *c*-4-1eq, 2ax, 4ax			
E(MP2/cc-pVTZ) = -1612.6835003 a.u.			
atom	X	Y	Z
C	-1.208797	-0.681802	0.331726
C	-0.532862	0.559372	0.921064
C	0.837673	0.175971	1.499022
C	1.732400	-0.675292	0.589224
C	0.960547	-1.831967	-0.048364
C	-0.337898	-1.365989	-0.715860
H	1.367456	1.077406	1.820709
H	1.601589	-2.350302	-0.767822
H	0.714263	-2.547007	0.749057
H	-0.130928	-0.674940	-1.538301
H	-0.873209	-2.228974	-1.122967
H	0.641947	-0.429458	2.395432
H	-1.355343	-1.375379	1.169946
Cl	-2.838579	-0.322949	-0.291396
Cl	2.543962	0.296068	-0.680443
H	2.547794	-1.075580	1.199143
H	-1.154126	0.951200	1.732215
Cl	-0.415137	1.884015	-0.269236

Table S34 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-4-1eq, 2ax, 4eq - trichlorocyclohexane.

r-1, *c*-2, *t*-4-1eq, 2ax, 4eq			
E(MP2/cc-pVTZ) = -1612.6899900 a.u.			
atom	X	Y	Z
C	-1.171205	-0.704955	0.424572
C	-0.640271	0.700192	0.718739
C	0.873138	0.639975	0.952990
C	1.593678	-0.000152	-0.233190
C	1.040459	-1.391635	-0.532403
C	-0.475709	-1.340482	-0.775218
H	1.256788	1.647740	1.137576
H	1.546535	-1.813411	-1.406927
H	1.258206	-2.046314	0.320755
H	-0.706572	-0.764271	-1.676671
H	-0.859825	-2.354809	-0.920435
H	1.062083	0.036090	1.849771
H	-0.955879	-1.303234	1.318810
Cl	-2.943370	-0.718407	0.235172
H	-1.139428	1.100730	1.606188
Cl	-1.007758	1.839678	-0.611628
Cl	3.346847	-0.095271	0.114891
H	1.490336	0.637824	-1.115407

Table S35 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-4-1eq, 2eq, 4ax -

trichlorocyclohexane.

r-1, *t*-2, *c*-4-1eq, 2eq, 4ax			
E(MP2/cc-pVTZ) = -1612.6903962 a.u.			
atom	X	Y	Z
C	-0.869772	-0.704009	0.420602
C	-0.495555	0.677187	-0.116707
C	0.703108	1.246081	0.648102
C	1.905634	0.304396	0.632917
C	1.520564	-1.081262	1.146435
C	0.329890	-1.654019	0.373520
H	0.974641	2.219185	0.228563
H	2.377426	-1.759029	1.080820
H	1.258256	-0.976967	2.207845
H	0.606091	-1.829524	-0.670861
H	0.032118	-2.616499	0.800785
H	0.409426	1.402645	1.694037
H	-0.268040	0.595718	-1.183671
Cl	-1.857261	1.823006	0.036988
H	-1.222361	-0.592162	1.453018
Cl	-2.218508	-1.416338	-0.507716
Cl	2.579486	0.187384	-1.028517
H	2.706044	0.727515	1.247411

Table S36 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-4-1eq, 2eq, 4eq - trichlorocyclohexane.

r-1, *t*-2, *t*-4-1eq, 2eq, 4eq			
E(MP2/cc-pVTZ) = -1612.6896384 a.u.			
atom	X	Y	Z
C	1.079412	-0.642739	-0.341298
C	0.640970	0.649706	0.347475
C	-0.816474	0.979972	0.008831
C	-1.739209	-0.178416	0.381315
C	-1.318771	-1.456147	-0.335877
C	0.133767	-1.790656	0.020506
H	-1.112265	1.890243	0.539122
H	-1.975046	-2.284658	-0.050819
H	-1.422241	-1.306434	-1.417359
H	0.220373	-1.992229	1.095308
H	0.455024	-2.695309	-0.505166
H	-0.902944	1.177273	-1.066051
H	0.762632	0.527558	1.430177
Cl	1.668320	2.027760	-0.134093
Cl	-3.430733	0.244042	-0.016569
H	-1.709002	-0.341819	1.465068
H	1.080310	-0.479695	-1.425211
Cl	2.746237	-1.087404	0.118262

Table S37 Optimized cartesian coordinates and total energies of *r*-1, *c*-3, *c*-5-1ax, 3ax, 5ax -

trichlorocyclohexane.

r-1, *c*-3, *c*-5-1ax, 3ax, 5ax			
E(MP2/cc-pVTZ) = -1612.6755200 a.u.			
atom	X	Y	Z
C	0.646300	1.351845	0.776641
C	-0.827880	1.206887	1.164868
C	-1.493923	-0.116196	0.776565
C	-0.631315	-1.320387	1.164859
C	0.847550	-1.235662	0.776632
C	1.459085	0.113480	1.164937
H	-2.433618	-0.189285	1.332276
H	-0.861387	1.255679	2.263138
H	-1.406606	2.050619	0.778209
H	1.052828	2.202170	1.332396
H	-0.656874	-1.373781	2.263128
H	-1.072624	-2.243452	0.778193
H	1.380666	-2.012908	1.332382
H	1.518043	0.118062	2.263210
H	2.479159	0.192820	0.778328
Cl	0.861051	1.800906	-0.942479
Cl	-1.990115	-0.154782	-0.942577
Cl	1.129153	-1.646108	-0.942490

Table S38 Optimized cartesian coordinates and total energies of *r*-1, *c*-3, *t*-5-1ax, 3ax, 5eq - trichlorocyclohexane.

r-1, *c*-3, *t*-5-1ax, 3ax, 5eq			
E(MP2/cc-pVTZ) = -1612.6866329 a.u.			
atom	X	Y	Z
C	1.036575	-0.232649	1.297221
C	1.837367	-0.388908	0.000000
C	1.036575	-0.232649	-1.297221
C	0.105337	0.981374	-1.253290
C	-0.764245	0.971099	0.000000
C	0.105337	0.981374	1.253290
H	1.744556	-0.106925	-2.121714
H	2.581922	0.419932	0.000000
H	2.380652	-1.338372	0.000000
H	1.744556	-0.106925	2.121714
H	0.723109	1.889173	-1.238574
H	-0.514096	1.007844	-2.154321
H	0.723109	1.889173	1.238574
H	-0.514096	1.007844	2.154321
Cl	0.105337	-1.709448	1.709864
Cl	0.105337	-1.709448	-1.709864
Cl	-1.833861	2.405129	0.000000
H	-1.417212	0.094441	0.000000

Table S39 Optimized cartesian coordinates and total energies of *r*-1, *c*-3, *t*-5-1eq, 3eq, 5ax -

trichlorocyclohexane.

r-1, *c*-3, *t*-5-1eq, 3eq, 5ax			
E(MP2/cc-pVTZ) = -1612.6921889 a.u.			
atom	X	Y	Z
C	0.122560	-0.465624	1.252551
C	0.811122	-1.008100	0.000000
C	0.122560	-0.465624	-1.252551
C	0.122560	1.061259	-1.267179
C	-0.520078	1.628237	0.000000
C	0.122560	1.061259	1.267179
H	1.861798	-0.694208	0.000000
H	0.786125	-2.102304	0.000000
H	1.161773	1.411972	-1.306727
H	-0.396920	1.436526	-2.153788
H	1.161773	1.411972	1.306727
H	-0.396920	1.436526	2.153788
H	-0.905592	-0.836413	-1.301985
Cl	0.948923	-1.083144	-2.713898
Cl	-2.287692	1.294860	0.000000
H	-0.426768	2.718198	0.000000
H	-0.905592	-0.836413	1.301985
Cl	0.948923	-1.083144	2.713898

Table S40 Optimized cartesian coordinates and total energies of *r*-1, *c*-3, *c*-5-1eq, 3eq, 5eq - trichlorocyclohexane.

r-1, *c*-3, *c*-5-1eq, 3eq, 5eq			
E(MP2/cc-pVTZ) = -1612.6906529 a.u.			
atom	X	Y	Z
C	-1.260857	-0.699672	0.409059
C	-1.251102	0.750945	-0.072073
C	0.024493	1.441769	0.409061
C	1.275888	0.708014	-0.072069
C	1.236363	-0.742099	0.409061
C	-0.024787	-1.458959	-0.072070
H	-1.284083	0.770741	-1.167417
H	-2.132444	1.279947	0.303074
H	1.309526	0.726677	-1.167413
H	2.174690	1.206773	0.303080
H	-0.025440	-1.497424	-1.167414
H	-0.042249	-2.486722	0.303081
H	0.025235	1.485492	1.504893
Cl	0.053299	3.137226	-0.156618
H	-1.299093	-0.720886	1.504892
Cl	-2.743569	-1.522455	-0.156618
Cl	2.690271	-1.614770	-0.156615
H	1.273853	-0.764600	1.504893

Table S41 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, t-4-1ax, 2ax,

3ax, 4ax-tetrachlorocyclohexane.

r-1, *t*-2, *c*-3, t-4-1ax, 2ax, 3ax, 4ax			
E(MP2/cc-pVTZ) = -2071.7994369 a.u.			
atom	X	Y	Z
C	1.001844	1.118797	0.471101
C	0.324332	0.700179	-0.845617
C	-0.324245	-0.699864	-0.845906
C	-1.001889	-1.118967	0.470592
C	-0.176283	-0.743742	1.698118
C	0.176108	0.743132	1.698405
H	-1.050683	-0.743587	-1.660307
H	1.050855	0.744196	-1.659927
H	1.158486	2.199171	0.435366
H	-1.158517	-2.199329	0.434447
H	-0.743968	-0.998785	2.597112
H	0.739530	-1.343988	1.694644
H	-0.739704	1.343381	1.695053
H	0.743700	0.997849	2.597550
Cl	2.643879	0.405713	0.585524
Cl	0.917487	-1.935676	-1.233092
Cl	-2.643946	-0.405946	0.585106
Cl	-0.917355	1.936138	-1.232485

Table S42 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *c*-4-1ax, 2ax, 3ax, 4eq-tetrachlorocyclohexane.

r-1, *t*-2, *c*-3, *c*-4-1ax, 2ax, 3ax, 4eq			
E(MP2/cc-pVTZ) = -2071.8011986 a.u.			
atom	X	Y	Z
C	1.678530	0.018113	0.511309
C	0.946331	0.637003	-0.693185
C	-0.551495	0.292554	-0.814593
C	-1.250515	0.435299	0.540837
C	-0.568579	-0.389872	1.625492
C	0.867163	0.115800	1.803003
H	-1.001831	0.983744	-1.532045
H	1.456015	0.363966	-1.620794
H	2.628286	0.546567	0.625542
H	-1.116940	-0.270802	2.564678
H	-0.583163	-1.450150	1.356237
H	0.844786	1.167941	2.111700
H	1.379162	-0.448522	2.587840
Cl	2.123757	-1.684706	0.182353
Cl	-0.758100	-1.335817	-1.510414
Cl	1.084019	2.424127	-0.545476
Cl	-2.987631	0.064592	0.418073
H	-1.189685	1.494545	0.812570

Table S43 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-3, *t*-4-1ax, 2ax, 3eq,

4ax-tetrachlorocyclohexane.

r-1, *t*-2, *t*-3, *t*-4-1ax, 2ax, 3eq, 4ax			
E(MP2/cc-pVTZ) = -2071.8009607 a.u.			
atom	X	Y	Z
C	-1.648588	-0.082230	0.633275
C	-0.425506	-0.966333	0.340031
C	0.357479	-0.428596	-0.863948
C	0.692450	1.066858	-0.835817
C	-0.576722	1.877068	-0.550909
C	-1.286510	1.398806	0.716743
H	-0.762278	-1.978455	0.099210
H	-2.108263	-0.421617	1.565020
H	-0.307935	2.933339	-0.459790
H	-1.248627	1.777282	-1.411047
H	-0.634993	1.539980	1.585712
H	-2.198744	1.980309	0.879822
Cl	-2.879576	-0.357488	-0.648296
Cl	0.531060	-1.112402	1.837195
H	-0.324504	-0.543553	-1.714930
Cl	1.769627	-1.437712	-1.236351
Cl	1.980330	1.506850	0.320497
H	1.085242	1.332072	-1.822012

Table S44 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *c*-4-1ax, 2eq, 3ax, 4eq-tetrachlorocyclohexane.

r-1, *c*-2, *c*-3, *c*-4-1ax, 2eq, 3ax, 4eq			
E(MP2/cc-pVTZ) = -2071.7965581 a.u.			
atom	X	Y	Z
C	1.289711	1.063789	-0.545563
C	0.835908	-0.341610	-0.962629
C	-0.494914	-0.823889	-0.361821
C	-1.556043	0.249676	-0.643994
C	-1.155635	1.609564	-0.083192
C	0.144882	2.060433	-0.756958
H	2.135095	1.335060	-1.184936
H	-1.947986	2.333589	-0.294804
H	-1.034190	1.544942	1.002000
H	-0.024179	2.158676	-1.838138
H	0.453144	3.041287	-0.383253
Cl	1.903763	1.174131	1.124623
H	0.646500	-0.261560	-2.041737
Cl	2.121965	-1.552597	-0.791394
Cl	-3.167579	-0.254842	-0.081373
H	-1.634943	0.328886	-1.735941
Cl	-0.399340	-1.227816	1.364319
H	-0.776632	-1.749560	-0.873225

Table S45 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *t*-4-1ax, 2eq, 3eq,

4ax-tetrachlorocyclohexane.

r-1, *c*-2, *t*-3, *t*-4-1ax, 2eq, 3eq, 4ax			
E(MP2/cc-pVTZ) = -2071.8041579 a.u.			
atom	X	Y	Z
C	1.289711	1.063789	-0.545563
C	0.835908	-0.341610	-0.962629
C	-0.494914	-0.823889	-0.361821
C	-1.556043	0.249676	-0.643994
C	-1.155635	1.609564	-0.083192
C	0.144882	2.060433	-0.756958
H	2.135095	1.335060	-1.184936
H	-1.947986	2.333589	-0.294804
H	-1.034190	1.544942	1.002000
H	-0.024179	2.158676	-1.838138
H	0.453144	3.041287	-0.383253
Cl	1.903763	1.174131	1.124623
H	0.646500	-0.261560	-2.041737
Cl	2.121965	-1.552597	-0.791394
Cl	-3.167579	-0.254842	-0.081373
H	-1.634943	0.328886	-1.735941
Cl	-0.399340	-1.227816	1.364319
H	-0.776632	-1.749560	-0.873225

Table S46 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *c*-4-1ax, 2eq, 3eq, 4eq-tetrachlorocyclohexane.

r-1, *c*-2, *t*-3, *c*-4-1ax, 2eq, 3eq, 4eq			
E(MP2/cc-pVTZ) = -2071.8028550 a.u.			
atom	X	Y	Z
C	1.528799	-0.840337	0.608231
C	0.871708	0.542948	0.610934
C	-0.469431	0.555780	-0.135797
C	-1.399525	-0.528015	0.429384
C	-0.747082	-1.909812	0.462372
C	0.578889	-1.867000	1.222179
H	2.459013	-0.782984	1.181265
H	-1.437650	-2.606826	0.946633
H	-0.586994	-2.261394	-0.560683
H	0.404971	-1.586036	2.269455
H	1.054400	-2.852480	1.217129
Cl	1.990658	-1.346686	-1.043712
H	-0.303810	0.389340	-1.204398
Cl	-1.238617	2.154154	0.043423
H	0.680886	0.801240	1.660226
Cl	1.992109	1.774105	-0.014020
Cl	-2.906640	-0.616448	-0.523200
H	-1.688642	-0.229368	1.444215

Table S47 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *t*-4-1eq, 2ax, 3ax,

4eq-tetrachlorocyclohexane.

r-1, *c*-2, *t*-3, *t*-4-1eq, 2ax, 3ax, 4eq			
E(MP2/cc-pVTZ) = -2071.8056612 a.u.			
atom	X	Y	Z
C	-1.330253	0.609705	0.422414
C	-0.769302	-0.025509	-0.853961
C	0.769307	0.025511	-0.853957
C	1.330251	-0.609706	0.422420
C	0.767616	0.037895	1.683488
C	-0.767625	-0.037900	1.683483
H	1.162105	-0.484428	2.560394
H	1.101089	1.079262	1.739175
H	-1.101099	-1.079268	1.739165
H	-1.162120	0.484420	2.560389
Cl	-3.111645	0.592187	0.421022
H	-1.038144	1.663973	0.398414
Cl	-1.278629	-1.729005	-1.037406
H	-1.146490	0.507093	-1.731356
H	1.038142	-1.663975	0.398415
Cl	3.111643	-0.592188	0.421038
Cl	1.278635	1.729008	-1.037394
H	1.146499	-0.507087	-1.731352

Table S48 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *t*-4-1eq, 2ax, 3eq, 4eq-tetrachlorocyclohexane.

r-1, *c*-2, *c*-3, *t*-4-1eq, 2ax, 3eq, 4eq			
E(MP2/cc-pVTZ) = -2071.8029258 a.u.			
atom	X	Y	Z
C	1.517987	-0.607194	-0.572145
C	0.720207	0.687635	-0.384705
C	-0.771158	0.384702	-0.602110
C	-1.268283	-0.679254	0.379201
C	-0.416199	-1.947701	0.260237
C	1.084693	-1.676122	0.423562
H	-0.751982	-2.669364	1.011519
H	-0.604648	-2.395165	-0.723473
H	1.318696	-1.346185	1.439711
H	1.642676	-2.597935	0.233822
Cl	3.271924	-0.308502	-0.501551
H	1.310699	-0.958603	-1.590688
Cl	-1.725695	1.882402	-0.536063
H	-0.880403	-0.007807	-1.620894
Cl	1.009728	1.399915	1.222985
H	1.041605	1.432411	-1.118917
H	-1.233336	-0.276669	1.395328
Cl	-2.970473	-1.100467	0.046943

Table S49 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-3, *c*-4-1eq, 2eq, 3ax,

4ax-tetrachlorocyclohexane.

r-1, *t*-2, *t*-3, *c*-4-1eq, 2eq, 3ax, 4ax			
E(MP2/cc-pVTZ) = -2071.8058533 a.u.			
atom	X	Y	Z
C	-0.994265	-0.625743	0.605842
C	-0.530959	0.237656	-0.568193
C	0.792000	0.949509	-0.253065
C	1.885347	-0.043242	0.162282
C	1.426436	-0.940826	1.308748
C	0.097280	-1.630385	0.989518
H	2.196535	-1.691484	1.510046
H	1.323880	-0.319849	2.204937
H	0.227573	-2.337839	0.164302
H	-0.243232	-2.201326	1.858794
H	-0.354286	-0.414640	-1.429426
Cl	-1.756538	1.422218	-1.075774
Cl	0.606637	2.139886	1.069199
H	1.112969	1.510876	-1.135058
H	2.780876	0.517661	0.443166
Cl	2.342972	-1.025732	-1.267854
Cl	-2.478567	-1.522541	0.183821
H	-1.245924	0.019651	1.452779

Table S50 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *t*-4-1eq, 2eq, 3eq, 4eq-tetrachlorocyclohexane.

r-1, *t*-2, *c*-3, *t*-4-1eq, 2eq, 3eq, 4eq			
E(MP2/cc-pVTZ) = -2071.8023087 a.u.			
atom	X	Y	Z
C	-0.252467	1.454629	-0.783310
C	0.190272	0.746234	0.501460
C	-0.190272	-0.746234	0.501460
C	0.252467	-1.454629	-0.783310
C	-0.252467	-0.720799	-2.021351
C	0.252467	0.720799	-2.021351
H	0.094207	-1.247136	-2.915910
H	-1.348984	-0.741957	-2.031828
H	1.348984	0.741957	-2.031828
H	-0.094207	1.247136	-2.915910
H	1.277510	0.840405	0.603943
Cl	-0.544518	1.538845	1.919268
Cl	0.345756	3.135747	-0.803835
H	-1.347158	1.506682	-0.799354
H	1.347158	-1.506682	-0.799354
Cl	-0.345756	-3.135747	-0.803835
Cl	0.544518	-1.538845	1.919268
H	-1.277510	-0.840405	0.603943

Table S51 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *c*-5-1ax, 2ax,

3ax, 5ax-tetrachlorocyclohexane.

r-1, *t*-2, *c*-3, *c*-5-1ax, 2ax, 3ax, 5ax			
E(MP2/cc-pVTZ) = -2071.7945633 a.u.			
atom	X	Y	Z
C	-0.595462	-1.300844	0.148053
C	-1.350266	0.000000	0.462370
C	-0.595462	1.300844	0.148053
C	0.076503	1.269141	-1.226129
C	0.867886	0.000000	-1.552459
C	0.076503	-1.269142	-1.226129
H	-1.330033	2.110141	0.149958
H	-1.676426	0.000000	1.505578
H	-1.330033	-2.110141	0.149958
H	-0.726821	1.337242	-1.970620
H	0.713826	2.150021	-1.341707
H	1.060729	0.000000	-2.629267
H	-0.726821	-1.337242	-1.970620
H	0.713826	-2.150021	-1.341706
Cl	0.539802	-1.709708	1.466664
Cl	-2.845757	0.000000	-0.541036
Cl	0.539802	1.709709	1.466664
Cl	2.496951	0.000000	-0.808418

Table S52 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *t*-5-1ax, 2ax, 3ax, 5eq-tetrachlorocyclohexane.

r-1, *t*-2, *c*-3, *t*-5-1ax, 2ax, 3ax, 5eq			
E(MP2/cc-pVTZ) = -2071.8044259 a.u.			
atom	X	Y	Z
C	-0.668210	0.119067	-1.301068
C	-1.390433	0.507858	-0.000004
C	-0.668209	0.119089	1.301066
C	0.830198	0.422781	1.254570
C	1.475994	-0.156869	0.000001
C	0.830197	0.422760	-1.254578
H	-1.129266	0.679799	2.117916
H	-2.405943	0.103036	0.000000
H	-1.129267	0.679764	-2.117927
H	0.969294	1.509812	1.252701
H	1.306348	0.019901	2.152720
H	0.969293	1.509791	-1.252727
H	1.306347	0.019865	-2.152721
Cl	-0.946633	-1.606358	-1.694039
Cl	-1.550744	2.298408	-0.000019
Cl	-0.946632	-1.606330	1.694066
Cl	3.224282	0.215268	-0.000003
H	1.391346	-1.246857	0.000010

Table S53 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *c*-5-1ax, 2eq,

3ax, 5ax-tetrachlorocyclohexane.

r-1, *c*-2, *c*-3, *c*-5-1ax, 2eq, 3ax, 5ax			
E(MP2/cc-pVTZ) = -2071.7891329 a.u.			
atom	X	Y	Z
C	0.418508	-1.299323	0.564162
C	1.170007	0.000000	0.870777
C	0.418508	1.299323	0.564162
C	-0.955462	1.268938	1.246004
C	-1.783920	0.000000	1.022673
C	-0.955462	-1.268938	1.246004
H	0.996024	-2.115541	1.008870
H	-0.770012	1.333652	2.327862
H	-1.529856	2.153429	0.956526
H	-0.770012	-1.333652	2.327862
H	-1.529856	-2.153429	0.956526
Cl	0.315440	-1.698070	-1.167465
H	1.281479	0.000000	1.964032
Cl	2.820280	0.000000	0.220278
H	0.996024	2.115541	1.008870
Cl	0.315440	1.698070	-1.167465
Cl	-2.625033	0.000000	-0.555619
H	-2.591009	0.000000	1.761366

Table S54 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *t*-5-1ax, 2eq, 3ax, 5eq-tetrachlorocyclohexane.

r-1, *c*-2, *c*-3, *t*-5-1ax, 2eq, 3ax, 5eq			
E(MP2/cc-pVTZ) = -2071.8000125 a.u.			
atom	X	Y	Z
C	-0.479161	0.364563	1.299572
C	-1.070744	0.923877	0.000000
C	-0.479161	0.364563	-1.299572
C	-0.479161	-1.167770	-1.254668
C	0.215318	-1.689747	0.000000
C	-0.479161	-1.167770	1.254668
H	-1.117581	0.700360	2.122119
H	-1.519279	-1.519364	-1.251187
H	0.004965	-1.556009	-2.155144
H	-1.519279	-1.519364	1.251187
H	0.004965	-1.556009	2.155144
Cl	1.153213	0.972940	1.684482
H	-2.112007	0.573463	0.000000
Cl	-1.155342	2.696242	0.000000
Cl	0.186608	-3.477217	0.000000
H	1.267442	-1.393130	0.000000
H	-1.117581	0.700360	-2.122119
Cl	1.153213	0.972940	-1.684482

Table S55 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *c*-5-1ax, 2eq,

3eq, 5ax-tetrachlorocyclohexane.

r-1, *c*-2, *t*-3, *c*-5-1ax, 2eq, 3eq, 5ax			
E(MP2/cc-pVTZ) = -2071.7992042 a.u.			
atom	X	Y	Z
C	0.263281	1.253050	0.800798
C	-0.980388	0.370432	0.619462
C	-0.658157	-0.880175	-0.199494
C	0.417914	-1.691410	0.526837
C	1.701033	-0.898615	0.770027
C	1.410920	0.453480	1.427605
H	-0.000800	2.071855	1.476798
H	0.012780	-1.997034	1.500617
H	0.640846	-2.599520	-0.039967
H	1.118193	0.238673	2.465077
H	2.314786	1.068593	1.459229
Cl	0.750785	2.036518	-0.727510
H	-0.331269	-0.593231	-1.202716
Cl	-2.097885	-1.916381	-0.389021
Cl	2.637927	-0.750905	-0.749913
H	2.344876	-1.472618	1.442786
H	-1.291007	0.044687	1.620736
Cl	-2.334122	1.313004	-0.039083

Table S56 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *t*-5-1ax, 2eq, 3eq, 5eq-tetrachlorocyclohexane.

r-1, *c*-2, *t*-3, *t*-5-1ax, 2eq, 3eq, 5eq			
E(MP2/cc-pVTZ) = -2071.8055229 a.u.			
atom	X	Y	Z
C	0.151991	-1.356456	0.619142
C	1.033048	-0.100660	0.634541
C	0.569793	0.915552	-0.410583
C	-0.908494	1.261711	-0.194397
C	-1.790036	0.014533	-0.198002
C	-1.315394	-0.989519	0.848317
H	0.496438	-2.032267	1.407382
H	-1.015613	1.772329	0.769967
H	-1.232609	1.956854	-0.974856
H	-1.412748	-0.539008	1.844243
H	-1.928562	-1.894985	0.822749
Cl	0.319076	-2.260366	-0.917592
H	0.735839	0.506483	-1.411539
Cl	1.521428	2.420734	-0.301944
H	0.923052	0.354243	1.626942
Cl	2.748625	-0.529681	0.459413
Cl	-3.484778	0.478405	0.131247
H	-1.785225	-0.449186	-1.188102

Table S57 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *t*-5-1eq, 2ax, 3ax,

5ax-tetrachlorocyclohexane.

r-1, *c*-2, *t*-3, *t*-5-1eq, 2ax, 3ax, 5ax			
E(MP2/cc-pVTZ) = -2071.8038244 a.u.			
atom	X	Y	Z
C	0.734085	-0.690730	-0.473427
C	0.900409	0.817051	-0.282651
C	-0.441453	1.464633	0.090874
C	-1.123357	0.756425	1.265325
C	-1.147334	-0.774544	1.197180
C	0.204828	-1.364787	0.786614
H	-0.255725	2.505318	0.369093
H	1.287178	1.271817	-1.198521
H	-0.554235	1.022361	2.164633
H	-2.138708	1.143463	1.387875
H	-1.412608	-1.153907	2.188177
H	0.920367	-1.217102	1.602583
H	0.098679	-2.439253	0.616230
Cl	2.077137	1.196521	1.011029
Cl	-1.469582	1.540676	-1.374000
Cl	-2.438993	-1.384565	0.109048
H	0.021181	-0.829717	-1.291718
Cl	2.259132	-1.443882	-1.001480

Table S58 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *t*-5-1eq, 2ax, 3ax, 5eq-tetrachlorocyclohexane.

r-1, *c*-2, *t*-3, *t*-5-1eq, 2ax, 3ax, 5eq			
E(MP2/cc-pVTZ) = -2071.8080431 a.u.			
atom	X	Y	Z
C	0.898183	-0.413766	-0.779870
C	1.154211	0.647493	0.293158
C	-0.097527	1.512873	0.504733
C	-1.347165	0.674329	0.777437
C	-1.549129	-0.393089	-0.296059
C	-0.314388	-1.282437	-0.451824
H	0.083640	2.195169	1.339433
H	1.996745	1.279901	-0.000675
H	-1.232186	0.185619	1.750491
H	-2.220405	1.330950	0.826905
H	-0.136878	-1.842270	0.471380
H	-0.475506	-2.000801	-1.261034
Cl	1.584516	-0.085308	1.864199
Cl	-0.334544	2.551509	-0.941200
Cl	-2.971614	-1.395045	0.113468
H	-1.779524	0.084488	-1.253521
Cl	2.344138	-1.414157	-1.062547
H	0.716568	0.125534	-1.715071

Table S59 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *t*-5-1eq, 2ax,

3eq, 5ax-tetrachlorocyclohexane.

r-1, *c*-2, *c*-3, *t*-5-1eq, 2ax, 3eq, 5ax			
E(MP2/cc-pVTZ) = -2071.8070496 a.u.			
atom	X	Y	Z
C	-1.239136	-0.043274	-0.432841
C	0.000001	-0.946693	-0.463145
C	1.239136	-0.043272	-0.432841
C	1.274132	0.827271	0.820175
C	-0.000001	1.667638	0.938670
C	-1.274134	0.827269	0.820175
H	0.000001	-1.544523	-1.379596
H	1.356672	0.185648	1.703845
H	2.147650	1.483959	0.790385
H	-1.356673	0.185646	1.703845
H	-2.147652	1.483956	0.790385
Cl	0.000002	-2.100045	0.895705
H	1.185709	0.597043	-1.319797
Cl	2.741179	-0.985245	-0.593993
Cl	-0.000002	2.957813	-0.317594
H	-0.000002	2.193922	1.897463
H	-1.185710	0.597042	-1.319797
Cl	-2.741178	-0.985249	-0.593993

Table S60 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *c*-5-1eq, 2ax, 3eq, 5eq-tetrachlorocyclohexane.

r-1, *c*-2, *c*-3, *c*-5-1eq, 2ax, 3eq, 5eq			
E(MP2/cc-pVTZ) = -2071.8044316 a.u.			
atom	X	Y	Z
C	0.801517	0.150446	1.237638
C	0.673234	1.047703	0.000000
C	0.801517	0.150446	-1.237638
C	-0.274056	-0.933906	-1.271769
C	-0.181925	-1.778911	0.000000
C	-0.274056	-0.933906	1.271769
H	1.473073	1.794433	0.000000
H	-1.264063	-0.475521	-1.348307
H	-0.122580	-1.570106	-2.148523
H	-1.264063	-0.475521	1.348307
H	-0.122580	-1.570106	2.148523
Cl	-0.864864	1.941865	0.000000
Cl	-1.463360	-3.023926	0.000000
H	0.769579	-2.324931	0.000000
H	1.790749	-0.321250	-1.180123
Cl	0.801517	1.101414	-2.742376
Cl	0.801517	1.101414	2.742376
H	1.790749	-0.321250	1.180123

Table S61 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *t*-5-1eq, 2eq, 3eq,

5ax-tetrachlorocyclohexane.

r-1, *t*-2, *c*-3, *t*-5-1eq, 2eq, 3eq, 5ax			
E(MP2/cc-pVTZ) = -2071.8058878 a.u.			
atom	X	Y	Z
C	0.001653	0.070428	1.265200
C	-0.370007	0.854812	0.000000
C	0.001653	0.070428	-1.265200
C	-0.590071	-1.338907	-1.254131
C	-0.195204	-2.111160	0.000000
C	-0.590071	-1.338907	1.254131
H	-1.684770	-1.266177	-1.277435
H	-0.269468	-1.874220	-2.152448
H	-1.684770	-1.266177	1.277435
H	-0.269468	-1.874220	2.152448
H	1.091503	0.025946	-1.347121
Cl	-0.590071	0.918781	-2.720458
Cl	1.568926	-2.447631	0.000000
H	-0.686411	-3.088634	0.000000
H	-1.449090	1.049788	0.000000
Cl	0.453172	2.435220	0.000000
H	1.091503	0.025946	1.347121
Cl	-0.590071	0.918781	2.720458

Table S62 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *c*-5-1eq, 2eq, 3eq, 5eq-tetrachlorocyclohexane.

r-1, *t*-2, *c*-3, *c*-5-1eq, 2eq, 3eq, 5eq			
E(MP2/cc-pVTZ) = -2071.8042903 a.u.			
atom	X	Y	Z
C	0.302142	1.261117	0.299433
C	1.032558	0.000000	-0.180239
C	0.302143	-1.261117	0.299433
C	-1.176946	-1.251184	-0.090087
C	-1.856392	0.000000	0.453797
C	-1.176947	1.251184	-0.090087
H	-1.270525	-1.268357	-1.182021
H	-1.657297	-2.152375	0.302386
H	-1.270525	1.268356	-1.182021
H	-1.657297	2.152375	0.302386
H	0.404638	-1.329058	1.388940
Cl	1.063604	-2.725028	-0.379060
H	1.076899	0.000000	-1.275425
Cl	2.708836	0.000000	0.423023
Cl	-3.587489	0.000000	0.014728
H	-1.815299	0.000000	1.549586
Cl	1.063603	2.725028	-0.379060
H	0.404637	1.329058	1.388940

Table S63 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-4, *c*-5-1ax, 2ax, 4ax,

5ax-tetrachlorocyclohexane.

r-1, *t*-2, *t*-4, *c*-5-1ax, 2ax, 4ax, 5ax			
E(MP2/cc-pVTZ) = -2071.7993462 a.u.			
atom	X	Y	Z
C	-0.000004	-0.767316	1.297418
C	-0.000004	0.767313	1.297429
C	0.557820	1.355800	0.000000
C	-0.000004	0.767313	-1.297429
C	-0.000004	-0.767316	-1.297418
C	-0.557872	-1.355779	0.000000
H	0.422584	2.441065	0.000000
H	0.614125	1.117023	2.130874
H	-0.614096	-1.117045	2.130883
H	0.614125	1.117023	-2.130874
H	-0.614096	-1.117045	-2.130883
H	-1.635527	-1.149873	0.000000
H	-0.422673	-2.441048	0.000000
H	1.635483	1.149936	0.000000
Cl	1.660181	-1.336245	1.665276
Cl	-1.660166	1.336242	1.665392
Cl	-1.660166	1.336242	-1.665392
Cl	1.660181	-1.336245	-1.665276

Table S64 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-4, *c*-5-1ax, 2ax, 4ax, 5eq-tetrachlorocyclohexane.

r-1, *t*-2, *t*-4, *c*-5-1ax, 2ax, 4ax, 5eq			
E(MP2/cc-pVTZ) = -2071.8032098 a.u.			
atom	X	Y	Z
C	-1.392089	-0.671398	-0.586318
C	-1.583046	0.541584	0.332406
C	-0.525348	0.613227	1.438909
C	0.925614	0.374361	0.995037
C	1.001408	-0.889391	0.135737
C	0.053986	-0.827181	-1.057693
H	-0.597193	1.574435	1.955542
H	-2.569994	0.480217	0.798375
H	-2.062578	-0.584534	-1.445038
H	1.540831	0.232231	1.888710
H	0.314767	0.025234	-1.693585
H	0.143593	-1.742263	-1.649346
H	-0.771486	-0.173420	2.163377
Cl	-1.920899	-2.142255	0.303755
Cl	-1.630502	2.012896	-0.686946
Cl	1.618070	1.794491	0.162814
Cl	2.663572	-1.249728	-0.388421
H	0.704799	-1.721003	0.783064

Table S65 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-4, *t*-5-1ax, 2ax, 4eq,

5eq-tetrachlorocyclohexane.

r-1, *t*-2, *c*-4, *t*-5-1ax, 2ax, 4eq, 5eq			
E(MP2/cc-pVTZ) = -2071.8091573 a.u.			
atom	X	Y	Z
C	0.665017	0.379666	-1.630542
C	-0.665017	-0.379666	-1.630542
C	-0.855772	-1.195165	-0.354417
C	-0.679197	-0.349862	0.910381
C	0.679197	0.349862	0.910381
C	0.855772	1.195165	-0.354417
H	-1.852687	-1.644793	-0.352347
H	-0.714214	-1.034826	-2.504707
H	0.714214	1.034826	-2.504707
H	0.120677	2.006797	-0.346698
H	1.852687	1.644793	-0.352347
H	-0.120677	-2.006797	-0.346698
Cl	1.993579	-0.811556	-1.820108
Cl	-1.993579	0.811556	-1.820108
Cl	0.855772	1.417179	2.330020
H	1.468426	-0.404709	0.982716
H	-1.468426	0.404709	0.982716
Cl	-0.855772	-1.417179	2.330020

Table S66 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-4, *t*-5-1ax, 2eq, 4ax, 5eq-tetrachlorocyclohexane.

r-1, *c*-2, *t*-4, *t*-5-1ax, 2eq, 4ax, 5eq			
E(MP2/cc-pVTZ) = -2071.8073740 a.u.			
atom	X	Y	Z
C	1.013988	-0.736682	0.799953
C	1.259033	0.683415	0.286046
C	0.488785	0.967151	-1.001363
C	-1.013988	0.736682	-0.799953
C	-1.259033	-0.683415	-0.286046
C	-0.488785	-0.967151	1.001363
H	0.656897	2.001353	-1.313679
H	1.542342	-0.877096	1.747596
H	-0.849480	-0.305737	1.796770
H	-0.656897	-2.001353	1.313679
H	0.849480	0.305737	-1.796770
Cl	1.673006	-1.970169	-0.319443
H	-1.542342	0.877096	-1.747596
Cl	-1.673006	1.970169	0.319443
Cl	2.992931	1.026918	0.072870
H	0.908185	1.360224	1.071928
H	-0.908185	-1.360224	-1.071928
Cl	-2.992931	-1.026918	-0.072870

Table S67 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-4, *c*-5-1ax, 2eq,

4eq, 5ax-tetrachlorocyclohexane.

r-1, *c*-2, *c*-4, *c*-5-1ax, 2eq, 4eq, 5ax			
E(MP2/cc-pVTZ) = -2071.7986391 a.u.			
atom	X	Y	Z
C	0.619753	-0.821164	1.302877
C	-0.870607	-0.477025	1.234166
C	-1.216204	0.353511	0.000000
C	-0.870607	-0.477025	-1.234166
C	0.619753	-0.821164	-1.302877
C	1.049849	-1.513392	0.000000
H	-2.287282	0.573620	0.000000
H	0.783664	-1.516773	2.131513
H	0.585476	-2.509552	0.000000
H	2.134183	-1.656766	0.000000
H	-0.664615	1.297995	0.000000
Cl	1.618536	0.607810	1.675549
Cl	-1.457466	0.296228	2.725182
H	-1.401544	-1.435739	1.168277
Cl	-1.457466	0.296228	-2.725182
H	-1.401544	-1.435739	-1.168277
H	0.783664	-1.516773	-2.131513
Cl	1.618536	0.607810	-1.675549

Table S68 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-4, *t*-5-1ax, 2eq, 4eq, 5eq-tetrachlorocyclohexane.

r-1, *c*-2, *c*-4, *t*-5-1ax, 2eq, 4eq, 5eq			
E(MP2/cc-pVTZ) = -2071.8060877 a.u.			
atom	X	Y	Z
C	-1.235892	-1.068389	-0.408189
C	-1.414892	0.412341	-0.742796
C	-0.428310	1.286395	0.025625
C	1.012342	0.860173	-0.278709
C	1.230515	-0.623158	0.019454
C	0.202684	-1.479816	-0.726139
H	-0.557352	2.332078	-0.267717
H	-1.934007	-1.666830	-1.001173
H	0.365798	-1.371657	-1.806022
H	0.351582	-2.532864	-0.470938
H	-0.622136	1.210858	1.099517
Cl	-1.609137	-1.413108	1.305460
Cl	-3.087800	0.963672	-0.486254
H	-1.223482	0.507458	-1.819094
H	1.157022	-0.787029	1.098315
Cl	2.864849	-1.142479	-0.475264
Cl	2.127535	1.882703	0.665934
H	1.241291	1.039331	-1.336258

Table S69 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-4, *c*-5-1eq, 2eq, 4eq,

5eq-tetrachlorocyclohexane.

r-1, *t*-2, *t*-4, *c*-5-1eq, 2eq, 4eq, 5eq			
E(MP2/cc-pVTZ) = -2071.8056158 a.u.			
atom	X	Y	Z
C	-0.604985	0.465306	1.268979
C	0.604985	-0.465306	1.268979
C	0.610323	-1.320212	0.000000
C	0.604985	-0.465306	-1.268979
C	-0.604985	0.465306	-1.268979
C	-0.610323	1.320212	0.000000
H	1.493487	-1.965475	0.000000
H	0.271298	1.971949	0.000000
H	-1.493487	1.965475	0.000000
H	-0.271298	-1.971949	0.000000
Cl	0.604985	-1.543427	2.688720
H	1.515815	0.141740	1.328461
H	-1.515815	-0.141740	-1.328461
Cl	-0.604985	1.543427	-2.688720
Cl	0.604985	-1.543427	-2.688720
H	1.515815	0.141740	-1.328461
H	-1.515815	-0.141740	1.328461
Cl	-0.604985	1.543427	2.688720

Table S70 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *t*-4, c-5-1ax, 2ax, 3ax, 4ax, 5ax-pentachlorocyclohexane.

r-1, *t*-2, *c*-3, *t*-4, c-5-1ax, 2ax, 3ax, 4ax, 5ax			
E(MP2/cc-pVTZ) = -2530.9064277 a.u.			
atom	X	Y	Z
C	-0.267852	-0.950181	1.294586
C	-0.267852	0.586512	1.304673
C	0.198759	1.260220	0.000000
C	-0.267852	0.586512	-1.304673
C	-0.267852	-0.950181	-1.294586
C	-0.839684	-1.525521	0.000000
H	-0.171961	2.287666	0.000000
H	0.363714	0.943789	2.121042
H	-0.902075	-1.278683	2.121108
H	0.363714	0.943789	-2.121042
H	-0.902075	-1.278683	-2.121108
H	-1.913130	-1.299453	0.000000
H	-0.723143	-2.612615	0.000000
Cl	1.357513	-1.585363	1.685430
Cl	-1.932744	1.128619	1.701185
Cl	-1.932744	1.128619	-1.701185
Cl	1.357513	-1.585363	-1.685430
Cl	1.983342	1.398784	0.000000

Table S71 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *t*-4, *t*-5-1ax, 2ax,

3ax, 4ax, 5eq-pentachlorocyclohexane.

r-1, *t*-2, *c*-3, *t*-4, *t*-5-1ax, 2ax, 3ax, 4ax, 5eq			
E(MP2/cc-pVTZ) = -2530.9146514 a.u.			
atom	X	Y	Z
C	-1.111588	-0.437107	-1.195918
C	-1.414021	0.665497	-0.166185
C	-0.513061	0.669644	1.086683
C	0.967496	0.318862	0.842035
C	1.085730	-0.891980	-0.083231
C	0.385931	-0.649121	-1.414198
H	-0.570043	1.657564	1.549365
H	-2.453410	0.582488	0.159470
H	-1.586063	-0.153901	-2.138159
H	1.426902	0.090770	1.807104
H	0.810671	0.235515	-1.899697
H	0.531335	-1.509214	-2.072625
Cl	-1.892848	-1.978409	-0.715232
Cl	-1.290743	2.243550	-1.007273
Cl	1.843434	1.736317	0.203703
Cl	-1.159754	-0.478415	2.302760
Cl	2.783943	-1.359828	-0.328102
H	0.609129	-1.732646	0.429877

Table S72 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *c*-4, *c*-5-1ax, 2ax, 3ax, 4eq, 5ax-pentachlorocyclohexane.

r-1, *t*-2, *c*-3, *c*-4, *c*-5-1ax, 2ax, 3ax, 4eq, 5ax			
E(MP2/cc-pVTZ) = -2530.9073053 a.u.			
atom	X	Y	Z
C	1.671618	0.537387	-0.482527
C	1.426077	-0.687943	0.412231
C	-0.046074	-0.971212	0.763380
C	-0.922619	-0.894203	-0.490742
C	-0.776490	0.375801	-1.333146
C	0.703342	0.604032	-1.665796
H	-0.103120	-1.995163	1.142278
H	2.006482	-0.599041	1.333870
H	2.685937	0.448689	-0.879413
H	0.999308	-0.188387	-2.364919
H	0.819103	1.561708	-2.180357
Cl	1.689076	2.038221	0.485973
Cl	2.069030	-2.127224	-0.456787
Cl	-0.583601	0.062308	2.106806
H	-0.556280	-1.699792	-1.138169
Cl	-2.614240	-1.291813	-0.140324
Cl	-1.553240	1.818044	-0.634488
H	-1.305998	0.196701	-2.273757

Table S73 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *c*-4, *t*-5-1ax, 2ax,

3ax, 4eq, 5eq-pentachlorocyclohexane.

r-1, *t*-2, *c*-3, *c*-4, *t*-5-1ax, 2ax, 3ax, 4eq, 5eq			
E(MP2/cc-pVTZ) = -2530.9163350 a.u.			
atom	X	Y	Z
C	-1.573524	0.983394	0.107127
C	-1.538321	-0.487537	0.550884
C	-0.274005	-1.263273	0.144017
C	1.003711	-0.465228	0.444930
C	0.955461	0.919368	-0.200899
C	-0.243997	1.692035	0.353772
H	-0.244601	-2.192604	0.718994
H	-2.421434	-1.014749	0.180930
H	-2.359937	1.483501	0.677624
H	-0.106221	1.815194	1.433987
H	-0.276867	2.688341	-0.094937
Cl	-2.061603	1.137221	-1.607336
Cl	-1.639918	-0.511385	2.344539
Cl	-0.374264	-1.750785	-1.568410
Cl	2.430196	1.851141	0.166100
H	0.898816	0.821755	-1.288649
H	1.058845	-0.332313	1.530879
Cl	2.438262	-1.405113	-0.014764

Table S74 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-3, *t*-4, *c*-5-1ax, 2ax, 3eq, 4ax, 5ax-pentachlorocyclohexane.

r-1, *t*-2, *t*-3, *t*-4, *c*-5-1ax, 2ax, 3eq, 4ax, 5ax			
E(MP2/cc-pVTZ) = -2530.9123900 a.u.			
atom	X	Y	Z
C	-0.089338	-1.152887	1.297356
C	-0.089338	0.384672	1.299953
C	0.511562	0.926178	0.000000
C	-0.089338	0.384672	-1.299953
C	-0.089338	-1.152887	-1.297356
C	-0.649978	-1.738596	0.000000
H	0.528689	0.737660	2.129478
H	-0.710142	-1.493377	2.129418
H	-1.726890	-1.529426	0.000000
H	-0.518193	-2.824124	0.000000
Cl	1.563466	-1.734682	1.674256
Cl	-1.742798	0.955914	1.648264
H	1.549189	0.571236	0.000000
Cl	0.595925	2.697938	0.000000
H	0.528689	0.737660	-2.129478
Cl	-1.742798	0.955914	-1.648264
Cl	1.563466	-1.734682	-1.674256
H	-0.710142	-1.493377	-2.129418

Table S75 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-3, *t*-4, *t*-5-1ax, 2ax,

3eq, 4ax, 5eq-pentachlorocyclohexane.

r-1, *t*-2, *t*-3, *t*-4, *t*-5-1ax, 2ax, 3eq, 4ax, 5eq			
E(MP2/cc-pVTZ) = -2530.9154706 a.u.			
atom	X	Y	Z
C	-0.061583	1.710645	0.634711
C	-1.252989	0.833410	0.219095
C	-0.851238	-0.129496	-0.906075
C	0.431545	-0.942092	-0.667854
C	1.554857	0.044423	-0.321299
C	1.207025	0.897743	0.893732
H	-2.054396	1.474161	-0.158352
H	-0.337287	2.272279	1.530501
H	1.046652	0.253583	1.764456
H	2.031948	1.580386	1.114064
Cl	0.229058	2.939210	-0.645239
Cl	-1.902887	0.043686	1.677300
H	-0.625815	0.516791	-1.763036
Cl	-2.206450	-1.152423	-1.418039
Cl	3.115328	-0.778849	-0.099876
H	1.682613	0.694969	-1.192736
H	0.680855	-1.452874	-1.603081
Cl	0.259641	-2.217923	0.556107

Table S76 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-3, *c*-4, *c*-5-1ax, 2ax, 3eq, 4eq, 5ax-pentachlorocyclohexane.

r-1, *t*-2, *t*-3, *c*-4, *c*-5-1ax, 2ax, 3eq, 4eq, 5ax			
E(MP2/cc-pVTZ) = -2530.9150963 a.u.			
atom	X	Y	Z
C	-1.523816	-1.102582	0.283081
C	-0.122187	-1.497900	-0.196218
C	0.707259	-0.271557	-0.601535
C	0.832171	0.698694	0.575628
C	-0.554737	1.179473	1.031082
C	-1.475020	-0.005062	1.348440
H	-0.200924	-2.175565	-1.050207
H	-2.000588	-1.986763	0.713508
H	-1.099215	-0.470968	2.267574
H	-2.484956	0.362112	1.549922
Cl	-2.518674	-0.672919	-1.140568
Cl	0.666576	-2.426538	1.116231
H	1.285477	0.166346	1.418120
Cl	1.897911	2.074087	0.227140
Cl	-1.296594	2.295624	-0.150759
H	-0.422117	1.768937	1.943073
H	0.185487	0.227168	-1.424574
Cl	2.283417	-0.793647	-1.232060

Table S77 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-3, *c*-4, *t*-5-1ax, 2ax,

3eq, 4eq, 5eq-pentachlorocyclohexane.

r-1, *t*-2, *t*-3, *c*-4, *t*-5-1ax, 2ax, 3eq, 4eq, 5eq			
E(MP2/cc-pVTZ) = -2530.9208532 a.u.			
atom	X	Y	Z
C	1.051710	-1.651615	0.028658
C	1.609190	-0.228188	0.124749
C	0.651438	0.785059	-0.509912
C	-0.756864	0.715944	0.095491
C	-1.302255	-0.716927	0.012281
C	-0.349023	-1.744261	0.623398
H	2.576568	-0.169016	-0.381993
H	1.727706	-2.333614	0.551269
H	-0.282645	-1.579652	1.703167
H	-0.752831	-2.747178	0.459818
Cl	1.051268	-2.163812	-1.690360
Cl	1.907086	0.128129	1.850036
H	-0.733303	1.048225	1.137984
Cl	-1.841263	1.818038	-0.789615
H	0.581986	0.545419	-1.575776
Cl	1.338847	2.421171	-0.407352
Cl	-2.870631	-0.837101	0.854736
H	-1.492882	-0.953484	-1.039045

Table S78 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *t*-4, *t*-5-1ax, 2eq, 3ax, 4ax, 5eq-pentachlorocyclohexane.

r-1, *c*-2, *c*-3, *t*-4, *t*-5-1ax, 2eq, 3ax, 4ax, 5eq			
E(MP2/cc-pVTZ) = -2530.9164275 a.u.			
atom	X	Y	Z
C	0.762286	0.908600	-1.081624
C	1.090041	-0.546899	-0.729164
C	0.405728	-1.103379	0.526154
C	-1.107968	-0.827723	0.485867
C	-1.376800	0.655369	0.226087
C	-0.756574	1.122059	-1.086005
H	0.562872	-2.185202	0.543547
H	1.154566	1.098486	-2.084965
H	-1.550693	-1.127545	1.439261
H	-1.198369	0.563343	-1.918189
H	-0.966594	2.183699	-1.238808
Cl	1.551849	2.112905	-0.025877
Cl	-1.846276	-1.870653	-0.766158
Cl	1.061073	-0.488151	2.064671
Cl	-3.120076	1.010217	0.263649
H	-0.930067	1.207941	1.058207
Cl	2.833028	-0.873456	-0.729802
H	0.674840	-1.133550	-1.557139

Table S79 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *c*-4, *c*-5-1ax,

2eq, 3ax, 4eq, 5ax-pentachlorocyclohexane.

r-1, *c*-2, *c*-3, *c*-4, *c*-5-1ax, 2eq, 3ax, 4eq, 5ax			
E(MP2/cc-pVTZ) = -2530.9014923 a.u.			
atom	X	Y	Z
C	1.301421	0.926841	-0.868652
C	1.240216	-0.604479	-0.845127
C	0.000000	-1.214607	-0.174664
C	-1.240216	-0.604479	-0.845127
C	-1.301422	0.926841	-0.868652
C	0.000000	1.485030	-1.459760
H	0.000000	-2.284417	-0.405974
H	2.118195	1.201915	-1.542817
H	0.000000	1.228973	-2.528790
H	0.000000	2.575823	-1.383253
Cl	1.720599	1.671290	0.691495
Cl	0.000000	-1.110006	1.593144
H	-1.160114	-0.894035	-1.901941
Cl	-2.744525	-1.340611	-0.265142
Cl	-1.720599	1.671290	0.691495
H	-2.118195	1.201915	-1.542817
H	1.160114	-0.894034	-1.901941
Cl	2.744525	-1.340611	-0.265142

Table S80 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *c*-4, *t*-5-1ax, 2eq, 3ax, 4eq, 5eq-pentachlorocyclohexane.

r-1, *c*-2, *c*-3, *c*-4, *t*-5-1ax, 2eq, 3ax, 4eq, 5eq			
E(MP2/cc-pVTZ) = -2530.9115752 a.u.			
atom	X	Y	Z
C	1.109311	1.353935	-0.455978
C	1.277574	-0.073396	-0.987477
C	0.311592	-1.112191	-0.400633
C	-1.131361	-0.604698	-0.572289
C	-1.317514	0.764591	0.083525
C	-0.359690	1.768273	-0.564289
H	0.419378	-2.034855	-0.979018
H	1.711091	2.012523	-1.089085
H	-0.621955	1.857025	-1.626667
H	-0.493461	2.752338	-0.107103
Cl	1.709312	1.609121	1.202426
Cl	0.666943	-1.545545	1.284700
Cl	-2.981012	1.364043	-0.143148
H	-1.143539	0.687186	1.160334
H	-1.311611	-0.491137	-1.649145
Cl	-2.292330	-1.820717	-0.003821
Cl	2.961111	-0.627845	-0.944573
H	1.012220	-0.006130	-2.051403

Table S81 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *t*-4, *t*-5-1ax, 2eq,

3eq, 4ax, 5eq-pentachlorocyclohexane.

r-1, *c*-2, *t*-3, *t*-4, *t*-5-1ax, 2eq, 3eq, 4ax, 5eq			
E(MP2/cc-pVTZ) = -2530.9189554 a.u.			
atom	X	Y	Z
C	-0.574519	1.418982	0.742327
C	-1.181768	0.016132	0.591633
C	-0.574614	-0.712270	-0.611757
C	0.956023	-0.798587	-0.475094
C	1.528055	0.618443	-0.368843
C	0.952907	1.360155	0.833163
H	-0.983735	1.876355	1.647677
H	1.242333	0.845698	1.755461
H	1.349026	2.378280	0.868660
Cl	-1.052055	2.493228	-0.610896
H	-0.797161	-0.142273	-1.520378
Cl	-1.265705	-2.330396	-0.848227
Cl	3.306209	0.607163	-0.323466
H	1.250522	1.144057	-1.288295
H	1.362116	-1.296951	-1.360327
Cl	1.428065	-1.794435	0.927364
Cl	-2.953101	0.102203	0.509842
H	-0.937619	-0.544270	1.500149

Table S82 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *c*-4, *c*-5-1ax, 2eq, 3eq, 4eq, 5ax-pentachlorocyclohexane.

r-1, *c*-2, *t*-3, *c*-4, *c*-5-1ax, 2eq, 3eq, 4eq, 5ax			
E(MP2/cc-pVTZ) = -2530.9098770 a.u.			
atom	X	Y	Z
C	1.291993	-1.069382	0.796647
C	1.244635	0.450655	0.601930
C	-0.000001	0.912592	-0.171902
C	-1.244636	0.450654	0.601931
C	-1.291991	-1.069383	0.796647
C	0.000001	-1.562448	1.454229
H	2.128372	-1.292051	1.465849
H	0.000001	-1.185930	2.486765
H	0.000002	-2.655082	1.500086
Cl	1.656826	-1.930523	-0.721380
H	-1.189979	0.896450	1.603901
Cl	-2.757666	1.040523	-0.116025
Cl	-1.656824	-1.930525	-0.721380
H	-2.128371	-1.292054	1.465849
H	-0.000001	0.506945	-1.188036
Cl	-0.000002	2.688773	-0.290788
H	1.189979	0.896451	1.603901
Cl	2.757665	1.040525	-0.116027

Table S83 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *c*-4, *t*-5-1ax, 2eq,

3eq, 4eq, 5eq-pentachlorocyclohexane.

r-1, *c*-2, *t*-3, *c*-4, *t*-5-1ax, 2eq, 3eq, 4eq, 5eq			
E(MP2/cc-pVTZ) = -2530.9179527 a.u.			
atom	X	Y	Z
C	-0.895752	-1.573546	-0.453133
C	-1.359058	-0.132253	-0.665593
C	-0.513170	0.863955	0.135040
C	0.989421	0.687889	-0.157117
C	1.455212	-0.767352	-0.040620
C	0.569017	-1.704401	-0.857242
H	-1.515739	-2.235212	-1.065072
H	0.663562	-1.457986	-1.922340
H	0.903277	-2.736584	-0.719817
Cl	-1.116650	-2.098698	1.241812
H	1.192668	1.043683	-1.174176
Cl	1.929942	1.714000	0.954892
H	-0.702964	0.733804	1.204470
Cl	-0.989402	2.527996	-0.289751
Cl	3.135621	-0.921543	-0.620858
H	1.456315	-1.062975	1.011622
H	-1.236773	0.087640	-1.733532
Cl	-3.090944	0.036002	-0.307811

Table S84 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *c*-4, *c*-5-1eq, 2ax, 3ax, 4ax, 5eq-pentachlorocyclohexane.

r-1, *c*-2, *t*-3, *c*-4, *c*-5-1eq, 2ax, 3ax, 4ax, 5eq			
E(MP2/cc-pVTZ) = -2530.9155210 a.u.			
atom	X	Y	Z
C	0.722174	0.601920	1.233904
C	-0.695235	0.026386	1.306730
C	-1.463857	0.310145	0.000000
C	-0.695235	0.026386	-1.306730
C	0.722174	0.601920	-1.233904
C	1.478667	0.115928	0.000000
H	-2.395064	-0.261827	0.000000
H	-1.238542	0.503050	2.126916
H	-1.238542	0.503050	-2.126916
H	1.568581	-0.974133	0.000000
H	2.482873	0.548621	0.000000
Cl	-0.695235	-1.717634	1.668500
Cl	-0.695235	-1.717634	-1.668500
Cl	-1.933711	2.045045	0.000000
Cl	1.638017	0.289354	-2.725742
H	0.613544	1.690429	-1.174530
Cl	1.638017	0.289354	2.725742
H	0.613544	1.690429	1.174530

Table S85 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *t*-4, *c*-5-1eq, 2ax,

3ax, 4eq, 5eq-pentachlorocyclohexane.

r-1, *c*-2, *t*-3, *t*-4, *c*-5-1eq, 2ax, 3ax, 4eq, 5eq			
E(MP2/cc-pVTZ) = -2530.9207306 a.u.			
atom	X	Y	Z
C	-1.489229	0.236150	-0.702794
C	-1.246758	-0.913885	0.276658
C	0.227518	-1.344069	0.230106
C	1.169785	-0.160503	0.493171
C	0.907962	0.990033	-0.479440
C	-0.564444	1.417787	-0.428069
H	0.403014	-2.111551	0.988863
H	-1.878874	-1.767552	0.016974
H	-0.788667	1.846135	0.553527
H	-0.733245	2.194416	-1.179436
Cl	-1.653944	-0.465646	1.956289
Cl	0.541426	-2.113190	-1.353421
Cl	1.920832	2.401240	-0.078155
H	1.186256	0.679295	-1.491298
H	0.973230	0.193473	1.510054
Cl	2.861006	-0.704410	0.465167
Cl	-3.192599	0.750868	-0.697633
H	-1.294949	-0.157942	-1.704684

Table S86 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *c*-4, *c*-5-1eq, 2ax, 3eq, 4ax, 5eq-pentachlorocyclohexane.

r-1, *c*-2, *c*-3, *c*-4, *c*-5-1eq, 2ax, 3eq, 4ax, 5eq			
E(MP2/cc-pVTZ) = -2530.9102710 a.u.			
atom	X	Y	Z
C	1.103648	-0.544726	1.235427
C	0.101418	0.616266	1.303970
C	0.225243	1.423757	0.000000
C	0.101418	0.616266	-1.303970
C	1.103648	-0.544726	-1.235427
C	0.894781	-1.417759	0.000000
H	0.379307	1.277526	2.130440
H	-0.106143	-1.858673	0.000000
H	1.632408	-2.224776	0.000000
Cl	-1.544398	0.055994	1.655374
H	1.253697	1.809792	0.000000
Cl	-0.819819	2.856243	0.000000
Cl	1.103648	-1.513382	-2.726062
H	2.101458	-0.090397	-1.179682
H	0.379307	1.277526	-2.130440
Cl	-1.544398	0.055994	-1.655374
Cl	1.103648	-1.513382	2.726062
H	2.101458	-0.090397	1.179682

Table S87 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *t*-4, *c*-5-1eq, 2ax,

3eq, 4eq, 5eq-pentachlorocyclohexane.

r-1, *c*-2, *c*-3, *t*-4, *c*-5-1eq, 2ax, 3eq, 4eq, 5eq			
E(MP2/cc-pVTZ) = -2530.9172843 a.u.			
atom	X	Y	Z
C	1.556173	-0.513980	-0.767849
C	1.171333	0.877516	-0.261454
C	-0.312916	1.106908	-0.575459
C	-1.213093	0.055027	0.087780
C	-0.754545	-1.357493	-0.304671
C	0.739665	-1.595985	-0.072343
H	1.764323	1.640093	-0.775147
H	0.961931	-1.601504	0.997879
H	1.003372	-2.576825	-0.477625
Cl	1.502753	1.051504	1.478826
H	-1.184976	0.172552	1.174931
Cl	-2.899498	0.294621	-0.433382
H	-0.432528	1.027182	-1.663402
Cl	-0.790050	2.761764	-0.140402
Cl	-1.677690	-2.587487	0.597944
H	-0.991653	-1.506134	-1.365069
Cl	3.300587	-0.818003	-0.601974
H	1.346077	-0.528125	-1.844813

Table S88 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-3, *t*-4, *c*-5-1eq, 2eq, 3ax, 4eq, 5eq-pentachlorocyclohexane.

r-1, *t*-2, *t*-3, *t*-4, *c*-5-1eq, 2eq, 3ax, 4eq, 5eq			
E(MP2/cc-pVTZ) = -2530.9179808 a.u.			
atom	X	Y	Z
C	0.849334	0.367691	1.282717
C	-0.331352	-0.601875	1.254797
C	-1.186275	-0.377006	0.000000
C	-0.331352	-0.601875	-1.254797
C	0.849334	0.367691	-1.282717
C	1.674377	0.218954	0.000000
H	-2.013890	-1.092406	0.000000
H	2.146058	-0.770673	0.000000
H	2.477603	0.961662	0.000000
Cl	-1.917128	1.249647	0.000000
Cl	1.915302	0.037550	-2.673131
H	0.478492	1.389173	-1.402205
H	0.061318	-1.625371	-1.207462
Cl	-1.334202	-0.511423	-2.717220
Cl	-1.334202	-0.511423	2.717220
H	0.061318	-1.625371	1.207462
Cl	1.915302	0.037550	2.673131
H	0.478492	1.389173	1.402205

Table S89 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *t*-4, *c*-5-1eq, 2eq,

3eq, 4eq, 5eq-pentachlorocyclohexane.

r-1, *t*-2, *c*-3, *t*-4, *c*-5-1eq, 2eq, 3eq, 4eq, 5eq			
E(MP2/cc-pVTZ) = -2530.9165407 a.u.			
atom	X	Y	Z
C	-1.254130	-1.096806	0.336981
C	-1.285661	0.336024	-0.196009
C	-0.000001	1.097647	0.168137
C	1.285660	0.336026	-0.196009
C	1.254132	-1.096804	0.336981
C	0.000001	-1.821946	-0.138288
H	0.000001	-1.882050	-1.232956
H	0.000002	-2.844192	0.250421
H	1.399620	0.310530	-1.285817
Cl	2.689898	1.208668	0.465970
H	-0.000001	1.298362	1.245788
Cl	-0.000003	2.675591	-0.660153
Cl	2.688138	-2.004549	-0.207283
H	1.289614	-1.071506	1.432413
H	-1.399620	0.310528	-1.285817
Cl	-2.689899	1.208666	0.465970
Cl	-2.688136	-2.004552	-0.207282
H	-1.289612	-1.071507	1.432413

Table S90 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *t*-4, *c*-5, *t*-6-1ax, 2ax, 3ax, 4ax, 5ax, 6ax-hexachlorocyclohexane.

r-1, *t*-2, *c*-3, *t*-4, *c*-5, *t*-6-1ax, 2ax, 3ax, 4ax, 5ax, 6ax			
E(MP2/cc-pVTZ) = -2990.0132979 a.u.			
atom	X	Y	Z
C	-0.162776	0.376446	-1.455726
C	0.162771	1.448921	-0.401852
C	-0.162773	1.072475	1.053874
C	0.162776	-0.376446	1.455726
C	-0.162770	-1.448921	0.401852
C	0.162773	-1.072475	-1.053874
H	0.406337	1.736989	1.706860
H	-0.406345	2.346678	-0.650840
H	0.406330	0.609696	-2.357706
H	-0.406330	-0.609696	2.357706
H	0.406346	-2.346678	0.650840
H	-0.406338	-1.736988	-1.706859
Cl	-1.883643	0.500513	-1.935492
Cl	1.883633	1.926461	-0.534294
Cl	-1.883639	1.425940	1.401205
Cl	1.883644	-0.500512	1.935492
Cl	-1.883633	-1.926461	0.534295
Cl	1.883638	-1.425940	-1.401206

Table S91 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *t*-4, *c*-5, *c*-6-1ax,

2ax, 3ax, 4ax, 5ax, 6eq-hexachlorocyclohexane.

r-1, *t*-2, *c*-3, *t*-4, *c*-5, *c*-6-1ax, 2ax, 3ax, 4ax, 5ax, 6eq			
E(MP2/cc-pVTZ) = -2990.0187913 a.u.			
atom	X	Y	Z
C	-0.509453	-0.338518	-1.297152
C	0.944901	0.166361	-1.304962
C	1.425531	0.830155	-0.000020
C	0.944912	0.166405	1.304949
C	-0.509442	-0.338475	1.297168
C	-0.806234	-1.092267	0.000022
H	2.517306	0.817983	-0.000024
H	1.063799	0.883471	-2.119508
H	-0.614085	-1.048843	-2.120485
H	1.063817	0.883542	2.119470
H	-0.614068	-1.048772	2.120526
Cl	-1.640734	0.984098	-1.667212
Cl	2.012224	-1.217540	-1.712224
Cl	0.969885	2.560052	-0.000047
Cl	2.012239	-1.217483	1.712248
Cl	-1.640721	0.984154	1.667192
Cl	-2.433263	-1.793817	0.000040
H	-0.111767	-1.940203	0.000033

Table S92 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *t*-4, *c*-5, *c*-6-1ax, 2ax, 3ax, 4ax, 5ax, 6eq-hexachlorocyclohexane.

r-1, *t*-2, *c*-3, *t*-4, *c*-5, *c*-6-1ax, 2ax, 3ax, 4ax, 5ax, 6eq			
E(MP2/cc-pVTZ) = -2990.0253165 a.u.			
atom	X	Y	Z
C	0.237408	-1.338131	0.671125
C	1.551464	-0.548984	0.540842
C	1.551481	0.548922	-0.540871
C	0.237463	1.338134	-0.671119
C	-0.988372	0.415067	-0.642812
C	-0.988389	-0.415014	0.642808
H	2.361181	1.248606	-0.322353
H	2.361129	-1.248706	0.322318
H	0.252425	-1.870198	1.625418
H	0.252493	1.870232	-1.625393
Cl	0.151304	-2.599583	-0.589816
Cl	1.936726	0.159020	2.140484
Cl	1.936691	-0.159081	-2.140528
Cl	0.151437	2.599537	0.589876
Cl	-2.470298	-1.363874	0.863896
H	-0.919517	0.259302	1.502197
H	-0.919525	-0.259249	-1.502202
Cl	-2.470243	1.363985	-0.863902

Table S93 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *c*-4, *c*-5, *c*-6-1ax,

2ax, 3ax, 4eq, 5ax, 6eq-hexachlorocyclohexane.

r-1, *t*-2, *c*-3, *c*-4, *c*-5, *c*-6-1ax, 2ax, 3ax, 4eq, 5ax, 6eq			
E(MP2/cc-pVTZ) = -2990.0188975 a.u.			
atom	X	Y	Z
C	0.903880	-0.229911	1.304129
C	1.721560	-0.280408	0.000000
C	0.903880	-0.229911	-1.304129
C	-0.148129	0.882647	-1.239088
C	-1.054710	0.874167	0.000000
C	-0.148129	0.882647	1.239088
H	1.594454	0.020058	-2.113820
H	2.341864	-1.179813	0.000000
H	1.594454	0.020058	2.113820
Cl	0.260231	-1.836088	1.709553
Cl	2.854588	1.117043	0.000000
Cl	0.260231	-1.836088	-1.709553
H	0.428588	1.812357	-1.163906
Cl	-1.069623	1.015844	-2.746050
Cl	-1.069623	1.015844	2.746050
H	0.428588	1.812357	1.163906
H	-1.609007	1.817913	0.000000
Cl	-2.285747	-0.399986	0.000000

Table S94 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *c*-4, *t*-5, *c*-6-1ax, 2ax, 3ax, 4eq, 5eq, 6eq-hexachlorocyclohexane.

r-1, *t*-2, *c*-3, *c*-4, *t*-5, *c*-6-1ax, 2ax, 3ax, 4eq, 5eq, 6eq			
E(MP2/cc-pVTZ) = -2990.0263958 a.u.			
atom	X	Y	Z
C	-1.295839	-1.028913	0.135263
C	0.000000	-1.725438	0.579134
C	1.295839	-1.028913	0.135263
C	1.244164	0.477505	0.417794
C	0.000000	1.150088	-0.181435
C	-1.244164	0.477505	0.417794
H	2.123364	-1.455131	0.708391
H	0.000000	-2.756708	0.217649
H	-2.123364	-1.455131	0.708391
Cl	-1.651217	-1.386655	-1.573163
Cl	0.000000	-1.810671	2.372872
Cl	1.651217	-1.386655	-1.573163
H	0.000000	1.071870	-1.272823
Cl	0.000000	2.878316	0.240742
H	1.196124	0.601560	1.505438
Cl	2.757321	1.248744	-0.098214
Cl	-2.757321	1.248744	-0.098214
H	-1.196124	0.601560	1.505438

Table S95 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-3, *t*-4, *c*-5, *c*-6-1ax,

2ax, 3eq, 4ax, 5ax, 6eq-hexachlorocyclohexane.

r-1, *t*-2, *t*-3, *t*-4, *c*-5, *c*-6-1ax, 2ax, 3eq, 4ax, 5ax, 6eq			
E(MP2/cc-pVTZ) = -2990.0247097 a.u.			
atom	X	Y	Z
C	0.000003	0.769954	1.300141
C	0.000003	-0.769957	1.300137
C	-0.603027	-1.310158	0.000000
C	0.000003	-0.769957	-1.300137
C	0.000003	0.769954	-1.300141
C	0.603020	1.310164	0.000000
H	-0.624829	-1.113830	2.128076
H	0.624846	1.113821	2.128074
Cl	-1.646285	1.354030	1.657713
Cl	1.646297	-1.354033	1.657678
H	-1.639265	-0.951103	0.000000
Cl	-0.693202	-3.080278	0.000000
H	-0.624829	-1.113830	-2.128076
Cl	1.646297	-1.354033	-1.657678
Cl	0.693175	3.080284	0.000000
H	1.639262	0.951122	0.000000
H	0.624846	1.113821	-2.128074
Cl	-1.646285	1.354030	-1.657713

Table S96 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-3, *t*-4, *t*-5, *c*-6-1ax, 2ax, 3eq, 4ax, 5eq, 6eq-hexachlorocyclohexane.

r-1, *t*-2, *t*-3, *t*-4, *t*-5, *c*-6-1ax, 2ax, 3eq, 4ax, 5eq, 6eq			
E(MP2/cc-pVTZ) = -2990.0267453 a.u.			
atom	X	Y	Z
C	-0.512711	-1.500514	0.295095
C	1.006939	-1.299199	0.193949
C	1.330075	-0.217015	-0.842423
C	0.565160	1.103539	-0.678082
C	-0.945117	0.807270	-0.613651
C	-1.251675	-0.173869	0.521063
H	1.458705	-2.235061	-0.144988
H	-0.728381	-2.174114	1.128214
Cl	-1.074857	-2.334205	-1.186110
Cl	1.659481	-1.003083	1.823416
H	0.990067	-0.630882	-1.799103
Cl	3.075094	0.035765	-1.019046
H	-1.233572	0.345952	-1.564088
Cl	-1.872114	2.314210	-0.495228
H	0.754337	1.711527	-1.567935
Cl	1.113309	2.077337	0.704207
Cl	-2.989279	-0.477534	0.715488
H	-0.894956	0.248989	1.465829

Table S97 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *t*-3, *c*-4, *t*-5, *c*-6-1ax,

2ax, 3eq, 4eq, 5eq, 6eq-hexachlorocyclohexane.

r-1, *t*-2, *t*-3, *c*-4, *t*-5, *c*-6-1ax, 2ax, 3eq, 4eq, 5eq, 6eq			
E(MP2/cc-pVTZ) = -2990.0323191 a.u.			
atom	X	Y	Z
C	0.755338	-1.544781	0.127317
C	-0.755338	-1.544781	-0.127318
C	-1.403640	-0.289206	0.459828
C	-0.766620	0.995357	-0.080351
C	0.766620	0.995357	0.080351
C	1.403640	-0.289205	-0.459828
H	-1.201833	-2.427676	0.338400
H	1.201833	-2.427676	-0.338401
Cl	1.036627	-1.690433	1.885171
Cl	-1.036626	-1.690432	-1.885171
H	-1.022098	1.116871	-1.137632
Cl	-1.437373	2.397956	0.789022
H	-1.261175	-0.322920	1.543838
Cl	-3.158250	-0.315436	0.182989
Cl	3.158250	-0.315435	-0.182989
H	1.261175	-0.322919	-1.543839
H	1.022098	1.116871	1.137632
Cl	1.437373	2.397957	-0.789022

Table S98 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *c*-4, *t*-5, *c*-6-1ax, 2eq, 3ax, 4eq, 5eq, 6eq-hexachlorocyclohexane.

r-1, *c*-2, *c*-3, *c*-4, *t*-5, *c*-6-1ax, 2eq, 3ax, 4eq, 5eq, 6eq			
E(MP2/cc-pVTZ) = -2990.0211220 a.u.			
atom	X	Y	Z
C	0.251690	-0.883153	1.293991
C	0.708539	-1.567926	0.000000
C	0.251690	-0.883153	-1.293991
C	0.684609	0.590573	-1.245800
C	0.162851	1.323599	0.000000
C	0.684609	0.590573	1.245800
H	0.776640	-1.359704	2.127390
Cl	-1.479107	-1.063556	1.639361
H	1.803830	-1.483294	0.000000
Cl	0.363122	-3.305632	0.000000
H	1.781535	0.603132	-1.199857
Cl	0.251690	1.413151	-2.757127
H	0.776640	-1.359704	-2.127390
Cl	-1.479107	-1.063556	-1.639361
Cl	0.251690	1.413151	2.757127
H	1.781535	0.603132	1.199857
H	-0.930665	1.361465	0.000000
Cl	0.770920	2.995379	0.000000

Table S99 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *t*-4, *t*-5, *c*-6-1ax,

2eq, 3eq, 4ax, 5eq, 6eq-hexachlorocyclohexane.

r-1, *c*-2, *t*-3, *t*-4, *t*-5, *c*-6-1ax, 2eq, 3eq, 4ax, 5eq, 6eq			
E(MP2/cc-pVTZ) = -2990.0299833 a.u.			
atom	X	Y	Z
C	0.000000	-1.388184	-0.488080
C	-1.261967	-0.513692	-0.567432
C	-1.261967	0.513692	0.567432
C	0.000000	1.388184	0.488080
C	1.261967	0.513692	0.567432
C	1.261967	-0.513692	-0.567432
H	0.000000	-2.084713	-1.331508
Cl	0.000000	-2.387191	0.991246
H	-1.244232	-0.015601	1.525874
Cl	-2.718510	1.526156	0.576480
H	0.000000	2.084713	1.331508
Cl	0.000000	2.387191	-0.991246
H	-1.244232	0.015601	-1.525874
Cl	-2.718510	-1.526156	-0.576480
Cl	2.718510	-1.526156	-0.576480
H	1.244232	0.015601	-1.525874
H	1.244232	-0.015601	1.525874
Cl	2.718510	1.526156	0.576480

Table S100 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *t*-3, *c*-4, *t*-5, *c*-6-1ax, 2eq, 3eq, 4eq, 5eq, 6eq-hexachlorocyclohexane.

r-1, *c*-2, *t*-3, *c*-4, *t*-5, *c*-6-1ax, 2eq, 3eq, 4eq, 5eq, 6eq			
E(MP2/cc-pVTZ) = -2990.0290398 a.u.			
atom	X	Y	Z
C	-0.307335	-1.576533	0.000000
C	-0.671513	-0.763045	1.243170
C	0.117705	0.546541	1.297656
C	-0.062149	1.355128	0.000000
C	0.117705	0.546541	-1.297656
C	-0.671513	-0.763045	-1.243170
H	-0.881023	-2.507951	0.000000
Cl	1.416046	-2.026837	0.000000
H	1.176364	0.333225	1.466970
Cl	-0.448479	1.536142	2.665962
H	-1.741801	-0.528797	1.183222
Cl	-0.448479	-1.735056	2.711570
H	1.176364	0.333225	-1.466970
Cl	-0.448479	1.536142	-2.665962
H	-1.071608	1.782746	0.000000
Cl	1.080582	2.721302	0.000000
Cl	-0.448479	-1.735056	-2.711570
H	-1.741801	-0.528797	-1.183222

Table S101 Optimized cartesian coordinates and total energies of *r*-1, *c*-2, *c*-3, *c*-4, *c*-5, *c*-6-

1eq, 2ax, 3eq, 4ax, 5eq, 6ax-hexachlorocyclohexane.

r-1, *c*-2, *c*-3, *c*-4, *c*-5, *c*-6-1eq, 2ax, 3eq, 4ax, 5eq, 6ax			
E(MP2/cc-pVTZ) = -2990.0125342 a.u.			
atom	X	Y	Z
C	-0.636247	-1.284450	-0.916867
C	0.832996	-1.251470	-0.467636
C	1.430578	0.091159	-0.916830
C	0.667427	1.347075	-0.467600
C	-0.794111	1.193333	-0.916862
C	-1.500285	-0.095579	-0.467867
H	1.356077	-2.037364	-1.021364
Cl	1.083374	-1.627637	1.243574
H	1.349472	0.086007	-2.012409
Cl	3.165184	0.201676	-0.576386
H	-0.749033	1.125806	-2.012446
Cl	-1.757121	2.640266	-0.576319
Cl	-1.951767	-0.124342	1.243204
H	-2.442285	-0.155593	-1.021846
H	1.086547	2.193022	-1.021288
Cl	0.868001	1.751903	1.243633
Cl	-1.407835	-2.841898	-0.576308
H	-0.600123	-1.211752	-2.012451

Table S102 Optimized cartesian coordinates and total energies of *r*-1, *t*-2, *c*-3, *t*-4, *c*-5, *t*-6-1eq, 2eq, 3eq, 4eq, 5eq, 6eq-hexachlorocyclohexane.

r-1, *t*-2, *c*-3, *t*-4, *c*-5, *t*-6-1eq, 2eq, 3eq, 4eq, 5eq, 6eq			
E(MP2/cc-pVTZ) = -2990.0269697 a.u.			
atom	X	Y	Z
C	-0.794140	1.234355	0.220114
C	0.671920	1.304919	-0.220118
C	1.466051	0.070563	0.220113
C	0.794140	-1.234355	-0.220114
C	-0.671920	-1.304919	0.220118
C	-1.466051	-0.070563	-0.220113
H	1.569573	0.075546	1.311413
Cl	3.105687	0.149476	-0.470001
H	0.719379	1.397070	-1.311417
Cl	1.423424	2.764313	0.470027
H	-0.719379	-1.397070	1.311417
Cl	-1.423423	-2.764314	-0.470027
H	0.850229	-1.321524	-1.311414
Cl	1.682334	-2.614826	0.470031
Cl	-3.105688	-0.149475	0.470002
H	-1.569573	-0.075546	-1.311413
H	-0.850229	1.321524	1.311414
Cl	-1.682336	2.614826	-0.470031