Supplementary data for

Dehydrochlorination mechanism of γ-hexachlorocyclohexane degraded by dehydrochlorinase LinA from *Sphingomonas paucimobilis* UT26

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Twenty pages

Contains additional details on the methods, three Figures, and the coordinates of the docked structures, MD snapshots, QM-optimized structures and QM/MM-optimized structures.

Figure S1. Root-mean-square deviations (RMSD) of the backbone for molecular dynamic simulation of γ-HCH reaction system (A) and γ-PCCH-1 reaction system (B). Key distance variations along the molecular dynamic simulation of γ-HCH reaction system (C) and γ-PCCH-1 reaction system (D).

Figure S2. The three dimensional structures of the docked structure, the MD snapshot, and the QM/MM-optimised structure in the γ-HCH reaction system. The key residues are shown in ball and stick representation. The values exhibited in MD snapshot and QM/MM-optimised structure are the average distance in the molecular dynamic simulation and the five pathways QM/MM optimizations. The unit of distance is in Å.

Figure S3. The three dimensional structures of the docked structure, the MD snapshot, and the QM/MM-optimised structure in the γ-PCCH-1 reaction system. The key residues are shown in ball and stick representation. The values exhibited in MD snapshot and QM/MM-optimised structure are the average distance in the molecular dynamic simulation and the five pathways QM/MM optimizations. The unit of distance is in Å.

Additional details on the methods

The protonation states of ionizable residues were determined on the basis of the pKa values obtained via the PROPKA procedure and were manually verified through visual inspection, especially for the residues around the active site. The pH value used (pH=8.3) during pKa calculation is same as experimentally used pH value in determining the $k$cat (*1*). The protonation states of the ionizable residues (Glu, Asp, Arg, Cys, Lys, and His residues) are all set in the standard state. For three histidine residues of enzyme LinA, the protonation states are listed as follows: Hsd69, Hsd73, and Hsd143. This was carefully determined based on the manual visual inspection and the results given by MolProbity software (*http://molprobity.biochem.duke.edu/*), especially for the active site residue Hsd73. The MolProbity software is also used to check the flipped residues, finding that Gln28 and Asn77 are flipped. Note that we follow the nomenclature in CHARMM and the CHARMM22 force field is used for the simulation. Important CHARMM simulation parameters are listed as follows (for explanation of the nomenclatures, see *http://www.charmm.org/documentation/c34b1/dynamc.html*):

The relevant codes for cutoff: "update group noextend fswitch cdie vdw vswitched eps 1.0 cutnb 14.0 ctofnb 13.0 ctonnb 12.0 vgroup WMIN 1.2 inbf 25"; time step for dynamics in picoseconds: timestp 0.001; the frequency for checking whether an atom is in the Langevin region: ilbfrq 50; a Gaussian distribution of velocities: iasvel 1; simulation temperature: 298.15 K.

Optimization parameters for QM/MM calculations are listed as follows

(most are set in default; for explanation of the nomenclatures, see http://yfaat.ch.huji.ac.il/chemshell-31/manual/hdlcopt.html):

Optimization parameters for reactants, intermediates, and products: Memory=100; mode=1; contyp=0; reghdl=60; cfact=0.5; recalc=0; toler=0.00045; printl=0; maxfun=100000; update_procedure=hdlcopt_update; theory=hybrid. Optimization parameters for transition states: Memory=100; contyp=0; ctfirst=1; reghdl=200; cfact=1; maxfun= 100000; toler=0.00045; mode=1; lockon=0; update_procedure=hdlcopt_update; theory=hybrid.

In our QM/MM calculations, each residue of the protein, each water molecule, and substrates (γ-HCH and γ-PCCH-1) are defined as HDLC residues. The transition state structure was determined by scanning the potential energy profile from the reactant to the product, reaction coordinates were defined as "$d(C^2-Cl^2)-d(N^\varepsilon-H^1)$" for γ-HCH reaction system and "$d(C^5-Cl^5)-d(N^\varepsilon-H^4)$" for γ-PCCH-1 reaction system. For microiterative TS optimisations, all the QM atoms are considered in the inner region.

References:

1. D. R. B. Brittain, R. Pandey, K. Kumari, P. Sharma, G. Pandey, R. Lal, M. L. Coote, J. G. Oakeshott and C. J. Jackson, *Chem. Commun.*, 2011, **47**, 976-978.
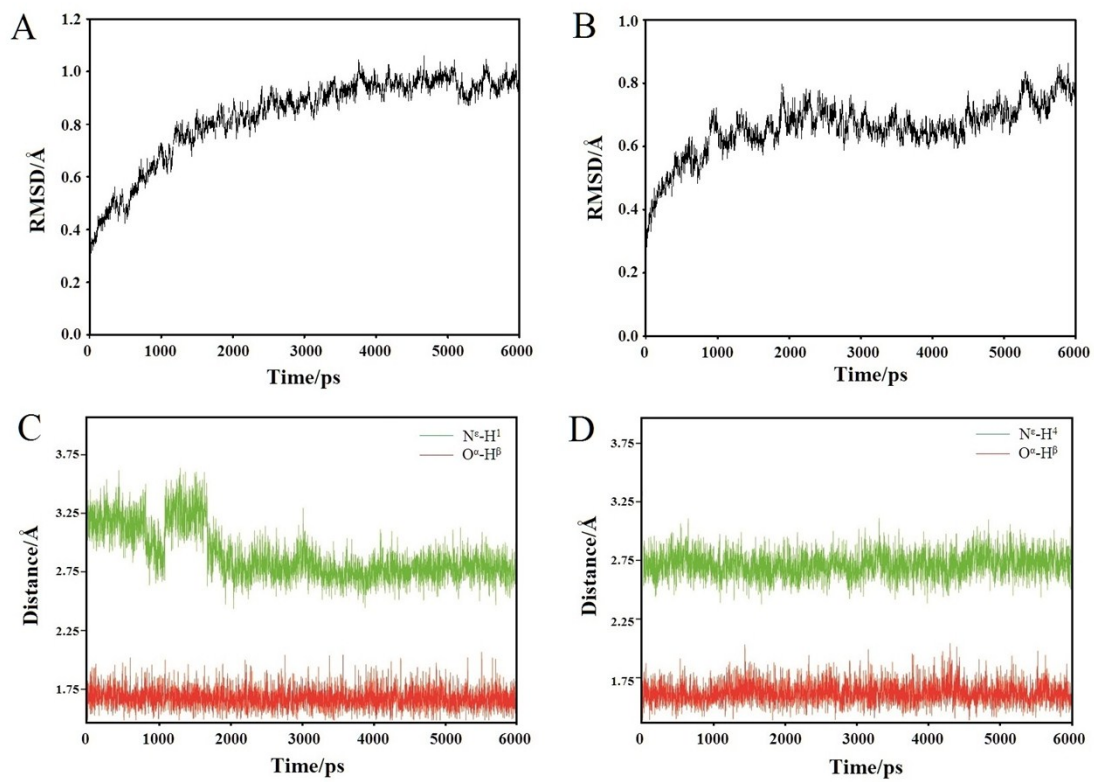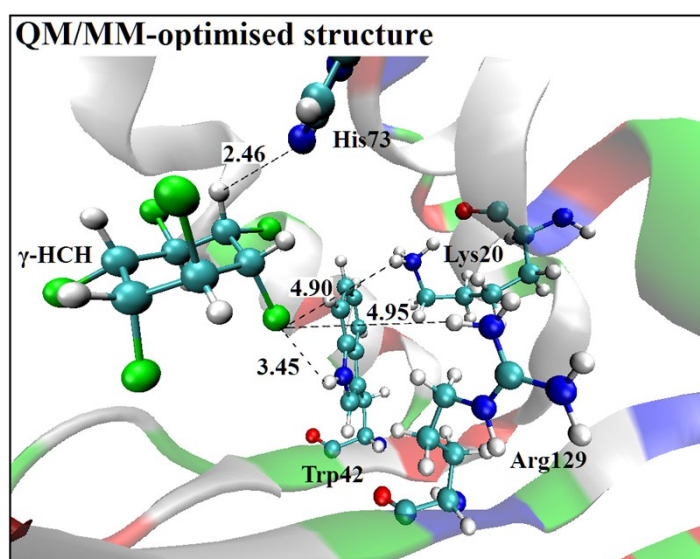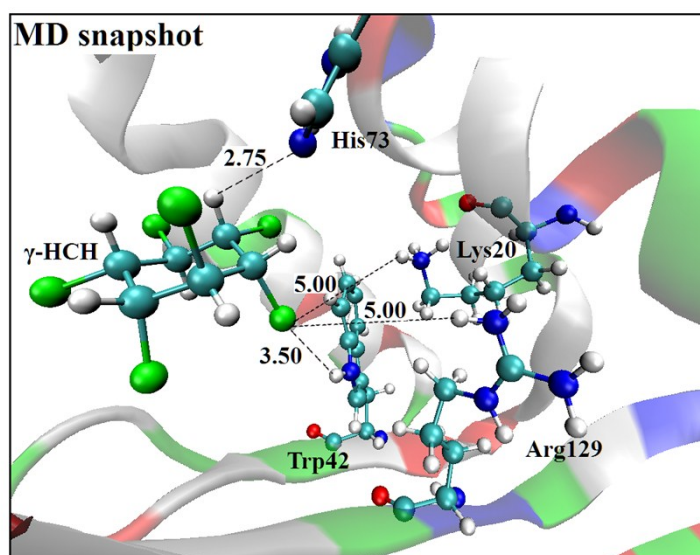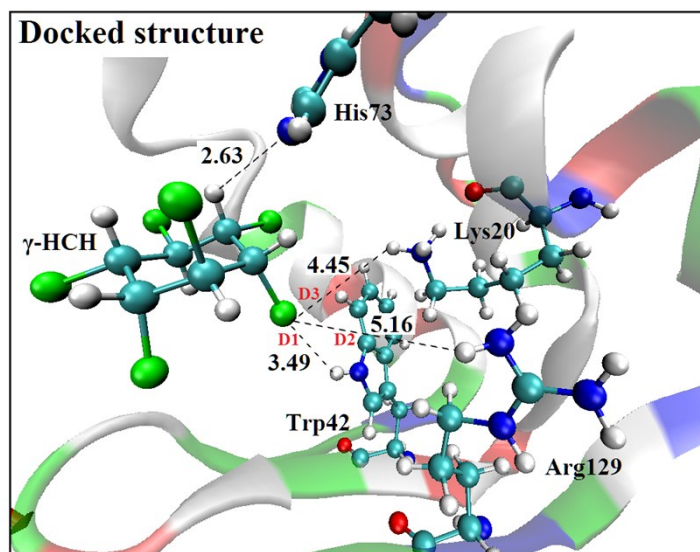
Figure S1

Figure S2
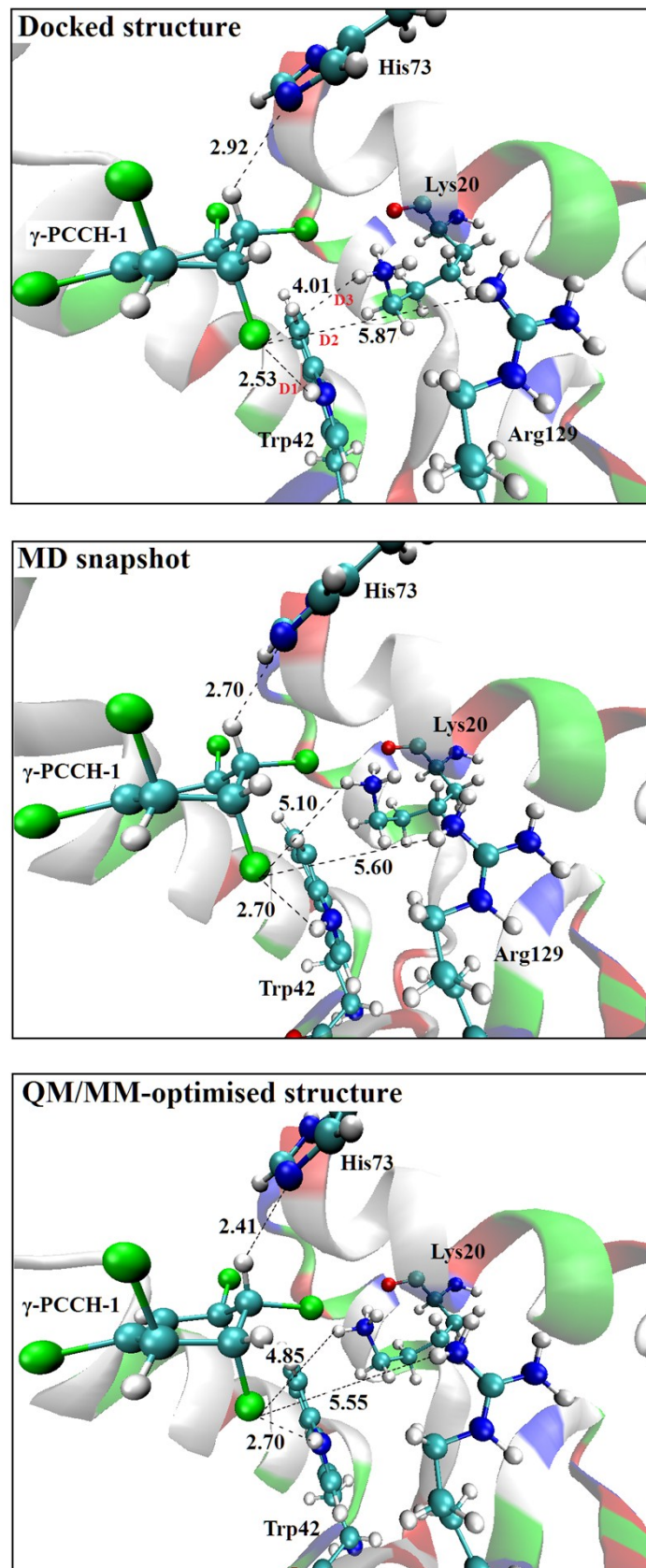
Figure S3

Docked structure (His73 and γ-HCH)

N	-7.269000	4.256000	-4.120000
HN	-6.850000	3.606000	-4.752000
CA	-6.371000	4.791000	-3.085000
HA	-6.964000	5.213000	-2.283000
CB	-5.344000	3.746000	-2.643000
HB1	-4.792000	3.380000	-3.536000
HB2	-4.592000	4.223000	-1.976000
ND1	-6.509000	1.499000	-2.597000
HD1	-6.611000	1.407000	-3.588000
CG	-5.907000	2.546000	-1.933000
CE1	-6.841000	0.561000	-1.731000
HE1	-7.347000	-0.369000	-2.004000
NE2	-6.452000	0.950000	-0.529000
CD2	-5.866000	2.188000	-0.626000
HD2	-5.493000	2.737000	0.230000
C	-5.574000	5.924000	-3.704000
O	-4.984000	5.758000	-4.772000
C1	-6.693000	1.014000	4.828000
H1	-7.026000	1.974000	5.219000
CL1	-5.769000	0.274000	6.170000
C2	-7.967000	0.232000	4.413000
H2	-8.556000	0.900000	3.783000
CL2	-9.038000	-0.076000	5.833000
C3	-7.650000	-1.029000	3.567000
H3	-7.116000	-1.757000	4.171000
CL3	-9.187000	-1.816000	3.060000
C4	-6.800000	-0.621000	2.331000
H4	-7.400000	0.077000	1.763000
CL4	-6.466000	-1.916000	1.132000
C5	-5.485000	0.102000	2.715000
H5	-5.013000	0.474000	1.803000
CL5	-4.254000	-1.025000	3.392000
C6	-5.726000	1.305000	3.663000
H6	-4.770000	1.678000	4.033000
CL6	-6.393000	2.716000	2.802000

MD snapshot-5.5 ns (His73 and γ-HCH)

N	-7.764000	4.210000	-4.269000
HN	-7.499000	3.353000	-4.747000
CA	-6.787000	4.853000	-3.411000
HA	-7.347000	5.092000	-2.486000
CB	-5.563000	3.874000	-2.926000
HB1	-4.892000	3.711000	-3.720000
HB2	-5.072000	4.570000	-2.192000
ND1	-6.434000	1.629000	-2.588000
HD1	-6.788000	1.534000	-3.521000
CG	-5.860000	2.700000	-2.075000
CE1	-6.417000	0.714000	-1.613000
HE1	-6.755000	-0.325000	-1.818000
NE2	-6.012000	1.119000	-0.472000
CD2	-5.693000	2.462000	-0.707000
HD2	-5.507000	3.174000	0.003000
C	-6.183000	6.123000	-3.975000
O	-6.279000	6.468000	-5.177000
C1	-6.693000	1.014000	4.828000
H1	-7.026000	1.974000	5.219000
L1	-5.769000	0.274000	6.170000
C2	-7.967000	0.232000	4.413000
H2	-8.556000	0.900000	3.783000
L2	-9.038000	-0.076000	5.833000
C3	-7.650000	-1.029000	3.567000
H3	-7.116000	-1.757000	4.171000
L3	-9.187000	-1.816000	3.060000
C4	-6.800000	-0.621000	2.331000
H4	-7.400000	0.077000	1.763000
L4	-6.466000	-1.916000	1.132000
C5	-5.485000	0.102000	2.715000
H5	-5.013000	0.474000	1.803000
L5	-4.254000	-1.025000	3.392000
C6	-5.726000	1.305000	3.663000
H6	-4.770000	1.678000	4.033000
L6	-6.393000	2.716000	2.802000

Docked structure (His73 and γ-PCCH-1)

N	-7.276000	4.294000	-4.093000
HN	-6.858000	3.645000	-4.727000
CA	-6.377000	4.824000	-3.057000
HA	-6.969000	5.245000	-2.253000
CB	-5.350000	3.778000	-2.618000
HB1	-4.800000	3.413000	-3.513000
HB2	-4.598000	4.252000	-1.951000
ND1	-6.518000	1.532000	-2.578000
HD1	-6.621000	1.442000	-3.569000
CG	-5.914000	2.577000	-1.911000
CE1	-6.851000	0.592000	-1.714000
HE1	-7.357000	-0.337000	-1.989000
NE2	-6.460000	0.977000	-0.511000
CD2	-5.873000	2.214000	-0.605000
HD2	-5.498000	2.761000	0.252000
C	-5.579000	5.959000	-3.673000
O	-4.990000	5.795000	-4.742000
C1	-7.031000	-3.993000	2.207000
H1	-7.544000	-4.920000	2.010000
C6	-7.379000	-3.248000	3.273000
L6	-8.517000	-3.748000	4.449000
C2	-6.006000	-3.584000	1.179000
H2	-5.153000	-4.254000	1.271000
L2	-6.680000	-3.854000	-0.459000
C3	-5.561000	-2.120000	1.394000
H3	-6.376000	-1.504000	1.026000
L3	-4.151000	-1.625000	0.400000
C4	-5.371000	-1.771000	2.889000
H4	-5.066000	-0.743000	3.010000
L4	-4.039000	-2.688000	3.666000
C5	-6.686000	-1.962000	3.668000
H5	-6.495000	-1.927000	4.743000
L5	-7.772000	-0.573000	3.324000

MD snapshot-6.0 ns (His73 and γ-PCCH-1)

N	-7.743000	3.885000	-3.795000
HN	-7.302000	3.329000	-4.502000
CA	-6.906000	4.478000	-2.843000
HA	-7.392000	4.711000	-1.908000
CB	-5.743000	3.551000	-2.552000
HB1	-5.050000	3.349000	-3.440000
HB2	-5.068000	4.197000	-1.939000
ND1	-6.589000	1.263000	-2.414000
HD1	-6.661000	1.094000	-3.456000
CG	-6.200000	2.378000	-1.780000
CE1	-6.848000	0.323000	-1.483000
HE1	-7.236000	-0.685000	-1.711000
NE2	-6.581000	0.789000	-0.260000
CD2	-6.165000	2.081000	-0.442000
HD2	-5.913000	2.769000	0.427000
C	-6.317000	5.726000	-3.374000
O	-5.986000	5.972000	-4.525000
C1	-7.031000	-3.993000	2.207000
H1	-7.544000	-4.920000	2.010000
C6	-7.379000	-3.248000	3.273000
CL6	-8.517000	-3.748000	4.449000
C2	-6.006000	-3.584000	1.179000
H2	-5.153000	-4.254000	1.271000
CL2	-6.680000	-3.854000	-0.459000
C3	-5.561000	-2.120000	1.394000
H3	-6.376000	-1.504000	1.026000
CL3	-4.151000	-1.625000	0.400000
C4	-5.371000	-1.771000	2.889000
H4	-5.066000	-0.743000	3.010000
CL4	-4.039000	-2.688000	3.666000
C5	-6.686000	-1.962000	3.668000
H5	-6.495000	-1.927000	4.743000
CL5	-7.772000	-0.573000	3.324000

R

C	0.553637 -3.927913 -1.330043		N	-6.127369 1.131943 -0.626888
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C	-6.978956 0.408433 -7.548313		H	2.586460 -0.419516 3.170629
H	-6.016018 0.247933 -8.042188		C	1.752527 0.205640 1.436255
H	-7.653914 0.823652 -8.301467		N	2.603376 1.223073 1.312767
C	-6.804732 1.484915 -6.456104		H	2.326769 2.002027 0.728997
O	-7.381129 1.381645 -5.343889		H	3.355737 1.369843 2.020279
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H	-1.022367 -8.435190 4.246562		C	-6.820087 1.170736 4.745602
C	-1.012148 -6.316053 3.760943		H	-7.200636 2.108472 5.146412
C	-1.035143 -5.112837 4.426621		Cl	-5.896606 0.457504 6.117725
H	-0.558653 -4.820176 5.351218		C	-8.040835 0.347047 4.285137
N	-1.809867 -4.186309 3.747456		H	-8.699702 1.050983 3.771086
H	-2.140811 -3.331564 4.166471		Cl	-8.988089 -0.291830 5.673876
C	-2.362040 -4.797399 2.644986		C	-7.738518 -0.815658 3.328650
C	-1.859015 -6.129969 2.604183		H	-7.307031 -1.655053 3.872303
C	-2.289197 -6.972009 1.567064		Cl	-9.323709 -1.402686 2.669799
H	-1.975746 -8.005372 1.545131		C	-6.831265 -0.395134 2.174387
C	-3.174173 -6.494301 0.607410		H	-7.317696 0.305713 1.503245
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C	-3.265894 -4.315185 1.697829		C	-5.558976 0.308983 2.630166
H	-3.706099 -3.327581 1.794282		H	-5.056217 0.688895 1.740778
C	-3.653215 -5.173122 0.673378		Cl	-4.419339 -0.888174 3.394220
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C	-5.655286 3.876079 -3.113511		H	-4.901882 1.843617 4.005211
H	-5.180259 3.585796 -4.051404		Cl	-6.521490 2.837196 2.624935
H	-4.940527 4.479833 -2.547756		h	0.923018 -2.904605 -1.396856
N	-6.414406 1.473844 -2.807835		h	-7.355037 -0.556601 -7.208697
H	-6.726737 1.345330 -3.787306		h	0.302615 -7.573413 5.035016
C	-5.968760 2.670185 -2.288348		h	-6.510830 4.484915 -3.405792
C	-6.512263 0.598623 -1.778125		h	2.398883 -3.074540 3.959668
H	-6.890984 -0.401924 -1.906824			

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C	0.578591 -3.967734 -1.320136			N	-6.692583 1.039492 -0.599313
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H	1.379030 -4.554735 -0.872140			H	-5.733518 2.908619 -0.132304
C	-0.669281 -4.130678 -0.465620			C	1.493295 -2.500487 3.918704
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O	-7.425655 1.341563 -5.376562			H	3.364260 1.385966 2.030313
O	-5.828234 2.259909 -6.646174			N	0.817678 0.054571 0.463363
C	-0.304568 -7.588515 4.141047			H	0.664540 0.902962 -0.100416
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H	-1.011372 -8.418082 4.250944			C	-6.775548 1.147084 4.476544
C	-1.012895 -6.301931 3.763760			H	-7.180561 2.074488 4.877330
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H	-0.595579 -4.796684 5.355253			C	-7.952144 0.343863 3.891377
N	-1.851228 -4.187119 3.744962			H	-8.570054 1.069244 3.364776
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C	-2.388784 -4.812304 2.642256			C	-7.561463 -0.765314 2.900280
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H	-1.930036 -8.011106 1.549956			C	-6.609203 -0.278964 1.810659
C	-3.161679 -6.529976 0.606971			H	-6.820720 0.544706 0.534143
H	-3.496718 -7.197489 -0.178917			Cl	-6.084020 -1.755952 0.843387
C	-3.305237 -4.351038 1.696757			C	-5.411186 0.361691 2.401863
H	-3.772234 -3.376157 1.793173			H	-4.723455 0.731961 1.642442
C	-3.670144 -5.219535 0.672684			Cl	-4.265752 -0.893912 3.325691
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C	-5.754502 3.619061 -3.097955			H	-4.805503 1.820365 3.880352
H	-5.316053 3.262362 -4.034985			Cl	-6.345508 2.917354 2.483202
H	-4.989727 4.162503 -2.538368			h	0.932027 -2.938897 -1.388280
N	-6.833431 1.347261 -2.762953			h	-7.312603 -0.600224 -7.234240
H	-7.062379 1.235013 -3.777961			h	0.309647 -7.554128 5.040838
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C	-7.120557 0.515787 -1.749271			h	2.423222 -3.068833 3.935606
H	-7.682746 -0.397603 -1.855667				

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C	0.578715 -3.986337 -1.321407	N	-6.633514 1.033306 -0.934456
H	0.411547 -4.406607 -2.319912	C	-6.077423 2.284513 -1.111344
H	1.387118 -4.558750 -0.869557	H	-5.690050 2.854850 -0.282801
C	-0.674476 -4.179166 -0.482072	C	1.464772 -2.500143 3.940688
H	-0.867816 -5.223497 -0.240783	H	0.659855 -3.162007 4.266304
H	-0.651805 -3.638165 0.464261	H	1.538473 -1.678476 4.661194
N	-1.897532 -3.684761 -1.245284	C	1.104091 -1.898869 2.583977
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H	-2.538505 -4.448631 -1.540129	H	0.034840 -1.644336 2.583650
H	-2.414620 -2.980773 -0.683327	N	1.900646 -0.682614 2.393491
C	-6.925085 0.363708 -7.598190	H	2.575710 -0.428126 3.156774
H	-5.976506 0.207579 -8.116368	C	1.752351 0.198650 1.423288
H	-7.628206 0.797028 -8.315514	N	2.606990 1.218617 1.303574
C	-6.728658 1.383653 -6.469474	H	2.300462 2.017983 0.764624
O	-7.507970 1.353130 -5.464865	H	3.346278 1.365307 2.022969
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H	0.376933 -7.897170 3.377299	H	-0.088180 -0.352771 0.838191
H	-1.012142 -8.419332 4.284810	C	-6.913948 1.115974 4.648321
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C	-1.156115 -5.083571 4.361253	Cl	-5.929718 0.284928 5.898932
H	-0.726076 -4.737453 5.290858	C	-8.152910 0.317976 4.217282
N	-1.956646 -4.232080 3.622389	H	-8.786013 1.015985 3.666823
H	-2.319825 -3.320990 3.895936	Cl	-9.125204 -0.239877 5.621280
C	-2.432170 -4.913857 2.531091	C	-7.871324 -0.889394 3.315489
C	-1.869554 -6.219854 2.565149	H	-7.574864 -1.761462 3.901248
C	-2.237631 -7.131295 1.565329	Cl	-9.464195 -1.374904 2.547576
H	-1.882436 -8.145777 1.619485	C	-6.823989 -0.598826 2.291567
C	-3.114887 -6.746921 0.560059	H	-6.744609 0.550583 -0.050460
H	-3.419224 -7.464417 -0.192191	Cl	-6.604927 -1.807381 1.042143
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C	-3.647093 -5.443715 0.547355	Cl	-3.738740 -1.505262 3.074098
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C	-5.706628 3.754510 -3.227530	H	-4.978800 1.634113 3.825914
H	-5.233671 3.435453 -4.160385	Cl	-6.510412 2.989130 2.654624
H	-4.968335 4.293025 -2.630261	h	0.913016 -2.950653 -1.381971
N	-6.790740 1.479540 -3.039107	h	-7.299685 -0.603375 -7.262793
H	-7.059117 1.436557 -4.100437	h	0.304209 -7.529143 5.049548
C	-6.171887 2.566712 -2.447908	h	-6.525517 4.418017 -3.505461
C	-7.080366 0.575776 -2.110969	h	2.391709 -3.073579 3.945627
H	-7.642580 -0.333889 -2.253148		

γ-PCCH

C	-1.16581400	-0.80861800	0.35994900
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C	1.57285300	-0.01990500	0.22861200
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C	-0.88519800	0.65509700	0.11554300
H	1.83883100	-2.11826300	0.67743600
H	-0.51770100	-2.80164900	0.53526300
H	2.56085300	0.17981800	-0.18172700
H	0.53653600	0.60809400	-1.50583500
H	-1.02916800	1.21971100	1.03836200
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Cl	-2.09091700	1.36571600	-1.06273900
Cl	1.00013600	2.61327200	-0.37248100
Cl	1.70852200	0.32057700	2.01723200
Cl	1.63420400	-2.01864100	-1.67216800
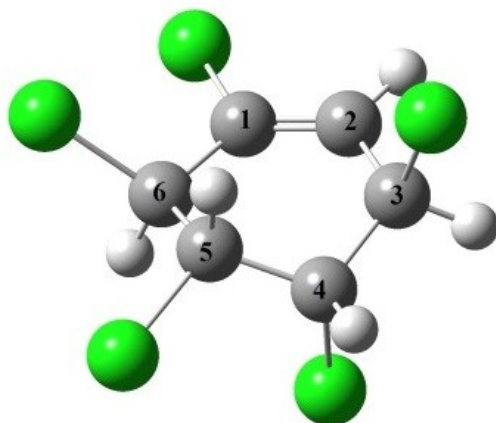
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C	-0.52729200	0.70280000	-1.38935000
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C	1.44229700	0.52078000	0.23398300
C	0.67335700	-0.66380500	0.92695900
C	-0.83254400	-0.77797700	0.58478200
C	-1.17326800	-0.30107900	-0.79056900
H	1.23951100	1.89771700	-1.41412700
H	-0.81762900	1.05369500	-2.37268600
H	-1.14783900	-1.80735700	0.72774100
H	1.87549000	1.13853200	1.01693600
Cl	-2.52374800	-1.10009100	-1.56356700
Cl	-1.83785900	0.14022500	1.83638900
Cl	2.88703700	0.00190400	-0.75326600
Cl	-0.08664900	2.85338400	0.26736200
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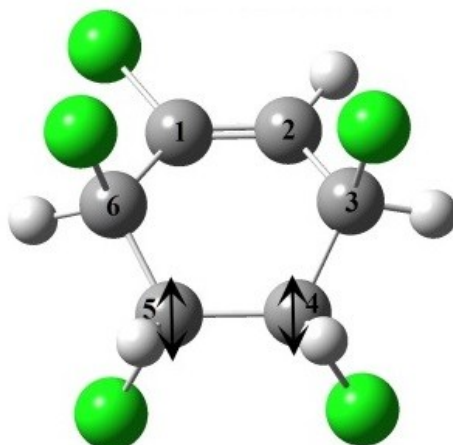
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C	1.16432600	-0.20090800	0.43191500
C	0.19146300	-1.33022500	0.09042600
C	-1.26140900	-0.84646600	0.22093500
C	-1.45980500	0.50426400	-0.39466100
H	1.48946600	0.83560800	-1.44988800
H	-0.67281500	2.27494600	-1.21551300
H	-1.93845900	-1.58203400	-0.21033100
H	0.95501000	0.09735000	1.46098400
Cl	-3.12667200	0.94829800	-0.70598400
Cl	-1.71264800	-0.80965200	2.01001100
Cl	2.87697900	-0.78801600	0.43851700
Cl	1.81759100	2.47071000	0.21492100
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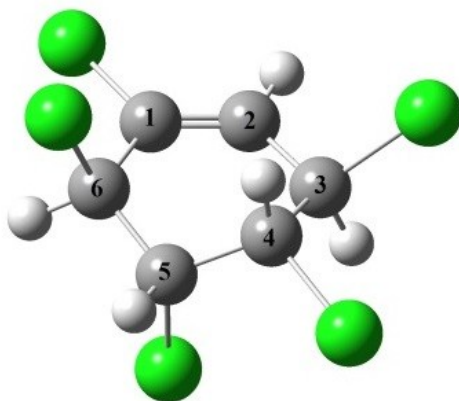
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H	1.959351 -3.263587 -0.847094	C	-5.774129 1.886505 -0.383522
C	-0.143874 -2.906692 -0.453369	H	-5.273141 2.463573 0.375536
H	-0.118849 -3.715647 0.276437	C	2.026937 -2.049531 4.009669
H	-0.301259 -1.972917 0.091402	H	1.271264 -2.650620 4.522964
N	-1.410439 -3.155781 -1.266305	H	2.257254 -1.204009 4.666128
H	-1.327772 -2.795053 -2.238611	C	1.421082 -1.470711 2.729983
H	-1.601805 -4.169077 -1.298942	H	1.447553 -2.171266 1.884375
H	-2.241590 -2.742171 -0.825488	H	0.364499 -1.232383 2.912652
C	-7.007213 0.760872 -7.148857	N	2.148848 -0.252471 2.381462
H	-6.118221 0.886809 -7.771136	H	2.971063 -0.001113 2.989900
H	-7.844516 1.227146 -7.675387	C	1.872889 0.582392 1.393211
C	-6.835528 1.517138 -5.813492	N	2.758375 1.502043 1.029413
O	-7.359056 1.031777 -4.773129	H	2.446871 2.252208 0.419833
O	-6.255630 2.641989 -5.866150	H	3.651326 1.619868 1.559908
C	1.459609 -7.414130 3.258795	N	0.698610 0.477535 0.697081
H	2.151936 -7.402794 2.409601	H	0.596148 1.228606 -0.004017
H	1.027490 -8.421078 3.274476	H	-0.118716 0.402068 1.295583
C	0.389349 -6.376384 3.056976	C	-7.153659 -3.823031 2.184047
C	0.057638 -5.220831 3.723233	H	-7.803716 -4.632784 1.881375
H	0.454258 -4.795267 4.634176	C	-7.323051 -3.270356 3.384839
N	-0.967258 -4.558062 3.056178	Cl	-8.502839 -3.892523 4.492279
H	-1.499820 -3.793582 3.443116	C	-6.020144 -3.455934 1.267914
C	-1.350470 -5.314333 1.966518	H	-5.209235 -4.171089 1.402982
C	-0.512528 -6.457024 1.940674	Cl	-6.518674 -3.690767 -0.457579
C	-0.685641 -7.420651 0.938421	C	-5.492720 -2.052199 1.542973
H	-0.072958 -8.312026 0.954395	H	-6.129147 -1.249241 1.152795
C	-1.660954 -7.233699 -0.027851	Cl	-3.911086 -1.739140 0.670627
H	-1.821332 -8.005354 -0.772102	C	-5.276073 -1.860994 3.043298
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C	-2.466644 -6.072449 -0.017929	C	-6.575158 -2.059918 3.830585
H	-3.277590 -5.979145 -0.737283	H	-6.377922 -2.048221 4.902438
C	-5.738393 3.510296 -2.430385	Cl	-7.652715 -0.623277 3.511673
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H	-5.030963 4.086532 -1.826969	h	-7.202322 -0.302702 -7.011713
N	-6.744256 1.193872 -2.210784	h	2.120508 -7.339909 4.122374
H	-7.037436 1.143735 -3.215816	h	-6.578408 4.151663 -2.697012
C	-6.096060 2.276258 -1.662581	h	2.924033 -2.659544 3.903987
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TS-3

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H	0.923997 -3.572937 -2.259789		N	-6.164091 0.234744 -0.241195
H	1.968759 -3.318921 -0.881651		C	-5.651917 1.510953 -0.402334
C	-0.131169 -2.960298 -0.467594		H	-5.009388 1.954290 0.337631
H	-0.100751 -3.775383 0.254978		C	2.011702 -2.088835 4.018980
H	-0.282180 -2.033257 0.089895		H	1.258178 -2.694992 4.529087
N	-1.405994 -3.195984 -1.267310		H	2.235142 -1.242066 4.676189
H	-1.332059 -2.823106 -2.234391		C	1.410876 -1.511853 2.736601
H	-1.602232 -4.207518 -1.308180		H	1.443515 -2.211418 1.891062
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H	-6.206933 0.932683 -7.766523		H	2.956900 -0.036646 3.003321
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C	-0.656477 -7.430699 0.918901		C	-5.401526 -1.874187 1.340500
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H	-5.044517 4.108789 -1.822613	h	-7.236391 -0.315397 -7.036007
N	-6.728142 1.213436 -2.285913	h	2.089519 -7.398679 4.084901
H	-6.991279 1.158518 -3.371891	h	-6.591626 4.180600 -2.698668
C	-6.124255 2.306838 -1.687273	h	2.957769 -2.682449 3.989525
C	-6.861635 0.243495 -1.383335		