Supporting Information

Cytochrome P-450-Catalyzed Dealkylation of Atrazine in *Rhodococcus* sp. strain NI86/21 Involves Hydrogen Atom Transfer rather than Single Electron Transfer

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1. Material and methods

a) Chemicals

Atrazine (1-chloro-3-ethylamino-5-isopropylamino-2,4,6-triazine, CAS: 1912-24-9) was purchased from Tropitzsch (97.7 %), simazine (2-chloro-4,6-bis(ethylamino)-s-triazine, CAS: 122-34-9, 99,0%), d_{10}-simazine (99.0%) from Dr. Ehrenstorfer GmbH (Augsburg, Germany). Ethyl acetate (99.8% Riedel-de Haën, supplied by Sigma Aldrich, Taufkirchen, Germany) was used as a solvent for standard solutions (GC-IRMS). Aqueous HPLC standards contained atrazine, simazine, hydroxyatrazine (CAS: 2163-68-0), desethylatrazine (CAS: 6190-65-4), and desisopropylatrazine (CAS: 1007-28-9) (96.0%, 99.9%, and 96.3%, respectively; all Riedel de Haën, supplied by Sigma-Aldrich, Seelze, Germany) and had

concentrations of 4.7, 11.6, 23.3, 46.6 and 93.2 µM of the analytes. Potassium permanganate (99%) as oxidative agent was from Sigma Aldrich (Seelze, Germany). Propazine (98.5%, CAS: 139-40-2) as control substance for selective oxidation of permanganate was supplied form Dr. Ehrenstorfer GmbH (Augsburg, Germany). Acetonitrile used as HPLC eluent and reaction medium for the metalloporphyrine system was from Roth (Karlsruhe, Germany), $Na_3PO_4 \cdot 12H_2O$ and $Na_2HPO_4 \cdot 2H_2O$ (for aqueous puffer solution), and dichloromethane for extraction were purchased form Merck (Darmstadt, Germany). 5,10,15,20-tetrakis(pentafluoro-phenyl)porphyrin-iron(III)-chloride (97%, CAS: 36965-71-6 Fluka supplied by Sigma-Aldrich, Seelze, Germany) and sodium periodate (99.8%, CAS:7790-28-5, Sigma-Aldrich) was used as a system biomimicking the cytochrome P450-monoxygenase enzyme.

b) Oxidative degradation with potassium permanganate

Figure S1 shows that during the time of 230 min no propazine was transformed after the addition of permanganate. In comparison to the results for atrazine and simazine, where degradation started immediately, this result shows that attack by permanganate was selective to the ethyl-group of the triazines.

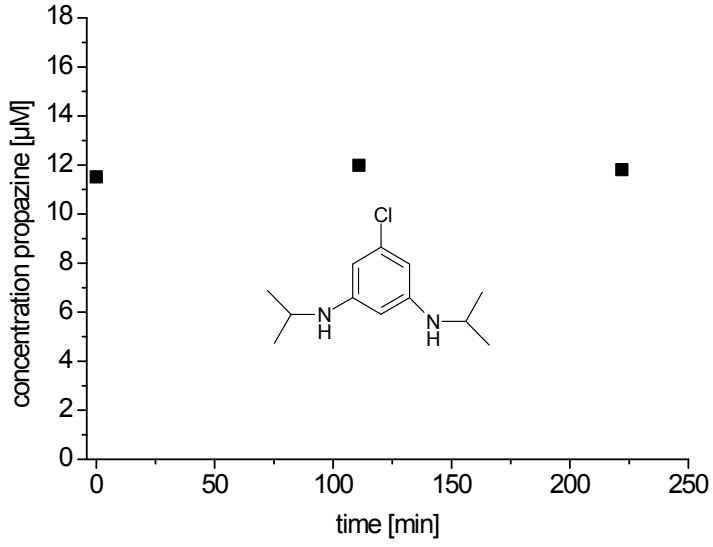


Figure S1. Time course of propazine concentration after adding permanganate.

c) Synthesis of the β-oxidized standard (2-((4-cloro-6-(isopropylamino)-1,3,5-triazine-2-yl)amino)ethanol

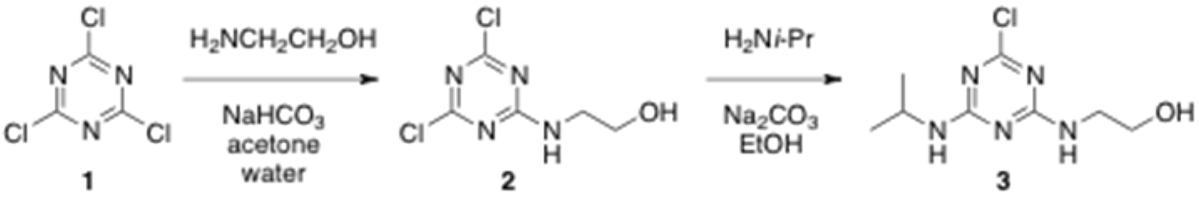


Figure S2. Synthesis of 2-((4-chloro-6-(isopropylamino)-1,3,5-triazine-2-yl)amino)ethanol (**3**) from cyanuric chloride (**1**).

Figure S2 indicates the synthesis of the standard 2-((4-chloro-6-(isopropylamino)-1,3,5-triazine-2-yl)amino)ethanol (β-AETOH) from cyanuric chloride via the intermediate 2-((4,6-dichloro-1,3,5-triazine-2-yl)amino) ethanol.

d) Quantification and identification of atrazine, simazine and its metabolites

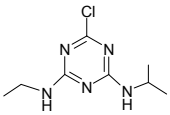
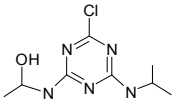
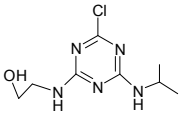
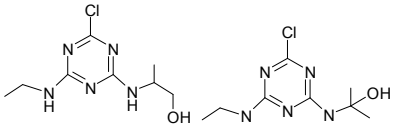
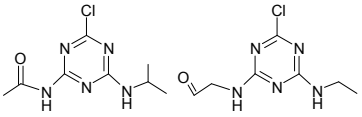
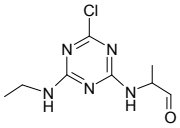
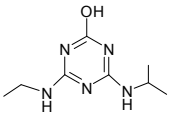
Separation was performed on an ODS (30) (Ultracarb 5µM, 150 x 4.6 mm, Phenomenex, Aschaffenburg) column using gradient elution at a flow rate of 0.8 mL/min. Initial conditions (15% acetonitrile and 85% buffer of KH_2PO_4 0.001 M, pH 7.0) were maintained isocratic for 1 min followed by a linear gradient to 55% acetonitrile within 9 min and a gradient to 75 % acetonitrile within 14 min after which conditions remained 2 min isocratically; a subsequent gradient led to initial conditions within 2 min. The oven-temperature was set to 45°C. Compounds were detected by their UV absorbance at 220 nm and quantified by CLASS-VP V6.10 software (Shimadzu). The relative standard deviation of atrazine, simazine, desethylatrazine, desisopropylatrazine and hydroxyatrazine quantification was less than 5%. Concentrations of the other metabolites could not be determined accurately, since no standards were available. Their relative amounts are indicated by the ratio of their UV absorbance and the absorbance of atrazine or simazine, respectively, at time 0.

e) Identification of further metabolites

Chromatographic separation was carried out by the same analytical column as used for HPLC UV/VIS analysis. The flow rate was 0.4 mL/min. Initial conditions were 15 % acetonitrile and 85 % acetic acid solution (0.1 M) for 1 min, followed by a linear gradient to 55 % acetonitrile within 18 min, a gradient to 75 % within 28 min after which conditions remained isocratic for 4 min; a subsequent gradient led to initial conditions within 3 min. To assign the obtained peaks by their retention time to the analysis of the HPLC UV/VIS we reanalyzed samples on

the HPLC UV/VIS at flow and eluent conditions given for the Q-Trap LC-MS/MS system. Retention times, precursor ($M+H^+$) and MS/MS spectrum ions are shown in Table S1 and S2

Table S1: Identification of biotic and abiotic atrazine degradation products by LC-MS/MS. Scan was done for target molecule-ion. Target molecule ions with no successful hit are in brackets. n.d. = not detected.

Name/abbreviation	structure	target molecule-ion [m/z]	fragment-ions [m/z]	Matches retention time of
Atrazine		216	174, 146, 104	Standard
α−AETOH		232	214, 188, 172, 146	
β−AETOH		232	214,188 172,146	synthesized standard
AIPOH		232	214, 174, 146	
AETOxo		230	188, 146	
AIPOxo		(230)	n.d.	
HAT		(198)	n.d.	

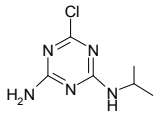
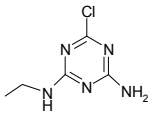
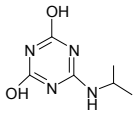
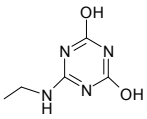
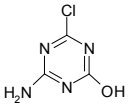
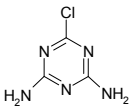
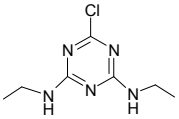
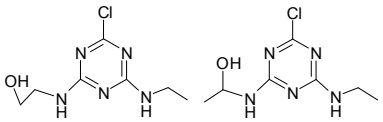
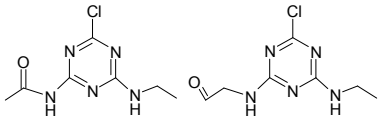
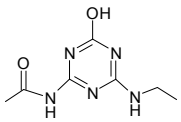
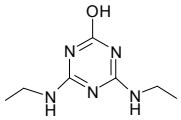
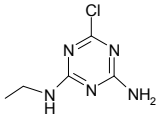
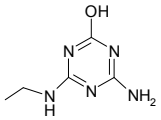
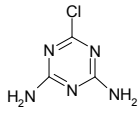
DEA		188	146, 104	Standard
DIA		174	146, 132, 104	Standard
2,6-Dihydroxy-4-(N'-isopropylamino)-1,3,5-triazine		(170)	n.d.	
2,4-Dihydroxy-6-(N'-ethylamino)-1,3,5-triazine		(157)	n.d.	
2-Chloro-4-hydroxy-6-amino-1,3,5-triazine		(147)	n.d.	
2-Chloro-4,6-diamino-1,3,5-triazine		(146)	n.d.	

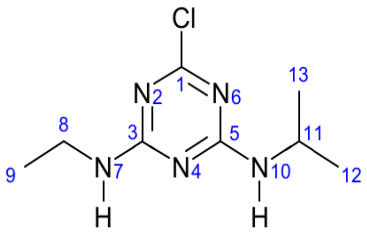
Table S2: Identification of biotic and abiotic simazine degradation products by LC-MS/MS. Scan was done for target molecule-ion. Target molecule ions with no successful hit are in brackets. n.d. = not detected.

Name/abbreviation	structure	target molecule-ion [m/z]	fragment-ions [m/z]	Matches retention time of
Simazine		202	174, 132, 104	Standard

SETOH		218	200, 174, 146, 104	
SETOxo		216	174, 146, 104	
ODET		(198)	n.d.	
OEET		(184)	n.d.	
DES		174	146, 132, 104	Standard
OEAT		(154)	n.d.	
CAAT		(146)	n.d.	

f) Computational methods

In the following section all coordinates optimized for single electron transfer (SET) and hydrogen atom abstraction (either in α- or in β- position) at the alkyl chain of atrazine are



given.

SET mechanism

Table S3. SET mechanism (KIEs data listed for the estimated low limit of atrazine redox potential of 0.8 V and λ=300 kJ/mol).

	KIE	EIE
Averaged ^{15}N KIE over 5 N positions	0.9986	0.9993
^{15}N KIE reactive position[a]	1.0011	0.9960
^{15}N KIE reactive position [b]	0.9953	1.0063

[a] N7 nitrogen atom adjacent to ethyl side-chain
[b] N10 - nitrogen atom adjacent to isopropyl side-chain

	KIE
Averaged ^{13}C KIE over 8 C positions	0.9965
^{13}C KIE reactive position[a]	0.9875

[a] C11

Table S4. Position specific isotope effects associated to SET

Nitrogen

N2	0.9994
N4	0.9988
N6	1.0001
N7	1.0011
N10	0.9953

Carbon

C1	0.9991

C3	0.9974
C5	0.9914
C8	0.9997
C9	1.0009
C11	0.9875
C12	0.9917
C13	1.0051

Table S5. SET mechanism, differences in geometries of neutral and radical cation form

bond	neutral	radical cation
C5-N10	1.34	1.39
N10-C11	1.46	1.43
C3-N7	1.34	1.32
N7-C8	1.46	1.46

HAT mechanism

α-C oxidation

Table S6. HAT mechanism: atrazine + $OOH^{\bullet}$. All N KIEs were calculated using small curvature semiclassical ground state approximation by Skodje&Truhlar for tunneling effect.

	isopropyl	ethyl
Average ^{15}N KIE over 5 N positions	1.0024	1.0016
^{15}N KIE reactive position*	1.0088	1.0061
$\Delta G^{\neq}$ (kcal/mol)	19.5	20.3
ΔG (kcal/mol)	7.7	9.0

*reactive position: nitrogen atom adjacent to carbon atom which hydrogen atom is abstracted from

Table S7. HAT mechanism: atrazine + $OOH^{\bullet}$. All C KIEs were calculated using small curvature semiclassical ground state approximation by Skodje&Truhlar for tunneling effect.

	isopropyl	ethyl
Average ^{13}C KIE over 8 C positions	1.0087	1.0068
^{13}C KIE reactive position*	1.0558	1.0451

*reactive position: carbon atom which hydrogen atom is abstracted from

Table S8. Position specific isotope effects associated to HAT at the αC-atom (C11 or C8)

Nitrogen:

	isopropyl	ethyl
N2	1.0002	1.0006
N4	1.0010	1.0005
N6	1.0010	1.0006
N7	1.0013	**1.0061**
N10	**1.0088**	1.0000

Carbon:

	isopropyl	ethyl
C1	1.0006	1.0008
C3	1.0009	1.0039
C5	1.0030	1.0013
C8	0.9995	**1.0451**
C9	0.9999	1.0034
C11	**1.0558**	0.9997
C12	1.0030	1.0004
C13	1.0070	0.9998

β-C oxidation

Table S9. HAT mechanism: atrazine + $OOH^{\bullet}$. All C KIEs were calculated using small curvature semiclassical ground state approximation by Skodje&Truhlar for tunneling effect.

	isopropyl	ethyl
$\Delta G^{\neq}$ (kcal/mol)	23.1	21.4
ΔG (kcal/mol)	13.1	12.3
Average ^{15}N KIE	1.0002	1.0000
^{15}N KIE reactive position[a]	1.0009	1.0001
Average ^{13}C KIE	1.0065	1.0061
^{13}C KIE reactive position[b]	1.0210	1.0456

^{13}C KIE reactive position[c]	1.0278	n/a

[a] nitrogen atom adjacent to carbon atom which hydrogen atom is abstracted from: N10 and N7 in the case of isopropyl and ethyl side chain, respectively
[b] hydrogen abstracted from C12 position
[c] hydrogen abstracted from C13 position

Table S10. Position specific isotope effects associated to HAT at the βC-atom (C9, C12 or C13)

Nitrogen

N2	1.0001	1.0003
N4	1.0000	0.9997
N6	1.0001	0.9996
N7	0.9999	**1.0001**
N10	**1.0009**	1.0000

Carbon

	isopropyl	ethyl
C1	1.0001	0.9999
C3	1.0000	1.0003
C5	1.0003	1.0005
C8	1.0000	1.0030
C9	0.9998	**1.0456**
C11	1.0034	1.0000
C12	**1.0210**	0.9998
C13	**1.0278**	0.9999

HAT reaction PROMOTED BY permanganate at ethyl site chain

α-C oxidation

Table S11. HAT mechanism: atrazine + MnO_4^-. All N KIEs were calculated using small curvature semiclassical ground state approximation by Skodje&Truhlar for tunneling effect.

Average ^{15}N KIE over 5 N positions	1.0024
^{15}N KIE reactive position*	1.0112
$\Delta G^{\neq}$ (kcal/mol)	19.5
ΔG (kcal/mol)	-82.3

*reactive position: nitrogen atom adjacent to carbon atom which hydrogen atom is abstracted from

Table S12. HAT mechanism: atrazine + MnO_4^-. All C KIEs were calculated using small curvature semiclassical ground state approximation by Skodje&Truhlar for tunneling effect.

Average ^{13}C KIE over 8 C positions	1.0053
^{13}C KIE reactive position*	1.0335

*reactive position: carbon atom which hydrogen atom is abstracted from

Table S13. Position specific isotope effects associated to permanganate HAT reaction at the αC-atom (C8)

Nitrogen:

N2	0.9998
N4	1.0015
N6	0.9999
N7	**1.0112**
N10	1.0024

Carbon:

C1	1.0001
C3	1.0052
C5	1.0004
C8	**1.0335**
C9	1.0036
C11	1.0001
C12	0.9993
C13	1.0001

β-C oxidation

Table S14. HAT mechanism: atrazine + MnO_4^-. All N KIEs were calculated using small curvature semiclassical ground state approximation by Skodje&Truhlar for tunneling effect.

Average ^{15}N KIE over 5 N positions	1.0003
^{15}N KIE reactive position*	1.0017
$\Delta G^{\neq}$ (kcal/mol)	25.3
ΔG (kcal/mol)	-77.1

*reactive position: N7 position

Table S15. HAT mechanism: atrazine + MnO_4^-. All C KIEs were calculated using small curvature semiclassical ground state approximation by Skodje&Truhlar for tunneling effect.

Average ^{13}C KIE over 8 C positions	1.0056
^{13}C KIE reactive position*	1.0314

*reactive position: carbon atom which hydrogen atom is abstracted from

Table S16. Position specific isotope effects associated to permanganate HAT reaction at the βC-atom (C9)

Nitrogen:

N2	1.0000
N4	1.0001
N6	1.0000
N7	**1.0017**
N10	0.9998

Carbon:

C1	1.0000
C3	1.0008
C5	0.9999

C8	1.0128
C9	**1.0314**
C11	0.9998
C12	1.0001
C13	0.9999

hydride transfer reaction at ethyl site chain

α-C oxidation

Table S17. Hydride mechanism: atrazine + H_3O^+. All N KIEs were calculated using small curvature semiclassical ground state approximation by Skodje&Truhlar for tunneling effect.

Average ^{15}N KIE over 5 N positions	0.9980
^{15}N KIE reactive position*	0.9966
$\Delta G^{\neq}$ (kcal/mol)	35.1
ΔG (kcal/mol)	10.5

*reactive position: nitrogen atom adjacent to carbon atom which hydrogen atom is abstracted from

Table S18. Hydride mechanism: atrazine + H_3O^+. All C KIEs were calculated using small curvature semiclassical ground state approximation by Skodje&Truhlar for tunneling effect.

Average ^{13}C KIE over 8 C positions	1.0039
^{13}C KIE reactive position*	1.0315

*reactive position: carbon atom which hydrogen atom is abstracted from

Table S19. Position specific isotope effects associated to hydride reaction at the αC-atom (C8)

Nitrogen:

N2	0.9983
N4	0.9979
N6	0.9989
N7	**0.9966**

N10	0.9985

Carbon:

C1	0.9987
C3	1.0007
C5	0.9995
C8	**1.0315**
C9	0.9998
C11	1.0008
C12	1.0001
C13	0.9999

2 Results and Discussion

a) Degradation products in oxidation of atrazine and simazine with MnO_4^-

Analog to atrazine, the α-position of the ethylgroup of simazine was mainly oxidized by permanaganate. A futher description can be found in the SI. Oxidation by permanganate gave the main product desethylsimazine, together with the products identified by LC-MS/MS analysis mass spectra as SETOH and SETOXO (structures see Figure 1). Considering the evolution of their concentrations with time and assuming the same regioselectivity as for atrazine, they can tentatively be attributed to α-SETOH (different retention times as SETOH of biotic experiment) and α–SETOXO as intermediates of simazine desethylation. This is also confirmed from the biotic experiment, where the SETOH had a different retention time, whereas the SETOXO eluted at the same time. Two other metabolites denoted as PS1 and PS2 did not match any of the scanned mass spectra (Table S2). Thus we expected them to be products of mixed oxidation in both ethyl groups.

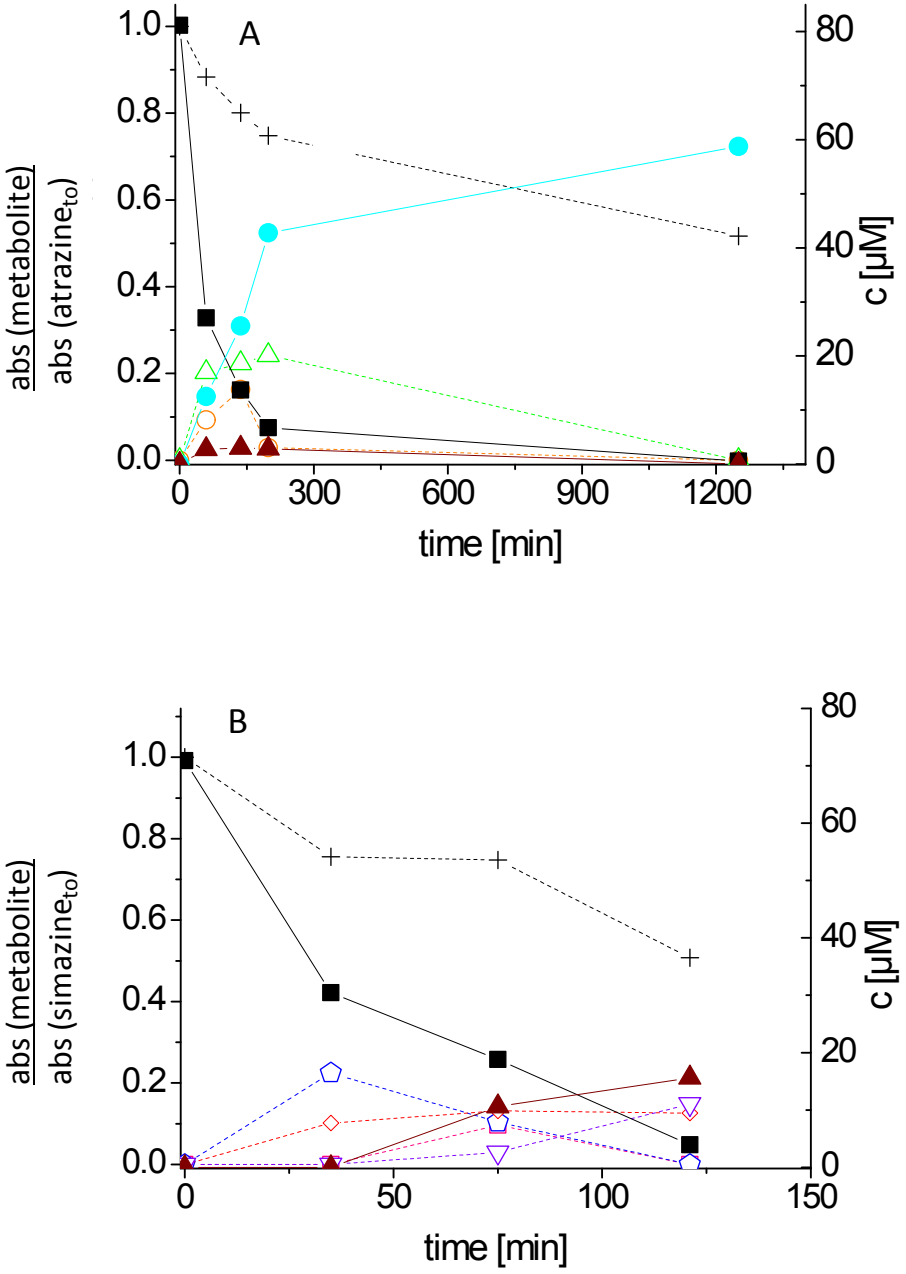


Figure S3. Time course of atrazine (A) and simazine (B) concentrations and formation of products during transformation by permanganate. Data with solid lines and solid symbols can be read on the right ordinate, giving the concentration of atrazine (black squares), DEA (cyan circles), DIA (brown triangles) and of simazine (black squares) and DES (brown triangles), respectively. Data with dashed lines and open symbols correspond to the left ordinate giving the relative amount by the ratio of UV/VIS absorbances at 220 nm, (abs (metabolite)$_{220nm}$/abs (triazine$_{t=0}$)$_{220nm}$). Crosses represent the molar balance based on the assumption that metabolites have nearly the same UV absorbance as atrazine or simazine, respectively. In

panel A, open orange circles denote α-AETOH and open green triangles α-AETOXO. In panel B, open blue pentagons represent α-SETOH, open pink squares metabolite α-SETOXO, and open violet triangles and open red rhombs represent unidentified products.

b) Atrazine degradation products in oxidation with an iron porpyhrine model system (FeP)

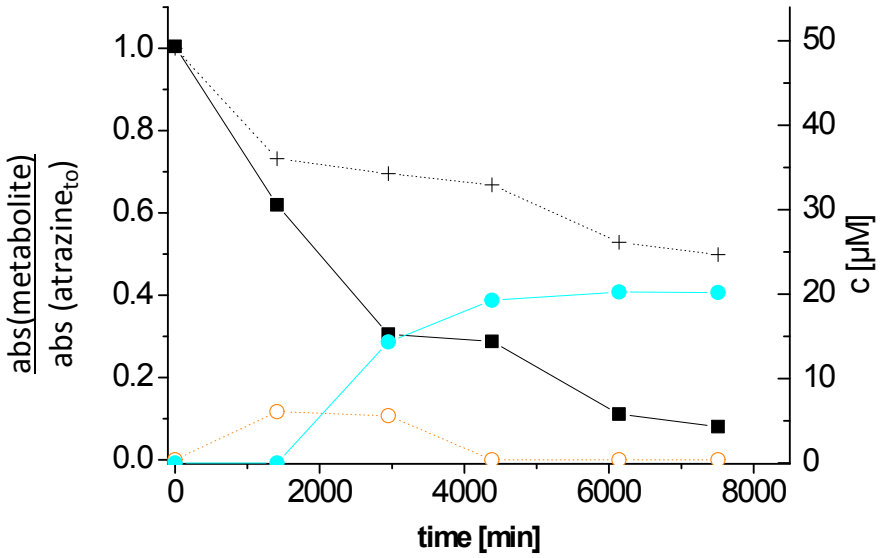


Figure S4. Time course of atrazine concentration and formation of products during transformation by FeP for one (the one which was sacrified as last) of 8 batches. Atrazine concentration and metabolite formation were continuously measured until sample was sacrified for istotpe analysis. For data with solid lines and filled symbols the right y-axis give the concentrations were determined according to their standards: Black squares indicate atrazine, cyan circles denote DEA. Open green circles repsresent relative amount of α-AETOH by the ratio of UV/VIS absorbances at 220 nm, (abs (metabolite)$_{220nm}$/abs (triazine$_{t=0}$)$_{220nm}$). Crosses represent the molar balance based on the assumption that metabolites have nearly the same UV absorbance as atrazine (both left y-axis).

c) Atrazine and simazine degradation products with Rhodococcus sp. NI86/21

For simazine a similiar picture as for atrazine degradation was observed and is illustrated in Figure S6. Besides the dealkylated product desethlysimazine (DES=DIA), we found evidence for metabolites which contained a hydroxyl- or an oxo-group either in the α- or in the β-position of the alkyl side chain. One of them was characterized as hydroxyethylsimazine

(SETOH, Table S2). During the degradation this product accumulated in small amounts besides DES. Thus we assumed that this product was oxidized in the β-position. The other metabolite identified as oxoethylsimazine decreased after its initial formation during the degradation process, suggesting that this product was an intermediate of the dealkylation pathway (see also permanganate oxidation). Identification of the third transformation product was not possible. Monitoring characteristic masses of possible follow up products of DES such as desethylhydroxysimazine, 2,4-dihydroxy-6-(N'-ethyl)amino-1,3,5-s-triazine, 2-chloro-4-hydroxy-6-amino-1,3,5-s-triazine and 2-chloro-4,6-diamino-s-triazine did not match (SI Table). Also, we did not detect a peak which was related to the mass of hydroxysimazine, the product of the alternative hydrolytic pathway.

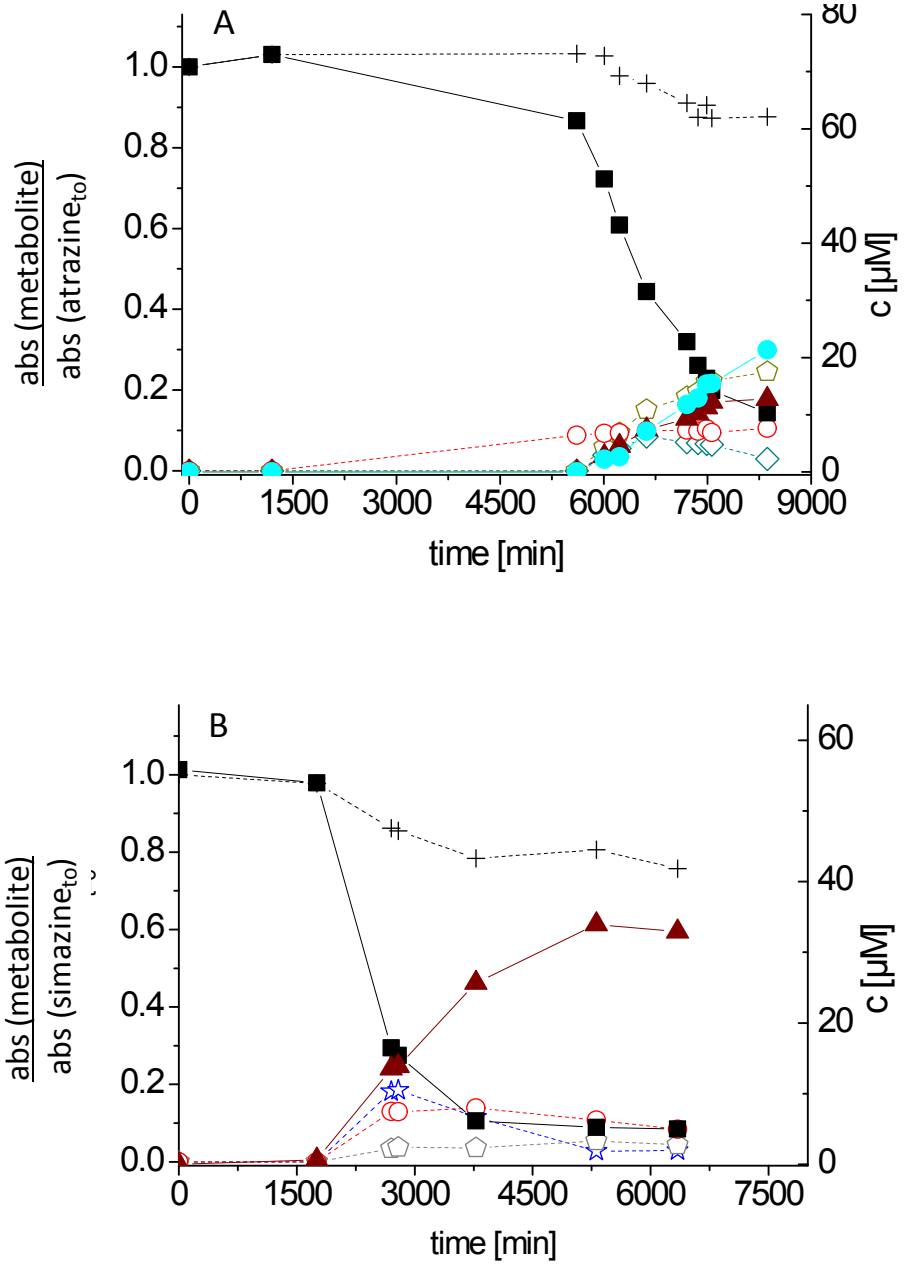


Figure S5. Time course of atrazine (A) and simazine (B) concentrations and formation of products during transformation by *Rhodococcus* sp. NI86/21. Data with solid lines and solid symbols can be read on the right ordinate, giving the concentration of atrazine (black squares), DEA (cyan circles), DIA (brown triangles) and of simazine (black squares) and DES (brown triangles), respectively. Data with dashed lines and open symbols correspond to the left ordinate giving the relative amount by the ratio of UV/VIS absorbances at 220 nm, (abs (metabolite)$_{220nm}$/abs (triazine$_{t=0}$)$_{220nm}$). Crosses represent the molar balance based on the assumption that metabolites have nearly the same UV absorbance as atrazine or simazine, respectively. In panel A, open red circles represent metabolite β-AETOH, open green pentagons β-AIPOH and open turqoise rhombs α-AETOxo.

d) Theoretical isotope effect computations for SET or HAT in atrazine

HAT in α- versus β- position. When HAT was assumed exclusively in α-position of the isopropyl group, ε_{carbon} was slightly greater (-8.8 ‰) than for the same scenario the ethyl group (-6.8 ‰), and the same was true for $\varepsilon_{nitrogen}$ (-2.4‰ compared to -1.4‰). The numbers changed drastically for βC-atom oxidation by HAT where, nitrogen isotope effects decreased to being practically non-existent, and also average carbon isotope effects became smaller (ε_{arbon} = -6.1 ‰ for βC-atom oxidation in the ethyl chain, ε_{arbon} = -6.5 ‰ in the isopropyl chain). These results show that HAT-associated isotope fractionation in the compound average of atrazine may change with the contribution of αC- versus βC- oxidation and must, therefore, be interpreted in the context of product distribution. Applying the product distribution derived above (α-C in ethyl group: 35%, β-C in ethyl group: 34%, α-C in isopropyl group:17%, β-C in isopropyl goup: 14%) theoretical $\varepsilon_{\alpha+\beta}$ values of -6,9‰ for carbon and -1.0‰ for nitrogen are obtained. Figure S7 visualizes the difference between αC- and βC-oxidation even more clearly in predicted dual element isotope plots. For the αC-oxidation we obtain a slopes up to Λ=0.27, whereas for βC-oxidation the slope tends to be 0. Considering the product distribution in the biotic experiment we would expect a slope which should lay with $\Lambda = \varepsilon_{\alpha+\beta\_nitrogen} / \varepsilon_{\alpha+\beta\_carbon}$ =0.15 in between that range.

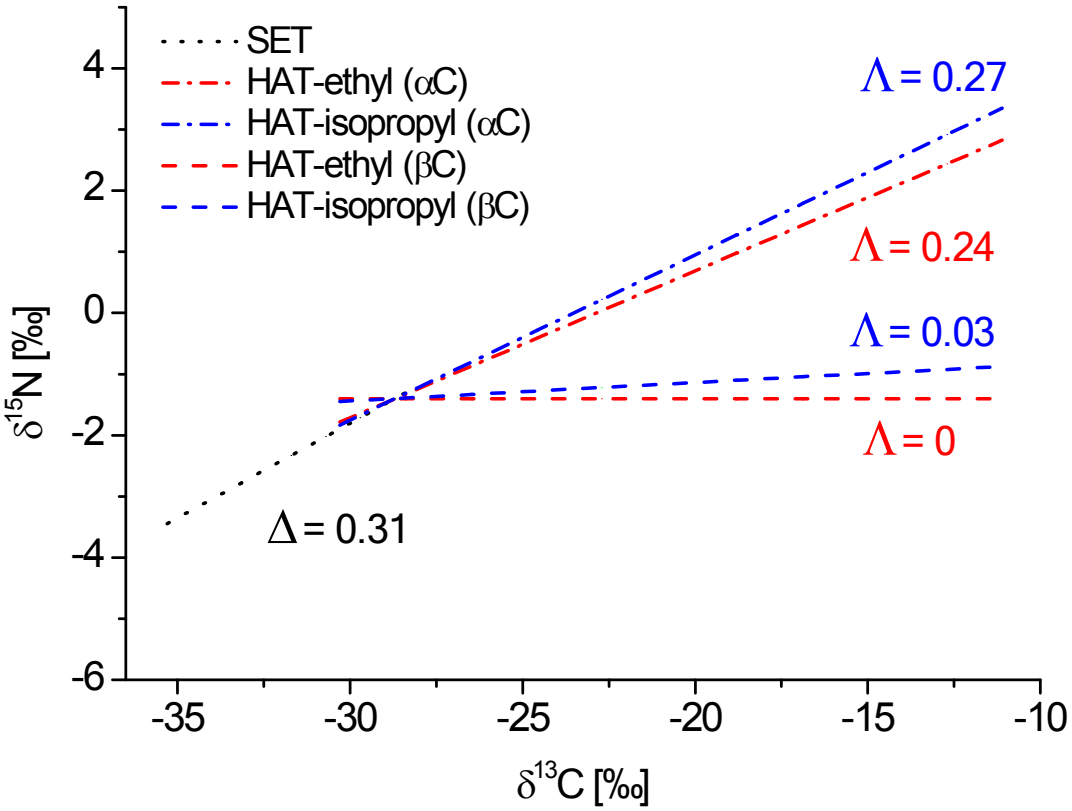


Figure S6. Theoretical C and N dual isotope plots according to HAT or SET. For HAT four different slopes were derived considering either αC or βC-oxidation of the ethyl- or isopropyl-group. Slopes Λ were estimated according to equation 7 from calculated $\varepsilon_{average}$ for carbon and nitrogen. Observed isotope effects during biotic and abiotic oxidation of atrazine and simazine

e) Observed isotope effects during biotic and abiotic oxidation of atrazine and simazine

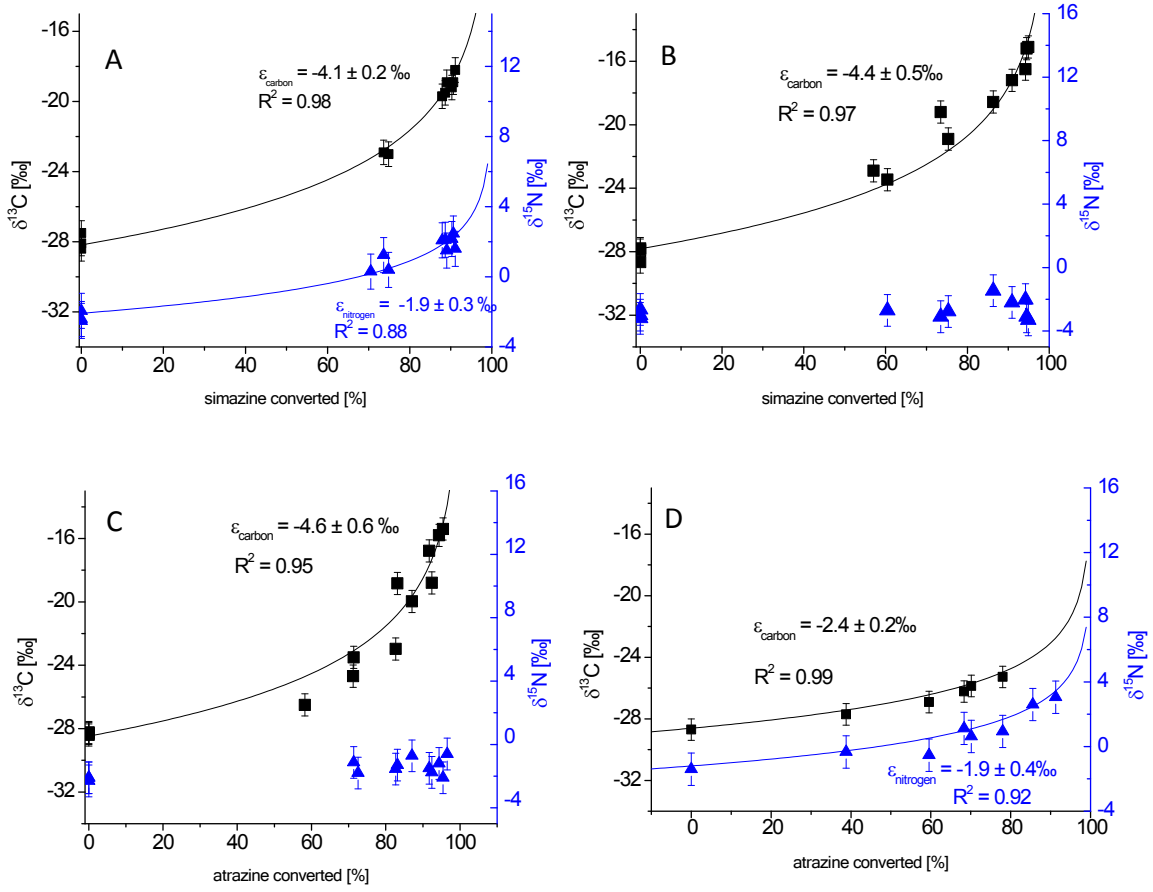


Figure S7. C and N isotope shifts of simazine and atrazine associated to degradation caused by *Rhodococcus* sp. NI86/21 (A), permanganate (B and C) or FeP (D), together with Rayleigh fits and corresponding enrichment factors ε. Error bars indicate the total uncertainity of carbon (± 0.7 ‰) and nitrogen isotope values (± 1.0 ‰).

f) Observed intermolecular $KIE_{H,\ ethyl\ side\ chain}$ of competition experiment of degradation experiment with *Rhodococcus* sp. NI86/21 fed with simazine and $simazine_{d10}$

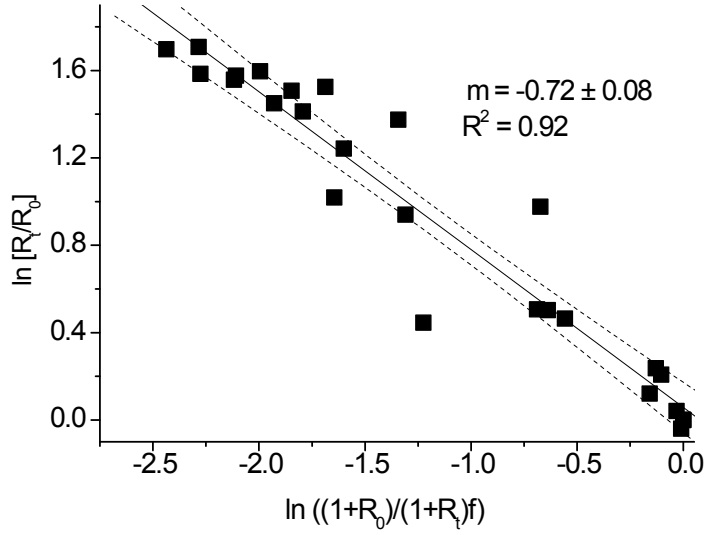


Figure S8. Logarithmic plot according to equation 5 to determine position-specifc hydrogen isotope effects in the ethyl side chain of simazine related to the competitive degradation of simazine and simazine$_{d10}$ by Rhodoccous sp. NI86/21. slope $m=1/\varepsilon_H$. Regressions is given together with 95% confidence intervals. According to equation 6 the $KIE_{H,\ ethyl\ side\ chain}$ of this transformation reaction is 3.6 ± 0.8.

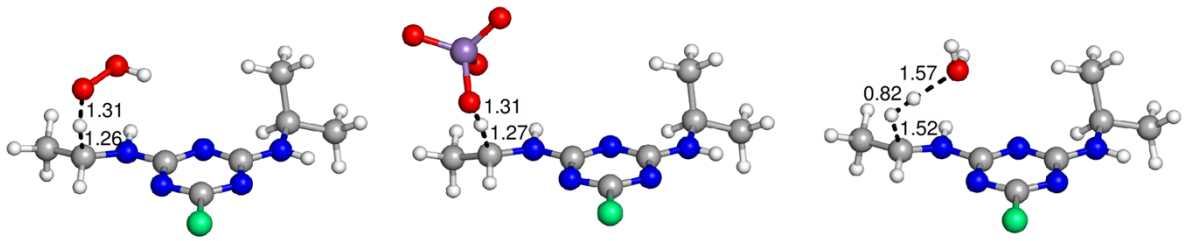


Figure S9. Samples of the located transition states for the reaction with (from left) $OOH^{\bullet}$, MnO_4^-, and H_3O^+.

Optimized Cartesian coordinates of all stationary points described in this study

SET mechanism

NEUTRAL SPECIES

N	0.759186	0.829832	-0.143846
C	0.862250	-0.523699	-0.034229
N	-0.171221	-1.348666	0.184341
C	-1.369503	-0.758016	0.293090
N	-1.582844	0.583433	0.197180
C	-0.475120	1.256974	-0.014431
CL	-0.670365	2.994729	-0.143047
N	-2.426898	-1.544440	0.540165
N	2.075929	-1.072537	-0.181222
C	-3.813996	-1.094757	0.506654
C	-4.364488	-0.973445	-0.908360
C	3.332970	-0.323110	-0.255843
C	3.757038	0.181027	1.121099
C	4.395538	-1.223314	-0.870751
H	-4.391621	-1.822831	1.079427
H	-3.878835	-0.139938	1.030698
H	-3.783590	-0.252998	-1.491645
H	-4.332026	-1.939857	-1.419832
H	-5.403891	-0.634002	-0.877773
H	-2.246916	-2.540177	0.502343
H	2.968198	0.784540	1.578752
H	3.978711	-0.663924	1.782191
H	4.657837	0.796125	1.034499
H	5.346904	-0.687604	-0.921196
H	4.541086	-2.118272	-0.255066
H	4.119767	-1.534985	-1.881835
H	3.159949	0.531065	-0.914683
H	2.133421	-2.070849	-0.013772

RADICAL CATION SPECIES

N	0.751010	0.888739	-0.126608
C	0.843440	-0.441115	-0.033830
N	-0.119507	-1.322554	0.148339
C	-1.361976	-0.766702	0.253068
N	-1.583210	0.568723	0.170424
C	-0.504241	1.296290	-0.005601
CL	-0.739695	3.008872	-0.096605
N	-2.377039	-1.589300	0.455246
N	2.110726	-0.997053	-0.145688
C	-3.778504	-1.176734	0.512214
C	-4.388326	-1.006605	-0.872014
C	3.343592	-0.273866	-0.226378
C	3.834927	-0.095692	1.242974
C	4.352089	-1.059513	-1.053044
H	-4.303161	-1.951644	1.072175
H	-3.837975	-0.249112	1.083849
H	-3.859937	-0.237244	-1.441777
H	-4.349443	-1.945918	-1.429967
H	-5.434817	-0.705087	-0.774872

H	-2.157676	-2.579631	0.464761
H	3.102966	0.461483	1.829600
H	4.019547	-1.071756	1.696553
H	4.769453	0.467029	1.180536
H	5.288888	-0.499132	-1.065721
H	4.535662	-2.041556	-0.607268
H	3.998262	-1.184621	-2.078297
H	3.128342	0.711144	-0.642559
H	2.154843	-2.021042	-0.061062

HAT mechanism

α-oxidation

ISOPROPYL SIDECHAIN

REACTANTS

C	1.426106000	-1.658270000	-0.109924000
N	1.943477000	-0.450915000	-0.198216000
C	1.016736000	0.534095000	-0.142353000
C	-0.693653000	-0.975371000	0.076564000
N	0.177478000	-2.024747000	0.030345000
Cl	2.584465000	-2.964862000	-0.185216000
N	-0.317786000	0.312221000	-0.018096000
N	1.431021000	1.795723000	-0.230761000
H	0.724089000	2.523233000	-0.141879000
N	-1.974961000	-1.303581000	0.242338000
C	-3.116744000	-0.388697000	0.283433000
C	2.833813000	2.192338000	-0.320151000
H	2.840351000	3.197105000	-0.745830000
H	3.337395000	1.529442000	-1.026104000
C	3.542174000	2.184537000	1.028079000
H	3.538486000	1.183016000	1.465935000
H	4.581402000	2.500695000	0.900628000
H	3.057030000	2.873283000	1.725298000
H	-2.168456000	-2.298952000	0.262991000
C	-4.252152000	-1.080208000	1.025636000
H	-2.813602000	0.489425000	0.861229000
C	-3.541052000	0.022903000	-1.125000000
H	-5.123209000	-0.421427000	1.060986000
H	-4.540752000	-2.000802000	0.506284000
H	-3.962691000	-1.329600000	2.049814000
H	-4.330231000	0.778460000	-1.073809000
H	-2.703862000	0.433752000	-1.696893000
H	-3.927990000	-0.849004000	-1.662649000
O	-1.868796000	2.432008000	-0.196356000
H	-1.289015000	1.561304000	-0.131085000
O	-1.038807000	3.435975000	-0.089046000

TRANSITION STATE

C	-1.4473880	1.5215020	-0.0189390
N	-2.0359750	0.3719780	-0.2698030
C	-1.1565880	-0.6315260	-0.5166230
C	0.6216590	0.7379900	-0.2460240
N	-0.1680030	1.8130730	0.0228120
Cl	-2.5273610	2.8560980	0.3078140
N	0.1849870	-0.4863260	-0.5158550
N	-1.6381000	-1.8437950	-0.8046100
H	-0.9501480	-2.5795100	-0.9114800
N	1.9552540	0.9845430	-0.2133030
C	2.9955490	0.0308740	-0.4180720
C	-3.0463480	-2.2168960	-0.7234490
H	-3.1776440	-3.0834050	-1.3737500
H	-3.6423670	-1.4018060	-1.1363080
C	-3.4921550	-2.5440600	0.6958010
H	-3.3459210	-1.6860590	1.3579470
H	-4.5540870	-2.8056220	0.6999360
H	-2.9271770	-3.3914050	1.0943170
H	2.2084210	1.8772690	0.1986260
C	4.3283800	0.6040430	0.0077300
H	2.7688570	-0.8884270	0.4098120

C	3.0185420	-0.6396370	-1.7791330
H	5.0995880	-0.1662450	-0.0585060
H	4.6122710	1.4325670	-0.6531860
H	4.2895470	0.9754490	1.0360830
H	3.7560660	-1.4460660	-1.7729400
H	2.0470560	-1.0470780	-2.0565930
H	3.3225760	0.0981690	-2.5324270
O	1.7121420	-0.8829500	2.2264790
H	0.8047900	-1.0224200	1.8999180
O	2.4923910	-1.6756890	1.4014300

PRODUCTS

C	-1.7145860	-1.4673530	-0.0348820
N	-2.0886950	-0.2444880	0.2839120
C	-1.0456910	0.6073930	0.4341060
C	0.4690260	-1.0334060	0.0084130
N	-0.5094210	-1.9575630	-0.1969260
CL	-3.0219340	-2.6027020	-0.2757030
N	0.2498530	0.2498820	0.3074710
N	-1.3001070	1.8834420	0.7417250
H	-0.4973150	2.5028780	0.7439090
N	1.7330630	-1.4819640	-0.1383710
C	2.9286250	-0.8083610	0.1518130
C	-2.6265480	2.4913660	0.6881140
H	-2.5947620	3.3710000	1.3334640
H	-3.3414910	1.7902250	1.1200300
C	-3.0316470	2.8820480	-0.7267060
H	-3.0505760	2.0072940	-1.3830590
H	-4.0298920	3.3286620	-0.7197050
H	-2.3299130	3.6114960	-1.1414860
H	1.8032780	-2.4013850	-0.5663100
C	4.1357020	-1.4272160	-0.4704110
H	3.5653770	1.6547480	-0.6988310
C	3.0735880	-0.1297230	1.4768930
H	4.9741740	-0.7263280	-0.4455350
H	4.4474260	-2.3302370	0.0797940
H	3.9511500	-1.7164070	-1.5090420
H	4.0073600	0.4375740	1.5009900
H	2.2492650	0.5462120	1.7070730
H	3.1219940	-0.8856740	2.2775500
O	1.7734280	2.0643790	-1.1632210
H	1.3200260	1.4576310	-0.5229750
O	2.9832120	2.4061930	-0.4914840

ETHYL SIDECHAIN, PATHWAY 1

REACTANTS

C	0.6791970	2.1395900	-0.0882180
N	-0.5524750	1.6947150	-0.2217620
C	-0.6297420	0.3403340	-0.1661040
C	1.6056240	0.1227800	0.1278230
N	1.7949180	1.4772700	0.0869760
CL	0.8449480	3.8828090	-0.1531170
N	0.4213180	-0.4806100	0.0063770
N	-1.8334350	-0.2279610	-0.3162760
H	-1.8675990	-1.2322110	-0.1902310
N	2.7081040	-0.6121540	0.3304130
C	2.7691450	-2.0706340	0.2175010
C	-3.0923210	0.5064260	-0.3644840
H	-3.8222800	-0.1536400	-0.8379110
H	-2.9627160	1.3708180	-1.0176310
C	-3.5810640	0.9413380	1.0110030
H	-2.8427040	1.5837450	1.4994750
H	-4.5160470	1.5008700	0.9145550
H	-3.7638150	0.0731490	1.6512970
H	3.5861410	-0.1052090	0.3186840
C	3.9972840	-2.5608930	0.9713460
H	1.8697910	-2.4667190	0.6950210
C	2.8011860	-2.5085070	-1.2452270
H	4.0727420	-3.6480640	0.8887420
H	4.9066460	-2.1230530	0.5439080

H	3.9467200	-2.2957630	2.0308110
H	2.7834490	-3.6003830	-1.3115770
H	1.9414160	-2.1151960	-1.7941850
H	3.7165510	-2.1477990	-1.7267320
O	-3.6491340	-2.8458740	-0.5665760
H	-4.2201000	-2.4367130	-1.2512410
O	-4.1330120	-2.4832510	0.5925830

TRANSITION STATE

C	0.1190140	1.9910330	-0.0477700
N	1.1064390	1.1668960	-0.3532330
C	0.6736390	-0.0915930	-0.5756400
C	-1.4838550	0.4409110	-0.1794720
N	-1.1606450	1.7470870	0.0613840
CL	0.5982590	3.6430440	0.2571850
N	-0.5930100	-0.5080630	-0.4969750
N	1.5964640	-1.0241370	-0.9296030
H	1.2514250	-1.9792980	-0.9549550
N	-2.7803450	0.1325800	-0.1025630
C	-3.3308970	-1.2203000	-0.2135850
C	2.9943070	-0.8400960	-0.8521030
H	3.2715380	-0.8523410	0.3722640
H	3.2950290	0.1600600	-1.1647300
C	3.7763180	-1.9737180	-1.4641540
H	3.6160420	-2.0134140	-2.5472810
H	4.8422660	-1.8316260	-1.2768720
H	3.4715890	-2.9325970	-1.0330200
H	-3.4012970	0.8790120	0.1896890
C	-4.8045660	-1.1111770	-0.5782800
H	-2.7946530	-1.7201450	-1.0241870
C	-3.1300990	-1.9997310	1.0835030
H	-5.2363880	-2.1112540	-0.6660680
H	-5.3526360	-0.5703980	0.2014310
H	-4.9425640	-0.5909260	-1.5298890
H	-3.4954420	-3.0241170	0.9658620
H	-2.0731380	-2.0384520	1.3604980
H	-3.6876110	-1.5251640	1.8980110
O	2.1340040	-1.7549530	1.8941230
H	1.4767180	-1.0662930	2.0958610
O	3.3064000	-1.0559570	1.6625240

PRODUCTS

C	0.4069850	1.8404700	-0.2584050
N	1.2983170	0.9033460	-0.5201400
C	0.7309750	-0.3158180	-0.6700960
C	-1.3559480	0.4694450	-0.3258500
N	-0.8930210	1.7437600	-0.1368350
CL	1.0655770	3.4458010	-0.0361180
N	-0.5795220	-0.5824120	-0.6006120
N	1.5523840	-1.3662290	-0.9068430
H	1.0902510	-2.2688880	-0.9729610
N	-2.6817050	0.3054260	-0.2405730
C	-3.3504980	-0.9970510	-0.1939000
C	2.9350330	-1.3437820	-0.8892680
H	2.9001140	-1.0405690	1.3066940
H	3.3977010	-0.3692840	-0.9675900
C	3.6450940	-2.5875130	-1.2876740
H	3.5812920	-2.7611710	-2.3724060
H	4.7024210	-2.5191270	-1.0253950
H	3.2210980	-3.4660290	-0.7894190
H	-3.2126990	1.1173630	0.0543690
C	-4.8210340	-0.7950820	-0.5295170
H	-2.8869340	-1.6245990	-0.9592370
C	-3.1696240	-1.6514610	1.1735790
H	-5.3444410	-1.7535530	-0.4875360
H	-5.2888160	-0.1204290	0.1964160
H	-4.9474880	-0.3739420	-1.5305640
H	-3.6105940	-2.6526680	1.1724440
H	-2.1098680	-1.7415900	1.4286340
H	-3.6659360	-1.0543590	1.9460690
O	1.2880450	-0.8082640	2.2844730

H	1.0606910	0.1312940	2.1781010
O	2.7116210	-0.7946790	2.2353020

ETHYL SIDECHAIN, PATHWAY 2

REACTANTS

C	-0.5181080	-1.3307390	-0.0652620
N	-1.1427760	-0.1616640	0.0345900
C	-0.2909320	0.9034210	0.0920130
C	1.5285200	-0.4397060	-0.1030980
N	0.7571520	-1.5750330	-0.1349870
CL	-1.5686890	-2.7225780	-0.1135410
N	1.0451330	0.7970070	0.0202560
N	-0.7990300	2.1269310	0.2490360
H	-0.1265020	2.8835820	0.2231370
N	2.8437860	-0.6289860	-0.2170950
C	3.8490550	0.4323080	-0.1187190
C	-2.2183540	2.4603790	0.2797580
H	-2.2982840	3.4204300	0.7919310
H	-2.7349950	1.7277110	0.9038630
C	-2.8371400	2.5503120	-1.1092670
H	-2.6918520	1.6231460	-1.6721000
H	-3.9112460	2.7388980	-1.0267560
H	-2.3835120	3.3685710	-1.6753910
H	3.1593840	-1.5916100	-0.2611390
C	5.1229210	-0.0458260	-0.8007690
H	3.4523080	1.2971970	-0.6567950
C	4.0976740	0.8170680	1.3372900
H	5.8885690	0.7313200	-0.7372720
H	5.5071000	-0.9442640	-0.3049610
H	4.9474690	-0.2745390	-1.8554180
H	4.7902640	1.6624010	1.3871580
H	3.1658210	1.1040640	1.8321020
H	4.5394260	-0.0239200	1.8821310
O	-3.7694340	-0.3172120	-0.2051730
H	-2.7439840	-0.1933020	-0.1617500
O	-4.1335560	-0.5874050	1.0210700

TRANSITION STATE

C	0.4384030	1.4712170	-0.1502840
N	1.1585350	0.3590800	-0.1578970
C	0.3963660	-0.7605820	-0.1685760
C	-1.5317260	0.4238430	-0.1312760
N	-0.8568390	1.6163570	-0.1440300
CL	1.3779120	2.9437450	-0.1312010
N	-0.9396100	-0.7767310	-0.1403550
N	1.0107540	-1.9662300	-0.1892800
H	0.4006500	-2.7544430	-0.0029540
N	-2.8624360	0.5051100	-0.1338630
C	-3.7760070	-0.6352270	-0.0320850
C	2.4084990	-2.2087160	-0.2699960
H	2.5899250	-3.2625650	-0.0606200
H	2.9537980	-1.6122700	0.7174970
C	3.1366020	-1.7077690	-1.4961940
H	2.9896330	-0.6404070	-1.6665990
H	4.2062800	-1.9040210	-1.3919630
H	2.7712450	-2.2516350	-2.3756230
H	-3.2556450	1.4378330	-0.0715060
C	-5.1064680	-0.2427200	-0.6592370
H	-3.3304960	-1.4509300	-0.6064150
C	-3.9428200	-1.0694640	1.4216410
H	-5.8056730	-1.0802410	-0.5963570
H	-5.5446800	0.6073970	-0.1244250
H	-4.9844480	0.0296470	-1.7109500
H	-4.5765620	-1.9594420	1.4765730
H	-2.9759070	-1.3040990	1.8751700
H	-4.4157090	-0.2700220	2.0018710
O	3.8265800	0.2802450	0.7697840
H	2.9755150	0.6055540	0.3938740
O	3.4068770	-0.7828230	1.5610740

PRODUCTS

C	0.5432910	1.4663010	-0.2400180
N	1.2398290	0.3475160	-0.3660060
C	0.4556840	-0.7590830	-0.4061220
C	-1.4446590	0.4491070	-0.1895670
N	-0.7485960	1.6316040	-0.1592320
Cl	1.5084260	2.9200290	-0.1498780
N	-0.8818090	-0.7563550	-0.3113010
N	1.0480040	-1.9680430	-0.5238780
H	0.4236020	-2.7504840	-0.3529530
N	-2.7731430	0.5524130	-0.1110170
C	-3.6964750	-0.5822410	-0.0462830
C	2.3836900	-2.2639470	-0.7597020
H	2.6070600	-3.3111400	-0.6061910
H	2.8269920	-1.7427580	1.7503990
C	3.2505120	-1.4305390	-1.6406870
H	3.6771660	-0.5532610	-1.1436590
H	4.0789740	-2.0445440	-2.0004810
H	2.6882680	-1.0633580	-2.5094750
H	-3.1477410	1.4859480	0.0151750
C	-5.0704980	-0.1111400	-0.5008650
H	-3.3229200	-1.3365680	-0.7439490
C	-3.7403700	-1.1723570	1.3607760
H	-5.7773620	-0.9436550	-0.4627340
H	-5.4414000	0.6811350	0.1590430
H	-5.0403670	0.2717860	-1.5245440
H	-4.3768320	-2.0620980	1.3743990
H	-2.7404660	-1.4572910	1.6990370
H	-4.1521740	-0.4415180	2.0648910
O	3.3803570	0.0414510	1.4303660
H	2.7511600	0.2541650	0.6994400
O	2.6228650	-0.8981270	2.1901820

β-oxidation

ISOPROPYL SIDECHAIN, PATHWAY 1

REACTANTS

C	-2.0693710	-1.2393910	0.0245530
N	-2.2806710	0.0515930	0.1744410
C	-1.1299570	0.7731820	0.1830890
C	0.1519150	-1.0754000	-0.0843110
N	-0.9435880	-1.8948520	-0.1039590
Cl	-3.5162440	-2.2285740	-0.0099480
N	0.1025600	0.2516710	0.0469760
N	-1.2199320	2.0971350	0.3565530
H	-0.3498490	2.6120060	0.3077090
N	1.3362180	-1.6833920	-0.2322660
C	2.6335170	-1.0181250	-0.1122130
C	-2.4707610	2.8367420	0.4754750
H	-2.2324290	3.7685720	0.9915520
H	-3.1459740	2.2683490	1.1180740
C	-3.1271170	3.1294130	-0.8675460
H	-3.3583810	2.2029900	-1.4001580
H	-4.0602150	3.6787200	-0.7122010
H	-2.4715620	3.7384070	-1.4965330
H	1.3178750	-2.6965090	-0.2537470
C	3.6890130	-1.8876460	-0.7801990
H	2.5571170	-0.0698240	-0.6509010
C	2.9766790	-0.7432230	1.3503570
H	4.6648560	-1.3995820	-0.7133330
H	3.7593190	-2.8588020	-0.2772460
H	3.4559210	-2.0560080	-1.8351240
H	3.9281300	-0.2043980	1.4200000
H	2.1975190	-0.1453210	1.8328830
H	3.0790860	-1.6857210	1.8987130
O	3.5215110	2.3718040	0.0087070
H	3.1470130	1.8521990	0.7527850
O	4.5287530	1.6872320	-0.4638060

TRANSITION STATE

C	-2.1444760	-1.2839220	-0.0345560
N	-2.5086650	-0.0342090	0.1598980
C	-1.4511030	0.8090550	0.2800700
C	0.0437690	-0.8644920	-0.0186620
N	-0.9447080	-1.7997480	-0.1403080
Cl	-3.4636810	-2.4277830	-0.1756980
N	-0.1611420	0.4351300	0.1961120
N	-1.7003400	2.1014060	0.5287520
H	-0.8940870	2.7141520	0.5187120
N	1.2977330	-1.3268140	-0.1477540
C	2.5018120	-0.5268910	0.0842360
C	-3.0225580	2.7146570	0.4751830
H	-2.9838230	3.6035210	1.1079680
H	-3.7383940	2.0234530	0.9216560
C	-3.4383340	3.0893410	-0.9410770
H	-3.4658230	2.2065440	-1.5863400
H	-4.4344450	3.5408930	-0.9323330
H	-2.7367840	3.8106190	-1.3704060
H	1.4022370	-2.3331550	-0.2106160
C	3.6117390	-1.1088720	-0.7574300
H	2.2796190	0.4841470	-0.2677190
C	2.8658670	-0.4877040	1.5650200
H	4.6348060	-0.2671210	-0.6109550
H	4.0427990	-2.0423690	-0.3875830
H	3.4483780	-1.0882800	-1.8356800
H	3.7393390	0.1511460	1.7251560
H	2.0341930	-0.0949460	2.1560270
H	3.1047940	-1.4950650	1.9213510
O	4.7947880	1.7613890	-0.4086550
H	4.5968080	1.8951620	0.5347200
O	5.4767780	0.5493890	-0.4401830

PRODUCTS

C	-2.2211880	-1.2305660	-0.0350800
N	-2.5116860	0.0360410	0.1750820
C	-1.4066150	0.8144360	0.3037240
C	-0.0115220	-0.9417600	-0.0096940
N	-1.0545530	-1.8156860	-0.1462200
Cl	-3.6087480	-2.2881110	-0.1968100
N	-0.1415470	0.3657490	0.2232830
N	-1.5815660	2.1184450	0.5578610
H	-0.7409880	2.6832520	0.5512240
N	1.2128540	-1.4705630	-0.1415860
C	2.4678260	-0.7248570	0.0336330
C	-2.8684700	2.8034710	0.5009040
H	-2.7742100	3.7016940	1.1139750
H	-3.6177540	2.1635270	0.9684800
C	-3.2795710	3.1714770	-0.9186840
H	-3.3593050	2.2789840	-1.5458240
H	-4.2507410	3.6744500	-0.9082290
H	-2.5477070	3.8480690	-1.3694230
H	1.2667950	-2.4746500	-0.2665160
C	3.5257640	-1.3661380	-0.8056400
H	2.2788830	0.2857190	-0.3382280
C	2.8693940	-0.6613420	1.5054420
H	5.3835870	-0.0306060	-0.4244560
H	4.1040930	-2.1904640	-0.3988470
H	3.5447100	-1.1932210	-1.8760730
H	3.7712640	-0.0522520	1.6242620
H	2.0685840	-0.2232380	2.1072010
H	3.0809430	-1.6675420	1.8818110
O	4.6516420	1.7066230	-0.5653830
H	4.1511160	1.7845540	0.2645390
O	5.7322600	0.8538000	-0.2052050

ISOPROPYL SIDECHAIN, PATHWAY 2

REACTANTS

C	-1.0775710	1.4334370	-0.3031970
N	-2.1122430	0.6190430	-0.2727890
C	-1.7495040	-0.6829460	-0.1429520
C	0.4582220	-0.1730690	-0.1084790
N	0.2014200	1.1672930	-0.2279750
Cl	-1.4803020	3.1313110	-0.4739200
N	-0.4813470	-1.1215640	-0.0626730
N	-2.7201440	-1.6076490	-0.1194020
H	-2.4178720	-2.5542470	0.0736540
N	1.7492230	-0.5073890	-0.0104520
C	2.2622710	-1.8772520	-0.0169040
C	-4.1434840	-1.3076480	-0.0158290
H	-4.6766510	-2.1835710	-0.3901230
H	-4.3683600	-0.4751660	-0.6841240
C	-4.5828290	-0.9907910	1.4086050
H	-4.0447050	-0.1228410	1.7996770
H	-5.6540480	-0.7703970	1.4280190
H	-4.3945530	-1.8416090	2.0698680
H	2.4201140	0.2513370	-0.1056300
C	3.6525160	-1.8717220	0.6048210
H	1.5914470	-2.4791780	0.6018920
C	2.2910180	-2.4448350	-1.4343520
H	4.0585640	-2.8864980	0.6093710
H	4.3292120	-1.2369020	0.0213110
H	3.6280230	-1.5039010	1.6342580
H	2.6226950	-3.4872650	-1.4164130
H	1.3014940	-2.4043730	-1.8971530
H	2.9880250	-1.8707280	-2.0544220
O	4.0593290	1.5712780	1.2585490
H	4.7383440	2.2311650	1.5132700
O	3.9308210	1.6465610	-0.0390560

TRANSITION STATE

C	1.3422700	1.4584720	0.1210590
N	2.2680150	0.5283610	0.2253240
C	1.7580770	-0.7289130	0.1608680
C	-0.3618120	0.0336580	-0.0674400
N	0.0460030	1.3378580	-0.0239630
Cl	1.9360980	3.1060270	0.1762370
N	0.4515970	-1.0190810	0.0233860
N	2.6109180	-1.7556140	0.2546170
H	2.2127500	-2.6791280	0.1409070
N	-1.6784150	-0.1576310	-0.2422640
C	-2.3344620	-1.4579990	-0.1245360
C	4.0616200	-1.6204620	0.3297160
H	4.4380210	-2.5531120	0.7535350
H	4.2970490	-0.8205200	1.0344870
C	4.7103660	-1.3528220	-1.0223310
H	4.3320250	-0.4252030	-1.4604030
H	5.7935240	-1.2603410	-0.9013240
H	4.5110980	-2.1731540	-1.7176960
H	-2.2672810	0.6692720	-0.1985070
C	-3.6153120	-1.4467450	-0.9152170
H	-1.6702060	-2.1992110	-0.5861410
C	-2.5643010	-1.8387840	1.3372400
H	-4.2316690	-2.3364440	-0.7814400
H	-4.3791380	-0.5043130	-0.3976260
H	-3.5345060	-1.1175640	-1.9527800
H	-2.9809540	-2.8478240	1.4029400
H	-1.6239010	-1.8116720	1.8934960
H	-3.2658160	-1.1392030	1.8029210
O	-4.2308090	1.5453390	-0.2403270
H	-4.5462950	1.8267860	-1.1163580
O	-5.0021730	0.4238480	0.0543400

PRODUCTS

C	-1.2312110	1.4579760	-0.0948080
N	-2.2083230	0.5860290	-0.2301590
C	-1.7748020	-0.6997330	-0.1751750
C	0.3792880	-0.0687570	0.1233180
N	0.0505190	1.2586520	0.0838110

Cl	-1.7232340	3.1384960	-0.1587640
N	-0.4925100	-1.0698630	-0.0095030
N	-2.6830640	-1.6727260	-0.3159770
H	-2.3407720	-2.6185850	-0.2043620
N	1.6748200	-0.3384640	0.3337920
C	2.2606190	-1.6739940	0.2277230
C	-4.1226110	-1.4537980	-0.3978770
H	-4.5473640	-2.3516280	-0.8502790
H	-4.3074660	-0.6226940	-1.0813290
C	-4.7646850	-1.1866250	0.9574370
H	-4.3409150	-0.2906690	1.4195310
H	-5.8409680	-1.0345360	0.8351080
H	-4.6112190	-2.0324670	1.6336190
H	2.3151430	0.4525110	0.3313090
C	3.5384650	-1.7126090	0.9965750
H	1.5468820	-2.3718690	0.6880060
C	2.4640160	-2.0800320	-1.2330980
H	4.2656140	-2.4803490	0.7567180
H	4.7308340	-0.1078130	-0.0808100
H	3.6102200	-1.2149300	1.9580070
H	2.8529840	-3.1008080	-1.2884630
H	1.5178410	-2.0359780	-1.7784910
H	3.1805600	-1.4057800	-1.7136900
O	3.9994640	1.6038680	0.2732340
H	4.3883550	1.8186340	1.1375830
O	4.9993730	0.7964530	-0.3384560

ISOPROPYL SIDECHAIN, PATHWAY 3

REACTANTS

C	-0.9462990	1.4521150	-0.4685880
N	-1.6400990	0.3495780	-0.6589770
C	-0.8669500	-0.7666420	-0.6333850
C	1.0245760	0.4257950	-0.2803770
N	0.3377400	1.6107430	-0.2713390
Cl	-1.8895100	2.9306940	-0.4843120
N	0.4679800	-0.7717080	-0.4772900
N	-1.4717160	-1.9497390	-0.8101270
H	-0.8850710	-2.7653960	-0.6859020
N	2.3426950	0.5189610	-0.0710390
C	3.2762120	-0.6076870	-0.0723320
C	-2.9176530	-2.1424430	-0.8207020
H	-3.1024430	-3.0911460	-1.3278790
H	-3.3670910	-1.3539420	-1.4260010
C	-3.5255150	-2.1616610	0.5758450
H	-3.3614520	-1.2089250	1.0876580
H	-4.6034640	-2.3357760	0.5101280
H	-3.0838900	-2.9604490	1.1787720
H	2.7169990	1.4553080	0.0289430
C	4.5100600	-0.2079250	0.7245730
H	2.7759030	-1.4391400	0.4324060
C	3.6376760	-1.0250890	-1.4953650
H	5.2235750	-1.0355330	0.7411180
H	5.0015310	0.6558110	0.2626480
H	4.2499630	0.0471040	1.7557340
H	4.2905610	-1.9028100	-1.4749540
H	2.7425580	-1.2747360	-2.0712040
H	4.1655630	-0.2117990	-2.0047480
O	-0.9193560	-0.1912440	2.3424720
H	-1.3883730	0.6684460	2.4015780
O	0.3366010	0.0446900	2.6160770

TRANSITION STATE

C	-1.3344570	1.3931440	-0.4654960
N	-2.2053480	0.4288870	-0.2528410
C	-1.6213530	-0.7913190	-0.1389410
C	0.4509040	0.0593570	-0.4638440
N	-0.0317040	1.3332170	-0.5843770
Cl	-2.0264610	2.9964070	-0.6046730
N	-0.2991720	-1.0201700	-0.2395400

N	-2.4140880	-1.8499570	0.0683860
H	-1.9424590	-2.7327880	0.2184830
N	1.7798840	-0.0695300	-0.5796940
C	2.5084450	-1.3229730	-0.4012430
C	-3.8423050	-1.7664340	0.3524230
H	-4.2529080	-2.7606950	0.1684460
H	-4.2996110	-1.0839750	-0.3665440
C	-4.1395000	-1.3246570	1.7795840
H	-3.7271050	-0.3305450	1.9723940
H	-5.2208310	-1.2870110	1.9401710
H	-3.7083890	-2.0268720	2.4989230
H	2.3085840	0.7930250	-0.6464870
C	3.9444730	-1.0063940	-0.0839120
H	2.0579910	-1.8615740	0.4387120
C	2.4322210	-2.2058980	-1.6530580
H	4.5467730	-1.8702270	0.1964700
H	4.4404090	-0.3355060	-0.7915400
H	3.9381810	-0.2637580	1.0072580
H	2.9412280	-3.1563710	-1.4713810
H	1.3883480	-2.4114870	-1.9042320
H	2.9107070	-1.7047970	-2.4996430
O	3.6782610	1.7475980	1.3144000
H	4.5819190	2.0909540	1.2089830
O	3.8579170	0.5069790	1.9197010

PRODUCTS

C	-1.1625390	1.3654530	-0.5291380
N	-2.0876160	0.4579130	-0.2945850
C	-1.5719910	-0.7886630	-0.1397470
C	0.5479190	-0.0627550	-0.4683150
N	0.1358070	1.2304840	-0.6339660
Cl	-1.7617230	3.0000720	-0.7283440
N	-0.2628840	-1.0912770	-0.2184060
N	-2.4219300	-1.7962260	0.0905450
H	-2.0031970	-2.7018670	0.2598050
N	1.8690300	-0.2729620	-0.5791330
C	2.5108350	-1.5446440	-0.2333270
C	-3.8577060	-1.6402850	0.2955050
H	-4.3067560	-2.6142490	0.0927010
H	-4.2400050	-0.9412710	-0.4508380
C	-4.2165910	-1.1741680	1.7003170
H	-3.7591930	-0.2056120	1.9197230
H	-5.3018210	-1.0707970	1.7899310
H	-3.8776050	-1.8970810	2.4477440
H	2.4455770	0.5631860	-0.5881090
C	3.9249060	-1.2876800	0.1689340
H	1.9647740	-1.9798120	0.6107890
C	2.4547340	-2.5328100	-1.4083900
H	4.4395730	-2.0354760	0.7605950
H	4.5221610	-0.5814100	-0.4012080
H	3.4675870	0.2572110	1.7749990
H	2.8801530	-3.4939060	-1.1070030
H	1.4203180	-2.6907230	-1.7252230
H	3.0294090	-2.1449070	-2.2547190
O	3.4043820	1.9206630	0.8740730
H	4.2891610	2.2888320	1.0325690
O	3.1674810	1.1473920	2.0451620

ISOPROPYL SIDECHAIN, PATHWAY 4

REACTANTS

C	-2.2103020	-1.2079080	-0.0083890
N	-2.4608750	0.0705840	0.1837520
C	-1.3313600	0.8192700	0.2673500
C	0.0076180	-0.9819080	-0.0411380
N	-1.0638900	-1.8286840	-0.1277810
Cl	-3.6299850	-2.2290680	-0.1242850
N	-0.0822780	0.3362070	0.1505570
N	-1.4603940	2.1309390	0.5125150
H	-0.6035180	2.6689270	0.4676470

N	1.2119600	-1.5482830	-0.1840290
C	2.4876640	-0.8462340	-0.0396260
C	-2.7271210	2.8540190	0.4943680
H	-2.5867100	3.7512480	1.1000170
H	-3.4794110	2.2383010	0.9889710
C	-3.1745220	3.2298230	-0.9119600
H	-3.3106740	2.3379800	-1.5300560
H	-4.1250380	3.7694040	-0.8696770
H	-2.4341580	3.8758500	-1.3925750
H	1.2265740	-2.5564400	-0.2850440
C	3.5703460	-1.6689670	-0.7230770
H	2.3845500	0.1119100	-0.5567490
C	2.8180400	-0.5956090	1.4294880
H	4.5349220	-1.1634290	-0.6275570
H	3.6568310	-2.6546190	-0.2518190
H	3.3541780	-1.8071780	-1.7861110
H	3.7456340	-0.0194860	1.5124890
H	2.0173540	-0.0394140	1.9242040
H	2.9567520	-1.5480880	1.9522590
O	4.5405240	1.7255950	-0.6229000
H	3.8496140	1.8629980	0.0601270
O	5.5680990	1.1901460	-0.0196610

TRANSITION STATE

C	2.1106370	-1.2457720	-0.1529210
N	2.4103920	0.0278410	-0.2937210
C	1.3314050	0.8410770	-0.1616340
C	-0.0596810	-0.9041160	0.2146450
N	0.9540720	-1.8105750	0.0968240
Cl	3.4610370	-2.3478490	-0.3210450
N	0.0791230	0.4145370	0.0844140
N	1.5152870	2.1596740	-0.3111330
H	0.7104820	2.7400740	-0.1084370
N	-1.2676070	-1.4163860	0.5163280
C	-2.5234710	-0.6642620	0.4348460
C	2.8243530	2.8028360	-0.3570360
H	2.6760470	3.7834800	-0.8127350
H	3.4685310	2.2252140	-1.0212480
C	3.4555980	2.9456530	1.0218800
H	3.5809680	1.9666380	1.4937210
H	4.4389560	3.4167820	0.9364420
H	2.8303460	3.5668250	1.6697910
H	-1.3391550	-2.4276540	0.4728990
C	-3.5686270	-1.3380240	1.3107210
H	-2.3204580	0.3424180	0.8054880
C	-2.9567490	-0.6011950	-1.0140750
H	-4.5152890	-0.7963050	1.2367780
H	-3.7371580	-2.3688100	0.9804350
H	-3.2536430	-1.3498680	2.3569460
H	-4.0390130	0.1618640	-1.0249010
H	-2.2819880	-0.0693940	-1.6867310
H	-3.3299870	-1.5444750	-1.4207580
O	-4.6636010	1.7367550	0.1265320
H	-4.1762730	2.4745700	-0.2781910
O	-4.9701070	0.9069020	-0.9476920

PRODUCTS

C	2.2131440	-1.2156220	-0.1315170
N	2.4870700	0.0631530	-0.2811260
C	1.3880050	0.8529020	-0.1733670
C	0.0281360	-0.9197620	0.1932640
N	1.0663400	-1.8036610	0.1043360
Cl	3.5913650	-2.2890700	-0.2642480
N	0.1416080	0.4020210	0.0574910
N	1.5462270	2.1738010	-0.3337330
H	0.7264880	2.7397630	-0.1517610
N	-1.1731600	-1.4558730	0.4634750
C	-2.4449150	-0.7195690	0.3646220
C	2.8429230	2.8409250	-0.3834440
H	2.6777730	3.8143970	-0.8486000
H	3.4982620	2.2683360	-1.0413740

C	3.4717620	3.0089280	0.9937810
H	3.6118260	2.0372900	1.4765350
H	4.4478580	3.4939160	0.9023860
H	2.8378990	3.6281700	1.6350980
H	-1.2197630	-2.4686500	0.4430780
C	-3.5275920	-1.5725240	1.0191590
H	-2.3250610	0.2107270	0.9244410
C	-2.7715380	-0.4129990	-1.0654420
H	-4.4796620	-1.0362420	1.0081980
H	-3.6551020	-2.5122800	0.4708790
H	-3.2691420	-1.8020840	2.0565770
H	-5.0599450	0.1743780	-0.9310220
H	-2.5570660	0.5574290	-1.4969520
H	-3.0216640	-1.2364340	-1.7285760
O	-4.9164950	1.5873530	0.3179150
H	-4.3840170	2.2230240	-0.1886600
O	-5.6532580	0.9117340	-0.6945990

ISOPROPYL SIDECHAIN, PATHWAY 5

REACTANTS

C	0.9784380	1.3883290	-0.4087580
N	1.6952380	0.3219940	-0.1241580
C	0.9682410	-0.8246650	-0.1618390
C	-0.9413500	0.2866790	-0.6561830
N	-0.2928350	1.4889460	-0.7099920
CL	1.8586840	2.9037380	-0.3749150
N	-0.3515300	-0.8846200	-0.4160000
N	1.6025070	-1.9780110	0.0798860
H	1.0485450	-2.8192780	-0.0189910
N	-2.2641280	0.3233840	-0.8895980
C	-3.1769670	-0.7747970	-0.5604200
C	3.0432360	-2.1057250	0.2650940
H	3.2062740	-3.0455130	0.7956510
H	3.3785740	-1.2972620	0.9174160
C	3.8161350	-2.0947780	-1.0471100
H	3.6481080	-1.1607220	-1.5904390
H	4.8874860	-2.1895950	-0.8477480
H	3.5099860	-2.9291540	-1.6846470
H	-2.6683150	1.2519650	-0.9440340
C	-4.5179400	-0.4981420	-1.2240690
H	-2.7494370	-1.6897200	-0.9781170
C	-3.3189340	-0.9273080	0.9530180
H	-5.2182820	-1.3047630	-0.9936090
H	-4.9436280	0.4400730	-0.8503170
H	-4.4157180	-0.4276000	-2.3103720
H	-3.9798040	-1.7667570	1.1890170
H	-2.3470640	-1.1148490	1.4208180
H	-3.7494500	-0.0162780	1.3841240
O	-0.4361690	0.9841800	2.3463280
H	-1.3946920	0.9038390	2.1477820
O	-0.0188470	-0.2088470	2.6783800

TRANSITION STATE

C	1.0344670	1.3036530	-0.4706960
N	1.8476710	0.3809380	-0.0160690
C	1.2622310	-0.8440730	0.0768270
C	-0.7182960	-0.0650890	-0.6883810
N	-0.2297280	1.2014380	-0.8275070
CL	1.7172470	2.9060850	-0.6096520
N	-0.0103650	-1.1090390	-0.2710320
N	1.9894290	-1.8537630	0.5605030
H	1.5350510	-2.7584650	0.5796600
N	-2.0166580	-0.2317580	-1.0368580
C	-2.8620130	-1.2260170	-0.3643750
C	3.4049940	-1.7773040	0.9056580
H	3.5879260	-2.5620110	1.6418060
H	3.5880670	-0.8186630	1.3934190
C	4.3187650	-1.9559090	-0.2997940
H	4.1376200	-1.1775810	-1.0463000

H	5.3646290	-1.8953600	0.0140550
H	4.1559940	-2.9312780	-0.7671820
H	-2.4906620	0.6457120	-1.2360700
C	-3.9907500	-1.6674790	-1.2941030
H	-2.2298140	-2.0820440	-0.1302810
C	-3.4311340	-0.6383060	0.9080440
H	-4.6429390	-2.3784250	-0.7806080
H	-4.5914550	-0.8049440	-1.6004630
H	-3.5803030	-2.1489340	-2.1860200
H	-3.8068700	-1.3590980	1.6353320
H	-2.4382660	-0.0158930	1.5408100
H	-4.0930110	0.2198740	0.7546510
O	-1.8688030	1.9652010	1.5565530
H	-1.3804720	2.0472300	0.7115280
O	-1.5662870	0.6754070	1.9856240

PRODUCTS

C	0.9754930	1.2606750	-0.5290580
N	1.7768920	0.3165720	-0.0952400
C	1.1566310	-0.8875010	0.0326510
C	-0.8256800	-0.0534250	-0.6700800
N	-0.2999160	1.1956320	-0.8456960
Cl	1.7037430	2.8401750	-0.7062120
N	-0.1382140	-1.1147350	-0.2577290
N	1.8708220	-1.9162870	0.4955040
H	1.3881500	-2.8044050	0.5513170
N	-2.1354690	-0.1819000	-0.9634950
C	-2.9525690	-1.2824920	-0.4315320
C	3.2937640	-1.8714980	0.8153290
H	3.4753940	-2.6773340	1.5285360
H	3.5028870	-0.9288440	1.3238590
C	4.1863670	-2.0358070	-0.4079310
H	4.0013730	-1.2419100	-1.1365560
H	5.2373660	-1.9904810	-0.1089540
H	4.0080860	-3.0005550	-0.8913270
H	-2.6223670	0.6991720	-1.1008470
C	-4.2821410	-1.3027560	-1.1862890
H	-2.4157980	-2.2121810	-0.6266870
C	-3.1698670	-1.1200060	1.0413260
H	-4.9147510	-2.1039770	-0.7968150
H	-4.8094350	-0.3521350	-1.0524430
H	-4.1197750	-1.4714720	-2.2546860
H	-3.1394590	-1.9792290	1.7013970
H	-1.4811750	0.2872040	2.1174560
H	-3.6308190	-0.2023460	1.3985490
O	-1.6278820	2.1116080	1.6215780
H	-1.3128350	2.1342150	0.6961020
O	-0.8647780	1.0412910	2.1705220

ISOPROPYL SIDECHAIN, PATHWAY 6

REACTANTS

C	-1.3081310	-1.8787620	0.0667560
N	-1.9423570	-0.7242190	0.0411030
C	-1.1124600	0.3362120	-0.0929020
C	0.7392540	-1.0055120	-0.1359980
N	-0.0268110	-2.1284560	-0.0164140
Cl	-2.3334370	-3.2823240	0.2398460
N	0.2384570	0.2413670	-0.1707210
N	-1.6667750	1.5458390	-0.1555180
H	-1.0563020	2.3491580	-0.2441500
N	2.0518840	-1.2146070	-0.2386540
C	3.0907500	-0.1829690	-0.2686780
C	-3.1074030	1.7910200	-0.1052660
H	-3.4971040	1.4797880	0.8685750
H	-3.5979810	1.1828440	-0.8694630
C	-3.3794570	3.2655280	-0.3426020
H	-3.0154910	3.5783070	-1.3255350
H	-4.4551700	3.4494830	-0.3019380
H	-2.8974540	3.8826040	0.4214990

H	2.3456670	-2.1826820	-0.1676400
C	4.3697190	-0.8096810	-0.8051540
H	2.7653430	0.5898280	-0.9714360
C	3.3009890	0.4222420	1.1173560
H	5.1653050	-0.0609690	-0.8201270
H	4.6896590	-1.6355460	-0.1603190
H	4.2318290	-1.1894590	-1.8209050
H	3.9908440	1.2690280	1.0555100
H	2.3600760	0.7743620	1.5499680
H	3.7300900	-0.3285370	1.7890280
O	1.5028770	2.5662540	-0.3039700
H	1.0683550	1.6237160	-0.2932460
O	1.2096740	3.1024510	0.8531130

TRANSITION STATE

C	1.3160480	1.7807600	0.1429620
N	1.9991260	0.6638440	-0.0064920
C	1.2056010	-0.4106160	-0.2348880
C	-0.6908160	0.8490930	-0.1649360
N	0.0241180	1.9859340	0.0845150
CL	2.2855630	3.2010310	0.4581450
N	-0.1419600	-0.3628740	-0.3143350
N	1.7929350	-1.5971470	-0.3935610
H	1.1885190	-2.3927880	-0.5648570
N	-2.0134180	1.0167370	-0.2726630
C	-3.0006270	-0.0034170	-0.6166820
C	3.2356170	-1.8193500	-0.3394820
H	3.6124040	-1.5237260	0.6441630
H	3.7241320	-1.1868570	-1.0859400
C	3.5359140	-3.2832580	-0.6079510
H	3.1740710	-3.5826040	-1.5959600
H	4.6152130	-3.4470000	-0.5757380
H	3.0693200	-3.9259080	0.1442970
H	-2.3488120	1.9656180	-0.1448170
C	-3.9845020	0.5753160	-1.6393360
H	-2.4659880	-0.8380940	-1.0778450
C	-3.7526820	-0.4865130	0.5999970
H	-4.7352740	-0.1745860	-1.8981460
H	-4.4959660	1.4487460	-1.2220800
H	-3.4570120	0.8732560	-2.5494250
H	-4.4483940	-1.3043010	0.4045030
H	-2.8512790	-1.0739660	1.3844930
H	-4.1589120	0.2993070	1.2404780
O	-1.4533170	-2.4701260	0.8860760
H	-0.9216480	-1.8338330	0.3358140
O	-1.9426680	-1.6396680	1.8954560

PRODUCTS

C	-1.3457110	-1.8783470	0.0793650
N	-1.9423750	-0.7045660	0.0219990
C	-1.0731280	0.3209000	-0.1465200
C	0.7251600	-1.0769160	-0.1493520
N	-0.0723760	-2.1740890	0.0054150
CL	-2.4173590	-3.2437300	0.2887620
N	0.2682550	0.1774110	-0.2338670
N	-1.5727870	1.5536460	-0.2361330
H	-0.9129130	2.3172360	-0.3384060
N	2.0368400	-1.3182940	-0.2344160
C	3.0821610	-0.2980420	-0.2990380
C	-2.9948430	1.8749050	-0.1533660
H	-3.3832500	1.5674280	0.8223040
H	-3.5352420	1.3111620	-0.9189420
C	-3.1859250	3.3672660	-0.3538290
H	-2.8189290	3.6817520	-1.3351510
H	-4.2477170	3.6145360	-0.2904900
H	-2.6559300	3.9359170	0.4162890
H	2.3191010	-2.2871290	-0.1412270
C	4.3940520	-0.9888360	-0.6848230
H	2.8237600	0.4047030	-1.1015920
C	3.2214000	0.4454470	0.9908560
H	5.1918470	-0.2464720	-0.7526580

H	4.6709310	-1.7273910	0.0743760
H	4.2971570	-1.4893320	-1.6526690
H	3.8826580	1.3056620	1.0208630
H	2.0078890	2.5972390	1.4595650
H	2.9228510	-0.0207150	1.9234630
O	1.4473600	2.6550200	-0.3522490
H	1.1319780	1.7078930	-0.3862680
O	1.2325170	2.9867180	1.0186050

ISOPROPYL SIDECHAIN, PATHWAY 7

REACTANTS

C	-1.1868960	1.4664120	0.1036200
N	-2.1490750	0.6262950	-0.2164210
C	-1.7270380	-0.6637820	-0.2561900
C	0.3897650	-0.0964810	0.3170050
N	0.0706930	1.2326250	0.3825950
CL	-1.6643630	3.1515380	0.1602700
N	-0.4697940	-1.0666850	-0.0007270
N	-2.6137920	-1.6080890	-0.6003670
H	-2.2857010	-2.5629880	-0.5234280
N	1.6550660	-0.4052650	0.6328530
C	2.2660750	-1.7178830	0.4199890
C	-4.0493600	-1.3842750	-0.7293920
H	-4.4375320	-2.1888060	-1.3566310
H	-4.2040290	-0.4474020	-1.2660560
C	-4.7698060	-1.3647650	0.6128520
H	-4.3744130	-0.5743410	1.2570900
H	-5.8377210	-1.1835210	0.4607870
H	-4.6531670	-2.3225960	1.1280980
H	2.2863740	0.3828730	0.7316760
C	3.5077880	-1.8131450	1.2954430
H	1.5383960	-2.4673550	0.7404540
C	2.6009320	-1.9261830	-1.0554300
H	3.9930000	-2.7816350	1.1497890
H	4.2243420	-1.0289300	1.0252880
H	3.2548130	-1.7058990	2.3537900
H	3.0021340	-2.9313710	-1.2155140
H	1.7124930	-1.8030330	-1.6811610
H	3.3545040	-1.1970480	-1.3737340
O	3.8743160	1.6306530	-0.2652380
H	3.4916010	2.2157430	-0.9527510
O	4.8242640	0.9404230	-0.8391610

TRANSITION STATE

C	-1.3815480	1.4647410	0.0973080
N	-2.2216380	0.5141300	-0.2531360
C	-1.6490380	-0.7166370	-0.2638190
C	0.3591400	0.1032060	0.3854010
N	-0.1162180	1.3837610	0.4277820
CL	-2.0621970	3.0783800	0.1239320
N	-0.3623120	-0.9643490	0.0412830
N	-2.4075330	-1.7593730	-0.6261680
H	-1.9756370	-2.6702210	-0.5316550
N	1.6407500	-0.0546070	0.7535260
C	2.3869870	-1.3006230	0.5995260
C	-3.8553160	-1.7068020	-0.7953260
H	-4.1286830	-2.5719310	-1.4021430
H	-4.1044460	-0.8119230	-1.3673680
C	-4.6047400	-1.7286190	0.5303740
H	-4.3348940	-0.8649570	1.1448680
H	-5.6833150	-1.7008630	0.3506800
H	-4.3717280	-2.6391520	1.0899770
H	2.1864160	0.7952340	0.8507250
C	3.5530830	-1.3177410	1.5819330
H	1.7021380	-2.1201430	0.8491440
C	2.8396520	-1.5028560	-0.8270810
H	4.1304020	-2.2362900	1.4511280
H	4.2169870	-0.4654860	1.4044150
H	3.1918740	-1.2750640	2.6121400

H	3.3928290	-2.4275650	-1.0021190
H	2.0977840	-1.2806430	-1.5962210
H	3.7635490	-0.5884400	-1.0585600
O	4.1304380	1.3680150	-0.5178590
H	3.5747630	1.8471290	-1.1565900
O	4.5918940	0.2661010	-1.2319110

PRODUCTS

C	-1.2336870	1.4647860	0.0957710
N	-2.1737530	0.6014660	-0.2277560
C	-1.7196450	-0.6775340	-0.2704760
C	0.3779670	-0.0590730	0.3176610
N	0.0280700	1.2605140	0.3819120
Cl	-1.7479660	3.1382380	0.1499560
N	-0.4523380	-1.0487010	-0.0133740
N	-2.5810460	-1.6429160	-0.6192900
H	-2.2293180	-2.5894070	-0.5415700
N	1.6476980	-0.3399720	0.6517350
C	2.2817270	-1.6369950	0.4208080
C	-4.0233360	-1.4581830	-0.7365530
H	-4.3942500	-2.2735490	-1.3601360
H	-4.2084880	-0.5263420	-1.2722190
C	-4.7314930	-1.4585750	0.6123480
H	-4.3555720	-0.6542370	1.2510340
H	-5.8059550	-1.3115490	0.4701560
H	-4.5793040	-2.4111560	1.1281110
H	2.2787740	0.4559070	0.7021500
C	3.4945880	-1.7624930	1.3398280
H	1.5509210	-2.4066050	0.7012380
C	2.6536030	-1.8018820	-1.0184930
H	3.9905030	-2.7212220	1.1700990
H	4.2128230	-0.9614110	1.1332940
H	3.1913680	-1.7040700	2.3880260
H	3.3537320	-2.5821550	-1.2985810
H	2.0351830	-1.3562790	-1.7909680
H	4.1481430	-0.0620600	-1.1286470
O	3.9772070	1.5124850	-0.0856870
H	3.4288480	2.1092590	-0.6219480
O	4.6752020	0.7589910	-1.0714690

ETHYL SIDECHAIN, PATHWAY 1

REACTANTS

C	-0.8452880	1.3042270	-0.6234710
N	-1.4781850	0.1654510	-0.8089330
C	-0.6814530	-0.9152040	-0.6121440
C	1.1308540	0.3695650	-0.1785550
N	0.4076530	1.5231530	-0.3099660
Cl	-1.8246980	2.7404970	-0.8373150
N	0.6322430	-0.8593540	-0.3331080
N	-1.2356620	-2.1306360	-0.7361570
H	-0.6404870	-2.9083790	-0.4780640
N	2.4192880	0.5260740	0.1556710
C	3.4122640	-0.5497000	0.1685830
C	-2.6766290	-2.3592240	-0.7757390
H	-2.8213840	-3.3787860	-1.1370700
H	-3.1144170	-1.6840440	-1.5128880
C	-3.3369990	-2.1754670	0.5852170
H	-3.1943170	-1.1545320	0.9518410
H	-4.4112020	-2.3676070	0.5094280
H	-2.9132080	-2.8705400	1.3161770
H	2.7590590	1.4811720	0.1748410
C	4.5801540	-0.1215750	1.0458390
H	2.9298300	-1.4240180	0.6124010
C	3.8719330	-0.8868930	-1.2479590
H	5.3400520	-0.9070000	1.0570280
H	5.0410940	0.7910000	0.6511650
H	4.2594250	0.0650540	2.0742070
H	4.5606790	-1.7366760	-1.2290900
H	3.0232400	-1.1436460	-1.8876820

H	4.3925860	-0.0299610	-1.6889750
O	-0.9870200	-0.0300760	2.3548710
H	-0.0871140	0.3204340	2.5289320
O	-1.7692720	1.0040610	2.1887440

TRANSITION STATE

C	-0.4824870	1.5401280	-0.4161370
N	-1.2053930	0.4733270	-0.7003410
C	-0.4972880	-0.6816740	-0.6045770
C	1.3938250	0.4066060	-0.0003010
N	0.7745830	1.6262640	-0.0645290
Cl	-1.3413520	3.0617190	-0.5202740
N	0.7996060	-0.7600030	-0.2648740
N	-1.1292510	-1.8310040	-0.8791410
H	-0.5951000	-2.6795490	-0.7376390
N	2.6774030	0.4254870	0.3772570
C	3.5720900	-0.7333210	0.3459960
C	-2.5388220	-1.9487050	-1.2128130
H	-2.6390780	-2.8011850	-1.8957980
H	-2.8478960	-1.0615120	-1.7670740
C	-3.4333180	-2.1878580	-0.0262260
H	-3.4575950	-1.1091550	0.7302280
H	-4.4886760	-2.3009680	-0.2801960
H	-3.0752890	-2.9322420	0.6884050
H	3.0978710	1.3425340	0.4789980
C	4.7288610	-0.4768180	1.3016170
H	2.9947460	-1.5911530	0.6988700
C	4.0641690	-1.0030640	-1.0740470
H	5.4172580	-1.3256020	1.2864980
H	5.2846880	0.4171930	0.9970530
H	4.3735930	-0.3356290	2.3258620
H	4.6630310	-1.9182870	-1.0989000
H	3.2249110	-1.1191240	-1.7653750
H	4.6874990	-0.1721400	-1.4216150
O	-2.3078900	-0.2808050	2.2192970
H	-1.6795960	0.2506590	1.6990920
O	-3.4943860	-0.1871100	1.4990230

PRODUCTS

C	-0.4147500	1.3624530	-0.0844020
N	-1.0754260	0.2175000	-0.1633390
C	-0.2538650	-0.8679600	-0.1411040
C	1.5981560	0.4169280	0.0968880
N	0.8663330	1.5739800	0.0423800
Cl	-1.4100470	2.7973760	-0.1631220
N	1.0810770	-0.8083160	-0.0089120
N	-0.7946440	-2.0833040	-0.2846050
H	-0.1597830	-2.8641130	-0.1727070
N	2.9130940	0.5690250	0.2817370
C	3.8943590	-0.5156860	0.2078610
C	-2.2201810	-2.3593190	-0.3731420
H	-2.3327130	-3.2995610	-0.9217560
H	-2.6779030	-1.5869520	-1.0058130
C	-2.8888730	-2.4483960	0.9555810
H	-4.8306520	-0.9083940	-0.0794960
H	-3.8698890	-2.9027060	1.0344980
H	-2.4286950	-2.0114780	1.8338230
H	3.2565380	1.5230890	0.2862460
C	5.1601730	-0.0731010	0.9278990
H	3.4625460	-1.3737380	0.7290140
C	4.1757230	-0.8957710	-1.2436290
H	5.9095540	-0.8669260	0.8771200
H	5.5785860	0.8207940	0.4518560
H	4.9626780	0.1501640	1.9798270
H	4.8513830	-1.7552770	-1.2831420
H	3.2516020	-1.1576910	-1.7665780
H	4.6493540	-0.0590280	-1.7681950
O	-3.8419310	0.5653140	0.5798880
H	-2.9256110	0.3791760	0.2651260
O	-4.6535290	-0.0202930	-0.4340500

ETHYL SIDECHAIN, PATHWAY 2

REACTANTS

C	0.352399	1.806059	-0.070123
N	-0.640738	0.941229	-0.077667
C	-0.214771	-0.346035	-0.002809
C	1.963830	0.270394	0.067043
N	1.643244	1.598815	-0.005578
CL	-0.131971	3.488097	-0.158595
N	1.073584	-0.724141	0.072795
N	-1.136731	-1.317416	-0.027924
H	-0.788890	-2.257900	0.110576
N	3.270141	-0.007092	0.164076
C	3.847462	-1.351787	0.126995
C	-2.576308	-1.093697	0.039071
H	-3.049512	-1.989176	-0.368396
H	-2.825281	-0.260499	-0.621596
C	-3.076015	-0.827419	1.453456
H	-2.591545	0.055794	1.878925
H	-4.156358	-0.654689	1.440143
H	-2.871637	-1.682625	2.104082
H	3.899936	0.783984	0.094958
C	5.243105	-1.291752	0.732525
H	3.212168	-1.991431	0.745498
C	3.882520	-1.900984	-1.297245
H	5.697861	-2.285215	0.710692
H	5.880483	-0.613452	0.154018
H	5.214591	-0.946345	1.769392
H	4.258763	-2.928318	-1.293261
H	2.885970	-1.900201	-1.746105
H	4.546074	-1.292234	-1.920777
O	-5.772150	-1.267931	-0.870997
H	-5.181696	-0.577011	-1.239305
O	-6.463756	-0.705415	0.083982

TRANSITION STATE

C	0.3439870	1.8318630	-0.0997900
N	-0.6536740	0.9907410	-0.2810450
C	-0.2560530	-0.3047960	-0.2561150
C	1.9054950	0.2525440	0.1077060
N	1.6144230	1.5889510	0.1007830
CL	-0.1021910	3.5243980	-0.1310570
N	1.0068300	-0.7197390	-0.0757180
N	-1.1936940	-1.2481790	-0.4546410
H	-0.8931330	-2.2057190	-0.3203190
N	3.1839670	-0.0655730	0.3415760
C	3.7379170	-1.4168100	0.2397460
C	-2.6284770	-0.9747660	-0.4538870
H	-3.1154550	-1.8532300	-0.8805020
H	-2.8277340	-0.1252310	-1.1088680
C	-3.1386790	-0.7108890	0.9430080
H	-2.8313930	0.2353220	1.3899560
H	-4.4423330	-0.5478880	0.7946140
H	-3.0883750	-1.5605900	1.6260750
H	3.8332430	0.7105000	0.4029840
C	5.0472550	-1.4595370	1.0149980
H	3.0184730	-2.0944990	0.7067660
C	3.9339860	-1.8169140	-1.2202880
H	5.4877470	-2.4569230	0.9409250
H	5.7616430	-0.7400670	0.5989250
H	4.8914280	-1.2268660	2.0718510
H	4.2932780	-2.8483520	-1.2831680
H	2.9951540	-1.7425990	-1.7760530
H	4.6737530	-1.1626250	-1.6938750
O	-5.8605240	-1.6554330	-0.1775490
H	-5.6812200	-1.4170170	-1.1034770
O	-5.6038980	-0.4828870	0.5266970

PRODUCTS

C	0.3565020	1.8147250	-0.0907920
N	-0.6389380	0.9544310	-0.1596550
C	-0.2199500	-0.3349720	-0.1108820
C	1.9539500	0.2669110	0.0733220
N	1.6423730	1.5981530	0.0224410
Cl	-0.1171990	3.4998560	-0.1553810
N	1.0602010	-0.7236660	0.0045180
N	-1.1498400	-1.2972160	-0.2067810
H	-0.8262520	-2.2455380	-0.0628060
N	3.2515370	-0.0234130	0.2228710
C	3.8127090	-1.3752980	0.1947310
C	-2.5945960	-1.0428500	-0.1702040
H	-3.0706000	-1.9546190	-0.5350720
H	-2.8185120	-0.2391880	-0.8748710
C	-3.0816180	-0.7070050	1.2024290
H	-2.9861010	0.3039350	1.5826310
H	-5.2166850	-0.1478550	0.5767050
H	-3.2981650	-1.5053540	1.9036010
H	3.8915100	0.7623910	0.2182220
C	5.1721680	-1.3482130	0.8791050
H	3.1334840	-2.0149840	0.7647520
C	3.9187550	-1.9005050	-1.2349660
H	5.6165680	-2.3463160	0.8547540
H	5.8485380	-0.6618320	0.3572510
H	5.0890440	-1.0315140	1.9222180
H	4.2652720	-2.9381470	-1.2280520
H	2.9514910	-1.8618800	-1.7427460
H	4.6363270	-1.3012820	-1.8056850
O	-5.8836500	-1.7222510	-0.2280980
H	-5.3779890	-1.7743260	-1.0562390
O	-5.9801500	-0.3197260	-0.0060780

ETHYL SIDECHAIN, PATHWAY 3

REACTANTS

C	0.7523640	2.1470120	-0.0807780
N	-0.4926610	1.7479200	-0.2330610
C	-0.6164670	0.3961440	-0.2249040
C	1.6077200	0.0949210	0.0829570
N	1.8446600	1.4428070	0.0783990
Cl	0.9738910	3.8854960	-0.0904760
N	0.4044530	-0.4641180	-0.0676840
N	-1.8362590	-0.1286510	-0.4167280
H	-1.9121540	-1.1279930	-0.2558520
N	2.6787480	-0.6850240	0.2727070
C	2.6659950	-2.1477510	0.2127430
C	-3.0777320	0.6355570	-0.3554850
H	-3.8177100	0.0922160	-0.9476530
H	-2.9138870	1.5968380	-0.8431380
C	-3.5741200	0.8275030	1.0716780
H	-2.8382930	1.3749870	1.6681300
H	-4.5098300	1.3940130	1.0727760
H	-3.7557580	-0.1399740	1.5498900
H	3.5736360	-0.2138100	0.3380420
C	3.9070670	-2.6669090	0.9249950
H	1.7741400	-2.4843630	0.7486960
C	2.6008070	-2.6422640	-1.2299210
H	3.9175980	-3.7594230	0.8998730
H	4.8130860	-2.3056930	0.4254180
H	3.9298130	-2.3436510	1.9692600
H	2.5371630	-3.7344110	-1.2479600
H	1.7266930	-2.2373580	-1.7464620
H	3.5015380	-2.3400380	-1.7747180
O	-4.3498620	-2.5641590	-0.4108340
H	-3.9055630	-2.2403870	-1.2232430
O	-3.4580160	-2.5408660	0.5435710

TRANSITION STATE

C	-0.4686470	2.0884940	-0.0417890
N	0.6598940	1.5200800	0.3327860

C	0.5534990	0.1724340	0.4443850
C	-1.6291030	0.1866030	-0.1549890
N	-1.6310020	1.5464730	-0.3044760
Cl	-0.3978810	3.8306470	-0.2090970
N	-0.5643890	-0.5329570	0.2093200
N	1.6389230	-0.5099760	0.8419590
H	1.5584620	-1.5191280	0.8356350
N	-2.7863470	-0.4329280	-0.4219220
C	-3.0594680	-1.8433860	-0.1367260
C	2.9618470	0.0744450	0.9927320
H	3.5535610	-0.6156040	1.5989340
H	2.8797270	1.0047310	1.5671150
C	3.6493920	0.3560050	-0.3146040
H	3.0414600	0.8484300	-1.0753770
H	4.6564480	0.7641520	-0.2191200
H	3.8658560	-0.8280240	-0.8604320
H	-3.5804150	0.1692810	-0.6085400
C	-4.2581260	-2.2814770	-0.9665630
H	-2.1790780	-2.4104010	-0.4486440
C	-3.3012540	-2.0629460	1.3548460
H	-4.4826010	-3.3316080	-0.7634510
H	-5.1416710	-1.6881620	-0.7052740
H	-4.0640290	-2.1686680	-2.0365960
H	-3.4349600	-3.1289100	1.5613920
H	-2.4584560	-1.6978350	1.9481220
H	-4.2060210	-1.5329060	1.6715370
O	4.1578150	-2.7066570	-0.0854920
H	3.2519120	-3.0181990	0.0829390
O	4.0416090	-1.9488470	-1.2471360

PRODUCTS

C	-0.6615130	2.1457120	-0.0404680
N	0.5365460	1.7226750	0.3101070
C	0.5955000	0.3747500	0.4437820
C	-1.5831760	0.1155130	-0.1121370
N	-1.7542240	1.4633730	-0.2697650
Cl	-0.8096120	3.8802380	-0.2300280
N	-0.4331700	-0.4641110	0.2442710
N	1.7616590	-0.1683740	0.8377750
H	1.8069710	-1.1789750	0.7736140
N	-2.6568960	-0.6413020	-0.3672290
C	-2.7449550	-2.0795320	-0.1069580
C	3.0286000	0.5540290	0.8165380
H	3.7227760	0.0159700	1.4664120
H	2.8703610	1.5363950	1.2784190
C	3.5937650	0.6943610	-0.5556860
H	2.9261470	0.8690910	-1.3940220
H	4.6490500	0.9125770	-0.6761400
H	3.6328620	-1.4014000	-1.2232090
H	-3.5167690	-0.1401790	-0.5604270
C	-3.8790490	-2.6532090	-0.9449240
H	-1.7981420	-2.5220100	-0.4265840
C	-2.9525750	-2.3538420	1.3802090
H	-3.9745380	-3.7249160	-0.7534620
H	-4.8286050	-2.1743850	-0.6800620
H	-3.6992180	-2.5066450	-2.0133240
H	-2.9455680	-3.4314940	1.5685050
H	-2.1623100	-1.8921150	1.9784170
H	-3.9177220	-1.9521220	1.7069770
O	4.1258470	-2.5798730	0.1654680
H	3.3124180	-2.9506880	0.5448260
O	3.7652420	-2.3695860	-1.1964320

HAT TRANSFER WITH PERMANGANATE, ETHYL SIDE CHAIN

H15

REACTANTS

C	-0.7972740	1.5814280	-0.8748180
N	-0.1197840	0.5211790	-1.2630870
C	-0.7770100	-0.6407390	-1.0107800

C	-2.5728960	0.4398850	-0.1535850
N	-1.9833770	1.6634660	-0.3267920
Cl	0.0154710	3.1130680	-1.1331860
N	-2.0041010	-0.7262580	-0.4646020
N	-0.1668070	-1.7842960	-1.3359390
H	-0.6741420	-2.6391760	-1.1415370
N	-3.8129800	0.4594400	0.3523190
C	-4.5968710	-0.7260040	0.6993380
C	1.1960610	-1.8791120	-1.8475120
H	1.8125020	-1.1394370	-1.3318940
H	1.2108820	-1.6395090	-2.9169870
C	1.7364320	-3.2777390	-1.6086880
H	1.1192330	-4.0307810	-2.1088670
H	2.7525170	-3.3539460	-2.0031350
H	1.7643050	-3.5055370	-0.5388100
H	-4.1669970	1.3665020	0.6333260
C	-6.0671900	-0.3327410	0.7421320
H	-4.4430830	-1.4562180	-0.0997810
C	-4.1375610	-1.3261640	2.0254300
H	-6.6766410	-1.2044650	0.9933770
H	-6.2367460	0.4330510	1.5075790
H	-6.4024080	0.0574680	-0.2227450
H	-4.6941050	-2.2446210	2.2348720
H	-3.0713460	-1.5666810	1.9997570
H	-4.3164230	-0.6196390	2.8429510
O	3.6174570	0.0961020	-0.5974540
Mn	3.2347740	0.0817150	0.9300300
O	4.3881210	-0.6116990	1.7467450
O	3.0466570	1.5641040	1.4260470
O	1.8974260	-0.7222090	1.1250270

TRANSITION STATE

C	1.2175180	1.8316010	0.4315570
N	0.3401090	0.9273860	0.8272200
C	0.8416070	-0.3270900	0.7919260
C	2.8605190	0.3664290	0.0570110
N	2.4546030	1.6721980	0.0392440
Cl	0.6333920	3.4791170	0.4279930
N	2.0807660	-0.6612110	0.4145180
N	0.0240900	-1.3349070	1.1759790
H	0.3562650	-2.2741910	0.9809700
N	4.1293520	0.1431460	-0.2959240
C	4.7451910	-1.1782920	-0.4320710
C	-1.3435730	-1.1605530	1.5131620
H	-1.8970820	-0.9499360	0.3892830
H	-1.4841260	-0.2703640	2.1172870
C	-1.9666170	-2.4163070	2.0662930
H	-1.4578200	-2.7176290	2.9895210
H	-3.0203520	-2.2416900	2.2871380
H	-1.8919730	-3.2393400	1.3485120
H	4.6584390	0.9518390	-0.6019880
C	6.2556300	-1.0137010	-0.3378940
H	4.3944640	-1.7842510	0.4076490
C	4.3342500	-1.8426720	-1.7435220
H	6.7401170	-1.9885590	-0.4332460
H	6.6203830	-0.3721150	-1.1479630
H	6.5492050	-0.5713990	0.6178990
H	4.7419070	-2.8565510	-1.7944520
H	3.2460960	-1.9019470	-1.8307360
H	4.7213420	-1.2699450	-2.5930120
O	-3.6669880	0.0751520	0.8674460
Mn	-3.6948640	-0.1289240	-0.7361910
O	-4.8832570	-1.0768230	-1.1384700
O	-3.6413140	1.2640620	-1.4713800
O	-2.2512550	-0.9147140	-0.8593480

PRODUCTS

C	1.4955840	2.1049770	-0.0141600
N	0.4050430	1.5611300	0.4894080
C	0.5492470	0.2367370	0.7339000
C	2.6927050	0.2230540	0.0065190

N	2.6518860	1.5574740	-0.2912020
Cl	1.3703560	3.8160710	-0.3635650
N	1.6651670	-0.4712720	0.5063830
N	-0.5017160	-0.4304210	1.2454110
H	-0.3442420	-1.4095310	1.4599150
N	3.8594120	-0.3926320	-0.2113240
C	4.1031090	-1.8211880	-0.0062010
C	-1.7862900	0.1702220	1.6147970
H	-1.3097410	-1.4412670	-0.4784220
H	-1.5626170	1.0820110	2.1822170
C	-2.5169270	-0.8215700	2.5057830
H	-1.9476780	-1.0094040	3.4202930
H	-3.4920670	-0.4116630	2.7768300
H	-2.6688460	-1.7691070	1.9782410
H	4.5967040	0.1665920	-0.6245640
C	5.5893100	-2.0269190	0.2523140
H	3.5394680	-2.1149740	0.8827820
C	3.6194560	-2.6403500	-1.1999690
H	5.7917100	-3.0883400	0.4163560
H	6.1780520	-1.6971960	-0.6110430
H	5.9183070	-1.4708470	1.1344550
H	3.7448640	-3.7080470	-0.9966660
H	2.5628040	-2.4488680	-1.4060410
H	4.2003430	-2.3877260	-2.0934020
O	-2.5509410	0.5832220	0.5161770
Mn	-3.4101390	-0.5049510	-0.7131680
O	-4.6300250	-1.1635110	0.0075430
O	-3.5071810	0.3500380	-2.0232650
O	-2.0975240	-1.7523460	-0.9454290

H16

Reactants

C	1.2756630	1.5391930	0.2173170
N	0.4823430	0.4905100	0.2640650
C	1.1619170	-0.6846600	0.2237710
C	3.1664930	0.3627950	0.1017390
N	2.5818810	1.5990400	0.1429070
Cl	0.4591540	3.0898040	0.2626880
N	2.5004210	-0.7929660	0.1319390
N	0.4522810	-1.8176040	0.2619430
H	0.9852340	-2.6773780	0.2825050
N	4.5068160	0.3573750	0.0561900
C	5.3262070	-0.8262680	-0.2058810
C	-1.0003200	-1.8881070	0.3935920
H	-1.2856480	-2.8913310	0.0718890
H	-1.4507330	-1.1768930	-0.3036550
C	-1.4917610	-1.6275050	1.8118370
H	-1.2467560	-0.6105960	2.1303580
H	-2.5779810	-1.7491790	1.8553930
H	-1.0378590	-2.3336090	2.5135810
H	4.9468550	1.2628290	-0.0643670
C	6.7321180	-0.5645890	0.3165190
H	4.8802910	-1.6540490	0.3501640
C	5.3351980	-1.1615300	-1.6954210
H	7.3720350	-1.4261760	0.1096120
H	7.1669940	0.3090810	-0.1824320
H	6.7290030	-0.3844170	1.3949010
H	5.8905580	-2.0874320	-1.8717190
H	4.3177140	-1.2895650	-2.0755930
H	5.8177580	-0.3555250	-2.2589240
O	-4.1077460	-1.6517560	-0.3464670
Mn	-4.2967500	-0.0888150	-0.3411010
O	-5.4753720	0.2941120	-1.3131280
O	-4.6501070	0.3827780	1.1192680
O	-2.9659800	0.6008020	-0.8184270

TRANSITION STATE

C	1.3214920	1.8201600	-0.0061370
N	0.4119600	0.9861240	0.4612510
C	0.8960510	-0.2615370	0.6409590

C	2.9666070	0.3133010	-0.0624940
N	2.5793070	1.6046340	-0.2951480
Cl	0.7526570	3.4511890	-0.2828530
N	2.1533690	-0.6484500	0.3893920
N	0.0598500	-1.2169700	1.1090470
H	0.4301830	-2.1596170	1.0698340
N	4.2519520	0.0332450	-0.2958590
C	4.8621850	-1.2885060	-0.1403330
C	-1.3075810	-1.0639600	1.4734100
H	-1.6526570	-2.0319990	1.8239900
H	-1.8980130	-0.8432210	0.3660000
C	-1.6512230	0.0751310	2.4121130
H	-1.9038500	0.9942420	1.8793080
H	-2.5157050	-0.2154760	3.0118990
H	-0.8080810	0.2896980	3.0779110
H	4.8172620	0.7828470	-0.6776340
C	6.3571440	-1.1065880	0.0806180
H	4.4184300	-1.7411750	0.7504020
C	4.5783800	-2.1745230	-1.3500490
H	6.8342120	-2.0832360	0.1944750
H	6.8131740	-0.6035700	-0.7795390
H	6.5592350	-0.5167120	0.9786800
H	4.9799370	-3.1779420	-1.1801290
H	3.5040180	-2.2578990	-1.5342690
H	5.0550680	-1.7585520	-2.2440230
O	-3.9473220	-1.0645740	0.9309790
Mn	-3.9445060	-0.4448450	-0.5628130
O	-4.6563990	-1.4376750	-1.5600720
O	-4.4774890	1.0340470	-0.5438460
O	-2.3124270	-0.4589760	-0.7929830

PRODUCTS

C	0.8653120	1.9813990	-0.1107520
N	-0.0307800	1.3156800	0.5878950
C	0.4055270	0.0932050	0.9718510
C	2.4378930	0.4093970	0.0130970
N	2.0835720	1.6449400	-0.4526740
Cl	0.3401870	3.5566180	-0.6719200
N	1.6325210	-0.3928530	0.7135370
N	-0.3982040	-0.7157040	1.6906610
H	0.0030070	-1.6354700	1.8364950
N	3.6869720	0.0135380	-0.2585850
C	4.2390480	-1.2966200	0.0896410
C	-1.8439180	-0.6563550	1.9580840
H	-1.9466430	-1.2754610	2.8574730
H	-0.7530670	-1.4549520	-0.6890720
C	-2.3684500	0.7298010	2.2969750
H	-2.4015650	1.3769060	1.4230030
H	-3.3820060	0.6113170	2.6896420
H	-1.7514040	1.2005680	3.0673660
H	4.2415400	0.6324060	-0.8389650
C	5.7567980	-1.1871110	0.1249420
H	3.8717110	-1.5403500	1.0900120
C	3.7762650	-2.3705080	-0.8915360
H	6.1908770	-2.1566560	0.3817820
H	6.1418440	-0.8904160	-0.8572710
H	6.0864480	-0.4533230	0.8654210
H	4.1374010	-3.3520840	-0.5701890
H	2.6850250	-2.4054650	-0.9499520
H	4.1734880	-2.1651070	-1.8912860
O	-2.6015770	-1.3098340	0.9768170
Mn	-2.9411170	-0.7481340	-0.7681350
O	-3.8714310	-1.8702220	-1.3402800
O	-3.2684270	0.7778720	-0.7923800
O	-1.2562300	-1.0390060	-1.4026690

H17

REACTANTS

C	0.6254930	1.7345720	1.2451610
N	0.1237060	2.1475760	0.1011770

C	0.5818250	1.4335870	-0.9571710
C	1.9153200	0.1540730	0.3484160
N	1.4949540	0.7856810	1.4861000
Cl	0.0461310	2.5932510	2.6592230
N	1.4936100	0.4494930	-0.8826610
N	0.1253790	1.7591490	-2.1773430
H	0.3966100	1.1288100	-2.9223430
N	2.7993570	-0.8390110	0.5272570
C	3.5248090	-1.5138040	-0.5504140
C	-1.0453810	2.6013440	-2.3988430
H	-0.9983050	2.9427280	-3.4345590
H	-0.9633850	3.4804880	-1.7584320
C	-2.3485610	1.8570430	-2.1401290
H	-2.3885140	1.4941790	-1.1081130
H	-3.2033700	2.5185700	-2.3087650
H	-2.4384160	0.9986940	-2.8125650
H	3.1645790	-0.9397940	1.4677730
C	4.0785710	-2.8251670	-0.0100930
H	2.8014600	-1.7278560	-1.3411480
C	4.6358450	-0.6247240	-1.1031850
H	4.6256070	-3.3484120	-0.7983810
H	4.7717450	-2.6353100	0.8173420
H	3.2780830	-3.4778180	0.3486270
H	5.1375730	-1.1223180	-1.9384970
H	4.2378900	0.3295100	-1.4586900
H	5.3787870	-0.4240570	-0.3236320
O	-3.2724220	-1.1681190	-1.0467180
Mn	-2.4321810	-1.5841820	0.2175390
O	-3.3621860	-1.5527510	1.4862480
O	-1.8617640	-3.0370940	0.0147070
O	-1.2344550	-0.5820200	0.4135080

TRANSITION STATE

C	-1.2450550	2.0576090	-0.4738100
N	-0.5030180	1.8977760	0.6016520
C	-0.7352680	0.7170880	1.2253290
C	-2.3460050	0.1315500	-0.2539730
N	-2.1567510	1.2699110	-0.9865970
Cl	-0.9819970	3.5561590	-1.3427030
N	-1.6609260	-0.1787870	0.8509590
N	-0.0259320	0.4298250	2.3349040
H	-0.1822050	-0.5069310	2.6915400
N	-3.2694770	-0.7166710	-0.7234370
C	-3.7580410	-1.9046230	-0.0211870
C	1.2645770	1.0199070	2.6496790
H	1.3065640	1.2193070	3.7281720
H	1.3459590	1.9765690	2.1360550
C	2.4240320	0.0987590	2.2984830
H	2.1636540	-0.0284740	1.0394720
H	3.3842740	0.5554290	2.5238160
H	2.3314020	-0.8912130	2.7459450
H	-3.8012360	-0.3930520	-1.5235980
C	-4.3805840	-2.8464480	-1.0430320
H	-2.8912630	-2.3884610	0.4353260
C	-4.7568880	-1.5233640	1.0686090
H	-4.7627190	-3.7374680	-0.5386730
H	-5.2185460	-2.3571510	-1.5525990
H	-3.6505460	-3.1602990	-1.7936970
H	-5.0797970	-2.4163240	1.6120270
H	-4.3134060	-0.8256640	1.7843040
H	-5.6393910	-1.0510460	0.6237750
O	3.9026720	-0.9586850	0.6705140
Mn	3.1132600	-0.9375320	-0.7445670
O	3.8732760	-0.0398590	-1.7867270
O	2.7486650	-2.3983470	-1.1989020
O	1.7731130	-0.1567170	-0.1492230

PRODUCTS

C	-1.003995	2.333218	-0.342309
N	-0.043419	2.192726	0.545637
C	-0.095382	1.000692	1.192381

C	-1.920836	0.337959	0.028764
N	-1.953420	1.499140	-0.691389
Cl	-1.012539	3.871132	-1.184632
N	-1.054403	0.082745	1.013532
N	0.837127	0.738418	2.137472
H	0.793115	-0.223618	2.459893
N	-2.820964	-0.594476	-0.304154
C	-2.857163	-1.943886	0.264901
C	2.189631	1.282294	2.058609
H	2.615143	1.321391	3.064422
H	2.129469	2.300703	1.676100
C	3.075254	0.422110	1.155359
H	0.859215	0.325041	-1.650151
H	4.053646	0.912178	1.051072
H	3.242722	-0.555931	1.629121
H	-3.445789	-0.371230	-1.069852
C	-3.469332	-2.886101	-0.762203
H	-1.818625	-2.236508	0.446966
C	-3.622084	-1.973942	1.584802
H	-3.507078	-3.900394	-0.356663
H	-4.492729	-2.579093	-1.005200
H	-2.880608	-2.904456	-1.683606
H	-3.554367	-2.970241	2.032028
H	-3.211084	-1.249119	2.292734
H	-4.679213	-1.741308	1.417792
O	2.461600	0.277872	-0.104970
Mn	2.017719	-1.390197	-0.671639
O	3.233919	-2.013922	-1.439795
O	1.234173	-2.143678	0.458058
O	0.837229	-0.625981	-1.833851

H18

Reactants

C	2.033247	1.796542	-0.102319
N	1.079021	0.897578	-0.225409
C	1.546462	-0.375704	-0.161667
C	3.686453	0.315677	0.109911
N	3.321510	1.633467	0.064214
Cl	1.495362	3.462538	-0.174956
N	2.838067	-0.709509	0.005281
N	0.668405	-1.379452	-0.305884
H	1.043087	-2.306740	-0.145907
N	4.990492	0.078101	0.299485
C	5.614757	-1.245230	0.253134
C	-0.781434	-1.216631	-0.255773
H	-1.213919	-2.091827	-0.744566
H	-1.050079	-0.343611	-0.851833
C	-1.314056	-1.086829	1.165209
H	-0.863687	-0.229142	1.673802
H	-2.398368	-0.942959	1.142156
H	-1.094415	-1.988259	1.745300
H	5.595960	0.890626	0.309227
C	6.967867	-1.161853	0.945627
H	4.966404	-1.927968	0.809196
C	5.751220	-1.740201	-1.184291
H	7.459431	-2.137321	0.913758
H	7.613981	-0.438547	0.435270
H	6.862515	-0.860599	1.991433
H	6.167806	-2.751870	-1.194155
H	4.780235	-1.761885	-1.686234
H	6.422662	-1.083505	-1.747835
MN	-5.310202	-0.486453	1.193673
O	-4.393119	-0.741622	2.447283
O	-4.437171	-0.623009	-0.108673
O	-6.481254	-1.538894	1.167617
O	-5.911789	0.964159	1.279567

TRANSITION STATE

C	-1.971874	1.850173	0.127623

N -1.007204 1.082739 0.592906
C -1.356969 -0.225930 0.638424
C -3.416152 0.183354 -0.206241
N -3.169391 1.525591 -0.290092
CL -1.591031 3.557766 0.060863
N -2.543964 -0.719140 0.252924
N -0.461034 -1.097606 1.138072
H -0.704041 -2.075584 1.032244
N -4.615891 -0.217111 -0.647552
C -5.171776 -1.557998 -0.452869
C 0.946292 -0.778896 1.345906
H 1.352003 -1.538073 2.016028
H 1.019303 0.188515 1.843427
C 1.695203 -0.775306 0.015359
H 1.333815 -0.001214 -0.658243
H 2.859007 -0.516021 0.505333
H 1.694295 -1.755452 -0.458702
H -5.264925 0.523917 -0.888563
C -6.298065 -1.763105 -1.455972
H -4.371392 -2.272162 -0.659652
C -5.657304 -1.740530 0.983043
H -6.736465 -2.755242 -1.322031
H -7.087922 -1.018900 -1.302937
H -5.935100 -1.681017 -2.484000
H -6.011537 -2.764345 1.134960
H -4.853119 -1.541761 1.696989
H -6.484494 -1.053095 1.190406
MN 4.895965 -0.205555 -0.323853
O 3.657164 -0.458820 -1.331694
O 3.975908 -0.299393 1.058572
O 5.921874 -1.392878 -0.393977
O 5.473392 1.242924 -0.508934

PRODUCTS

C -1.953581 1.897258 0.073587
N -0.894235 1.137381 0.261199
C -1.193818 -0.186149 0.262476
C -3.390590 0.202966 -0.121147
N -3.202777 1.558462 -0.119417
CL -1.638999 3.621125 0.089178
N -2.422224 -0.696637 0.068837
N -0.197856 -1.052493 0.495813
H -0.439097 -2.034781 0.463803
N -4.644465 -0.207868 -0.348287
C -5.096378 -1.598650 -0.283798
C 1.193687 -0.675270 0.675852
H 1.631720 -1.437114 1.323615
H 1.239292 0.286427 1.190545
C 1.943775 -0.572287 -0.660880
H 1.249705 -0.138918 -1.395864
H 3.464786 -1.087352 1.611562
H 2.204645 -1.580459 -1.014640
H -5.347784 0.519013 -0.413754
C -6.406079 -1.711152 -1.052011
H -4.334823 -2.207077 -0.778768
C -5.253882 -2.067903 1.160758
H -6.769884 -2.740986 -1.014469
H -7.168390 -1.064592 -0.602576
H -6.279229 -1.426094 -2.099861
H -5.514804 -3.130197 1.181604
H -4.327622 -1.929195 1.724509
H -6.052456 -1.506354 1.657223
O 4.765187 -0.312659 -0.162387
MN 3.077381 0.262926 -0.612377
O 4.337452 -1.337301 1.285212
O 5.250570 -1.263795 -1.307253
O 5.540764 0.941951 0.368752

H19

REACTANTS

C 3.157561 -1.599917 0.047826
N 1.920792 -1.896672 0.388185
C 1.133696 -0.797292 0.518799
C 2.830734 0.604338 -0.021092
N 3.708940 -0.433631 -0.176281
CL 4.225523 -2.978243 -0.135235
N 1.548582 0.466615 0.324801
N -0.141121 -0.972448 0.895598
H -0.730538 -0.147790 0.851482
N 3.321933 1.825949 -0.262603
C 2.579998 3.074634 -0.082328
C -0.830164 -2.258540 0.871168
H -1.693031 -2.167767 1.534173
H -0.168061 -3.014465 1.295230
C -1.281478 -2.651370 -0.529782
H -0.423670 -2.750084 -1.201735
H -1.810864 -3.608209 -0.500911
H -1.959323 -1.895729 -0.939381
H 4.309985 1.882324 -0.480659
C 3.222676 4.148301 -0.949313
H 1.559323 2.892199 -0.428594
C 2.545538 3.490805 1.386365
H 2.688689 5.093545 -0.823750
H 4.265897 4.305549 -0.652661
H 3.197949 3.875053 -2.007688
H 1.923072 4.382012 1.508923
H 2.136145 2.693330 2.012224
H 3.556887 3.723718 1.736653
MN -4.151398 0.392390 -0.031071
O -4.655852 -1.030286 -0.480465
O -2.794744 0.237472 0.756948
O -3.924741 1.292600 -1.301862
O -5.226215 1.055458 0.906284

TRANSITION STATE

C -1.046616 1.769129 -0.572179
N -0.294085 1.593583 0.495125
C -0.649469 0.497869 1.210852
C -2.340548 -0.009773 -0.205039
N -2.058167 1.061748 -1.007635
CL -0.623237 3.156170 -1.554726
N -1.660067 -0.328721 0.899952
N 0.038062 0.230792 2.335156
H -0.166678 -0.664411 2.763481
N -3.362672 -0.779011 -0.594674
C -3.864662 -1.938847 0.143980
C 1.299221 0.865602 2.679323
H 1.469425 0.695015 3.743979
H 1.201544 1.946645 2.532481
C 2.479072 0.366603 1.858486
H 2.309049 0.418042 0.783911
H 3.405251 0.857687 2.146876
H 2.421589 -0.868219 2.224733
H -3.866063 -0.477033 -1.420492
C -4.658524 -2.809736 -0.819321
H -2.992525 -2.495173 0.498883
C -4.709138 -1.512271 1.342043
H -5.046885 -3.684770 -0.292355
H -5.509810 -2.251383 -1.225061
H -4.035684 -3.152193 -1.650278
H -5.002778 -2.391092 1.923737
H -4.150746 -0.835883 1.994596
H -5.617314 -1.002259 1.003529
MN 3.640666 -2.702457 1.992876
O 4.140437 -1.321567 1.312468
O 2.256594 -2.047485 2.642343
O 3.298731 -3.768656 0.890359
O 4.640690 -3.151116 3.117897

PRODUCTS

C 2.595282 -1.884088 -0.068891
N 1.318132 -1.977024 0.231383

C	0.725975	-0.765977	0.406347
C	2.647018	0.343638	-0.059861
N	3.343679	-0.822513	-0.233113
Cl	3.418455	-3.418747	-0.276957
N	1.354512	0.416365	0.265942
N	-0.561987	-0.733995	0.767992
H	-1.003238	0.179262	0.836570
N	3.346830	1.467859	-0.253637
C	2.810389	2.824072	-0.130798
C	-1.442453	-1.890933	0.807013
H	-2.036833	-1.858871	1.726193
H	-0.820137	-2.784219	0.854840
C	-2.366853	-1.997593	-0.404249
H	-1.773247	-1.788728	-1.309334
H	-2.702290	-3.042201	-0.464526
H	-2.993721	-0.008697	1.876576
H	4.325605	1.352103	-0.487725
C	3.709459	3.765212	-0.920513
H	1.812113	2.816877	-0.578221
C	2.699002	3.254571	1.329521
H	3.333442	4.788299	-0.843011
H	4.728820	3.745023	-0.518588
H	3.745281	3.489066	-1.977885
H	2.217224	4.234791	1.393045
H	2.105939	2.540630	1.906748
H	3.694270	3.329573	1.780463
O	-3.589046	0.644765	-0.271603
Mn	-3.531031	-1.205309	-0.375160
O	-2.897859	0.834819	1.412887
O	-2.571852	1.205616	-1.319638
O	-5.111245	0.997177	-0.205364

HYDRIDE TRANSFER WITH H_3O^+

REACTANTS

C	0.020243	1.894885	-0.079854
N	1.001052	1.063143	-0.369282
C	0.574770	-0.219229	-0.503078
C	-1.576033	0.335707	-0.065950
N	-1.255848	1.658238	0.087610
Cl	0.503812	3.568857	0.106920
N	-0.698492	-0.626498	-0.357992
N	1.490313	-1.148960	-0.794793
H	1.153376	-2.097266	-0.909057
N	-2.871759	0.030114	0.074144
C	-3.416352	-1.327922	0.048549
C	2.908339	-0.876100	-0.996091
H	3.313121	-0.387601	-0.104031
H	3.034140	-0.183747	-1.834262
C	3.643548	-2.175895	-1.272158
H	3.249075	-2.666215	-2.167139
H	4.704399	-1.971109	-1.436597
H	3.553171	-2.867328	-0.428469
H	-3.483574	0.786839	0.357222
C	-4.905533	-1.242324	-0.254799
H	-2.913289	-1.858721	-0.764272
C	-3.151825	-2.054174	1.365092
H	-5.334421	-2.247078	-0.284858
H	-5.422690	-0.674122	0.526581
H	-5.086960	-0.758200	-1.218338
H	-3.501182	-3.088948	1.300161
H	-2.084423	-2.063089	1.601465
H	-3.686780	-1.559966	2.183154
H	5.160138	-1.462498	1.082493
O	5.132724	-1.020214	1.955813
H	5.202804	-1.698687	2.659061
H	4.276694	-0.553079	2.044662

TRANSITION STATE

C	0.560656	1.883886	-0.048586
N	1.450017	0.918102	-0.250356

C	0.862166	-0.262775	-0.457516
C	-1.219377	0.540154	-0.232388
N	-0.742109	1.799893	-0.016959
Cl	1.233058	3.465693	0.215322
N	-0.429322	-0.525724	-0.478744
N	1.693815	-1.358329	-0.682243
H	1.222477	-2.260966	-0.719030
N	-2.536723	0.373684	-0.203315
C	-3.212411	-0.925929	-0.311900
C	3.025088	-1.337874	-0.517251
H	3.461536	-1.314358	0.948257
H	3.493336	-0.363885	-0.621062
C	3.791059	-2.554412	-0.912496
H	3.847635	-2.547891	-2.006650
H	4.803018	-2.517507	-0.511174
H	3.284290	-3.464741	-0.587061
H	-3.094656	1.191210	0.019690
C	-4.669904	-0.680229	-0.672524
H	-2.724441	-1.472974	-1.122863
C	-3.079038	-1.720470	0.984588
H	-5.191386	-1.636463	-0.758903
H	-5.163272	-0.091936	0.108971
H	-4.762641	-0.149248	-1.623590
H	-3.523711	-2.711724	0.857456
H	-2.029362	-1.846114	1.264991
H	-3.601810	-1.208381	1.799048
H	2.767620	-1.386930	1.383132
O	1.407037	-1.436033	2.159375
H	0.922876	-2.255583	1.973368
H	1.671015	-1.498528	3.089698

PRODUCTS

C	1.021059	1.911057	-0.055934
N	1.765225	0.804861	-0.025961
C	1.015697	-0.284795	-0.121386
C	-0.928533	0.817113	-0.204542
N	-0.276995	2.012079	-0.152035
Cl	1.903065	3.399040	0.058157
N	-0.287408	-0.376524	-0.221692
N	1.672857	-1.548759	-0.112249
H	1.016556	-2.367018	-0.161703
N	-2.251712	0.829856	-0.247159
C	-3.097307	-0.371352	-0.181051
C	2.948164	-1.719415	-0.038767
H	-0.403630	0.565352	2.553919
H	3.572585	-0.830221	0.013420
C	3.554839	-3.053401	-0.027476
H	4.253099	-3.111987	-0.870459
H	4.162452	-3.139848	0.880448
H	2.815810	-3.852484	-0.079238
H	-2.701530	1.738855	-0.202333
C	-4.497561	0.011671	-0.634593
H	-2.676222	-1.101247	-0.879022
C	-3.097908	-0.955177	1.229145
H	-5.146365	-0.866555	-0.599225
H	-4.918471	0.775399	0.028643
H	-4.492634	0.397421	-1.657461
H	-3.695504	-1.871248	1.247450
H	-2.084450	-1.199186	1.560973
H	-3.534766	-0.240279	1.934114
H	0.296376	0.806072	2.590472
O	-0.390125	-3.370291	-0.270050
H	-0.493139	-4.016160	0.442291
H	-1.065734	-2.693014	-0.109263