

2,4-二氯苯氧乙酸代谢中的水解反应机理

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Hydrolysis Reaction Mechanism of 2,4-Dichlorophenoxy Acetic Acid Metabolism

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2,4-D:

0 1

C	-0.59742500	1.06507900	-0.13178100
C	-1.91817300	0.77131100	0.21085200
C	-2.38397200	-0.53289000	0.05055000
C	-1.55669000	-1.53968000	-0.44747400
C	-0.23751700	-1.23136900	-0.77705700
C	0.26034500	0.06498200	-0.61814600
H	-2.56983900	1.55200200	0.58416800
H	-1.93657900	-2.54702900	-0.57407700
H	0.43293400	-1.98956200	-1.16472600
O	1.54268100	0.34973400	-1.02923600
C	2.52948900	0.52770900	-0.02194800
H	3.28657800	1.19982500	-0.43726700
H	2.12365100	1.00279200	0.87689100
C	3.25622400	-0.73750800	0.41876100
O	4.07455000	-0.72936900	1.31277500
O	2.93239800	-1.84354900	-0.28209200
H	3.47055000	-2.57016100	0.07792900
Cl	-0.03088900	2.71563600	0.02524600
Cl	-4.04664100	-0.90317800	0.47610500

COM1-1:

0 1

C	0.77324400	0.98879800	-0.26656300
C	2.14707600	0.76800600	-0.37442200
C	2.68772100	-0.39965100	0.16287900
C	1.88275900	-1.34109500	0.80499000
C	0.51100100	-1.10947900	0.89786000
C	-0.05829200	0.04679900	0.35904700
H	2.77978900	1.50133700	-0.85964400
H	2.32047400	-2.23957300	1.22470200
H	-0.14389800	-1.81995100	1.38865800
O	-1.40727300	0.28217100	0.53100500
C	-2.26840400	0.05568300	-0.58744400
H	-3.14888000	0.68420700	-0.42163400
H	-1.79977200	0.36035300	-1.52731900
C	-2.76240600	-1.37461300	-0.75130900
O	-3.36876600	-1.73471000	-1.73639000
O	-2.50183800	-2.17955100	0.29924700
H	-2.89837300	-3.04447300	0.09489700

Cl	0.10049700	2.47622900	-0.90042100
Cl	4.41535900	-0.67756700	0.03242400
O	-3.41636200	1.67101400	2.04920200
H	-2.54128700	1.30846900	1.83769400
H	-3.25989300	2.55427200	2.40386600

TS1-1:

0 1

C	1.01198000	1.14499500	-0.03847100
C	2.22356200	0.50162600	-0.26272800
C	2.36530400	-0.85451700	0.04978900
C	1.29852100	-1.56801100	0.58183100
C	0.07147000	-0.92830700	0.79786200
C	-0.08915600	0.42147400	0.46005300
H	3.05370400	1.06453100	-0.67354800
H	1.40874600	-2.61632400	0.83651400
H	-0.76218600	-1.48310700	1.21672700
O	-1.61065400	0.78670000	-0.49475100
C	-2.18938700	-0.29923400	-1.14517000
H	-2.55546100	-0.00250400	-2.13557500
H	-1.44519400	-1.10082400	-1.30433400
C	-3.35917800	-0.94786700	-0.41717600
O	-4.17180400	-1.67973500	-0.93477200
O	-3.39499700	-0.64670600	0.91421300
H	-4.17107000	-1.10501200	1.28046800
O	-1.00531200	1.30736400	1.56175100
H	-1.77614900	1.22371900	0.82886200
H	-1.18198200	0.72420300	2.31833600
Cl	0.84847200	2.84485700	-0.41088800
Cl	3.90994200	-1.64877700	-0.22999000

INT1-1:

0 1

C	-0.91362000	-0.38597400	0.00001900
C	0.39704600	-0.86124100	-0.00005800
C	1.45522400	0.04713000	-0.00004600
C	1.21782000	1.42033300	0.00002400
C	-0.09800900	1.88329400	0.00007000
C	-1.17767900	0.99319600	0.00008200
H	0.58229600	-1.92870500	-0.00011000
H	2.04537600	2.12051500	0.00002500
H	-0.28941700	2.95373600	0.00008600

Cl	-2.24093600	-1.52248500	0.00001200
Cl	3.10625300	-0.55519200	-0.00012200
O	-2.47682400	1.40324100	0.00008800
H	-2.51873700	2.36861300	0.00063300

COM2-1:

0 1

C	0.02162300	-2.34218000	0.02110000
C	1.12586400	-1.48333500	0.01013200
C	0.89802400	-0.09868500	-0.00864200
C	-0.39475200	0.42324800	-0.01561900
C	-1.47541300	-0.45926300	-0.00428300
C	-1.27910000	-1.83890300	0.01426700
H	0.18184800	-3.41765500	0.03528300
H	-0.54838000	1.49760400	-0.02840200
H	-2.12746200	-2.51375300	0.02295500
Cl	2.27633800	0.98821700	-0.02442700
H	1.01230400	3.47664700	0.04309200
O	0.07613500	3.70777500	-0.02853700
H	-0.04604900	4.50461200	0.50185000
O	2.41377400	-1.93060800	0.01663900
H	2.42623500	-2.89670100	0.02545300
Cl	-3.11135300	0.18393700	-0.01126600

TS2-1:

0 1

C	-0.34660200	1.98905300	-0.16694800
C	0.80854700	1.24321400	0.07870600
C	0.62098000	-0.12603900	0.25027100
C	-0.59195400	-0.78000700	0.22872300
C	-1.72092200	0.01374800	-0.02577500
C	-1.60978200	1.39013700	-0.20632800
H	-0.22984100	3.05451100	-0.33923000
H	-0.67294800	-1.85334100	0.34832200
H	-2.49335600	1.98815900	-0.39432000
Cl	2.38979300	-1.16313000	-0.93524800
O	1.68254900	-0.74876500	1.64477000
H	2.28019700	-1.32891800	1.10412200
H	1.12184200	-1.28862400	2.22761800
Cl	-3.29255300	-0.76414300	-0.10344200
O	2.02893000	1.83050000	0.09501300
H	2.68758200	1.15733400	-0.15893800

INT2-1:

0 1

C	-1.06152100	0.79776800	0.00000200
C	0.31894000	1.00052500	0.00000900
C	1.18431100	-0.09661600	0.00000600
C	0.69440800	-1.39698400	-0.00001900
C	-0.69210000	-1.59154800	-0.00004200
C	-1.57603100	-0.51414800	-0.00001800
H	0.71969000	2.00968100	0.00002800
H	1.37059400	-2.24347300	-0.00002900
H	-1.08905300	-2.60413700	-0.00008000
Cl	2.92142000	0.18764500	0.00002800
O	-2.93630400	-0.65028100	-0.00005900
H	-3.16922300	-1.58771200	0.00027300
O	-1.96430700	1.82190500	0.00001200
H	-1.49929300	2.66869900	0.00007500

COM3-1:

0 1

C	-1.70636400	-1.49131200	-0.00032000
C	-2.08603700	-0.15148900	-0.00001800
C	-1.09486900	0.84407900	0.00073500
C	0.25641800	0.51093300	0.00142800
C	0.60799500	-0.84031800	0.00068500
C	-0.35344800	-1.84672900	-0.00009300
H	-2.47921500	-2.25262400	-0.00105400
H	1.01407400	1.28864700	0.00307800
H	-0.05875000	-2.88967600	-0.00065800
Cl	2.32236100	-1.27840500	0.00044500
O	-3.40963300	0.18094700	-0.00047200
H	-3.48712700	1.14709300	-0.00142500
O	3.13094400	2.13837000	-0.00928900
H	3.94746700	2.64798900	0.05777000
H	3.39305700	1.20630700	-0.00798000
O	-1.56190900	2.13914700	0.00133300
H	-0.82702800	2.76644800	-0.00436800

TS3-1:

0 1

C	-1.00858000	-1.62181700	-0.05555300
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C	-1.88199200	-0.54037300	-0.10564800
C	-1.37604100	0.76138900	0.06084800
C	-0.01832900	0.98293200	0.29342800
C	0.79997500	-0.13271300	0.27786500
C	0.36660900	-1.43723500	0.16303800
H	-1.40300100	-2.62144700	-0.20550200
H	0.38353600	1.97920000	0.43535800
H	1.05201700	-2.27528900	0.14688800
Cl	2.74354500	0.22821000	-1.01490100
O	-3.21558700	-0.75219300	-0.32183900
H	-3.66542900	0.10504600	-0.35933400
O	2.09977100	0.08927800	1.61623900
H	2.14689500	-0.74848600	2.10690400
H	2.85968800	0.13581300	0.96926200
O	-2.31108800	1.76749600	0.00041700
H	-1.88858800	2.63584600	-0.00266300

COM1-2:

0 1

C	-0.11483300	-1.96486900	-0.27826200
C	0.41084700	-0.67045700	-0.30588900
C	-0.46620500	0.41686000	-0.17229700
C	-1.83833300	0.22648900	-0.00373800
C	-2.32806700	-1.07938400	0.02658600
C	-1.48247900	-2.18020900	-0.11351100
H	0.56637200	-2.80043800	-0.40377800
H	-2.50187200	1.07973300	0.09454900
H	-1.88583400	-3.18623400	-0.09722700
Cl	-4.05289800	-1.33846700	0.23523500
O	1.75680000	-0.49358100	-0.53238000
C	2.54273400	-0.29211500	0.63753300
H	2.24172600	0.61679800	1.17284000
H	2.44483200	-1.14029400	1.32857800
C	4.01580600	-0.14953000	0.30774400
O	4.84522500	0.04238400	1.17234900
O	4.30990100	-0.25807300	-0.99878600
H	5.27336000	-0.14778700	-1.07960000
Cl	0.16935200	2.05371700	-0.24067100
H	-2.38483100	3.70254200	-0.03595300
O	-3.19263600	3.22381800	0.19160900
H	-3.92463000	3.75934200	-0.13832500

TS1-2:

0 1

C	0.09573900	-1.46306700	0.33758000
C	-0.27011900	-0.12823600	0.52280300
C	0.73476000	0.82762400	0.35321500
C	2.06274400	0.52072000	0.10432100
C	2.37806000	-0.83166500	-0.07346700
C	1.41206900	-1.82888600	0.03931600
H	-0.67585800	-2.21582200	0.45668600
H	2.80894200	1.29306300	-0.03610600
H	1.68064500	-2.87014900	-0.09154700
Cl	0.03911600	2.58050400	-0.97768000
O	0.54085500	2.10198400	1.63835500
H	0.27219600	2.84104900	1.02926900
H	1.42949600	2.28658200	1.98867400
Cl	4.03874400	-1.26023100	-0.44638700
O	-1.53604500	0.24932100	0.89490500
C	-2.51728000	0.36112000	-0.13466600
H	-3.13495300	1.23256900	0.09946700
H	-2.05681000	0.54379100	-1.11109000
C	-3.46137400	-0.82517100	-0.26392100
O	-4.43495700	-0.79767200	-0.98525600
O	-3.12594700	-1.90039900	0.48279500
H	-3.80611500	-2.57622300	0.31630600

INT1-2:

0 1

C	-0.44872000	1.22443300	-0.13716700
C	-1.76811300	1.00759000	0.26844000
C	-2.35887300	-0.23766500	0.05271400
C	-1.65780200	-1.27534100	-0.55660800
C	-0.33361200	-1.05267200	-0.94132500
C	0.28301300	0.18008200	-0.73441700
H	-2.33570200	1.80815100	0.73387700
H	-2.12993900	-2.23657100	-0.72196100
H	0.24728400	-1.83780100	-1.41193400
O	1.56019200	0.37366300	-1.21770600
C	2.57663100	0.70752700	-0.28356500
H	3.39602900	1.13984600	-0.86630100
H	2.24773300	1.46188700	0.43604200
C	3.16064600	-0.46140700	0.49923100
O	3.94665700	-0.30277300	1.40923200

O	2.75506200	-1.67511600	0.07324400
H	3.20041700	-2.33283000	0.63524000
Cl	-4.02405900	-0.48662700	0.56030600
O	0.17492600	2.43467600	0.01613100
H	-0.43053100	3.07109300	0.41882200

COM2A-2:

0 1

C	-0.72530800	-0.57131400	1.12549700
C	-2.08482500	-0.65696600	0.81490500
C	-2.60029700	0.11080800	-0.22992400
C	-1.78723900	0.96150500	-0.97547600
C	-0.42615800	1.02666200	-0.66838500
C	0.11195900	0.26721100	0.36755700
H	-2.73853100	-1.30500600	1.39116700
H	-2.20314500	1.55516200	-1.78084700
H	0.24022700	1.67125400	-1.23048600
O	1.44784300	0.42760600	0.69693700
C	2.30856100	-0.70215800	0.56051800
H	3.20087200	-0.47495800	1.15126700
H	1.85308700	-1.60655200	0.97096800
C	2.77692700	-1.00310000	-0.85681800
O	3.41158300	-2.00039000	-1.12513300
O	2.45185200	-0.05785000	-1.75914000
H	2.82493700	-0.33766900	-2.61310600
Cl	-4.31436900	-0.00373600	-0.59938200
O	2.90952400	2.93637600	0.83078900
H	2.33887500	2.15054600	0.79275000
H	2.72294900	3.35373800	1.68026600
O	-0.15913100	-1.27282500	2.15571400
H	-0.83007600	-1.80221400	2.60694800

TS2A-2:

0 1

C	1.00397000	1.39345300	-0.21072600
C	2.24544800	0.79123500	-0.37243300
C	2.45816400	-0.52720700	0.06015800
C	1.43773100	-1.25030300	0.65349100
C	0.17263000	-0.65281900	0.81156500
C	-0.04875000	0.64111300	0.35316500
H	3.05619100	1.34986800	-0.83171200
H	1.60213900	-2.26435500	0.99926100

H	-0.63295900	-1.20945300	1.27970500
O	-1.59215700	0.87742500	-0.65480700
C	-2.14337700	-0.29569800	-1.15343000
H	-2.52237000	-0.14438100	-2.17206200
H	-1.37941300	-1.09410500	-1.21181200
C	-3.29236900	-0.87936500	-0.34109200
O	-4.10252900	-1.67464700	-0.76101200
O	-3.31270300	-0.43963600	0.95247700
H	-4.07462600	-0.87027600	1.37718000
O	-1.02248400	1.62202500	1.36650700
H	-1.76249000	1.46556900	0.62626400
H	-1.22902800	1.08314600	2.14762800
Cl	4.05012500	-1.24892000	-0.15477900
O	0.72643400	2.67768800	-0.58245500
H	1.51727400	3.09033000	-0.95308100

COM2B-2:

0 1

C	-0.02079100	-1.79954400	-0.09089800
C	0.55431600	-0.53695500	-0.23100100
C	-0.27718200	0.59943500	-0.24301300
C	-1.65864700	0.45961200	-0.09010600
C	-2.20006700	-0.81682000	0.05137900
C	-1.40230200	-1.95767900	0.04762700
H	0.63599100	-2.66323400	-0.10219200
H	-2.29726700	1.33801900	-0.09530700
H	-1.84183400	-2.94242600	0.15371600
Cl	-3.94935800	-0.98582100	0.23496100
O	1.91248300	-0.45095400	-0.43947200
O	-4.20968600	2.54699100	-0.04050100
H	-4.88146000	3.23760600	0.01252700
H	-4.67752100	1.70608100	0.06155000
C	2.65318000	0.26456800	0.54323200
H	2.35380200	1.31761600	0.58300000
H	2.50470700	-0.17228600	1.53981100
C	4.14002200	0.22904800	0.25553400
O	4.94840500	0.72887900	1.01094000
O	4.47712200	-0.38462800	-0.89255300
H	5.44603200	-0.32992700	-0.96313600
O	0.31283100	1.82271000	-0.41496400
H	-0.36379400	2.51354600	-0.42842600

TS2B-2:

0 1

C	-0.00931400	-0.48342700	1.35119500
C	-0.63688300	0.56149800	0.67816000
C	0.11810200	1.37380500	-0.19273400
C	1.48108200	1.12496400	-0.38607300
C	2.02527500	0.03642600	0.27176600
C	1.35567500	-0.75625600	1.18459500
H	-0.60921800	-1.09966700	2.01147400
H	2.08045100	1.73798800	-1.04932800
H	1.82420500	-1.60354500	1.66955400
Cl	3.33784400	-1.27434500	-1.15844200
O	-1.95975000	0.84604200	0.95416300
O	3.72900400	0.50056100	0.84244200
H	3.80316300	0.22803600	1.77291000
H	4.19363700	-0.16592600	0.26112000
O	-0.52592700	2.40940600	-0.81063300
H	0.07942000	2.87386600	-1.40369600
C	-2.89241500	0.68979900	-0.10557800
H	-3.76755200	1.28940000	0.16380600
H	-2.50811400	1.07402700	-1.05480500
C	-3.38789700	-0.73049700	-0.34626300
O	-2.98455900	-1.62716800	0.57763000
O	-4.10810000	-1.01432200	-1.27961000
H	-3.36642900	-2.48434200	0.32014600

COM1-3:

0 1

C	-0.01864800	-1.88104700	-0.25172200
C	0.52472400	-0.59463500	-0.30349500
C	-0.33681600	0.51000200	-0.21165000
C	-1.71430300	0.34037900	-0.05898100
C	-2.22014600	-0.95771600	-0.00374600
C	-1.39132600	-2.07479300	-0.10253500
H	0.65308600	-2.72830600	-0.34535900
H	-2.37136000	1.20133200	0.00985400
H	-1.80900300	-3.07441900	-0.06713200
Cl	-3.95661600	-1.20006600	0.18573900
O	1.87602500	-0.44595700	-0.51471600
O	-4.34625900	2.28850200	0.22226700
H	-4.81581300	3.02923000	0.62472700
H	-4.90667700	1.51101200	0.34708200

Cl	0.31123300	2.13409900	-0.31106900
C	2.64671300	-0.19697000	0.65643400
H	2.34293800	0.73622700	1.14652800
H	2.53515400	-1.01363900	1.38216000
C	4.12470500	-0.07485700	0.34121000
O	4.94723400	0.11157700	1.21366400
O	4.43030400	-0.18858700	-0.96199600
H	5.39534200	-0.08645000	-1.03407600

TS1-3:

0 1

C	0.02831000	-0.95355800	-1.08607600
C	0.58622600	0.26156300	-0.68225300
C	-0.25349300	1.23715600	-0.11590700
C	-1.61835800	1.00353300	0.06547100
C	-2.09238400	-0.24557200	-0.29785900
C	-1.33433800	-1.22197400	-0.92397600
H	0.68318900	-1.69709300	-1.52565400
H	-2.26452600	1.75559500	0.49785500
H	-1.75131800	-2.18489800	-1.19349900
Cl	-3.42973700	-1.19821900	1.34626200
O	1.91651700	0.51741300	-0.93520800
O	-3.74738500	-0.02707200	-1.05846200
H	-3.76054400	-0.51685400	-1.89890600
H	-4.24147700	-0.54049600	-0.35797400
C	2.81774300	0.42059500	0.15945100
H	3.63801600	1.11638300	-0.04161800
H	2.35307300	0.72123100	1.10442500
C	3.44790800	-0.94988200	0.37706600
O	3.09557700	-1.88250200	-0.53268100
O	4.21861200	-1.16492100	1.28717200
H	3.56866500	-2.69827600	-0.29195200
Cl	0.39554000	2.79762500	0.33875300

INT1-3:

0 1

C	-1.05507900	0.87791900	-0.08097500
C	-2.31518300	0.44343200	0.32300400
C	-2.63531500	-0.91431700	0.23288300
C	-1.69794900	-1.82605800	-0.26279700
C	-0.43716100	-1.37618300	-0.65540300
C	-0.09434000	-0.02598700	-0.56464000

H	-3.05095100	1.14653000	0.69494500
H	-1.94676700	-2.88134100	-0.34283400
H	0.30472400	-2.06472900	-1.04295500
O	1.13190100	0.40134300	-1.03378000
C	2.12352700	0.69975000	-0.06364100
H	2.78735700	1.44795600	-0.50880300
H	1.69660900	1.13677800	0.84490300
C	3.00441700	-0.46863400	0.36296700
O	3.82529900	-0.36770800	1.24962600
O	2.81754700	-1.60139200	-0.34645700
H	3.44965700	-2.25416900	0.00188600
O	-3.88917500	-1.28231300	0.64261700
H	-4.00846200	-2.23474800	0.53305900
Cl	-0.68672000	2.59086800	-0.00144900

COM2-3:

0 1

C	-0.20028300	-2.08477100	-0.20652600
C	0.18177800	-0.74053800	-0.27421700
C	-0.81223900	0.23835200	-0.15248400
C	-2.15042600	-0.10336300	0.04130200
C	-2.50503800	-1.45399700	0.10922900
C	-1.53040100	-2.44973700	-0.01700300
H	0.56862700	-2.84214300	-0.32313800
H	-2.90357200	0.67366900	0.13383800
H	-1.82559700	-3.49228800	0.02823500
O	1.49836700	-0.41447900	-0.52780800
C	2.27603900	-0.13717200	0.62965500
H	1.90434900	0.74600100	1.16375300
H	2.25976400	-0.98504700	1.32885800
C	3.72823300	0.12839700	0.28350300
O	4.53324500	0.46908100	1.12561600
O	4.03854300	-0.06046100	-1.01049300
H	4.98721600	0.13566800	-1.10221300
Cl	-0.37596500	1.94065300	-0.26667400
H	-2.98646500	3.09124900	-0.04890400
O	-3.86572300	2.72636100	0.12309600
H	-4.38955400	3.45119800	0.48571800
O	-3.80030600	-1.85412900	0.29536400
H	-4.38235100	-1.08342000	0.34036300

TS2-3:

0 1			
C	0.17885100	-1.62840200	0.27162600
C	0.01232700	-0.25916300	0.50807900
C	1.13585900	0.53711800	0.30361200
C	2.39253500	0.05376500	-0.02411900
C	2.51111300	-1.32519700	-0.25960900
C	1.40761800	-2.16917700	-0.10591400
H	-0.68755300	-2.26470700	0.41591800
H	3.22255200	0.73056800	-0.19918200
H	1.52330300	-3.23236500	-0.28098100
Cl	0.68309400	2.44785200	-0.94449100
O	1.18876700	1.79976200	1.64446500
H	1.02191000	2.58563700	1.05911300
H	2.10822000	1.82975700	1.95864100
O	-1.16996500	0.27619700	0.96391800
C	-2.14711100	0.61622300	-0.01626500
H	-2.64040000	1.53223800	0.32203700
H	-1.68625400	0.83535800	-0.98472300
C	-3.24505700	-0.41530700	-0.23137300
O	-4.19853400	-0.20114100	-0.94905300
O	-3.07544300	-1.57552700	0.44053600
H	-3.84255000	-2.13391300	0.22436300
O	3.69518900	-1.89188900	-0.64479800
H	4.37126000	-1.21442500	-0.77562000

INT2-3:

0 1			
C	-0.90728100	1.14465200	-0.09007700
C	-2.18841800	0.85910700	0.38301400
C	-2.70387800	-0.43503100	0.26610800
C	-1.93945200	-1.44829900	-0.31756100
C	-0.65106500	-1.15566500	-0.77309400
C	-0.12055500	0.12669800	-0.66271600
H	-2.80266200	1.63549000	0.83083600
H	-2.33793700	-2.45482100	-0.41448500
H	-0.03429200	-1.92370900	-1.22598400
O	1.12032200	0.39853900	-1.21234600
C	2.14805300	0.78896300	-0.31673100
H	2.91147400	1.28887800	-0.92213100
H	1.79719600	1.50622700	0.43062100
C	2.84801100	-0.34521200	0.42125800
O	3.63441300	-0.14641300	1.32369900

O	2.54950300	-1.57823300	-0.03856800
H	3.06652700	-2.20638700	0.49502500
O	-0.36642100	2.40214600	-0.02332400
H	-1.00168400	3.01083400	0.37606800
O	-3.97287800	-0.63948000	0.74561700
H	-4.23063600	-1.56026500	0.60821200

COM3-3:

0 1

C	-1.10600900	0.19074400	1.12951000
C	-2.45162900	-0.11169300	0.91996000
C	-2.94851900	-0.21478700	-0.38299100
C	-2.10339400	-0.02215700	-1.47940000
C	-0.75357700	0.26291600	-1.25988100
C	-0.24457100	0.36526500	0.03094400
H	-3.12788700	-0.25555300	1.75798500
H	-2.48800600	-0.09571900	-2.49309100
H	-0.07416300	0.41272900	-2.09134900
O	1.08056200	0.73995700	0.21534900
C	1.95163600	-0.21019200	0.82139000
H	2.82664200	0.35351600	1.16042500
H	1.49187200	-0.67880300	1.69508300
C	2.46176000	-1.31318800	-0.09587800
O	3.05711700	-2.28139500	0.32684500
O	2.22939800	-1.09659300	-1.40565300
H	2.62362500	-1.84318600	-1.88919900
O	2.44577200	3.12964300	-0.66571000
H	1.89467300	2.36786400	-0.41684700
H	2.10438200	3.87393300	-0.15584300
O	-0.57049200	0.33151700	2.38216900
H	-1.25538300	0.19532700	3.05016400
O	-4.28119800	-0.50561100	-0.51200400
H	-4.51920000	-0.55169900	-1.44721800

TS3-3:

0 1

C	1.48834900	1.11476100	-0.20647600
C	2.64917900	0.36714000	-0.39893900
C	2.71308400	-0.98326900	-0.01611900
C	1.60651700	-1.58994500	0.56151300
C	0.42531200	-0.84841700	0.74986500

C	0.36495700	0.47501800	0.34121900
H	3.51502600	0.84980800	-0.85073900
H	1.65634600	-2.62894900	0.86728500
H	-0.44029900	-1.31786000	1.20604700
O	-1.18874000	0.95201000	-0.63198000
C	-1.88363200	-0.12936700	-1.15095800
H	-2.26063100	0.09299000	-2.15795400
H	-1.22321700	-1.01320500	-1.24753400
C	-3.08145200	-0.60026900	-0.33503000
O	-3.99575400	-1.26686000	-0.76711500
O	-3.02019100	-0.22415500	0.97693000
H	-3.82166100	-0.57688800	1.40048200
O	-0.50185600	1.55838600	1.41947100
H	-1.24733800	1.50348500	0.67459300
H	-0.77326500	1.01047900	2.17327700
O	3.85051800	-1.74155400	-0.19103200
H	4.54338600	-1.21129100	-0.60387300
O	1.37451800	2.43491200	-0.53544400
H	2.20981300	2.75560100	-0.89868000

PRO:

0 1

C	-0.14025300	-1.59530800	0.00003700
C	-1.11811500	-0.60711900	0.00007100
C	-0.72268300	0.74062100	0.00000900
C	0.62321100	1.09365900	-0.00010100
C	1.59682800	0.08813700	-0.00009200
C	1.21812200	-1.25519000	-0.00001800
H	-0.45042500	-2.63504700	0.00010400
H	0.93217900	2.13512900	-0.00023600
H	1.97137700	-2.03877900	0.00002900
O	-2.44425700	-0.95293500	0.00014200
H	-2.97393700	-0.14214800	0.00039200
O	-1.75392500	1.65534100	-0.00002500
H	-1.40994200	2.55740100	0.00082500
O	2.91015200	0.49844000	-0.00008200
H	3.49232900	-0.27213000	-0.00083700