

Electronic Supplementary Information (ESI)

Molecular mechanism of oxidized lignin compound to N-substituted aromatics

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1. The Gibbs free diagram for the hydroxy addition process of **Z-Int7**.

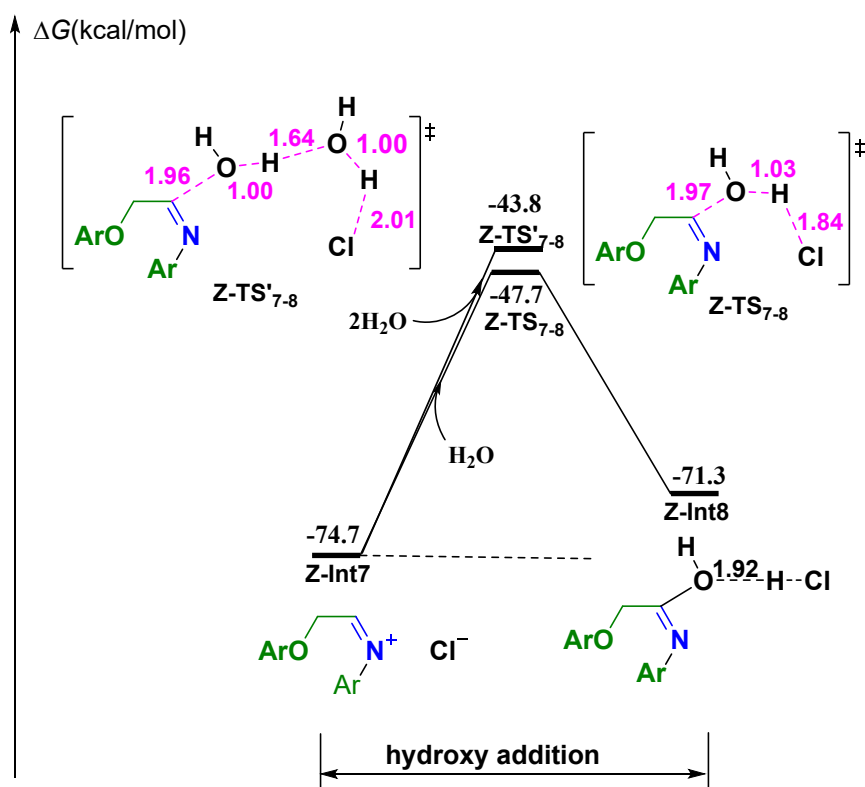


Fig. S1 The Gibbs free diagram for the hydroxy addition process of **Z-Int7**. Bond distance are given

in

angstroms

(Å).

2. The cartesian coordinates of optimized reactants, intermediates, transition states and products.

Lignin

C	1.38099200	-0.94917900	-1.27522400
C	0.43743900	0.06934400	-1.33099600
C	0.61461800	1.22122000	-0.56009900
C	1.75339900	1.34695600	0.24182600
C	2.69593200	0.33675900	0.29245700
C	2.49867400	-0.83432000	-0.45864800
H	1.26359600	-1.85657400	-1.85547400
H	-0.43852600	-0.05383400	-1.95421700
H	1.90609300	2.24646600	0.82651100
C	-0.33929000	2.37007600	-0.56429500
O	-0.06621300	3.42324500	-0.03657500
O	3.41037800	-1.85016900	-0.42674700
C	3.48412600	-2.53668200	0.82378500
H	4.24421000	-3.30624900	0.70375100
H	3.76316500	-1.85480700	1.62910900
H	2.52097700	-3.00372600	1.04904000
O	3.79842100	0.47476200	1.09289800
C	5.01373700	0.66559800	0.37045800
H	4.95421100	1.57702000	-0.23147900
H	5.79990900	0.77202100	1.11576500
H	5.22318900	-0.19124700	-0.27450100
C	-1.68357000	2.26692600	-1.29523500
H	-2.33067800	3.05294000	-0.89621400
O	-2.29757600	1.00030200	-1.25621500
C	-2.54459600	0.45808200	-0.02981300
C	-2.73835000	-0.93827100	-0.01949400
C	-2.60822700	1.17698900	1.15248400
C	-3.01768500	-1.57813800	1.17938900
C	-2.88370400	0.52138600	2.35587200
C	-3.09178200	-0.84453300	2.36720700
H	-3.17203500	-2.64834200	1.20405900
H	-2.92938600	1.09305800	3.27408300
H	-3.30609000	-1.35886700	3.29565400
H	-1.50895400	2.47390500	-2.35421700
O	-2.62039600	-1.55213400	-1.22351800
C	-2.78432400	-2.95397400	-1.25529700
H	-2.64502500	-3.24940300	-2.29289500
H	-2.03759300	-3.45323200	-0.62907800

H	-3.78766500	-3.24331900	-0.92716300
H	-2.44065400	2.24668900	1.15226500

NH₂OH

N	0.67799000	-0.00002300	0.15175800
H	1.04424300	-0.81338500	-0.33597000
H	1.04424500	0.81348000	-0.33573200
O	-0.71397300	0.00002700	-0.13988400
H	-1.12263100	-0.00014700	0.72846900

Int1

C	1.69341500	1.77315300	-0.82547000
C	0.75807700	0.75969700	-1.01655100
C	1.11613500	-0.55654400	-0.74467500
C	2.39612800	-0.84837800	-0.25418800
C	3.30896100	0.16565800	-0.01577100
C	2.95675000	1.49618500	-0.32899500
H	1.45262400	2.80746400	-1.03960100
H	-0.23302400	1.00458700	-1.37055300
H	2.63830700	-1.88106100	-0.04416400
C	0.21025900	-1.71762700	-0.96511800
O	0.65115300	-2.84203800	-1.10336700
O	3.81195900	2.52812200	-0.09084700
C	5.00126600	2.52891600	-0.87766000
H	5.53529100	3.44046000	-0.61665700
H	5.62004000	1.65936500	-0.65469100
H	4.74597900	2.54600800	-1.94160500
O	4.53839600	-0.02124800	0.52527400
C	4.86767500	-1.33242200	0.94882300
H	4.91570800	-2.01943300	0.09874900
H	5.84842700	-1.25800200	1.41293000
H	4.14002100	-1.70425000	1.67643400
C	-1.29374200	-1.53117900	-1.09398700
H	-1.53226500	-1.38018000	-2.15740900
O	-1.73481300	-0.43719100	-0.32850300
C	-3.06340000	-0.16271700	-0.32355800
C	-3.43182000	0.98654600	0.41120000
C	-4.03578400	-0.90914400	-0.96939300
C	-4.76769100	1.34892100	0.48648100
C	-5.38076500	-0.53212900	-0.88842600
C	-5.74337300	0.58653300	-0.16518000
H	-5.06352700	2.22518400	1.04759700
H	-6.13048000	-1.12519200	-1.39672400
H	-6.78237400	0.88369200	-0.09715700

H	-1.74724300	-2.46722500	-0.75766500
O	-2.40669600	1.65541000	0.99253600
C	-2.72257400	2.81622300	1.73114200
H	-1.77591000	3.20143400	2.10336400
H	-3.20004600	3.57055300	1.09742900
H	-3.37838000	2.58168100	2.57580100
H	-3.76185400	-1.78824600	-1.53725800
N	-0.01662200	-2.10748800	1.70926500
H	-0.65772300	-2.36759300	2.45398000
H	0.43666900	-1.24258400	1.99722100
O	0.99620000	-3.09910100	1.71993700
H	0.97943000	-3.43603400	0.81282100

TS'1-2

C	1.80223500	-1.53770900	-0.90775500
C	0.87796100	-0.49593000	-0.87338100
C	1.23623500	0.71005200	-0.27576700
C	2.50929000	0.87116800	0.27279500
C	3.42725500	-0.17219300	0.24109500
C	3.06466800	-1.39328300	-0.35557400
H	1.56038700	-2.48773300	-1.36968000
H	-0.11634000	-0.64117400	-1.28017400
H	2.74426400	1.83639400	0.70192900
C	0.30056400	1.91541200	-0.19831600
O	0.89712800	3.08871400	0.12964500
O	3.95949800	-2.42098500	-0.44952500
C	4.26346300	-3.05402600	0.78875400
H	4.97214200	-3.84848600	0.56138800
H	4.71322000	-2.34866200	1.48949700
H	3.35611100	-3.48544400	1.22345000
O	4.68860500	-0.09861800	0.73771600
C	5.09594200	1.13428200	1.29892600
H	4.48245100	1.39668800	2.16600400
H	6.12849300	0.99427800	1.61090100
H	5.04154800	1.93904500	0.56013900
C	-0.98260800	1.64997100	0.57227600
H	-0.70197400	1.38267400	1.59713900
O	-1.67582400	0.59747400	-0.06078000
C	-2.80417300	0.12681100	0.52398400
C	-3.38450700	-0.99559000	-0.10419200
C	-3.39166200	0.66456900	1.65725800
C	-4.54282800	-1.54789900	0.42045600
C	-4.55949700	0.09920200	2.17897100
C	-5.13036600	-0.99809700	1.56501700

H	-4.99889600	-2.40876500	-0.04933800
H	-5.00832400	0.52884400	3.06560300
H	-6.03414700	-1.44190000	1.96325700
H	-1.58807000	2.56090900	0.59558500
O	-2.72851700	-1.45021800	-1.20288900
C	-3.27679400	-2.57031400	-1.86533000
H	-2.61965200	-2.77412900	-2.70800600
H	-3.30568800	-3.44420300	-1.20683500
H	-4.28523700	-2.35687100	-2.23356500
H	-2.94978100	1.52413100	2.14342400
N	0.01466400	2.32644000	-1.67285500
H	0.07114500	1.61463300	-2.40186400
H	0.84779200	3.07993900	-1.28463600
O	-1.18591200	3.01396400	-1.87107100
H	-1.08298200	3.81352000	-1.33430700

TS₁₋₂

C	-2.24500000	-0.78122100	-1.48063500
C	-0.87676800	-0.53187900	-1.42622100
C	-0.16578800	-0.80444500	-0.25488900
C	-0.83168700	-1.34389100	0.84494900
C	-2.19191100	-1.60387300	0.78788400
C	-2.91213100	-1.30142200	-0.37938200
H	-2.82212200	-0.55219300	-2.36898900
H	-0.39222500	-0.05227100	-2.26917000
H	-0.28411600	-1.54486400	1.75829700
C	1.31896700	-0.55383900	-0.12342900
O	1.85569700	-0.76740200	0.99763700
O	-4.25650600	-1.53479500	-0.46625800
C	-5.05624900	-0.72918600	0.39930700
H	-6.09175000	-0.98277600	0.18004800
H	-4.83131700	-0.93345500	1.44751800
H	-4.88560600	0.33051700	0.18733900
O	-2.82415800	-2.12179900	1.88596600
C	-3.25988700	-3.46965000	1.72171700
H	-2.40298900	-4.12053300	1.52409000
H	-3.72643300	-3.75827900	2.66186500
H	-3.98168600	-3.55182000	0.90555800
C	1.90123100	0.56534800	-1.02618600
H	2.83053900	0.91529900	-0.56896600
O	0.99449000	1.63000100	-1.23908400
C	0.38965700	2.19136800	-0.15010900
C	-0.91346500	2.68097000	-0.36409600
C	0.97367700	2.29111600	1.10118900

C	-1.60550800	3.25883500	0.69230900
C	0.27231800	2.87726700	2.15626000
C	-1.00896100	3.35622900	1.95174200
H	-2.61007200	3.63343700	0.54924500
H	0.73562300	2.94452500	3.13240900
H	-1.56172000	3.80701600	2.76676300
H	2.12921100	0.19211100	-2.02549000
O	-1.40029300	2.53013300	-1.62241300
C	-2.75709400	2.85099900	-1.83138600
H	-2.96667400	2.61621900	-2.87325300
H	-3.40391600	2.25016100	-1.18235700
H	-2.94974500	3.91419500	-1.65644800
H	1.96524800	1.88911800	1.26831200
C	5.02526000	-0.60489100	0.37577500
O	4.58094200	-1.14903800	-0.62249400
C	6.49183600	-0.33534200	0.57228000
H	7.04762500	-0.63672500	-0.31144700
H	6.64287300	0.72514200	0.77749500
H	6.84060100	-0.89011700	1.44499700
O	4.28328100	-0.19608800	1.37580500
H	3.29053800	-0.43039800	1.22063900
N	1.93681200	-2.07414400	-1.10121500
H	1.78246800	-2.82814400	-0.42894200
H	2.94798200	-1.91286800	-1.19172700
O	1.43503000	-2.44078100	-2.34985500
H	0.50113400	-2.18109200	-2.31618900

Z-Int2

C	-1.83512400	0.98521300	-0.50217200
C	-0.70590100	0.18779100	-0.42410300
C	-0.45435000	-0.57755600	0.71515600
C	-1.33405100	-0.49758900	1.78668900
C	-2.46209200	0.31647400	1.72988200
C	-2.73069700	1.05388400	0.57997100
H	-0.03449000	0.17243700	-1.27473400
H	-1.16503600	-1.10520200	2.66877900
C	0.72972700	-1.52659100	0.80712800
O	0.18179300	-2.79048200	1.24563400
O	-3.82107000	1.84257200	0.40380900
C	-4.78800700	1.86199700	1.43435800
H	-5.58469200	2.51546000	1.08606500
H	-5.18946800	0.86009400	1.61473600
H	-4.36972500	2.26139300	2.36358700
C	1.76412600	-1.11791900	1.88981600

H	1.23974500	-0.63928400	2.72240800
O	2.82625000	-0.31000300	1.41446500
C	2.51244300	0.84267700	0.74853700
C	3.09453400	1.00829300	-0.51274000
C	1.69063100	1.83099400	1.27177100
C	2.83673100	2.15327300	-1.24987700
C	1.43224100	2.97848600	0.52766600
C	1.99909300	3.13893400	-0.73169800
H	3.28525800	2.24882800	-2.23184000
H	0.78122100	3.74297900	0.93481200
H	1.79340400	4.02991600	-1.31287700
H	2.25440500	-2.01808200	2.25782000
O	3.89884700	0.01569400	-1.02092900
C	5.21896600	0.04012700	-0.47830900
H	5.76835300	-0.76807000	-0.95962200
H	5.70305300	0.99514000	-0.70141800
H	5.19036100	-0.11909900	0.60278200
H	1.23541300	1.68949000	2.24538800
C	-2.18572000	-2.63492100	-1.28312800
O	-2.36877900	-2.94582900	-0.00081400
C	-3.44988600	-2.18851800	-1.95735800
H	-3.35193600	-2.31010500	-3.03326900
H	-4.31049000	-2.73381500	-1.57315600
H	-3.58359300	-1.12600500	-1.73273100
O	-1.10594100	-2.67980600	-1.82425300
H	0.87865900	-3.44784900	1.11621500
N	1.37094300	-1.62363400	-0.47486400
H	0.71797800	-2.05237000	-1.13278200
H	-1.49403200	-3.06595000	0.42383700
O	2.46189300	-2.52080000	-0.37139000
H	3.21018700	-1.93669100	-0.55863500
H	-3.13887700	0.34347100	2.57298000
O	-2.10688700	1.65049300	-1.66472100
C	-1.92140600	3.06011200	-1.59311100
H	-2.16590200	3.45234000	-2.57889200
H	-2.58467600	3.50247700	-0.84660700
H	-0.87812500	3.28826500	-1.35408600

E-Int2

C	-1.69877600	0.80244400	1.97081500
C	-0.40045200	0.37719600	1.70457900
C	0.15826800	0.60016100	0.45062900
C	-0.58712500	1.26753100	-0.52390600
C	-1.88811700	1.66935700	-0.27076900

C	-2.45511600	1.42557000	0.98817300
H	-2.15141900	0.65068700	2.94433400
H	0.17600600	-0.14130400	2.45914700
H	-0.17666600	1.46646700	-1.50837400
C	1.54668800	0.09748100	0.09062000
O	2.30883200	1.18980600	-0.47362100
O	-3.73565000	1.82687700	1.26247700
C	-4.73038700	1.04554000	0.60437800
H	-5.68935200	1.50368100	0.84137700
H	-4.56989800	1.04159000	-0.47634700
H	-4.70845800	0.01783800	0.98082100
O	-2.61542100	2.27839700	-1.25999900
C	-2.83412300	3.66938900	-1.03726500
H	-1.87865400	4.20280500	-1.01804200
H	-3.43302900	4.02541200	-1.87393100
H	-3.36830300	3.83512000	-0.09885000
C	1.51898300	-0.92786400	-1.05692500
H	1.21222000	-0.39619100	-1.96116600
O	0.70528600	-2.04773400	-0.80198500
C	-0.63446100	-1.91754000	-1.07699300
C	-1.53981900	-2.20517800	-0.04090800
C	-1.10072200	-1.55281500	-2.32828000
C	-2.90520000	-2.07864500	-0.28329300
C	-2.46786200	-1.41255500	-2.56089600
C	-3.36334100	-1.67139300	-1.53646500
H	-3.61799200	-2.28790000	0.50330600
H	-2.82094100	-1.10621500	-3.53719000
H	-4.42894000	-1.56787400	-1.70375300
H	2.53233400	-1.30810300	-1.21585700
O	-0.99429900	-2.57991400	1.13653000
C	-1.87155300	-2.80813400	2.21702400
H	-1.24056700	-3.05583800	3.06794800
H	-2.45797700	-1.91109100	2.44366500
H	-2.54757700	-3.64414000	2.00901000
H	-0.38758400	-1.36573900	-3.12307100
C	5.56500200	0.45001200	-0.20805100
O	4.83134100	0.69589100	-1.28389300
C	7.00096100	0.16288300	-0.53472000
H	7.54360800	-0.07833800	0.37485000
H	7.05466900	-0.66359100	-1.24438400
H	7.43953900	1.03830500	-1.01633900
O	5.11327600	0.45831600	0.91762900
H	3.90401400	0.89953300	-1.00672900
N	2.19647600	-0.49387400	1.23382000

H	3.03340800	-0.99580800	0.94705200
H	2.22491800	1.93704900	0.13132600
O	2.58985400	0.50615100	2.14941200
H	3.47847300	0.77780300	1.86555800

Z-TS₂₋₃

C	1.88521800	-1.00271200	-0.62084500
C	0.75861400	-0.20859800	-0.51437800
C	0.46801300	0.45828100	0.67918300
C	1.31484400	0.30163600	1.77052700
C	2.45111600	-0.49217400	1.67365500
C	2.75232500	-1.14365400	0.47877100
H	0.10990200	-0.12682900	-1.37848700
H	1.11964900	0.84439800	2.68704000
C	-0.77059400	1.27978200	0.79154500
O	0.02765900	2.81394900	1.71407500
O	3.84641800	-1.91462200	0.28002600
C	4.79786300	-1.99118400	1.32421400
H	5.60722300	-2.61159300	0.94655500
H	5.18358000	-0.99878300	1.57493600
H	4.36862800	-2.45563300	2.21730600
C	-1.75208500	0.98973900	1.92081900
H	-1.20680900	0.56190500	2.76405400
O	-2.79986700	0.12726000	1.48836200
C	-2.43047000	-0.99302400	0.78737000
C	-2.90111700	-1.10386800	-0.52323700
C	-1.63071500	-1.99184800	1.32727600
C	-2.56963800	-2.21167800	-1.29069600
C	-1.29352600	-3.09738800	0.55436200
C	-1.76156200	-3.20787900	-0.75158500
H	-2.93908700	-2.26746500	-2.30786800
H	-0.66046000	-3.86998800	0.97358600
H	-1.49912300	-4.06986700	-1.35319100
H	-2.24883000	1.90499300	2.22943700
O	-3.67454200	-0.09474600	-1.05428600
C	-5.04550600	-0.17534900	-0.65212900
H	-5.56235600	0.65005200	-1.13955600
H	-5.47558200	-1.12437800	-0.98207700
H	-5.12753100	-0.08184700	0.43354500
H	-1.26042200	-1.88700100	2.34069300
C	1.72158100	3.06394800	-1.13067000
O	1.82128100	3.22730900	0.12317900
C	2.97791800	3.29315800	-1.94252800
H	2.72281500	3.70081300	-2.91934300

H	3.66907900	3.94392100	-1.41094500
H	3.45513500	2.32153800	-2.09629300
O	0.69179200	2.70309100	-1.74202200
H	-0.60173700	3.53993300	1.63536400
N	-1.25587400	1.72850600	-0.34652700
H	-0.54064600	2.13970300	-1.04346300
H	0.83113900	3.02360300	0.98232300
O	-2.47793700	2.38294000	-0.29679100
H	-3.09596800	1.71028800	-0.63143200
H	3.11197900	-0.57318700	2.52562100
O	2.17467900	-1.59624500	-1.81493500
C	2.02578900	-3.01150400	-1.82554700
H	2.26253200	-3.33620100	-2.83729300
H	2.71098300	-3.48294200	-1.11828800
H	0.99276600	-3.28057800	-1.58402500

E-TS₂₋₃

C	1.89558200	-0.64316700	2.01906400
C	0.54940800	-0.33354400	1.86489300
C	-0.10618000	-0.63997300	0.67497000
C	0.60889300	-1.26152600	-0.35176900
C	1.94784800	-1.57793400	-0.20227600
C	2.60566600	-1.25104400	0.99288000
H	2.42218100	-0.41245400	2.93779000
H	0.02089000	0.17300600	2.65864400
H	0.14970900	-1.49450500	-1.30584300
C	-1.50054000	-0.18374900	0.41579300
O	-2.31251600	-1.79015100	-0.22294600
O	3.92746500	-1.54821000	1.16574900
C	4.80770500	-0.74800700	0.37613000
H	5.80980900	-1.13886600	0.54317200
H	4.54799400	-0.81098400	-0.68297700
H	4.75759900	0.29456900	0.70521900
O	2.61879800	-2.16999800	-1.23670000
C	2.97602200	-3.53032200	-0.98961100
H	2.07598900	-4.13389000	-0.83920400
H	3.50327600	-3.87490200	-1.87730900
H	3.62464800	-3.61019200	-0.11465900
C	-1.73632800	0.65012000	-0.84444900
H	-1.45674500	0.06465000	-1.72065800
O	-1.01167400	1.86322000	-0.77478600
C	0.31073300	1.81271400	-1.13919800
C	1.26497100	2.22051200	-0.19160500
C	0.71027400	1.40464500	-2.40053500

C	2.61493700	2.17743000	-0.53065100
C	2.06334900	1.34683100	-2.72924200
C	3.00890600	1.73016600	-1.79209200
H	3.36649900	2.48801100	0.18289500
H	2.36746800	1.01091100	-3.71221700
H	4.06423200	1.69563900	-2.03572000
H	-2.79226000	0.91019200	-0.91252400
O	0.77987200	2.61705300	1.00778200
C	1.71715800	3.00237400	1.98970600
H	1.13708300	3.26958900	2.87060700
H	2.39529700	2.17668300	2.23220800
H	2.29953000	3.86992200	1.66325900
H	-0.04537100	1.12446700	-3.12595400
C	-5.23135700	-0.35633300	-0.37284700
O	-4.53780600	-1.22025500	-0.99575200
O	-4.80041100	0.40132900	0.52130700
H	-3.33582700	-1.53649900	-0.57194700
N	-2.32805800	0.14821800	1.38985300
H	-3.33765300	0.32178800	1.08934000
H	-1.87056100	-2.37368900	-0.84652600
O	-2.24635200	-0.59771900	2.56369900
H	-2.50122400	0.02142100	3.25633700
C	-6.69107900	-0.26957900	-0.75876000
H	-6.80280000	-0.39109400	-1.83550000
H	-7.21951700	-1.09373700	-0.27361400
H	-7.11866300	0.67259700	-0.42300900

Z-Int3

C	0.13322000	1.32065600	1.72099100
C	0.51899000	0.01295200	1.45071400
C	0.50977400	-0.46413800	0.14117300
C	0.13955700	0.38934000	-0.90111000
C	-0.22977800	1.69640400	-0.63568300
C	-0.25665900	2.16195300	0.68664500
H	0.11286100	1.70636700	2.73399000
H	0.79640200	-0.65485400	2.25759900
H	0.16234000	0.06045400	-1.93363400
C	0.88503300	-1.87228000	-0.14311700
O	2.16174800	-1.11368500	-2.66692800
O	-0.64242300	3.44481300	0.96383300
C	-2.03710700	3.67080900	0.76259000
H	-2.21564000	4.72028900	0.99031500
H	-2.32047700	3.45483700	-0.26985700
H	-2.61913900	3.04088600	1.44350500

O	-0.57471100	2.53200600	-1.66441900
C	0.46281600	3.45356700	-1.99554700
H	1.36139100	2.91147000	-2.30527200
H	0.09148500	4.05573300	-2.82306400
H	0.69282300	4.09650000	-1.14143100
C	0.03703100	-2.69432700	-1.09051100
H	0.00082300	-2.17993400	-2.05429800
O	-1.27046700	-2.91055200	-0.56474500
C	-2.11148500	-1.82661900	-0.58426200
C	-2.47420400	-1.24257200	0.64143000
C	-2.60206900	-1.31469300	-1.77291700
C	-3.29928900	-0.12088300	0.63969000
C	-3.42341400	-0.18855700	-1.77219100
C	-3.76211600	0.40576800	-0.56700200
H	-3.57696900	0.35587000	1.57031600
H	-3.78870500	0.21684100	-2.70723700
H	-4.39581100	1.28479400	-0.55218400
H	0.47467700	-3.67799000	-1.22780600
O	-1.95243100	-1.81806500	1.75075600
C	-2.27662400	-1.23914800	2.99614400
H	-1.77002800	-1.84121100	3.74780400
H	-1.92068200	-0.20456200	3.05424200
H	-3.35617300	-1.26695100	3.17571800
H	-2.31502200	-1.79587200	-2.70145600
C	3.76218200	0.64741900	0.45356200
O	3.43288700	0.49908000	-0.70262200
C	4.34452900	1.92034400	0.99783200
H	3.56560600	2.42814400	1.57170700
H	5.17096700	1.70195200	1.67327800
H	4.66617700	2.55822200	0.17883300
O	3.63036800	-0.28974000	1.38135000
H	2.85438400	-1.49535300	-3.20896200
N	1.92793200	-2.30072300	0.45386900
H	3.10115000	-1.04971000	1.02744000
H	2.62213900	-0.57704800	-2.00185900
O	2.23825100	-3.62383200	0.18012800
H	3.00178500	-3.79999300	0.73582900

E-Int3

C	-1.70885900	0.98669400	1.96310700
C	-0.45863200	0.40831300	1.78412200
C	0.12402700	0.38612900	0.51698500
C	-0.54317900	0.97792700	-0.55662300
C	-1.78302800	1.56948200	-0.37815200

C	-2.38277900	1.55397400	0.88804000
H	-2.18779100	1.00578300	2.93531900
H	0.05995400	-0.04832400	2.61758600
H	-0.11480200	0.99491700	-1.55160400
C	1.39886400	-0.33871900	0.28990200
O	2.41108200	2.52382000	0.01811600
O	-3.61325500	2.11838900	1.08152500
C	-4.67990500	1.37966400	0.48793900
H	-5.58909200	1.94872300	0.67410200
H	-4.52053900	1.26058800	-0.58616900
H	-4.75890700	0.39523100	0.95993900
O	-2.42624400	2.12946100	-1.44961600
C	-2.46508400	3.55469400	-1.41185700
H	-1.44898000	3.95939500	-1.44215900
H	-3.01100600	3.87140100	-2.29896200
H	-2.97805600	3.90605700	-0.51347500
C	1.50894600	-1.29794000	-0.87540600
H	1.32378900	-0.76044800	-1.81243800
O	0.62943000	-2.40658000	-0.75480200
C	-0.69781000	-2.16272800	-1.00671200
C	-1.60454600	-2.26930000	0.06166200
C	-1.14667300	-1.84179800	-2.27582600
C	-2.95519700	-2.02222400	-0.17134600
C	-2.49692500	-1.57960200	-2.50199100
C	-3.39250600	-1.66784900	-1.44821900
H	-3.67101700	-2.09522700	0.63643200
H	-2.83849200	-1.31124600	-3.49338800
H	-4.44545000	-1.47010200	-1.61093900
H	2.51626000	-1.71091200	-0.90008700
O	-1.07129200	-2.59185400	1.26232400
C	-1.94940000	-2.66296700	2.36537000
H	-1.33133900	-2.91251900	3.22525100
H	-2.44373700	-1.70023600	2.53466300
H	-2.70349200	-3.44325800	2.22107200
H	-0.42614100	-1.78626800	-3.08461100
C	5.44244800	0.24417100	-0.34937400
O	4.75732100	1.19610300	-0.67309300
C	6.88546000	0.09761700	-0.74483500
H	7.03087900	-0.85928000	-1.24733400
H	7.17788700	0.91952100	-1.39244800
H	7.50018500	0.09102100	0.15692100
O	5.00912000	-0.76221100	0.37895000
H	3.23939300	2.10295000	-0.27692700
N	2.45234500	-0.24423500	1.00525400

H	4.04654600	-0.62383900	0.64220300
H	2.54179400	3.46849600	-0.08071800
O	2.44322700	0.67916500	2.03765500
H	2.17929700	1.52364500	1.62179700

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C	-2.08147600	-0.16966000	-1.04503000
C	-0.75837200	-0.56317000	-1.06130400
C	-0.24362100	-1.39545600	-0.06075400
C	-1.08965400	-1.82222400	0.95622500
C	-2.43123300	-1.44425200	0.97621400
C	-2.93719000	-0.61350600	-0.01855300
H	-0.11375200	-0.20184700	-1.85453700
H	-0.72193900	-2.47485000	1.73976400
C	1.19159500	-1.76430800	-0.08894000
O	-4.21988400	-0.17997800	-0.08639700
C	-5.11974400	-0.63630500	0.90234400
H	-6.08361700	-0.19563300	0.65777300
H	-5.20333400	-1.72725800	0.88466800
H	-4.81135600	-0.30886100	1.90027100
C	2.02128900	-1.70782200	1.17882400
H	1.37297600	-1.79823300	2.05443000
O	2.75861600	-0.48575700	1.25308800
C	1.97102100	0.63856600	1.12993900
C	1.95541100	1.33816400	-0.08248200
C	1.17671900	1.06020600	2.18932800
C	1.11736400	2.44266700	-0.21530400
C	0.33775700	2.15845600	2.04673300
C	0.30446900	2.84543600	0.83713200
H	1.11220100	2.96135500	-1.16692100
H	-0.28451000	2.47466900	2.87477100
H	-0.34811200	3.70199600	0.71582000
H	2.76673500	-2.50064200	1.18717900
O	2.67475300	0.93934400	-1.16848300
C	4.08711900	0.83677800	-0.98919100
H	4.50550200	0.71511400	-1.98726300
H	4.47570900	1.75758400	-0.54346300
H	4.34233800	-0.02112500	-0.36871500
H	1.21640900	0.50234000	3.11847100
N	1.70055600	-2.01413100	-1.23072300
O	3.06562400	-2.23096200	-1.16254800
H	3.30459700	-2.41718000	-2.07426600
H	-3.07079900	-1.80464100	1.77035800
O	-2.56241300	0.62879300	-2.04363000

C	-2.77149400	1.97914800	-1.64610800
H	-3.11689300	2.51140000	-2.53086300
H	-3.52772700	2.04112700	-0.86004400
H	-1.83164300	2.41575200	-1.29306200

Z-Int4

C	1.20825000	-2.11642400	0.64468000
C	0.14111800	-1.49841800	0.00265900
C	0.37915200	-0.62186400	-1.05403100
C	1.69047300	-0.39837000	-1.47957100
C	2.75566300	-1.01819400	-0.84579900
C	2.51413300	-1.86615000	0.24363200
H	1.04841600	-2.78796000	1.48074200
H	-0.87445300	-1.65253800	0.34735400
H	1.91757200	0.26967300	-2.30249800
C	-0.74975600	0.09045700	-1.70532400
O	3.55671500	-2.45758600	0.90737500
C	4.31052800	-1.54071200	1.69699500
H	5.13902800	-2.10493600	2.12230900
H	4.68788100	-0.71862600	1.08384100
H	3.68636000	-1.14105500	2.50315800
O	4.03398500	-0.76184300	-1.26720000
C	4.66782800	-1.87838200	-1.88871100
H	4.10847000	-2.17993000	-2.77937900
H	5.66301700	-1.54548500	-2.17863100
H	4.74208200	-2.71978700	-1.19604900
C	-0.63316200	1.57968000	-1.96156100
H	0.21999000	1.78571200	-2.61636600
O	-0.50736100	2.30465200	-0.73891400
C	0.72797200	2.28707100	-0.13845100
C	0.85525200	1.65675700	1.11170000
C	1.82536000	2.88707800	-0.73173500
C	2.10361600	1.62330200	1.72782300
C	3.07675400	2.83455200	-0.12118300
C	3.20975900	2.20012500	1.10370200
H	2.22428200	1.14284700	2.68961900
H	3.93392900	3.28913600	-0.60115900
H	4.17638300	2.15296700	1.59105900
H	-1.53893200	1.94791100	-2.43382000
O	-0.27036900	1.10250300	1.61668400
C	-0.15530500	0.37289600	2.82060800
H	-1.13165700	-0.07546200	2.99409100
H	0.58975300	-0.42320200	2.72521800
H	0.10823700	1.03012700	3.65574200

H	1.69319500	3.38331300	-1.68715200
N	-1.78009000	-0.60776900	-1.98203900
O	-2.78958300	0.12521800	-2.58700600
H	-3.51605300	-0.50293100	-2.63393400
S	-3.99201400	-0.58623400	1.23609000
O	-2.87138400	-1.43385800	1.58506100
Cl	-4.86951600	-1.39962800	-0.52228400
Cl	-3.20851200	1.15793700	0.44299500

Z-TS₄₋₅

C	1.69336200	-1.94124800	1.23214000
C	0.49712900	-1.56993800	0.63688400
C	0.50413200	-0.92607400	-0.60297500
C	1.71923800	-0.70335200	-1.25473400
C	2.91488000	-1.08785400	-0.66929100
C	2.90529400	-1.68236600	0.60035800
H	1.71580600	-2.41643700	2.20592700
H	-0.44946600	-1.73159800	1.13903300
H	1.77607100	-0.22265000	-2.22352700
C	-0.77457800	-0.45616600	-1.18002700
O	4.07330400	-2.02663100	1.21810600
C	4.84618700	-0.90483000	1.64674400
H	5.75092600	-1.30998200	2.09606100
H	5.09953100	-0.26034600	0.80198600
H	4.28727600	-0.33236900	2.39363200
O	4.08994700	-0.83789900	-1.32311000
C	4.76450000	-2.01221100	-1.77512600
H	4.13250600	-2.56092200	-2.47949700
H	5.66553600	-1.67154100	-2.28192800
H	5.02965100	-2.65812900	-0.93545100
C	-0.82527100	0.82950000	-1.98962100
H	-0.07606400	0.75258100	-2.78693900
O	-0.61104600	2.00906200	-1.23270600
C	0.60565200	2.14018100	-0.60734800
C	0.69772500	1.79410700	0.75159200
C	1.70666300	2.62424400	-1.28832100
C	1.92529800	1.91844400	1.39683900
C	2.93653100	2.74161600	-0.64176600
C	3.03754500	2.38498100	0.69386800
H	2.02529200	1.64963400	2.44006500
H	3.80139100	3.10694600	-1.18034100
H	3.98735200	2.47304900	1.20833300
H	-1.80874000	0.94530500	-2.43635300
O	-0.43737800	1.32451700	1.31626200

C	-0.39424600	1.00082400	2.69210700
H	-1.39159500	0.65167300	2.94631700
H	0.33272300	0.20498800	2.88517700
H	-0.14234400	1.88179100	3.29070000
H	1.58968200	2.89713500	-2.33145000
N	-1.76339500	-1.25073800	-0.97879600
O	-2.97993100	-0.74363300	-1.44225300
H	-3.53078600	-1.54774100	-1.53370000
S	-4.04564500	-0.12033300	0.51546000
O	-2.98392300	-0.49430000	1.40410300
Cl	-4.92260800	-2.32863100	-0.00605400
Cl	-3.45908000	1.86280900	-0.11071000

Z-Int5

C	1.87608400	-0.10413900	-2.25830900
C	0.67869400	-0.63532700	-1.79925100
C	0.03626400	-0.03052600	-0.72605500
C	0.57249700	1.11413300	-0.12853800
C	1.77526300	1.63785800	-0.58143800
C	2.45109000	0.99806600	-1.64185900
H	2.41263000	-0.55832900	-3.08255700
H	0.27844000	-1.53595200	-2.24745200
H	0.05261600	1.56213100	0.70774200
C	-1.16762800	-0.65664700	-0.14170300
O	3.64192200	1.43796600	-2.12487900
C	4.66947500	1.75334300	-1.18624300
H	5.61097000	1.49456800	-1.67028700
H	4.65444100	2.81269900	-0.93500100
H	4.54846400	1.16620900	-0.27124200
O	2.36282700	2.74600100	-0.07001800
C	1.72223800	3.37063500	1.03084900
H	1.66009800	2.68386800	1.88126800
H	2.34297000	4.22448100	1.29224500
H	0.71991500	3.71145400	0.75898200
C	-1.17346700	-2.16114900	0.10460600
H	-1.79369400	-2.39236400	0.97099800
O	0.12981700	-2.68048000	0.23829000
C	0.94790200	-2.02951600	1.12385100
C	2.31099900	-1.95979000	0.77190900
C	0.49172400	-1.40618100	2.27289500
C	3.17669900	-1.22100700	1.56989400
C	1.37064900	-0.67118300	3.07137200
C	2.70298500	-0.57199300	2.71279600
H	4.22280400	-1.14017500	1.30631500

H	1.00042600	-0.17987600	3.96238700
H	3.39157500	0.00261100	3.32029800
H	-1.61728000	-2.65527500	-0.76380500
O	2.66312100	-2.61018600	-0.35892800
C	3.97850500	-2.41768000	-0.83642000
H	4.04150700	-2.97050300	-1.77126400
H	4.17377500	-1.35612700	-1.02645500
H	4.71832700	-2.81101800	-0.13231000
H	-0.55731500	-1.46139300	2.53941400
N	-2.13518100	0.12358400	0.15051900
O	-3.18275600	-0.59914600	0.80086700
H	-2.42976700	2.17331300	0.25587600
S	-4.66944300	-0.27741800	0.19875400
O	-4.75958300	1.12753600	-0.12014300
Cl	-2.27968400	3.38361900	0.70018800
Cl	-4.37538500	-1.30265700	-1.66492200

Z-TS_{5,6}

C	1.57214700	-2.04501300	-1.44138000
C	0.30109300	-1.78083900	-0.97014200
C	-0.04668900	-0.44777600	-0.75247200
C	0.79761400	0.61474500	-1.11073000
C	2.05792700	0.34368900	-1.60412300
C	2.46949200	-1.01122000	-1.72149000
H	1.92090800	-3.05957500	-1.58778100
H	-0.39436800	-2.57467000	-0.72689300
H	0.44149800	1.62757000	-0.97424900
C	-1.28261300	-0.14456100	0.07216600
O	3.68348800	-1.38763800	-2.15064400
C	4.84654600	-0.61694900	-1.82672700
H	5.66948200	-1.32929400	-1.82915500
H	5.01461200	0.16023800	-2.56878800
H	4.74237100	-0.16501800	-0.83832800
O	2.93555000	1.28737900	-2.01112800
C	2.53257500	2.64453300	-1.89589100
H	2.32689500	2.89679100	-0.85148400
H	3.36911300	3.23478900	-2.26163600
H	1.64883700	2.84020800	-2.50966100
C	-1.48885400	-0.20949000	1.56549700
H	-1.84073100	0.77142000	1.89535100
O	-0.33332100	-0.65994700	2.21245800
C	0.78863700	0.12115400	2.09540200
C	2.00475900	-0.56927600	1.92426400
C	0.76631400	1.50452900	2.11955900

C	3.18034900	0.15942800	1.77475500
C	1.95008400	2.22736800	1.95592600
C	3.14873400	1.55594700	1.78369100
H	4.12563100	-0.35230600	1.65220000
H	1.92134700	3.30988600	1.97774800
H	4.07378600	2.10751200	1.66467000
H	-2.27928200	-0.94350000	1.73486200
O	1.91886400	-1.91634400	1.88984800
C	3.10484300	-2.64087700	1.63522200
H	2.81551900	-3.68914900	1.61222400
H	3.53733900	-2.35995700	0.66751500
H	3.84308500	-2.48482700	2.42768900
H	-0.17047000	2.03229600	2.24852700
N	-1.91534100	0.07334100	-0.94822900
O	-3.66383200	0.66457100	-0.02452600
H	-2.90781300	2.31784400	-0.02399600
S	-4.87545500	-0.15576300	-0.44951100
O	-4.97596000	-0.24378200	-1.89269300
Cl	-2.00829300	3.24635800	0.17474700
Cl	-4.06106900	-2.21975200	0.19662200

Z-Int6

C	2.00576400	-0.81597500	-2.06702800
C	0.67545100	-1.08516200	-1.91567100
C	-0.14478900	-0.10075600	-1.31716300
C	0.38009500	1.16405300	-0.95174600
C	1.72679700	1.41305800	-1.05710200
C	2.56551800	0.39919600	-1.61378400
H	2.68730300	-1.53684500	-2.49991500
H	0.24669000	-2.03328900	-2.21641000
H	-0.30769100	1.88096600	-0.51468200
C	-1.30491500	-0.63235500	-0.40889000
O	3.87357800	0.48122500	-1.78634000
C	4.70470300	1.50884600	-1.22229300
H	5.71853100	1.16877400	-1.41893000
H	4.51987300	2.46290900	-1.71009400
H	4.52585400	1.59156900	-0.15241000
O	2.30459400	2.56843500	-0.67212400
C	1.45917500	3.52364400	-0.02880300
H	0.96108500	3.08012600	0.83716400
H	2.11457900	4.33382700	0.27983400
H	0.70502600	3.90047500	-0.72486600
C	-1.35101300	-1.28005900	0.94193600
H	-1.61124900	-0.51280500	1.67308700

O	-0.13472100	-1.93170700	1.18629300
C	0.96259600	-1.15364000	1.47732900
C	2.20340800	-1.69254000	1.08495100
C	0.90611100	0.07116200	2.12196200
C	3.37003300	-0.98530300	1.36046000
C	2.08207000	0.77631200	2.38520500
C	3.30574300	0.24794600	2.01330900
H	4.33257200	-1.38709400	1.07309700
H	2.02135000	1.73037200	2.89440200
H	4.22318600	0.77996200	2.23641500
H	-2.14414300	-2.02831800	0.91049600
O	2.15547600	-2.87892300	0.43438600
C	3.38456000	-3.45282600	0.03985700
H	3.13334500	-4.38340800	-0.46406200
H	3.92566300	-2.79519700	-0.65010300
H	4.01672000	-3.66741200	0.90687300
H	-0.04171400	0.51710300	2.39782700
N	-1.71754600	-0.24224800	-1.48062200
O	-3.83702700	0.32936000	1.06674100
H	-3.11682600	1.13115500	1.08451100
S	-4.90830900	0.28373400	-0.07506300
O	-4.52684300	1.18006100	-1.14524100
Cl	-1.80620500	2.23731100	1.36209500
Cl	-4.40689500	-1.79602200	-0.77984500

Z-TS₆₋₇

C	0.25106300	1.11599400	-1.64030600
C	0.18421500	-0.25106100	-1.80325300
C	-0.94143300	-0.93334200	-1.32555800
C	-2.01670600	-0.23492300	-0.75025600
C	-1.93984100	1.13307300	-0.57736600
C	-0.76902900	1.81640200	-0.99075900
H	1.11391900	1.68310300	-1.96614600
H	0.99399400	-0.80630200	-2.25996600
H	-2.87408800	-0.80592200	-0.42419000
C	-0.71806000	-2.46936200	-0.53742200
O	-0.58509800	3.13772600	-0.84931100
C	-1.03760300	3.80568200	0.33280100
H	-0.37226100	4.65925500	0.45068300
H	-2.06753100	4.13791900	0.22096800
H	-0.95009900	3.14621800	1.19754300
O	-2.93303800	1.88209700	-0.03948600
C	-4.07185800	1.18710700	0.44790400
H	-3.78551900	0.45128700	1.20540100

H	-4.71715100	1.94362200	0.88751000
H	-4.59922100	0.68505400	-0.36794400
C	0.50066400	-2.84645300	0.30288400
H	0.23202600	-2.87919900	1.35342400
O	1.59754100	-2.02226800	0.04418600
C	1.63605300	-0.81603400	0.69703700
C	2.74586300	-0.00916700	0.37535400
C	0.65970000	-0.34830400	1.56054400
C	2.85879600	1.25180600	0.94445500
C	0.78668600	0.92337100	2.12873400
C	1.87561700	1.71763600	1.82172700
H	3.70300700	1.88443000	0.70575900
H	0.02164900	1.27363800	2.81122400
H	1.97798100	2.70410000	2.25774500
H	0.76214900	-3.85037100	-0.04106200
O	3.61470300	-0.54035600	-0.51746600
C	4.74400000	0.23359400	-0.86603000
H	5.31521800	-0.36897500	-1.56830200
H	4.44714000	1.17199800	-1.34610600
H	5.35929300	0.45259600	0.01209200
H	-0.22209400	-0.93948500	1.78234200
N	-1.09397100	-2.41571700	-1.70799400
Cl	-2.27777900	-2.87921500	1.01286200

Z-Int7

C	-2.43657000	-2.13390800	-0.04962200
C	-1.21160400	-1.47387500	-0.05842700
C	-1.17530600	-0.11307000	0.21366800
C	-2.34340400	0.57931100	0.54913900
C	-3.55838700	-0.09372300	0.58555800
C	-3.60632900	-1.46440300	0.26710900
H	-2.50307700	-3.19337300	-0.26586500
H	-0.28804300	-1.99511700	-0.27631200
H	-2.28095400	1.62969400	0.79461400
C	0.38863100	1.56959700	-0.37660800
O	-4.78287800	-2.15404100	0.33461800
C	-5.70544500	-1.84679500	-0.70496600
H	-6.58631400	-2.46051400	-0.52457000
H	-5.98196800	-0.79104600	-0.68305600
H	-5.27455900	-2.09999500	-1.67899300
O	-4.73987300	0.48266700	0.91955000
C	-4.72512900	1.85325100	1.26485800
H	-4.37141200	2.46655100	0.42977800
H	-5.75465400	2.11454400	1.49875000

H	-4.09583600	2.03135700	2.14217700
C	1.76733100	2.19271300	-0.34658100
H	2.08318100	2.40228400	-1.37532600
O	2.69973200	1.41889100	0.34253900
C	3.16259100	0.28513500	-0.25791000
C	4.15272000	-0.41084200	0.46628300
C	2.74372300	-0.19445900	-1.48813700
C	4.69661100	-1.57157100	-0.06619900
C	3.30013000	-1.36266500	-2.01656300
C	4.26961600	-2.04691100	-1.30916900
H	5.45755800	-2.11437900	0.47803800
H	2.95932600	-1.72557900	-2.97804200
H	4.70387500	-2.95454200	-1.70944300
H	1.69934200	3.14591200	0.18204300
O	4.50032300	0.13445300	1.65533400
C	5.47234900	-0.54225300	2.42237200
H	5.59546200	0.04122200	3.33198600
H	5.13977700	-1.55279200	2.68029400
H	6.42841400	-0.59680300	1.89172500
H	1.96928500	0.31745200	-2.04499400
N	0.08182600	0.52200000	0.21030600
Cl	-0.70822300	2.54542200	-1.40883000

Z-TS₇₋₈

C	2.98164300	-2.29922300	-1.13791600
C	1.70245200	-1.86058400	-1.45996100
C	1.31229800	-0.61717400	-0.99206700
C	2.14401900	0.18820700	-0.21240800
C	3.41736600	-0.26519200	0.10406700
C	3.83962300	-1.53146100	-0.35983700
H	3.34353800	-3.26053200	-1.47994900
H	1.02850900	-2.46494000	-2.05214400
H	1.76714600	1.14048800	0.14875700
C	-0.64563200	0.80504400	-1.51833200
O	5.07982100	-2.02263800	-0.12762900
C	5.59119800	-1.97700100	1.20628100
H	6.29241000	-2.80636100	1.28229200
H	6.09852000	-1.03309600	1.39608300
H	4.78447900	-2.11080800	1.93106300
O	4.30056800	0.45380200	0.82522600
C	3.87351100	1.73013700	1.29555200
H	2.99398100	1.64242900	1.93816200
H	4.71214300	2.13158000	1.85853700
H	3.63162700	2.39381900	0.46147100

C	-1.99912800	1.42513400	-1.57083700
H	-1.96597100	2.30144300	-0.91096600
O	-2.97871300	0.49660100	-1.24365700
C	-3.11141900	0.13023300	0.07782400
C	-4.14378200	-0.79508000	0.32610500
C	-2.32506300	0.60741700	1.11112600
C	-4.36463200	-1.22430300	1.62738300
C	-2.56157100	0.16679500	2.41679300
C	-3.57120000	-0.74124800	2.67140500
H	-5.15297000	-1.93344100	1.84022000
H	-1.94356100	0.55049300	3.21829200
H	-3.75749400	-1.08570700	3.68110400
H	-2.17411500	1.75807500	-2.59336000
O	-4.85399500	-1.19229300	-0.75677000
C	-5.92159300	-2.09046800	-0.53940200
H	-6.37247300	-2.26093900	-1.51436400
H	-5.56218800	-3.04092000	-0.13218100
H	-6.66693300	-1.66174100	0.13781200
H	-1.52903900	1.32648000	0.94367100
N	0.03715400	-0.11264100	-1.27806100
Cl	0.39604000	3.10113800	0.66398000
O	0.27839800	2.44879400	-2.09605300
H	1.16157000	2.23508500	-2.41830300
H	0.40089000	2.86621800	-1.16102400

Z-TS'₇₋₈

C	-2.30638700	-2.59016200	-0.62234700
C	-1.07313800	-2.01002600	-0.90654000
C	-0.93069500	-0.65129900	-0.67962200
C	-1.97492500	0.14461800	-0.21112600
C	-3.20356700	-0.44234200	0.05275400
C	-3.36663500	-1.82967900	-0.15155100
H	-2.47362600	-3.65023900	-0.76804200
H	-0.24681400	-2.59159400	-1.29444900
H	-1.80733700	1.20853700	-0.10709500
C	0.94202300	0.89178800	-0.55909200
O	-4.54245200	-2.44885700	0.14484400
C	-5.63485800	-2.10559300	-0.70662000
H	-6.47829700	-2.70757000	-0.37446100
H	-5.87868600	-1.04611100	-0.62233400
H	-5.39265200	-2.35378600	-1.74447500
O	-4.27002100	0.24204100	0.51252400
C	-4.10041900	1.64374700	0.70751900
H	-3.83098200	2.13861200	-0.23026500

H	-5.06169500	2.00925000	1.05989900
H	-3.32747800	1.84578600	1.45400900
C	2.14817300	1.74525600	-0.73643900
H	2.48382400	1.59057300	-1.76748500
O	3.15178100	1.43082900	0.20436100
C	3.76063100	0.20480600	0.00772000
C	3.28294500	-0.90116700	0.72306000
C	4.83078100	0.07757300	-0.85928100
C	3.88266300	-2.14271900	0.53719800
C	5.43498800	-1.16491700	-1.03871900
C	4.95496600	-2.26653100	-0.34444500
H	3.52325000	-3.00737900	1.07995400
H	6.27198900	-1.26598400	-1.71744300
H	5.41710400	-3.23682500	-0.48023600
H	1.84357700	2.77948900	-0.59794200
O	2.24734000	-0.65745500	1.56406200
C	1.43607700	-1.75470100	1.95962700
H	0.54031100	-1.31964600	2.39901700
H	1.15628200	-2.35525700	1.08964600
H	1.95055800	-2.37709100	2.69663000
H	5.18145200	0.95897500	-1.38428400
N	0.29321400	-0.01591400	-0.93221400
Cl	-0.65512100	3.18703300	-1.35531900
O	0.45824500	1.35390700	1.28080000
H	-0.02180100	2.20378400	1.47902800
H	1.28079000	1.28308600	1.78193800
O	-1.10595000	3.43751700	1.55183800
H	-1.09439700	3.56990300	0.56699500
H	-0.95809600	4.29955600	1.94732500

Z-Int8

C	3.21217900	-2.18173400	-0.95069800
C	1.87195700	-1.99067300	-1.28226400
C	1.20150200	-0.88405500	-0.77894600
C	1.86503400	0.02465900	0.05926800
C	3.20200300	-0.17671900	0.39050000
C	3.88263600	-1.29633300	-0.12523800
H	3.76618300	-3.02990100	-1.33551000
H	1.34418700	-2.69168000	-1.91588100
H	1.30724700	0.86254700	0.46066300
C	-0.48999700	0.30878100	-1.78237800
O	5.20741400	-1.48913200	0.14651800
C	5.47195900	-1.92847400	1.47484300
H	6.55262600	-2.03118800	1.55600400

H	5.11574300	-1.19909900	2.20492100
H	4.99631600	-2.89809900	1.65327200
O	3.92055000	0.64596400	1.18819900
C	3.28329300	1.81697300	1.66634800
H	2.42698500	1.56919800	2.30105100
H	4.03124400	2.34551200	2.25249700
H	2.95040800	2.44917500	0.83807900
C	-1.91889800	0.67082000	-2.10800400
H	-2.06859200	1.74192800	-1.91898500
O	-2.84993500	-0.12014200	-1.43672100
C	-3.02724200	0.08513000	-0.09983500
C	-3.95978800	-0.77371200	0.51759000
C	-2.38342800	1.05463800	0.65024500
C	-4.22090400	-0.63369100	1.87367500
C	-2.65649500	1.19009100	2.01401300
C	-3.56856800	0.35003300	2.62239400
H	-4.93330900	-1.28666300	2.35926200
H	-2.14353900	1.95561400	2.58291100
H	-3.78466200	0.44487900	3.67919800
H	-2.07860900	0.50054800	-3.17474600
O	-4.53960800	-1.69018500	-0.29328800
C	-5.43141400	-2.60923600	0.29818000
H	-5.75580300	-3.26979000	-0.50269600
H	-4.93377400	-3.19593600	1.07708900
H	-6.30205700	-2.10073100	0.72528100
H	-1.65569700	1.71453500	0.19722900
N	-0.16769800	-0.67955600	-1.07595100
Cl	0.34442100	3.68274600	-0.37290800
O	0.36605700	1.19678400	-2.37496000
H	1.27557500	0.88144700	-2.25409300
H	0.36945700	2.88261000	-1.39059400

Z-TS₈₋₉

C	-1.38801000	-2.62810700	-0.75215300
C	-0.00300900	-2.52092700	-0.66183300
C	0.55087800	-1.58780600	0.20178900
C	-0.26819000	-0.77110200	0.98412800
C	-1.65068600	-0.87185400	0.87970000
C	-2.21584000	-1.82241100	0.00927600
H	-1.85248500	-3.36024600	-1.40179800
H	0.64258700	-3.16663000	-1.24507600
H	0.19875100	-0.05177900	1.64497700
C	2.76565900	-0.99152000	-0.54017100
O	-3.56850300	-2.02286900	-0.03611200

C	-4.31097700	-0.98710300	-0.66224800
H	-5.34355100	-1.33050800	-0.70322100
H	-4.25370700	-0.06166500	-0.08567500
H	-3.94037300	-0.81840300	-1.67901100
O	-2.52394400	-0.10500800	1.58408200
C	-1.99217500	0.69849500	2.62316600
H	-1.32099500	1.46735000	2.22811200
H	-2.84702200	1.16959900	3.10390600
H	-1.45526100	0.08307600	3.35124100
C	2.31624700	-0.30808800	-1.82504600
H	3.13894800	0.33552900	-2.14932200
O	1.10882500	0.39866800	-1.71735800
C	1.06296200	1.44103500	-0.84397300
C	-0.20741800	2.03912000	-0.69154600
C	2.13968200	1.90912200	-0.10771100
C	-0.36105500	3.09014000	0.20205700
C	1.97063800	2.96567700	0.79350500
C	0.72898100	3.55017600	0.94869200
H	-1.32832700	3.55722400	0.33145400
H	2.82076800	3.31435100	1.36600200
H	0.58966000	4.36801300	1.64481100
H	2.14944000	-1.06954200	-2.58884100
O	-1.19695500	1.51523000	-1.44911600
C	-2.49588100	2.03445000	-1.25816000
H	-3.13999600	1.48885900	-1.94378800
H	-2.83361400	1.86768200	-0.22901800
H	-2.53597000	3.10237300	-1.49588500
H	3.11931500	1.45881900	-0.21132000
N	1.96083200	-1.49352200	0.35421200
O	4.03907500	-1.04111600	-0.37393500
H	2.73200800	-1.94998600	1.28902300
O	3.83994200	-2.09244800	1.73678900
H	4.10400000	-3.00724000	1.86004500
H	4.19165500	-1.59765300	0.68227000

Z-Int9

C	-1.38767700	-2.61873400	-0.80460400
C	-0.00309300	-2.49236300	-0.73562200
C	0.54724400	-1.57561100	0.14400300
C	-0.26590800	-0.79072600	0.96242100
C	-1.64819100	-0.91784700	0.88930500
C	-2.21240200	-1.85235800	0.00026600
H	-1.85357500	-3.33813600	-1.46706600
H	0.64363000	-3.11113000	-1.34595700

H	0.20238400	-0.07320600	1.62427700
C	2.80832200	-0.94450600	-0.67743000
O	-3.56057900	-2.07402100	-0.02620300
C	-4.33340100	-1.03008200	-0.60189700
H	-5.36169200	-1.38714300	-0.62519700
H	-4.27251200	-0.12137900	-0.00000100
H	-3.99256100	-0.82755700	-1.62277100
O	-2.52001400	-0.19008400	1.63360000
C	-1.97850100	0.61458100	2.66716400
H	-1.33995500	1.40560500	2.26147700
H	-2.83062100	1.05700900	3.17878200
H	-1.40385600	0.00492200	3.37077800
C	2.22801200	-0.26697600	-1.92223600
H	3.01532100	0.38914800	-2.30343800
O	1.01787100	0.42313000	-1.73661000
C	1.00500300	1.46178500	-0.85992100
C	-0.26188000	2.05039500	-0.64951300
C	2.10975800	1.93594800	-0.16999400
C	-0.38531200	3.09501600	0.25610700
C	1.97128400	2.98706200	0.74271400
C	0.73294800	3.56011700	0.95651600
H	-1.34928400	3.55511600	0.42828700
H	2.84302900	3.34103300	1.27826500
H	0.61806300	4.37382000	1.66186500
H	2.01959600	-1.03144900	-2.67291400
O	-1.27958500	1.52344600	-1.36835300
C	-2.57075300	2.04077000	-1.12844200
H	-3.23850000	1.50113300	-1.79601800
H	-2.87355100	1.86526000	-0.08976400
H	-2.61947400	3.11060200	-1.35538300
H	3.08705100	1.49363200	-0.31953500
N	1.96612900	-1.44182500	0.25298800
O	4.02786000	-1.00411100	-0.56667000
H	2.42551900	-1.81514000	1.08421500
O	4.19812300	-2.08960500	1.96173900
H	4.79158700	-2.78947300	2.23784900
H	4.52437100	-1.75876500	1.10826300

Z-Int10

C	2.06166500	-2.00697500	0.86718100
C	0.80211800	-2.59472300	0.80882900
C	-0.13981100	-2.10762000	-0.08623800
C	0.17710200	-1.04075400	-0.92939300
C	1.41309200	-0.41243000	-0.82044500

C	2.37406600	-0.91813600	0.07463800
H	2.81412500	-2.36558000	1.55989100
H	0.54565600	-3.41618800	1.46656100
H	-0.55375200	-0.68779800	-1.64403700
C	-2.67556400	-2.27902300	-0.23731900
O	3.58223500	-0.29222000	0.22743400
C	4.47440500	-0.45625800	-0.87056300
H	5.38452800	0.08170000	-0.61097100
H	4.70313200	-1.51671600	-1.01485800
H	4.04786300	-0.03926500	-1.78462000
O	1.77804100	0.68893900	-1.52021800
C	0.81246800	1.28622700	-2.36886400
H	1.28879400	2.17168200	-2.78378600
H	0.53438500	0.60793400	-3.18193100
H	-0.07669500	1.58350700	-1.80534500
C	-2.91061000	-0.77555800	-0.21956500
H	-2.75440300	-0.39542900	-1.23689100
O	-2.05094700	-0.14094300	0.69628400
C	-1.71091700	1.15146500	0.44160200
C	-0.51122700	1.60317500	1.03518500
C	-2.45713900	2.00794400	-0.35341800
C	-0.07790100	2.89830000	0.77707300
C	-2.01508400	3.31154300	-0.59853300
C	-0.82763400	3.74837400	-0.04140700
H	0.85041500	3.25300100	1.20331600
H	-2.60916100	3.96897000	-1.22083300
H	-0.47062900	4.75353900	-0.22875800
H	-3.96073100	-0.63035000	0.04479900
O	0.13359100	0.71034000	1.81280900
C	1.39379400	1.09294400	2.33461700
H	1.77129000	0.22099900	2.86434000
H	2.09066600	1.35168100	1.53122300
H	1.28972500	1.93216400	3.03001500
H	-3.39391600	1.66961000	-0.77831600
N	-1.39802400	-2.76068900	-0.15741900
O	-3.62179100	-3.02856600	-0.35406100
H	-1.38109200	-3.77000600	-0.08613600

Z-Int11

C	-0.48626100	-2.79862900	-0.20175600
C	0.68973400	-2.12742200	0.12451300
C	0.59014700	-0.96828100	0.87379200
C	-0.63790900	-0.46327600	1.29926300
C	-1.80406000	-1.14100700	0.96440700
C	-1.72081800	-2.32881900	0.21467500

H	-0.46484400	-3.71717200	-0.77615600
H	1.67581000	-2.46329000	-0.19723200
H	-0.65797100	0.46573900	1.85484800
C	2.70941000	0.21466400	0.39145000
O	-2.84211000	-3.06540800	-0.05372700
C	-3.71653100	-2.49513700	-1.01660600
H	-4.51629600	-3.21779100	-1.17113000
H	-4.13547600	-1.55355700	-0.65469800
H	-3.18468700	-2.33113000	-1.96001300
O	-3.05411400	-0.73346700	1.31579300
C	-3.15326400	0.39152500	2.16759100
H	-2.73372900	1.28685700	1.69617700
H	-4.21602400	0.53704000	2.35067600
H	-2.64154400	0.20791900	3.11753200
C	2.33963600	0.43302700	-1.06865900
H	2.98039400	1.24168100	-1.43440000
O	0.98042200	0.69644900	-1.32021700
C	0.41666200	1.78704800	-0.74623300
C	-0.98167600	1.89917700	-0.91999200
C	1.09581900	2.74386500	-0.00765300
C	-1.65819400	2.96406200	-0.34120000
C	0.40295600	3.81206500	0.57193600
C	-0.96446000	3.91977900	0.40937000
H	-2.72854200	3.06112400	-0.46577900
H	0.94863600	4.54906600	1.14765400
H	-1.50787100	4.74379000	0.85521800
H	2.60053300	-0.50284400	-1.57352800
O	-1.55903800	0.91949000	-1.65183100
C	-2.96279400	0.95895900	-1.78686700
H	-3.22731600	0.10957600	-2.41208000
H	-3.45271600	0.85852000	-0.81119100
H	-3.29049700	1.88334200	-2.27374500
H	2.16655500	2.66703200	0.13582300
N	1.78586800	-0.26518000	1.24014400
O	3.85084800	0.49807200	0.77292500
H	2.11571600	-0.36438300	2.19231400
O	3.81254300	-2.20561700	-0.83493300
H	3.77983500	-2.99519100	-1.37408600
Na	5.23001500	-1.11780100	0.15277400
Z-TS₁₁₋₁₂			
C	-1.27230100	-2.43618300	-0.72623500
C	0.03740500	-2.05220800	-0.45336700
C	0.27573500	-1.11501400	0.54520500
C	-0.80093400	-0.54239900	1.23507700

C	-2.10469100	-0.93093800	0.95359600
C	-2.34258800	-1.91103600	-0.02504400
H	-1.48092300	-3.18513200	-1.48141000
H	0.85985100	-2.47455700	-1.01485400
H	-0.59278000	0.22885100	1.96613700
C	2.69190300	-0.54693500	0.11665700
O	-3.60668400	-2.40082700	-0.23338700
C	-4.46793200	-1.54074200	-0.96106500
H	-5.43220600	-2.04376500	-1.01978100
H	-4.58641400	-0.58082600	-0.45217100
H	-4.07859900	-1.38175000	-1.97268100
O	-3.20426900	-0.41292800	1.56607800
C	-2.99260500	0.59453500	2.53414900
H	-2.48062100	1.46034300	2.09855600
H	-3.97989200	0.88930900	2.88344700
H	-2.40717000	0.21462700	3.37727500
C	2.43968300	-0.15393900	-1.35841600
H	3.29426700	0.46506800	-1.65095500
O	1.21892400	0.52990000	-1.56509600
C	0.94306100	1.64638900	-0.84605300
C	-0.41651400	2.03035800	-0.84111600
C	1.87137700	2.38982800	-0.13455900
C	-0.80967100	3.14838200	-0.11726400
C	1.46462400	3.51575000	0.58786900
C	0.13436700	3.89168300	0.59900800
H	-1.84835600	3.45155000	-0.10302300
H	2.20064000	4.08336400	1.14375900
H	-0.18635000	4.76128100	1.15979700
H	2.39445400	-1.03087600	-1.99376800
O	-1.24746200	1.24104000	-1.56151200
C	-2.62621900	1.51729000	-1.48451300
H	-3.11501500	0.77314600	-2.10873000
H	-2.99108900	1.42159400	-0.45451800
H	-2.85614800	2.51870600	-1.86443600
H	2.90662200	2.07424100	-0.10478700
N	1.56947600	-0.70815900	0.90895700
O	3.72686700	-0.10146400	0.67876000
H	1.72558400	-0.43389000	1.86749000
O	3.27561200	-2.41056500	-0.27738900
H	2.59707500	-3.04739200	-0.04607500
Na	5.05623900	-1.79972300	0.61862000

Z-Int12

C	-1.27743200	-2.51993100	-0.63502000
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C	0.04436100	-2.14299600	-0.41718800
C	0.33630300	-1.15699300	0.52679100
C	-0.72405300	-0.53699300	1.20678400
C	-2.04070500	-0.91205800	0.97261200
C	-2.32364200	-1.93919600	0.05756100
H	-1.51597800	-3.29957100	-1.34944600
H	0.82596100	-2.59968100	-1.01161300
H	-0.49189000	0.26202900	1.90038300
C	2.77785800	-0.69767100	-0.05583700
O	-3.60344700	-2.41190800	-0.10300400
C	-4.45416200	-1.57072900	-0.86311700
H	-5.41972200	-2.07228300	-0.91883700
H	-4.57554300	-0.59683400	-0.38174700
H	-4.05350300	-1.43821600	-1.87426000
O	-3.11420400	-0.33616700	1.58070800
C	-2.85825000	0.71177100	2.49415900
H	-2.33319200	1.54171600	2.00789200
H	-3.83122100	1.04775000	2.84697300
H	-2.26640000	0.35758300	3.34398100
C	2.39475400	-0.15761900	-1.48267900
H	3.19889400	0.52648700	-1.77149600
O	1.13639800	0.47902400	-1.58158600
C	0.86904000	1.58278900	-0.84615500
C	-0.48558800	1.98746500	-0.85925000
C	1.79330200	2.29202500	-0.09404800
C	-0.87839800	3.09247100	-0.11632300
C	1.38405600	3.40458800	0.64955000
C	0.05996600	3.80217000	0.64123300
H	-1.91275800	3.41068700	-0.11713700
H	2.11539200	3.94527600	1.23787700
H	-0.26044000	4.66174500	1.21763500
H	2.33907000	-0.97477200	-2.19917300
O	-1.31280700	1.22788300	-1.61538500
C	-2.69172100	1.50304400	-1.53524100
H	-3.17978800	0.77767600	-2.18211000
H	-3.05895000	1.37840700	-0.50946300
H	-2.92041000	2.51466900	-1.88806100
H	2.81914900	1.94674100	-0.04173200
N	1.64230700	-0.78636200	0.86325500
O	3.77271100	-0.03884500	0.48466200
H	1.70409300	-0.01055300	1.50848500
O	3.23638900	-2.13756200	-0.28259000
H	2.54501000	-2.72042900	0.04539800
Na	5.11832800	-1.62419200	0.76074700

Z-TS₁₂₋₁₃

C	-2.17631600	-2.49515100	-1.12276200
C	-0.89045700	-2.82995800	-0.70497600
C	-0.32600800	-2.19206600	0.40112400
C	-1.09945300	-1.25147300	1.10220000
C	-2.37884600	-0.92373000	0.68448600
C	-2.92730700	-1.54796600	-0.44974300
H	-2.62866800	-2.97802600	-1.98129600
H	-0.31581300	-3.58026100	-1.23644500
H	-0.64012100	-0.72974100	1.93191200
C	2.48635500	-1.39551600	-0.16786100
O	-4.20393600	-1.27720300	-0.87524600
C	-4.41266800	0.04233300	-1.35701700
H	-5.33209400	0.01814300	-1.94173800
H	-4.52261100	0.74613000	-0.52974900
H	-3.57942400	0.35374500	-1.99566000
O	-3.16622900	0.00476500	1.30050700
C	-2.65595700	0.60764800	2.47093700
H	-1.73076000	1.15385600	2.26095300
H	-3.42348000	1.30033300	2.81316200
H	-2.47069800	-0.14143800	3.24754400
C	1.68344200	-0.64147400	-1.20916600
H	2.37886300	-0.20676500	-1.93882000
O	0.85101700	0.33803200	-0.63523900
C	1.28323600	1.60943200	-0.46932000
C	0.26475100	2.54588300	-0.18107000
C	2.59843900	2.03466300	-0.56233500
C	0.58956200	3.88624900	-0.02671200
C	2.91422700	3.38714000	-0.40738200
C	1.91739800	4.30797400	-0.14542200
H	-0.18330500	4.61441100	0.17990400
H	3.94688200	3.70497100	-0.48339000
H	2.15464300	5.35762000	-0.02410400
H	1.02426200	-1.33535400	-1.72851100
O	-0.98853900	2.03218600	-0.07686500
C	-2.04774200	2.93846400	0.14048100
H	-2.95050700	2.33199200	0.18381800
H	-1.92408600	3.47577600	1.08778500
H	-2.12373100	3.66237600	-0.67773400
H	3.38299900	1.30610500	-0.71327600
N	1.01197400	-2.41225100	0.73296100
O	3.18852500	-0.79236000	0.67207600
H	1.19731000	-2.15477500	1.69718500

O	2.90398700	-2.66195900	-0.57543800
H	1.98806800	-3.04256600	-0.03864800
Na	4.64126600	-2.41937900	0.75502200

Z-TS₁₂₋₁₃

C	-1.02462600	-3.06437100	-0.21166400
C	0.33701700	-2.78025000	-0.31861800
C	0.84942100	-1.71245000	0.39184400
C	0.04575300	-0.92261200	1.21396800
C	-1.31337800	-1.19148300	1.28907900
C	-1.84756000	-2.28434000	0.57650100
H	-1.46916100	-3.89732600	-0.74302100
H	0.98573100	-3.37735900	-0.94860700
H	0.49867100	-0.07578000	1.71450600
C	2.68999700	0.10412900	-0.06086600
O	-3.17569100	-2.59287300	0.69001600
C	-4.02358700	-1.70690500	-0.02793700
H	-5.04681200	-2.01369100	0.18496500
H	-3.87022800	-0.67393100	0.29628800
H	-3.82547200	-1.78907200	-1.10153200
O	-2.19602000	-0.46706600	2.01661800
C	-1.70821700	0.70408600	2.64887100
H	-1.28293200	1.39768100	1.91761500
H	-2.56935600	1.16214900	3.13082000
H	-0.95667700	0.45472800	3.40461100
C	1.93018300	0.55106600	-1.33243200
H	2.29688900	1.55542700	-1.57105800
O	0.51560000	0.52570900	-1.28921800
C	-0.19157500	1.55092500	-0.76126400
C	-1.57905800	1.52653600	-1.03146200
C	0.33719000	2.58833100	-0.00527300
C	-2.39257500	2.54083400	-0.54268000
C	-0.49036300	3.60868600	0.47055600
C	-1.84867500	3.58621800	0.20809800
H	-3.45473700	2.52895100	-0.74889900
H	-0.05986400	4.40933400	1.05993700
H	-2.49737400	4.36986300	0.57965800
H	2.19594900	-0.12256000	-2.14910100
O	-2.02601400	0.48765000	-1.78366700
C	-3.27833200	0.64765600	-2.41506900
H	-3.38548500	-0.19805300	-3.09194200
H	-4.10326000	0.63684100	-1.69523500
H	-3.31031900	1.58202000	-2.98494400
H	1.38537600	2.55682800	0.25816200

N	2.25959600	-1.40103200	0.26006300
O	2.56015600	0.84690300	1.00961300
H	2.73202400	-1.56247000	1.15019300
O	4.04198300	-0.05264900	-0.45250000
H	4.13078400	-0.99728600	-1.03840300
Na	4.66915200	1.24862300	1.15192900
O	3.89085000	-2.23805700	-1.41423400
H	3.78361400	-2.42598100	-2.34713900
H	2.80819000	-2.00121300	-0.53146800

Z-Int13

C	3.45144500	-2.05794300	0.80480900
C	2.38605600	-2.19326700	1.69182300
C	1.12352800	-1.71085800	1.33892200
C	0.94680000	-1.11985100	0.07777600
C	2.01417000	-0.99564500	-0.80097900
C	3.29023400	-1.45784200	-0.43224400
H	4.43838300	-2.42461300	1.06372100
H	2.53808500	-2.65223500	2.66242300
H	-0.04065400	-0.75373800	-0.17353800
C	-3.22131900	-0.10137700	0.54611900
O	4.35120800	-1.35858000	-1.29989800
C	4.84015300	-0.03396000	-1.44319000
H	5.65688500	-0.07617300	-2.16311300
H	4.05778700	0.63304700	-1.81537700
H	5.21875400	0.33786200	-0.48390800
O	1.91069300	-0.43550800	-2.03558600
C	0.60575500	-0.18073500	-2.51654200
H	0.06868700	0.52627600	-1.88080200
H	0.72888500	0.24867700	-3.50920300
H	0.03773600	-1.11589500	-2.58446100
C	-2.94327000	1.03641500	1.53092900
H	-3.51872900	1.92029700	1.24434900
O	-1.57564300	1.31074000	1.68322400
C	-0.93367900	1.89679800	0.64017500
C	0.47156300	1.98556700	0.77764500
C	-1.54743100	2.40475300	-0.49522900
C	1.21850900	2.59059800	-0.22396700
C	-0.78519600	3.03599000	-1.48666100
C	0.58638300	3.12939700	-1.35016500
H	2.29551100	2.64661700	-0.13538300
H	-1.28014300	3.44010600	-2.36110900
H	1.18352400	3.60628600	-2.11780300
H	-3.29226200	0.71001400	2.51290400

O	0.97154200	1.45407400	1.90897400
C	2.37596400	1.33785900	2.01781800
H	2.55640800	0.78672900	2.93805500
H	2.78900400	0.77469000	1.17464600
H	2.84831500	2.32469000	2.07836100
H	-2.61901700	2.31878400	-0.62471500
N	0.05431600	-1.74771700	2.21926200
O	-2.31509900	-0.94806100	0.34248800
H	-0.84421600	-1.50131000	1.82075900
O	-4.36468500	-0.14283800	0.02842900
H	-5.73618600	-1.09228400	-0.86832000
Na	-3.60423200	-2.09638800	-1.03677900
O	-5.78448600	-1.90681800	-1.39933700
H	-6.68904000	-2.04108100	-1.68239700
H	0.04239300	-2.50193400	2.88607000

E-lignin^{oxime}

C	1.15525500	-0.22502600	-1.69758900
C	0.06363300	0.55474700	-1.34197000
C	0.10579000	1.32559100	-0.18135700
C	1.27099300	1.34763300	0.58459000
C	2.37391700	0.59016700	0.21728500
C	2.30476600	-0.22724000	-0.91669200
H	1.13130000	-0.86179100	-2.57414900
H	-0.83924600	0.54219400	-1.94033300
H	1.34482300	1.94570400	1.48641300
C	-1.10400100	2.03793900	0.31137800
O	3.36310600	-1.02299900	-1.26755800
C	3.52670400	-2.14857800	-0.40691200
H	4.38800500	-2.70077200	-0.77928200
H	3.70536600	-1.82604400	0.62219000
H	2.63515500	-2.78224600	-0.44577600
O	3.49417000	0.60972300	1.00490000
C	4.62875500	1.21440200	0.38536600
H	4.41344300	2.26060500	0.14884500
H	5.43805700	1.16293200	1.11163400
H	4.90725800	0.67791100	-0.52410700
C	-1.61708900	1.72552000	1.70020200
H	-0.77747400	1.65827500	2.40084000
O	-2.38864200	0.52726900	1.74591200
C	-1.79313300	-0.60836800	1.26025300
C	-2.38438600	-1.22672400	0.14510600
C	-0.65516500	-1.15114400	1.83246500
C	-1.81493300	-2.38824200	-0.37080600

C	-0.07120400	-2.29753600	1.29650400
C	-0.65644300	-2.91308000	0.20067500
H	-2.25370900	-2.88072800	-1.22803300
H	0.82728800	-2.70451100	1.74405100
H	-0.21859700	-3.81007400	-0.22127400
H	-2.29432900	2.51431800	2.02068200
O	-3.47496600	-0.60978400	-0.36811800
C	-4.08841100	-1.20057400	-1.49277400
H	-4.93447100	-0.56424300	-1.74211600
H	-3.40087600	-1.24266000	-2.34450400
H	-4.44648100	-2.20987000	-1.26535300
H	-0.21317900	-0.65739700	2.69067400
N	-1.79368000	2.88672500	-0.34151400
O	-1.29841800	3.12280300	-1.61124400
H	-1.88886500	3.79831200	-1.95527500

E-Int4

C	-0.87297900	0.95273200	1.99069800
C	-0.01554200	0.01364300	1.44064100
C	0.06869000	-0.12904800	0.05512000
C	-0.68766200	0.70784100	-0.76501000
C	-1.51235000	1.67752200	-0.22133600
C	-1.63954800	1.78028200	1.17249300
H	-0.97437400	1.06422900	3.06364000
H	0.55758500	-0.63850600	2.08704700
H	-0.62718200	0.65078500	-1.84567600
C	0.89702500	-1.18959400	-0.55375000
O	-2.45235700	2.68642700	1.77106600
C	-3.77804900	2.82814100	1.25615700
H	-3.82563300	3.60985500	0.49698700
H	-4.12184500	1.88661000	0.82273800
H	-4.40147200	3.10083700	2.10639200
O	-2.19332000	2.52522100	-1.05342300
C	-1.62635400	3.83443400	-1.08517200
H	-0.60025500	3.79298800	-1.46158300
H	-2.24431300	4.42416500	-1.76014800
H	-1.62976300	4.28526400	-0.08738700
C	0.30496300	-2.07400500	-1.63238100
H	0.02040600	-1.44428100	-2.48364000
O	-0.79503000	-2.82971700	-1.16247300
C	-1.98145100	-2.15659100	-0.99184100
C	-2.48021900	-2.02608300	0.31518600
C	-2.68264500	-1.63978900	-2.06642500
C	-3.67861200	-1.34557900	0.51522500

C	-3.87569200	-0.94925200	-1.86149700
C	-4.36529000	-0.80529800	-0.57294900
H	-4.08047600	-1.22565800	1.51268200
H	-4.41435100	-0.53557900	-2.70423500
H	-5.29674700	-0.27877500	-0.40169500
H	1.06026200	-2.78678500	-1.95716600
O	-1.72312300	-2.57095500	1.29489100
C	-2.18884300	-2.44608400	2.62287500
H	-1.45009900	-2.94382500	3.24744200
H	-2.26781800	-1.39328000	2.91422600
H	-3.15934500	-2.93606600	2.74826900
H	-2.28197700	-1.77491500	-3.06534100
N	2.10884700	-1.49588800	-0.27196900
O	2.67202300	-0.55542700	0.63558800
H	3.28301200	-1.05014400	1.22471700
S	4.18184000	0.61026200	-0.28629300
O	4.83134900	-0.28193500	-1.19237800
Cl	5.23961600	-0.17238700	1.73416100
Cl	2.56944600	1.40247900	-1.61811100

E-TS₄₋₅

C	-0.84789600	0.90769100	1.98607300
C	0.04800900	0.04546000	1.37579100
C	0.08768700	-0.05073500	-0.01634800
C	-0.75279700	0.75941300	-0.78121800
C	-1.62136500	1.65175100	-0.17647700
C	-1.70234500	1.70202500	1.22373600
H	-0.91643400	0.97770800	3.06507900
H	0.68318900	-0.58759900	1.98169800
H	-0.73727500	0.73459500	-1.86459300
C	0.95104400	-1.04161300	-0.68934000
O	-2.56157800	2.52240500	1.87915100
C	-3.91931100	2.54351700	1.43211000
H	-4.07447000	3.31234600	0.67436300
H	-4.19955100	1.57174700	1.01925600
H	-4.52042400	2.76597200	2.31237100
O	-2.40079800	2.46207700	-0.95652700
C	-1.96841000	3.82170100	-0.95014100
H	-0.95489200	3.89811200	-1.35437400
H	-2.66065100	4.37010100	-1.58667000
H	-1.98707300	4.23391600	0.06366000
C	0.37445200	-1.91390700	-1.78763500
H	0.02032900	-1.27266800	-2.60315100
O	-0.65984400	-2.75195700	-1.30888900

C	-1.87951400	-2.16107900	-1.07836400
C	-2.34057200	-2.10079900	0.24750500
C	-2.64793700	-1.66020000	-2.11373900
C	-3.57233600	-1.50406100	0.50629500
C	-3.87473000	-1.05414700	-1.84982300
C	-4.32835200	-0.97868900	-0.54243400
H	-3.94667700	-1.43719300	1.51928100
H	-4.46777400	-0.65359400	-2.66174000
H	-5.28468800	-0.51703200	-0.32657500
H	1.15847200	-2.56743200	-2.16455900
O	-1.51984700	-2.62662600	1.18452200
C	-1.95011300	-2.57487300	2.52948200
H	-1.16218700	-3.04457000	3.11431200
H	-2.08616800	-1.53931500	2.85870900
H	-2.88372100	-3.12935500	2.66567900
H	-2.27417000	-1.74302200	-3.12859100
N	2.18237800	-1.30553700	-0.45029300
O	2.71389600	-0.40305000	0.51709800
H	3.38180700	-0.89363600	1.11733200
S	4.16371700	0.73969900	-0.25855300
O	4.77924700	-0.03630400	-1.28532300
Cl	5.14403200	-0.57190400	1.73713700
Cl	2.61329400	1.81563400	-1.35747100

E-Int5

C	0.95537000	0.99393400	-1.96964400
C	-0.12520800	0.46430600	-1.28055300
C	-0.17171900	0.54869200	0.11132500
C	0.84751200	1.21552000	0.79228300
C	1.91003400	1.77951300	0.10329400
C	1.98986100	1.63241800	-1.28936500
H	1.02842300	0.91619900	-3.04804700
H	-0.91551600	-0.05131800	-1.81150700
H	0.83928300	1.31820700	1.87172200
C	-1.24545200	-0.12776200	0.87592400
O	3.02388700	2.12656000	-2.02107900
C	4.34632100	1.87554600	-1.54322000
H	4.70784700	2.70466600	-0.93304400
H	4.37230400	0.95947900	-0.94973300
H	4.97328500	1.77068700	-2.42788700
O	2.87804900	2.45947200	0.79437300
C	2.81148700	3.87070000	0.60261100
H	1.86419600	4.26093900	0.98554300
H	3.63927300	4.29999200	1.16474500

H	2.90752100	4.12776700	-0.45709400
C	-0.85702400	-1.07941700	1.98705500
H	-0.38256300	-0.53051300	2.80541200
O	0.00832800	-2.09672600	1.49266000
C	1.34881800	-1.80661600	1.43002700
C	1.98343100	-1.98486000	0.19050100
C	2.07784300	-1.38074500	2.52690100
C	3.33608400	-1.69156400	0.06281300
C	3.43105100	-1.07404600	2.39435300
C	4.05265100	-1.22406400	1.16496400
H	3.83392500	-1.81877100	-0.88970200
H	3.99091900	-0.72629300	3.25304400
H	5.10434600	-0.98930100	1.05404400
H	-1.75222300	-1.57496400	2.35731800
O	1.19205500	-2.43745000	-0.81387800
C	1.74010900	-2.51429900	-2.11789700
H	0.91941400	-2.81999500	-2.76462900
H	2.11814400	-1.53777900	-2.43563900
H	2.53967600	-3.25937600	-2.16000300
H	1.58410600	-1.27925700	3.48660400
N	-2.50145300	-0.04465000	0.69106200
O	-2.80949600	0.87060900	-0.33498400
H	-0.73995500	-2.71957600	-0.71270200
S	-4.41122200	0.93485700	-0.69514300
O	-4.93768900	-0.40382600	-0.80838000
Cl	-1.86505800	-2.80166600	-1.35543400
Cl	-5.07439800	1.69410000	1.18946300

E-TS₅₋₆

C	-0.83287200	0.60284800	2.11271200
C	0.15559900	0.03815500	1.32659200
C	0.11341700	0.22792400	-0.05471900
C	-0.87152900	1.01819900	-0.63863100
C	-1.83658200	1.61057200	0.15435700
C	-1.84803300	1.36955800	1.53975800
H	-0.84365100	0.46170000	3.18649100
H	0.94051600	-0.56380500	1.76534000
H	-0.88821400	1.23948200	-1.69884500
C	1.12420800	-0.44237100	-0.85290500
O	-2.77620100	1.89354000	2.36985900
C	-4.13980600	1.91439800	1.94164300
H	-4.38152600	2.85247300	1.44145600
H	-4.34126400	1.08318300	1.26324900
H	-4.73557300	1.81454900	2.84748200

O	-2.75382700	2.44574700	-0.42072600
C	-2.43037200	3.82465400	-0.22113300
H	-1.45368500	4.05024000	-0.65793800
H	-3.20644200	4.39942900	-0.72304800
H	-2.41621900	4.06665000	0.84652300
C	0.76346700	-1.10223600	-2.39468400
H	0.28406100	-0.19317200	-2.77660500
O	-0.02196200	-2.19388100	-2.28076000
C	-1.28899100	-2.00169500	-1.73369900
C	-1.47455900	-2.36636600	-0.39382600
C	-2.30786500	-1.46662500	-2.49441600
C	-2.72680500	-2.15397200	0.17839300
C	-3.55715000	-1.25425000	-1.91364000
C	-3.75356300	-1.59745600	-0.58426800
H	-2.90456500	-2.41146100	1.21385000
H	-4.36192100	-0.82890000	-2.49847000
H	-4.72226600	-1.44063900	-0.12452900
H	1.66564100	-1.33768200	-2.94871500
O	-0.39093900	-2.85431600	0.23913900
C	-0.54068200	-3.27118200	1.58768000
H	0.43977200	-3.62290200	1.89752600
H	-0.84543200	-2.43379100	2.22233500
H	-1.27291000	-4.08047800	1.66126500
H	-2.11617400	-1.21855300	-3.53272800
N	2.25789200	-0.82841400	-0.93448400
O	3.11086000	0.36159800	0.63443900
H	3.30806400	-1.07527500	1.68232800
S	3.90186200	1.49480400	0.02548800
O	4.87592900	1.01753300	-0.93585700
Cl	3.07957000	-2.08982200	2.47452200
Cl	2.21328600	2.44619200	-1.36495800

E-Int6

C	3.25834400	0.43152600	-1.54366000
C	1.96452400	0.86007100	-1.77598500
C	0.99690700	0.55180100	-0.82053500
C	1.29413700	-0.18316700	0.33565000
C	2.58958200	-0.61918600	0.54919100
C	3.59247200	-0.28730200	-0.39292300
H	4.05821300	0.65733100	-2.23702300
H	1.70980100	1.44042300	-2.65278000
H	0.49256200	-0.39941100	1.03242400
C	-0.36630000	0.85698300	-1.00534700
O	4.87509500	-0.67192000	-0.27923400

C	5.51681200	-0.64617700	1.00144800
H	5.13113400	0.17599000	1.60655400
H	5.37180100	-1.58832200	1.52542000
H	6.57226100	-0.48561100	0.79059100
O	2.94974600	-1.37822400	1.60666100
C	1.93310500	-1.67306800	2.56155900
H	1.12161700	-2.24640700	2.10304100
H	2.41773600	-2.26452900	3.33399200
H	1.52256700	-0.75528300	2.99033100
C	-2.92335000	0.74839300	-1.17067800
H	-3.27251000	0.83040500	-0.13846400
O	-3.11448800	-0.50318400	-1.73577700
C	-2.68604000	-1.55226900	-0.92905300
C	-1.43727900	-2.13918700	-1.18239600
C	-3.48668300	-2.00179000	0.10170100
C	-1.00341500	-3.17084200	-0.35256000
C	-3.05181800	-3.03602500	0.92445100
C	-1.81114600	-3.60931800	0.69585500
H	-0.04184800	-3.63845300	-0.51900000
H	-3.67307900	-3.37316000	1.74352900
H	-1.45700700	-4.40971700	1.33432700
H	-3.37724100	1.50167100	-1.80922900
O	-0.72703900	-1.63906000	-2.22717200
C	0.50105400	-2.26817100	-2.54759200
H	0.87982600	-1.75094600	-3.42653900
H	1.22347800	-2.16881200	-1.72988200
H	0.34769400	-3.32566300	-2.78145600
H	-4.44287900	-1.51814300	0.26534700
N	-1.49506000	1.02976900	-1.09690000
O	-0.14171100	2.62676000	1.25087000
H	0.18672600	3.48520500	-0.22199400
S	-1.45976900	2.51169900	1.91504600
O	-2.56486900	2.74793100	0.98745600
Cl	0.40595200	4.01941000	-1.40663800
Cl	-1.60880100	0.06328500	2.13082500

E-Int7

C	2.14987600	-1.81927900	-1.09946200
C	0.87977100	-1.60093900	-1.59119300
C	0.32690300	-0.32542900	-1.42094300
C	1.00345000	0.70133700	-0.74472400
C	2.25913900	0.45391500	-0.21966500
C	2.85601500	-0.81246300	-0.42701500
H	2.64498600	-2.77465200	-1.21975500

H	0.32957700	-2.38155000	-2.10097000
H	0.47707600	1.64831100	-0.60736900
C	-1.01063200	-0.05259500	-1.74192600
O	4.06768100	-1.15683800	0.03569300
C	5.12893900	-0.19497900	0.07042900
H	5.06916700	0.47101300	-0.79186500
H	5.09460900	0.38921100	0.98699100
H	6.04468000	-0.78088800	0.02451700
O	2.93248200	1.35574200	0.52210500
C	2.27808100	2.60743100	0.75229800
H	1.32161300	2.45773800	1.25968000
H	2.95737700	3.18115900	1.37720200
H	2.09304500	3.13049300	-0.18899100
C	-3.37275800	0.56834400	-1.29280900
H	-3.18695000	1.62792200	-1.06744700
O	-3.55464500	-0.23551400	-0.17782000
C	-2.53182600	-0.19423900	0.75851500
C	-1.74320200	-1.34673500	0.90467900
C	-2.27554000	0.94223600	1.50322100
C	-0.70908100	-1.34431300	1.83701700
C	-1.22921000	0.94442800	2.42172000
C	-0.45789000	-0.19592000	2.58765600
H	-0.08310500	-2.21650200	1.96760200
H	-1.01908200	1.84363600	2.98631900
H	0.35967500	-0.20203700	3.29905400
H	-4.20567200	0.40444000	-1.96859400
O	-2.01993200	-2.38022300	0.06601800
C	-1.38312100	-3.61562500	0.33223000
H	-1.79428500	-4.32540000	-0.38260000
H	-0.29920000	-3.54263900	0.19522000
H	-1.59885600	-3.95386300	1.35002900
H	-2.86351500	1.83518700	1.33360600
N	-2.11880200	0.18247100	-1.97192100
Cl	-1.23104100	3.11498400	-0.70572500

E-TS₇₋₈

C	3.16480000	-1.95669700	0.09653000
C	1.86018900	-2.37811700	-0.09783400
C	0.93891200	-1.46636200	-0.60956600
C	1.29833700	-0.14053500	-0.89894600
C	2.59988800	0.28017600	-0.67536700
C	3.55441000	-0.65033300	-0.19375500
H	3.92162400	-2.62960400	0.47901800
H	1.56072900	-3.39149800	0.13548000

H	0.54057600	0.54913000	-1.24821700
C	-0.42483500	-1.81962300	-0.77152700
O	4.83083200	-0.32644800	0.07164600
C	5.56000400	0.51293300	-0.83279900
H	5.24306400	0.33210800	-1.86171900
H	5.42205300	1.56244100	-0.58327900
H	6.60279300	0.22671300	-0.71299700
O	3.02476100	1.54783400	-0.85221400
C	2.09616800	2.49205300	-1.37209300
H	1.23585900	2.59931500	-0.70643000
H	2.63547800	3.43367500	-1.43315300
H	1.76155000	2.19459100	-2.36988300
C	-3.07908400	-1.43423800	-0.50731400
H	-3.21529000	-0.76040300	-1.34857400
O	-2.91219200	-0.91376400	0.70536700
C	-2.26857800	0.31721200	0.76404600
C	-1.06639000	0.37314700	1.48483500
C	-2.82008800	1.43691800	0.16843900
C	-0.42035600	1.60229700	1.60347700
C	-2.15787800	2.65862900	0.28816400
C	-0.97441500	2.73669600	1.00764300
H	0.50429000	1.68564400	2.15925500
H	-2.58844800	3.54378700	-0.16224600
H	-0.47084900	3.68992700	1.12388800
H	-3.71703300	-2.30633800	-0.50881100
O	-0.60797800	-0.79640800	1.99713400
C	0.61143700	-0.75690200	2.71431600
H	0.80641600	-1.77964100	3.03000400
H	1.43270000	-0.40867200	2.07722400
H	0.52878200	-0.11296500	3.59462500
H	-3.76799800	1.32674800	-0.35995200
N	-1.54398800	-2.05556200	-0.90734400
Cl	-5.47922900	-0.13525000	-1.37281000

E-Int8

C	-1.98380500	-2.20875400	-0.57425700
C	-0.84521100	-2.50790200	0.15968800
C	-0.41561400	-1.61125300	1.13224600
C	-1.09851400	-0.41215200	1.36140800
C	-2.22136600	-0.10754800	0.60514200
C	-2.67998700	-1.02815600	-0.35888000
H	-2.35407100	-2.88104200	-1.33802500
H	-0.29533700	-3.42252300	-0.01780600
H	-0.70747100	0.28719800	2.08900500

C	0.77201300	-1.88243200	1.88904600
O	-3.74563900	-0.76371600	-1.15874500
C	-4.97355500	-0.38705700	-0.53312400
H	-5.07613000	-0.87976400	0.43705900
H	-5.02764900	0.69248200	-0.40138200
H	-5.76572700	-0.72647100	-1.19870700
O	-2.90497200	1.06109300	0.69127200
C	-2.57609200	1.93608600	1.75903300
H	-1.55331800	2.30836600	1.66118100
H	-3.27597500	2.76587900	1.68946800
H	-2.69874400	1.43132400	2.72203600
C	3.29432700	-1.22868200	-0.16112900
H	3.41929100	-1.13159600	0.91479400
O	2.10417100	-0.70233200	-0.62023300
C	1.73717900	0.55561500	-0.22510500
C	0.59309200	1.07124800	-0.87028000
C	2.38578800	1.30151900	0.74319100
C	0.14275900	2.34267100	-0.53883300
C	1.91308800	2.57267600	1.08227500
C	0.80511600	3.09155000	0.43868000
H	-0.72562900	2.75638000	-1.03414800
H	2.43462800	3.14942400	1.83540600
H	0.44686100	4.08532500	0.68029700
H	3.31452100	-2.26930800	-0.46626700
O	0.00431200	0.25276600	-1.76722900
C	-1.09572400	0.76494300	-2.49684800
H	-1.44019400	-0.05111800	-3.12847100
H	-1.91112300	1.06956000	-1.83401800
H	-0.78657500	1.61166600	-3.11828100
H	3.27331800	0.91890100	1.22886700
N	1.73040900	-2.08912700	2.49292900
Cl	4.73132500	-0.43809000	-0.92973800