

Supporting Information

Elucidating mechanism and reactivity of reaction between donor-acceptor-acceptor 1,3-bisdiazo compound and cinnamyl alcohol catalyzed by $\text{Rh}_2(\text{OAc})_4$: a DFT study

Yan Zhang, Yongsheng Yang, Ying Xue*

College of Chemistry,
Key Lab of Green Chemistry and Technology in Ministry of Education,
Sichuan University, Chengdu 610064,
People's Republic of China

**The Cartesian Coordinates (Å) for Ground state and Transition State Geometries
Optimized in the Gas Phase and CHCl₃ Solvent**

1a

0 1

Br	5.33634400	-0.03319400	-0.31624100
O	-1.37188900	2.17883200	-0.01915900
N	-1.29185100	-1.11009000	1.13201100
C	1.36380900	1.17932000	0.11422900
H	0.82056500	2.11355700	0.10165800
O	-3.20169900	-1.54210500	-0.75634900
N	-1.68433800	-2.02439900	1.67999900
C	2.74314000	1.17329500	-0.08273900
H	3.27122800	2.10578500	-0.24679600
O	-5.16121500	-0.42496800	-0.49427800
N	-3.98170900	1.74436900	0.19949000
C	3.44241500	-0.03052700	-0.05705500
N	-4.62483000	2.66260700	0.33627600
C	2.77614800	-1.23587000	0.15598800
H	3.32560100	-2.17018000	0.16748300
C	1.39770600	-1.22730400	0.34069900
H	0.88943700	-2.17619400	0.48344200
C	0.66846700	-0.02410300	0.32613000
C	-0.79792300	-0.04716000	0.52784000
C	-1.73836800	1.02058900	0.16990600
C	-3.19208700	0.69015100	0.06511700
C	-3.81508500	-0.54496100	-0.43246900
C	-5.85249700	-1.57852300	-1.01171900
H	-5.66175300	-2.45163600	-0.38310900
H	-5.52475300	-1.79609100	-2.03114200
H	-6.90917100	-1.31438500	-0.99480900

1a-h

0 1

Br	3.66852200	-2.12450500	0.06952600
O	-3.37672600	-2.26218600	0.51511100
N	-2.49420100	0.57988200	-1.30089300
C	-0.49356400	-2.12936000	0.11819500
H	-1.26508200	-2.84691000	0.35838000
O	-4.02266000	1.89749300	0.51815000
N	-2.66614600	1.44464400	-2.01633800
C	0.84820300	-2.47016400	0.26192100
H	1.11838800	-3.46179700	0.60658600
O	-6.23119900	1.37239500	0.57381800

N	-5.77359900	-1.13807800	0.30433200
C	1.85240400	-1.56296100	-0.06708600
N	-6.65676700	-1.83699600	0.38647000
C	1.53202800	-0.26794000	-0.51197800
C	0.17672200	0.06187600	-0.63509100
H	-0.06456100	1.07323900	-0.94794400
C	-0.84930100	-0.85039100	-0.34311400
C	-2.26280500	-0.44428400	-0.50240400
C	-3.42540600	-1.10533800	0.10165100
C	-4.71334200	-0.35376600	0.18540100
C	-4.91794000	1.08072700	0.43554600
C	-6.52098200	2.75386600	0.86556600
H	-6.15954100	3.39775600	0.06030300
H	-6.04549400	3.05484400	1.80212100
H	-7.60564600	2.81071500	0.94799400
C	2.56378800	0.74485900	-0.85040600
C	3.55934600	1.29971000	0.07960000
C	3.45856200	1.02533900	1.45507300
C	4.61385800	2.11620700	-0.36735000
C	4.38719000	1.54946400	2.35019900
H	2.65174600	0.39899900	1.81952900
C	5.53367200	2.64221000	0.53541300
H	4.71978200	2.33696100	-1.42555700
C	5.42909700	2.36176500	1.89949500
H	4.29164100	1.32225400	3.40800800
H	6.34029800	3.27021100	0.16833900
H	6.15035600	2.76997100	2.60063900
N	2.51091300	1.22320600	-2.06573600
N	2.49198900	1.65004400	-3.12958000

1-int2

0 1

Rh	-1.10004900	-1.16549200	-0.44109400
C	-2.85480900	-2.54139400	-2.28126000
O	-1.61529500	-2.35588600	-2.03970700
C	-2.23392100	1.10183800	-1.83433600
O	-3.35304600	0.77608400	-1.32212600
C	-1.67792800	0.54397700	1.82876900
O	-2.91016000	0.40754300	1.53855000
C	-2.29660200	-3.07758600	1.37435600
O	-1.18911500	-2.80992900	0.79372900
Rh	-3.43319900	-0.81556300	-0.03255300
O	-3.38302000	-2.43739800	1.23027900
O	-1.12313200	0.50451900	-1.63134700

O	-0.71497000	0.00100400	1.18803000
O	-3.82554500	-2.05626300	-1.61755400
C	-3.19824900	-3.38558600	-3.48428700
H	-2.41909900	-4.12833400	-3.66314900
H	-4.16860900	-3.86438300	-3.34620500
H	-3.25685400	-2.73247400	-4.36159300
C	-2.29359300	-4.26448100	2.30615900
H	-2.04851700	-5.16694300	1.73825500
H	-1.51427200	-4.12976000	3.06154900
H	-3.26554700	-4.38019600	2.78510700
C	-1.31293700	1.41296100	3.00226100
H	-0.24001800	1.60589200	3.00888500
H	-1.87348900	2.34889800	2.94213900
H	-1.60851900	0.90258500	3.92463800
C	-2.19515500	2.30011300	-2.74773600
H	-1.86139800	1.98376500	-3.74036800
H	-3.17540000	2.77098400	-2.80496200
H	-1.46681500	3.01733600	-2.36008500
Br	7.92022100	0.63393900	-1.27939300
O	2.01456200	-0.04804200	3.16891100
C	4.59177800	1.14562800	1.17799100
H	4.38618600	1.47003700	2.19355000
O	1.20854100	-1.50564600	-0.77462200
C	5.89914900	1.10687600	0.70024400
H	6.73133400	1.39160300	1.33411800
O	1.75954900	-3.52617600	0.07031300
N	1.98631500	-2.58658900	2.46281300
C	6.12773400	0.69282100	-0.61385600
N	2.05315400	-3.29110800	3.34115900
C	5.07565200	0.32575200	-1.45053800
H	5.27274800	0.01667500	-2.47079400
C	3.76916200	0.36989300	-0.95914700
H	2.94061400	0.08250800	-1.59859200
C	3.51970700	0.77537700	0.35550200
C	2.10351200	0.82798400	0.91759500
C	1.96729700	-0.27752500	1.97524200
C	1.89855800	-1.68840000	1.49201000
C	1.59812900	-2.20624700	0.16766900
C	1.30420300	-4.12545600	-1.16860400
H	1.90575200	-3.75722700	-2.00230700
H	0.25379300	-3.88268500	-1.33751100
H	1.44827700	-5.19603600	-1.03087900
C	-0.53319400	4.43590800	0.56306900
C	0.14191000	3.29101800	0.38044000

H	0.01926500	5.30254000	0.93028400
H	-0.34638600	2.40403600	-0.01729000
C	1.60359000	3.14731200	0.69297300
H	2.19414800	3.01550500	-0.22648200
H	1.98062000	4.04264100	1.19767600
O	1.84836400	2.05009400	1.58600100
H	1.38220900	0.64675700	0.11855900
C	-1.95838100	4.67562600	0.28600900
C	-2.41018800	5.98830300	0.06215600
C	-2.89986700	3.63308100	0.23456700
C	-3.74768600	6.24492800	-0.23701600
H	-1.70024800	6.81053400	0.11128100
C	-4.23528200	3.88638000	-0.06770300
H	-2.59943400	2.61543100	0.44266100
C	-4.66553200	5.19408500	-0.30910200
H	-4.07373800	7.26603000	-0.41438500
H	-4.93305900	3.05565400	-0.11180500
H	-5.70765200	5.39378700	-0.54147400

1-int3

0 1

Rh	1.45768400	2.96015700	-0.15486100
C	2.18286100	0.95326800	-2.11911200
O	2.50235400	2.10838800	-1.70878900
C	-0.89617400	3.01006400	-1.78280900
O	-1.14646000	1.83997900	-1.33582900
C	-0.55011200	2.89126700	1.93193600
O	-0.82817000	1.69697500	1.56571300
C	2.55937100	0.95342300	1.59028100
O	2.76705300	2.13639900	1.18604400
Rh	0.15378500	0.88787800	-0.05413200
O	1.58779400	0.20043400	1.23423400
O	0.10825100	3.72431100	-1.48914800
O	0.31396500	3.65549900	1.40977300
O	1.23971700	0.21966500	-1.66015500
C	2.99998200	0.35153600	-3.23580600
H	3.70605200	-0.36059500	-2.79725500
H	2.35035300	-0.19719000	-3.92066300
H	3.55326600	1.12865600	-3.76338000
C	3.54664700	0.35228100	2.55748400
H	4.10347000	1.14181700	3.06318200
H	3.02545400	-0.27948600	3.27912200
H	4.24806800	-0.27824200	2.00212700
C	-1.35125700	3.41819000	3.09888600

H	-1.25923500	2.72878000	3.94264800
H	-1.00446200	4.41128000	3.38388100
H	-2.40793100	3.45912000	2.81786900
C	-1.91626400	3.57266500	-2.74244300
H	-2.87085800	3.68860500	-2.22066100
H	-1.58479100	4.53663300	-3.12838400
H	-2.07207000	2.86496900	-3.56070100
Br	5.44976500	-2.62896800	0.78902000
O	-1.64623500	-1.16423900	-2.23033800
C	2.06586100	-2.86286500	-1.63204700
H	1.85784900	-2.87556200	-2.69810700
O	-1.57930600	-1.65315500	1.98127100
C	3.38603500	-2.77931700	-1.19397300
H	4.20620400	-2.74326500	-1.90211700
O	-3.00317200	-0.15594000	1.02102800
C	3.63836200	-2.75621500	0.17707900
C	2.60340600	-2.82102400	1.10708000
H	2.81833500	-2.79600300	2.16861600
C	1.28728000	-2.90205700	0.65531600
H	0.46898200	-2.93052300	1.36616800
C	1.01226600	-2.92520000	-0.71598400
C	-0.41384700	-2.98422600	-1.20812200
C	-1.07431200	-1.58408400	-1.23554100
C	-0.99679900	-0.69103600	-0.06245800
C	-1.90568900	-0.89881300	1.08210800
C	-3.83683500	-0.14857900	2.20026100
H	-3.33370500	0.41947300	2.98664600
H	-4.03264900	-1.16641900	2.53922600
H	-4.76276600	0.33241500	1.89251400
C	-4.27819400	-2.54256800	-0.93547000
C	-3.53518200	-3.42568400	-0.25245200
H	-4.03819800	-2.36668400	-1.98357400
H	-3.67774300	-3.55901300	0.81831000
C	-2.44373200	-4.24646000	-0.87547900
H	-2.56340100	-5.30285300	-0.60860000
H	-2.47760300	-4.16799900	-1.97074100
O	-1.13631700	-3.88790600	-0.38936000
H	-0.44079400	-3.30307300	-2.26228800
C	-5.36141600	-1.71825800	-0.37933900
C	-5.59373900	-0.43880100	-0.91288900
C	-6.16631000	-2.15878400	0.68521500
C	-6.58049200	0.38735400	-0.37809200
H	-4.97078400	-0.08683900	-1.73046200
C	-7.15816600	-1.33518700	1.21585100

H	-6.02227200	-3.15901000	1.08319400
C	-7.36637300	-0.05710300	0.68983500
H	-6.73802800	1.37822500	-0.79441400
H	-7.77560400	-1.69372700	2.03460500
H	-8.14187600	0.58278400	1.10078400

1-int4

0 1

Rh	3.30535500	-1.90776000	-0.42045100
C	2.95734500	0.78155600	-1.78080600
O	3.67288300	-0.20976100	-1.67619200
C	3.30963800	-0.29533400	1.99765800
O	2.08192400	-0.01811500	1.77537800
C	1.44826400	-3.36493400	1.23734600
O	0.60129100	-2.41976500	1.08033800
C	1.18895500	-2.47758000	-2.29017300
O	2.40304200	-2.77518200	-2.04462100
Rh	1.16204900	-0.76905000	0.06740200
O	0.46440200	-1.65243300	-1.64633100
O	4.07511100	-0.98526900	1.25940900
O	2.62452600	-3.42242100	0.75857100
O	1.93550100	0.94851600	-0.89755600
C	3.14594000	1.78972300	-2.87073800
H	2.18905300	2.00824400	-3.35317500
H	3.53893400	2.72441100	-2.46364000
H	3.84730100	1.37836900	-3.59533600
C	0.52150100	-3.18025300	-3.44866600
H	1.26714400	-3.54069100	-4.15861200
H	-0.03631000	-4.03798300	-3.05809400
H	-0.19100600	-2.50858700	-3.93066400
C	0.99397100	-4.51147200	2.10788300
H	1.58824500	-5.40211500	1.90143900
H	1.12979500	-4.22990500	3.15751900
H	-0.06814000	-4.70349200	1.94544400
C	3.89096300	0.25019000	3.28339400
H	3.63829000	-0.43838100	4.09671200
H	4.97714300	0.32036900	3.21262700
H	3.44961000	1.22044300	3.52106800
Br	-8.21837500	-0.63344500	-0.12032500
O	-1.32870700	0.42435300	-2.02399800
C	-4.49844700	0.61890200	-1.53210900
H	-3.93490200	0.54892900	-2.45747900
O	-2.21226100	-0.70596700	1.41673700
C	-5.76781600	0.05085200	-1.44764800

H	-6.20773900	-0.44941300	-2.30276200
O	-0.76415500	0.51168100	2.66007000
C	-6.46812500	0.13491500	-0.24488400
C	-5.91753400	0.76796900	0.86712400
H	-6.47361500	0.81854400	1.79636200
C	-4.64352900	1.32723400	0.77220500
H	-4.19857900	1.81296300	1.63182200
C	-3.92954200	1.26035200	-0.42602400
C	-2.54900600	1.86578800	-0.55661000
C	-1.46311700	0.79234600	-0.87483600
C	-0.52490300	0.55622600	0.29459300
C	-1.27127800	0.06636300	1.47874100
C	-1.35711800	-0.07723300	3.82397500
H	-1.19720900	-1.15916800	3.82810100
H	-2.43276200	0.11815700	3.85390600
H	-0.85904800	0.38610000	4.67668700
C	1.14724300	2.22370500	-0.69061700
C	0.17466200	1.92672900	0.46913700
H	0.60037000	2.37828400	-1.62487700
H	0.75103800	1.88573900	1.39259000
C	-0.88302700	3.08299300	0.57271500
H	-0.73879000	3.64672300	1.49526700
H	-0.78757600	3.78989000	-0.26957700
O	-2.20859200	2.58051700	0.62310800
H	-2.53515300	2.55096100	-1.42284500
C	2.08013000	3.36433700	-0.38735300
C	1.97631500	4.57114900	-1.08742500
C	3.03434200	3.23522500	0.63253400
C	2.81589500	5.64181300	-0.77193600
H	1.24030600	4.67290900	-1.88094500
C	3.88274900	4.29845600	0.93380700
H	3.10073700	2.30110100	1.18025900
C	3.77362900	5.50439600	0.23407100
H	2.72641000	6.57659900	-1.31689200
H	4.62506500	4.18914400	1.71872500
H	4.43301300	6.33314300	0.47351400

1-int5

O 1

Rh	2.29820200	-2.49497700	-0.46588200
C	4.76648900	-1.01786900	-0.76628400
O	4.27353600	-2.18216700	-0.91493300
C	2.84529800	-1.92706700	2.31666500
O	2.62006800	-0.69857400	2.05641700

C	-0.33248900	-1.68393300	0.34468400
O	0.17974400	-0.53151100	0.54149900
C	1.50383200	-0.77074400	-2.63042800
O	1.73700000	-1.99592000	-2.37104600
Rh	2.14794700	-0.18573700	0.12827900
O	1.67655900	0.20274600	-1.82614700
O	2.80715600	-2.88687800	1.48078000
O	0.31804900	-2.71726200	-0.02394000
O	4.14320100	0.00879900	-0.33621800
C	6.20874000	-0.82362600	-1.16554200
H	6.23886600	-0.47804100	-2.20450400
H	6.67428700	-0.06117500	-0.53866500
H	6.75194600	-1.76698000	-1.09812900
C	0.93742900	-0.43403700	-3.98406500
H	1.06674600	-1.26516900	-4.67754700
H	-0.12892200	-0.22840600	-3.84539200
H	1.40841800	0.47192500	-4.37217500
C	-1.81833300	-1.81502900	0.53378900
H	-2.09409000	-2.85829500	0.68965400
H	-2.15197400	-1.18115300	1.35561600
H	-2.30584500	-1.44529300	-0.37408200
C	3.15258400	-2.28190900	3.75078900
H	2.23012300	-2.62554500	4.23113800
H	3.87492600	-3.09927800	3.78732100
H	3.52594000	-1.40955100	4.28840800
Br	-6.98135300	-2.26628800	0.80440500
O	-1.36637800	0.61228500	-1.74202200
C	-4.48669600	-0.11075400	-1.74805200
H	-4.03576200	-0.25995500	-2.72441400
O	-2.03779800	1.21387400	1.63303800
C	-5.30335100	-1.10459900	-1.21011400
H	-5.50422500	-2.01544400	-1.76225700
O	0.07881300	1.97243000	1.84996400
C	-5.86290800	-0.90853100	0.05231300
C	-5.62022200	0.25754900	0.77643900
H	-6.05805900	0.38984400	1.75896300
C	-4.79539900	1.23967400	0.23066000
H	-4.57361600	2.13879100	0.79085000
C	-4.22780200	1.06394900	-1.03392800
C	-3.24910200	2.07987700	-1.58649700
C	-1.82406100	1.60144300	-1.20917000
C	-1.07500300	2.42594000	-0.17822400
C	-1.06473700	1.78749200	1.18338200
C	0.16748500	1.32800200	3.13520200

H	0.12317200	0.24675200	2.99628600
H	-0.64616200	1.65772000	3.78585300
H	1.13824000	1.61918800	3.53268100
C	-0.02690300	3.40469800	-0.72034700
C	-1.36133400	3.91937500	-0.25391500
H	0.08112700	3.32402500	-1.80165700
H	-1.39622200	4.43459600	0.70137800
C	-2.46330500	4.27769400	-1.23590000
H	-2.86336500	5.27441500	-1.03720800
H	-2.08889500	4.26520000	-2.27270800
O	-3.56039600	3.37381200	-1.09742300
H	-3.28340200	2.07064700	-2.68935600
C	1.26984800	3.68037900	-0.02437500
C	2.40594700	2.96014600	-0.42503700
C	1.39304500	4.60809200	1.01362900
C	3.62357400	3.12052600	0.24037700
H	2.33097900	2.27477800	-1.26183100
C	2.61366000	4.78235200	1.66878800
H	0.53423200	5.19378800	1.32574900
C	3.72854600	4.02937000	1.29598600
H	4.47303100	2.51806000	-0.06253600
H	2.69044100	5.50642200	2.47527400
H	4.67329100	4.15651800	1.81658400

1-TS1(2-TS1)

O 1

Rh	0.63629500	0.40872900	-0.00549500
C	0.59461000	2.11247200	2.35538800
O	-0.01937900	1.12849200	1.80895800
C	-0.19900800	2.91354100	-1.21676500
O	0.93028300	3.39977800	-0.90175900
C	2.39656000	0.52708500	-2.33120200
O	2.94749400	1.54696000	-1.81738100
C	3.17842400	-0.31681900	1.19645400
O	2.00450800	-0.77626300	0.97137200
Rh	2.30730500	2.18932800	0.02034100
O	3.58727300	0.85042200	0.92876900
O	-0.60332200	1.72436300	-0.98121300
O	1.45803400	-0.16562500	-1.80802900
O	1.57489500	2.74161300	1.86314200
C	0.09137700	2.52841200	3.71672900
H	0.29247200	1.72383000	4.43091200
H	0.58547100	3.44292900	4.04418200
H	-0.99171600	2.67197500	3.68109200

C	4.14730000	-1.28626500	1.83016800
H	4.26292800	-2.14731900	1.16597500
H	5.11161900	-0.80993200	2.00495400
H	3.72993700	-1.65022300	2.77356800
C	2.88040600	0.06906500	-3.68583800
H	3.29268400	-0.94029800	-3.60168900
H	2.03056700	0.01740700	-4.37185300
H	3.63888300	0.75037500	-4.07094100
C	-1.15899100	3.80540900	-1.96725000
H	-1.04490400	3.61535600	-3.03974400
H	-2.18803400	3.56830300	-1.69101800
H	-0.93349500	4.85455300	-1.77236800
Br	-6.93097700	-0.00552000	-0.01780800
O	-0.76165400	-2.08342900	-2.13063200
N	-0.65476400	-1.71184000	1.64274500
C	-3.23237000	-1.83286900	-0.56006000
H	-2.87501300	-2.76370200	-0.98315300
O	0.71564400	-3.83726900	1.48516300
N	-0.63963000	-1.48944100	2.73069500
C	-4.59718300	-1.57141500	-0.56154300
H	-5.29755800	-2.29211800	-0.96714800
O	2.64165500	-4.10387700	0.32191700
N	1.60878100	-3.17396200	-1.82972200
C	-5.05887800	-0.36675400	-0.02648200
N	2.21317700	-3.29757100	-2.77568200
C	-4.17632900	0.57359500	0.50510500
H	-4.55302200	1.50193800	0.91876500
C	-2.81095000	0.30664300	0.49258800
H	-2.11930300	1.02840700	0.90520600
C	-2.31597200	-0.89558800	-0.04413700
C	-0.85566400	-1.16118400	-0.02519200
C	-0.32137300	-2.17210100	-0.98629000
C	0.87818700	-3.01012900	-0.73916400
C	1.36990700	-3.66125200	0.47581200
C	3.15697500	-4.86578100	1.42963400
H	2.52975800	-5.74044900	1.61903700
H	3.19181500	-4.25001700	2.33128900
H	4.16052900	-5.16839600	1.13169600

1-TS1'

O 1

Rh	1.40737000	0.05042000	0.18466700
C	-0.29115200	-2.23702100	0.73702300
O	-0.20503600	-0.97596100	0.94207000

C	3.11574900	-1.43046800	2.02383500
O	3.20945900	-2.34008700	1.14857100
C	3.93669600	0.19628400	-1.23644600
O	3.87912500	-1.06130900	-1.38014000
C	0.55879000	-0.69902300	-2.50783300
O	0.43774900	0.21139100	-1.61758300
Rh	2.25243500	-2.08553400	-0.64664800
O	1.26173300	-1.74796800	-2.40715100
O	2.45326900	-0.34111400	1.90252400
O	3.08078700	0.93011200	-0.63151400
O	0.55688900	-2.95524600	0.12770400
C	-1.53535300	-2.90697100	1.26812900
H	-2.40297000	-2.53108200	0.71716000
H	-1.46495700	-3.98860600	1.15571400
H	-1.67319300	-2.64082800	2.31953300
C	-0.24277500	-0.50360600	-3.77063400
H	-1.25337400	-0.89212400	-3.60333800
H	-0.32265700	0.55871800	-4.00653200
H	0.21032100	-1.05765600	-4.59346100
C	5.11175900	0.92222400	-1.84752700
H	4.76227500	1.48748300	-2.71760500
H	5.52088000	1.63587500	-1.12819800
H	5.87814900	0.21344700	-2.16102600
C	3.85090000	-1.61356900	3.32844300
H	4.65486600	-0.87355500	3.39053100
H	3.16928100	-1.42942600	4.16256500
H	4.27070900	-2.61729800	3.39174100
Br	-7.37964600	-0.78382600	0.15584500
O	-1.29497800	1.76282800	2.14887000
N	-1.42680100	2.23990000	-1.34164200
C	-3.39633600	0.21707900	0.89683700
H	-2.61751500	-0.10766600	1.57248700
O	0.96819700	3.50273700	-0.88965500
N	-1.25525800	2.60257100	-2.40216700
C	-4.65471300	-0.37435600	0.95691300
H	-4.85515400	-1.15520900	1.68203200
O	2.43007700	3.44794500	0.84017300
N	1.13142500	2.05132900	2.60084900
C	-5.65538500	0.03572000	0.07532200
N	1.67185300	1.69237600	3.49864900
C	-5.41029800	1.03546400	-0.86300100
H	-6.19315400	1.35223500	-1.54246800
C	-4.15056000	1.62976000	-0.91208800
H	-3.97432600	2.41497400	-1.64172000

C	-3.12625100	1.23183300	-0.03859800
C	-1.76798100	1.82235500	-0.13794700
C	-0.85407800	1.88516600	1.00941000
C	0.64027600	1.88562300	0.78219700
C	1.34232800	3.04923000	0.17476800
C	3.26244900	4.39221700	0.13597800
H	2.69056600	5.28192700	-0.13700000
H	3.66212000	3.92147200	-0.76503700
H	4.06342000	4.64386400	0.82973900

1-TS1-h

O 1

Rh	1.69111600	-0.40035200	-0.19338400
C	1.33440900	-1.01311800	2.63540000
O	0.94795800	-0.22138900	1.71331000
C	4.33225200	0.22895800	0.85697300
O	4.49184800	-1.00392800	1.10983000
C	3.33655100	-1.74802600	-2.17394600
O	3.71584000	-2.53086600	-1.25587700
C	0.32834100	-2.96211000	-0.36242200
O	0.16662300	-1.71963600	-0.62778200
Rh	2.97014200	-2.30589900	0.65403000
O	1.35734400	-3.48773000	0.15484600
O	3.31164800	0.76497300	0.30803600
O	2.51756200	-0.77048000	-2.04270900
O	2.15161400	-1.97547100	2.50593000
C	0.76002000	-0.74355200	4.00564800
H	-0.32569900	-0.64177200	3.93213800
H	1.02616700	-1.53958700	4.70104900
H	1.15403400	0.21181900	4.36652900
C	-0.82577800	-3.86900200	-0.71912100
H	-1.74638000	-3.48897600	-0.26905500
H	-0.96759200	-3.86026000	-1.80423300
H	-0.63057100	-4.88667600	-0.38137300
C	3.88183000	-1.96639200	-3.56559900
H	3.05216200	-2.17396900	-4.24782200
H	4.37068300	-1.05186800	-3.91330000
H	4.58820200	-2.79625200	-3.57426600
C	5.43652300	1.17647300	1.26352100
H	5.56827900	1.94687600	0.50078100
H	5.14229300	1.67472500	2.19323100
H	6.36616600	0.63167300	1.43039800
Br	1.13527900	3.09942600	1.65323500
O	-5.60548300	1.08613100	2.04315200

N	-4.00509600	-0.99459800	-0.25506400
C	-2.73777900	1.63552900	1.90418100
H	-3.53760300	1.70435700	2.62758600
O	-6.07483700	-0.33882200	-1.89241000
N	-3.85538400	-1.93088100	-0.88180800
C	-1.54180600	2.31525600	2.10295800
H	-1.40350400	2.90953100	2.99913000
O	-8.15398900	-0.96323800	-1.22697500
N	-7.71092000	-0.30938000	1.21486500
C	-0.49811200	2.22581200	1.18471800
N	-8.58039800	-0.36431600	1.93383200
C	-0.63640700	1.47116400	0.00141500
C	-1.85371000	0.80407600	-0.18346400
H	-1.98199300	0.20929900	-1.07948200
C	-2.89789300	0.85535600	0.74858900
C	-4.13499600	0.08367100	0.49186400
C	-5.45927900	0.37302800	1.05231600
C	-6.65985200	-0.24387600	0.41146600
C	-6.89699200	-0.51163000	-1.01437700
C	-8.48706000	-1.21176000	-2.60610400
H	-7.82491100	-1.97191100	-3.02799800
H	-8.39486100	-0.29491800	-3.19373300
H	-9.51896300	-1.56131600	-2.59663100
C	0.53110100	1.27743300	-0.91250700
C	1.13520500	2.49243100	-1.55081100
C	2.44458700	2.44754400	-2.05694600
C	0.39232500	3.68058300	-1.67944300
C	3.00491300	3.57751400	-2.64919200
H	3.01420200	1.53261000	-1.97406400
C	0.95551400	4.80691800	-2.27020900
H	-0.62276100	3.71853000	-1.29712100
C	2.26657400	4.75823600	-2.75357100
H	4.02164600	3.53649300	-3.02896600
H	0.37542400	5.72101000	-2.35466100
H	2.70852700	5.63773300	-3.21336400
N	-0.09003600	0.51400400	-2.30276700
N	0.01380100	-0.08985800	-3.23332300

1-TS2

O 1

Rh	-0.68553200	-0.75193600	0.08936600
C	0.31190000	-2.43503900	-2.04781400
O	0.70451200	-1.61367900	-1.15092800
C	-1.53966800	0.77354500	-2.26708200

O	-2.28097900	-0.20313000	-2.57914000
C	-3.44540500	-0.17893300	0.85731900
O	-3.81863500	-0.82390600	-0.17047100
C	-1.60422900	-3.34716000	1.01082700
O	-0.71217700	-2.45887500	1.23163200
Rh	-2.39813300	-1.79414900	-1.28360800
O	-2.44641900	-3.33425600	0.06160400
O	-0.83482400	0.86695800	-1.20075100
O	-2.23463000	0.00359800	1.22573000
O	-0.89250200	-2.72400900	-2.32206400
C	1.40018500	-3.13534100	-2.82231700
H	1.86874200	-3.87066600	-2.16146100
H	0.98908300	-3.63667200	-3.69836000
H	2.16548000	-2.41146800	-3.11154300
C	-1.64824600	-4.50137300	1.98041400
H	-0.66255700	-4.96978500	2.03666700
H	-1.88294200	-4.11726800	2.97749600
H	-2.39785100	-5.23037200	1.67332200
C	-4.50529600	0.44690000	1.72769500
H	-4.31594200	0.18648300	2.77197500
H	-4.43922400	1.53440200	1.63590100
H	-5.49610900	0.11115300	1.42184800
C	-1.48373400	1.95527700	-3.20440100
H	-0.44089600	2.19611800	-3.42786000
H	-2.02766100	1.74017700	-4.12398100
H	-1.92453500	2.82624700	-2.70960400
Br	5.70178700	3.54101400	-0.94579100
O	1.15374900	-1.31379300	3.33775100
C	3.35140200	1.19895500	1.56583000
H	3.42837200	0.79149400	2.57022900
O	3.67026700	-1.23857800	-0.23065800
C	4.38963100	1.97214000	1.06068400
H	5.27645100	2.16734300	1.65244000
O	3.46722500	-3.48686500	-0.04707700
N	2.08995400	-3.36535500	2.06008500
C	4.27649800	2.48801900	-0.23164300
N	1.88493300	-4.34792400	2.57881600
C	3.14281400	2.25355900	-1.00596700
H	3.07329000	2.66591900	-2.00605000
C	2.10426400	1.48334400	-0.48471200
H	1.22251600	1.29415100	-1.08082600
C	2.20195700	0.93762000	0.79868400
C	1.13217000	0.11447500	1.41689400
C	1.53687800	-1.11058600	2.19645000

C	2.29330500	-2.18943300	1.48880200
C	3.18679400	-2.20213900	0.31943100
C	4.51422300	-3.61622600	-1.02437600
H	5.44854300	-3.19658400	-0.64142000
H	4.24898300	-3.09885500	-1.94837800
H	4.61902700	-4.68703700	-1.19929700
C	-1.83994100	3.57191700	1.84041000
C	-0.75401900	2.88377100	1.46022300
H	-1.91392200	3.90314800	2.87710400
H	-0.63475500	2.56433000	0.42817000
C	0.32508200	2.46632600	2.40539800
H	1.31293800	2.80997000	2.08503000
H	0.13880500	2.82995400	3.41972300
O	0.36489600	1.01536800	2.57741600
H	-0.12816000	0.44452600	1.60591800
C	-2.97359800	3.92639400	0.97388500
C	-3.82673600	4.98605800	1.32317200
C	-3.25948000	3.19639900	-0.19588900
C	-4.91197500	5.32675500	0.51506700
H	-3.63122100	5.55031700	2.23170900
C	-4.34519900	3.53298500	-1.00000400
H	-2.64125700	2.34225400	-0.44228500
C	-5.17382400	4.60453000	-0.65076100
H	-5.55641400	6.15385600	0.79891700
H	-4.55554400	2.94683500	-1.89044000
H	-6.02345200	4.86420000	-1.27531800

1-TS3

O 1

Rh	1.68762900	2.85486700	0.10271000
C	2.11348600	1.14869400	-2.19111600
O	2.61118300	2.14543600	-1.58569000
C	-0.61943500	3.49801000	-1.48580400
O	-1.03437700	2.31413900	-1.23663300
C	-0.34290500	2.75683000	2.16906800
O	-0.80788100	1.70894700	1.60193000
C	2.41933100	0.49046000	1.56321500
O	2.83766100	1.65870700	1.29012000
Rh	0.09825000	1.01160100	-0.11090300
O	1.37413900	-0.06375300	1.08340300
O	0.46612900	4.00509100	-1.07640000
O	0.64469200	3.44720000	1.77775200
O	1.08916000	0.47686000	-1.82918800
C	2.81026100	0.69298100	-3.45115400

H	3.64336500	0.04078900	-3.17145300
H	2.12329900	0.13590200	-4.08959200
H	3.21908700	1.55424200	-3.98207700
C	3.23240900	-0.31023900	2.54936400
H	3.51592600	0.33475400	3.38433900
H	2.66548900	-1.17185300	2.89912700
H	4.14979700	-0.65640800	2.06541500
C	-1.03752500	3.18088500	3.44201300
H	-0.71735000	2.51861900	4.25341900
H	-0.77380500	4.20758700	3.69673900
H	-2.11892600	3.07595500	3.32957100
C	-1.52270500	4.34480500	-2.34927500
H	-2.51297100	4.40345800	-1.88907000
H	-1.10548800	5.34381700	-2.47454300
H	-1.64183800	3.86307500	-3.32410900
Br	5.62699100	-2.68914600	0.54336200
O	-1.55469600	-1.24546100	-2.49065700
C	2.10459500	-2.33247200	-1.65551800
H	1.82560600	-1.99734100	-2.64879500
O	-0.95871600	-1.83278500	1.73008300
C	3.44295400	-2.29321300	-1.27176800
H	4.20891100	-1.94351700	-1.95421000
O	-2.80788000	-0.53002000	1.56392700
N	-2.81474100	0.24876500	-0.84124100
C	3.78954000	-2.73600100	0.00333500
N	-3.43598700	1.10440600	-1.16687400
C	2.82656900	-3.21253500	0.88916800
H	3.11636300	-3.56029700	1.87396700
C	1.48835000	-3.22641700	0.49913600
H	0.72524000	-3.57077800	1.18300400
C	1.11929000	-2.78827200	-0.77408400
C	-0.31253800	-2.87209200	-1.25595000
C	-1.08908900	-1.51949300	-1.39601400
C	-1.26334600	-0.59147000	-0.24058600
C	-1.67108100	-1.07381900	1.10775300
C	-3.10154400	-0.77855000	2.94930000
H	-2.37983300	-0.25026900	3.57729400
H	-3.06061800	-1.84842800	3.16746600
H	-4.10862600	-0.39323600	3.10139700
C	-4.29988500	-2.64135500	-0.93931000
C	-3.40321100	-3.38799400	-0.27729800
H	-4.21313700	-2.58538800	-2.02443900
H	-3.40807500	-3.44026600	0.80925500
C	-2.31492700	-4.18138300	-0.93854800

H	-2.40921300	-5.24391400	-0.68329900
H	-2.36769700	-4.08912000	-2.03201100
O	-1.01917200	-3.79579600	-0.45425100
H	-0.30505100	-3.21163500	-2.30332600
C	-5.38227200	-1.83798300	-0.35481300
C	-6.07147600	-0.92697900	-1.17344000
C	-5.75104300	-1.92077300	1.00089500
C	-7.07386600	-0.10745500	-0.65556800
H	-5.80544200	-0.85390400	-2.22500100
C	-6.75265700	-1.10535700	1.51887500
H	-5.25656100	-2.63486300	1.65160000
C	-7.41626600	-0.19015900	0.69478800
H	-7.58666200	0.59421400	-1.30687800
H	-7.02558100	-1.18877700	2.56733400
H	-8.19834100	0.44402800	1.10148300

1-TS4

O 1

Rh	2.86331000	-2.11084200	-0.73420400
C	0.33464100	-2.27675900	-2.08909600
O	1.49623300	-2.78967300	-2.09859200
C	2.80497000	0.44220000	-2.10754900
O	1.85743200	0.79810100	-1.32809000
C	3.71647700	-0.46085000	1.50013400
O	2.56689200	0.10481400	1.47466100
C	1.23048100	-3.12513300	1.41651200
O	2.17143300	-3.47205200	0.64204400
Rh	1.16919400	-0.52507800	0.07827900
O	0.64072800	-1.99296000	1.43433800
O	3.43119600	-0.65971800	-2.07668800
O	4.13137900	-1.35260600	0.70693700
O	-0.07847000	-1.35327600	-1.31309800
C	-0.67577600	-2.78897800	-3.08700600
H	-1.56014200	-3.14594300	-2.55221000
H	-0.99313600	-1.96210700	-3.72862400
H	-0.24756200	-3.59071700	-3.68869000
C	0.74620800	-4.13044100	2.43597900
H	1.25291600	-5.08626500	2.30307400
H	0.94238900	-3.74549700	3.44159700
H	-0.33519000	-4.25485700	2.33408200
C	4.65076300	-0.00458300	2.59899800
H	5.62451400	-0.48301300	2.49563100
H	4.76322900	1.08337000	2.57027000
H	4.21383900	-0.26034200	3.56901500

C	3.23847300	1.45276300	-3.14292700
H	4.08527000	2.01996300	-2.74537700
H	3.56199200	0.93771500	-4.04893000
H	2.42729800	2.14878300	-3.35874100
Br	-7.95207500	-0.58757400	-0.77140500
O	-1.20797500	1.29162800	-1.50283000
C	-4.30573000	1.38851900	-1.21608800
H	-3.71175600	1.78194900	-2.03453000
O	-1.98133700	-0.67155100	1.68635900
C	-5.52726200	0.77237800	-1.48136600
H	-5.90007700	0.69914400	-2.49648400
O	-0.43186800	0.27205800	3.04511000
C	-6.26679500	0.25081000	-0.42079700
C	-5.80045100	0.32961400	0.88959600
H	-6.38370500	-0.08889000	1.70167600
C	-4.57366400	0.94264200	1.14213300
H	-4.19119300	0.99183400	2.15333700
C	-3.82247600	1.47956200	0.09427100
C	-2.48277800	2.14504000	0.34221200
C	-1.32726800	1.32127100	-0.29758800
C	-0.35494700	0.69668000	0.68254100
C	-1.03338600	0.07266700	1.85695200
C	-0.93258000	-0.55140200	4.11198500
H	-0.78120600	-1.60432600	3.86479200
H	-1.99772700	-0.36676800	4.27569200
H	-0.35467500	-0.27320700	4.99345900
C	0.72230400	3.31437300	0.37266000
C	0.21706800	2.54046400	1.42080500
H	-0.01675400	3.88575500	-0.19096200
H	0.92039600	2.07171100	2.10266900
C	-1.10163800	3.05439800	2.04354500
H	-1.00983200	3.00671200	3.12996300
H	-1.25285500	4.10533200	1.75361800
O	-2.27677100	2.31825900	1.73363600
H	-2.46857600	3.12281200	-0.16955200
C	2.07034700	3.52109600	-0.06122800
C	2.29770600	4.40693800	-1.14192500
C	3.18437000	2.93891500	0.58589400
C	3.58880400	4.70234700	-1.55844300
H	1.44699900	4.85698100	-1.64635700
C	4.47164900	3.22852400	0.15828500
H	3.01705400	2.23770000	1.39129200
C	4.67955200	4.11303700	-0.90932500
H	3.75086900	5.38413300	-2.38729700

H	5.32169400	2.76796300	0.65242000
H	5.69051200	4.34079300	-1.23428700

2a

0 1

C	0.82771700	-0.61610700	0.18333900
C	1.88019900	0.21214700	0.22008300
H	1.02308400	-1.68829200	0.22507000
H	1.75493300	1.29079800	0.15114600
C	3.29842300	-0.24265000	0.36965100
H	3.66946600	0.05645000	1.36652000
H	3.35086300	-1.34274900	0.32256000
O	4.07763500	0.37074500	-0.65809800
H	5.00867800	0.21110800	-0.45693200
C	-0.59346200	-0.25255900	0.08513700
C	-1.54729000	-1.27420100	-0.06552500
C	-1.05386100	1.07671400	0.13499900
C	-2.90671400	-0.98463400	-0.17235500
H	-1.21318800	-2.30815600	-0.10290900
C	-2.41023500	1.36720100	0.02686400
H	-0.34600300	1.88911500	0.26557000
C	-3.34491200	0.33890200	-0.12800600
H	-3.62264500	-1.79304000	-0.28980400
H	-2.74246300	2.40065300	0.06789000
H	-4.40300100	0.56927300	-0.20944900

2-int2

0 1

Rh	-0.72898500	-0.12532700	-0.07623000
C	0.21212700	-1.81703200	2.08484700
O	0.46169200	-0.71336000	1.49334500
C	0.18079300	-2.43191100	-1.56161600
O	-0.74593300	-3.10508800	-1.01283000
C	-2.99189700	-0.48738500	-1.87582300
O	-3.21588300	-1.59509800	-1.30075000
C	-2.97955800	0.16022500	1.75802200
O	-2.00926400	0.83101900	1.25538900
Rh	-2.02710500	-2.15911500	0.28281200
O	-3.23139000	-1.06071900	1.55355100
O	0.42335200	-1.19149700	-1.38022900
O	-2.06922200	0.34544200	-1.57984500
O	-0.74889900	-2.60625300	1.83110800
C	1.18157700	-2.23113900	3.16713800
H	0.68051500	-2.85898400	3.90542700

H	1.98591900	-2.81400000	2.70576400
H	1.62615900	-1.35261800	3.63749000
C	-3.88499300	0.90663200	2.71401200
H	-3.98132600	1.95151800	2.41071100
H	-4.86444500	0.42926900	2.75713700
H	-3.44399700	0.87751100	3.71668300
C	-3.87679000	-0.10730400	-3.04042600
H	-4.16272300	0.94468600	-2.96398500
H	-3.30609600	-0.22672600	-3.96698800
H	-4.76151900	-0.74322400	-3.07534400
C	1.08410900	-3.14320100	-2.54042500
H	2.12325100	-2.86800700	-2.34533500
H	0.95034000	-4.22283900	-2.47038600
H	0.83701400	-2.81175300	-3.55414400
Br	6.47301200	-0.18575800	0.01620200
O	0.15292800	2.10059800	-2.67201300
C	2.67795700	0.85196800	-1.38121400
H	2.15145400	0.83382500	-2.32673100
O	0.17602000	2.51774900	0.84953900
C	3.99790100	0.41517300	-1.31036400
H	4.50755500	0.06957900	-2.20272100
O	-1.53024600	3.90223800	1.40673400
N	-2.13169500	3.65480100	-1.49236400
C	4.66061800	0.42361200	-0.08365400
N	-2.98656800	3.97303500	-2.16078400
C	4.02109600	0.86701100	1.07249100
H	4.54580000	0.86598800	2.02128700
C	2.70000500	1.30006900	0.99684800
H	2.19092700	1.61484600	1.89981100
C	2.01303800	1.30287400	-0.22739000
C	0.59289900	1.67896300	-0.30294600
C	-0.02681300	2.28951300	-1.48549800
C	-1.07396300	3.20726800	-0.86670700
C	-0.84377500	3.24181000	0.51845700
C	-1.23576700	3.60383800	2.80386200
H	-0.22350900	3.93441500	3.04510600
H	-1.34135400	2.52876300	2.95589900
H	-1.97411500	4.16812400	3.36942300

2-int3

0 1

Br	-6.47306900	-0.18578100	0.01617700
O	-0.15296200	2.10050500	-2.67203400
C	-2.67801500	0.85198500	-1.38123600

H	-2.15151800	0.83371500	-2.32674900
O	-0.17607300	2.51769900	0.84953000
C	-3.99793200	0.41508800	-1.31034700
H	-4.50757500	0.06945400	-2.20269600
O	1.53016700	3.90222400	1.40668500
N	2.13168500	3.65469600	-1.49236500
C	-4.66067400	0.42355200	-0.08365100
N	2.98655800	3.97294700	-2.16077800
C	-4.02116800	0.86703800	1.07247200
H	-4.54587700	0.86604500	2.02126600
C	-2.70008800	1.30013900	0.99682900
H	-2.19103300	1.61489300	1.89981000
C	-2.01310900	1.30290200	-0.22740600
C	-0.59290300	1.67879600	-0.30294900
C	0.02678600	2.28941200	-1.48552300
C	1.07393700	3.20717000	-0.86673600
C	0.84373300	3.24173600	0.51843000
C	1.23563100	3.60391900	2.80382500
H	1.34140900	2.52887900	2.95598300
H	0.22329300	3.93433200	3.04495100
H	1.97382900	4.16840400	3.36938200
Rh	0.72902600	-0.12528900	-0.07626900
C	-0.18077900	-2.43199100	-1.56146800
O	-0.42310900	-1.19148800	-1.38037100
C	-0.21206700	-1.81695300	2.08488700
O	0.74905900	-2.60610000	1.83131200
C	2.97964200	0.16038700	1.75788600
O	3.23152800	-1.06054600	1.55340400
C	2.99193000	-0.48736700	-1.87582700
O	2.06940600	0.34559000	-1.57972700
Rh	2.02714800	-2.15908400	0.28288200
O	3.21578000	-1.59514500	-1.30082800
O	-0.46174200	-0.71339500	1.49321500
O	2.00919600	0.83108900	1.25543000
O	0.74582500	-3.10519600	-1.01252500
C	-1.08430400	-3.14336600	-2.54004300
H	-2.12339900	-2.86819600	-2.34464300
H	-0.83750400	-2.81200600	-3.55385800
H	-0.95050300	-4.22299500	-2.46992500
C	3.87665800	-0.10754500	-3.04063800
H	4.16162400	0.94476800	-2.96525000
H	4.76188600	-0.74280400	-3.07492700
H	3.30615800	-0.22843600	-3.96714400
C	3.88523100	0.90681100	2.71372000

H	4.86527600	0.43050700	2.75523000
H	3.98002900	1.95215100	2.41154300
H	3.44543600	0.87590400	3.71686800
C	-1.18149600	-2.23100100	3.16722200
H	-1.62631600	-1.35246100	3.63731100
H	-1.98566200	-2.81419000	2.70595900
H	-0.68032600	-2.85852900	3.90571000

2-TS2

O 1

Rh	-0.74385400	-0.19434800	-0.11652600
C	-0.94628800	-1.41480400	2.53428800
O	-0.27786700	-0.54859100	1.87203000
C	0.02910700	-2.92636200	-0.71095700
O	-1.15121600	-3.28607300	-0.41734700
C	-2.35089900	-0.69777300	-2.48564700
O	-3.00986600	-1.55105900	-1.81814400
C	-3.32792900	0.86062400	0.74660900
O	-2.12783700	1.22268600	0.48189000
Rh	-2.52292700	-1.86717500	0.15190100
O	-3.77881700	-0.31829300	0.70885800
O	0.49028600	-1.73495200	-0.67725900
O	-1.38946200	0.02362200	-2.05251000
O	-1.92806900	-2.09173700	2.11007700
C	-0.48801400	-1.66472300	3.95352500
H	-1.29793400	-2.09460300	4.54400000
H	0.34399600	-2.37694800	3.93199100
H	-0.12674000	-0.73843900	4.40476000
C	-4.29296300	1.96657700	1.11195700
H	-3.75389400	2.86479300	1.41790000
H	-4.90271600	2.20359700	0.23372800
H	-4.96556400	1.62927600	1.90296900
C	-2.70178400	-0.52353300	-3.94440500
H	-2.59899800	0.52424600	-4.23296100
H	-1.99393400	-1.10537200	-4.54412900
H	-3.71170000	-0.88624100	-4.13884100
C	0.99330500	-3.99372500	-1.17290600
H	1.99432900	-3.78436300	-0.79037800
H	0.65201500	-4.97898900	-0.85363300
H	1.04145800	-3.97214000	-2.26673700
Br	6.70778900	-0.49469300	0.10112200
O	0.54250800	2.19379000	-2.54342600
C	3.17611400	1.31532000	-1.16200100
H	2.87731500	1.97514900	-1.96788800

O	0.49095500	2.28670100	1.20129200
C	4.50428900	0.90930500	-1.07160700
H	5.23908300	1.26257300	-1.78590400
O	-1.00461400	3.94670400	1.59470500
N	-1.19657800	4.13818500	-1.23720400
C	4.88318900	0.04885600	-0.04121200
N	-1.86629900	4.80951400	-1.85554000
C	3.95332300	-0.42489600	0.88690300
H	4.26865400	-1.09330300	1.67999100
C	2.62241600	-0.04448300	0.76865700
H	1.88352700	-0.41320100	1.46895000
C	2.21279400	0.83921900	-0.25030600
C	0.80245700	1.21362200	-0.35988800
C	0.37684400	2.25500900	-1.33721000
C	-0.37938900	3.32102600	-0.62263300
C	-0.29078000	3.17545300	0.79727800
C	-0.97479600	3.58171500	2.99991300
H	0.03419000	3.70443100	3.39870100
H	-1.29398200	2.54307900	3.10763700
H	-1.67045200	4.26437200	3.48444200

2-TS3

O 1

Rh	2.69224400	-0.43127100	-0.14899100
C	3.76669400	-0.01250800	2.52198100
O	2.65919700	-0.06783400	1.89220800
C	4.16365000	2.03374000	-0.53912800
O	5.23931300	1.37725600	-0.34132300
C	4.03154900	-1.02363400	-2.63242900
O	5.13067100	-1.01114800	-1.98799000
C	3.63648600	-3.10550400	0.45596700
O	2.55652900	-2.44522700	0.27542900
Rh	5.08542000	-0.62916200	0.02471600
O	4.81291500	-2.63493500	0.40971100
O	2.98703900	1.54954200	-0.53469400
O	2.87215500	-0.83839200	-2.13786900
O	4.91958300	-0.21950400	2.02956000
C	3.70232100	0.36840300	3.98254800
H	4.54415200	-0.06197900	4.52673900
H	3.76488600	1.45936900	4.05752100
H	2.75346700	0.05191600	4.41962800
C	3.48770500	-4.58580300	0.71701600
H	2.53288200	-4.79108100	1.20497700
H	3.50555000	-5.11398800	-0.24239400

H	4.31923400	-4.94919500	1.32247800
C	4.10661400	-1.24774400	-4.12232200
H	3.16464300	-1.65614600	-4.49037200
H	4.27993100	-0.28235500	-4.60972400
H	4.94296500	-1.90622100	-4.36305600
C	4.28254000	3.50913200	-0.82924400
H	3.38626900	4.03191900	-0.49027000
H	5.17807300	3.91687500	-0.35794200
H	4.36950100	3.64591400	-1.91252600
Br	0.67248200	5.87570100	0.10513500
O	-0.24583900	-0.95139400	-2.41266600
C	0.01326100	1.96464900	-1.19901100
H	-0.16484500	1.45853600	-2.13962000
O	0.01244700	-0.99189600	1.13464500
C	0.16174400	3.34627300	-1.15971200
H	0.10279700	3.92749200	-2.07310200
O	-0.13076400	-3.13390200	1.85169300
N	-0.59020100	-3.62067500	-1.06179300
C	0.40277700	3.97726000	0.06012200
N	-0.83437600	-4.53383900	-1.68328800
C	0.47308900	3.24733700	1.24611000
H	0.65708700	3.75173200	2.18839000
C	0.31881500	1.86611700	1.20606800
H	0.39516100	1.28908400	2.11847700
C	0.10579500	1.20848800	-0.01586000
C	0.00877700	-0.23960300	-0.09622000
C	-0.19665100	-1.13912900	-1.20490500
C	-0.31945100	-2.48456300	-0.48449000
C	-0.15197100	-2.25879500	0.88705700
C	0.05600900	-2.59057800	3.19013800
H	-0.79795400	-1.95494300	3.43233200
H	0.98412300	-2.01539000	3.22004200
H	0.10236100	-3.46066600	3.84157700
Rh	-2.77875900	-0.28174300	-0.12968600
C	-3.66642500	1.83008300	1.63927300
O	-2.61539400	1.28457900	1.17052000
C	-3.90662600	-1.87836000	2.01790200
O	-5.04104000	-1.42868800	1.67394900
C	-4.30994100	-2.20863700	-1.66946600
O	-5.35990300	-1.65642900	-1.21010900
C	-4.04328800	1.48611500	-2.02304100
O	-2.90902500	1.00191100	-1.70405500
Rh	-5.16428400	-0.09592600	0.10624700
O	-5.15515800	1.21744300	-1.46073800

O	-2.78614400	-1.58589200	1.47583000
O	-3.10967500	-1.88614700	-1.38419600
O	-4.86335300	1.47145800	1.39458800
C	-3.46113400	2.98607500	2.58685800
H	-2.50201300	3.46510300	2.38429100
H	-4.28228900	3.69861400	2.49334300
H	-3.45507100	2.60513700	3.61387700
C	-4.05254500	2.48565400	-3.15192700
H	-3.38109500	2.15046400	-3.94516800
H	-5.06442600	2.62630000	-3.53263300
H	-3.67352500	3.44081800	-2.77369900
C	-4.48927300	-3.32874300	-2.66487900
H	-3.71853200	-4.08844300	-2.51873400
H	-5.48519000	-3.76409300	-2.57775900
H	-4.36728100	-2.91873100	-3.67294800
C	-3.86270400	-2.82210900	3.19712700
H	-3.03614600	-3.52685600	3.08688900
H	-3.70214100	-2.23789500	4.10995300
H	-4.81066600	-3.35275600	3.29325400

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O 1

Rh	-2.29198300	-0.78159500	-0.12989500
C	-3.47879100	-2.04596900	-2.44092500
O	-2.36480100	-1.88328100	-1.84369700
C	-3.98984000	-2.76203000	1.14865700
O	-4.99506700	-2.11922500	0.70534000
C	-3.50390900	0.77485100	1.99648000
O	-4.60929100	0.65074300	1.37911300
C	-3.01820800	1.59290300	-1.65372900
O	-1.99232100	0.94529000	-1.24856000
Rh	-4.65198100	-0.41505800	-0.37093200
O	-4.22846300	1.27458800	-1.44120200
O	-2.76975400	-2.43554200	0.98395100
O	-2.36966100	0.35613800	1.58809400
O	-4.59217100	-1.54028600	-2.08430000
C	-3.44982900	-2.90269200	-3.68108000
H	-4.45802500	-3.21129600	-3.95826500
H	-2.80790900	-3.76938600	-3.50432100
H	-3.01290400	-2.32355800	-4.50126200
C	-2.77721300	2.86452100	-2.43191400
H	-2.48189700	3.66243900	-1.74305000
H	-3.68893400	3.16166300	-2.95014600
H	-1.96290300	2.71764500	-3.14372200

C	-3.54616300	1.46821900	3.33637200
H	-3.99132800	2.46000500	3.22462500
H	-2.54607600	1.54544700	3.76262400
H	-4.18913900	0.89127000	4.00760500
C	-4.25565400	-4.03730800	1.90792200
H	-3.38737200	-4.30464900	2.51161300
H	-4.44294200	-4.83882900	1.18549000
H	-5.14655800	-3.92701500	2.52892600
Br	-0.42713100	-5.24697200	-1.93768700
O	0.57021500	0.52226900	2.36149000
C	0.19747700	-1.87136300	0.42836600
H	0.03255000	-1.60988200	1.46483100
O	1.21777000	1.32577600	-1.04579600
C	-0.14069800	-3.16218500	-0.00407200
H	-0.63750300	-3.83461500	0.67995000
O	0.15484100	3.26773200	-1.47473300
N	-0.81306100	2.95300200	1.28834500
C	0.13279700	-3.53013400	-1.30975600
N	-1.58330200	3.51077100	1.89697700
C	0.78261100	-2.65838700	-2.18825600
H	0.99315700	-2.96754500	-3.20584200
C	1.15840500	-1.39699600	-1.74376000
H	1.68672700	-0.72637500	-2.41200400
C	0.86326300	-0.98804200	-0.43290500
C	1.37764400	0.33493400	0.05575400
C	0.64500500	0.94873900	1.23162000
C	0.06357900	2.19639600	0.67814500
C	0.50060000	2.33028300	-0.65984400
C	0.87928500	3.34354900	-2.73932500
H	1.92965400	3.51059100	-2.49552300
H	0.73114700	2.42125100	-3.30317500
H	0.43865700	4.19348900	-3.25652300
C	2.75141000	-2.05026200	2.71139800
C	3.63706600	-1.78671200	1.73876500
H	2.57382400	-1.28294500	3.46423800
H	3.78463000	-2.48987800	0.91915700
C	4.40669400	-0.49980700	1.61106800
H	5.49091700	-0.71517500	1.66108900
H	4.18156200	0.14961800	2.47611900
O	4.09235300	0.11726700	0.38259600
H	2.51757400	0.27309700	0.25455800
C	1.89878600	-3.24458500	2.81780400
C	0.70746400	-3.16854900	3.56306700
C	2.18281400	-4.45112900	2.15114300

C	-0.18491600	-4.23998800	3.60915600
H	0.46902500	-2.24307100	4.08128700
C	1.29476600	-5.52321100	2.19939700
H	3.10751900	-4.54612300	1.59043600
C	0.10213700	-5.42305200	2.92357200
H	-1.10373300	-4.15014600	4.18263000
H	1.53150400	-6.44103700	1.66871100
H	-0.58828700	-6.26079700	2.95996200
C	8.03381200	1.54000100	-0.51876000
C	6.70189000	1.46739100	-0.64412800
H	8.48509400	2.52163200	-0.36475000
H	6.20241100	0.51196300	-0.79332500
C	5.76633700	2.64449600	-0.56417700
H	5.33156700	2.81694500	-1.57026800
H	6.33513700	3.55526400	-0.31546600
O	4.74520600	2.43479900	0.39144300
H	4.44354900	1.27657400	0.40522900
C	8.98644400	0.42018900	-0.58010100
C	10.36442000	0.69287100	-0.64418200
C	8.58392700	-0.92972600	-0.56835000
C	11.30507400	-0.33482700	-0.70879000
H	10.69773300	1.72809800	-0.64684400
C	9.52179700	-1.95618900	-0.63249300
H	7.52868700	-1.17484200	-0.49521900
C	10.88835000	-1.66646700	-0.70557500
H	12.36363300	-0.09446600	-0.76027200
H	9.18675800	-2.98998500	-0.61894000
H	11.61734200	-2.47040600	-0.75308900
C	0.36501400	5.81636100	0.92947400
C	1.36366900	5.54406200	0.07835400
H	0.53227100	5.62640400	1.99063900
H	1.24499900	5.74376300	-0.98503400
C	2.63909300	4.84261200	0.44412300
H	3.50769400	5.47150500	0.18044700
H	2.68323900	4.68418000	1.53456800
O	2.66672400	3.62103700	-0.26971000
H	3.54699700	3.11103400	-0.00088300
C	-0.98218600	6.29517000	0.58450300
C	-1.84419100	6.73172300	1.60625400
C	-1.48664300	6.25764000	-0.73104600
C	-3.15168700	7.13070000	1.32819400
H	-1.47976300	6.75565300	2.63006400
C	-2.79125200	6.65608900	-1.00979700
H	-0.85608300	5.89502200	-1.53631000

C	-3.63212200	7.09519900	0.01868000
H	-3.79598000	7.46514700	2.13613100
H	-3.15894200	6.61653700	-2.03146500
H	-4.65139900	7.39860000	-0.20028500

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Br	-5.72090700	3.50149000	0.13786400
O	1.01786100	2.36687700	-2.37407200
C	-1.84486000	2.74042900	-1.20734500
H	-1.34358300	2.63761800	-2.16148200
O	0.59588000	1.02583400	0.89025900
C	-3.20496800	3.04022300	-1.16244300
H	-3.77043600	3.17198800	-2.07829300
O	2.57468300	0.00743700	1.44995900
N	3.20589700	0.55251800	-1.36723700
C	-3.83804900	3.15440500	0.07456600
N	4.04450900	0.17784900	-2.03050200
C	-3.12945700	3.00721800	1.26562600
H	-3.63452800	3.10722500	2.21949300
C	-1.76893800	2.72182600	1.20874100
H	-1.20898100	2.58898400	2.12892500
C	-1.11681600	2.56149400	-0.02234600
C	0.31721400	2.21926700	-0.02477800
C	1.10195300	1.91110800	-1.24738600
C	2.17999900	1.01275300	-0.70877400
C	1.87055100	0.73609500	0.65164100
C	2.13963200	-0.03714900	2.84649500
H	1.22422700	-0.62558800	2.92103600
H	2.00181500	0.99245100	3.17868500
H	2.96138500	-0.52205200	3.36966300
Rh	-0.65483400	-1.03241000	0.29421700
C	-1.47204600	-0.79830000	-2.46418400
O	-0.85198900	-0.17513800	-1.53927600
C	-3.52397000	-0.91439000	0.63423100
O	-3.58546800	-2.04414200	0.04664900
C	-1.02289500	-3.16215000	2.21389900
O	-1.63892200	-3.79168500	1.29749100
C	1.02320400	-3.05728500	-0.92379500
O	1.08835000	-1.91256500	-0.36012100
Rh	-1.84299900	-2.92592100	-0.55200600
O	-0.03903600	-3.72258800	-1.13066200
O	-2.45365700	-0.27553400	0.90119800
O	-0.48518800	-2.00872300	2.09765400

O	-1.98805500	-1.95598600	-2.35558200
C	-1.62347400	-0.06889800	-3.77359800
H	-2.54352900	0.52415800	-3.73002400
H	-0.78384600	0.61366100	-3.91763500
H	-1.70656000	-0.77708600	-4.59903900
C	2.33305500	-3.66960400	-1.35552700
H	2.85808000	-4.04006700	-0.46893800
H	2.16110800	-4.49827000	-2.04247500
H	2.96374400	-2.90835100	-1.82055800
C	-0.94161900	-3.81663400	3.57103700
H	-1.09491800	-4.89268000	3.48505500
H	0.02134300	-3.59862800	4.03716500
H	-1.72796500	-3.39777900	4.20796200
C	-4.82303300	-0.25973100	1.02674400
H	-4.70954000	0.24447000	1.98805100
H	-5.07199600	0.50669800	0.28649500
H	-5.62575500	-0.99656800	1.06445700
C	5.34397700	2.40767700	0.04388800
C	4.54551700	2.69747000	1.08177700
H	5.08292500	2.82917600	-0.92833200
H	4.74257000	2.28448300	2.07003200
C	3.29658300	3.53470300	0.99419400
H	3.44088000	4.47286500	1.56113100
H	3.13449200	3.83500500	-0.05944200
O	2.20008000	2.83070300	1.51914000
H	1.17968100	2.90502300	0.70703200
C	6.53878900	1.55068900	0.04240300
C	7.13636600	1.21973500	-1.18705700
C	7.11028000	1.02311900	1.21625400
C	8.25313000	0.38665200	-1.24747000
H	6.71271700	1.61884500	-2.10501500
C	8.22447300	0.19135800	1.15701900
H	6.68499900	1.27486000	2.18292900
C	8.80193100	-0.13361000	-0.07499300
H	8.69426900	0.14583000	-2.21055400
H	8.65022600	-0.20197300	2.07607500
H	9.67308300	-0.78081700	-0.11699900

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O 1

Rh	-1.33385100	-1.45496800	-0.26672500
C	-3.17339600	-1.52610900	1.96563400
O	-2.66691900	-0.74163500	1.09931700
C	-3.41731300	-3.16764600	-1.33949600

O	-3.07251300	-4.04176400	-0.48072000
C	0.26066400	-3.56807800	-1.45068600
O	-0.21084600	-4.34442300	-0.55991000
C	0.53939100	-1.92912800	1.90320600
O	0.22802200	-1.04929100	1.03103000
Rh	-1.54648500	-3.59491100	0.80116300
O	-0.01218000	-3.06387800	2.04866200
O	-2.87816400	-2.02288100	-1.49394300
O	0.01163300	-2.32296500	-1.56498300
O	-2.89854700	-2.76339800	2.09526900
C	-4.16432400	-0.91484100	2.92321100
H	-4.78318700	-1.68877200	3.37826800
H	-4.77625700	-0.18046400	2.39450100
H	-3.61376000	-0.39137200	3.71212100
C	1.67379300	-1.58557900	2.83893900
H	2.59028200	-1.44872200	2.25879100
H	1.81451300	-2.37482000	3.57684600
H	1.45416800	-0.63872200	3.33991700
C	1.21568600	-4.17337100	-2.45149300
H	2.17163400	-4.38008100	-1.96000400
H	1.37446100	-3.49100600	-3.28693000
H	0.81600300	-5.12568300	-2.80686300
C	-4.58143100	-3.49392600	-2.24086100
H	-4.35743700	-3.18101700	-3.26302300
H	-5.45526200	-2.92790600	-1.90176000
H	-4.80760300	-4.55967400	-2.20426600
Br	-5.38313200	1.82583700	0.07300900
O	0.75534900	-0.05383100	-3.35467000
C	-1.81210600	0.85084800	-1.86182300
H	-1.52423700	0.33650900	-2.77129400
O	1.43089400	1.41498700	-0.17596600
C	-3.17251700	0.99541400	-1.54772600
H	-3.91954400	0.52266400	-2.17187700
O	3.27111500	0.36141300	0.63593900
N	3.14836800	-1.11401600	-1.86037900
C	-3.53634700	1.69172800	-0.40593800
N	3.80263400	-1.95533400	-2.24239200
C	-2.57835700	2.26957500	0.43037300
H	-2.87506800	2.82449600	1.31152000
C	-1.23652500	2.13984400	0.10946300
H	-0.49590900	2.60348400	0.74661200
C	-0.83374000	1.43521100	-1.03846400
C	0.60980000	1.44004200	-1.42067100
C	1.14785800	0.31632600	-2.27301500

C	2.33198900	-0.16006700	-1.50574400
C	2.41977900	0.59431600	-0.30770300
C	3.41660400	1.37747000	1.67858500
H	3.62652400	2.31880000	1.16994200
H	2.49976300	1.41772900	2.26848600
H	4.26143700	1.03396100	2.27113000
C	-0.41648400	5.41874900	-0.79101000
C	0.81859200	4.89952300	-0.86843500
H	-0.85018800	5.82982600	-1.70339600
H	1.28073800	4.42459800	-0.00198100
C	1.64284700	4.82949500	-2.13174100
H	2.57146600	5.41260700	-1.96995800
H	1.09811500	5.33881500	-2.94546300
O	1.94829100	3.50752900	-2.48424700
H	0.98446200	2.42796800	-1.95186700
C	-1.30079500	5.44089500	0.38309400
C	-2.67725000	5.66529800	0.20009700
C	-0.84425400	5.19980800	1.69313500
C	-3.56877100	5.61823100	1.27112200
H	-3.05165100	5.85311400	-0.80285300
C	-1.73324000	5.14738300	2.76450000
H	0.21780700	5.05836300	1.87139800
C	-3.10245100	5.35171200	2.56027600
H	-4.62907700	5.77645300	1.09690100
H	-1.35689800	4.95718900	3.76615800
H	-3.79341700	5.31233600	3.39718500
C	6.63915700	1.47954700	-0.05092400
C	5.71913900	1.39384000	-1.02158400
H	6.97872500	2.47165600	0.25016600
H	5.39795600	0.41144800	-1.36497800
C	4.97621700	2.56555500	-1.60344900
H	4.94607400	2.49007500	-2.70403000
H	5.51787200	3.49754300	-1.36333300
O	3.67540400	2.57142800	-1.06045500
H	2.93310900	3.04742800	-1.74268600
C	7.24758800	0.34954700	0.66962000
C	8.49657200	0.50848600	1.29527600
C	6.60362900	-0.89752700	0.78603400
C	9.09656400	-0.54533900	1.98322300
H	9.00326400	1.46808900	1.22834700
C	7.20249900	-1.95103900	1.47303600
H	5.61497400	-1.02768000	0.35681500
C	8.45427500	-1.78211700	2.07179000
H	10.06610700	-0.40080400	2.45159700

H	6.68708100	-2.90448600	1.55211300
H	8.91835300	-2.60307000	2.61042700
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Br	-5.62802400	1.21499000	-0.11685300
O	0.48792700	-1.44945300	2.23191900
C	-2.54653800	-1.24023700	1.24263100
H	-2.23806200	-1.67623900	2.18769700
O	0.59615800	1.42711600	1.00925000
C	-3.69043100	-0.44963700	1.18575200
H	-4.29169400	-0.28160700	2.07153600
O	1.79095700	1.41170700	-0.91231400
C	-4.05344200	0.13074400	-0.02976200
C	-3.29084600	-0.06368100	-1.17808700
H	-3.58745600	0.39648900	-2.11371700
C	-2.14347500	-0.85502600	-1.10808100
H	-1.54001600	-1.02072800	-1.99229700
C	-1.76959700	-1.45360300	0.09756100
C	-0.49720200	-2.28018600	0.20054400
C	0.51367300	-1.44707700	1.02142600
C	1.49102800	-0.64543900	0.19589900
C	1.22202500	0.82867800	0.16315600
C	1.74372800	2.84974600	-0.92319300
H	2.29729400	3.24712400	-0.06848600
H	0.71061300	3.20140900	-0.87724300
H	2.21689400	3.15056000	-1.85730200
C	2.94175400	-1.14506000	0.18102300
C	2.04948500	-1.39077600	-1.00222500
H	3.10165600	-1.99842400	0.84052300
H	2.22077400	-0.79316600	-1.89101800
C	1.38239900	-2.74248800	-1.19250600
H	1.58463400	-3.15137000	-2.18482100
H	1.74652500	-3.47060800	-0.44975200
O	-0.03719500	-2.61211500	-1.10463700
H	-0.68758400	-3.19628600	0.78058800
C	4.07575000	-0.16783900	0.15790400
C	4.28809100	0.66657100	1.26358100
C	4.93809900	-0.08047300	-0.93834500
C	5.34371200	1.57720600	1.26778500
H	3.60795400	0.60897700	2.10925000
C	5.99740700	0.82854800	-0.93390900
H	4.77422700	-0.72242100	-1.79907500
C	6.20174200	1.66010100	0.16805200

H	5.49469900	2.22388900	2.12714900
H	6.66009200	0.88898900	-1.79234300
H	7.02333400	2.37028700	0.17019600
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C	-0.88960000	2.20899300	0.09684900
C	0.70563200	0.75784800	0.94237700
H	0.50891100	0.71800800	2.02451600
C	2.11000000	0.30130500	0.63822200
C	2.61273600	-0.83432900	1.28195400
C	2.89422200	0.95838200	-0.31290100
C	3.88889700	-1.30856900	0.98777800
H	2.00200400	-1.35846800	2.01048100
C	4.17665800	0.49773600	-0.60988200
H	2.49960900	1.83416400	-0.81455500
C	4.66156600	-0.63272000	0.04411000
H	4.28088100	-2.18798600	1.48516800
H	4.79130600	1.00890300	-1.34186600
Br	6.42116300	-1.26784800	-0.35544600
O	0.46868500	2.07514600	0.44709400
C	-0.35824900	-0.12861100	0.23960400
O	-0.35851300	-1.33807200	0.19250600
C	-1.38496900	0.81396700	-0.28938000
N	-1.95325200	0.58576500	-1.49352000
N	-3.01794100	0.39435500	-1.92405800
O	-1.06369200	3.10653900	-0.92908700
C	-0.62621300	4.44364100	-0.63628200
H	0.45765900	4.47159100	-0.49049400
H	-0.89989500	5.04086800	-1.50628300
H	-1.12484300	4.82875200	0.25765200
O	-1.56320000	2.57983300	1.28344200
C	-2.95972400	2.26066100	1.19444100
H	-3.37275500	2.51210700	2.17563800
H	-3.44646100	2.88948000	0.43666200
C	-3.14397000	0.79615600	0.86166800
C	-4.17134600	0.37259100	0.01302900
H	-2.79371200	0.10262000	1.62306000
H	-4.82725700	1.13377900	-0.40411000
C	-4.67192600	-1.00983500	-0.03196200
C	-6.01455400	-1.25798900	-0.36384200
C	-3.83262000	-2.10973700	0.22771100
C	-6.51275600	-2.55854900	-0.40849400
H	-6.67190000	-0.41971900	-0.58069300
C	-4.33347900	-3.40856800	0.18238000

H	-2.77631200	-1.95210400	0.42582100
C	-5.67537400	-3.64049300	-0.13048200
H	-7.55568000	-2.72733100	-0.66127300
H	-3.66860400	-4.24475700	0.37910000
H	-6.06113800	-4.65490700	-0.16820700

3-TS-R

0 1

Rh	0.82708600	-0.96925600	0.23206800
C	3.41397400	-0.25590800	1.36654700
O	2.16062200	-0.00510000	1.46558500
C	2.10057200	0.14705300	-2.15053200
O	2.92330300	-0.81898500	-2.13080100
C	0.17612600	-2.99400800	-1.75799800
O	1.40789000	-3.28212800	-1.80724900
C	1.50015100	-3.37973800	1.70482200
O	0.67109100	-2.40449700	1.69082800
Rh	2.73176400	-2.22303300	-0.64730000
O	2.44708700	-3.56463900	0.88341900
O	1.14024200	0.33425400	-1.32870800
O	-0.35944800	-2.08446700	-1.03270200
O	3.94163100	-1.08274900	0.56598800
C	4.31515000	0.52721800	2.28754600
H	4.04520100	0.30983100	3.32526500
H	5.35901100	0.27037000	2.11049200
H	4.15478500	1.59488000	2.11580700
C	1.30792800	-4.38686500	2.81217400
H	1.37589800	-3.87862900	3.77826900
H	0.30406800	-4.81441200	2.73762000
H	2.05861600	-5.17427300	2.74808300
C	-0.77306300	-3.77577400	-2.63390000
H	-1.58117400	-4.18312000	-2.02051500
H	-1.22261800	-3.09946800	-3.36747900
H	-0.24512500	-4.57824400	-3.14867500
C	2.29690400	1.21396900	-3.19874200
H	1.35546800	1.72586200	-3.40055700
H	3.01425200	1.94596300	-2.81007900
H	2.71338700	0.77718600	-4.10785400
C	-1.18634400	1.52691800	0.59822000
C	-2.69153800	0.04482100	-0.48329600
H	-2.39805400	-0.55527400	-1.35106100
C	-4.18066900	0.25757700	-0.45433400
C	-4.94395100	-0.01860900	-1.59224900
C	-4.82030100	0.75445100	0.68963500

C	-6.32123100	0.20466300	-1.60496100
H	-4.45971000	-0.40694000	-2.48421600
C	-6.19330500	0.98354200	0.69350000
H	-4.23672600	0.96199900	1.58008300
C	-6.93251600	0.70766000	-0.45848600
H	-6.90956000	-0.00640600	-2.49051500
H	-6.68820600	1.36690500	1.57849100
Br	-8.81686800	1.02468400	-0.46086300
O	-1.95547500	1.29875700	-0.56967500
C	-2.10118000	-0.63816700	0.76119000
O	-2.59031300	-1.53149300	1.41068100
C	-0.79323500	0.07182000	0.93127300
N	-0.60201000	-0.02533200	2.81909400
N	-0.16295400	-0.51035500	3.71249000
O	-1.95820600	2.02681400	1.66712700
C	-2.58419300	3.28989100	1.39220400
H	-3.26235100	3.20422000	0.53828200
H	-3.14791700	3.54464000	2.29073200
H	-1.83862100	4.06331000	1.18694000
O	-0.21505000	2.40833900	0.19243000
C	0.78587900	2.76890900	1.16399400
H	0.51745000	3.72058000	1.64053900
H	0.84126900	1.99832300	1.94050300
C	2.09573800	2.83203300	0.45167100
C	3.03450300	3.77553300	0.59530200
H	2.25516700	1.98851200	-0.20519400
H	2.83346000	4.64046900	1.22857500
C	4.35566200	3.74547100	-0.05562800
C	5.13526300	4.91373300	-0.09830300
C	4.88297700	2.57605600	-0.64122300
C	6.38295900	4.92543700	-0.72188500
H	4.75135800	5.82385400	0.35621800
C	6.12708800	2.58837100	-1.26611400
H	4.33251300	1.64191400	-0.59310200
C	6.88327300	3.76372900	-1.31212200
H	6.96469600	5.84262600	-0.74549700
H	6.51153600	1.67294500	-1.70699500
H	7.85610500	3.76967700	-1.79483900
4			
O 1			
C	-0.52932600	0.71794700	-0.02883900
C	1.46452200	1.07913700	-1.27133400
H	1.47423600	1.38874000	-2.32286400

C	2.75686200	0.38348500	-0.90721700
C	3.94422300	0.73883300	-1.55311400
C	2.78813100	-0.56375300	0.12120300
C	5.15398100	0.14956300	-1.18916600
H	3.92861700	1.48384400	-2.34314900
C	3.99015000	-1.16403100	0.49081800
H	1.86893600	-0.82208800	0.63537200
C	5.16273100	-0.80156900	-0.17043500
H	6.07570300	0.42024400	-1.69101500
H	4.01911400	-1.90211000	1.28411700
Br	6.81480600	-1.62689900	0.33002900
O	0.32138800	0.25095700	-1.04879100
C	1.27345800	2.33694000	-0.39167500
O	1.99937200	3.30907600	-0.37591200
C	0.08643800	2.03567400	0.38961100
N	-0.32383600	2.75985600	1.38685100
N	-0.64481100	3.42323400	2.25271700
O	-0.53760100	-0.13805300	1.08103000
C	-1.03470400	-1.45940200	0.80507000
H	-0.44697200	-1.93243200	0.01269900
H	-0.92083700	-2.01690000	1.73556000
H	-2.08761400	-1.43357000	0.50879100
O	-1.78790100	0.79770700	-0.63040400
C	-2.85545300	1.27009800	0.21687800
H	-2.67754900	0.97682200	1.25781000
H	-2.87561400	2.36939300	0.16502000
C	-4.13625600	0.68449900	-0.28488800
C	-4.97080200	-0.02361800	0.48939000
H	-4.35209600	0.86871600	-1.33454600
H	-4.68449900	-0.17997700	1.53020500
C	-6.25607100	-0.62658300	0.10935400
C	-6.97398100	-1.35222800	1.07563500
C	-6.80702700	-0.51781200	-1.18126700
C	-8.19502900	-1.95065600	0.76930500
H	-6.56574800	-1.44668500	2.07881100
C	-8.02509100	-1.11559400	-1.48827100
H	-6.28076700	0.03841000	-1.95048700
C	-8.72592200	-1.83507500	-0.51536300
H	-8.73045400	-2.50619900	1.53359500
H	-8.43226700	-1.01993600	-2.49062600
H	-9.67696000	-2.29906000	-0.75883500

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0 1

C	-6.13244800	-0.29059600	-0.34462700
H	-6.50805100	0.71879000	-0.49181400
C	-7.02698000	-1.34511000	-0.15156000
H	-8.09577500	-1.15249900	-0.14743500
C	-6.54726800	-2.64196600	0.03298700
H	-7.24189800	-3.46348800	0.18119000
C	-5.17047300	-2.88144800	0.02352800
H	-4.79192800	-3.88993400	0.16089600
C	-4.27682200	-1.82949800	-0.16746700
H	-3.20628100	-2.02099300	-0.17746000
C	-4.75469000	-0.52315000	-0.34842700
C	-3.77162600	0.61237100	-0.54011700
H	-4.31322200	1.54164300	-0.74921900
N	-2.94134500	0.33452600	-1.75753200
N	-1.72815800	0.26886100	-1.52096100
C	-1.41630500	0.54541100	-0.09839000
C	-2.76096200	0.78474500	0.62533200
H	-2.95895400	0.05012200	1.40707500
C	-2.60778300	2.20157700	1.21894100
H	-3.51034500	2.81188500	1.13568400
H	-2.30925400	2.14443200	2.27229300
O	-1.58245300	2.84267300	0.45446100
C	-0.64530300	1.86591400	0.12060000
O	0.17857200	1.61302900	1.26736700
C	0.54964900	0.22783300	1.34964200
H	0.44686600	-0.07266500	2.39878700
C	-0.53005600	-0.51192000	0.53686100
O	0.07983000	2.24455100	-0.98131000
C	0.91251200	3.39855200	-0.78784200
H	1.66664100	3.20422400	-0.01987200
H	0.30985600	4.26672300	-0.50593900
H	1.39537400	3.57744000	-1.74880200
O	-0.67623600	-1.70786500	0.46401100
C	1.95877000	-0.07015500	0.88219300
C	2.32749800	0.09452600	-0.46074700
H	1.59907100	0.44977800	-1.18177800
C	3.62705900	-0.18229500	-0.87687300
H	3.91245300	-0.05667100	-1.91501200
C	4.56126300	-0.63129900	0.05706500
C	4.21651900	-0.80904400	1.39446200
H	4.95384600	-1.15957900	2.10733500
C	2.91151100	-0.52585100	1.79725600
H	2.63800600	-0.66082000	2.84013600
Br	6.34737200	-1.01093700	-0.50942100

Int1

0 1

Rh	0.75107300	-0.27920800	0.16508100
C	0.83831600	-1.46519800	-2.50299400
O	0.12491000	-0.71355500	-1.75089400
C	0.45001800	-3.09356600	0.82701600
O	1.63008200	-3.28262700	0.41122700
C	2.69216800	-0.52060000	2.32444000
O	3.37981100	-1.28567500	1.58475300
C	3.06845500	1.10000100	-0.96825100
O	1.87562500	1.29534500	-0.54870200
Rh	2.71321600	-1.69043600	-0.31412300
O	3.67819000	-0.00771600	-1.00415400
O	-0.18281200	-1.97940600	0.83712600
O	1.58027700	0.03225500	2.01760700
O	1.93907800	-2.00679100	-2.19437600
C	0.28293600	-1.72253500	-3.88443200
H	1.00873000	-2.26184200	-4.49305000
H	-0.63427700	-2.31357000	-3.79792800
H	0.01783900	-0.77220200	-4.35461000
C	3.80015600	2.31931900	-1.48153300
H	3.23315700	3.22561000	-1.26656100
H	4.79153500	2.36898600	-1.02478700
H	3.94107900	2.21963400	-2.56242400
C	3.21733500	-0.20316600	3.70417000
H	3.47927100	0.85842200	3.74960800
H	2.43089800	-0.37721800	4.44265600
H	4.09547600	-0.80909200	3.92744900
C	-0.30053600	-4.27704300	1.39010800
H	-1.32315600	-4.28678300	1.00566200
H	0.21322100	-5.20609200	1.14265200
H	-0.35748000	-4.17209500	2.47827400
Br	-6.76356400	-0.65926800	-0.15192900
O	-0.61957700	1.97915800	2.64335700
C	-3.27524400	1.23306600	1.06321600
H	-3.01619500	2.07150000	1.69954800
O	-0.70587300	2.56450600	-1.44520400
C	-4.60808200	0.89472200	0.89953200
H	-5.39155100	1.46661700	1.38266700
O	0.76247400	4.28855700	-1.23898300
N	0.68648200	4.07229600	1.41269700
C	-4.93468200	-0.20142300	0.09169700
N	1.23159200	4.80375500	2.08250500

C	-3.94839600	-0.96374400	-0.54024800
H	-4.22904900	-1.80451500	-1.16387900
C	-2.61422500	-0.63235600	-0.35605400
H	-1.84172800	-1.20473300	-0.84804700
C	-2.24213200	0.47787900	0.44496600
C	-0.86295700	0.82974200	0.61001200
C	-0.52511600	2.02844000	1.41959000
C	0.03063800	3.18446100	0.69646100
C	-0.01547200	3.29556600	-0.76056900
C	0.77084300	4.40969500	-2.67479100
H	-0.24107200	4.57375800	-3.05278500
H	1.17888500	3.50085800	-3.12405100
H	1.40800500	5.26679500	-2.89049600

Int1'

0 1

Rh	-1.50838500	0.20439100	-0.09769200
C	-0.27776500	-2.43044900	-0.09638100
O	0.00780500	-1.18047500	-0.09578300
C	-2.35765600	-0.80754100	-2.69958400
O	-3.07822500	-1.66157800	-2.10305800
C	-4.30663300	0.95240100	-0.04909600
O	-4.58812100	-0.28229500	-0.03647800
C	-2.29530400	-0.75413600	2.55348700
O	-1.58956600	0.13047200	1.95313800
Rh	-3.07942800	-1.67859900	-0.05442500
O	-3.01594200	-1.63121200	1.99552300
O	-1.61251600	0.06997200	-2.14146800
O	-3.13299200	1.46396700	-0.08681000
O	-1.43873100	-2.93195000	-0.07265800
C	0.89977600	-3.37246100	-0.16334800
H	1.77872800	-2.91712800	0.29603200
H	0.65201400	-4.31942600	0.31804800
H	1.12790000	-3.56845200	-1.21647300
C	-2.23293400	-0.72103300	4.05960700
H	-1.20175300	-0.90229400	4.37627000
H	-2.51211400	0.27567300	4.41159200
H	-2.89558700	-1.47431000	4.48521600
C	-5.44760100	1.94042700	-0.00513000
H	-5.40790300	2.48742800	0.94191800
H	-5.33221100	2.66800800	-0.81267100
H	-6.40346600	1.42418300	-0.09181300
C	-2.36394300	-0.79465800	-4.20820000
H	-2.78003900	0.15569800	-4.55535400

H	-1.33667200	-0.85644300	-4.57648300
H	-2.95793700	-1.62352100	-4.59300900
Br	8.05698000	-0.52358900	-0.32494800
O	1.47137700	1.88983100	-1.55049200
N	1.54544600	0.54874700	1.69047800
C	4.14153800	0.80569400	-0.90438100
H	3.56893900	1.23189400	-1.71712800
O	-0.61803200	3.39072900	1.41401200
N	1.11470800	0.21487300	2.68464700
C	5.48236400	0.48111500	-1.09712900
H	5.94833400	0.65708500	-2.05993700
O	-1.18234900	3.77406100	-0.75739000
C	6.22060900	-0.07383300	-0.05382400
C	5.63027300	-0.30513200	1.18784900
H	6.20921600	-0.73540000	1.99693800
C	4.29208800	0.02386300	1.37959400
H	3.85264500	-0.15795800	2.35590400
C	3.52443700	0.58132700	0.34038000
C	2.09987000	0.90566000	0.54010500
C	1.19166800	1.51934100	-0.40585000
C	-0.24724100	1.69247900	-0.09580300
C	-0.69332100	3.05500800	0.24391600
C	-1.71336300	5.06650600	-0.38896700
H	-0.94821800	5.66805600	0.10734000
H	-2.56753500	4.93849600	0.28013100
H	-2.02091000	5.52838700	-1.32572700

Rh-cata

O 1

Rh	0.00001100	0.00000000	1.19218600
C	1.86277000	-1.85366800	0.00000200
O	1.44691000	-1.44749400	1.13477800
C	1.86300600	1.85343200	0.00024100
O	1.44705500	1.44734100	-1.13455200
C	-1.86277700	1.85367400	0.00010300
O	-1.44778100	1.44665500	-1.13466500
C	-1.86300500	-1.85344500	0.00033200
O	-1.44798700	-1.44637800	1.13504500
Rh	-0.00002500	0.00000000	-1.19201300
O	-1.44709800	-1.44734900	-1.13447900
O	1.44801100	1.44638200	1.13497200
O	-1.44689000	1.44748700	1.13486000
O	1.44773200	-1.44664900	-1.13474700
C	2.96598000	-2.88203500	0.00025200

H	2.90448800	-3.50145000	0.89618600
H	2.91283500	-3.49345000	-0.90163300
H	3.92905200	-2.36030700	0.00747000
C	-2.96611100	-2.88192500	-0.00084000
H	-2.93066400	-3.47622100	0.91314200
H	-3.92878700	-2.36081000	-0.03871300
H	-2.88701600	-3.51816600	-0.88365000
C	-2.96592700	2.88210600	0.00027000
H	-3.92905000	2.36043900	0.00347800
H	-2.90667400	3.49929000	0.89787700
H	-2.91041900	3.49577600	-0.89995800
C	2.96615700	2.88186300	-0.00086000
H	2.92870800	3.47815100	0.91175900
H	3.92889200	2.36061300	-0.03523000
H	2.88907300	3.51617200	-0.88522100

1a-smd

O 1

Br	5.34124300	-0.03631700	-0.31573000
O	-1.37660600	2.18747500	-0.00648300
N	-1.29899800	-1.10440900	1.12458300
C	1.36316200	1.17822600	0.08854000
H	0.82361700	2.11404600	0.05582200
O	-3.18973900	-1.53548300	-0.78333600
N	-1.70683700	-2.01565000	1.66441300
C	2.74280700	1.17178600	-0.10922700
H	3.26436400	2.10405500	-0.29547800
O	-5.15217800	-0.43277500	-0.48671500
N	-3.98355900	1.73664500	0.20427800
C	3.44190400	-0.03089900	-0.05540000
N	-4.63408000	2.64753400	0.35020000
C	2.77941400	-1.23270100	0.18732500
H	3.32521500	-2.16885400	0.22094400
C	1.40084800	-1.22233100	0.37338500
H	0.89786400	-2.17012200	0.53874600
C	0.66894100	-0.02046700	0.33094500
C	-0.79793400	-0.04109200	0.52776900
C	-1.74128700	1.02441600	0.17328700
C	-3.18876900	0.68911800	0.05821500
C	-3.81130800	-0.54626200	-0.44235600
C	-5.85900200	-1.57954900	-1.00915400
H	-5.66774900	-2.45981100	-0.39061300
H	-5.55284800	-1.78252200	-2.03836300
H	-6.91412300	-1.30974500	-0.97252900

1-int2-smd

O 1

Rh	1.40291900	-2.99572400	0.16104700
C	2.15341400	-0.99556800	2.13347000
O	2.44572300	-2.16485500	1.73277600
C	-0.98375700	-2.98023600	1.75964500
O	-1.19027400	-1.80437300	1.30353900
C	-0.58671200	-2.88501100	-1.95708100
O	-0.83510900	-1.68409400	-1.59035600
C	2.58115600	-1.01089700	-1.57746600
O	2.75514100	-2.19837800	-1.16346700
Rh	0.15260000	-0.89291300	0.03302100
O	1.61375900	-0.24309800	-1.24388300
O	0.01023300	-3.71870000	1.48021700
O	0.25842800	-3.66551300	-1.42179200
O	1.24100300	-0.24260300	1.64613300
C	2.96185400	-0.41485200	3.26301900
H	3.71987700	0.25120800	2.83727300
H	2.32213400	0.17702600	3.92105200
H	3.45972300	-1.20701800	3.82397000
C	3.60155400	-0.42919300	-2.51716300
H	4.16469100	-1.22522100	-3.00652500
H	3.11406900	0.20716200	-3.25836200
H	4.29572900	0.19145100	-1.94072100
C	-1.39252200	-3.39427400	-3.12299300
H	-1.31366000	-2.68975000	-3.95582500
H	-1.04689900	-4.38109200	-3.43264500
H	-2.44622800	-3.44849100	-2.83058100
C	-2.03035600	-3.51290900	2.70132400
H	-2.98185800	-3.59699900	2.16669100
H	-1.73797000	-4.48897200	3.08980600
H	-2.17333800	-2.80603200	3.52352800
Br	5.52521500	2.58758600	-0.67144100
O	-1.59134100	1.21562300	2.17658300
C	2.05124800	2.89245900	1.61813100
H	1.80340900	2.92198300	2.67521100
O	-1.49968800	1.58256600	-2.08836800
C	3.38649500	2.78415400	1.23193800
H	4.17361900	2.73958800	1.97615100
O	-2.99536500	0.21670200	-1.04600600
C	3.69011900	2.74600800	-0.12849000
C	2.69482500	2.81889300	-1.10071000
H	2.94678000	2.78518900	-2.15417800

C	1.36338700	2.92178900	-0.69916400
H	0.57579500	2.95715500	-1.44379800
C	1.03493900	2.96360200	0.66027300
C	-0.41008800	3.04144100	1.09768000
C	-1.04573400	1.63302400	1.16387200
C	-0.96850000	0.71660800	0.01056500
C	-1.86747300	0.90181700	-1.14543700
C	-3.84161800	0.19089300	-2.22130000
H	-3.34380900	-0.37473600	-3.01278300
H	-4.05883500	1.20357700	-2.56265500
H	-4.75525600	-0.30717100	-1.90373700
C	-4.25369700	2.64611500	0.89160600
C	-3.52517000	3.47883100	0.13262800
H	-3.99164500	2.54404800	1.94435200
H	-3.70352000	3.55043500	-0.93889700
C	-2.41148000	4.32723500	0.67180200
H	-2.50748700	5.35698900	0.30985300
H	-2.43049700	4.35074600	1.76922700
O	-1.11231700	3.89250500	0.20898400
H	-0.47382500	3.41092900	2.13218200
C	-5.35073100	1.78760400	0.41906400
C	-5.57871000	0.55382400	1.05435900
C	-6.17125500	2.14628300	-0.66508600
C	-6.57412500	-0.31017500	0.59949700
H	-4.95130800	0.26653200	1.89405000
C	-7.17296400	1.28631800	-1.11428700
H	-6.03160500	3.11027900	-1.14577400
C	-7.37484000	0.05237600	-0.48839800
H	-6.72750000	-1.26462300	1.09553800
H	-7.80170700	1.58162900	-1.94981800
H	-8.15684500	-0.61589400	-0.83790900

1-int3-smd

O 1

Rh	1.40291900	-2.99572400	0.16104700
C	2.15341400	-0.99556800	2.13347000
O	2.44572300	-2.16485500	1.73277600
C	-0.98375700	-2.98023600	1.75964500
O	-1.19027400	-1.80437300	1.30353900
C	-0.58671200	-2.88501100	-1.95708100
O	-0.83510900	-1.68409400	-1.59035600
C	2.58115600	-1.01089700	-1.57746600
O	2.75514100	-2.19837800	-1.16346700
Rh	0.15260000	-0.89291300	0.03302100

O	1.61375900	-0.24309800	-1.24388300
O	0.01023300	-3.71870000	1.48021700
O	0.25842800	-3.66551300	-1.42179200
O	1.24100300	-0.24260300	1.64613300
C	2.96185400	-0.41485200	3.26301900
H	3.71987700	0.25120800	2.83727300
H	2.32213400	0.17702600	3.92105200
H	3.45972300	-1.20701800	3.82397000
C	3.60155400	-0.42919300	-2.51716300
H	4.16469100	-1.22522100	-3.00652500
H	3.11406900	0.20716200	-3.25836200
H	4.29572900	0.19145100	-1.94072100
C	-1.39252200	-3.39427400	-3.12299300
H	-1.31366000	-2.68975000	-3.95582500
H	-1.04689900	-4.38109200	-3.43264500
H	-2.44622800	-3.44849100	-2.83058100
C	-2.03035600	-3.51290900	2.70132400
H	-2.98185800	-3.59699900	2.16669100
H	-1.73797000	-4.48897200	3.08980600
H	-2.17333800	-2.80603200	3.52352800
Br	5.52521500	2.58758600	-0.67144100
O	-1.59134100	1.21562300	2.17658300
C	2.05124800	2.89245900	1.61813100
H	1.80340900	2.92198300	2.67521100
O	-1.49968800	1.58256600	-2.08836800
C	3.38649500	2.78415400	1.23193800
H	4.17361900	2.73958800	1.97615100
O	-2.99536500	0.21670200	-1.04600600
C	3.69011900	2.74600800	-0.12849000
C	2.69482500	2.81889300	-1.10071000
H	2.94678000	2.78518900	-2.15417800
C	1.36338700	2.92178900	-0.69916400
H	0.57579500	2.95715500	-1.44379800
C	1.03493900	2.96360200	0.66027300
C	-0.41008800	3.04144100	1.09768000
C	-1.04573400	1.63302400	1.16387200
C	-0.96850000	0.71660800	0.01056500
C	-1.86747300	0.90181700	-1.14543700
C	-3.84161800	0.19089300	-2.22130000
H	-3.34380900	-0.37473600	-3.01278300
H	-4.05883500	1.20357700	-2.56265500
H	-4.75525600	-0.30717100	-1.90373700
C	-4.25369700	2.64611500	0.89160600
C	-3.52517000	3.47883100	0.13262800

H	-3.99164500	2.54404800	1.94435200
H	-3.70352000	3.55043500	-0.93889700
C	-2.41148000	4.32723500	0.67180200
H	-2.50748700	5.35698900	0.30985300
H	-2.43049700	4.35074600	1.76922700
O	-1.11231700	3.89250500	0.20898400
H	-0.47382500	3.41092900	2.13218200
C	-5.35073100	1.78760400	0.41906400
C	-5.57871000	0.55382400	1.05435900
C	-6.17125500	2.14628300	-0.66508600
C	-6.57412500	-0.31017500	0.59949700
H	-4.95130800	0.26653200	1.89405000
C	-7.17296400	1.28631800	-1.11428700
H	-6.03160500	3.11027900	-1.14577400
C	-7.37484000	0.05237600	-0.48839800
H	-6.72750000	-1.26462300	1.09553800
H	-7.80170700	1.58162900	-1.94981800
H	-8.15684500	-0.61589400	-0.83790900

1-int4-smd

O 1

Rh	3.42741900	-1.82277800	-0.33595800
C	3.07915500	0.87902400	-1.66081800
O	3.81122700	-0.10281100	-1.53382300
C	3.21687300	-0.24664500	2.09596900
O	1.98235700	-0.07341100	1.82147900
C	1.52095400	-3.40166700	1.15368900
O	0.64843700	-2.49381900	0.92533300
C	1.48472400	-2.39489100	-2.39129600
O	2.65987600	-2.71879200	-2.01895200
Rh	1.21807200	-0.77428700	0.02686200
O	0.71102900	-1.56725400	-1.80815500
O	4.06335300	-0.86982400	1.38062300
O	2.74109800	-3.38368700	0.79125200
O	1.99103300	0.98260800	-0.85164000
C	3.35432600	1.93378600	-2.67953400
H	2.43399400	2.29656700	-3.14079200
H	3.85668900	2.78110300	-2.20411000
H	4.01428300	1.50706200	-3.43523800
C	0.93565800	-3.06671600	-3.62427400
H	1.74088100	-3.47678300	-4.23588400
H	0.27857300	-3.88459200	-3.30756100
H	0.33314900	-2.36205500	-4.20168900
C	1.03739800	-4.59050100	1.94191900

H	1.79366200	-5.37598100	1.96025600
H	0.81452200	-4.27146800	2.96557000
H	0.10931600	-4.96813400	1.50452800
C	3.70607300	0.32515900	3.40335300
H	3.70267200	-0.47356900	4.15403200
H	4.73227800	0.68475700	3.30003200
H	3.05052100	1.12678300	3.74720900
Br	-8.33278200	-0.66460600	-0.09368700
O	-1.63845000	-0.06596400	-1.88111400
C	-4.65308800	0.60871400	-1.60055400
H	-4.14461000	0.59311600	-2.55877900
O	-2.11682300	-0.86474800	1.43341200
C	-5.93133400	0.06273300	-1.49239200
H	-6.42099700	-0.36422500	-2.36043700
O	-0.77505000	0.50674200	2.62709400
C	-6.56955300	0.07847600	-0.25296000
C	-5.95341400	0.62360300	0.87134200
H	-6.45957600	0.62697800	1.83034700
C	-4.67075900	1.15921800	0.75003900
H	-4.17927200	1.57805300	1.61972700
C	-4.01301800	1.16004900	-0.48372100
C	-2.61458100	1.72332000	-0.62502100
C	-1.57473900	0.58000700	-0.85698300
C	-0.54208800	0.49247900	0.25271400
C	-1.23246100	-0.01762000	1.46392700
C	-1.33201900	-0.06353700	3.82083400
H	-1.11449700	-1.13406700	3.87856500
H	-2.41549300	0.08292500	3.85692700
H	-0.85387800	0.46165400	4.64923500
C	1.11197800	2.21486900	-0.71711400
C	0.10668700	1.88814600	0.40316400
H	0.60942000	2.31473500	-1.68299600
H	0.65352700	1.88742200	1.34484300
C	-0.97354400	3.02174600	0.44800300
H	-0.84317300	3.63706000	1.33933300
H	-0.90007700	3.68353400	-0.42980200
O	-2.28803500	2.48698300	0.52478300
H	-2.56749900	2.35825800	-1.52677700
C	1.95908600	3.41699000	-0.39609900
C	1.82486100	4.59336500	-1.14110100
C	2.86369900	3.37265900	0.67522200
C	2.58238600	5.72062000	-0.81542700
H	1.13160000	4.62515400	-1.97728800
C	3.63176100	4.49307600	0.98724900

H	2.96564100	2.46059900	1.25523100
C	3.48934600	5.67016100	0.24506700
H	2.46960500	6.63232900	-1.39444200
H	4.33702700	4.45040500	1.81206100
H	4.08538300	6.54362800	0.49273800

1-int5-smd

0 1

Rh	2.47044500	-2.48690500	-0.41658900
C	4.89963100	-0.92955300	-0.72708500
O	4.44603100	-2.11527800	-0.84933600
C	2.98629600	-1.82690100	2.36426800
O	2.73668200	-0.61335000	2.06118100
C	-0.20167100	-1.72711000	0.35323700
O	0.27503600	-0.56159800	0.54635500
C	1.64666600	-0.83867000	-2.63972100
O	1.92998700	-2.04812200	-2.34690600
Rh	2.23700500	-0.16491600	0.12313100
O	1.74976500	0.15324400	-1.84796000
O	2.96442100	-2.81119200	1.55365100
O	0.48444000	-2.74862900	0.00564500
O	4.22911400	0.08356100	-0.33793000
C	6.33784600	-0.69290300	-1.10453200
H	6.36800200	-0.30340300	-2.12856900
H	6.78297200	0.05449500	-0.44418700
H	6.90565400	-1.62379800	-1.06690100
C	1.10925300	-0.55898400	-4.01646200
H	1.34322100	-1.37520400	-4.70130700
H	0.02106200	-0.45805600	-3.93587000
H	1.50816000	0.38529800	-4.39426000
C	-1.68466600	-1.91040200	0.50896100
H	-1.91394900	-2.93174100	0.81881200
H	-2.08975200	-1.18020400	1.20868300
H	-2.14850600	-1.72832400	-0.46663900
C	3.30026000	-2.13155400	3.80467600
H	2.38716800	-2.49248500	4.29162700
H	4.05115500	-2.92205200	3.86741400
H	3.64399500	-1.23499400	4.32272700
Br	-7.17905200	-2.35461600	0.70810500
O	-1.52237800	0.58411700	-1.64989800
C	-4.62768600	-0.13367100	-1.73769400
H	-4.16299200	-0.25669400	-2.71098900
O	-2.07125400	1.10818600	1.66053900
C	-5.45523400	-1.14106700	-1.24171000

H	-5.64219400	-2.03579800	-1.82480600
O	-0.01172600	2.00189600	1.88573400
C	-6.04013300	-0.97514200	0.01326900
C	-5.81549300	0.17166200	0.77295100
H	-6.27564400	0.28566900	1.74805800
C	-4.97922400	1.16692500	0.26755500
H	-4.77989800	2.05575700	0.85349800
C	-4.38432300	1.02328700	-0.98944400
C	-3.40475300	2.06055800	-1.50118300
C	-1.97623400	1.58493100	-1.13341600
C	-1.21018000	2.41991800	-0.12638000
C	-1.14051100	1.75777300	1.21743100
C	0.11485200	1.35473800	3.16834700
H	0.11547900	0.27179200	3.03250500
H	-0.70345800	1.64914800	3.83080400
H	1.07170800	1.68987500	3.56699800
C	-0.20421000	3.42769600	-0.70368200
C	-1.52041300	3.91177900	-0.16723400
H	-0.15886300	3.36195900	-1.79001100
H	-1.52112300	4.41089000	0.79718800
C	-2.66000200	4.27162400	-1.10491700
H	-3.07820400	5.24947000	-0.85686900
H	-2.32006500	4.30236300	-2.15160500
O	-3.73155600	3.33227500	-0.96427900
H	-3.43423500	2.09136000	-2.60320300
C	1.12971800	3.71847800	-0.09032200
C	2.25937600	3.08396900	-0.63036800
C	1.30069900	4.59463600	0.98763200
C	3.52506700	3.28289900	-0.07266900
H	2.14051100	2.41835600	-1.47868400
C	2.56693100	4.80566000	1.53687500
H	0.44442100	5.10936900	1.41159500
C	3.68231000	4.14382800	1.01660100
H	4.37733500	2.75195400	-0.48431600
H	2.68104200	5.48879700	2.37421100
H	4.66505400	4.30241600	1.45178300

1-TS2-smd

O 1			
Rh	-0.71646100	-0.76912300	0.08634400
C	0.12269300	-2.50758700	-2.08319800
O	0.58239100	-1.71635300	-1.19192900
C	-1.51949400	0.81200900	-2.24676600
O	-2.34017500	-0.11207000	-2.53335500

C	-3.40739600	-0.01663200	0.93965400
O	-3.84904000	-0.63957600	-0.07722600
C	-1.75804300	-3.30969800	1.04350700
O	-0.81629500	-2.46899500	1.23854500
Rh	-2.52632700	-1.70245600	-1.23805900
O	-2.62345300	-3.24643500	0.11374100
O	-0.78597300	0.84983800	-1.19876400
O	-2.17741200	0.07493900	1.27522600
O	-1.10841900	-2.72297500	-2.32174800
C	1.13884400	-3.26492900	-2.89441600
H	1.53449700	-4.07766300	-2.27683300
H	0.68349400	-3.68449400	-3.79227000
H	1.96866100	-2.60574000	-3.15804900
C	-1.84743600	-4.45443500	2.01658300
H	-0.86456300	-4.91716100	2.13547500
H	-2.14776700	-4.06175500	2.99381100
H	-2.57529800	-5.19364900	1.68027200
C	-4.39689100	0.68775600	1.82755300
H	-4.19151800	0.44028100	2.87237400
H	-4.27012900	1.76800900	1.70795500
H	-5.41819200	0.40987200	1.56484100
C	-1.37350400	1.96196000	-3.20733300
H	-0.40816200	1.86984100	-3.71749700
H	-2.17347100	1.95345200	-3.94859600
H	-1.37392800	2.90718400	-2.65923000
Br	5.82751500	3.38877900	-0.92895800
O	1.10954400	-1.38777100	3.31311200
C	3.45667500	1.00521700	1.52936500
H	3.54870700	0.54822900	2.51070800
O	3.57457400	-1.44487800	-0.29985800
C	4.51080500	1.76325200	1.03216300
H	5.41829000	1.89320700	1.61075900
O	3.22981400	-3.67610700	-0.11277000
N	1.95440300	-3.47419600	2.04833600
C	4.37990800	2.34800400	-0.22871200
N	1.71605500	-4.44157400	2.57999800
C	3.21858200	2.19727700	-0.98335800
H	3.13171100	2.66289100	-1.95874500
C	2.16585300	1.44125100	-0.46860100
H	1.25953700	1.32137000	-1.04668300
C	2.27723100	0.82802800	0.78392100
C	1.17771000	0.04394500	1.39673600
C	1.51147900	-1.19849700	2.17108600
C	2.20539300	-2.31359400	1.46520500

C	3.05217600	-2.38425400	0.26105000
C	4.22447400	-3.89003700	-1.13489100
H	5.21261000	-3.59643300	-0.76899000
H	3.98946200	-3.32047700	-2.03555900
H	4.20258300	-4.95981400	-1.34365800
C	-1.61912200	3.68781900	1.82889300
C	-0.58262500	2.92252400	1.45564800
H	-1.67371700	4.02994500	2.86299100
H	-0.48175200	2.59078800	0.42498200
C	0.47020700	2.44199900	2.39944200
H	1.47527500	2.73830400	2.08658200
H	0.30281400	2.80404900	3.41755000
O	0.43321300	0.98504400	2.55525800
H	-0.05871100	0.44864900	1.57057200
C	-2.71580100	4.12566600	0.95069800
C	-3.49003000	5.24714200	1.29572900
C	-3.04322400	3.42519700	-0.22707700
C	-4.53537400	5.67442000	0.47526400
H	-3.26327700	5.78997800	2.21019900
C	-4.08745800	3.85032000	-1.04472300
H	-2.49037600	2.52873900	-0.47964400
C	-4.83599700	4.98087800	-0.69958800
H	-5.11784000	6.54781000	0.75531600
H	-4.32475600	3.29109800	-1.94586000
H	-5.65288400	5.31037700	-1.33531700

1-TS3-smd

O 1

Rh	1.61993700	2.86867300	-0.02027900
C	2.04665800	0.97774000	-2.17378000
O	2.53922400	2.03329100	-1.66077000
C	-0.74475400	3.30229400	-1.61748600
O	-1.11696400	2.13622600	-1.24837500
C	-0.37250300	2.89423100	2.09978000
O	-0.81404800	1.79018100	1.62961000
C	2.48141500	0.63378700	1.58110200
O	2.84236400	1.80317100	1.23001500
Rh	0.07651900	0.97357300	-0.03818700
O	1.42710800	0.03114000	1.19363200
O	0.33348700	3.87483400	-1.27027600
O	0.58947600	3.57304500	1.62378600
O	1.04421700	0.32595200	-1.72914300
C	2.70787000	0.46224800	-3.42625900
H	3.75722300	0.23920400	-3.21276700

H	2.20475500	-0.42920800	-3.79935300
H	2.68567000	1.24622800	-4.18952100
C	3.39206400	-0.10468700	2.52665700
H	3.80558700	0.59278000	3.25883200
H	2.85815700	-0.91308100	3.02568500
H	4.22473400	-0.52826000	1.95606000
C	-1.04713100	3.40346500	3.34692500
H	-0.64652600	2.85504600	4.20709600
H	-0.85037600	4.46754500	3.48559400
H	-2.12221800	3.21580700	3.29800500
C	-1.67355000	4.02742400	-2.55488500
H	-2.69200700	4.00107100	-2.15795400
H	-1.35086200	5.05877000	-2.70137300
H	-1.68039100	3.50539300	-3.51757800
Br	5.68984000	-2.45602600	0.14008200
O	-1.56005200	-1.44059300	-2.16880300
C	1.90331700	-2.55582100	-1.60860000
H	1.48413900	-2.37675400	-2.59323600
O	-0.81339700	-1.66358500	2.10635800
C	3.27620000	-2.41846400	-1.41618100
H	3.92197800	-2.13481700	-2.23878700
O	-2.75750800	-0.51778300	1.89413100
N	-2.86431000	0.12370100	-0.54874100
C	3.80134200	-2.65961600	-0.14782200
N	-3.51850400	0.94045300	-0.90642900
C	2.98721000	-3.03974800	0.91628400
H	3.41293900	-3.23137000	1.89425800
C	1.61179800	-3.14906600	0.71298800
H	0.96103800	-3.41065400	1.53638000
C	1.06251600	-2.90922600	-0.54805900
C	-0.42417200	-3.05411900	-0.80716000
C	-1.14303300	-1.68534900	-1.04705400
C	-1.26961300	-0.66410700	0.03903000
C	-1.60513000	-1.02361900	1.44469600
C	-2.99944100	-0.67344100	3.30851400
H	-2.23139900	-0.14594500	3.87960300
H	-3.00398900	-1.73000700	3.58694700
H	-3.97702600	-0.22631700	3.48496400
C	-4.24023300	-2.92806200	-0.70054400
C	-3.40983300	-3.43597100	0.22347300
H	-4.10074700	-3.23763200	-1.73650600
H	-3.48299500	-3.13667700	1.26643100
C	-2.29992900	-4.39277800	-0.09159500
H	-2.36606200	-5.28495100	0.54092200

H	-2.33949900	-4.71587600	-1.14126600
O	-1.00797400	-3.83299000	0.21220200
H	-0.56101700	-3.54128800	-1.78430300
C	-5.29735200	-1.93106600	-0.48382800
C	-5.89956600	-1.33212200	-1.60485200
C	-5.69368100	-1.49780400	0.79675800
C	-6.84684700	-0.31916400	-1.45703900
H	-5.60364900	-1.65358700	-2.60026000
C	-6.63998900	-0.48751900	0.94432400
H	-5.25794800	-1.95128100	1.68083800
C	-7.21760800	0.11106600	-0.18105700
H	-7.29267900	0.13535200	-2.33723300
H	-6.93151800	-0.16541100	1.94033300
H	-7.95410700	0.90057100	-0.06245600

1-TS4-smd

O 1

Rh	3.05767300	-1.96072700	-0.74085400
C	0.57787200	-2.33577300	-2.17363200
O	1.78778500	-2.72742400	-2.16462400
C	2.78025800	0.60099000	-2.08665500
O	1.78219400	0.84075000	-1.32897900
C	3.70233600	-0.27147200	1.53705700
O	2.49887800	0.16144700	1.49064000
C	1.47060300	-3.16749800	1.35787100
O	2.45215700	-3.41193300	0.58966100
Rh	1.19920400	-0.55691800	0.05700000
O	0.77476200	-2.09702900	1.36963200
O	3.53406800	-0.42166000	-2.03170700
O	4.21702100	-1.12050600	0.74936700
O	0.06009000	-1.47925500	-1.38243600
C	-0.34621800	-2.90891300	-3.21724900
H	-1.26834600	-3.25402400	-2.74179000
H	-0.61515600	-2.11686300	-3.92398500
H	0.13339300	-3.72921800	-3.75279700
C	1.08788100	-4.21552300	2.37218100
H	1.61421300	-5.15133400	2.17985400
H	1.35061000	-3.85269100	3.37177400
H	0.00698600	-4.37698700	2.34852400
C	4.58286200	0.32236400	2.60765000
H	5.42461900	-0.33789000	2.82181700
H	4.97461800	1.28057200	2.24682200
H	4.00507900	0.51222700	3.51475100
C	3.07236700	1.60757600	-3.16924700

H	4.14719400	1.79465000	-3.22625000
H	2.75390500	1.18149700	-4.12718200
H	2.53459700	2.53803300	-2.99395600
Br	-8.04479000	-0.62380100	-0.84052900
O	-1.31466200	1.15856400	-1.44365100
C	-4.41079800	1.40901500	-1.14203600
H	-3.84951800	1.91137900	-1.92304000
O	-1.96285900	-0.90808400	1.68442800
C	-5.63841600	0.82264200	-1.44749000
H	-6.03672600	0.87597100	-2.45439800
O	-0.45330300	0.08377600	3.05309300
C	-6.34571000	0.17270400	-0.43701100
C	-5.84525300	0.09359000	0.86090300
H	-6.40248700	-0.42029800	1.63618100
C	-4.61255000	0.67907400	1.15094700
H	-4.20849700	0.61150700	2.15285500
C	-3.88988600	1.34351800	0.15587600
C	-2.54550000	1.98216100	0.45003800
C	-1.39499400	1.18603800	-0.23200400
C	-0.40143700	0.52183500	0.69138300
C	-1.04131300	-0.12763700	1.86991400
C	-0.98825700	-0.68246200	4.15093200
H	-0.88907400	-1.75176700	3.95204900
H	-2.04118400	-0.43552600	4.31411400
H	-0.39482100	-0.39975400	5.02067000
C	0.52088300	3.35380500	0.52452300
C	0.10379200	2.51747100	1.54957400
H	-0.26118900	3.94592800	0.04745200
H	0.84459100	1.99728100	2.14857000
C	-1.22846400	2.87120600	2.21971900
H	-1.12901700	2.74227100	3.29876100
H	-1.46923600	3.92394500	2.01635700
O	-2.35062100	2.06630600	1.84894900
H	-2.52126200	2.98531500	-0.00481700
C	1.83896600	3.61505400	0.01803800
C	1.97170600	4.53554000	-1.04884300
C	3.00698700	3.05186300	0.57991200
C	3.22647700	4.87048200	-1.54409400
H	1.07873900	4.98056700	-1.47965300
C	4.25648100	3.37999800	0.07403900
H	2.91391600	2.35090300	1.39671500
C	4.37094000	4.28908600	-0.98738400
H	3.31712100	5.57815200	-2.36228200
H	5.14906400	2.93668000	0.50552800

H	5.35224700	4.54653600	-1.37513300
2a-smd			
0 1			
C	0.82878600	-0.61483800	0.20193500
C	1.87902800	0.21879600	0.21407200
H	1.02491900	-1.68550000	0.27059100
H	1.74562900	1.29510100	0.11798900
C	3.29857500	-0.22688300	0.37568800
H	3.67370400	0.11102200	1.35719400
H	3.35776500	-1.32693700	0.36879700
O	4.07762800	0.34885700	-0.67844500
H	5.00967000	0.21675400	-0.45329900
C	-0.59350700	-0.25272400	0.09532800
C	-1.54558400	-1.27642200	-0.06291100
C	-1.05562400	1.07701300	0.14432900
C	-2.90501200	-0.98695500	-0.18067600
H	-1.21037200	-2.31015100	-0.09817700
C	-2.41224000	1.36643900	0.02533900
H	-0.35007500	1.89003600	0.28502100
C	-3.34507700	0.33696000	-0.13890400
H	-3.61975100	-1.79583800	-0.30422400
H	-2.74562800	2.39975500	0.06651500
H	-4.40296600	0.56658700	-0.22804900

2-int2-smd

0 1			
Rh	-0.72837100	-0.14303000	-0.08527100
C	0.23994000	-1.84759000	2.05958900
O	0.48376900	-0.74573800	1.46415500
C	0.10320700	-2.47713600	-1.58941700
O	-0.84035300	-3.12133500	-1.02787100
C	-3.05526000	-0.45111200	-1.82092600
O	-3.30120500	-1.54631900	-1.22268600
C	-2.92318200	0.20421900	1.80585500
O	-1.96182600	0.84185000	1.25234700
Rh	-2.06200100	-2.14797900	0.31437300
O	-3.20019100	-1.02145600	1.62870400
O	0.38463200	-1.24600200	-1.40351100
O	-2.08176400	0.33605400	-1.57234200
O	-0.73673700	-2.62625100	1.81859100
C	1.22599100	-2.27424900	3.11693700
H	0.74579800	-2.92178200	3.85275800
H	2.03070900	-2.83748100	2.63049200
H	1.66864100	-1.40210500	3.60196300

C	-3.77402200	0.97928700	2.78078200
H	-3.75701800	2.04487600	2.54382100
H	-4.79909500	0.60380200	2.77339100
H	-3.36770600	0.83963600	3.78911300
C	-3.96913300	-0.04216800	-2.94851200
H	-4.12878100	1.03895700	-2.93063100
H	-3.48353800	-0.29220500	-3.89847600
H	-4.92196000	-0.57003600	-2.88841300
C	0.97483800	-3.21476300	-2.57333500
H	2.02523100	-3.08478800	-2.29723900
H	0.72209700	-4.27534400	-2.60022700
H	0.83822700	-2.77914700	-3.56850600
Br	6.48753700	-0.20314000	0.00947400
O	0.15877100	2.06431800	-2.69071400
C	2.67893000	0.79873800	-1.38764900
H	2.14832300	0.75395000	-2.32990200
O	0.19719400	2.51595600	0.82696200
C	3.99854500	0.35967400	-1.31580700
H	4.49427800	-0.01680200	-2.20386200
O	-1.49086600	3.93189600	1.36398100
N	-2.09256700	3.67316500	-1.52730300
C	4.67057000	0.40682500	-0.09496100
N	-2.94587500	4.01771800	-2.18031400
C	4.04389900	0.89197800	1.05140100
H	4.57337500	0.92486200	1.99733400
C	2.72320900	1.32841400	0.97248700
H	2.23164800	1.68606600	1.86947700
C	2.02268400	1.29135400	-0.24483600
C	0.60484000	1.67417100	-0.31980300
C	-0.02077000	2.27398000	-1.50145600
C	-1.04748700	3.20097500	-0.89515800
C	-0.81672200	3.25254200	0.49244100
C	-1.15686000	3.72974600	2.77513900
H	-0.16383400	4.13837600	2.97346900
H	-1.19609200	2.66333300	2.99913800
H	-1.91895700	4.28186500	3.32090600

2-int3-smd

O 1

Br	-6.48756700	-0.20310500	0.00946900
O	-0.15878700	2.06429100	-2.69071700
C	-2.67896400	0.79878000	-1.38765800
H	-2.14836700	0.75401800	-2.32991600
O	-0.19721300	2.51596900	0.82695200

C	-3.99858200	0.35972400	-1.31581600
H	-4.49432600	-0.01672300	-2.20387700
O	1.49088900	3.93186600	1.36396200
N	2.09266900	3.67297800	-1.52727800
C	-4.67059700	0.40684800	-0.09496400
N	2.94605900	4.01740600	-2.18024900
C	-4.04391300	0.89196400	1.05140700
H	-4.57338200	0.92482800	1.99734400
C	-2.72322100	1.32839200	0.97249400
H	-2.23164900	1.68601700	1.86948800
C	-2.02270600	1.29135900	-0.24483600
C	-0.60486200	1.67417100	-0.31980400
C	0.02076000	2.27395700	-1.50146200
C	1.04750400	3.20092900	-0.89516900
C	0.81672900	3.25251900	0.49242800
C	1.15688100	3.72972800	2.77512000
H	1.19600200	2.66330700	2.99910400
H	0.16390200	4.13846500	2.97346700
H	1.91904500	4.28175500	3.32088600
Rh	0.72836200	-0.14302600	-0.08526500
C	-0.10329800	-2.47720300	-1.58925600
O	-0.38466600	-1.24604000	-1.40345100
C	-0.23982600	-1.84753800	2.05968200
O	0.73689500	-2.62615100	1.81870600
C	2.92327400	0.20431100	1.80572300
O	3.20033200	-1.02134600	1.62854000
C	3.05514400	-0.45116400	-1.82106300
O	2.08170900	0.33604700	-1.57237100
Rh	2.06204100	-2.14794600	0.31436500
O	3.30111500	-1.54637100	-1.22283900
O	-0.48373900	-0.74573500	1.46419300
O	1.96183500	0.84189500	1.25230300
O	0.84027900	-3.12138100	-1.02771800
C	-0.97507400	-3.21491400	-2.57298300
H	-2.02539800	-3.08531700	-2.29643200
H	-0.83901100	-2.77907600	-3.56812800
H	-0.72203700	-4.27541700	-2.60014400
C	3.96887000	-0.04219900	-2.94875600
H	4.12956000	1.03876400	-2.93003100
H	4.92122700	-0.57101300	-2.88958600
H	3.48251500	-0.29088500	-3.89868500
C	3.77416000	0.97941400	2.78058300
H	4.79925000	0.60398000	2.77309700
H	3.75708200	2.04500500	2.54363600

H	3.36793900	0.83973300	3.78894800
C	-1.22582600	-2.27420800	3.11707500
H	-1.66858700	-1.40206900	3.60201000
H	-2.03047000	-2.83759700	2.63069100
H	-0.74555000	-2.92160100	3.85296500

2-TS1-smd

0 1

Rh	0.64571000	-0.41333800	0.01630500
C	0.55364500	-2.14113700	-2.32818500
O	-0.04204700	-1.14989800	-1.77752800
C	-0.11859200	-2.91569600	1.28948000
O	1.01436200	-3.38415400	0.95063400
C	2.49559500	-0.45313600	2.28192700
O	3.05103200	-1.47054500	1.75922100
C	3.13811300	0.34986100	-1.27358800
O	1.96713100	0.78832600	-1.00091600
Rh	2.34563200	-2.16475100	-0.04167800
O	3.57050400	-0.81531600	-1.01637100
O	-0.54807600	-1.73884400	1.03820800
O	1.50227500	0.18653600	1.79626200
O	1.55164400	-2.75917600	-1.84864100
C	0.01101400	-2.58234200	-3.66179300
H	0.14040600	-1.77069200	-4.38519800
H	0.52764300	-3.47521700	-4.01502400
H	-1.06165600	-2.77871900	-3.57501600
C	4.06760500	1.32846700	-1.94255600
H	4.25954000	2.15646100	-1.25316300
H	5.00797500	0.84892700	-2.21582000
H	3.58415000	1.74097300	-2.83263300
C	3.06835100	0.07411400	3.57199800
H	3.75700400	0.89423100	3.34140100
H	2.27230600	0.46924100	4.20622600
H	3.61991400	-0.71017500	4.09284000
C	-1.03465500	-3.80684000	2.08682600
H	-0.87232400	-3.60488000	3.15180600
H	-2.07828900	-3.58476600	1.85502500
H	-0.81172900	-4.85753300	1.89380800
Br	-6.95299000	-0.02833300	0.02805200
O	-0.77326700	2.02683200	2.15588300
N	-0.68192300	1.68773000	-1.63106400
C	-3.25811800	1.82372100	0.52231700
H	-2.90576900	2.77796800	0.89623500
O	0.62670800	3.84510700	-1.47281600

N	-0.67330600	1.45635100	-2.71674900
C	-4.62310400	1.56357400	0.52098300
H	-5.32406200	2.30616000	0.88425400
O	2.57004200	4.09255400	-0.33407400
N	1.55915500	3.18300700	1.83088400
C	-5.07670500	0.33421400	0.03695600
N	2.17469100	3.31043700	2.76819600
C	-4.19174300	-0.63083300	-0.44394500
H	-4.55955500	-1.57847800	-0.82065400
C	-2.82635800	-0.36181500	-0.43130300
H	-2.13437500	-1.10233900	-0.80842200
C	-2.33749800	0.86262800	0.05925800
C	-0.88011700	1.13384500	0.04553700
C	-0.35281000	2.14618200	1.00297400
C	0.81742200	3.01376500	0.74801800
C	1.29994900	3.66518800	-0.47421900
C	3.09069900	4.87127000	-1.43332900
H	2.50710700	5.78686200	-1.56060600
H	3.06951800	4.29252500	-2.35915500
H	4.11751600	5.11087600	-1.15781100

2-TS2-smd

O 1			
Rh	-0.76838200	-0.21385600	-0.12992200
C	-0.99727700	-1.37085500	2.55007600
O	-0.30038600	-0.55576500	1.85532200
C	-0.10896700	-2.99687000	-0.66725600
O	-1.30555800	-3.29552000	-0.36284300
C	-2.41985400	-0.69115300	-2.48509100
O	-3.10736400	-1.50582100	-1.79391400
C	-3.29741700	0.97232600	0.73054700
O	-2.08698400	1.26659900	0.44185300
Rh	-2.61888600	-1.80426400	0.18440700
O	-3.80208300	-0.19147700	0.72080100
O	0.39491100	-1.82220900	-0.67171700
O	-1.41834600	-0.01462100	-2.07116900
O	-2.01544700	-2.01323800	2.14696500
C	-0.53536200	-1.60474900	3.96656300
H	-1.35672100	-1.97301900	4.58345800
H	0.25695800	-2.36218700	3.95302700
H	-0.11986600	-0.68746100	4.38916700
C	-4.20225000	2.12569100	1.08486100
H	-3.61824500	3.00412600	1.36581300
H	-4.81207700	2.37320700	0.20860700

H	-4.87802100	1.84042400	1.89434300
C	-2.80005000	-0.48795500	-3.92969300
H	-3.02483600	0.56921000	-4.10118000
H	-1.94910600	-0.74954500	-4.56610500
H	-3.66375100	-1.09878300	-4.19475300
C	0.81786300	-4.11349700	-1.07566900
H	1.76446000	-4.02347000	-0.53592700
H	0.36301800	-5.08601100	-0.88329900
H	1.03678900	-4.02018800	-2.14469700
Br	6.71445800	-0.62283400	0.08702000
O	0.56888700	2.11334700	-2.56251200
C	3.22007700	1.30387000	-1.10526100
H	2.95397300	2.04883700	-1.84614700
O	0.55998200	2.25846000	1.22099200
C	4.54586500	0.89323200	-1.01215500
H	5.29983900	1.32095100	-1.66320700
O	-0.77462700	4.06661000	1.54854400
N	-0.91747600	4.23743200	-1.25976600
C	4.89076500	-0.06827700	-0.06116900
N	-1.49174200	4.99952400	-1.86551000
C	3.93479200	-0.63342700	0.78552900
H	4.22150100	-1.37624300	1.52141400
C	2.60751700	-0.24134100	0.66155000
H	1.85438700	-0.67411900	1.30699500
C	2.22479300	0.73687100	-0.28080200
C	0.82173800	1.12722700	-0.39405100
C	0.43185300	2.20180700	-1.34910600
C	-0.22149700	3.31781900	-0.63696300
C	-0.13701200	3.20021300	0.79159400
C	-0.71270700	3.83347900	2.98396100
H	0.31960200	3.91133400	3.33149700
H	-1.11569900	2.84493700	3.21307300
H	-1.32777600	4.61650000	3.42396900

2-TS3-smd

O 1

Rh	2.94037200	-0.34322800	-0.20414700
C	4.02906100	0.78082800	2.23997700
O	2.93306600	0.62324000	1.61019900
C	4.56581900	1.78428300	-1.29683700
O	5.58438300	1.13182900	-0.88775500
C	4.23796300	-1.77458900	-2.36975000
O	5.33103600	-1.63858300	-1.72571500
C	3.67228600	-2.77089000	1.21772500

O	2.65941700	-2.11603800	0.79979500
Rh	5.30579000	-0.65770100	0.07687900
O	4.88734000	-2.43496900	1.04423500
O	3.35251400	1.42121500	-1.16034800
O	3.09863000	-1.35123600	-1.98801800
O	5.16795300	0.34680700	1.86382500
C	3.97443800	1.57517500	3.51777900
H	4.82601900	1.33987000	4.15819100
H	4.01020600	2.64017600	3.26157900
H	3.03511500	1.38693700	4.04226100
C	3.40427000	-4.02668600	2.00412300
H	2.36116400	-4.33004400	1.90604300
H	4.06719500	-4.82728300	1.66710100
H	3.62609600	-3.83249600	3.05934300
C	4.29733500	-2.46292800	-3.70721600
H	3.40671300	-3.07810600	-3.85285400
H	4.30748900	-1.69643000	-4.49040500
H	5.20130600	-3.06778400	-3.79313500
C	4.81411900	3.07637300	-2.02734800
H	4.00371200	3.78058500	-1.82828100
H	5.77593600	3.50316700	-1.73823800
H	4.83128100	2.86994200	-3.10353900
Br	0.31786900	6.06985100	0.11538000
O	-0.17060600	-0.83326600	-2.35910000
C	0.05417400	2.10693900	-1.18876800
H	-0.00393200	1.58737300	-2.13804900
O	0.02958400	-0.80116300	1.19501500
C	0.12842600	3.49559200	-1.15766600
H	0.12406300	4.05856400	-2.08468200
O	-0.07903100	-2.94496000	1.94203500
N	-0.41620600	-3.49538000	-0.95619200
C	0.21147700	4.15206500	0.07100000
N	-0.60981100	-4.44144600	-1.54164400
C	0.21930300	3.43668700	1.26813800
H	0.28360200	3.95453100	2.21901000
C	0.14207200	2.04736600	1.23442000
H	0.14984200	1.49117300	2.16401700
C	0.06275200	1.36096300	0.00871800
C	-0.01818300	-0.08148700	-0.04891300
C	-0.13006700	-1.00194200	-1.13677500
C	-0.19704800	-2.33462500	-0.40189400
C	-0.08179800	-2.08138300	0.97318000
C	0.08847200	-2.42017300	3.29270500
H	-0.72139300	-1.72308400	3.51254800

H	1.05870000	-1.92520900	3.36934300
H	0.04343400	-3.29328400	3.94009200
Rh	-2.95714800	-0.25544700	-0.17069900
C	-4.13741800	1.86888900	1.40789900
O	-3.01836000	1.44298500	0.97277600
C	-3.82640200	-1.81185500	2.13022400
O	-5.01951800	-1.54521200	1.77885100
C	-4.18001700	-2.53421400	-1.50088800
O	-5.29927000	-2.11731100	-1.05471000
C	-4.48684300	1.13050800	-2.20644400
O	-3.29008600	0.87047700	-1.85428200
Rh	-5.34095100	-0.40974200	0.09093400
O	-5.54020200	0.73148900	-1.60531900
O	-2.77202100	-1.40980900	1.53229800
O	-3.04915100	-1.98250000	-1.29338700
O	-5.26780900	1.30662100	1.21919600
C	-4.12028200	3.12633600	2.23559100
H	-3.22210700	3.70874100	2.02472600
H	-5.01638400	3.71859500	2.03847900
H	-4.12197600	2.85022600	3.29618800
C	-4.66182700	2.00147400	-3.42162800
H	-3.97959700	1.67667200	-4.21114700
H	-5.69354600	1.97493500	-3.77431700
H	-4.39821300	3.03082700	-3.15495500
C	-4.19201200	-3.76311800	-2.37048800
H	-3.29047200	-4.35599300	-2.20277500
H	-5.08507200	-4.36088400	-2.18198300
H	-4.19571900	-3.44524200	-3.41924000
C	-3.63106100	-2.64915800	3.36708300
H	-2.80359100	-3.34671600	3.22000900
H	-3.37796400	-1.98931700	4.20440600
H	-4.54506800	-3.19158900	3.61286700

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O 1

Br	-5.75953200	-3.48174700	-0.14704600
O	0.99029600	-2.40776500	2.38135000
C	-1.89850600	-2.65936900	1.21230700
H	-1.41709900	-2.49763000	2.16827300
O	0.58972800	-1.06578900	-0.88913400
C	-3.26156500	-2.94791600	1.16491900
H	-3.83914400	-3.01261800	2.08060700
O	2.58281600	-0.07099300	-1.43684400
N	3.19099500	-0.59479200	1.38002500

C	-3.87345400	-3.13548500	-0.07386700
N	4.03365800	-0.21577400	2.03187300
C	-3.14594800	-3.06878600	-1.26126200
H	-3.63327400	-3.22370600	-2.21734100
C	-1.78250700	-2.79457000	-1.19891500
H	-1.20725600	-2.73313500	-2.11780100
C	-1.14800800	-2.56763500	0.03164200
C	0.29270400	-2.24456700	0.03389600
C	1.08145800	-1.94248300	1.25669700
C	2.16015400	-1.05333900	0.72317900
C	1.85932300	-0.77301200	-0.63763200
C	2.16820500	-0.01952300	-2.84268300
H	1.25938900	0.57692100	-2.93152300
H	2.02483300	-1.04526600	-3.18357300
H	3.00061600	0.45966400	-3.35417000
Rh	-0.65205700	1.03363500	-0.28801100
C	-1.43296000	0.87398100	2.48976900
O	-0.83917600	0.21843900	1.57059800
C	-3.53131800	0.96917200	-0.59426000
O	-3.55836700	2.11591300	-0.03347400
C	-0.97551100	3.13655600	-2.25153600
O	-1.57025400	3.79982500	-1.34098900
C	1.09829000	3.04056500	0.86228500
O	1.11864800	1.88572000	0.31727600
Rh	-1.78338600	2.97555900	0.52976400
O	0.05210400	3.73536300	1.07226900
O	-2.47741200	0.30157500	-0.85434400
O	-0.48924000	1.96291400	-2.11279400
O	-1.92982400	2.04044600	2.35550300
C	-1.58185800	0.19251400	3.82211100
H	-2.53514600	-0.34817000	3.82936800
H	-0.77480900	-0.52730500	3.97018500
H	-1.59842700	0.92793200	4.62867100
C	2.42790800	3.62433000	1.25771600
H	2.92650200	4.00035100	0.35727600
H	2.29754500	4.44748400	1.96133700
H	3.06284100	2.84748500	1.69139400
C	-0.81154000	3.78243200	-3.60093800
H	-1.37800500	4.71236100	-3.65905700
H	0.25046800	3.99212200	-3.76742000
H	-1.14035100	3.09049300	-4.38116300
C	-4.84770500	0.33536900	-0.95389100
H	-4.76286600	-0.19257100	-1.90574000
H	-5.10160000	-0.40360200	-0.18687700

H	-5.63815700	1.08579700	-0.99942400
C	5.28264300	-2.45610300	-0.01624700
C	4.50738400	-2.80522200	-1.05452200
H	5.00831900	-2.83257800	0.97054000
H	4.72248900	-2.44538200	-2.06010600
C	3.25340400	-3.63287900	-0.94278600
H	3.39979400	-4.59517000	-1.47101600
H	3.08557100	-3.89487000	0.12061400
O	2.16677500	-2.94000300	-1.49874100
H	1.12283000	-2.95804500	-0.66521400
C	6.46580600	-1.58202400	-0.03128300
C	7.08516700	-1.26002500	1.19105900
C	7.00260000	-1.02565300	-1.20958900
C	8.19224300	-0.41196700	1.23985500
H	6.68659400	-1.67887100	2.11168100
C	8.10708900	-0.17912700	-1.16112300
H	6.55331800	-1.25799300	-2.17037400
C	8.70912700	0.13318200	0.06329600
H	8.65100200	-0.17922600	2.19698600
H	8.50430600	0.23790000	-2.08276000
H	9.57120500	0.79336300	0.09653300

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0 1

Br	-1.46807400	5.43810600	-1.15847500
O	-0.86093500	-1.28379800	1.66752100
C	-1.12879300	1.55240700	0.34932400
H	-1.22549800	1.06474900	1.31220300
O	-0.17442600	-1.34870500	-1.85156700
C	-1.31904600	2.92384600	0.23915400
H	-1.57495100	3.50696600	1.11686000
O	0.93385300	-3.36653700	-2.15934100
N	0.29285400	-3.82308900	0.58274300
C	-1.19387400	3.54071000	-1.00840300
N	0.61717600	-4.71232200	1.22712700
C	-0.88177600	2.79770700	-2.14599100
H	-0.78703600	3.28321200	-3.11143300
C	-0.68302400	1.42341500	-2.03303800
H	-0.42453200	0.84676700	-2.91442200
C	-0.79268200	0.77331100	-0.78425900
C	-0.61186300	-0.65434700	-0.66711100
C	-0.55222200	-1.50265700	0.48192600
C	-0.11300100	-2.80795000	-0.09110800
C	-0.12170900	-2.71715400	-1.58446100

C	1. 14994100	-3. 06941300	-3. 55067700
H	1. 48200000	-2. 03526100	-3. 66657000
H	0. 23937700	-3. 24310600	-4. 13285400
H	1. 93187700	-3. 75315700	-3. 88286000
Rh	2. 35068400	-0. 03688500	0. 27338800
C	2. 80567900	1. 35541900	2. 77434600
O	1. 87488000	0. 87898000	2. 04883300
C	3. 35865600	2. 49225800	-0. 72831800
O	4. 48691300	2. 18226700	-0. 21812500
C	4. 21168900	-0. 98668200	-1. 73427800
O	5. 14906300	-0. 54388500	-0. 98998200
C	3. 66198900	-2. 13814900	1. 78394200
O	2. 54390800	-1. 83643800	1. 25487600
Rh	4. 66002500	0. 38893800	0. 77422400
O	4. 71854900	-1. 42336600	1. 73835700
O	2. 30510200	1. 78022100	-0. 67794900
O	2. 96537700	-0. 90386200	-1. 48721700
O	4. 05433800	1. 29334200	2. 51409400
C	2. 39439600	2. 08305400	4. 02660100
H	2. 16675600	3. 12258300	3. 76391700
H	1. 49249000	1. 63301700	4. 44615300
H	3. 20325700	2. 07793900	4. 75925800
C	3. 73665400	-3. 42669500	2. 55821000
H	2. 98739000	-4. 13293500	2. 19757500
H	4. 73854800	-3. 85531700	2. 48967600
H	3. 52770600	-3. 20777400	3. 61167600
C	4. 60851500	-1. 68969300	-3. 00672500
H	5. 66238100	-1. 52110200	-3. 23167400
H	4. 43393400	-2. 76374400	-2. 88284400
H	3. 98525700	-1. 34140000	-3. 83390200
C	3. 26305600	3. 79379800	-1. 48064000
H	3. 24836100	3. 57658400	-2. 55441500
H	2. 32784300	4. 30029500	-1. 23043000
H	4. 11616000	4. 43606700	-1. 25777100
C	-4. 39280500	1. 50711200	-0. 94252500
C	-4. 68232900	0. 24267400	-1. 29257500
H	-3. 57209500	2. 00636100	-1. 45601600
H	-5. 48982800	-0. 31235300	-0. 82272600
C	-3. 85294200	-0. 51662200	-2. 26364400
H	-4. 43417000	-1. 14368500	-2. 94238000
H	-3. 15460100	0. 10987800	-2. 82184200
O	-3. 05356600	-1. 49176500	-1. 46036200
H	-2. 31816900	-1. 01526500	-0. 91260400
C	-5. 06925100	2. 31191100	0. 08248000

C	-4.80120900	3.69151700	0.14208100
C	-5.94727600	1.75684400	1.03429600
C	-5.40171600	4.49730600	1.10873900
H	-4.10953600	4.13060300	-0.57072600
C	-6.54517900	2.56283500	1.99958800
H	-6.14337900	0.68872700	1.03752800
C	-6.27779400	3.93597600	2.04008500
H	-5.17875500	5.56015500	1.13777500
H	-7.21440500	2.11848700	2.73113000
H	-6.74204600	4.55926100	2.79913000
C	-4.01344500	-4.22605400	-0.67126100
C	-2.69833400	-4.46897000	-0.55924200
H	-4.47896800	-4.30723600	-1.65526200
H	-2.22882400	-4.44027500	0.41937600
C	-1.80316200	-4.57814300	-1.75800400
H	-0.90267700	-5.17285000	-1.58363300
H	-2.32872500	-4.99022700	-2.62312200
O	-1.38318700	-3.23166600	-2.18561500
H	-2.49198300	-2.20909500	-1.95787700
C	-4.89119600	-3.76073900	0.41295100
C	-6.27817900	-3.98322500	0.34321400
C	-4.38342100	-3.00483800	1.48860900
C	-7.13124300	-3.49497800	1.33288500
H	-6.68498200	-4.54717200	-0.49281600
C	-5.23825900	-2.51521600	2.47460000
H	-3.32522000	-2.76269100	1.53318600
C	-6.61372700	-2.75981500	2.40301800
H	-8.19932100	-3.68278700	1.26655900
H	-4.83111100	-1.92496000	3.29067100
H	-7.27772600	-2.37035000	3.16959800

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0 1

Rh	-2.39971400	-0.66899500	-0.05440300
C	-3.91351600	-1.82535700	-2.23442700
O	-2.72724200	-1.69980000	-1.78782900
C	-3.92562800	-2.68068300	1.37717000
O	-4.97284900	-2.00535000	1.10216300
C	-3.27525400	0.83384800	2.27604800
O	-4.45860500	0.74957100	1.80881400
C	-3.25181600	1.78471900	-1.36439800
O	-2.20582700	1.08767900	-1.13134600
Rh	-4.75880400	-0.25804300	0.04455600
O	-4.43457900	1.47527500	-1.00992300

O	-2.73833700	-2.37232100	1.03240000
O	-2.22322000	0.39248100	1.70550400
O	-4.95924400	-1.32139500	-1.70329800
C	-4.07737000	-2.61283200	-3.50614800
H	-5.10208100	-2.97295200	-3.60933100
H	-3.37243100	-3.44718000	-3.51494000
H	-3.84473200	-1.96162600	-4.35627600
C	-3.06326700	3.09102400	-2.08893800
H	-2.67661800	3.83595700	-1.38498400
H	-4.01386500	3.44644200	-2.48821300
H	-2.33176300	2.97553700	-2.89126000
C	-3.11640200	1.49550300	3.61892000
H	-3.60390300	2.47405300	3.61135700
H	-2.06304800	1.59632300	3.88163500
H	-3.61953400	0.87994200	4.37205000
C	-4.09082600	-3.92883200	2.20095500
H	-3.37953800	-4.69012300	1.87384600
H	-5.11341700	-4.30328000	2.13471300
H	-3.87126600	-3.68591600	3.24678200
Br	-0.86384900	-5.21269700	-2.25637900
O	0.75571100	0.38422400	2.06865200
C	0.31417900	-2.01460300	0.14658400
H	0.33861900	-1.80860100	1.20713000
O	1.19034100	1.25274500	-1.35343300
C	-0.14814900	-3.26108600	-0.28742300
H	-0.50182000	-3.97975400	0.43947200
O	0.12692700	3.22097700	-1.66122500
N	-0.70055900	2.85604600	1.10733000
C	-0.16734300	-3.53499800	-1.64677600
N	-1.44914300	3.43338000	1.71974700
C	0.28936900	-2.60498300	-2.58234900
H	0.27013300	-2.83372500	-3.64209200
C	0.76798500	-1.37556300	-2.14145400
H	1.13704500	-0.65900100	-2.86651400
C	0.77490400	-1.06396200	-0.77194900
C	1.38551700	0.22981300	-0.29535600
C	0.74588200	0.83855700	0.94650600
C	0.15124300	2.09840900	0.45796700
C	0.50088100	2.25548100	-0.90344200
C	0.71476200	3.30403700	-2.99966800
H	1.79311900	3.41176800	-2.87969300
H	0.45728700	2.41016400	-3.56969800
H	0.26863500	4.19162500	-3.44233900
C	2.83036700	-2.31105900	2.44192800

C	3.70151900	-1.99268800	1.47162500
H	2.62202000	-1.56374000	3.20714500
H	3.88726400	-2.67968800	0.64587200
C	4.41601600	-0.67235800	1.35941100
H	5.50407700	-0.84389200	1.49784800
H	4.11020700	-0.02199500	2.20196800
O	4.16368200	-0.09248000	0.10461600
H	2.50967500	0.12428000	-0.13970200
C	2.02181200	-3.53787200	2.53127400
C	0.85998700	-3.52904700	3.32680700
C	2.31190500	-4.70735300	1.80218400
C	0.00213800	-4.62912900	3.36647000
H	0.61798300	-2.63613200	3.89846900
C	1.45863800	-5.80823000	1.84494200
H	3.21158000	-4.75208900	1.19585700
C	0.29485600	-5.77458300	2.62132900
H	-0.89517500	-4.59062100	3.97840000
H	1.70050300	-6.69692400	1.26815800
H	-0.36976700	-6.63350200	2.65023800
C	8.23384400	1.44349500	-0.56118200
C	6.91488000	1.24975900	-0.70660400
H	8.60671700	2.46904000	-0.55076600
H	6.48678700	0.24865000	-0.70955200
C	5.89326600	2.34660200	-0.84968500
H	5.47944600	2.30837500	-1.87777700
H	6.37960100	3.33013800	-0.75130900
O	4.86580800	2.22129800	0.11658900
H	4.53025700	1.10683700	0.12924400
C	9.26904300	0.40771300	-0.40561800
C	10.61611400	0.79877900	-0.29014400
C	8.97851800	-0.97085200	-0.35751900
C	11.63388500	-0.14335300	-0.13427100
H	10.86349600	1.85745100	-0.32219500
C	9.99342700	-1.91131400	-0.20078300
H	7.95031600	-1.30958600	-0.44004700
C	11.32785300	-1.50476000	-0.08878800
H	12.66569600	0.18698300	-0.04750500
H	9.74319700	-2.96843200	-0.16475200
H	12.11675800	-2.24176200	0.03299300
C	0.56262200	5.70004700	0.83800000
C	1.49701200	5.41281900	-0.07963900
H	0.76955900	5.44483800	1.87828900
H	1.33969900	5.65977000	-1.12788800
C	2.76619500	4.66717700	0.20401600

H	3.63755400	5.30481900	-0.02994500
H	2.83072800	4.42384700	1.27697200
O	2.77337900	3.49734400	-0.60204500
H	3.60751500	2.96651100	-0.34635900
C	-0.76684000	6.28219500	0.59589000
C	-1.56640800	6.64323400	1.69652900
C	-1.31445900	6.43099200	-0.69495100
C	-2.85775100	7.14213700	1.51969200
H	-1.16674500	6.52614300	2.70075000
C	-2.60348500	6.92863700	-0.87154500
H	-0.73372000	6.14135100	-1.56497300
C	-3.38309400	7.28705600	0.23451900
H	-3.45362000	7.41328900	2.38671500
H	-3.00624400	7.03097500	-1.87556500
H	-4.38984900	7.66934400	0.09322500

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O 1

C	0.88752400	2.20524100	-0.10267600
C	-0.70107400	0.74336600	-0.96058600
H	-0.49687300	0.68906600	-2.03978800
C	-2.10918200	0.29909600	-0.65712800
C	-2.69305400	-0.71374900	-1.42416900
C	-2.81259400	0.83912200	0.42421800
C	-3.97046600	-1.18430800	-1.12325200
H	-2.15241200	-1.13980700	-2.26408100
C	-4.09398900	0.38352600	0.73148400
H	-2.35857900	1.62285000	1.02028200
C	-4.65763000	-0.62606400	-0.04672000
H	-4.42256200	-1.96754400	-1.72091400
H	-4.64203700	0.80720300	1.56545000
Br	-6.42112500	-1.25733300	0.36991400
O	-0.46664400	2.06734700	-0.47217700
C	0.35110000	-0.13536400	-0.23637800
O	0.33789100	-1.34454500	-0.15303500
C	1.37902200	0.80778500	0.28268500
N	1.94860200	0.57943400	1.48475300
N	3.01107000	0.38482000	1.91942400
O	1.04162900	3.09049900	0.93731300
C	0.64031200	4.44242800	0.64640000
H	-0.43354500	4.49344300	0.44177700
H	0.87105100	5.01885000	1.54320700
H	1.19649200	4.84241900	-0.20612700
O	1.57276900	2.58977300	-1.27469300

C	2.97134100	2.27099500	-1.17825600
H	3.39315900	2.53470300	-2.15250400
H	3.45097000	2.89008400	-0.40911200
C	3.15144200	0.80159400	-0.86894700
C	4.17405000	0.37200600	-0.01870000
H	2.79534100	0.11981900	-1.63835800
H	4.82712600	1.13099500	0.40700200
C	4.67371200	-1.01108600	0.02524400
C	6.01071200	-1.26229400	0.38196200
C	3.83981500	-2.11071800	-0.25611400
C	6.50719600	-2.56442000	0.42874900
H	6.66383100	-0.42552400	0.61651500
C	4.33870300	-3.41091000	-0.20974000
H	2.78842700	-1.94760200	-0.47524900
C	5.67518800	-3.64541800	0.12767700
H	7.54518200	-2.73509800	0.70094700
H	3.67809600	-4.24620000	-0.42540300
H	6.06007100	-4.66033200	0.16635800

