

Supporting Information

**Theoretical Insight to the Mechanism,
Regioselectivity, and Substituent Group Effect of Rh-
Catalyzed Synthesis of 1,2-Benzothiazines from NH-
Sulfoximines and Diazo Compounds**

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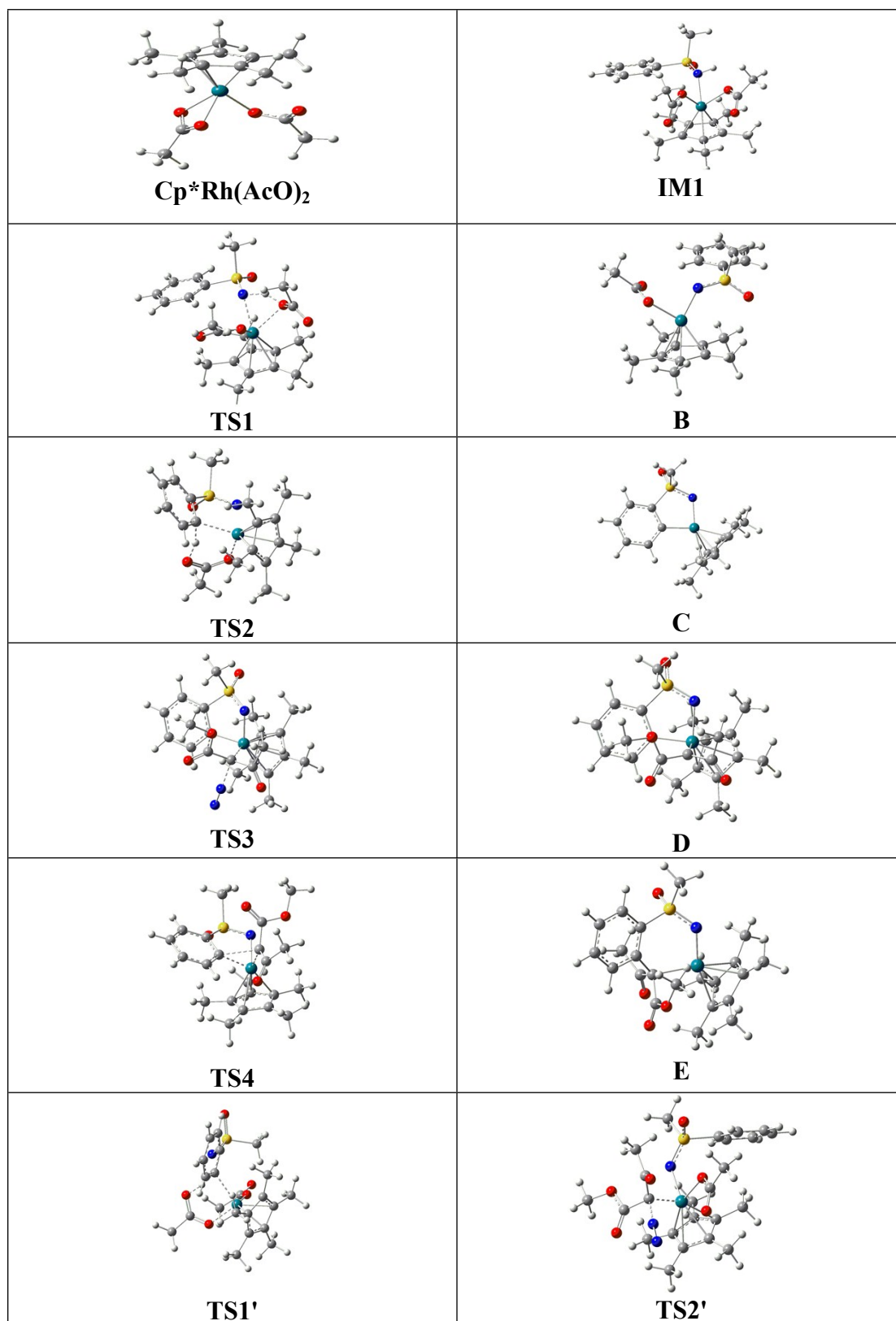
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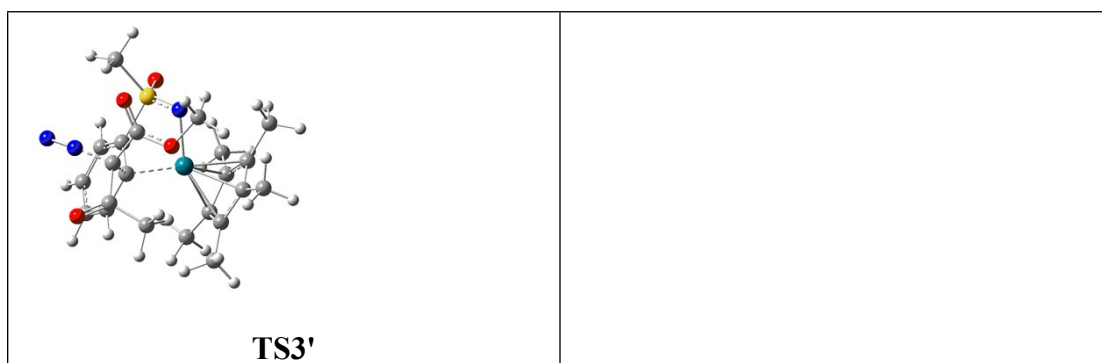


Fig. S1 Optimized geometries with selected structural parameters for the species shown in Figure 1.

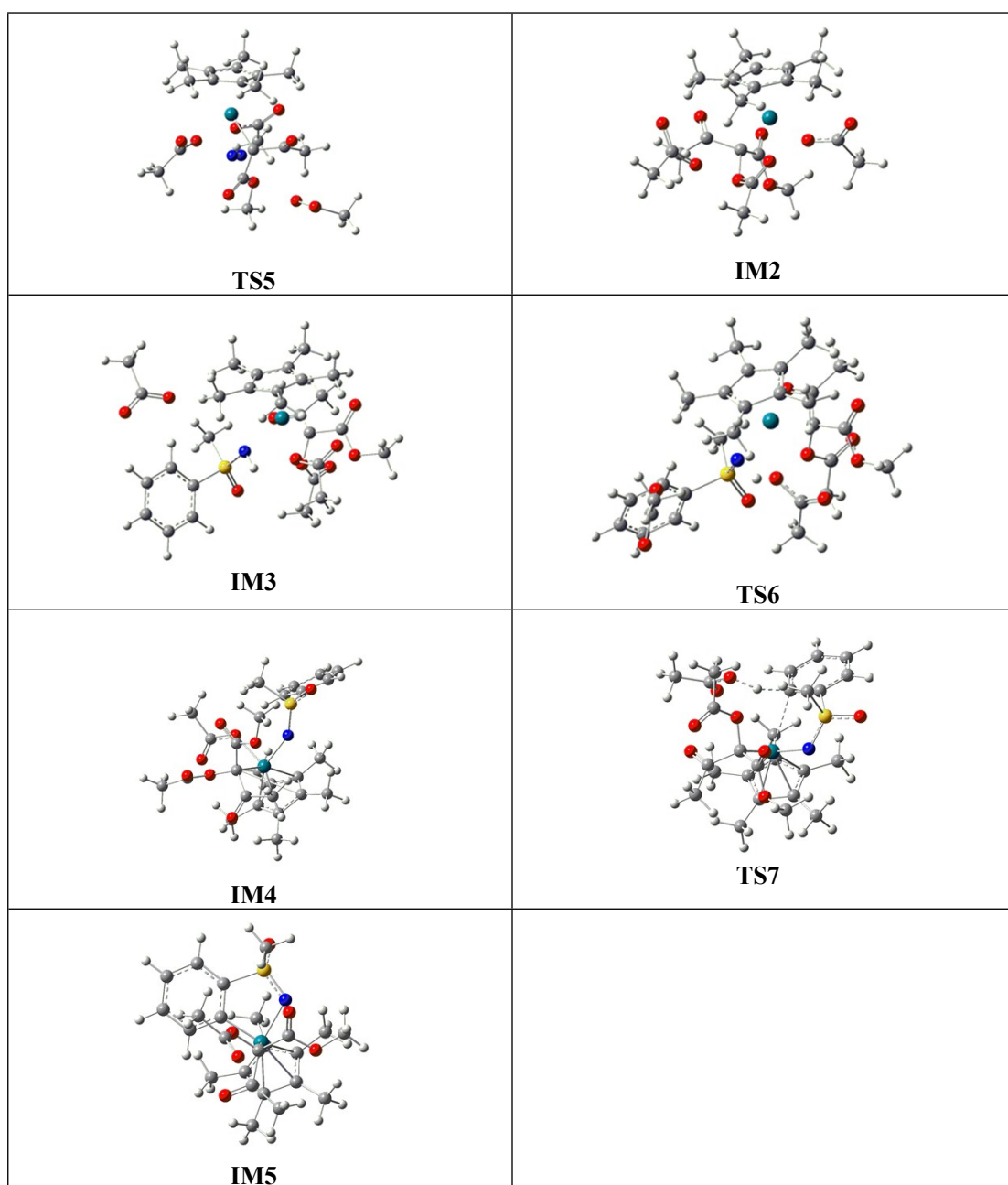


Fig. S2 Optimized geometries with selected structural parameters for the species shown in Figure 2.

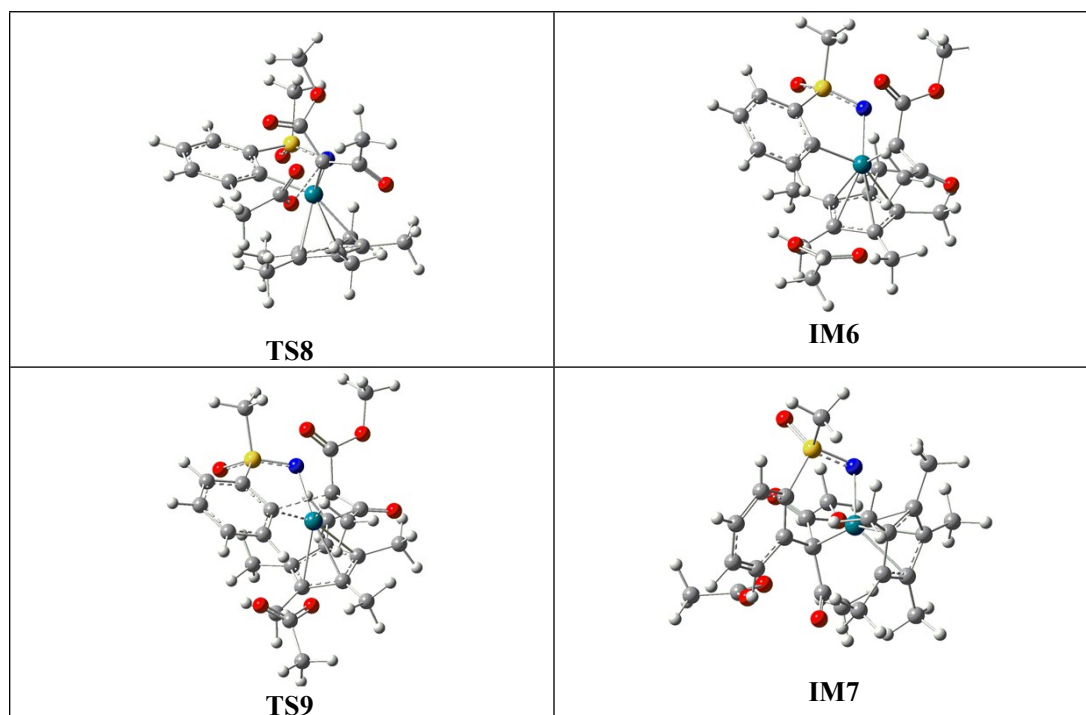


Fig. S3 Optimized geometries with selected structural parameters for the species shown in Figure 3.

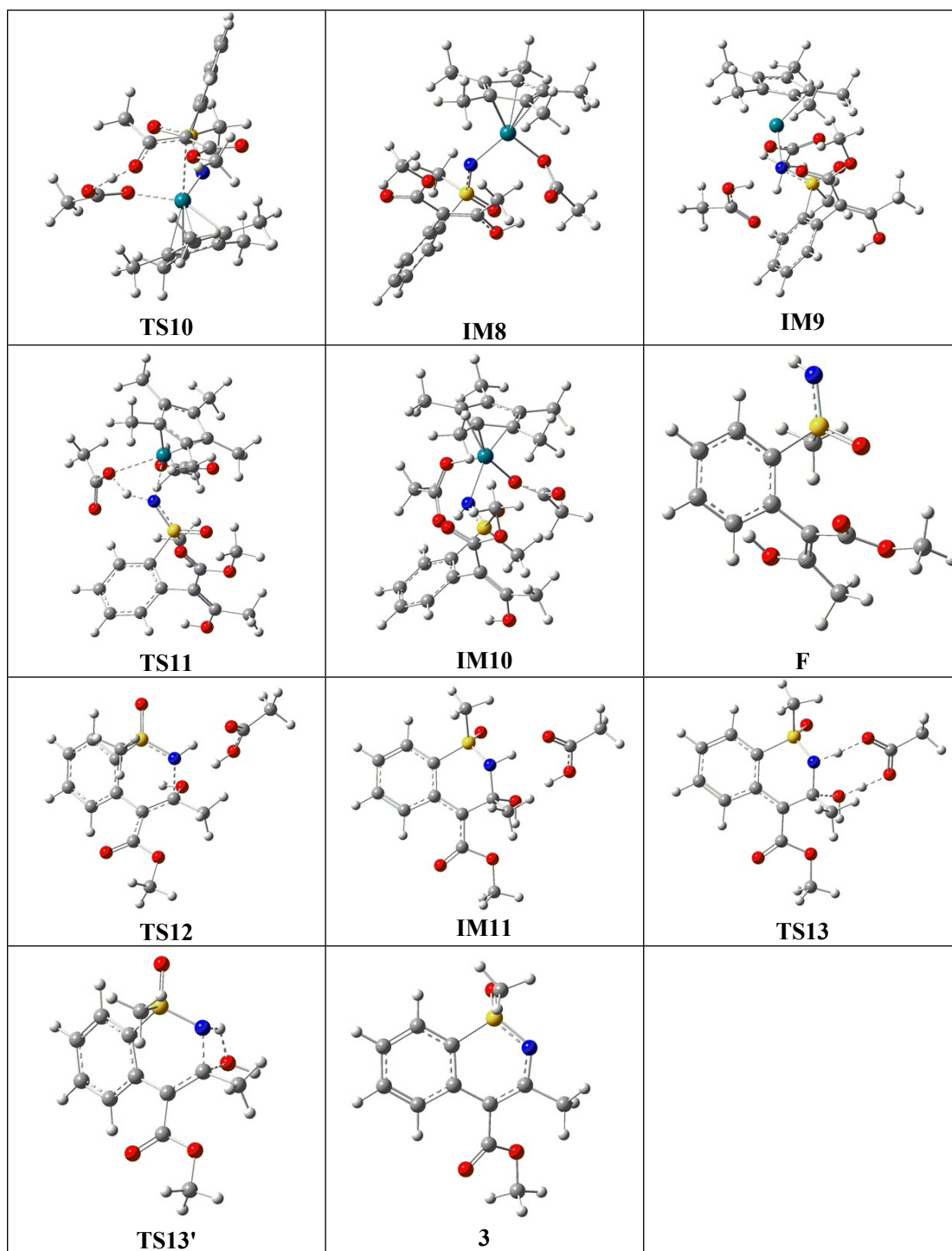


Fig. S4 Optimized geometries with selected structural parameters for the species shown in Figure 4.

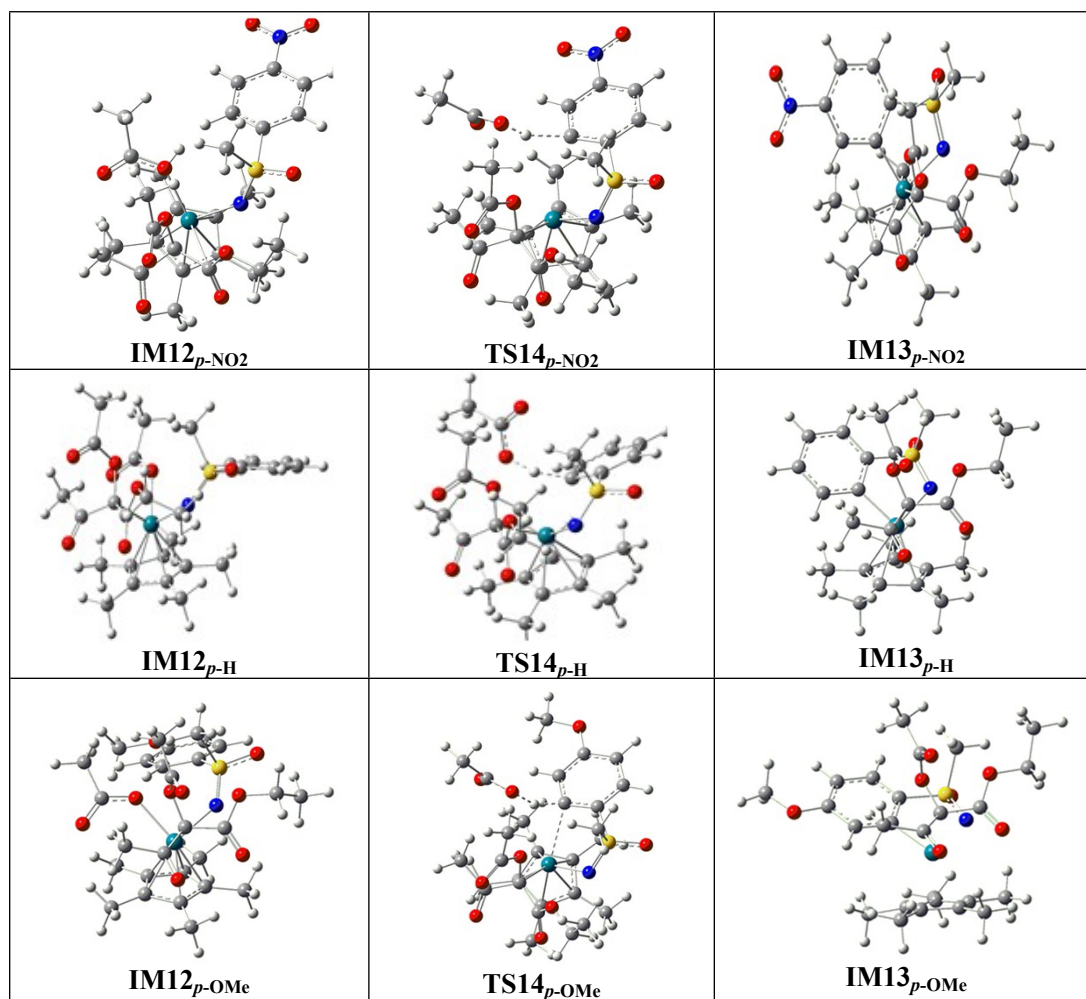


Fig. S5 Optimized geometries with selected structural parameters for the species shown in Figure 5.

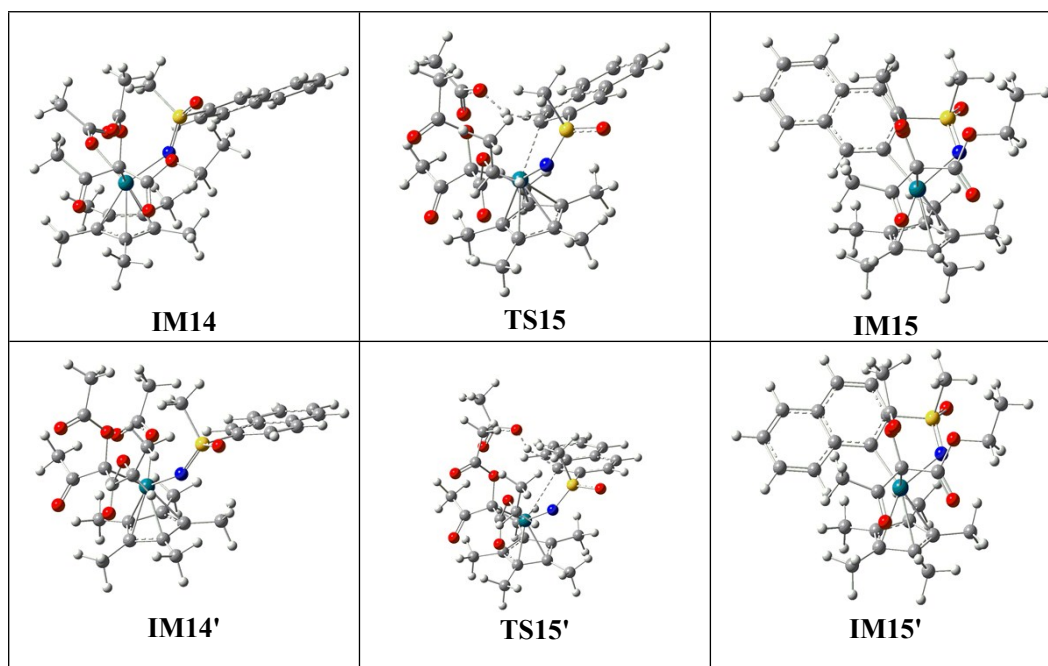


Fig. S6 Optimized geometries with selected structural parameters for the species shown in Figure 8.

Cartesian Coordinates for the Stationary Points Given in Fig. S1

Cp*Rh(AcO)₂

C	-3.01754200	-1.37220600	0.21829100
C	-3.03495700	-0.37794000	1.23586700
C	-2.93018500	0.92893800	0.59552100
C	-2.90430300	0.72172700	-0.82601500
C	-2.89681600	-0.69450500	-1.06965700
Rh	-1.14862100	-0.22869100	0.11625500
O	0.37701400	0.70489300	-0.90704300
C	0.53233900	1.99915800	-0.85533000
O	-0.23594500	2.81213500	-0.33530900
C	1.83133100	2.45810900	-1.51361500
H	2.66817300	2.23730300	-0.84228200
H	2.00864700	1.91774400	-2.44689500
H	1.79819700	3.53358600	-1.69466200
C	-3.08948400	-2.85831500	0.39359400
H	-2.33924000	-3.36397900	-0.22000600
H	-2.92098500	-3.15095000	1.43158600
H	-4.07714500	-3.23038700	0.09417400
C	-2.89588500	-1.37347400	-2.40516000
H	-3.92348300	-1.55404500	-2.74671700
H	-2.39266000	-0.76642800	-3.16050300
H	-2.38554100	-2.33874900	-2.35936100
C	-3.12698400	-0.59392300	2.71543400
H	-2.38623700	0.00961400	3.24633300
H	-4.12045800	-0.30641600	3.08066600
H	-2.95985000	-1.63896800	2.98294300
C	-2.95075100	2.25752100	1.28455700
H	-2.17764000	2.90172900	0.86017600
H	-3.93077800	2.73724700	1.16439100
H	-2.75873500	2.15093300	2.35449700
C	-2.87753400	1.80435800	-1.85924600
H	-3.89391000	2.18828600	-2.01570100
H	-2.23278700	2.62325800	-1.53690800
H	-2.50935400	1.43341700	-2.81809500
O	0.32244500	-1.85523900	0.17912700
C	0.87564300	-1.31970500	1.19205500

O	0.32558700	-0.30234700	1.72563400
C	2.17923700	-1.85159100	1.72628000
H	2.26154300	-2.92307600	1.53418400
H	3.00089200	-1.34587700	1.20791300
H	2.26766000	-1.64366700	2.79426700

IM1

C	-3.14744000	-0.89171100	0.71509300
C	-3.23604000	0.41362000	1.27488500
C	-3.13143600	1.38723400	0.19442400
C	-3.01753000	0.65805800	-1.03107700
C	-2.95779600	-0.75327600	-0.72070600
Rh	-1.27009700	0.23210400	0.23603400
O	0.13090400	1.09135600	-1.08615800
C	0.45028600	0.52273300	-2.21799700
O	-0.13521100	-0.41768600	-2.75241100
C	1.68508700	1.15230400	-2.86451300
H	1.63482800	2.24415600	-2.82345000
H	2.57757900	0.84283400	-2.30977300
H	1.77655700	0.81859200	-3.89926300
C	-3.29621900	-2.18643200	1.45157900
H	-2.60462400	-2.92695600	1.04871900
H	-3.09163900	-2.06440700	2.51804600
H	-4.32623600	-2.55307500	1.34818700
C	-2.91913600	-1.86779900	-1.71723600
H	-3.94033800	-2.13151800	-2.02613000
H	-2.34281500	-1.57197200	-2.59419000
H	-2.43007200	-2.74014500	-1.28430600
C	-3.51159800	0.75171400	2.70871100
H	-3.03973600	1.69116300	3.00326400
H	-4.59418600	0.86245900	2.85669000
H	-3.16479200	-0.03361400	3.38310700
C	-3.26305400	2.87335200	0.35136100
H	-2.83558400	3.40070300	-0.50434400
H	-4.32074700	3.15927500	0.42240400
H	-2.75687600	3.22866700	1.25215300
C	-2.95075400	1.23974100	-2.40809600
H	-3.94909500	1.21564400	-2.86389600

H	-2.61447300	2.27833700	-2.38884800
H	-2.26466300	0.66666200	-3.03283700
O	-0.66625700	-3.13506100	0.07934100
C	0.30223500	-2.41399700	0.32513200
O	0.29361900	-1.13940200	0.59197100
C	1.71554800	-3.00176300	0.32501800
H	1.67079100	-4.09010100	0.39357000
H	2.20680500	-2.72684800	-0.61455300
H	2.31773900	-2.59291500	1.14125300
C	-0.13802300	0.89461900	4.06483000
C	-0.64090800	1.22605600	5.32614800
C	0.25131400	-0.40432500	3.72949300
C	-0.73646300	0.22421600	6.29090500
H	-0.96466100	2.24102600	5.53133000
C	0.13620300	-1.39499900	4.70815900
H	0.58641400	-0.63410800	2.72000000
C	-0.34653700	-1.08236700	5.98118200
H	-1.12358800	0.46055000	7.27728400
H	0.41963000	-2.41493700	4.46725600
H	-0.42771700	-1.86107800	6.73403400
S	0.01189100	2.22012000	2.85859000
O	-0.99368000	3.27941000	3.19217800
C	1.65377300	2.94647500	3.17812400
H	2.41241300	2.17072900	3.07600200
H	1.79589500	3.73633000	2.43706800
H	1.64471600	3.37347100	4.18158900
N	0.09799600	1.48524600	1.47627000
H	0.58063400	2.01259200	0.74604700

TS1

C	0.30079800	-2.31975200	-0.04471300
C	0.14982000	-1.87153800	-1.42193900
C	1.42170700	-1.42016400	-1.87178800
C	2.40180800	-1.66558400	-0.81176400
C	1.71267800	-2.24491100	0.29269000
Rh	0.89956900	-0.25309500	-0.09410700
O	1.72554900	1.79954900	-0.89082000
C	2.77242900	2.40339200	-0.30874000

O	3.91280900	2.01479300	-0.48869400
C	2.42472600	3.58821200	0.56930500
H	1.77993800	4.29379100	0.03583100
H	1.87297400	3.21336900	1.43671700
H	3.33529300	4.09084500	0.89609500
C	-0.75195700	-2.93959400	0.81907900
H	-0.68377900	-2.54185800	1.83366600
H	-1.75414000	-2.72543900	0.44393400
H	-0.62438000	-4.02982600	0.84645400
C	2.29985600	-2.67234200	1.60174100
H	2.50909800	-3.74957900	1.58525800
H	3.23340700	-2.14744300	1.81263700
H	1.60331500	-2.46955300	2.41737500
C	-1.10801800	-1.91231400	-2.23431000
H	-1.26133100	-0.98574300	-2.79060900
H	-1.05955100	-2.74830200	-2.94354200
H	-1.98448900	-2.06276700	-1.60176800
C	1.74328500	-0.82653500	-3.20749400
H	2.46888000	-0.01635800	-3.10481300
H	2.17231900	-1.58993400	-3.86959300
H	0.84881000	-0.42259100	-3.68562100
C	3.86367700	-1.35289400	-0.91674200
H	4.39931500	-1.66060300	-0.01668800
H	4.30175400	-1.88529800	-1.76959600
H	4.03004400	-0.27825000	-1.05401300
O	-0.17254400	-0.52927400	2.92326400
C	0.74769300	0.29315200	2.82912100
O	1.41395600	0.57977700	1.75233600
C	1.18878100	1.10473700	4.04563600
H	0.88947500	0.59614600	4.96375300
H	2.26788400	1.27456100	4.03642300
H	0.69757500	2.08405900	4.01624200
C	-3.10914000	0.51919800	-0.13056500
C	-4.25720900	0.22724200	-0.87264000
C	-2.94705100	0.07453200	1.18256600
C	-5.27967300	-0.50869500	-0.27370000
H	-4.32900200	0.55857000	-1.90340300
C	-3.97812200	-0.66834400	1.76501600

H	-2.02347400	0.26075900	1.72285900
C	-5.14073400	-0.95206800	1.04507600
H	-6.17825100	-0.74246000	-0.83720200
H	-3.86149800	-1.02883700	2.78259800
H	-5.93760400	-1.52749100	1.50780600
S	-1.80525000	1.50409700	-0.92871100
O	-1.92348600	1.25833000	-2.40766200
C	-2.39244900	3.21252100	-0.66375700
H	-2.45732900	3.40678800	0.40652000
H	-1.65241700	3.86407900	-1.13261300
H	-3.36120300	3.32504700	-1.15235700
N	-0.49692900	1.37425100	-0.10219700
H	0.61253900	1.95336600	-0.53264400

B

C	-3.14877800	-0.85508700	0.80394600
C	-3.21265400	0.52752500	1.27112500
C	-2.98079400	1.37053700	0.14879300
C	-2.81299500	0.51518800	-1.02927300
C	-2.96552800	-0.84381100	-0.62469800
Rh	-1.23517600	0.06895600	0.42281000
C	-3.30855300	-2.08781100	1.63973300
H	-2.40994600	-2.70828200	1.56279100
H	-3.45270400	-1.83824300	2.69246900
H	-4.17739400	-2.66776300	1.30553800
C	-2.87003600	-2.05944600	-1.49591200
H	-3.84674500	-2.30009200	-1.93431900
H	-2.15858300	-1.91209400	-2.31159300
H	-2.53578600	-2.92409900	-0.91896100
C	-3.53343200	0.97003800	2.66605100
H	-3.01503900	1.89728800	2.91574500
H	-4.61468000	1.13037100	2.76853100
H	-3.23756100	0.21719000	3.40003400
C	-2.96899000	2.86907500	0.15709400
H	-2.40504200	3.26552700	-0.69069000
H	-3.99291800	3.25881100	0.08658400
H	-2.50989700	3.24712700	1.07293300
C	-2.57681200	1.00499600	-2.42418400

H	-2.11141800	0.23470800	-3.04271500
H	-3.52681400	1.28854100	-2.89596100
H	-1.92679700	1.88349000	-2.43436300
O	-0.04051100	-2.62997100	1.36264300
C	0.51975000	-2.25929800	0.32062800
O	0.21503500	-1.20791900	-0.37549100
C	1.69645000	-3.04740700	-0.25045800
H	1.70878900	-4.05879100	0.15961400
H	1.65468300	-3.07822300	-1.34206900
H	2.62823300	-2.54274200	0.02772500
C	-0.02614800	0.72643500	4.22405000
C	-0.35243400	1.36364900	5.42400500
C	0.14434900	-0.65685900	4.14598800
C	-0.48304100	0.59686600	6.58201500
H	-0.51975300	2.43586800	5.43812800
C	0.00038500	-1.41157100	5.31387100
H	0.34829500	-1.13509300	3.19131200
C	-0.30300600	-0.78866600	6.52633700
H	-0.73451200	1.07774900	7.52303000
H	0.12324900	-2.48961800	5.26809300
H	-0.40887100	-1.38323400	7.42951000
S	0.14620200	1.73880800	2.71043100
O	-0.81133400	2.89555000	2.87228300
C	1.81518300	2.44866000	2.91246700
H	2.54098500	1.63673800	2.94718000
H	1.98209700	3.07573300	2.03490800
H	1.83446500	3.04683700	3.82463700
N	0.25528900	0.79400500	1.47784200

TS2

Rh	0.06313800	-0.80090600	-0.57734900
N	-1.15361900	0.78426800	-0.02715300
C	0.54678500	-0.74090400	-2.74441500
C	1.07604600	-2.00646400	-2.23070900
C	-0.00795400	-2.75069600	-1.71042900
C	-1.22485100	-1.96311200	-1.88278900
C	-0.87833500	-0.77053000	-2.61162500
O	-0.45941000	-1.74432000	1.27120400

O	1. 50296800	-1. 17449300	2. 19578000
C	0. 35894200	-1. 71890200	2. 24149000
C	-0. 08074800	-2. 34539500	3. 54546200
H	0. 77622500	-2. 76412500	4. 07621800
H	-0. 51139600	-1. 54963000	4. 16250400
H	-0. 84375300	-3. 10587800	3. 37412400
C	1. 26147300	1. 81688500	0. 50584800
C	1. 77864200	0. 53129500	0. 23339500
C	2. 01160600	2. 97905400	0. 36178500
C	3. 11833500	0. 47115300	-0. 18756500
H	1. 52847900	-0. 43738900	1. 09313500
C	3. 33285800	2. 87885700	-0. 09149300
H	1. 59112800	3. 95395200	0. 59012900
C	3. 88644500	1. 62704200	-0. 36303300
H	3. 57984200	-0. 50060700	-0. 34654000
H	3. 92876700	3. 77873000	-0. 21733300
H	4. 91880200	1. 55134400	-0. 69391400
O	-0. 54765600	1. 61100600	2. 47931500
C	-1. 84978200	0. 28648500	-3. 03374400
H	-2. 18294200	0. 84645600	-2. 15038300
H	-1. 39747600	0. 98764600	-3. 73862100
H	-2. 72237700	-0. 16463500	-3. 51689700
C	-2. 60956200	-2. 39957300	-1. 51227000
H	-3. 26034400	-1. 53631700	-1. 35796200
H	-3. 04944700	-3. 02650400	-2. 29959500
H	-2. 60213500	-2. 97713000	-0. 58477300
C	0. 04170800	-4. 09914000	-1. 05954600
H	-0. 45840400	-4. 07398600	-0. 08686700
H	-0. 46574500	-4. 84696300	-1. 68112500
H	1. 06952100	-4. 43378100	-0. 90346200
C	2. 50216600	-2. 45905100	-2. 34168500
H	2. 79782000	-3. 08706500	-1. 49727300
H	2. 64836700	-3. 04490700	-3. 25868900
H	3. 18814000	-1. 61093100	-2. 38563300
C	1. 35050900	0. 29623800	-3. 47158800
H	2. 30966200	0. 47477800	-2. 97985300
H	1. 55365800	-0. 02250500	-4. 50230800
H	0. 82167200	1. 25057900	-3. 51247400

S	-0.49388800	1.75154300	0.98634300
C	-1.16649200	3.41163800	0.62892400
H	-0.77231800	4.12550100	1.35397700
H	-0.93242300	3.69659000	-0.39681800
H	-2.24541100	3.30860400	0.75601200

C

C	0.51921600	-0.87004600	-0.00450700
C	-0.09901700	0.36840800	-0.25246900
C	-1.52279400	0.11859300	-0.50513200
C	-1.77828400	-1.27195500	-0.30988500
C	-0.50997000	-1.91038200	-0.11102600
Rh	-0.39279200	-0.96242400	-2.08144700
N	1.09251100	-0.63731800	-3.29489100
S	0.90537100	-1.08025400	-4.80316100
C	0.67855200	0.44731100	-5.78129200
H	1.59154000	1.02914900	-5.64215700
H	0.55469900	0.17724000	-6.83163400
H	-0.18764400	0.99057800	-5.40363100
O	1.97372200	-1.86198400	-5.49278500
C	-0.68984900	-1.89167600	-4.90610700
C	-1.14656700	-2.51534000	-6.06492000
C	-1.38048900	-1.84447700	-3.68265700
C	-2.40618500	-3.11306100	-6.03537800
H	-0.52707700	-2.54526400	-6.95746900
C	-2.65087800	-2.44837600	-3.70332000
C	-3.15321800	-3.06596300	-4.85408100
H	-2.79804400	-3.61331700	-6.91618500
H	-3.26941700	-2.44913600	-2.81192400
H	-4.13833500	-3.52617900	-4.82603000
C	1.96731800	-1.12544100	0.28453200
H	2.32269900	-2.01737400	-0.23768200
H	2.59283500	-0.28996400	-0.03568600
H	2.12949500	-1.27859900	1.35940200
C	-0.28373300	-3.36781500	0.15213500
H	-0.31964900	-3.57576200	1.23030700
H	-1.04325900	-3.98381400	-0.33435400
H	0.69326900	-3.69001000	-0.21569100

C	0.55327900	1.71761100	-0.27841200
H	0.11646800	2.35564000	-1.05123200
H	0.42752600	2.23104700	0.68385800
H	1.62318000	1.63978000	-0.48175300
C	-2.55063300	1.18413800	-0.73755200
H	-3.42652400	0.78814000	-1.25630700
H	-2.88943000	1.61087500	0.21637600
H	-2.14812400	2.00255300	-1.33962800
C	-3.12164500	-1.93488500	-0.25038800
H	-3.49608200	-1.94228600	0.78164800
H	-3.86231000	-1.41235300	-0.86092100
H	-3.07808800	-2.97289000	-0.58890500

TS3

N	3.96132800	1.63514800	0.30612700
C	3.88981900	0.73923400	2.81565100
C	4.03979900	-0.21387500	3.82420300
H	4.74756800	-1.03158200	3.71570600
C	3.26911600	-0.09153100	4.98081100
H	3.35810300	-0.82549700	5.77655000
C	2.38669800	0.98484400	5.10811800
H	1.78122900	1.08152600	6.00593600
C	2.27332700	1.94234500	4.09400400
H	1.58102400	2.76921600	4.23137500
C	3.02843400	1.84681200	2.91744300
C	3.68707900	5.25945800	0.31273200
C	4.86327300	4.59909200	0.76793100
C	4.78514000	4.45312500	2.20465000
C	3.55922100	5.08025000	2.64008900
C	2.87600100	5.55113300	1.47498500
Rh	3.08948200	3.20593800	1.38308400
C	1.61944200	6.36926400	1.45071900
H	1.86726200	7.43481100	1.35747100
H	1.03958700	6.25476000	2.37017600
H	0.98281600	6.10209400	0.60356600
C	3.40237100	5.73310500	-1.08258000
H	3.69289600	6.78546400	-1.20416600
H	2.33943300	5.65870400	-1.32745600

H	3.96230200	5.15443600	-1.82134200
C	6.02137100	4.15066100	-0.06868100
H	5.73410900	4.01677000	-1.11348500
H	6.42114300	3.20065800	0.29202600
H	6.82171600	4.90200900	-0.03053900
C	5.88882800	3.95132600	3.09058500
H	6.65028600	4.72985900	3.23411900
H	6.37239800	3.07046300	2.66179200
H	5.50935500	3.67412200	4.07727400
C	3.16276000	5.32885900	4.06586500
H	3.62914800	6.24969400	4.44023600
H	3.47587900	4.51177100	4.71952500
H	2.08098900	5.44657100	4.17491100
C	1.26579800	2.54820300	0.64157200
N	0.03196000	3.38310700	1.56730700
N	-0.49868300	3.97429900	2.34046900
C	0.76716300	1.14454100	0.90952000
O	0.04896800	0.84875500	1.84238600
S	4.80308200	0.74399400	1.25940800
C	1.03719600	3.16816700	-0.70896800
O	0.37598000	4.19354900	-0.83189600
C	1.71646400	2.48261200	-1.87381000
H	1.04374500	1.71377000	-2.26913200
H	2.64751800	1.99725700	-1.56713700
H	1.88595400	3.23149800	-2.65021700
O	1.19391100	0.27849900	-0.01812300
C	0.76420200	-1.08292800	0.18265700
H	1.19576800	-1.64488600	-0.64490000
H	1.12715700	-1.45925200	1.14148000
H	-0.32630600	-1.14588100	0.16562800
C	4.72439200	-0.96523900	0.61877300
H	3.68612900	-1.29210900	0.58180400
H	5.14431300	-0.91571100	-0.38760700
H	5.33517900	-1.61659800	1.24557900
O	6.27095400	0.95308100	1.54492100

D

C	1.66262000	-2.07324000	0.50335800
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C	2.44274300	-1.55688600	-0.59419300
C	3.02078200	-0.31546300	-0.20347400
C	2.61035700	-0.05347900	1.15323300
C	1.79539100	-1.16192200	1.59926100
Rh	0.56971900	-0.06050200	-0.00343800
N	-0.23009300	-0.80842300	-1.71419400
S	-1.68479200	-1.38275400	-1.60206600
C	-2.21442900	-1.06251000	0.08221500
C	-3.45009500	-1.48271500	0.57582000
C	-1.25596200	-0.39245900	0.85589400
C	-3.77681300	-1.18091100	1.89684600
H	-4.13099100	-2.04327900	-0.05916000
C	-1.61984600	-0.08258600	2.17383300
C	-2.86343200	-0.47209900	2.68422700
H	-4.73167000	-1.49301400	2.30952000
H	-0.94244500	0.47930900	2.80842300
H	-3.11832600	-0.22232600	3.71105200
C	0.94526100	-3.39189700	0.49801800
H	0.29109900	-3.49348200	1.36708900
H	0.32727800	-3.50364400	-0.39824500
H	1.65797900	-4.22668700	0.52059600
C	1.34958400	-1.40495100	3.00977600
H	2.11323000	-1.98152000	3.54822000
H	1.19959700	-0.47103100	3.55636900
H	0.41615200	-1.96952700	3.04959200
C	2.53345100	-2.22149700	-1.92593600
H	3.30497800	-1.77622600	-2.55767600
H	2.74945700	-3.28955900	-1.81641600
H	1.56029700	-2.12108800	-2.42962100
C	3.99858500	0.51112200	-0.98530700
H	3.78256000	1.57997900	-0.90001200
H	5.02011700	0.35547500	-0.61403900
H	3.98963200	0.24564300	-2.04508400
C	3.13358800	1.05688100	2.01547800
H	4.13559300	0.80056300	2.38613300
H	3.19946900	1.99011300	1.45454000
H	2.49386300	1.22905700	2.88397300
C	0.19889000	1.79464400	-0.12414500

C	-1.00547200	2.48761500	0.40611200
O	-1.04290600	2.97741400	1.51683300
C	1.15480400	2.69006600	-0.84273100
O	2.19959300	3.09680700	-0.35245300
O	-2.02950600	2.53261800	-0.47487700
C	-3.22854100	3.16846500	0.01852900
H	-3.01876000	4.19315900	0.33268500
H	-3.92880100	3.15674700	-0.81613500
H	-3.62889000	2.60670500	0.86526400
C	0.73834700	3.02518400	-2.26464500
H	0.71386800	2.10682100	-2.86204600
H	1.45259300	3.73403700	-2.68843400
H	-0.27241600	3.44484200	-2.28454800
C	-2.81211500	-0.35436500	-2.61467500
H	-2.45617500	-0.45191700	-3.64242100
H	-3.83233000	-0.73385200	-2.53163000
H	-2.73323700	0.67868400	-2.27427500
O	-1.98092300	-2.79188400	-2.01345100

TS4

N	-0.87306900	-0.26484400	-1.63427700
C	-1.82517000	-1.31886700	0.65105400
C	-2.69808700	-2.05009600	1.45263200
H	-3.40951100	-2.73720900	1.00313100
C	-2.62441000	-1.90839500	2.84019200
H	-3.30606400	-2.46151400	3.47980900
C	-1.66369900	-1.06326800	3.39862300
H	-1.60650900	-0.94772100	4.47773900
C	-0.77083400	-0.35465200	2.58549400
H	-0.03905300	0.31089800	3.02922000
C	-0.83719900	-0.48352800	1.19627900
C	2.59553600	-0.04154700	-1.33263900
C	2.14218400	-1.40487400	-1.22674400
C	2.05050700	-1.72562700	0.15180600
C	2.54092900	-0.58105300	0.92176800
C	2.89943400	0.44144000	0.00743000
Rh	0.63992100	0.07812200	-0.23886600
C	3.54701100	1.74764800	0.35443900

H	4. 62610800	1. 61565000	0. 50686300
H	3. 12540600	2. 16537400	1. 27282900
H	3. 41664700	2. 48402800	-0. 44256600
C	2. 86690100	0. 68657700	-2. 61507500
H	3. 85557500	0. 41910300	-3. 01210800
H	2. 84811600	1. 76978200	-2. 47421400
H	2. 12231900	0. 43706500	-3. 37428900
C	1. 79329800	-2. 31314300	-2. 36719100
H	2. 60631800	-3. 03104300	-2. 53779900
H	1. 64417400	-1. 74942700	-3. 28969200
H	0. 87211100	-2. 86581200	-2. 16849900
C	1. 61499000	-3. 04826100	0. 70990400
H	2. 45357600	-3. 75704800	0. 72447000
H	0. 81375900	-3. 48057800	0. 10502000
H	1. 24639200	-2. 94877200	1. 73319400
C	2. 77526900	-0. 55897700	2. 40205800
H	3. 79780800	-0. 88895000	2. 62894700
H	2. 09069800	-1. 22897300	2. 92624800
H	2. 64005400	0. 44575800	2. 80525300
C	-0. 39618700	1. 58933400	0. 32447300
C	-1. 70878700	1. 91783900	-0. 33534100
O	-2. 82055000	1. 59277900	0. 03110700
O	-1. 47843200	2. 75945100	-1. 36738000
C	-2. 64541700	3. 17739400	-2. 09414000
H	-3. 07476200	2. 32603200	-2. 62762600
H	-2. 29653900	3. 92884400	-2. 80240500
H	-3. 39619900	3. 59777500	-1. 42057500
S	-1. 73719600	-1. 46408900	-1. 15117100
C	0. 12581800	2. 56747000	1. 31550900
O	0. 90446500	2. 23542300	2. 20896700
C	-0. 30029400	4. 02079700	1. 17436300
H	-1. 36457300	4. 12054800	1. 41905100
H	-0. 17032400	4. 37772800	0. 14948500
H	0. 28767100	4. 62473400	1. 86680200
O	-1. 44746300	-2. 91310000	-1. 45871100
C	-3. 43689900	-1. 17100800	-1. 73985900
H	-3. 79468700	-0. 24026600	-1. 29910300
H	-3. 36093500	-1. 08749000	-2. 82579400

H	-4.06211900	-2.02438700	-1.47293600
E			
C	1.22293800	-0.62703900	-0.34167000
C	0.07159800	0.28280100	-0.23350300
C	-1.04778200	-0.45359000	0.24391300
C	-0.65256100	-1.83572000	0.28838900
C	0.78308000	-1.92320500	0.00365000
Rh	-0.33461500	-1.26440200	-1.80133300
N	0.76458500	-2.08860000	-3.20286500
S	0.23149100	-2.84920100	-4.44990300
C	1.65274900	-2.85364100	-5.59785900
H	2.47479600	-3.24146700	-4.99511400
H	1.45710200	-3.51870900	-6.43897700
H	1.86983000	-1.83640300	-5.92475900
O	-0.22670000	-4.27448500	-4.35418700
C	-1.05650900	-1.92928100	-5.35735200
C	-1.12126000	-2.07812600	-6.74939600
C	-1.98832600	-1.14172300	-4.65404500
C	-2.09179100	-1.40961000	-7.48779600
H	-0.41660700	-2.72287400	-7.26231800
C	-2.96765600	-0.49078000	-5.43578100
C	-3.01853700	-0.60622400	-6.82109700
H	-2.12888000	-1.52302900	-8.56695600
H	-3.71311700	0.11618800	-4.92973500
H	-3.78995600	-0.08116100	-7.37682200
C	2.61371500	-0.22360900	-0.72313800
H	3.16190600	-1.05955500	-1.16192700
H	2.60843600	0.59017100	-1.45267600
H	3.16956400	0.12438500	0.15709300
C	1.60404600	-3.17451700	0.05114200
H	1.96913600	-3.35745900	1.06999700
H	1.01835200	-4.04380300	-0.25632100
H	2.46671100	-3.10871500	-0.61454900
C	0.11874300	1.76468700	-0.44529700
H	-0.81690800	2.13764900	-0.86652500
H	0.29104100	2.27402300	0.51212800
H	0.93110100	2.04837000	-1.11847000

C	-2.37519300	0.09098600	0.66915900
H	-3.18699700	-0.47723700	0.21359000
H	-2.45863000	0.03509700	1.76255300
H	-2.49762500	1.13148400	0.36773700
C	-1.51758200	-2.96557200	0.74894400
H	-1.52754500	-2.99916300	1.84719900
H	-2.54277100	-2.83702300	0.39763600
H	-1.14568600	-3.92849100	0.39111900
C	-2.09864300	-0.98938600	-3.14301600
C	-3.04037500	-2.03041600	-2.54124900
C	-3.31526900	-3.30246000	-3.33242900
H	-3.87568500	-3.07349000	-4.24535900
H	-2.39574900	-3.81230200	-3.63366500
H	-3.91460000	-3.96182300	-2.70288400
O	-3.57931300	-1.89213400	-1.44976000
C	-2.47204000	0.43623100	-2.78341400
O	-1.71304400	1.47947300	-3.27984900
C	-0.53442000	1.35839100	-4.07569000
H	0.08166900	0.50274500	-3.78549100
H	-0.78713200	1.28288600	-5.13745300
O	-3.40954800	0.77186100	-2.09318600
H	0.03031800	2.27966600	-3.90840600

TS1'

Rh	-0.75370600	-0.49839200	0.05560200
N	1.36407000	3.02053500	0.34930300
C	-0.13295800	-2.08944200	-1.40767400
C	-0.60376100	-2.75064000	-0.19912100
C	-1.97177400	-2.37758400	-0.00883800
C	-2.35013000	-1.47099500	-1.06349900
C	-1.21816500	-1.34462200	-1.96135500
O	-1.61855500	-0.02182400	1.94422300
O	0.13215000	1.16886300	2.68655600
C	-1.02573000	0.67170300	2.82773600
C	-1.76124500	0.95937800	4.11571600
H	-1.05683800	1.01491200	4.94729800
H	-2.24944600	1.93519000	4.02004000
H	-2.52609300	0.20449400	4.30259400

C	2.45356200	0.62867400	0.05844500
C	1.43545400	-0.02182400	0.79613600
C	3.75216700	0.12602600	-0.04338600
C	1.85804200	-1.17585700	1.49658300
H	0.63157300	0.73299800	1.64782100
C	4.09559500	-1.06036200	0.60732100
H	4.49155600	0.69935800	-0.59278600
C	3.14823000	-1.70077500	1.40598400
H	1.14838700	-1.66381000	2.16026100
H	5.10701700	-1.44883700	0.52855100
H	3.41714200	-2.59097800	1.96933800
O	3.67612500	2.77898300	-0.99645000
C	-1.23147100	-0.53506900	-3.21592600
H	-1.44014200	0.51256700	-2.97097900
H	-0.27836800	-0.58621400	-3.74510400
H	-2.01567800	-0.89860400	-3.88991300
C	-3.70375000	-0.86901800	-1.28186400
H	-3.61558200	0.14241200	-1.68513400
H	-4.28749700	-1.46963400	-1.99164200
H	-4.26649100	-0.81327600	-0.34706200
C	-2.87115600	-2.80767700	1.10874900
H	-3.19587700	-1.94054200	1.69251100
H	-3.76173100	-3.30606400	0.71016200
H	-2.36873200	-3.50129800	1.78533700
C	0.13306900	-3.81327700	0.55987500
H	-0.13660800	-3.82025600	1.61893500
H	-0.11085700	-4.80240600	0.15048200
H	1.21316200	-3.68108100	0.48990000
C	1.21988600	-2.28012800	-2.02157200
H	2.00358100	-2.31559800	-1.26198800
H	1.24867500	-3.22354000	-2.58195200
H	1.46188700	-1.47210800	-2.71368500
S	2.29081800	2.29989300	-0.67222300
C	1.53422100	2.04333100	-2.31361100
H	2.19615800	1.39546900	-2.89152900
H	0.52943700	1.64638000	-2.17782700
H	1.48934200	3.03258000	-2.77426700
H	1.08868200	3.92808100	-0.03167600

O	-1.10982500	1.35192800	-0.85679800
C	-1.51178500	2.58316100	-0.60869500
O	-1.45915000	3.43316500	-1.49302400
C	-2.04726100	2.92347600	0.76974000
H	-1.19926600	3.00325300	1.45575000
H	-2.56278000	3.88405600	0.72519800
H	-2.72330500	2.14748800	1.13670000

TS2'

N	-0.57552900	-0.71095400	-1.46897200
C	-3.39163500	-0.37901400	-0.84300000
C	-3.95097400	-0.53231600	0.42660500
H	-3.53306500	-1.27684400	1.09370200
C	-5.03713400	0.26180500	0.79840400
H	-5.47492200	0.14636000	1.78605000
C	-5.57256600	1.18894700	-0.09937000
H	-6.42618800	1.79575500	0.18888000
C	-5.01525900	1.32878800	-1.37260300
H	-5.43612100	2.04062600	-2.07742800
C	-3.91504100	0.55139700	-1.74411200
C	1.42738400	2.03772900	-1.18620600
C	0.00722600	2.25618000	-1.24602500
C	-0.47066800	2.45268700	0.08455100
C	0.68216200	2.48271800	0.96883600
C	1.84387000	2.25820500	0.18677600
Rh	0.46352700	0.36910100	-0.00100800
C	3.26251900	2.38662800	0.64932300
H	3.64442100	3.38045000	0.38013600
H	3.34353700	2.29135400	1.73394800
H	3.91275100	1.64361200	0.18275400
C	2.33134800	1.93893200	-2.37988300
H	2.55663200	2.93668300	-2.78080100
H	3.28212200	1.46709200	-2.12337200
H	1.86159800	1.36025300	-3.18006600
C	-0.78627700	2.24842600	-2.51270400
H	-0.33905200	2.93052400	-3.24461200
H	-0.79644400	1.23594800	-2.93218300
H	-1.81756600	2.56074500	-2.34141400

C	-1.87134800	2.75231000	0.52550400
H	-1.96324200	3.80215800	0.83257700
H	-2.59648400	2.56381600	-0.26640200
H	-2.15163900	2.12997000	1.37946100
C	0.63819100	2.87844400	2.41274200
H	0.66381300	3.97433700	2.49293000
H	-0.27221800	2.52464400	2.89766000
H	1.47576300	2.46686400	2.97432600
C	1.85453400	-1.16304600	0.16823900
N	2.89376800	-0.75261400	1.61824400
N	3.51597700	-0.32269500	2.42307000
C	1.47820400	-2.55360700	0.67991800
O	1.73116000	-2.86673800	1.82997400
S	-1.92896500	-1.43194800	-1.27229300
C	-2.36843800	-1.97209600	-2.96558100
H	-3.35784400	-2.43044700	-2.92763600
H	-2.33572700	-1.13893600	-3.66630400
H	-1.61272400	-2.71306700	-3.22883000
C	2.94821000	-1.08975500	-0.87143100
O	4.01252300	-0.51241000	-0.73687000
O	2.58737300	-1.73625400	-1.98876700
C	3.55563300	-1.72714800	-3.05655200
H	3.71116800	-0.71059600	-3.42267600
H	4.50782500	-2.13719200	-2.71320400
H	3.12349400	-2.35146200	-3.83740300
C	0.80613000	-3.50302100	-0.27264600
H	1.10192000	-4.51482900	0.01494700
H	-0.27793500	-3.38998300	-0.14739600
H	1.04173300	-3.30177100	-1.31518400
O	-2.16133500	-2.64933500	-0.41331800
H	-3.48069600	0.67107100	-2.73143900
C	-1.26651500	-1.38658000	3.59597500
H	-1.10163900	-2.45337900	3.41452700
H	-2.31418700	-1.17139900	3.36949800
H	-1.05179800	-1.16359800	4.64223700
C	-0.33529700	-0.58716100	2.69021100
O	0.66447000	-0.02355500	3.13908600
O	-0.70608900	-0.60452900	1.43836800

	TS3'		
Rh	0. 89603900	0. 04897500	−0. 05783200
C	2. 74003300	0. 12857500	1. 27941800
C	2. 27135000	1. 46586800	1. 11094800
C	3. 12146400	−0. 38734100	−0. 02541300
C	2. 28981500	1. 76439300	−0. 30435600
C	2. 86150200	0. 62386500	−0. 99097400
C	2. 90808200	−0. 59952200	2. 58024000
H	3. 96325800	−0. 62832300	2. 88103300
H	2. 55440300	−1. 63269600	2. 51061200
H	2. 34646800	−0. 11578300	3. 38242100
C	1. 92794600	2. 42257200	2. 21524100
H	2. 84096700	2. 82635000	2. 67200600
H	1. 35087200	1. 94191500	3. 01083100
H	1. 34859500	3. 27236400	1. 84709100
C	1. 97334600	3. 07851200	−0. 95161200
H	2. 86541900	3. 71802000	−1. 00321600
H	1. 20348300	3. 62781600	−0. 40383000
H	1. 61551300	2. 92864000	−1. 97315700
C	3. 10020400	0. 53203900	−2. 46865300
H	3. 79692400	1. 31095900	−2. 80152700
H	2. 15993000	0. 64144300	−3. 01790300
H	3. 52311000	−0. 43820100	−2. 73721600
C	3. 68217800	−1. 75107100	−0. 30989300
H	3. 66040800	−2. 38019900	0. 58281900
H	4. 72597700	−1. 68358900	−0. 64160300
H	3. 10442400	−2. 25940100	−1. 08754100
C	−0. 60143800	−1. 69805200	0. 22924300
C	−0. 34992700	−2. 89748000	0. 95512000
C	−0. 41167400	−2. 90371700	2. 32680800
C	−0. 69867000	−1. 69237600	3. 01277000
C	−0. 92773800	−0. 52153600	2. 33223100
C	−0. 88953100	−0. 43382300	0. 88713600
H	−0. 10638400	−3. 79183900	0. 39006000
H	−0. 24190400	−3. 81947500	2. 88484800
H	−0. 71164400	−1. 68409200	4. 09974800
H	−1. 12298200	0. 37748200	2. 90983700
O	0. 54086400	−2. 87834300	−1. 86394300

C	-2.45479800	0.52252100	0.34594300
C	-2.70396600	1.57731700	1.44318300
C	-2.48393100	1.01305900	-1.10218100
N	-3.48004400	-0.42697400	0.46387100
N	-3.92985700	-1.44201300	0.69621100
O	-3.60779400	1.41458700	2.23987000
O	-3.22352700	0.53436100	-1.93968700
O	-1.73384700	2.10255400	-1.26689000
C	-1.57286800	2.51902500	-2.63968100
H	-0.99930600	3.44445800	-2.59496000
H	-1.02436100	1.73633300	-3.16705300
H	-2.54695500	2.68753300	-3.10306300
C	-1.76751600	2.75683100	1.50248300
H	-1.80044500	3.16567500	2.51408000
H	-0.75520900	2.47142000	1.21315600
H	-2.10311800	3.52162900	0.79588400
S	-0.41259300	-1.74384900	-1.58953900
C	-1.95179700	-2.32620000	-2.39057600
H	-1.71071200	-2.40440700	-3.45279200
H	-2.17991700	-3.31587800	-1.99222000
H	-2.75722100	-1.61166400	-2.23219700
N	-0.14692600	-0.23884000	-1.87871200

Cartesian Coordinates for the Stationary Points Given in Fig. S2

TS5

C	2.58101300	-0.93462700	1.38698200
C	1.75240300	-2.04267100	0.95730700
C	2.06962600	-2.30150400	-0.42642100
C	2.98375700	-1.30141300	-0.87362000
C	3.32317300	-0.46751300	0.26393500
Rh	1.08479600	-0.24746800	-0.22346600
C	4.41663000	0.55579700	0.27914900
H	5.38033000	0.05263200	0.44713500
H	4.46665600	1.10351300	-0.66125000
H	4.26954000	1.29944800	1.06133100
C	2.73233200	-0.46491800	2.80247600

H	3.33227300	-1.18961500	3.36887300
H	3.24744100	0.49715700	2.85008700
H	1.76695500	-0.36131700	3.30277900
C	0.91123200	-2.90878200	1.84698800
H	0.56328400	-2.35074200	2.72003300
H	0.03564100	-3.26366500	1.30142500
H	1.48635200	-3.77227400	2.20952400
C	1.57310000	-3.45410900	-1.24317300
H	2.27774300	-4.29254600	-1.15070800
H	0.58462300	-3.77054900	-0.91406600
H	1.50637000	-3.19223200	-2.30193400
C	3.58668400	-1.18335200	-2.24157600
H	4.57608300	-1.65934800	-2.28268800
H	2.95443600	-1.65853700	-2.99487100
H	3.70664700	-0.13510600	-2.52621600
C	-0.30421400	0.81134700	0.89600700
N	0.70043900	2.06303900	1.82268600
N	1.43484500	2.73259600	2.30363900
C	-1.16300000	1.83800200	0.15734900
O	-0.95484700	3.03748000	0.17031300
C	-0.91923900	0.14507400	2.11815700
O	-0.38407500	0.28088900	3.21604400
O	-0.41782800	-0.72291100	-1.58522100
C	-1.28264000	-1.68318600	-1.41547000
O	-1.25591900	-2.54000700	-0.51972900
C	-2.41576900	-1.66356000	-2.42786000
H	-3.29640300	-1.20516900	-1.95095100
H	-2.15373300	-1.08791400	-3.31797500
H	-2.67604100	-2.69067400	-2.69914400
O	1.10362800	1.39651300	-1.53144800
C	1.76692700	2.49333100	-1.31544300
O	2.54599900	2.71634400	-0.38404600
C	1.45584100	3.57307000	-2.35120500
H	0.50556500	4.03827500	-2.06939200
H	2.24045200	4.33289000	-2.35056400
H	1.33607100	3.14291000	-3.34867700
O	-2.14995100	1.20779700	-0.43319600
C	-3.12897300	2.00538100	-1.15279000

H	-2.65012000	2.41199600	-2.04808500
H	-3.93559700	1.29830900	-1.36843900
H	-3.47377700	2.81612300	-0.50945800
C	-2.15684900	-0.66790800	1.90760600
H	-2.40079400	-1.12968200	2.86716700
H	-1.99434600	-1.43623900	1.14524900
H	-3.01728900	-0.06704100	1.55031400
C	-6.88605800	-0.78421300	0.50303100
H	-6.69822000	-1.78753400	0.90729900
H	-7.55863100	-0.88742200	-0.35408500
H	-7.36535800	-0.19768400	1.29357900
C	-5.53506800	-0.14441100	0.08452300
O	-4.89247400	0.43127000	1.00426000
O	-5.21258500	-0.28367400	-1.12951400

IM2

C	1.32008800	-2.47092300	0.66704500
C	0.56289000	-1.83199600	1.71577000
C	-0.81834800	-1.74849600	1.27176000
C	-0.87634000	-2.27594100	-0.05912500
C	0.44120300	-2.74019200	-0.43561700
Rh	0.52097200	-0.53038600	-0.04568500
C	0.81361500	-3.45478100	-1.69962500
H	0.93529500	-4.53157700	-1.51507500
H	0.03829700	-3.33604400	-2.46016700
H	1.74459900	-3.04604500	-2.09695500
C	2.77491200	-2.82501900	0.71774700
H	2.89209600	-3.87451000	1.02198400
H	3.23398900	-2.68400200	-0.26233000
H	3.30839600	-2.20481100	1.44158500
C	1.05214900	-1.46797000	3.08383600
H	2.14325100	-1.47436500	3.13164500
H	0.70593600	-0.46883100	3.36194600
H	0.67505000	-2.18798600	3.82337100
C	-2.00880400	-1.38998200	2.10802600
H	-2.32205000	-2.28810800	2.66160300
H	-1.76535000	-0.62386900	2.84621300
H	-2.86564300	-1.06454000	1.50362200
C	-2.11617900	-2.31477200	-0.89569600

H	-2.86969200	-2.95718400	-0.42607000
H	-2.56319200	-1.31520500	-0.97784500
H	-1.90778700	-2.69572700	-1.89784100
C	0.16992000	1.52578300	0.65283600
C	1.50433500	2.14691100	0.96445800
O	2.20571800	1.84027000	1.90523300
C	-0.78338800	1.61717900	1.82383500
O	-0.42464600	1.35470700	2.96726400
O	-0.33474600	0.41091500	-1.77140000
C	-0.71545200	1.57360400	-1.57492700
O	-0.46526900	2.23967200	-0.46798900
C	-1.56387500	2.30572500	-2.56317900
H	-1.31371200	1.98604800	-3.57592500
H	-2.59266900	1.99056800	-2.32155900
H	-1.45957100	3.38622400	-2.45345500
O	2.32614000	0.34219000	-0.76909600
C	3.12543000	-0.17826600	-1.64132000
O	3.09544700	-1.31933400	-2.11928300
C	4.23871800	0.78979600	-2.06657000
H	4.92033300	0.95578500	-1.22470000
H	4.80056000	0.37493600	-2.90586500
H	3.81312800	1.75969600	-2.33910500
O	1.83502600	3.14658700	0.10134700
C	3.12617700	3.70938500	0.33247300
H	3.90187000	2.94529200	0.23527200
H	3.25485500	4.48052700	-0.42985800
H	3.19220000	4.14924700	1.33241800
C	-2.20430300	2.04574100	1.53096300
H	-2.78081600	1.97391800	2.45478000
H	-2.66641000	1.44086200	0.73745900
H	-2.20972100	3.08226300	1.17323800
C	-5.96461700	0.66423600	-1.29928700
H	-6.07530800	1.74815400	-1.17304900
H	-6.85218900	0.16372800	-0.90299200
H	-5.88673500	0.47757300	-2.37671800
C	-4.67854000	0.18447500	-0.58353900
O	-3.59164300	0.66867900	-1.04111400
O	-4.80481500	-0.61889000	0.36641700

IM3

C	-1.82174700	-2.60020400	0.90810900
C	-1.34327200	-2.77271200	-0.44059100
C	0.07556800	-2.60011200	-0.44261400
C	0.50520000	-2.44288200	0.94787100
C	-0.64994300	-2.45114200	1.76196600
Rh	-0.86605500	-0.71432600	0.31610600
C	-0.68440600	-2.34874600	3.25609200
H	-0.73001900	-3.35380100	3.69839300
H	0.21431500	-1.86015300	3.63997100
H	-1.55932900	-1.78571200	3.58581600
C	-3.21898900	-2.83878000	1.39336000
H	-3.33304400	-3.88505700	1.71281600
H	-3.44174300	-2.17645500	2.23097000
H	-3.94708100	-2.63241800	0.60791100
C	-2.17808100	-3.20645800	-1.60392500
H	-3.17880200	-2.77678100	-1.54855700
H	-1.72228400	-2.92556200	-2.55524900
H	-2.27101200	-4.30153700	-1.59278100
C	0.96952200	-2.79450800	-1.63323800
H	0.96705700	-3.85579700	-1.92062400
H	0.60709800	-2.22403400	-2.49361400
H	2.00707500	-2.50934400	-1.43271600
C	1.91897500	-2.34051600	1.42784500
H	2.25390100	-3.32222000	1.79172400
H	2.60941300	-2.02887400	0.63895600
H	2.00412000	-1.63676600	2.26055500
C	-2.12625500	0.50999700	-1.02314900
C	-3.52959000	0.31187800	-0.53590600
O	-4.21752800	-0.67832300	-0.75458800
C	-1.83865100	0.10968100	-2.46734500
O	-0.71907400	0.28890500	-2.93177100
O	-3.00769900	2.63571600	-2.46115900
C	-2.22680800	2.83239300	-1.54959400
O	-1.67822300	1.85561100	-0.79567700
C	-1.74285200	4.18586600	-1.09684300
H	-0.65057400	4.18430600	-1.07926700
H	-2.12819800	4.95361700	-1.76860700

H	-2.09627400	4.37220900	-0.07746800
O	-1.25422900	0.75956100	1.80843200
C	-2.18673200	0.80695100	2.70114600
O	-3.05633300	-0.04445600	2.93194200
C	-2.15831000	2.10673200	3.51279600
H	-2.54396700	2.91907700	2.88716600
H	-2.78396200	2.01268300	4.40281000
H	-1.13478800	2.36856000	3.79503000
C	3.27539800	2.06589800	0.22874800
C	3.44449900	3.38884100	0.64407000
C	4.22500400	1.07815800	0.49114800
C	4.59306600	3.72121100	1.36339500
H	2.69500700	4.13049700	0.38981100
C	5.38377500	1.43511800	1.18346300
H	4.11616900	0.05031600	0.13889200
C	5.56115600	2.74660200	1.62960100
H	4.73836800	4.74413300	1.70142200
H	6.12763100	0.65836600	1.33240600
H	6.46141500	3.01832800	2.17591600
S	1.75576200	1.65054500	-0.67918000
N	0.89506500	0.69533600	0.26109300
H	0.59742900	1.24503400	1.07295200
O	-3.97883800	1.34000400	0.21647000
C	-5.25111400	1.13600300	0.84549600
H	-5.54697900	2.11481200	1.22729400
H	-5.98645100	0.76696500	0.12690300
H	-5.13649900	0.42978700	1.67067900
C	-2.93056200	-0.41594000	-3.38333500
H	-2.46227000	-0.89700600	-4.24477300
H	-3.63795800	-1.07514200	-2.88768300
H	-3.48428300	0.46627900	-3.72228500
O	1.23241400	2.95635100	-1.19890000
C	2.29649400	0.62290500	-2.04508700
H	2.89056800	-0.22433200	-1.67944700
H	1.37484400	0.32538700	-2.54693400
H	2.88877300	1.28226800	-2.68195900
C	5.65105400	-3.39313700	-1.43053200
H	5.42530000	-3.32415300	-2.50055500

H	5.07202100	-4.23819400	-1.03851700
H	6.71630100	-3.59332500	-1.28888600
C	5.22542600	-2.09300300	-0.71148400
O	6.06378000	-1.51956600	0.01135300
O	4.01530500	-1.73229400	-0.92644900

TS6

C	-1.95815900	-2.49112700	0.73802100
C	-2.17965200	-2.36372800	-0.66280200
C	-0.90003700	-2.54914200	-1.31835100
C	0.04767700	-3.02837100	-0.30933200
C	-0.58370300	-2.97015900	0.94468400
Rh	-0.64865100	-0.87381100	0.01991500
C	-0.00922200	-3.29026300	2.28854400
H	-0.58151500	-4.09386200	2.76699300
H	1.03242400	-3.60989900	2.21985500
H	-0.05221200	-2.40899700	2.93513100
C	-2.96601600	-2.31921000	1.83243500
H	-3.33967300	-3.29697300	2.16517000
H	-2.51818000	-1.81272800	2.69202600
H	-3.81081200	-1.71647000	1.49615700
C	-3.50902900	-2.23992500	-1.33659300
H	-4.16545700	-1.55446400	-0.80124000
H	-3.41249000	-1.89981000	-2.36837300
H	-3.98092900	-3.23142000	-1.35989200
C	-0.66689600	-2.57392300	-2.79797900
H	-1.06027500	-3.50298800	-3.23199500
H	-1.14714900	-1.72893900	-3.29474500
H	0.39972300	-2.52429200	-3.02798600
C	1.44606400	-3.46336000	-0.61006200
H	1.43837900	-4.39050600	-1.19626400
H	1.97585100	-2.70347200	-1.18984900
H	2.01573100	-3.64716200	0.30245700
C	-1.58567400	0.98128300	-0.67702500
C	-2.76011400	1.16844100	0.25295600
O	-3.78219400	0.49621900	0.23280100
C	-1.89675800	0.82704800	-2.16638200
O	-0.96484600	0.75166600	-2.96109900

O	-2.04057100	3.45702600	-1.57182200
C	-1.02173500	3.27489300	-0.93867700
O	-0.63092300	2.04199400	-0.50001900
C	-0.05520800	4.34670700	-0.52104200
H	0.97237400	4.00273600	-0.64532000
H	-0.25770200	5.25385800	-1.09075800
H	-0.20522800	4.55054900	0.54494900
O	0.03706000	-0.03643700	2.17282900
C	-0.36914900	0.92646800	3.01298300
O	-1.37843800	0.79888500	3.68171600
C	0.55117700	2.12892000	3.09404300
H	0.82502100	2.47307600	2.09282300
H	0.06822400	2.92644200	3.65939600
H	1.47735300	1.84266800	3.60559100
C	4.05368600	0.34455800	-0.16953200
C	5.06822600	1.29890600	-0.27126400
C	4.33225700	-0.96873000	0.20514900
C	6.38680600	0.91871100	-0.01778200
H	4.81393200	2.32220900	-0.52442400
C	5.65397200	-1.33873800	0.46187200
H	3.51470400	-1.67119300	0.31515800
C	6.67993100	-0.39837200	0.34503600
H	7.18327500	1.65323000	-0.09373200
H	5.88122200	-2.35836200	0.75985900
H	7.70698600	-0.68904200	0.54643400
S	2.33204600	0.86976900	-0.51306700
N	1.39138500	-0.14017300	0.19021400
H	0.90034900	0.11533800	1.42594400
O	-2.55917700	2.14383900	1.15520400
C	-3.61444000	2.33638400	2.11608000
H	-3.35390400	3.25002500	2.64947700
H	-4.57521000	2.44266200	1.60875700
H	-3.63840000	1.49587200	2.81032900
C	-3.31627100	0.84368100	-2.69747700
H	-3.33927400	0.35039400	-3.67170800
H	-4.04709000	0.42112200	-2.01377200
H	-3.56562700	1.90078000	-2.83570900
O	2.35635600	2.34761700	-0.24077000

C	2. 20187400	0. 65875200	-2. 31330300
H	2. 47263300	-0. 36608400	-2. 57169000
H	1. 15550000	0. 85598600	-2. 56655000
H	2. 87854100	1. 37142500	-2. 78703400
O	3. 97397118	-2. 62347045	2. 19007810
C	4. 35990342	-2. 76473444	3. 41805687
O	5. 19362988	-2. 08731159	4. 03114675
C	3. 64224172	-3. 91959391	4. 12673877
H	2. 58650014	-3. 66126667	4. 26245890
H	3. 67762480	-4. 82498080	3. 51367353
H	4. 09622179	-4. 10622016	5. 10193448

IM4

Rh	0. 24537800	-0. 65959300	-0. 20223600
N	-0. 92975400	0. 80405800	-1. 17585700
C	-1. 13419500	-2. 39547900	-0. 71617000
C	-0. 42161100	-2. 71956500	0. 47248000
C	0. 99234400	-2. 77514600	0. 15964200
C	1. 12323300	-2. 57794000	-1. 25708400
C	-0. 16308900	-2. 23268900	-1. 77943800
O	1. 05619200	-0. 93314200	3. 15348300
O	-0. 14573800	0. 29231600	1. 65501100
C	0. 44206500	0. 07833100	2. 79246300
C	0. 30684900	1. 27056800	3. 74539700
H	-0. 74596400	1. 54199300	3. 87910400
H	0. 81108600	2. 12845900	3. 29022200
H	0. 75006000	1. 03759600	4. 71602600
C	-3. 55303600	0. 89991800	0. 01921600
C	-3. 47027300	0. 21327800	1. 23515400
C	-4. 75469200	0. 94957000	-0. 68817000
C	-4. 60913800	-0. 41529400	1. 74556000
H	-2. 52091100	0. 16412900	1. 76260700
C	-5. 88391300	0. 30058200	-0. 18206300
H	-4. 78373400	1. 51000100	-1. 61741400
C	-5. 81440500	-0. 37781500	1. 03723400
H	-4. 55430300	-0. 93996100	2. 69669500
H	-6. 82156200	0. 33583800	-0. 73227200
H	-6. 69629000	-0. 87260400	1. 43694500

C	-0.52763100	-1.90656100	-3.19656700
H	-1.10784100	-0.97781800	-3.21995600
H	-1.13274300	-2.70548300	-3.64634600
H	0.35818100	-1.76262200	-3.81960300
C	2.35225600	-2.88935300	-2.05178800
H	2.21573100	-2.65816900	-3.11065900
H	2.55576700	-3.96558300	-1.97103000
H	3.23615700	-2.35111700	-1.69888700
C	2.10042200	-3.17971900	1.08657000
H	3.05164000	-2.76862200	0.73754800
H	2.20005800	-4.27431800	1.14284500
H	1.91808300	-2.77876600	2.08506500
C	-1.01553300	-3.01539200	1.81646600
H	-0.38421100	-2.59937300	2.60363100
H	-1.09805400	-4.10187100	1.96175500
H	-2.01707400	-2.58876300	1.91228000
C	-2.61524800	-2.34978200	-0.93137200
H	-3.16870100	-2.33603500	0.00839000
H	-2.94183800	-3.23097700	-1.50243100
H	-2.90018300	-1.46004400	-1.49819500
S	-2.05208200	1.72908100	-0.71951100
C	4.36794900	0.51787500	2.56193200
H	5.06123000	-0.29275900	2.31086400
H	4.92325200	1.29560300	3.08990200
H	3.56943200	0.10375000	3.18046400
C	3.80927200	1.07986000	1.27222500
O	2.66957000	0.42657100	0.95155100
O	4.31272600	1.97116600	0.62361500
C	2.03590500	0.70782100	-0.29529700
C	1.58380500	2.14179300	-0.32635500
O	1.35164000	2.81488000	0.66054400
O	1.48801800	2.62797000	-1.58755400
C	0.90419100	3.92157300	-1.75733800
H	-0.17887200	3.82087300	-1.87765800
H	1.33619300	4.33216200	-2.67337300
H	1.13783800	4.56548400	-0.90666000
C	2.88444800	0.20989500	-1.42236200
O	3.89980600	-0.44863900	-1.19042700

C	2.48336300	0.46557700	-2.86803900
H	2.96859600	1.38698700	-3.20416200
H	1.40854600	0.59422800	-2.99332900
H	2.86311000	-0.35978000	-3.47604400
O	-2.64964000	2.63386400	-1.77295900
C	-1.72161600	2.85790500	0.69633700
H	-1.35256800	2.26666700	1.53168000
H	-0.94152500	3.54875600	0.38407700
H	-2.65327400	3.38182900	0.91862900

TS7

Rh	-0.02669100	-0.36552500	0.64280800
N	-0.08869100	1.63681300	1.22765800
C	1.27602500	-1.08239100	2.38824500
C	1.37555800	-2.10595300	1.39740200
C	0.06351000	-2.63920700	1.12357600
C	-0.85411500	-1.95937300	1.98448700
C	-0.11502900	-0.96676700	2.74213900
O	1.69741900	-2.65162700	-2.31653700
O	0.93307300	-0.57603500	-2.80524800
C	1.02092200	-1.85800700	-2.98811900
C	0.16617100	-2.37218900	-4.14156300
H	0.20276700	-1.68954000	-4.99560800
H	-0.86836900	-2.41840900	-3.78632200
H	0.49082700	-3.37113400	-4.44112700
C	2.34515600	1.71269300	-0.10571200
C	2.16177000	0.48392300	-0.76512600
C	3.59241300	2.27108100	0.19025000
C	3.36907400	-0.16027700	-1.12499500
H	1.29543500	-0.10953200	-1.71773400
C	4.75128100	1.59124200	-0.17982400
H	3.62878400	3.21703500	0.72232300
C	4.63118100	0.36669900	-0.84078500
H	3.29965500	-1.10188800	-1.66430000
H	5.73007400	2.00989300	0.04461600
H	5.52386400	-0.17756500	-1.14534700
C	-0.65116500	-0.06135900	3.80747300
H	-0.40395300	0.97613300	3.55868000

H	-0.21083300	-0.31137200	4.78171100
H	-1.73684600	-0.14224000	3.89192600
C	-2.27164600	-2.35561800	2.25918900
H	-2.89969100	-1.48517300	2.45300500
H	-2.30414400	-3.00246900	3.14753600
H	-2.70190200	-2.91709800	1.42882900
C	-0.22346600	-3.80848900	0.22862100
H	-1.25577200	-3.79482100	-0.12594900
H	-0.05190400	-4.75924000	0.75559200
H	0.41684600	-3.78081200	-0.65671200
C	2.62721900	-2.66251200	0.79927700
H	2.51539200	-2.78734400	-0.28104600
H	2.81939900	-3.65116700	1.24085600
H	3.49201400	-2.02752000	0.99388100
C	2.38188100	-0.26922200	2.99062800
H	3.29292700	-0.32464200	2.39092300
H	2.62289800	-0.61283200	4.00669900
H	2.08897100	0.78348500	3.04780400
S	0.90936000	2.61656300	0.57528400
C	-1.32990200	1.48802700	-3.97208300
H	-1.93449300	1.42938000	-4.87815900
H	-1.11849700	2.53903600	-3.74798100
H	-0.37804200	0.96330800	-4.08634800
C	-2.08859700	0.87231600	-2.82233400
O	-1.26943900	0.69024300	-1.76362500
O	-3.26435100	0.56712700	-2.84570900
C	-1.81218000	0.14312200	-0.55172200
C	-2.54345500	1.26486800	0.14664800
O	-2.71788700	2.37984300	-0.30297200
O	-3.02093300	0.90412800	1.37216000
C	-3.52631400	1.99568500	2.14619100
H	-2.72574200	2.71670400	2.32821400
H	-3.86996300	1.56011900	3.08684600
H	-4.35391800	2.49486600	1.63373700
C	-2.60219700	-1.12029200	-0.87243600
O	-2.11763700	-1.98927300	-1.58552600
C	-4.03429300	-1.28167800	-0.38068000
H	-4.64983200	-0.64658700	-1.02653100

H	-4.18485000	-0.95858700	0.64739300
H	-4.33537300	-2.32324600	-0.51420700
O	1.42446200	3.75183500	1.42355400
C	0.27804000	3.46324100	-0.93154300
H	0.07591400	2.70371000	-1.68389200
H	-0.65188900	3.95364900	-0.64106100
H	1.02939500	4.18209100	-1.26414300

IM5

Rh	-0.02669100	-0.36552500	0.64280800
N	-0.08869100	1.63681300	1.22765800
C	1.27602500	-1.08239100	2.38824500
C	1.37555800	-2.10595300	1.39740200
C	0.06351000	-2.63920700	1.12357600
C	-0.85411500	-1.95937300	1.98448700
C	-0.11502900	-0.96676700	2.74213900
O	1.69741900	-2.65162700	-2.31653700
O	0.93307300	-0.57603500	-2.80524800
C	1.02092200	-1.85800700	-2.98811900
C	0.16617100	-2.37218900	-4.14156300
H	0.20276700	-1.68954000	-4.99560800
H	-0.86836900	-2.41840900	-3.78632200
H	0.49082700	-3.37113400	-4.44112700
C	2.34515600	1.71269300	-0.10571200
C	2.16177000	0.48392300	-0.76512600
C	3.59241300	2.27108100	0.19025000
C	3.36907400	-0.16027700	-1.12499500
H	1.29543500	-0.10953200	-1.71773400
C	4.75128100	1.59124200	-0.17982400
H	3.62878400	3.21703500	0.72232300
C	4.63118100	0.36669900	-0.84078500
H	3.29965500	-1.10188800	-1.66430000
H	5.73007400	2.00989300	0.04461600
H	5.52386400	-0.17756500	-1.14534700
C	-0.65116500	-0.06135900	3.80747300
H	-0.40395300	0.97613300	3.55868000
H	-0.21083300	-0.31137200	4.78171100
H	-1.73684600	-0.14224000	3.89192600

C	-2.27164600	-2.35561800	2.25918900
H	-2.89969100	-1.48517300	2.45300500
H	-2.30414400	-3.00246900	3.14753600
H	-2.70190200	-2.91709800	1.42882900
C	-0.22346600	-3.80848900	0.22862100
H	-1.25577200	-3.79482100	-0.12594900
H	-0.05190400	-4.75924000	0.75559200
H	0.41684600	-3.78081200	-0.65671200
C	2.62721900	-2.66251200	0.79927700
H	2.51539200	-2.78734400	-0.28104600
H	2.81939900	-3.65116700	1.24085600
H	3.49201400	-2.02752000	0.99388100
C	2.38188100	-0.26922200	2.99062800
H	3.29292700	-0.32464200	2.39092300
H	2.62289800	-0.61283200	4.00669900
H	2.08897100	0.78348500	3.04780400
S	0.90936000	2.61656300	0.57528400
C	-1.32990200	1.48802700	-3.97208300
H	-1.93449300	1.42938000	-4.87815900
H	-1.11849700	2.53903600	-3.74798100
H	-0.37804200	0.96330800	-4.08634800
C	-2.08859700	0.87231600	-2.82233400
O	-1.26943900	0.69024300	-1.76362500
O	-3.26435100	0.56712700	-2.84570900
C	-1.81218000	0.14312200	-0.55172200
C	-2.54345500	1.26486800	0.14664800
O	-2.71788700	2.37984300	-0.30297200
O	-3.02093300	0.90412800	1.37216000
C	-3.52631400	1.99568500	2.14619100
H	-2.72574200	2.71670400	2.32821400
H	-3.86996300	1.56011900	3.08684600
H	-4.35391800	2.49486600	1.63373700
C	-2.60219700	-1.12029200	-0.87243600
O	-2.11763700	-1.98927300	-1.58552600
C	-4.03429300	-1.28167800	-0.38068000
H	-4.64983200	-0.64658700	-1.02653100
H	-4.18485000	-0.95858700	0.64739300
H	-4.33537300	-2.32324600	-0.51420700

O	1.42446200	3.75183500	1.42355400
C	0.27804000	3.46324100	-0.93154300
H	0.07591400	2.70371000	-1.68389200
H	-0.65188900	3.95364900	-0.64106100
H	1.02939500	4.18209100	-1.26414300

Cartesian Coordinates for the Stationary Points Given in Fig. S3

TS8

Rh	0.30438300	0.62774200	-0.21152500
N	1.91264500	0.09207500	-1.39380500
C	-0.16267300	2.13214100	1.43996900
C	-0.78801400	2.71615500	0.26825100
C	0.23906400	3.07992100	-0.63776800
C	1.50679300	2.78496200	-0.01141500
C	1.26914400	2.22030000	1.26729700
C	2.04034400	-1.56277100	0.72892600
C	0.80051200	-0.95186600	0.96051700
C	2.57741000	-2.54711800	1.56359100
C	0.04681300	-1.42405900	2.04608100
C	1.82402700	-2.97798000	2.65310500
H	3.56633300	-2.95395000	1.36690600
C	0.55823600	-2.42079200	2.87991700
H	-0.95452000	-1.03444300	2.19928500
H	2.21282300	-3.74583500	3.31741000
H	-0.04206600	-2.77646200	3.71452700
C	2.32180400	1.83415000	2.26957000
H	1.93522800	1.10926100	2.99020800
H	2.67227200	2.70847600	2.83656400
H	3.18974400	1.37949500	1.78293700
C	2.84142300	3.01651000	-0.64537400
H	3.05855900	2.19230600	-1.33890300
H	3.64094700	3.04459200	0.09941100
H	2.85446900	3.95941900	-1.20273200
C	0.08086000	3.75903700	-1.96657300
H	-0.88341900	3.51614300	-2.41182700
H	0.85656700	3.43309100	-2.66602700

H	0.16153100	4.85207900	-1.87053500
C	-2.25369000	3.00609100	0.15813200
H	-2.52834000	3.29481000	-0.85697800
H	-2.51848800	3.83064400	0.83654800
H	-2.83924700	2.12494200	0.43781000
C	-0.89453200	1.80098100	2.70759700
H	-0.30300200	1.14883300	3.35513000
H	-1.83572500	1.29556100	2.47580400
H	-1.11117600	2.71899300	3.27382600
S	2.89801200	-0.89151000	-0.70204700
C	-4.36009200	-0.86836500	2.58165200
H	-5.37794200	-1.24944400	2.69997300
H	-3.65930900	-1.58948900	3.01893500
H	-4.24834400	0.07101300	3.13420100
C	-4.02125500	-0.67211300	1.08639500
O	-2.93442900	-0.03157100	0.86336900
O	-4.80674300	-1.15265200	0.24661800
C	-1.11017900	-0.37419000	-0.99687200
C	-1.15441400	-1.87503700	-0.98911600
O	-1.61429300	-2.61945600	-0.15545400
O	-0.57331600	-2.34577400	-2.14040100
C	-0.61052500	-3.77139300	-2.27896900
H	-0.14576900	-3.98671400	-3.24280900
H	-1.64109600	-4.13771700	-2.26126100
H	-0.05692000	-4.25762300	-1.47042500
C	-2.12297600	0.25439500	-1.93919900
O	-1.96520700	1.39739800	-2.35082100
C	-3.28993500	-0.58420500	-2.40702700
H	-3.91438000	-0.86434100	-1.54093100
H	-2.93277000	-1.49939200	-2.89232600
H	-3.86813300	0.00043200	-3.12636000
O	4.30267600	-0.49994900	-0.32032300
C	3.14932400	-2.34144200	-1.80219900
H	3.61903700	-1.94207200	-2.70362900
H	3.80825200	-3.06917300	-1.32399600
H	2.17409000	-2.76486000	-2.04066500

IM6

Rh	-0.69495200	0.01790100	-0.42295500
N	-0.59946600	1.60862300	-1.79056800
C	-1.92936800	-0.59588300	1.50864600
C	-1.93690900	-1.70743900	0.59730600
C	-2.62237500	-1.28647700	-0.60219200
C	-3.01659000	0.08236200	-0.42932000
C	-2.57133700	0.51981100	0.86458900
C	0.81654900	2.46653400	0.32668000
C	0.65923400	1.11900700	0.67619500
C	1.61060100	3.35248500	1.05840000
C	1.37719700	0.64169000	1.77830800
C	2.31195400	2.86339300	2.15962600
H	1.67189500	4.40027800	0.77485500
C	2.19518500	1.51322800	2.50655200
H	1.31437200	-0.39177500	2.11826800
H	2.94221600	3.52982400	2.74362200
H	2.73320200	1.11448100	3.36263200
C	-2.85396600	1.87117600	1.45880500
H	-2.24683800	2.04288700	2.35053900
H	-3.90912800	1.95697700	1.75520400
H	-2.63274600	2.67578400	0.75126000
C	-3.75436100	0.94308600	-1.41034900
H	-3.06153000	1.66338600	-1.86270300
H	-4.55427900	1.49967800	-0.90922200
H	-4.20348700	0.34705300	-2.20895600
C	-2.95209900	-2.17439800	-1.76772800
H	-2.08819600	-2.77908600	-2.05290600
H	-3.25456600	-1.58978500	-2.64005300
H	-3.77880000	-2.85271300	-1.51397500
C	-1.50132400	-3.10697600	0.91665900
H	-1.29066300	-3.67023600	0.00392200
H	-2.30527200	-3.63435000	1.45094100
H	-0.59924100	-3.14105900	1.54048700
C	-1.46294900	-0.65494100	2.93018300
H	-1.29057200	0.34445900	3.33638400
H	-0.53817200	-1.23112000	3.06148400
H	-2.24234800	-1.13023500	3.54352500
S	-0.12921500	2.93504900	-1.12529900

C	2.68066100	-3.82482900	4.31193600
H	2.26532300	-4.82280300	4.49034900
H	3.66598900	-3.96878700	3.85132500
H	2.80761200	-3.29791200	5.26172300
C	1.76898300	-3.03345900	3.34043900
O	1.47125300	-1.85634000	3.67469600
O	1.42448300	-3.65559100	2.29475500
C	0.63123700	-0.84668700	-1.45517900
C	1.44085500	-0.10094400	-2.46409300
O	2.45430500	0.52661800	-2.21944200
O	0.95175300	-0.30014500	-3.70487900
C	1.61073500	0.42381800	-4.75019400
H	1.17665600	0.05698500	-5.68089800
H	2.68913900	0.24560400	-4.73110100
H	1.42025500	1.49512000	-4.64334500
C	0.94560300	-2.30983300	-1.39053600
O	0.23762200	-3.10921600	-1.99549400
C	2.13366200	-2.70238700	-0.56221500
H	1.80498100	-2.93385100	0.47332700
H	2.87195400	-1.89605500	-0.51029800
H	2.57785300	-3.60936600	-0.98308600
C	1.10962300	3.71271000	-2.23146500
H	0.58716800	3.88768600	-3.17483000
H	1.44238400	4.66232600	-1.80802400
H	1.93413800	3.01186400	-2.36713400
O	-1.07157600	4.06569300	-0.79116100

TS9

Rh	-0.50601800	0.79405000	-0.00680100
N	-2.51904100	0.12839800	-0.12743800
C	1.09954000	1.88845600	-1.31197600
C	1.18027800	2.36831300	0.04632800
C	-0.08286000	2.98246600	0.36507400
C	-0.94175200	2.84691600	-0.78315300
C	-0.20330900	2.18448700	-1.82807600
C	-1.07800700	-1.91238800	-1.14500500
C	-0.03530400	-1.24778100	-0.47014600
C	-0.85056900	-3.07324300	-1.87708800

C	1. 25499400	-1. 77576900	-0. 55520000
C	0. 43958800	-3. 61679800	-1. 91067900
H	-1. 65878700	-3. 52679100	-2. 44526600
C	1. 48848000	-2. 96104500	-1. 26528300
H	2. 12106800	-1. 27583700	-0. 12048900
H	0. 62351600	-4. 53242000	-2. 46816300
H	2. 51609900	-3. 31590300	-1. 29508000
C	-0. 71832400	1. 91457000	-3. 21481400
H	0. 02324300	1. 37193100	-3. 80666300
H	-0. 93798200	2. 85294700	-3. 74303000
H	-1. 63024200	1. 30926100	-3. 19721300
C	-2. 34994300	3. 34350300	-0. 92848000
H	-3. 02125500	2. 51084900	-1. 15956100
H	-2. 41537500	4. 08450200	-1. 73572800
H	-2. 70675100	3. 81407200	-0. 00908600
C	-0. 40567100	3. 66673900	1. 66124000
H	-0. 03850200	3. 08459200	2. 51070300
H	-1. 48364000	3. 79423200	1. 78722500
H	0. 05853400	4. 66234200	1. 70385700
C	2. 40660900	2. 38664200	0. 91424200
H	2. 13720700	2. 30845900	1. 97166800
H	2. 94837900	3. 33501100	0. 78366100
H	3. 09224600	1. 56520000	0. 68236600
C	2. 23078000	1. 25120400	-2. 06246400
H	1. 86718000	0. 54467900	-2. 81256100
H	2. 90866700	0. 71774500	-1. 38931400
H	2. 80890300	2. 02508600	-2. 58734300
S	-2. 63676200	-0. 99079900	-1. 19094800
C	6. 25896400	-0. 72612300	-0. 04330500
H	6. 97219500	-1. 48044900	-0. 38633000
H	6. 34444900	0. 16680600	-0. 67425200
H	6. 51255700	-0. 41620200	0. 97710300
C	4. 80752500	-1. 26171500	-0. 08837700
O	3. 92495700	-0. 44199700	0. 34610000
O	4. 62191500	-2. 41084400	-0. 53522100
C	-0. 39290400	-0. 37073400	1. 50772700
C	-1. 56139200	-1. 15855400	2. 04007100
O	-1. 80127800	-2. 33668400	1. 85125400

O	-2.24312000	-0.39145200	2.91671800
C	-3.35825900	-1.02951000	3.54570600
H	-3.70779500	-0.32844800	4.30461200
H	-3.06377500	-1.97798900	4.00322600
H	-4.14922100	-1.21584800	2.81356100
C	0.72539900	-0.29962300	2.52731000
O	0.63487200	0.62112100	3.33245900
C	1.83430100	-1.30839700	2.57438600
H	2.63715700	-1.01743500	1.87161200
H	1.48926300	-2.30368200	2.28272500
H	2.24304200	-1.31717200	3.58859700
O	-2.98517400	-0.75884900	-2.64294800
C	-3.90240900	-2.18605900	-0.62145800
H	-3.57572000	-2.61241300	0.32671900
H	-4.81757800	-1.60313100	-0.49652900
H	-4.04721100	-2.95038800	-1.38713200

IM7

Rh	1.06587200	-0.24565400	-0.12528000
N	0.80790800	1.03873500	-1.78029500
C	3.17845000	-0.70539800	0.73264900
C	2.25862900	-1.73052100	1.19840500
C	1.77984200	-2.44606500	0.06358200
C	2.27895600	-1.78291500	-1.11497200
C	3.21175700	-0.74949400	-0.68283400
C	0.23194000	1.82672200	0.70863600
C	-0.68370000	0.74252500	1.00648700
C	0.73054900	2.62554700	1.77485100
C	-1.09227100	0.59129500	2.37091200
C	0.35160500	2.39899000	3.07947700
H	1.39056300	3.45509400	1.55498300
C	-0.59164900	1.39090500	3.37126500
H	-1.88215700	-0.12020900	2.56332200
H	0.73582700	3.03679300	3.87203400
H	-0.95647900	1.26960700	4.38773300
O	-0.16197500	3.51414000	-1.55069900
C	4.01007500	0.09423600	-1.62975800
H	3.33475300	0.64441800	-2.29609800

H	4. 63660400	0. 81873600	-1. 10233600
H	4. 67033800	-0. 52826600	-2. 24687400
C	2. 07003700	-2. 19347000	-2. 54158700
H	1. 99063600	-1. 31199000	-3. 18331300
H	2. 90150900	-2. 81395900	-2. 90574700
H	1. 14601300	-2. 76454900	-2. 65663200
C	0. 98196800	-3. 71113700	0. 10866200
H	0. 51177700	-3. 92717600	-0. 85311900
H	1. 64134400	-4. 55545200	0. 35426300
H	0. 19581100	-3. 65430000	0. 86560300
C	1. 95524700	-2. 05937900	2. 63089600
H	0. 89473700	-2. 29812400	2. 74231700
H	2. 54929100	-2. 91525600	2. 98118300
H	2. 17740400	-1. 21225900	3. 28614200
C	3. 93709900	0. 22246500	1. 63692300
H	3. 25783300	0. 79390100	2. 27939500
H	4. 61823300	-0. 33536700	2. 29226500
H	4. 53751000	0. 93686500	1. 06767400
S	0. 64419400	2. 37827000	-1. 01997200
C	2. 28574500	3. 23078400	-0. 74714200
H	2. 14971400	4. 21292300	-0. 29165800
H	2. 96859300	2. 60685200	-0. 17090300
H	2. 65629200	3. 35316700	-1. 76692200
C	-5. 94153400	0. 43089300	1. 14123300
H	-5. 77596200	1. 50520800	0. 99296400
H	-5. 98981500	0. 25150200	2. 22036400
H	-6. 89184600	0. 16263400	0. 66964100
C	-4. 76513000	-0. 34790000	0. 50404300
O	-3. 72390200	-0. 44102800	1. 21849200
O	-4. 94170100	-0. 79121300	-0. 66066200
C	-1. 10830000	-0. 22678200	-0. 02400900
C	-1. 86901200	0. 38487300	-1. 17326100
O	-2. 36634600	1. 49063600	-1. 12080600
O	-1. 99118800	-0. 43112700	-2. 23742300
C	-2. 98176900	-0. 00599200	-3. 18795700
H	-2. 73724600	0. 98468100	-3. 57924000
H	-2. 95520300	-0. 74974200	-3. 98739800
H	-3. 95764800	0. 00302100	-2. 69454100

C	-1.54715900	-1.59977400	0.46852500
O	-1.15070800	-2.01529500	1.56178200
C	-2.30945600	-2.53451300	-0.44415800
H	-3.26912200	-2.08626800	-0.72830700
H	-1.73549400	-2.73763800	-1.35414200
H	-2.47102000	-3.46207400	0.11060200

Cartesian Coordinates for the Stationary Points Given in Fig. S4

TS10

C	2.40032700	2.37813300	3.82773800
C	1.70889900	1.51659700	2.94911000
H	3.22431200	2.73912900	5.77743400
C	2.68425000	2.04075300	5.14489000
C	1.60307800	-0.07541800	4.80137500
C	2.29238800	0.79540400	5.63672100
H	1.31782800	-1.04889400	5.18231000
H	2.52489900	0.50113900	6.65592700
Rh	-0.33674800	0.75167300	-0.10347500
C	1.59148600	1.97866100	1.51707800
C	2.46016400	1.42055400	0.55356500
O	2.52559100	1.88025600	-0.65827800
C	-2.50778300	0.93928300	-0.47310100
C	-1.93615000	2.25084200	-0.35965200
C	-1.83255600	0.26991000	-1.55584300
C	-1.03323700	2.44990600	-1.49779100
C	-0.97186700	1.24776300	-2.22511500
C	-0.32202700	3.71531600	-1.86850700
H	0.75502100	3.62500300	-1.69910400
H	-0.48645800	3.94375700	-2.92765600
H	-0.68954700	4.56002500	-1.28284400
C	-2.39605400	3.31546800	0.58742600
H	-1.56766100	3.90684000	0.97980100
H	-3.09647100	3.98966600	0.07598200
H	-2.91105200	2.87902200	1.44517000
C	-3.53325900	0.33833500	0.43469200
H	-3.02914300	-0.13056800	1.29051500

H	-4.22179800	1.10137400	0.80650500
H	-4.11871200	-0.42406900	-0.08571300
C	-2.08988300	-1.12489600	-2.03466700
H	-1.15214700	-1.62677100	-2.28346800
H	-2.58763700	-1.71956000	-1.26666300
H	-2.72438600	-1.11399900	-2.93040500
C	-0.19823400	1.02658400	-3.48944400
H	0.82493300	1.39923500	-3.40713500
H	-0.14725600	-0.03287900	-3.74733600
H	-0.68566900	1.54772900	-4.32385200
C	1.95106700	-0.96415000	-1.72105100
O	2.72533300	-0.02422400	-2.11665800
O	1.03388500	-0.87136500	-0.86210800
C	2.20776300	-2.32970100	-2.33434500
H	1.38575200	-3.01459500	-2.12483500
H	2.37017000	-2.23271600	-3.41120000
H	3.12640600	-2.74012200	-1.90200600
H	2.67900700	1.01258900	-1.38678000
C	3.38919000	0.28198800	0.92385800
H	4.04078200	0.05344700	0.08047500
H	4.00426000	0.58652100	1.77726300
H	2.84716600	-0.62129600	1.21566500
C	1.11454700	3.38448800	1.43887100
O	0.29486900	3.87124900	2.20516500
O	1.75522900	4.15327100	0.51820200
C	1.45911400	5.55311600	0.58525600
H	2.06642200	6.01633100	-0.19315000
H	0.39905400	5.75073400	0.40676600
H	1.72180000	5.95860400	1.56630700
C	1.28519700	0.28281900	3.48229400
S	0.31184800	-0.94162800	2.50527700
N	-0.73307100	-0.28701300	1.57025200
O	1.30504200	-1.99795900	2.10752200
C	-0.76608500	-1.70295700	3.77725100
H	-1.26467000	-0.92763500	4.35819200
H	-1.49164200	-2.26975900	3.19364800
H	-0.18164700	-2.37420700	4.40623000
H	2.73640200	3.33833500	3.44911900

IM8

C	-4.78206200	0.24702300	0.24224700
C	-3.38822500	0.06488800	0.16408500
H	-6.75229600	-0.57169600	-0.00165900
C	-5.68521000	-0.75857700	-0.08106200
C	-3.84499600	-2.22121000	-0.57608000
C	-5.21572100	-2.01240100	-0.47466300
H	-3.46956700	-3.20236700	-0.84516900
H	-5.90552000	-2.82225900	-0.69252800
Rh	1.63399700	-0.25809200	-0.15737600
C	-2.51734600	1.17238100	0.66712200
C	-1.69983100	0.91435700	1.73685900
O	-1.72996400	-0.32579700	2.24523600
C	2.57530700	0.84537200	-1.81310100
C	2.26251200	1.77231900	-0.78200100
C	3.49256800	-0.14576600	-1.25462700
C	3.01324000	1.38274200	0.41320500
C	3.79917000	0.23598200	0.09743100
C	3.01120200	2.11955200	1.71703600
H	2.11376600	2.73071000	1.82675400
H	3.05220200	1.42969000	2.56296100
H	3.88045400	2.78771900	1.77769400
C	1.38122800	2.97817600	-0.89965100
H	0.71457900	3.07978900	-0.04059400
H	1.98750300	3.89030200	-0.97035400
H	0.75309400	2.92218600	-1.79057700
C	2.08507000	0.88044900	-3.22821200
H	1.08698300	1.31765400	-3.29414100
H	2.76155400	1.47910200	-3.85162500
H	2.03884700	-0.12215300	-3.65955900
C	4.11645800	-1.28829700	-1.99468800
H	4.32801600	-2.12261000	-1.32197700
H	3.46730600	-1.65533900	-2.79306400
H	5.06449100	-0.97590200	-2.45288500
C	4.70962800	-0.51697500	1.02115000
H	4.67382600	-0.10857100	2.03294300
H	4.41743600	-1.56998100	1.07763200

H	5.74800700	-0.46474500	0.67346700
C	1.20316800	-2.00741000	2.15285200
O	0.76445600	-0.99367400	2.74267600
O	1.72518100	-2.00607900	0.97662700
C	1.12070000	-3.37348500	2.80775700
H	1.97046000	-3.99891400	2.52587300
H	1.05528200	-3.27644700	3.89281500
H	0.21069200	-3.85255600	2.43188100
H	-0.84229900	-0.56944400	2.62359800
C	-0.78417500	1.84840400	2.47331100
H	0.20529200	1.38331000	2.52073200
H	-0.73043200	2.83627700	2.03001600
H	-1.14132600	1.93772400	3.50675500
C	-2.69278800	2.44938600	-0.03672400
O	-3.41244400	2.59521000	-1.01293700
O	-1.98551000	3.51203100	0.46387600
C	-2.20136800	4.74834100	-0.22668100
H	-1.58983300	5.48656700	0.29459300
H	-1.89931300	4.67239200	-1.27471800
H	-3.25547400	5.03570900	-0.19285100
C	-2.94189700	-1.18507600	-0.30086200
S	-1.19060200	-1.68597100	-0.58742000
N	-0.25407600	-0.43061100	-0.61720100
O	-0.97929100	-2.95435400	0.18041300
C	-1.27062300	-2.19311200	-2.35463600
H	-1.61285000	-1.34759000	-2.95074000
H	-0.24323700	-2.45773600	-2.61128400
H	-1.92513100	-3.05654400	-2.47302200
H	-5.14959100	1.20934100	0.58161700

IM9

C	4.51831900	1.81049300	-0.95672600
C	3.56385300	0.99565100	-0.31758900
H	4.97411700	3.68573900	-1.90781800
C	4.21064700	3.08926300	-1.41681400
C	1.95257500	2.81364600	-0.61455000
C	2.92310200	3.59341000	-1.24134600
H	0.95482000	3.21683500	-0.46838000

H	2.66744300	4.59040100	-1.58746000
Rh	-1.94329300	-0.53243400	-0.23100200
C	4.02569500	-0.34697400	0.17166900
C	4.69790700	-0.41263400	1.35524600
O	4.92420200	0.70219700	2.09307900
C	-1.19549200	-2.60083400	-0.45198000
C	-1.95595100	-2.40184100	0.77243500
C	-2.06515000	-2.29209000	-1.53201700
C	-3.34651600	-2.12572800	0.41268400
C	-3.40703100	-2.02313700	-0.99638800
C	-4.46770900	-1.96901700	1.39318100
H	-4.15832100	-1.34597600	2.23492400
H	-5.34429400	-1.51006200	0.93118400
H	-4.76780500	-2.95160800	1.77891400
C	-1.44723600	-2.57918200	2.16543000
H	-1.94763000	-1.88067600	2.83863400
H	-1.63664000	-3.60667400	2.50566100
H	-0.37433200	-2.38483200	2.21359300
C	0.23410400	-3.03041900	-0.53721100
H	0.81542500	-2.60717100	0.28284300
H	0.29225800	-4.12639300	-0.49366800
H	0.70463100	-2.69439600	-1.46280800
C	-1.71197000	-2.29250000	-2.98686300
H	-2.23468100	-1.49708600	-3.52472100
H	-0.64013100	-2.15164600	-3.13495600
H	-1.99933400	-3.24740900	-3.44604000
C	-4.60991500	-1.71406900	-1.83335300
H	-5.39415200	-1.23075000	-1.24773300
H	-4.35637100	-1.05179500	-2.66580800
H	-5.02649000	-2.63526700	-2.26096000
C	-3.00963100	1.31378700	1.81270000
O	-2.64832400	0.51873000	2.68952600
O	-2.85795800	1.14416400	0.53049600
C	-3.67222400	2.63982500	2.16555200
H	-4.63556200	2.73009200	1.65387800
H	-3.81764200	2.71356500	3.24403500
H	-3.03767100	3.45952300	1.81471200
H	4.56145700	1.47076500	1.62242400

C	5.25460100	-1.62251300	2.04934900
H	5.68685100	-1.31280100	3.00226800
H	4.46796500	-2.35921600	2.22520700
H	6.01962500	-2.11044900	1.44162000
C	3.72465900	-1.48325500	-0.70686300
O	3.07084500	-1.39957300	-1.73390900
O	4.27262900	-2.66210200	-0.29731700
C	4.05090600	-3.77438000	-1.17145300
H	4.64094900	-4.59428200	-0.75956000
H	2.99302000	-4.04886200	-1.19669200
H	4.37520000	-3.54146200	-2.18878500
C	2.26785700	1.52853100	-0.15852600
S	0.88982300	0.60116000	0.63646400
N	-0.23719300	0.55668400	-0.41771200
O	1.41945500	-0.64535700	1.28948300
C	0.48405200	1.70209200	2.04292100
H	0.12279700	2.65331400	1.64940300
H	-0.31387200	1.19227900	2.58801900
H	1.37228800	1.81882300	2.66681300
H	5.51882800	1.41032100	-1.09424500
H	-0.86441300	1.88680100	-1.25760100
O	-1.44985200	2.50848700	-1.80396300
C	-1.71385500	3.61481000	-1.11889300
O	-1.12068900	3.95703000	-0.10299600
C	-2.83769100	4.42022800	-1.73089400
H	-3.78591800	3.91844100	-1.51065000
H	-2.85393500	5.42322200	-1.30420300
H	-2.73331300	4.46645600	-2.81788200

TS11

C	4.63144800	1.78226600	-1.20887100
C	3.72247500	0.95281400	-0.52581500
H	4.96978600	3.60591300	-2.29908400
C	4.23981500	2.99430900	-1.77671200
C	1.98200200	2.61341500	-1.01009700
C	2.91332800	3.41030900	-1.67607600

H	0.94870400	2.94856200	-0.93183600
H	2.59377100	4.35142300	-2.11304100
Rh	-2.05487300	-0.30124600	-0.14360900
C	4.24042000	-0.31850300	0.07897400
C	4.94713600	-0.25171700	1.24141800
O	5.17726400	0.93735900	1.85634100
C	-1.61847900	-2.33648200	-0.85262300
C	-2.09013600	-2.31624000	0.52607100
C	-2.64209800	-1.77161100	-1.66226300
C	-3.48082100	-1.87342400	0.51706400
C	-3.80584700	-1.49644300	-0.81101300
C	-4.37622800	-1.83079600	1.71581200
H	-3.82972500	-1.47969700	2.59292100
H	-5.23338400	-1.17312400	1.55485100
H	-4.76133100	-2.83726800	1.92443300
C	-1.34451000	-2.84181300	1.71147900
H	-1.62339800	-2.28877300	2.60943400
H	-1.56714100	-3.90797800	1.85599600
H	-0.26806500	-2.72567200	1.57043400
C	-0.26856400	-2.81218400	-1.28970300
H	0.51948700	-2.40696900	-0.65133500
H	-0.23329000	-3.90811800	-1.24114400
H	-0.04347100	-2.50914400	-2.31286100
C	-2.59426100	-1.51931900	-3.13811100
H	-2.96407600	-0.51846000	-3.37705400
H	-1.57584800	-1.59568000	-3.52127300
H	-3.21713800	-2.24782400	-3.67231200
C	-5.11483500	-0.96428000	-1.30759900
H	-5.68989500	-0.49661800	-0.50584100
H	-4.96743600	-0.22192500	-2.09589600
H	-5.72265900	-1.77632800	-1.72751800
C	-2.45814100	1.02700100	2.54145300
O	-2.08736200	0.01997800	3.15431800
O	-2.43551900	1.18843800	1.25084700
C	-2.99773200	2.24727100	3.28361300
H	-4.06775100	2.35832700	3.07724000
H	-2.84974100	2.12965500	4.35792200
H	-2.50492700	3.15650800	2.92880000

H	4. 80695000	1. 65186600	1. 31214600
C	5. 53948600	-1. 37792200	2. 03937900
H	4. 75705800	-2. 06855100	2. 36247200
H	6. 24820500	-1. 95624600	1. 44368100
H	6. 04550600	-0. 96284800	2. 91260500
C	3. 91710300	-1. 54599700	-0. 66491400
O	3. 27454800	-1. 56190600	-1. 70072200
O	4. 42161800	-2. 68112500	-0. 11091600
C	4. 11580900	-3. 88624000	-0. 82225700
H	4. 61857200	-4. 68579000	-0. 27664000
H	3. 03680000	-4. 06063000	-0. 84294500
H	4. 48071500	-3. 83576100	-1. 85136500
C	2. 38894100	1. 40203000	-0. 44049200
S	1. 08148100	0. 46451100	0. 44144900
N	-0. 11287900	0. 39668800	-0. 54759600
O	1. 59690600	-0. 82539900	0. 99745400
C	0. 80622200	1. 52747700	1. 90201600
H	0. 37412800	2. 47283400	1. 57109700
H	0. 11228400	0. 97423200	2. 53772700
H	1. 76406600	1. 66717200	2. 40677100
H	5. 66042500	1. 44604600	-1. 29989000
H	-0. 74441600	1. 30902600	-1. 15018700
O	-1. 82662800	1. 73377000	-1. 52754600
C	-2. 03748100	2. 95575900	-1. 05230000
O	-1. 13312900	3. 68337800	-0. 65419200
C	-3. 49059800	3. 38003800	-1. 03571500
H	-3. 98321500	2. 84014600	-0. 22074100
H	-3. 56961200	4. 45353000	-0. 85980500
H	-3. 98640500	3. 11170100	-1. 97273600

IM10

C	4. 66823700	1. 73322900	-1. 16238300
C	3. 73875100	0. 94859800	-0. 45962900
H	5. 01470900	3. 40198600	-2. 47630000
C	4. 26981000	2. 81907700	-1. 94268500
C	1. 96627900	2. 38162100	-1. 36262100
C	2. 91840400	3. 14028000	-2. 04568400
H	0. 91550000	2. 63682400	-1. 45424000

H	2.59480800	3.97691600	-2.65705100
Rh	-2.23690500	-0.21404400	-0.17994700
C	4.24165900	-0.21826000	0.33970700
C	4.77567000	-0.00483700	1.57196700
O	4.81415200	1.24503600	2.11307000
C	-1.78651600	-2.17382300	-1.12969700
C	-2.04712500	-2.34511300	0.29383100
C	-2.94698100	-1.60525700	-1.72733400
C	-3.40778900	-1.93666000	0.53941100
C	-3.95511100	-1.43043100	-0.68584600
C	-4.10439700	-2.01040500	1.86206900
H	-3.40505500	-1.82037700	2.67770400
H	-4.91504500	-1.28206300	1.92969800
H	-4.53612200	-3.01037400	1.99806500
C	-1.13876500	-2.99606400	1.29089100
H	-1.25218100	-2.52578000	2.26929900
H	-1.37082300	-4.06627700	1.37756400
H	-0.09482200	-2.88578400	0.99660200
C	-0.51401500	-2.55174300	-1.82240300
H	0.35755700	-2.24472800	-1.24151000
H	-0.47478800	-3.64049900	-1.95527200
H	-0.44194200	-2.09126900	-2.80952300
C	-3.14578600	-1.20805800	-3.15733100
H	-3.49599500	-0.17308200	-3.21455700
H	-2.21945000	-1.28482000	-3.72936000
H	-3.89506400	-1.85198300	-3.63389700
C	-5.32522200	-0.87366400	-0.92192500
H	-5.84639800	-0.67778600	0.01723600
H	-5.25954900	0.06890900	-1.47319300
H	-5.93437800	-1.57356400	-1.50764400
C	-2.24635100	0.80155300	2.63564500
O	-1.52080000	-0.14323000	2.98526600
O	-2.66485900	1.04544900	1.43701600
C	-2.71193700	1.84056900	3.65605700
H	-3.78026500	2.04134400	3.54018700
H	-2.49909200	1.49577100	4.66922600
H	-2.18600900	2.78483600	3.47851400
H	4.47735100	1.88264300	1.46203300

C	5.35309400	-1.00527300	2.53064700
H	4.55180300	-1.55635800	3.03350400
H	5.97159700	-1.73954100	2.01696100
H	5.94099900	-0.47518100	3.28243000
C	4.15039200	-1.51731000	-0.35892800
O	3.85187800	-1.62464600	-1.53383400
O	4.43681100	-2.58929200	0.42152200
C	4.32473800	-3.85846900	-0.23771800
H	4.59465100	-4.60339600	0.51152700
H	3.30136800	-4.01876600	-0.58556100
H	4.99969100	-3.91400100	-1.09565200
C	2.37794100	1.30818800	-0.56837700
S	1.07399000	0.39033600	0.35066500
N	-0.28400300	0.68944600	-0.36639900
O	1.42720700	-1.04988000	0.47962900
C	1.19715500	1.13362700	2.00789800
H	0.96089700	2.19639700	1.91774600
H	0.44470900	0.61802300	2.61330700
H	2.20784900	0.98639300	2.39132600
H	5.71775900	1.46010500	-1.10410900
H	-0.54676400	1.70876400	-0.47564300
O	-2.94918200	1.49567700	-1.30350400
C	-2.46736100	2.68550800	-1.33110000
O	-1.34333700	3.04887600	-0.91415100
C	-3.40172400	3.73571500	-1.92208800
H	-4.11149800	4.04711900	-1.14773600
H	-2.83484100	4.60969600	-2.24751900
H	-3.97707000	3.32121800	-2.75316000

F

C	4.71366100	1.81281500	-1.10416600
C	3.78283500	0.99108300	-0.44804000
H	5.05520900	3.48121000	-2.42053600
C	4.30846700	2.87229100	-1.91945100
C	2.00559000	2.33304600	-1.45822100
C	2.95192400	3.12836300	-2.10661200
H	0.94121800	2.49171100	-1.60247900
H	2.62800100	3.93562600	-2.75650700

C	4.27701100	-0.16322000	0.37530500
C	4.81400000	0.07156000	1.60039000
O	4.84411100	1.33076000	2.12853500
H	4.50745600	1.95620800	1.46646300
C	5.43323700	-0.89562000	2.56118900
H	4.80940800	-0.97165400	3.45934900
H	5.54410100	-1.88447500	2.12771900
H	6.40573100	-0.50505300	2.87822500
C	4.21792200	-1.46794100	-0.33370600
O	4.15536800	-1.55329300	-1.54413200
O	4.23316200	-2.55068300	0.47889200
C	4.08830800	-3.80871600	-0.19985200
H	4.12078600	-4.56789100	0.58212700
H	3.13258100	-3.84078800	-0.72757000
H	4.89756400	-3.96086600	-0.91846100
C	2.41564700	1.29381800	-0.62560700
S	1.05730800	0.34206900	0.18135700
N	-0.33318900	0.74347100	-0.38759200
O	1.40387100	-1.09782500	0.08931700
C	1.22907800	0.88564100	1.92117600
H	0.99302600	1.94969600	1.99244200
H	0.51032800	0.29266000	2.49040700
H	2.24380700	0.69386900	2.26869300
H	5.77034300	1.58850000	-0.99099300
H	-0.70878100	1.55590900	0.09946200

TS12

C	2.50531600	-1.16456800	-1.53679900
C	1.51650800	-0.69758000	-0.63915500
H	3.38686700	-2.82803700	-2.55434500
C	2.62418800	-2.51402200	-1.84695000
C	0.81302900	-3.06303600	-0.35844600
C	1.76973900	-3.47084200	-1.28089200
H	0.15264600	-3.77455600	0.12622600
H	1.85601200	-4.51848800	-1.55099500
C	1.30671400	0.72232900	-0.31831200
C	-0.05671200	1.15575000	-0.23786800
O	-0.89007300	0.69380500	-1.26760100

H	-0.42211300	-0.00489900	-1.74914200
C	-0.50522000	2.53890300	0.15792900
H	-1.59522100	2.55296700	0.22760300
H	-0.07296800	2.83050100	1.11103400
H	-0.18612100	3.25292000	-0.60516800
C	2.47996900	1.54179700	-0.10060100
O	3.64123900	1.15706800	-0.21111900
O	2.21000900	2.84543000	0.23762800
C	3.36619000	3.66355100	0.43482300
H	2.98549200	4.65225300	0.69693300
H	3.99475600	3.27337200	1.24021900
H	3.97024100	3.71849600	-0.47510700
C	0.70700400	-1.70274000	-0.04739200
S	-0.33921100	-1.29027700	1.36138300
N	-0.89036000	0.21039900	1.22986800
O	-1.29018500	-2.39974500	1.63960600
C	0.87909000	-1.16280800	2.69243700
H	1.59428000	-0.38688400	2.41232000
H	0.32994500	-0.87973300	3.59178500
H	1.36572400	-2.13239700	2.80674600
H	3.17588700	-0.43845600	-1.97813100
H	-1.90339900	0.19497200	1.02722200
C	-5.79233700	0.61241500	-0.70082400
H	-6.29240500	0.49898800	0.26001500
H	-6.07087600	-0.20931200	-1.36742800
H	-6.10720400	1.54239800	-1.18320600
C	-4.29800000	0.61969000	-0.49992500
O	-3.75587700	0.49468900	0.58781700
O	-3.63161900	0.78091800	-1.64602500
H	-2.66245400	0.77717600	-1.45839300

IM11

C	3.46714800	-0.23254800	0.08994700
C	2.02959800	-0.27280800	0.11415200
H	5.32170500	-1.24648800	-0.09601100
C	4.24030000	-1.35738900	-0.09580100
C	2.30619600	-2.74918700	-0.27124400

C	3.67917900	-2.64031300	-0.28147200
H	1.83230100	-3.71378100	-0.43248500
H	4.30556200	-3.51273900	-0.43088500
C	1.21781800	0.89268900	0.25474700
C	-0.27444600	0.81361900	0.51077700
O	-1.05418200	1.27696800	-0.64212900
H	-0.66061500	2.14082000	-0.86667200
C	-0.73612200	1.59188600	1.76063400
H	-1.81675200	1.47821900	1.89966500
H	-0.22278200	1.20793600	2.64480700
H	-0.50554100	2.64950500	1.64456900
C	1.78725200	2.19641800	0.03211100
O	2.96094600	2.54607900	-0.02662900
O	0.79414400	3.16919800	-0.20603300
C	1.29130500	4.48900300	-0.45049100
H	0.40963900	5.11916500	-0.58144900
H	1.88956300	4.84321200	0.39271100
H	1.91306400	4.51336200	-1.34927700
C	1.51360700	-1.60282700	-0.05284400
S	-0.20587700	-1.81320800	-0.17579000
N	-0.73682200	-0.55806200	0.76230300
O	-0.78049600	-2.04307600	-1.52405500
C	-0.71969800	-3.19060800	0.88378100
H	-0.24403800	-3.09440300	1.85828100
H	-1.80745400	-3.12079800	0.95944900
H	-0.44130600	-4.11688900	0.38098700
H	3.93394300	0.73284000	0.21990000
H	-1.77476500	-0.58831200	0.81965000
C	-5.67538800	-0.15582900	-0.30164700
H	-6.05196300	-0.93042200	0.36519700
H	-5.86655200	-0.43518400	-1.34237100
H	-6.19556700	0.78856100	-0.11904400
C	-4.19239100	0.02608700	-0.09629800
O	-3.53520800	-0.68620700	0.66380600
O	-3.69446200	1.01850300	-0.81100500
H	-2.69873600	1.10227800	-0.70024700

TS13

C	3.43774500	-0.00615500	0.17689000
C	2.01552800	-0.15555700	0.14886000
H	5.36719300	-0.88934000	0.04543200
C	4.29702700	-1.07434000	0.00623900
C	2.46719600	-2.59018800	-0.25796500
C	3.83127800	-2.38483300	-0.21261100
H	2.06717600	-3.58173000	-0.45053000
H	4.52091700	-3.21064500	-0.34886700
C	1.10118000	0.94913200	0.31587200
C	-0.31802200	0.72443700	0.55526300
O	-1.18990200	1.21389200	-0.90357800
H	-0.93693200	2.14951100	-0.99346600
C	-1.02533600	1.54764200	1.63177800
H	-2.10598400	1.39968700	1.59157300
H	-0.66067900	1.20745400	2.60530700
H	-0.80152500	2.60522500	1.52312000
C	1.58159300	2.30999700	0.15112200
O	2.72936300	2.73070500	0.19679600
O	0.55468200	3.20140500	-0.16688500
C	0.97195500	4.56240900	-0.34470600
H	0.05903700	5.12819800	-0.53665000
H	1.47227700	4.93721200	0.55139300
H	1.65967800	4.64998200	-1.18940900
C	1.59424200	-1.50454000	-0.05932300
S	-0.11374700	-1.80543000	-0.25273000
N	-0.75658000	-0.61696700	0.68788900
O	-0.59293800	-2.01215100	-1.63884400
C	-0.60347000	-3.23961800	0.73535200
H	-0.14178200	-3.17911000	1.71969200
H	-1.69308700	-3.18144400	0.80185500
H	-0.30439700	-4.13647300	0.19275700
H	3.83092000	0.98654800	0.34010600
H	-1.86900000	-0.73095700	0.73920800
C	-5.47969700	-0.50646800	-0.12010500
H	-5.81672700	-1.12563800	0.71266600
H	-5.63528500	-1.06375600	-1.05077700
H	-6.06471800	0.41312300	-0.18200400
C	-4.00272500	-0.18510000	0.01193900

O	-3.28518000	-0.98048400	0.69253100
O	-3.58905400	0.85894200	-0.58348100
H	-2.27966500	1.07790300	-0.74609900

TS13'

C	-3.96301400	1.23377900	2.98736800
C	-2.77362600	0.70908400	2.41861900
H	-5.85502800	2.17213000	2.69297500
C	-4.95811100	1.80172000	2.20400400
C	-3.70134900	1.41152800	0.19975600
C	-4.84928300	1.89315800	0.80705100
H	-3.56079500	1.44660800	-0.87563800
H	-5.64649000	2.32797800	0.21338600
C	-1.71219400	0.03637900	3.18330100
C	-0.99867000	-1.03984300	2.57090200
O	-2.15706100	-2.45581300	2.11805200
H	-1.84946600	-3.28498000	2.51326100
C	0.12213000	-1.81631200	3.22980200
H	0.49453500	-2.55869400	2.52049000
H	0.94612000	-1.14365400	3.48567200
H	-0.20863700	-2.29879000	4.14658800
C	-1.61510700	0.36996600	4.60449500
O	-2.20749200	1.28823600	5.16084000
O	-0.73935800	-0.40259200	5.32002700
C	-0.60358400	-0.03660600	6.69709400
H	0.12193700	-0.73599700	7.11576700
H	-0.24436100	0.99112100	6.79793400
H	-1.55914800	-0.12012900	7.22137800
C	-2.70298100	0.85724500	1.01020900
S	-1.22932800	0.28479200	0.26089900
N	-0.74206900	-1.02426200	1.10832400
O	-1.32127500	0.05543300	-1.19702200
C	0.03160600	1.52703600	0.62561100
H	0.05516900	1.66780600	1.70809400
H	0.97902100	1.13388100	0.25366400
H	-0.24922800	2.44585800	0.10852100
H	-4.08675000	1.18163400	4.05880200
H	-1.43764100	-1.94166600	1.04103900

3

C	-1.83629100	0.44898400	0.08612700
C	-0.53134600	0.96785200	-0.12329500
C	-2.97110400	1.25571700	0.26914500
C	-0.45469800	2.38743400	-0.15874300
C	-2.84884100	2.63239200	0.21268900
H	-3.93461000	0.79731000	0.47114100
C	-1.57587500	3.18462400	-0.00018200
H	0.50898800	2.84297900	-0.33468300
H	-3.71755800	3.26900600	0.34516600
H	-1.45989400	4.26406100	-0.04173600
S	-2.00296900	-1.29457800	0.27001200
O	-2.37846400	-1.70747100	1.64753600
C	-3.33146700	-1.83583100	-0.83152400
H	-3.17781600	-1.41189700	-1.82349600
H	-3.25276500	-2.92406000	-0.86064000
H	-4.28895100	-1.53660900	-0.40415800
N	-0.71442500	-1.95567900	-0.41025400
C	0.62990100	0.09260800	-0.28919600
C	0.47234600	-1.28337900	-0.45957000
C	1.97960600	0.70681700	-0.32225400
O	2.26713100	1.81136600	-0.75620500
O	2.92666200	-0.08987100	0.24029900
C	1.59142500	-2.22876200	-0.84322400
H	2.34875300	-1.75771400	-1.46936600
H	2.09072000	-2.60584500	0.05462900
H	1.15172400	-3.07878000	-1.36875200
C	4.26177100	0.43427800	0.20882600
H	4.32261600	1.36799500	0.77350000
H	4.58363600	0.62727500	-0.81802400
H	4.88730800	-0.33130600	0.66866800

Cartesian Coordinates for the Stationary Points Given in Fig. S5**IM12_{p-NO2}**

Rh	0.73604300	-0.89606000	-0.29663900
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N	-0.20463500	0.92010000	-0.98164600
C	-0.59664600	-2.12442100	-1.65113400
C	-0.27380300	-2.91721300	-0.52015300
C	1.16743300	-3.11371300	-0.48916000
C	1.71305700	-2.47274700	-1.65014000
C	0.64992500	-1.77563200	-2.31580200
O	0.72775300	-2.19154100	2.96235000
O	-0.11617600	-0.51632700	1.68975300
C	0.01906900	-1.18182600	2.78513400
C	-0.78300300	-0.61204600	3.95936700
H	-0.35762300	0.35503100	4.25579800
H	-0.74961900	-1.29141600	4.81489100
H	-1.82434000	-0.43351700	3.66957800
C	-2.88447100	1.37245200	-0.15815300
C	-3.11893100	0.29952800	0.71038200
C	-3.92828900	1.94648300	-0.88869900
C	-4.41307600	-0.18922700	0.86848100
H	-2.28999600	-0.15025000	1.25140900
C	-5.22487800	1.45557800	-0.74974200
H	-3.72100100	2.78037000	-1.55382100
C	-5.44688100	0.39746100	0.13306800
H	-4.62691100	-1.01114900	1.54546900
H	-6.05383200	1.88731600	-1.30286500
C	0.75109500	-1.02847800	-3.60960500
H	0.01122600	-0.22389400	-3.65234500
H	0.56730500	-1.70562100	-4.45659300
H	1.74252000	-0.58560800	-3.73355600
C	3.10175300	-2.61146900	-2.18276500
H	3.48461200	-1.65489300	-2.54426800
H	3.08218500	-3.31947100	-3.02436000
H	3.79552600	-2.99036600	-1.43137300
C	1.88576400	-4.05538300	0.43098700
H	2.96392900	-3.87085800	0.42577100
H	1.72180000	-5.09669400	0.11747900
H	1.52723200	-3.94012200	1.45597500
C	-1.24317600	-3.52627200	0.44602400
H	-0.81735200	-3.57694000	1.45053100
H	-1.48953600	-4.55009900	0.12920700

H	-2.17624700	-2.95721800	0.49136500
C	-1.95743000	-1.76041300	-2.15468300
H	-2.73116200	-1.94569600	-1.40524900
H	-2.19735200	-2.35912900	-3.04502600
H	-2.00061600	-0.70435600	-2.43973400
S	-1.14634400	1.97773100	-0.43401000
C	2.57260900	2.66911900	3.16332000
H	1.89027700	2.04536500	3.74810900
H	3.39348900	3.03098500	3.78654200
H	2.00531700	3.53109800	2.78916400
C	3.13034400	1.90557100	1.98925100
O	2.19296000	1.10842400	1.42895800
O	4.27810100	1.99543700	1.59071900
C	2.54666200	0.36318900	0.23728300
C	2.74880500	1.26612500	-0.94282200
O	3.15604200	0.90606500	-2.03958700
O	2.43172400	2.55358100	-0.68702700
C	2.54173800	3.47804000	-1.79778800
H	3.59651600	3.54547600	-2.09461600
H	1.96999100	3.07800400	-2.64348900
C	3.68308600	-0.57702400	0.53242700
O	4.54333200	-0.87971500	-0.29302500
C	3.75346500	-1.17291000	1.93020000
H	4.26702200	-0.46919500	2.59685600
H	4.35764800	-2.08329400	1.87879100
H	2.77040900	-1.39895800	2.34524700
C	-0.79497500	2.62219800	1.24205100
H	-0.68586900	1.77479300	1.91771800
H	0.15164700	3.15887500	1.15511000
H	-1.60321500	3.29675700	1.53363700
O	-1.35899100	3.22456900	-1.27505700
C	1.99490600	4.81545200	-1.33549900
H	2.09961500	5.55087400	-2.14181900
H	0.93335600	4.72879000	-1.08327800
H	2.54250700	5.18497400	-0.46100500
N	-6.80805000	-0.11169100	0.29777400
O	-6.99189500	-1.04640100	1.08247900
O	-7.71360300	0.41536100	-0.35409100

TS14_{p-NO2}

Rh	-0.40222600	0.82878900	-0.58969600
N	-0.74011900	-0.99086400	-1.56898700
C	0.84129200	1.76073700	-2.25075100
C	1.28552900	2.35650100	-1.04119600
C	0.17043700	3.03983400	-0.40538600
C	-0.95723700	2.91024200	-1.26262700
C	-0.57932800	2.03186000	-2.35996900
O	2.05383100	1.17897200	3.15466800
O	1.04492500	-0.81820100	2.84119500
C	1.50786900	0.16780500	3.59189700
C	1.28482400	-0.07078500	5.06985100
H	1.69463100	-1.04475300	5.36000700
H	0.20828200	-0.09233000	5.27886700
H	1.75462500	0.72305900	5.65407200
C	1.85463900	-1.78061600	-0.82374400
C	1.95114300	-0.89758300	0.26088800
C	2.93455000	-2.34468600	-1.51892500
C	3.28180200	-0.60207300	0.62872100
H	1.20695300	-0.68298500	1.80825600
C	4.22931900	-2.01874900	-1.13439600
H	2.75905800	-3.02512400	-2.35163300
C	4.37636600	-1.14258000	-0.05493000
H	3.48627900	0.06019300	1.46868200
H	5.09784700	-2.42432100	-1.64331100
C	-1.44559700	1.68572200	-3.52906900
H	-1.10071200	0.76943500	-4.01528500
H	-1.41832600	2.49986700	-4.26839600
H	-2.48301000	1.54155300	-3.21640900
C	-2.24533900	3.66259200	-1.19379300
H	-3.09680900	3.01426100	-1.41075000
H	-2.21652700	4.46276900	-1.94823400
H	-2.40414700	4.11671400	-0.21500200
C	0.29157900	3.90839400	0.81103500
H	-0.69014100	4.16134200	1.21995100
H	0.80433800	4.84861900	0.56111300
H	0.87246800	3.41455200	1.59733100

C	2.68616300	2.42749000	-0.52757700
H	2.72312000	2.27260000	0.55472900
H	3.08214600	3.43385300	-0.73127000
H	3.34158400	1.69918500	-1.00775400
C	1.66518500	1.03243000	-3.26783300
H	2.63161500	0.72679500	-2.85787900
H	1.85368700	1.67580900	-4.13877700
H	1.14798900	0.13365700	-3.62018200
S	0.18059300	-2.21025200	-1.44999200
C	-2.08771600	-2.50315400	3.08502900
H	-2.66275500	-2.68205700	3.99638900
H	-2.18002300	-3.37900200	2.43002800
H	-1.02841100	-2.35996000	3.31357500
C	-2.64263200	-1.30006300	2.36997200
O	-1.76450000	-0.80978500	1.46024400
O	-3.74184100	-0.81768700	2.57439400
C	-2.19333400	0.29299800	0.62453100
C	-3.23809000	-0.12868900	-0.36544700
O	-3.81649500	0.62787000	-1.13523800
O	-3.48378300	-1.45397500	-0.34671300
C	-4.41444900	-1.94611300	-1.34313800
H	-5.35649000	-1.39149500	-1.25361800
H	-3.99124900	-1.75128600	-2.33664500
C	-2.53507000	1.48959400	1.46885200
O	-3.41687000	2.29481500	1.17790300
C	-1.71724500	1.70148400	2.73531700
H	-0.66513200	1.44835600	2.59518100
H	-2.11994900	1.07728600	3.54202700
H	-1.81428600	2.74780100	3.03612900
O	0.35844300	-3.06310900	-2.69407700
C	-0.33122500	-3.43594300	-0.17931700
H	-0.33007500	-2.94264200	0.79200700
H	-1.34153200	-3.75611000	-0.44583500
H	0.36374800	-4.27872800	-0.20030500
C	-4.61180700	-3.42923600	-1.09336600
H	-5.01021700	-3.60817100	-0.08830800
H	-5.32441300	-3.83109400	-1.82298800
H	-3.66829400	-3.97598500	-1.19921900

N	5.73176800	−0.78966000	0.36986900
O	6.68877600	−1.31650700	−0.21028000
O	5.87332100	0.02081400	1.29145700

IM13_{p-NO2}

Rh	0.25178900	−0.65796700	−1.22610100
N	0.87382100	1.15651700	−2.11474400
C	−0.75918900	−1.44547900	−3.05824300
C	−1.26712200	−2.21691200	−1.96062100
C	−0.17479800	−2.94317500	−1.38872700
C	0.99819600	−2.71316800	−2.22248000
C	0.64346800	−1.79809700	−3.23407900
C	−1.19916200	1.83504300	−0.53116000
C	−1.10332500	0.46463300	−0.21502200
C	−2.14110100	2.70737700	0.01949400
C	−2.02877000	0.00429100	0.73773100
C	−3.04178800	2.23171200	0.96634100
H	−2.18102600	3.74549300	−0.30042200
C	−2.96116500	0.87758100	1.30559800
H	−2.03812900	−1.02992800	1.05735700
H	−3.78982500	2.86608100	1.42470300
C	1.51404100	−1.22516000	−4.31064200
H	1.49001100	−0.13108500	−4.25672900
H	1.16644700	−1.53257000	−5.30569100
H	2.55262200	−1.54486300	−4.19891600
C	2.30438900	−3.42434800	−2.04564000
H	3.06270700	−3.04369200	−2.73205200
H	2.17514800	−4.49846900	−2.24031800
H	2.68008700	−3.29662800	−1.02782500
C	−0.25619500	−3.98411200	−0.31116100
H	0.64887500	−3.98462700	0.30316100
H	−0.36285700	−4.98934900	−0.74370100
H	−1.11662900	−3.82126400	0.34436900
C	−2.70852200	−2.32368200	−1.55760200
H	−2.82200000	−2.59656900	−0.50527500
H	−3.21056600	−3.09971700	−2.15103900
H	−3.24768500	−1.38650200	−1.71648000

C	-1.54560700	-0.58699700	-4.00572200
H	-2.55129600	-0.38893400	-3.62481600
H	-1.65416300	-1.07493600	-4.98417900
H	-1.05180800	0.37724300	-4.15779900
S	-0.02291000	2.36274500	-1.80657600
C	1.55834200	2.54767400	2.82538500
H	1.77900300	2.58077800	3.89369500
H	2.08560400	3.37689800	2.34027900
H	0.48899600	2.67438500	2.64645900
C	2.06327600	1.24720600	2.24313100
O	1.34352600	0.89474600	1.15786400
O	2.99494800	0.61005600	2.69525400
C	1.76559500	-0.26576600	0.39518400
C	3.03038700	0.01194200	-0.35361900
O	3.66694500	-0.80245600	-0.99818300
O	3.42628900	1.31004600	-0.24676900
C	4.58479800	1.66547500	-1.01849600
H	5.40032500	0.97042800	-0.79171500
H	4.34490100	1.56033700	-2.08241500
C	1.73451800	-1.51026500	1.21580600
O	2.44201200	-2.49749500	1.00571800
C	0.73647000	-1.56858100	2.37005000
H	-0.04442100	-0.81178000	2.31044800
H	1.28980000	-1.42787500	3.30467600
H	0.29005200	-2.56572400	2.39262000
O	-0.78457700	3.11951300	-2.87480700
C	0.92465600	3.70777200	-0.97826700
H	1.47464600	3.26991200	-0.14716900
H	1.61623600	4.08158400	-1.73716200
H	0.25733100	4.51086600	-0.65847300
C	4.95943500	3.09348200	-0.66351500
H	5.18397400	3.18323300	0.40413300
H	5.84741400	3.39694600	-1.22786800
H	4.14710200	3.78582300	-0.90354400
N	-3.90433200	0.35342300	2.29708300
O	-4.70826700	1.13828300	2.81225400
O	-3.86140500	-0.84927400	2.57362400

IM12_{p-H}			
Rh	0.29833900	-0.83072800	-0.29365200
N	-0.72143600	0.97735100	-0.84385000
C	-1.00137400	-2.03395600	-1.70361200
C	-0.63695900	-2.87359100	-0.61998400
C	0.81125900	-3.02291100	-0.61665200
C	1.31960700	-2.29663500	-1.74087300
C	0.22386300	-1.60077300	-2.35647100
O	0.40419000	-2.34684200	2.89178400
O	-0.49483400	-0.61124800	1.74324100
C	-0.32921700	-1.34333100	2.78911700
C	-1.12605900	-0.86993700	4.00940300
H	-0.72104500	0.08785600	4.35952700
H	-1.06107000	-1.60006800	4.82021100
H	-2.17610400	-0.70107700	3.74664400
C	-3.43095000	1.13674600	0.07307900
C	-3.54746600	0.00060200	0.87994600
C	-4.54925200	1.67508400	-0.56686400
C	-4.80237600	-0.58923800	1.05579500
H	-2.66309400	-0.41303500	1.35623100
C	-5.79851600	1.06993900	-0.39829300
H	-4.43513000	2.56148100	-1.18505900
C	-5.92735800	-0.05876100	0.41524500
H	-4.90136500	-1.46797100	1.69201400
H	-6.67202700	1.48622400	-0.89827300
C	0.28197900	-0.78652900	-3.61193600
H	-0.48066500	-0.00216300	-3.60085200
H	0.10279900	-1.42400200	-4.49021600
H	1.25828600	-0.30924500	-3.72837300
C	2.70728300	-2.35035900	-2.29151400
H	3.05037100	-1.36008400	-2.59778700
H	2.70757400	-3.00746800	-3.17365200
H	3.42218800	-2.74603900	-1.56890800
C	1.57469500	-3.98684900	0.24259100
H	2.64437400	-3.75740700	0.24218500
H	1.45203100	-5.01418500	-0.13046200
H	1.22065700	-3.94630000	1.27461700
C	-1.57165700	-3.56758500	0.32333300

H	-1.13353800	-3.64933100	1.32049900
H	-1.78054100	-4.58446600	-0.03971500
H	-2.52562300	-3.03904500	0.40397400
C	-2.37885000	-1.69102000	-2.17668800
H	-3.14070800	-1.96051800	-1.44121500
H	-2.59743600	-2.23240300	-3.10829800
H	-2.46561500	-0.61939400	-2.38238100
S	-1.76463900	1.89634100	-0.22306100
C	2.00249300	2.69150600	3.26734600
H	1.33887800	2.03016100	3.83197100
H	2.80866200	3.06349500	3.90364100
H	1.40778300	3.54339000	2.91320100
C	2.58848600	1.97928600	2.07481200
O	1.67943800	1.16870300	1.48967200
O	3.73443300	2.11858100	1.68425800
C	2.04863700	0.48910800	0.26459600
C	2.21311600	1.45225800	-0.87332400
O	2.63712800	1.15277900	-1.98155700
O	1.87629300	2.72307100	-0.55495800
C	2.12230700	3.74171700	-1.56160200
H	2.19170500	4.66785000	-0.98013400
H	3.09249600	3.54127200	-2.02997800
C	3.22677700	-0.41587500	0.50904000
O	4.09354000	-0.64655000	-0.33281100
C	3.33033400	-1.07327900	1.87700500
H	3.79567300	-0.37362900	2.58188800
H	3.98995700	-1.94084900	1.78383400
H	2.36205800	-1.38145300	2.27329200
C	-1.40298800	2.50707600	1.46647300
H	-1.19075500	1.64760900	2.10114100
H	-0.51428700	3.13346100	1.36523400
H	-2.25573500	3.09119900	1.81986400
O	-2.10065400	3.16084500	-0.99973800
C	1.01373300	3.82964900	-2.60060800
H	1.20563600	4.68853300	-3.25605900
H	0.97982800	2.92437900	-3.21288700
H	0.03956900	3.95873500	-2.12215100
H	-6.90231400	-0.52441700	0.55141800

TS14 _{p-H}			
Rh	0.64086200	-0.79987400	-0.05090000
N	-0.08071500	-0.29616400	1.87092500
C	2.74761100	-1.60796400	0.23491300
C	2.48187000	-1.59579100	-1.19757700
C	1.40601500	-2.47754200	-1.46632900
C	0.95758000	-3.02577500	-0.19867700
C	1.82600800	-2.51690600	0.83272800
O	-0.31713200	3.94555600	-1.14003600
O	0.30953800	2.01597600	-2.12763800
C	-0.12467700	3.24054900	-2.14327900
C	-0.42662300	3.77351000	-3.53968400
H	-1.34958300	3.30812900	-3.90948700
H	0.37435300	3.51065800	-4.23835500
H	-0.56437200	4.85739600	-3.51484500
C	1.60333900	1.80632000	1.39910500
C	1.61605700	1.47858300	0.03095800
C	2.59126200	2.55234900	2.04407600
C	2.74399800	1.97182300	-0.66787700
H	0.65135900	1.55669300	-0.97682300
C	3.68080300	3.01790100	1.30693700
H	2.50805800	2.75100100	3.11313300
C	3.75243900	2.72132200	-0.05722600
H	2.80132600	1.80821300	-1.74170700
H	4.46122300	3.60340300	1.79058800
C	1.79517100	-2.91844300	2.27420600
H	2.15959600	-2.11542900	2.92047500
H	2.43773200	-3.79780300	2.42696900
H	0.78246100	-3.17925200	2.59310000
C	0.02054000	-4.18277000	-0.05071200
H	-0.35179000	-4.27186500	0.97163700
H	0.55728100	-5.10927900	-0.30576400
H	-0.83745300	-4.08154100	-0.71635000
C	0.97890700	-2.94130400	-2.82426200
H	1.53592900	-3.85211700	-3.09076300
H	1.19272000	-2.18880900	-3.58952500
H	-0.08580300	-3.18128300	-2.85597600
C	3.32555600	-0.93718400	-2.24818300

H	2.71299500	-0.44816600	-3.01337200
H	3.93776200	-1.69871100	-2.75277500
H	3.99967300	-0.19415300	-1.82012200
C	3.91869200	-0.97808700	0.92635800
H	4.24315200	-0.06488400	0.42474400
H	4.76783500	-1.67703700	0.93962200
H	3.68003700	-0.72704100	1.96430600
S	0.28023200	1.10015000	2.41339000
C	-3.51051500	2.59841700	-0.77224100
H	-4.34862000	2.90597500	-1.40229300
H	-3.80080400	2.72463900	0.27952100
H	-2.63323000	3.22161500	-0.95488000
C	-3.22224700	1.13837700	-1.00101500
O	-1.95720400	0.80715100	-0.64652500
O	-4.03589800	0.34072500	-1.43348400
C	-1.61642500	-0.60085900	-0.59064000
C	-2.33993500	-1.25961400	0.55228000
O	-2.30901000	-2.45124900	0.81446100
O	-3.08194900	-0.39374300	1.28305400
C	-3.78988800	-0.96497000	2.40896600
H	-4.39595700	-1.80898800	2.05780000
H	-3.05181300	-1.34739100	3.12573600
C	-1.78695900	-1.26837400	-1.91736800
O	-2.07870100	-2.46247100	-2.04160600
C	-1.56893500	-0.43943000	-3.17416000
H	-0.96699300	0.45217600	-3.00308900
H	-2.55187200	-0.13749700	-3.55610500
H	-1.10294200	-1.07784100	-3.93074800
O	0.66506400	1.21398700	3.87681000
C	-1.03143300	2.37130700	2.23237600
H	-1.21997100	2.51797100	1.16933500
H	-1.92103100	1.98331800	2.73414200
H	-0.68710400	3.29407800	2.70500800
C	-4.65139100	0.12755500	3.01427000
H	-5.36812700	0.51313100	2.28042300
H	-5.21294200	-0.27798100	3.86396800
H	-4.03915400	0.96121000	3.37629200
H	4.59329300	3.08445300	-0.65180100

IM13_{p-H}

Rh	0.73604300	-0.89606000	-0.29663900
N	-0.20463500	0.92010000	-0.98164600
C	-0.59664600	-2.12442100	-1.65113400
C	-0.27380300	-2.91721300	-0.52015300
C	1.16743300	-3.11371300	-0.48916000
C	1.71305700	-2.47274700	-1.65014000
C	0.64992500	-1.77563200	-2.31580200
O	0.72775300	-2.19154100	2.96235000
O	-0.11617600	-0.51632700	1.68975300
C	0.01906900	-1.18182600	2.78513400
C	-0.78300300	-0.61204600	3.95936700
H	-0.35762300	0.35503100	4.25579800
H	-0.74961900	-1.29141600	4.81489100
H	-1.82434000	-0.43351700	3.66957800
C	-2.88447100	1.37245200	-0.15815300
C	-3.11893100	0.29952800	0.71038200
C	-3.92828900	1.94648300	-0.88869900
C	-4.41307600	-0.18922700	0.86848100
H	-2.28999600	-0.15025000	1.25140900
C	-5.22487800	1.45557800	-0.74974200
H	-3.72100100	2.78037000	-1.55382100
C	-5.44688100	0.39746100	0.13306800
H	-4.62691100	-1.01114900	1.54546900
H	-6.05383200	1.88731600	-1.30286500
C	0.75109500	-1.02847800	-3.60960500
H	0.01122600	-0.22389400	-3.65234500
H	0.56730500	-1.70562100	-4.45659300
H	1.74252000	-0.58560800	-3.73355600
C	3.10175300	-2.61146900	-2.18276500
H	3.48461200	-1.65489300	-2.54426800
H	3.08218500	-3.31947100	-3.02436000
H	3.79552600	-2.99036600	-1.43137300
C	1.88576400	-4.05538300	0.43098700
H	2.96392900	-3.87085800	0.42577100
H	1.72180000	-5.09669400	0.11747900

H	1. 52723200	-3. 94012200	1. 45597500
C	-1. 24317600	-3. 52627200	0. 44602400
H	-0. 81735200	-3. 57694000	1. 45053100
H	-1. 48953600	-4. 55009900	0. 12920700
H	-2. 17624700	-2. 95721800	0. 49136500
C	-1. 95743000	-1. 76041300	-2. 15468300
H	-2. 73116200	-1. 94569600	-1. 40524900
H	-2. 19735200	-2. 35912900	-3. 04502600
H	-2. 00061600	-0. 70435600	-2. 43973400
S	-1. 14634400	1. 97773100	-0. 43401000
C	2. 57260900	2. 66911900	3. 16332000
H	1. 89027700	2. 04536500	3. 74810900
H	3. 39348900	3. 03098500	3. 78654200
H	2. 00531700	3. 53109800	2. 78916400
C	3. 13034400	1. 90557100	1. 98925100
O	2. 19296000	1. 10842400	1. 42895800
O	4. 27810100	1. 99543700	1. 59071900
C	2. 54666200	0. 36318900	0. 23728300
C	2. 74880500	1. 26612500	-0. 94282200
O	3. 15604200	0. 90606500	-2. 03958700
O	2. 43172400	2. 55358100	-0. 68702700
C	2. 54173800	3. 47804000	-1. 79778800
H	3. 59651600	3. 54547600	-2. 09461600
H	1. 96999100	3. 07800400	-2. 64348900
C	3. 68308600	-0. 57702400	0. 53242700
O	4. 54333200	-0. 87971500	-0. 29302500
C	3. 75346500	-1. 17291000	1. 93020000
H	4. 26702200	-0. 46919500	2. 59685600
H	4. 35764800	-2. 08329400	1. 87879100
H	2. 77040900	-1. 39895800	2. 34524700
C	-0. 79497500	2. 62219800	1. 24205100
H	-0. 68586900	1. 77479300	1. 91771800
H	0. 15164700	3. 15887500	1. 15511000
H	-1. 60321500	3. 29675700	1. 53363700
O	-1. 35899100	3. 22456900	-1. 27505700
C	1. 99490600	4. 81545200	-1. 33549900
H	2. 09961500	5. 55087400	-2. 14181900
H	0. 93335600	4. 72879000	-1. 08327800

H	2.54250700	5.18497400	-0.46100500
N	-6.80805000	-0.11169100	0.29777400
O	-6.99189500	-1.04640100	1.08247900
O	-7.71360300	0.41536100	-0.35409100

IM12_{p-OMe}

Rh	0.57842800	-0.81610600	-0.33838800
N	-0.19186100	1.10284300	-0.90040800
C	-0.70432600	-1.80219000	-1.92817000
C	-0.53429600	-2.73618600	-0.87481500
C	0.88366700	-3.04145300	-0.74990200
C	1.56850300	-2.31896000	-1.77733700
C	0.61624500	-1.47098600	-2.43973800
O	0.18620800	-2.50726200	2.73615500
O	-0.34664400	-0.59262900	1.64429000
C	-0.37746500	-1.39802000	2.64845600
C	-1.19764500	-0.87815900	3.83458500
H	-2.21365400	-0.61930800	3.51528500
H	-0.73899900	0.03779100	4.22641400
H	-1.24332800	-1.62595600	4.63038000
C	-2.94061000	1.50730000	-0.16497500
C	-3.21657200	0.38199000	0.61234500
C	-3.97921100	2.15962500	-0.83989400
C	-4.52616200	-0.09448400	0.73083100
H	-2.40686500	-0.12892400	1.12519200
C	-5.28350700	1.68585000	-0.73806200
H	-3.75828200	3.03823000	-1.43974700
C	-5.56471000	0.55798800	0.05059500
H	-4.72088300	-0.96899600	1.34914200
H	-6.10480000	2.18070200	-1.25816100
C	0.88538700	-0.59585100	-3.62386900
H	0.23594700	0.28460700	-3.60902400
H	0.69793700	-1.14398600	-4.55880700
H	1.92215400	-0.25058100	-3.63110800
C	2.98453600	-2.50689600	-2.21463100
H	3.46146600	-1.55126800	-2.44115400
H	2.98689900	-3.12059500	-3.12752800
H	3.58688100	-3.01351900	-1.45934900

C	1.46165600	-4.11819600	0.11926700
H	2.54887400	-4.02414900	0.19562500
H	1.24013600	-5.11142300	-0.29788800
H	1.04412300	-4.06135900	1.12644500
C	-1.62232700	-3.38525400	-0.07525800
H	-1.29782000	-3.56198800	0.95288900
H	-1.88359200	-4.35599700	-0.52114900
H	-2.52766200	-2.77186300	-0.05530900
C	-1.98927900	-1.28747500	-2.49561200
H	-2.83349100	-1.47412900	-1.82674800
H	-2.19792600	-1.78284300	-3.45479900
H	-1.93082400	-0.21022000	-2.67890800
S	-1.20352700	2.10701500	-0.36725600
C	2.28148400	2.33424700	3.53114300
H	1.51961500	1.70759200	4.00426400
H	3.05588800	2.60876300	4.25087100
H	1.78969800	3.24697800	3.17110300
C	2.90881200	1.62296600	2.35944200
O	1.98489100	0.94112100	1.64883000
O	4.09589100	1.65799200	2.08573900
C	2.40009900	0.27617000	0.43039300
C	2.78726000	1.26521100	-0.62961800
O	3.31672700	0.97793500	-1.69506900
O	2.51611500	2.54544700	-0.28632300
C	3.00050800	3.58409700	-1.17793000
H	3.09057200	4.46303300	-0.52970200
H	3.99671100	3.30066900	-1.53565600
C	3.43780800	-0.77011200	0.73737500
O	4.34697600	-1.07150000	-0.03418600
C	3.34116200	-1.48465400	2.07772300
H	3.89842800	-2.42245900	1.99868000
H	2.31394100	-1.68742100	2.38197000
H	3.82429400	-0.87224800	2.84900400
C	-0.88480300	2.72008500	1.33282800
H	-0.80829000	1.85970900	1.99756400
H	0.07118800	3.24566400	1.28150600
H	-1.69091000	3.39743100	1.62368800
O	-1.37969600	3.37900700	-1.18394500

O	-6.87458000	0.17608700	0.09389600
C	-7.22261400	-0.95929700	0.88679700
H	-6.97175400	-0.80056000	1.94390400
H	-8.30407700	-1.07669600	0.78293000
H	-6.72039500	-1.86739100	0.52777300
C	2.05395200	3.85263800	-2.33665400
H	2.42512600	4.70968000	-2.91270500
H	1.99473200	2.98575900	-3.00056100
H	1.04671700	4.08035000	-1.97691500

TS14_{p-OMe}

Rh	0.07361500	-0.32887800	0.80739000
N	-0.03448100	1.75642800	1.09205400
C	1.40221800	-1.07906600	2.48812500
C	1.14713400	-2.21218700	1.61459000
C	-0.24594400	-2.48267200	1.60568000
C	-0.88635300	-1.50308800	2.45793300
C	0.14457200	-0.66144900	3.02100900
O	1.82304200	-2.42117900	-2.69120300
O	1.22894400	-0.23955300	-2.79655800
C	1.48517300	-1.40450100	-3.31718700
C	1.30726200	-1.45123600	-4.83040500
H	1.77927800	-0.58203700	-5.30037800
H	0.23738200	-1.41485000	-5.07248900
H	1.72967400	-2.37378000	-5.23622000
C	2.51774300	1.57429200	0.07419400
C	2.25926300	0.31011400	-0.48500900
C	3.80008600	2.04209400	0.38212400
C	3.40903700	-0.48123700	-0.71798700
H	1.43845500	-0.07104100	-1.58779600
C	4.90548900	1.24137500	0.12562200
H	3.92232200	3.02705700	0.82757800
C	4.70458300	-0.03101700	-0.43294800
H	3.27265100	-1.44844400	-1.19152400
H	5.91943100	1.57841300	0.34384200
C	-0.07872700	0.41692000	4.03541600
H	0.69254600	1.18888700	3.97401400
H	-0.05250600	-0.01502900	5.04651000

H	-1.05185700	0.89554500	3.89575600
C	-2.30028900	-1.59154600	2.93434100
H	-2.62448600	-0.66979100	3.41984500
H	-2.36967900	-2.41190600	3.66516900
H	-2.97979000	-1.80211100	2.10762700
C	-0.89857700	-3.69747300	1.02209100
H	-1.90183800	-3.47892400	0.64640000
H	-0.99637500	-4.47315800	1.79637800
H	-0.30119200	-4.11989800	0.20824300
C	2.17679900	-3.08319200	0.96393600
H	1.92731100	-3.28599300	-0.08224900
H	2.21935400	-4.04721600	1.49118200
H	3.16926800	-2.63213100	0.99964100
C	2.74672100	-0.57195100	2.91275100
H	3.48304200	-0.65883600	2.11124400
H	3.11507500	-1.14768500	3.77460900
H	2.69798200	0.47915200	3.21196700
S	1.11988100	2.61898800	0.55196400
C	-1.39819600	1.81986300	-3.83369500
H	-1.98469700	1.75584500	-4.75294100
H	-1.35543000	2.86796900	-3.51042400
H	-0.37445500	1.47183200	-3.99554700
C	-2.05772400	1.00415400	-2.75324800
O	-1.20935000	0.77111900	-1.72678500
O	-3.20637000	0.59854400	-2.79170400
C	-1.71858700	0.09987300	-0.55380400
C	-2.59396200	1.03342600	0.23590400
O	-3.19940400	0.74614200	1.25654000
O	-2.67262300	2.26836400	-0.31172100
C	-3.42833100	3.24629700	0.44145700
H	-4.43941500	2.85889800	0.61741900
H	-2.93987200	3.38679200	1.41418700
C	-2.30782400	-1.23368800	-0.87370600
O	-3.20973100	-1.75755800	-0.21042700
C	-1.73366600	-2.01754100	-2.04590200
H	-1.03108000	-1.44830500	-2.64851800
H	-2.56851400	-2.35901000	-2.66696100
H	-1.22174100	-2.90513900	-1.66006600

O	1.63930800	3.74439700	1.43034300
C	0.73466200	3.48503000	-1.01998500
H	0.46894400	2.73483000	-1.76380600
H	-0.11565200	4.14145100	-0.81729100
H	1.60729700	4.06560000	-1.32845700
O	5.84382100	-0.75133500	-0.67509400
C	5.72005600	-2.02537100	-1.30720500
H	5.22582000	-1.94292100	-2.28399800
H	6.74086600	-2.39167600	-1.44319000
H	5.15925500	-2.73242300	-0.68223900
C	-3.45482500	4.53000700	-0.36698800
H	-3.92493100	4.36887400	-1.34366900
H	-4.03226000	5.29009000	0.17208900
H	-2.44249000	4.91789900	-0.52571300

IM13_{p-OMe}

Rh	0.12161000	0.41220500	0.61587200
N	0.13038700	-1.62282000	1.28682100
C	-1.14718400	1.00074500	2.40165200
C	-1.46527100	1.88532900	1.33997900
C	-0.26743500	2.63211600	0.98373700
C	0.77150600	2.22611800	1.87949700
C	0.27174000	1.14675400	2.68562300
O	-1.28997000	1.72634900	-2.34168200
O	-0.97804300	-0.20043200	-1.18750000
C	-1.43251400	0.49940200	-2.16813400
C	-2.21042000	-0.31889300	-3.20500700
H	-3.01907700	-0.88042400	-2.72335600
H	-1.54202300	-1.05204400	-3.67253900
H	-2.62667900	0.33207900	-3.97801400
C	-2.40827200	-2.94231400	1.01439300
C	-3.16098000	-2.00979700	0.29986800
C	-3.05124600	-3.86479700	1.84826600
C	-4.55573800	-1.99564100	0.40254900
H	-2.65838200	-1.28773600	-0.33707300
C	-4.43755200	-3.85062400	1.96647900
H	-2.45958600	-4.59143300	2.39828300
C	-5.19777400	-2.91798100	1.24165600

H	-5.12458300	-1.26518800	-0.17003300
H	-4.95510600	-4.56097200	2.61258100
C	0.99944100	0.46821300	3.80388100
H	0.68504900	-0.57611700	3.89179600
H	0.79109600	0.97027100	4.76003400
H	2.07935800	0.48284100	3.63740400
C	2.09531800	2.88949700	2.07734900
H	2.89161400	2.15561400	2.21637200
H	2.03828700	3.51456000	2.98070800
H	2.36815700	3.52747100	1.23563400
C	-0.22431600	3.79429600	0.03696400
H	0.80600000	4.05832000	-0.21888800
H	-0.69379200	4.67936800	0.49064600
H	-0.75299600	3.55374300	-0.88748400
C	-2.81884600	2.10115000	0.73529200
H	-2.73814600	2.32324800	-0.33137900
H	-3.31329000	2.95340500	1.22376700
H	-3.46061400	1.22459800	0.86205400
C	-2.08190700	0.12195800	3.17110100
H	-3.03470700	-0.01201200	2.65231600
H	-2.28863600	0.56848900	4.15437900
H	-1.64132300	-0.86604700	3.33609600
S	-0.56179800	-2.92838500	0.92286900
C	2.13871400	-2.19345700	-3.49997600
H	1.14752300	-1.87561100	-3.83687000
H	2.83624800	-2.23421500	-4.33953200
H	2.04090800	-3.19792000	-3.06864200
C	2.67149400	-1.25853700	-2.44431800
O	1.69837600	-0.88299200	-1.58669200
O	3.83044400	-0.88870400	-2.37114700
C	2.05661900	-0.05902100	-0.45008400
C	2.91224200	-0.81248000	0.52558400
O	3.47782100	-0.31493100	1.49026800
O	3.03035600	-2.12621100	0.22469300
C	3.96624700	-2.90294600	1.01790400
H	4.23903400	-3.73478000	0.35875400
H	4.85534100	-2.29110800	1.20734100
C	2.62627300	1.25309500	-0.91873000

O	3.49387100	1.87388200	-0.30666400
C	2.08757200	1.82894400	-2.22051400
H	2.30736500	2.90033700	-2.22953300
H	1.01684700	1.66826400	-2.34932800
H	2.61810500	1.37134500	-3.06459300
C	-0.33076100	-3.48664400	-0.80995900
H	-0.64998800	-2.68288500	-1.47331500
H	0.74079100	-3.66641900	-0.92060600
H	-0.90184900	-4.40444200	-0.96715600
O	-0.17474000	-4.14559600	1.75025300
O	-6.54954600	-2.98940200	1.41799500
C	-7.37509000	-2.07179100	0.70009500
H	-7.25621300	-2.19176400	-0.38483700
H	-8.40344900	-2.31053100	0.98225500
H	-7.15239000	-1.03257800	0.97613400
C	3.35807700	-3.40916300	2.31582500
H	4.07856400	-4.06736700	2.81761300
H	3.12045400	-2.57781000	2.98526200
H	2.43992800	-3.97215600	2.12654400

Cartesian Coordinates for the Stationary Points Given in Fig. S6

IM14

Rh	-0.54630000	-0.13232400	-0.92249900
N	-0.27049500	-2.04569600	0.02867800
C	0.34255300	-0.92345600	-2.84599500
C	0.53836400	0.48432300	-2.82776500
C	-0.75977000	1.13326300	-2.79133200
C	-1.75640800	0.09998000	-2.85355500
C	-1.08960500	-1.16718900	-2.79301600
O	0.99159100	2.92288900	-0.14919200
O	0.94713600	0.73242600	0.43561500
C	1.37790800	1.94382200	0.51914800
C	2.45993100	2.14350300	1.58547700
H	3.24506400	1.38549300	1.49210900
H	2.01282900	2.02650300	2.58074000
H	2.89766300	3.14210200	1.50897700

C	2.39689300	-2.79565700	0.70958600
C	3.03577300	-4.05747800	0.79668500
C	3.08069400	-1.68278200	0.27084100
C	4.36258400	-4.17897600	0.44408000
C	4.45342700	-1.77973200	-0.08624000
H	2.57099200	-0.72443600	0.19786200
H	4.86021500	-5.14649700	0.50733900
C	-1.73975600	-2.51317400	-2.87267000
H	-1.13405700	-3.26733600	-2.36312500
H	-1.85953500	-2.81918700	-3.92224200
H	-2.72765700	-2.49897700	-2.40457600
C	-3.21590700	0.27867300	-3.11905200
H	-3.81467000	-0.40796700	-2.51810400
H	-3.40050400	0.06594700	-4.18256700
H	-3.55142000	1.29391800	-2.90736600
C	-1.00461300	2.60479100	-2.94388000
H	-2.00713400	2.87534500	-2.60050300
H	-0.91940000	2.90442200	-3.99871000
H	-0.28041000	3.18100600	-2.36316400
C	1.85541100	1.19229500	-2.91790800
H	1.84157800	2.12609800	-2.35236500
H	2.07383700	1.43059600	-3.96910500
H	2.67238300	0.56994200	-2.54114100
C	1.38351200	-1.98910700	-2.98525600
H	2.38740900	-1.60557900	-2.78498200
H	1.37304300	-2.39409900	-4.00735500
H	1.19051000	-2.81574600	-2.29432600
S	0.59520600	-2.64541500	1.12645400
C	-1.40418700	1.03298300	4.18040900
H	-1.93950300	1.64021500	4.91407200
H	-1.22614600	0.03876200	4.61019600
H	-0.43338500	1.47789600	3.94470100
C	-2.24792100	0.88397000	2.93995000
O	-1.49525000	0.55893400	1.86563400
O	-3.45677500	1.03379800	2.90802600
C	-2.16808100	0.31457800	0.60731900
C	-2.99615000	-0.93295400	0.65593300
O	-3.76515900	-1.30300200	-0.22264700

O	-2.81745800	-1.65067300	1.78625400
C	-3.52592700	-2.91367500	1.85485000
H	-4.60486600	-2.71256700	1.84052700
H	-3.27411500	-3.50469500	0.96616900
C	-2.87370300	1.55667800	0.14067500
O	-3.90201400	1.53685600	-0.53503800
C	-2.26940700	2.89947900	0.52605700
H	-1.18151600	2.91049700	0.44936000
H	-2.55381800	3.14764500	1.55586400
H	-2.69825000	3.66039300	-0.13200600
C	5.10934200	-3.05284100	-0.00032000
C	6.48256800	-3.14309100	-0.36046200
C	7.17445400	-2.02932100	-0.78501700
H	6.97954700	-4.11051600	-0.29396900
C	5.19631700	-0.64926200	-0.53039700
C	6.52573100	-0.77042100	-0.87124600
H	8.22560400	-2.11111500	-1.05710000
H	4.69342200	0.31534400	-0.59293400
H	7.08491800	0.10099300	-1.20815100
C	-3.09651700	-3.61186400	3.13109100
H	-3.64405700	-4.55636500	3.23187300
H	-2.02553100	-3.83576200	3.10367800
H	-3.31169500	-2.99491500	4.01100400
C	0.72365200	-1.66756400	2.66979800
H	1.04148200	-0.65965100	2.40564900
H	-0.28139300	-1.64982400	3.09304000
H	1.42621100	-2.16563400	3.34205400
O	0.23452800	-4.04651200	1.59837900
H	2.46607500	-4.91469300	1.14456100

TS15

Rh	-0.54630000	-0.13232400	-0.92249900
N	-0.27049500	-2.04569600	0.02867800
C	0.34255300	-0.92345600	-2.84599500
C	0.53836400	0.48432300	-2.82776500
C	-0.75977000	1.13326300	-2.79133200

C	-1.75640800	0.09998000	-2.85355500
C	-1.08960500	-1.16718900	-2.79301600
O	0.99159100	2.92288900	-0.14919200
O	0.94713600	0.73242600	0.43561500
C	1.37790800	1.94382200	0.51914800
C	2.45993100	2.14350300	1.58547700
H	3.24506400	1.38549300	1.49210900
H	2.01282900	2.02650300	2.58074000
H	2.89766300	3.14210200	1.50897700
C	2.39689300	-2.79565700	0.70958600
C	3.03577300	-4.05747800	0.79668500
C	3.08069400	-1.68278200	0.27084100
C	4.36258400	-4.17897600	0.44408000
C	4.45342700	-1.77973200	-0.08624000
H	2.57099200	-0.72443600	0.19786200
H	4.86021500	-5.14649700	0.50733900
C	-1.73975600	-2.51317400	-2.87267000
H	-1.13405700	-3.26733600	-2.36312500
H	-1.85953500	-2.81918700	-3.92224200
H	-2.72765700	-2.49897700	-2.40457600
C	-3.21590700	0.27867300	-3.11905200
H	-3.81467000	-0.40796700	-2.51810400
H	-3.40050400	0.06594700	-4.18256700
H	-3.55142000	1.29391800	-2.90736600
C	-1.00461300	2.60479100	-2.94388000
H	-2.00713400	2.87534500	-2.60050300
H	-0.91940000	2.90442200	-3.99871000
H	-0.28041000	3.18100600	-2.36316400
C	1.85541100	1.19229500	-2.91790800
H	1.84157800	2.12609800	-2.35236500
H	2.07383700	1.43059600	-3.96910500
H	2.67238300	0.56994200	-2.54114100
C	1.38351200	-1.98910700	-2.98525600
H	2.38740900	-1.60557900	-2.78498200
H	1.37304300	-2.39409900	-4.00735500
H	1.19051000	-2.81574600	-2.29432600
S	0.59520600	-2.64541500	1.12645400
C	-1.40418700	1.03298300	4.18040900

H	-1.93950300	1.64021500	4.91407200
H	-1.22614600	0.03876200	4.61019600
H	-0.43338500	1.47789600	3.94470100
C	-2.24792100	0.88397000	2.93995000
O	-1.49525000	0.55893400	1.86563400
O	-3.45677500	1.03379800	2.90802600
C	-2.16808100	0.31457800	0.60731900
C	-2.99615000	-0.93295400	0.65593300
O	-3.76515900	-1.30300200	-0.22264700
O	-2.81745800	-1.65067300	1.78625400
C	-3.52592700	-2.91367500	1.85485000
H	-4.60486600	-2.71256700	1.84052700
H	-3.27411500	-3.50469500	0.96616900
C	-2.87370300	1.55667800	0.14067500
O	-3.90201400	1.53685600	-0.53503800
C	-2.26940700	2.89947900	0.52605700
H	-1.18151600	2.91049700	0.44936000
H	-2.55381800	3.14764500	1.55586400
H	-2.69825000	3.66039300	-0.13200600
C	5.10934200	-3.05284100	-0.00032000
C	6.48256800	-3.14309100	-0.36046200
C	7.17445400	-2.02932100	-0.78501700
H	6.97954700	-4.11051600	-0.29396900
C	5.19631700	-0.64926200	-0.53039700
C	6.52573100	-0.77042100	-0.87124600
H	8.22560400	-2.11111500	-1.05710000
H	4.69342200	0.31534400	-0.59293400
H	7.08491800	0.10099300	-1.20815100
C	-3.09651700	-3.61186400	3.13109100
H	-3.64405700	-4.55636500	3.23187300
H	-2.02553100	-3.83576200	3.10367800
H	-3.31169500	-2.99491500	4.01100400
C	0.72365200	-1.66756400	2.66979800
H	1.04148200	-0.65965100	2.40564900
H	-0.28139300	-1.64982400	3.09304000
H	1.42621100	-2.16563400	3.34205400
O	0.23452800	-4.04651200	1.59837900
H	2.46607500	-4.91469300	1.14456100

IM15

Rh	0.49409200	-0.71772700	1.27207100
N	0.67491400	-2.48270900	0.13827900
C	0.10286900	-1.69445500	3.23769800
C	-0.25723800	-0.31441400	3.41295900
C	0.92223400	0.47246000	3.24836600
C	2.04993900	-0.43814200	3.08801200
C	1.55058100	-1.75551000	3.09154300
C	-1.81096100	-1.58347200	-0.39171800
C	-1.33053400	-0.50047400	0.40610100
C	-3.06061900	-1.63046100	-0.96427700
C	-2.20966400	0.56119800	0.56082000
C	-3.95115300	-0.53691100	-0.80454600
H	-3.38058900	-2.50318200	-1.53038500
H	-1.91795500	1.42614200	1.15221100
C	2.31942200	-3.03031100	2.92642700
H	1.88514300	-3.61729200	2.10976900
H	2.29327200	-3.63278300	3.84425200
H	3.36519300	-2.83577100	2.67775000
C	3.47964300	0.00183700	3.01040700
H	4.14196700	-0.83275900	2.77317200
H	3.80136700	0.42982900	3.97079000
H	3.60486400	0.75644400	2.23006800
C	1.05163000	1.95155500	3.46482400
H	1.79516500	2.38215600	2.78783100
H	1.37011600	2.17229000	4.49384900
H	0.10102600	2.46834800	3.30191200
C	-1.61260000	0.19057000	3.81098900
H	-1.76426900	1.23043600	3.51161300
H	-1.72953900	0.14386700	4.90240200
H	-2.41457100	-0.40113200	3.36378800
C	-0.79668400	-2.88477400	3.40323500
H	-1.84495500	-2.61247500	3.25259000
H	-0.70790100	-3.32040100	4.40874900
H	-0.55452700	-3.65886200	2.67024300
S	-0.62762900	-2.94403800	-0.53395400

C	-0.29755100	0.92163600	-3.72220800
H	-1.03651500	1.70856600	-3.53350400
H	0.11113300	1.06689600	-4.72336500
H	-0.80999500	-0.03845100	-3.64790200
C	0.81051000	1.04087300	-2.69894100
O	0.50043600	0.36047700	-1.57979400
O	1.81632400	1.70702200	-2.85699000
C	1.44547400	0.35216600	-0.48056600
C	2.64440100	-0.48002200	-0.80050200
O	3.63974700	-0.58747900	-0.10527800
O	2.52286500	-1.13678900	-1.98667200
C	3.57890300	-2.05929400	-2.29280200
H	4.54623600	-1.56537900	-2.15679400
H	3.52838200	-2.89420400	-1.58521800
C	1.69853800	1.71839900	0.04770700
O	2.73073600	2.05974200	0.63125700
C	0.59168600	2.75564000	-0.13433500
H	-0.38907400	2.31618700	-0.31335500
H	0.85433500	3.38664700	-0.99052100
H	0.56301800	3.39174100	0.75367400
C	-3.50751200	0.58289100	-0.02416000
C	-4.39700400	1.68186100	0.14234600
C	-5.65186700	1.67572400	-0.42614400
H	-4.06635300	2.53400600	0.73227600
C	-5.25203000	-0.51475800	-1.37640500
C	-6.08684800	0.56595500	-1.19428300
H	-6.31602600	2.52489200	-0.28679700
H	-5.57851300	-1.37024000	-1.96392500
H	-7.07912600	0.57227200	-1.63707500
C	3.38954100	-2.52389700	-3.72624200
H	4.18474400	-3.22516000	-4.00051000
H	2.42794100	-3.02925000	-3.85375400
H	3.42558100	-1.67598500	-4.41726400
C	-0.38499100	-3.10902700	-2.35287600
H	0.06232700	-2.18609500	-2.71938500
H	0.31154200	-3.94114800	-2.47910700
H	-1.32953600	-3.33847300	-2.85046100
O	-1.32296900	-4.24678100	-0.18703800

IM14'

Rh	-0.54630000	-0.13232400	-0.92249900
N	-0.27049500	-2.04569600	0.02867800
C	0.34255300	-0.92345600	-2.84599500
C	0.53836400	0.48432300	-2.82776500
C	-0.75977000	1.13326300	-2.79133200
C	-1.75640800	0.09998000	-2.85355500
C	-1.08960500	-1.16718900	-2.79301600
O	0.99159100	2.92288900	-0.14919200
O	0.94713600	0.73242600	0.43561500
C	1.37790800	1.94382200	0.51914800
C	2.45993100	2.14350300	1.58547700
H	3.24506400	1.38549300	1.49210900
H	2.01282900	2.02650300	2.58074000
H	2.89766300	3.14210200	1.50897700
C	2.39689300	-2.79565700	0.70958600
C	3.03577300	-4.05747800	0.79668500
C	3.08069400	-1.68278200	0.27084100
C	4.36258400	-4.17897600	0.44408000
C	4.45342700	-1.77973200	-0.08624000
H	2.57099200	-0.72443600	0.19786200
H	4.86021500	-5.14649700	0.50733900
C	-1.73975600	-2.51317400	-2.87267000
H	-1.13405700	-3.26733600	-2.36312500
H	-1.85953500	-2.81918700	-3.92224200
H	-2.72765700	-2.49897700	-2.40457600
C	-3.21590700	0.27867300	-3.11905200
H	-3.81467000	-0.40796700	-2.51810400
H	-3.40050400	0.06594700	-4.18256700
H	-3.55142000	1.29391800	-2.90736600
C	-1.00461300	2.60479100	-2.94388000
H	-2.00713400	2.87534500	-2.60050300
H	-0.91940000	2.90442200	-3.99871000
H	-0.28041000	3.18100600	-2.36316400
C	1.85541100	1.19229500	-2.91790800
H	1.84157800	2.12609800	-2.35236500
H	2.07383700	1.43059600	-3.96910500

H	2.67238300	0.56994200	-2.54114100
C	1.38351200	-1.98910700	-2.98525600
H	2.38740900	-1.60557900	-2.78498200
H	1.37304300	-2.39409900	-4.00735500
H	1.19051000	-2.81574600	-2.29432600
S	0.59520600	-2.64541500	1.12645400
C	-1.40418700	1.03298300	4.18040900
H	-1.93950300	1.64021500	4.91407200
H	-1.22614600	0.03876200	4.61019600
H	-0.43338500	1.47789600	3.94470100
C	-2.24792100	0.88397000	2.93995000
O	-1.49525000	0.55893400	1.86563400
O	-3.45677500	1.03379800	2.90802600
C	-2.16808100	0.31457800	0.60731900
C	-2.99615000	-0.93295400	0.65593300
O	-3.76515900	-1.30300200	-0.22264700
O	-2.81745800	-1.65067300	1.78625400
C	-3.52592700	-2.91367500	1.85485000
H	-4.60486600	-2.71256700	1.84052700
H	-3.27411500	-3.50469500	0.96616900
C	-2.87370300	1.55667800	0.14067500
O	-3.90201400	1.53685600	-0.53503800
C	-2.26940700	2.89947900	0.52605700
H	-1.18151600	2.91049700	0.44936000
H	-2.55381800	3.14764500	1.55586400
H	-2.69825000	3.66039300	-0.13200600
C	5.10934200	-3.05284100	-0.00032000
C	6.48256800	-3.14309100	-0.36046200
C	7.17445400	-2.02932100	-0.78501700
H	6.97954700	-4.11051600	-0.29396900
C	5.19631700	-0.64926200	-0.53039700
C	6.52573100	-0.77042100	-0.87124600
H	8.22560400	-2.11111500	-1.05710000
H	4.69342200	0.31534400	-0.59293400
H	7.08491800	0.10099300	-1.20815100
C	-3.09651700	-3.61186400	3.13109100
H	-3.64405700	-4.55636500	3.23187300
H	-2.02553100	-3.83576200	3.10367800

H	-3.31169500	-2.99491500	4.01100400
C	0.72365200	-1.66756400	2.66979800
H	1.04148200	-0.65965100	2.40564900
H	-0.28139300	-1.64982400	3.09304000
H	1.42621100	-2.16563400	3.34205400
O	0.23452800	-4.04651200	1.59837900
H	2.46607500	-4.91469300	1.14456100

TS15'

Rh	-0.37993000	1.04667800	-0.40931700
N	-0.68723100	-0.42003700	-1.85129000
C	1.17373800	2.47594000	-1.27761000
C	0.97228800	2.82683900	0.12140700
C	-0.37357400	3.23481900	0.31028400
C	-1.05881100	3.05374100	-0.95162400
C	-0.07364900	2.63215000	-1.93784100
O	1.23483600	-0.46008900	3.56811700
O	1.27529900	-2.17450900	2.09538900
C	1.24980300	-1.66260700	3.31576600
C	1.23749300	-2.72374600	4.39626800
H	2.02567700	-3.46167100	4.21168600
H	0.27848700	-3.25614000	4.38087100
H	1.37509300	-2.26004400	5.37532500
C	1.95527900	-1.34492600	-1.42920200
C	3.00068600	-1.64713800	-2.34154800
C	2.11467400	-0.84547100	-0.14928400
C	4.30259800	-1.42007900	-1.96464200
H	1.37340200	-1.46529300	1.32344100
C	3.49410200	-0.61438200	0.22435100
H	5.12633400	-1.63826100	-2.64412900
C	-0.33035000	2.45462800	-3.40027300
H	0.33289900	1.70103300	-3.83321000
H	-0.15625800	3.40668100	-3.92255700
H	-1.36355500	2.14995200	-3.58887700
C	-2.43833400	3.54342900	-1.25224700
H	-2.84115800	3.08590600	-2.15805700
H	-2.40064700	4.63331800	-1.40204400
H	-3.11932600	3.32782500	-0.42748700

C	-0.91767100	3.92762400	1.52109700
H	-1.97914800	3.71868600	1.66887400
H	-0.80294200	5.01507800	1.40032900
H	-0.37551300	3.63853100	2.42654700
C	2.04159500	2.90995900	1.16396600
H	1.67416900	2.58253700	2.14188100
H	2.36932400	3.95549400	1.26432000
H	2.91227400	2.30730300	0.90459100
C	2.48706600	2.18675200	-1.93634100
H	3.18701700	1.70814900	-1.24931800
H	2.94302900	3.12459600	-2.28643600
H	2.36400300	1.53158600	-2.80342000
S	0.25842300	-1.61202900	-2.07336100
C	-2.08570300	-3.29943700	2.12536900
H	-2.56986400	-3.69600400	3.02131300
H	-2.35583300	-3.93709800	1.27299800
H	-0.99936500	-3.31238200	2.22741200
C	-2.60011600	-1.91233200	1.84782700
O	-1.70872200	-1.17089900	1.14206800
O	-3.69392000	-1.50486700	2.19475800
C	-2.16722000	0.09439800	0.60222700
C	-3.17860400	-0.11645900	-0.48791700
O	-3.76755000	0.77711600	-1.07658700
O	-3.40421800	-1.42030000	-0.76380800
C	-4.35880600	-1.69076900	-1.81839900
H	-5.28745900	-1.14787200	-1.60508100
H	-3.94804000	-1.31254500	-2.76338000
C	-2.56699700	1.04175800	1.68585800
O	-3.42022100	1.92173700	1.53714800
C	-1.84986100	0.91870500	3.02177400
H	-1.84659900	1.89898900	3.50533600
H	-0.83154200	0.53857500	2.93000300
H	-2.41631900	0.23149700	3.66213300
C	4.58731700	-0.89773900	-0.67381900
C	5.92710200	-0.65745000	-0.25889700
C	6.20327700	-0.15946400	0.99576900
H	6.73575100	-0.87842700	-0.95604600
C	3.83348000	-0.10460600	1.51344000

C	5.14210300	0.11996500	1.89094700
H	7.23344000	0.01889900	1.30105500
H	3.02609100	0.11536400	2.20430300
H	5.36279500	0.51254900	2.88271100
C	-4.58478100	-3.19058600	-1.86029700
H	-5.31566200	-3.42879200	-2.64182200
H	-3.65546400	-3.72511200	-2.08699200
H	-4.97370400	-3.55475800	-0.90266200
H	2.76153200	-2.05012700	-3.32483900
C	-0.22552100	-3.14370700	-1.17760300
H	-0.21802400	-2.94111200	-0.10812000
H	-1.23458100	-3.39354800	-1.51400200
H	0.48017800	-3.93630400	-1.43744500
O	0.37931800	-2.09352800	-3.51076500

IM15'

Rh	-0.10208900	1.21390800	-0.86984000
N	-0.63700800	-0.09752900	-2.41206600
C	0.75830100	2.74011200	-2.26447700
C	1.21245200	3.12869600	-0.95841400
C	0.06676000	3.48071300	-0.18133000
C	-1.09845700	3.41824700	-1.05148400
C	-0.67537400	2.97845100	-2.32154800
C	1.60444200	-1.14160200	-1.35596400
C	2.67674400	-2.06112600	-1.31816900
C	1.40511500	-0.11174700	-0.44162600
C	3.58805100	-1.99719700	-0.29264400
C	2.35625100	-0.06274900	0.64429300
H	4.42706200	-2.68780700	-0.24242700
C	-1.50923500	2.73975100	-3.54248200
H	-1.42793500	1.68538500	-3.83288400
H	-1.16565100	3.36105600	-4.38049100
H	-2.56267900	2.96329800	-3.35910600
C	-2.47268700	3.85516600	-0.64320700
H	-3.19519400	3.70030500	-1.44607200
H	-2.46666400	4.92510500	-0.38760600
H	-2.81490900	3.28645200	0.22481800
C	0.03753900	4.06841400	1.19985900

H	-0.79468700	3.65641300	1.78047900
H	-0.09903700	5.15922200	1.16004200
H	0.96805100	3.88107000	1.74465000
C	2.65373800	3.27557600	-0.56360400
H	2.78376100	3.31210900	0.51911600
H	3.06468600	4.20623200	-0.98005200
H	3.26398800	2.44970500	-0.93806800
C	1.61333200	2.38740700	-3.44802500
H	2.62933900	2.12325000	-3.14193300
H	1.68757000	3.23192800	-4.14897300
H	1.20196000	1.53045000	-3.98798200
S	0.39722500	-1.20244900	-2.69072600
C	-1.05646300	-3.47310800	1.48486900
H	-1.33580200	-4.00862600	2.39380100
H	-1.41839600	-4.04165000	0.62116900
H	0.02865900	-3.38745700	1.40010200
C	-1.71587000	-2.10924900	1.47872800
O	-1.01553600	-1.25398600	0.70691600
O	-2.73088200	-1.84194200	2.08840000
C	-1.55272200	0.07120100	0.45245200
C	-2.77876700	0.00455100	-0.40439300
O	-3.49030900	0.94353100	-0.70362200
O	-3.04379200	-1.26285200	-0.84013100
C	-4.12770300	-1.36668000	-1.77088800
H	-4.99550900	-0.82402000	-1.38336900
H	-3.82863600	-0.89073800	-2.71134300
C	-1.67131100	0.88008700	1.70101700
O	-2.39259000	1.87062900	1.81344400
C	-0.84222700	0.46042300	2.91485400
H	-0.53019900	1.36294000	3.44630200
H	0.02782200	-0.14699600	2.66992000
H	-1.49692300	-0.11520900	3.57682300
C	3.44535200	-1.00559000	0.71586700
C	4.36645700	-0.92524900	1.79621900
C	4.23491000	0.02739800	2.78181000
H	5.18516900	-1.64172600	1.83044400
C	2.25866700	0.89708600	1.68854200
C	3.16294600	0.94783900	2.72871100

H	4.94873000	0.06973500	3.60119200
H	1.43161200	1.59471800	1.64531800
H	3.04902400	1.69277700	3.51229200
C	-4.43234900	-2.84356500	-1.95897800
H	-5.26438200	-2.97066700	-2.66086100
H	-3.56382200	-3.37694100	-2.35692100
H	-4.71100500	-3.30448700	-1.00595200
H	2.77875400	-2.79288100	-2.11595400
C	-0.37256200	-2.86780800	-2.47589600
H	-0.89158500	-2.87397800	-1.51899600
H	-1.08509900	-2.96164800	-3.29853700
H	0.38065700	-3.65594600	-2.54573400
O	1.10805000	-1.35439500	-4.01539800