

Theoretical Study of the Mechanism of Two Successive N-methylene C–H Bond Activations on a Phosphine-Tethered N-Heterocyclic Carbene on a Triruthenium Carbonyl Cluster

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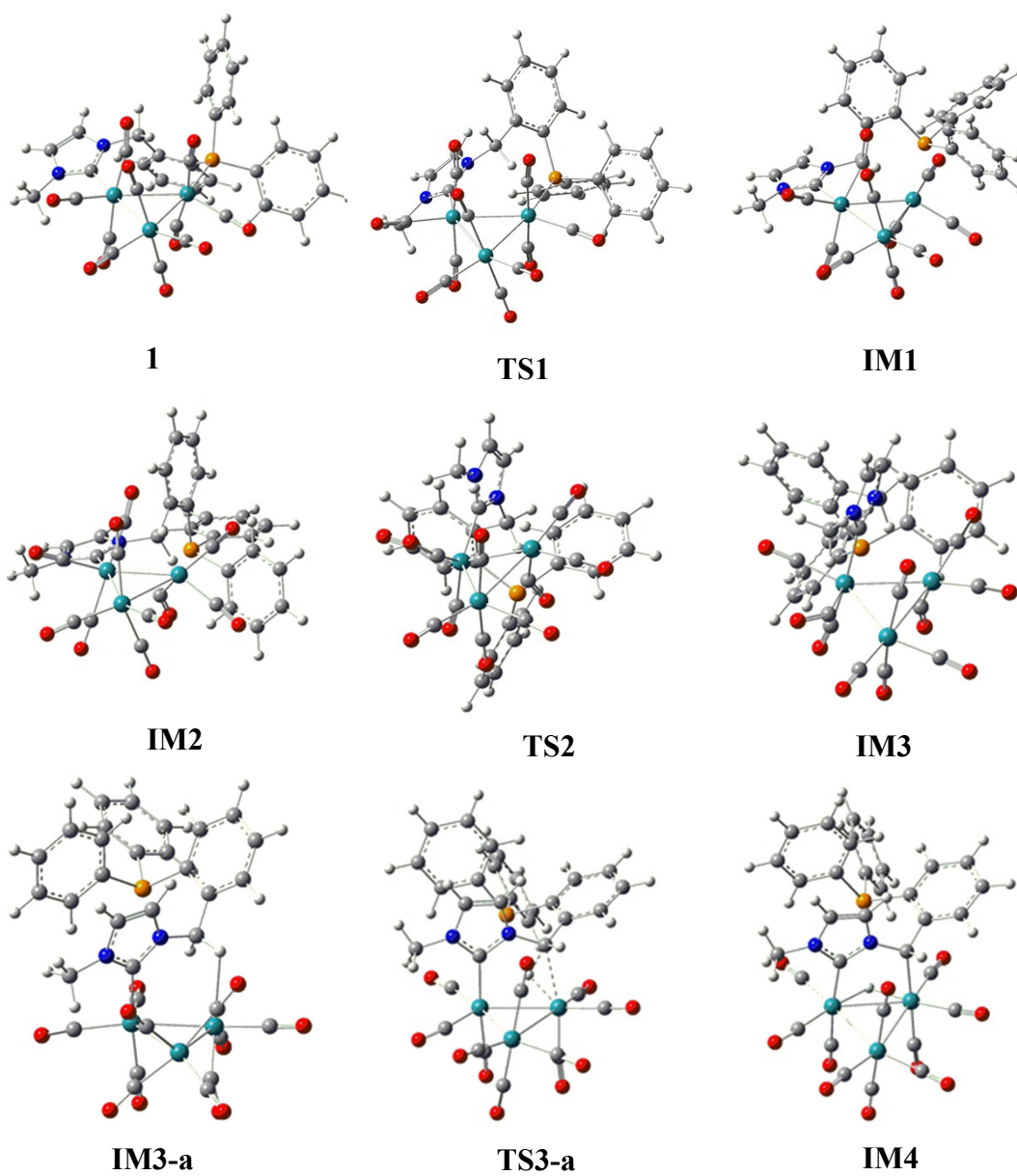


Fig. S1 Optimized geometries for the species shown in Fig.1.

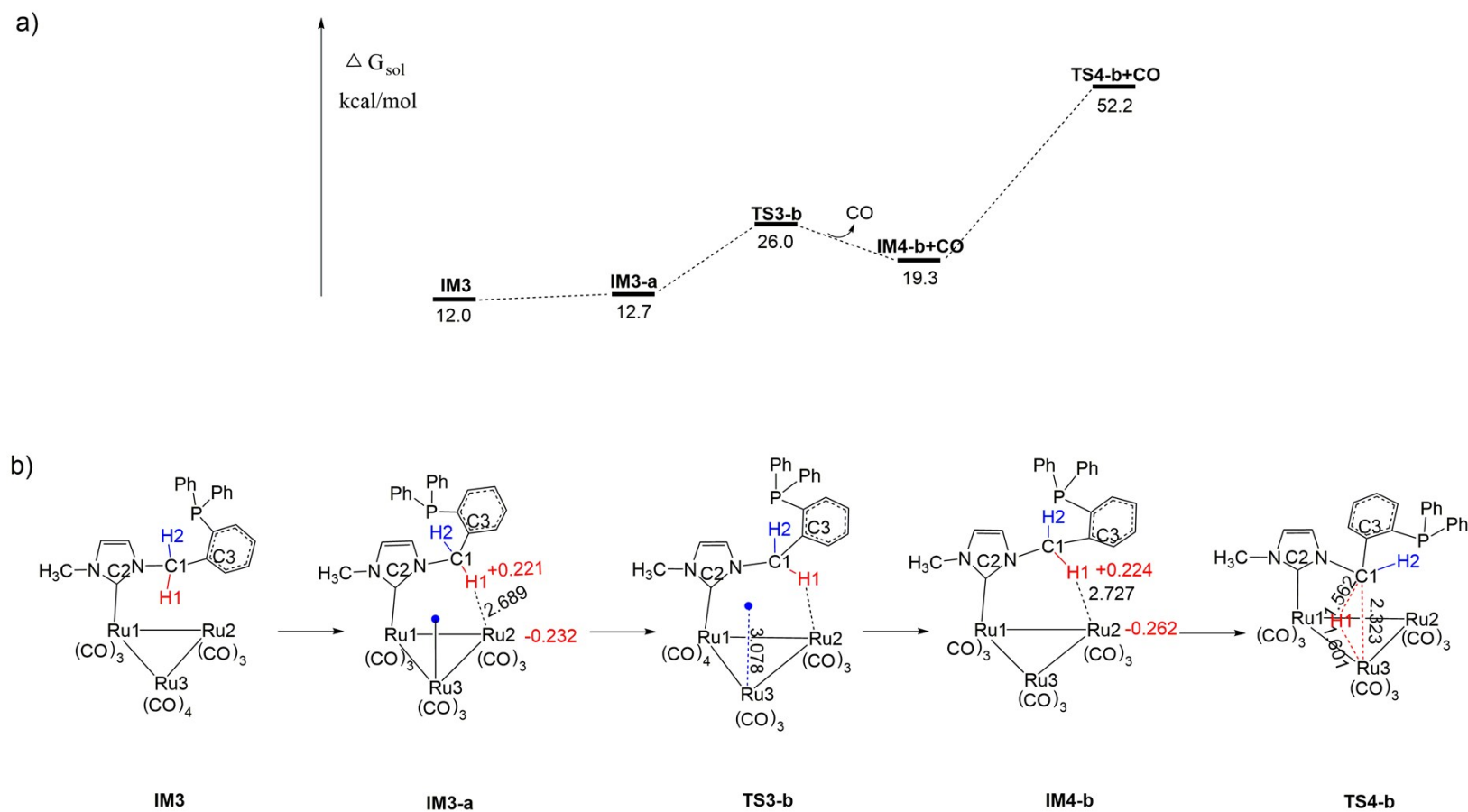


Fig. S2 Calculated free energy profile (a) and the schematic diagrams for the oxidative addition of C1–H1 bond on Ru3 (b). The blue point denotes the CO that will be released from the metal center. Bond lengths in angstroms.

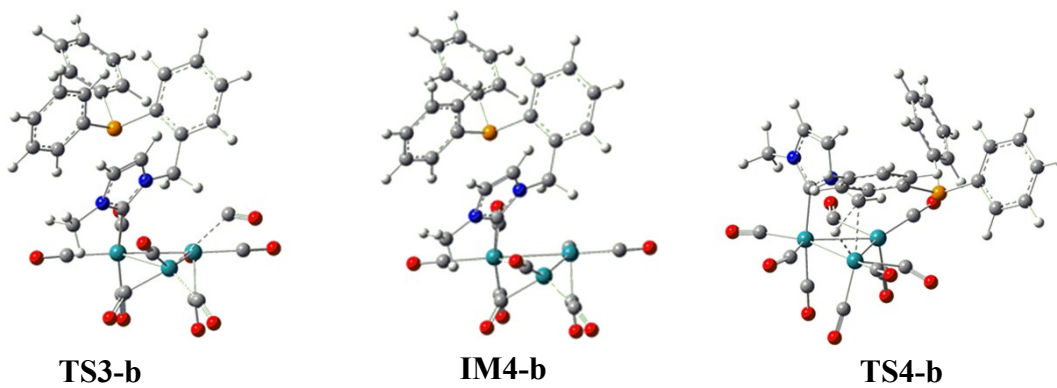


Fig. S3 Optimized geometries for the species shown in Fig. S2.

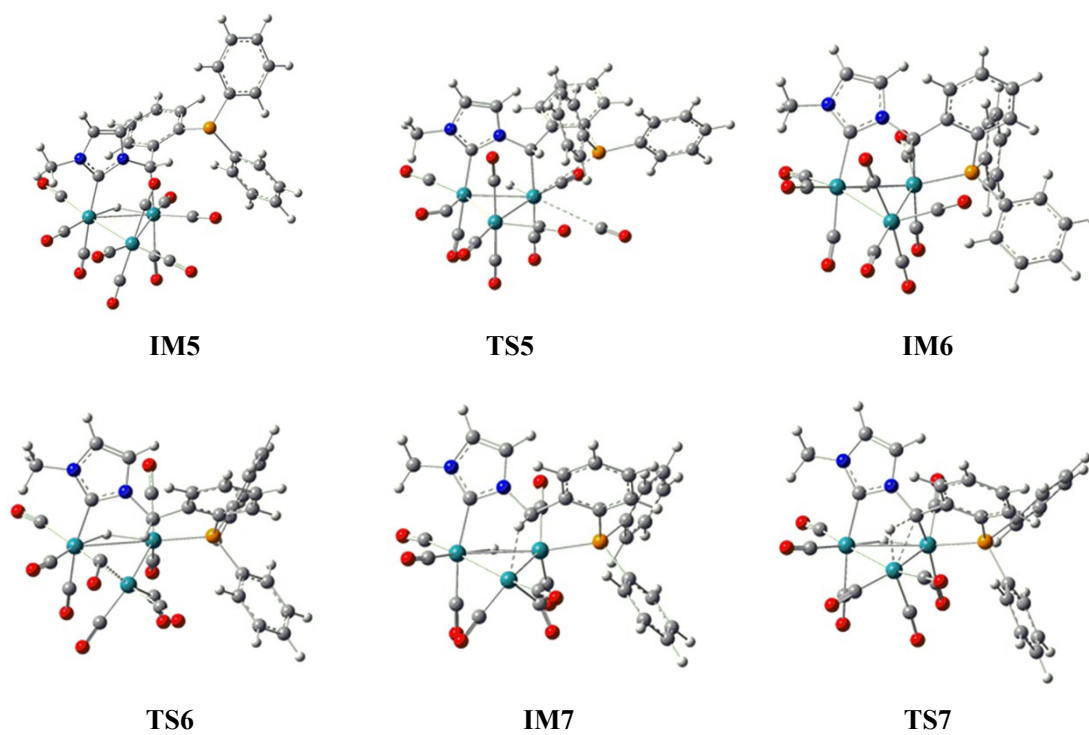


Fig. S4 Optimized geometries for the species shown in Fig. 2.

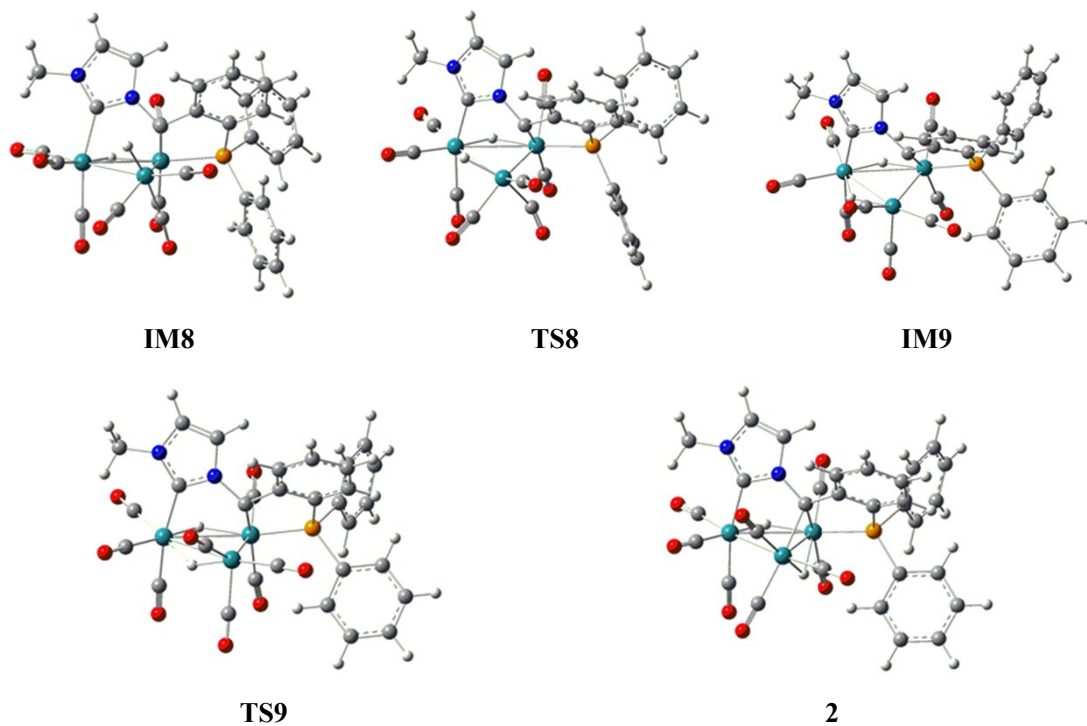


Fig. S5 Optimized geometries for the species shown in Fig. 3.

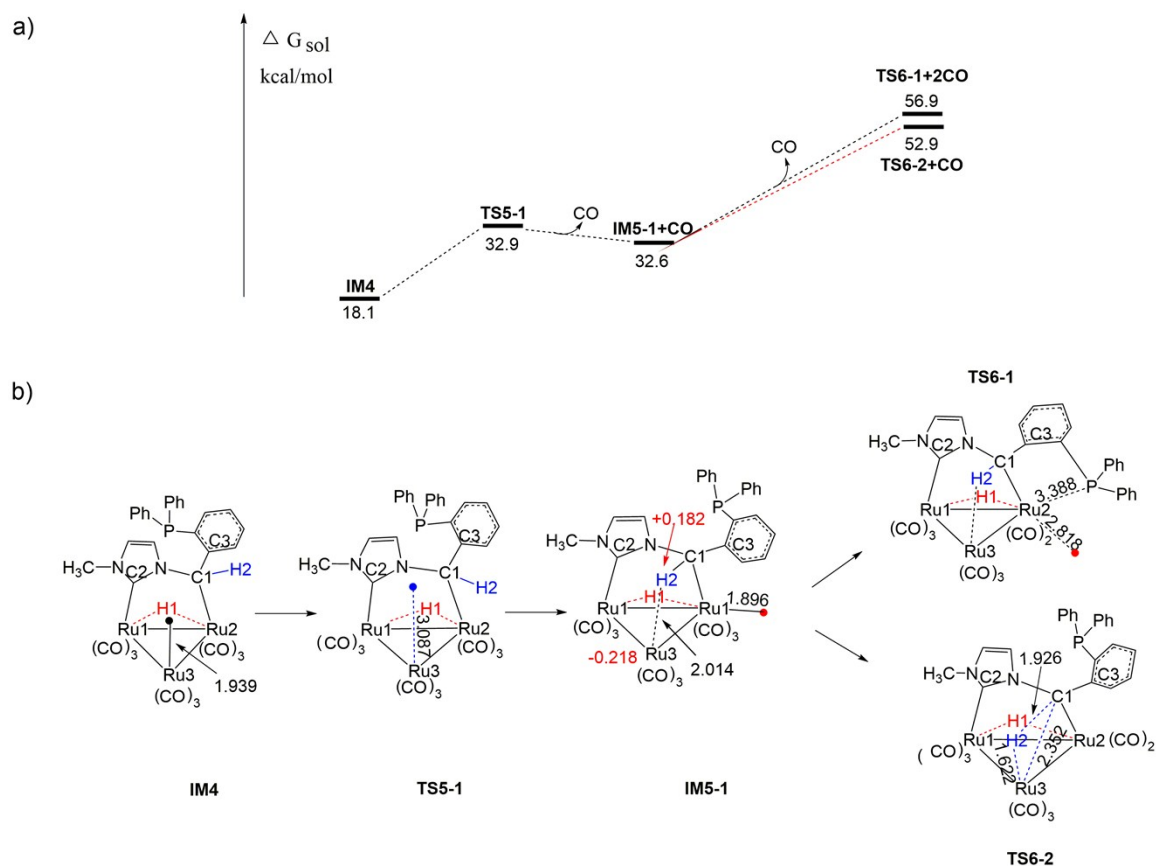
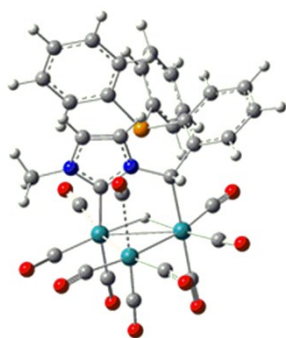
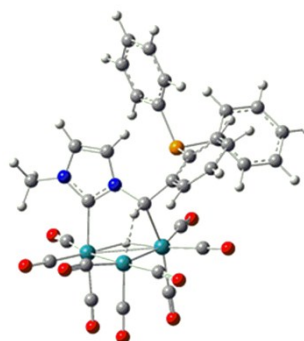


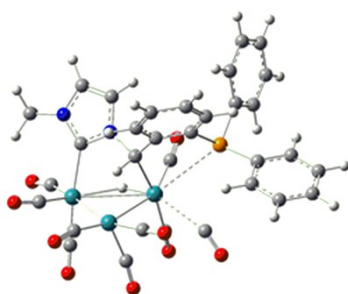
Fig. S6 Calculated free energy profile (a) and the schematic diagrams of the alternative pathways for the second C–H bond activation (b). The red and blue points denote the CO that will be released or is being released from the metal center. Bond lengths in angstroms.



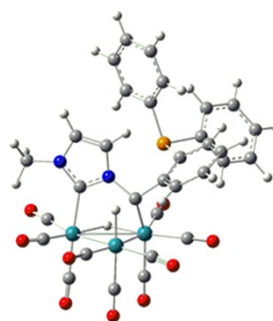
TS5-1



IM5-1



TS6-1



TS6-2

Fig. S7 Optimized geometries for the species shown in Fig. S6.

Cartesian Coordinates for the Stationary Points Given in Fig. S1

	1		
C	0.84177900	2.98404000	-0.69665900
C	0.69398100	5.12138000	-1.43025500
C	-0.48441600	4.52104800	-1.70610400
C	-1.51808700	2.30735500	-1.22146900
C	2.85546900	4.46327300	-0.40909900
C	-3.13476400	-0.64294200	-1.54821400
C	-3.91649400	0.33244600	-2.17388100
C	-4.41129800	0.11883200	-3.45931200
C	-4.14684800	-1.07682100	-4.12128000
C	-3.39670700	-2.06796600	-3.48979000
C	-2.89333300	-1.85284600	-2.21078800
C	-3.67295400	-1.46617000	1.13931900
C	-4.86942800	-1.93797900	0.59026000
C	-5.75104900	-2.68867000	1.36642900
C	-5.45571600	-2.96101000	2.69916800
C	-4.27382900	-2.47884700	3.25924400
C	-3.38558500	-1.74211600	2.48246600
C	-0.47438600	-2.52647700	1.62646200
C	-0.30575900	0.27377100	2.09467600
C	0.08994300	-1.99664000	-1.01744000
C	1.07335600	0.41349900	-1.75913400
C	1.89169900	1.86813600	1.73308500
C	3.39629100	1.48268600	-0.67540000
C	2.89389300	-1.60870100	-1.00880000
C	2.16975100	-0.87638700	2.73421300
C	2.62496300	-3.27375100	1.30242900
C	4.41380400	-0.84425000	1.14428900
N	-0.38303100	3.22272000	-1.23684000
N	1.48448700	4.17361400	-0.80822000
P	-2.48004000	-0.44144200	0.16363900
Ru	-0.21575800	-0.98228900	0.60957100
Ru	1.66486500	1.15515400	-0.07236900
Ru	2.61500600	-1.38935500	0.90713900
O	-0.62447500	-3.47963100	2.25567000
O	-0.55330900	0.89364300	3.03773800
O	0.20856500	-2.67592800	-1.93948800
O	0.81295200	0.20416000	-2.86495700
O	2.08072400	2.39694300	2.73494200
O	4.47078600	1.60584700	-1.07290100
O	3.17109000	-1.78689600	-2.10816100

O	2.00305800	-0.64672100	3.84603100
O	2.73786700	-4.39299700	1.52698800
O	5.50809300	-0.55136300	1.33727000
H	1.04592400	6.12382600	-1.61685400
H	-1.38157100	4.88965400	-2.17899000
H	3.54970400	4.19360400	-1.20759600
H	2.93291800	5.53256400	-0.21111400
H	3.10483400	3.91566900	0.49818500
H	-4.15505000	1.25797800	-1.65797300
H	-5.01019200	0.88726600	-3.93815500
H	-4.53228600	-1.24091500	-5.12269500
H	-3.20302100	-3.01037300	-3.99227600
H	-2.33268800	-2.64049300	-1.71608000
H	-5.12049300	-1.72528500	-0.44416100
H	-6.67158500	-3.05849900	0.92560300
H	-6.14343500	-3.54670900	3.30118100
H	-4.03866100	-2.68127300	4.29939900
H	-2.47022200	-1.36329100	2.92940500
C	-2.35818600	2.42117100	0.04116000
C	-2.95393000	1.29280300	0.64389800
C	-2.61511500	3.68800100	0.56983300
C	-3.82029500	1.48695500	1.72717700
C	-3.45565800	3.86234200	1.66427200
H	-2.15070200	4.55989800	0.11998400
C	-4.07223200	2.75712100	2.23606200
H	-4.30228900	0.63769600	2.19681600
H	-3.63118700	4.85846200	2.05785000
H	-4.74483300	2.87352000	3.07974500
H	-2.13020400	2.54743300	-2.09684900
H	-1.14061900	1.29575400	-1.35544500

TS1

C	1.18359700	2.67671400	-0.80530600
C	1.02646600	4.72539100	-1.76102200
C	-0.14653500	4.09287700	-1.97943400
C	-1.16840100	1.94548800	-1.30059500
C	3.18323200	4.18909100	-0.65238900
C	-4.12358700	0.56166900	-2.58570500
C	-4.87743900	1.74190300	-2.63920600
C	-5.41777200	2.17993000	-3.84563000
C	-5.21499600	1.44314200	-5.01137200
C	-4.46977400	0.26702800	-4.96796900
C	-3.92224700	-0.16883900	-3.76203600
C	-4.85973200	-0.92190900	-0.22415300
C	-6.14390500	-0.93819300	-0.77660600

C	-7.18428600	-1.59226000	-0.11654600
C	-6.95456500	-2.22817700	1.10052800
C	-5.67630700	-2.21769300	1.65749200
C	-4.63438200	-1.57731900	0.99394300
C	-0.90760000	-2.21123500	1.79843600
C	-0.59076800	0.48149900	1.83507500
C	0.32004600	-2.48263900	-0.54763500
C	1.42508200	-0.05801900	-1.37519000
C	1.80370800	2.00965300	1.85227000
C	3.72395500	1.22571500	-0.27449900
C	3.09217300	-1.87364600	-0.03752600
C	1.61870900	-0.53978100	3.31640800
C	2.27919600	-3.21946500	2.44571900
C	4.09231600	-0.90889800	2.24696200
N	-0.03651000	2.84955500	-1.38370900
N	1.81991700	3.85241700	-1.03900900
P	-3.40243600	-0.09487200	-1.00605800
Ru	-0.20748600	-1.01231900	0.59025900
Ru	1.92027900	0.98509900	0.17850400
Ru	2.36360100	-1.40553800	1.71843700
O	-1.22992600	-2.96436300	2.61401100
O	-0.96787700	1.19955200	2.64893400
O	0.58198200	-3.40477600	-1.17845200
O	1.33230500	-0.41048900	-2.48056500
O	1.80235200	2.71924900	2.75685200
O	4.84074800	1.28389000	-0.55368600
O	3.61859300	-2.20460200	-0.99957500
O	1.22827700	-0.11121000	4.30138000
O	2.40255400	-4.26445900	2.89288800
O	5.14500900	-0.60168100	2.58807400
H	1.37182300	5.70576000	-2.04903200
H	-1.04772700	4.40333200	-2.48564700
H	3.89758200	3.73758000	-1.34354500
H	3.28681800	5.27350400	-0.68926300
H	3.37855400	3.84495100	0.36288600
H	-5.04923900	2.31743800	-1.73352100
H	-6.00147600	3.09524500	-3.87447400
H	-5.63689900	1.78641100	-5.95122400
H	-4.30795900	-0.30800500	-5.87446100
H	-3.33510600	-1.08362500	-3.73539100
H	-6.34144700	-0.44065500	-1.72145900
H	-8.17816900	-1.59780900	-0.55475600
H	-7.76770200	-2.73323100	1.61271500
H	-5.48928400	-2.71376700	2.60486300

H	-3.63650500	-1.57405100	1.42956200
C	-2.17031100	2.31810400	-0.22445900
C	-3.27801600	1.47057300	-0.00762800
C	-2.01192000	3.45731000	0.56221300
C	-4.21314200	1.81354700	0.97259800
C	-2.94887200	3.78188600	1.54146800
H	-1.14824100	4.10072300	0.41873500
C	-4.05542400	2.96613900	1.74028800
H	-5.08027200	1.18103000	1.13755400
H	-2.80812900	4.67335500	2.14483600
H	-4.79783300	3.21930500	2.49085400
H	-1.64763600	1.91817000	-2.28563200
H	-0.78202300	0.94531200	-1.09337400

IM1

C	-0.73687600	2.92909100	-0.38017400
C	-0.05099700	5.00308100	-0.98193800
C	1.05198600	4.23087700	-0.88610600
C	1.53898100	1.85121400	-0.39780100
C	-2.49530000	4.70658500	-0.66398400
C	3.24648700	-1.41698000	-0.11819600
C	2.78222400	-1.49854100	1.20023800
C	2.33158600	-2.71766600	1.71337300
C	2.33830800	-3.86098200	0.91898300
C	2.78218900	-3.78359700	-0.40143600
C	3.22114800	-2.56902900	-0.91937600
C	5.81523200	-0.34097300	-0.74859800
C	6.32485900	-1.38523800	0.03071000
C	7.69342200	-1.64636600	0.04756700
C	8.56706100	-0.86517200	-0.70636700
C	8.06864600	0.17812600	-1.48360600
C	6.69984800	0.43242100	-1.51022800
C	-0.42082000	-2.95683200	-0.86104400
C	-0.32603300	-0.40921200	-1.88163700
C	-0.79368700	-2.06836700	1.62723700
C	-0.92433400	0.75825200	1.52338300
C	-2.61851200	1.45045000	-1.88342800
C	-3.26888000	2.24337800	0.92149500
C	-3.36776900	-0.73001500	1.95876600
C	-3.12216700	-1.42198600	-1.87987700
C	-4.04804100	-3.02586600	0.33502200
C	-4.90573400	-0.18740900	-0.20697700
N	0.61624500	2.97131200	-0.51079100
N	-1.13055400	4.19607300	-0.67348800

P	4.02008100	0.09497800	-0.86433700
Ru	-0.49308400	-1.27038800	-0.09685700
Ru	-1.97169500	1.28513600	-0.01799500
Ru	-3.36493900	-1.21359600	0.05046000
O	-0.49203500	-3.99304700	-1.36335200
O	-0.08342300	-0.04805900	-2.94579500
O	-0.92970300	-2.60083100	2.63592000
O	-0.39040500	0.81067900	2.55901500
O	-3.04271200	1.67421000	-2.92686500
O	-4.07957200	2.75175000	1.56449700
O	-3.44304300	-0.47362100	3.07061500
O	-3.00928200	-1.59309700	-3.00491900
O	-4.62821800	-3.99225500	0.53433100
O	-5.86659900	0.41242300	-0.40682600
H	-0.17388600	6.04356300	-1.23866800
H	2.09663000	4.45120900	-1.04216600
H	-2.84389300	4.84954800	0.36040000
H	-2.49801900	5.66681400	-1.17930300
H	-3.16054200	4.02079000	-1.18794300
H	2.80169200	-0.62241600	1.84336600
H	1.98386900	-2.76860100	2.74083200
H	1.99259600	-4.80766400	1.32309600
H	2.78326700	-4.66961600	-1.02879200
H	3.57377800	-2.51734600	-1.94738100
H	5.65521000	-1.99836700	0.62776200
H	8.07712300	-2.46135300	0.65379800
H	9.63250000	-1.07294900	-0.69247500
H	8.74219800	0.78695400	-2.07883700
H	6.31367700	1.23668400	-2.13253500
C	2.64084500	2.06768600	0.61664600
C	3.83092900	1.31826900	0.52501900
C	2.46713800	2.96324300	1.67346500
C	4.82619700	1.51110000	1.48994200
C	3.46597500	3.14151400	2.62606200
H	1.54366400	3.52981700	1.75048700
C	4.65124700	2.41907400	2.53051400
H	5.75007700	0.94403400	1.42918700
H	3.31608800	3.84560900	3.43832200
H	5.43664700	2.55423600	3.26742700
H	0.94592700	0.97168500	-0.12868000
H	1.96687700	1.66434900	-1.38855300

IM2

C	-0.02403700	-2.31770700	-0.50824500
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C	-1.42742800	-3.95622100	-1.18597100
C	-2.18164700	-2.99582300	-0.60780300
C	-1.76114900	-0.74849300	0.41562400
C	0.99484000	-4.34844200	-1.57543900
C	-4.06821500	1.54334100	-0.81158900
C	-3.93764000	2.32459900	0.34237400
C	-3.48295600	3.63842200	0.25411600
C	-3.15621700	4.18515600	-0.98587500
C	-3.28509900	3.41531400	-2.13991700
C	-3.73378500	2.09990900	-2.05178900
C	-6.46858200	-0.06499700	-0.77549300
C	-7.20486300	-1.21323200	-1.09459900
C	-8.59695200	-1.18986200	-1.08110100
C	-9.26902000	-0.01039900	-0.76621500
C	-8.54502800	1.14040700	-0.46078200
C	-7.15187600	1.11403600	-0.46099700
C	2.08441900	3.28528100	0.32706400
C	0.81353700	0.69931600	-0.68406300
C	0.23669300	2.00524800	1.65313900
C	1.37486100	-1.19601000	1.75887000
C	2.21757700	-1.22145300	-2.05038600
C	3.02687300	-2.65445100	0.16467400
C	4.21655800	-0.26908000	1.68961300
C	3.54286900	1.31395000	-1.71426400
C	5.31241800	1.83074800	0.28048700
C	5.46437300	-0.87171200	-0.99835600
N	-1.30797300	-2.00548000	-0.19566800
N	-0.11666600	-3.52570000	-1.11785400
P	-4.62567200	-0.22097000	-0.80510700
Ru	1.81893900	1.51265600	0.77924000
Ru	1.77655200	-1.23787800	-0.14222900
Ru	4.20701900	0.37763300	-0.14286500
O	2.20994000	4.36261700	-0.06112000
O	0.11596600	1.04845200	-1.56598800
O	-0.71576700	2.29721700	2.22689800
O	1.11350700	-1.28983500	2.87201500
O	2.41651900	-1.25370800	-3.17631000
O	3.80066100	-3.48550000	0.33172800
O	4.26409800	-0.61509600	2.78591200
O	3.21745600	1.89932800	-2.64724300
O	5.98526400	2.72046300	0.55920500
O	6.26388800	-1.51416300	-1.50809600
H	-1.69669300	-4.89961700	-1.63435100
H	-3.24568500	-2.93133400	-0.44664500

H	1.51126100	-4.79896800	-0.72520400
H	0.59320500	-5.14015600	-2.20818100
H	1.69475500	-3.75495600	-2.16285900
H	-4.18883200	1.90525200	1.31332400
H	-3.38304900	4.23473400	1.15607900
H	-2.79840100	5.20804300	-1.05154200
H	-3.02574500	3.83409000	-3.10737800
H	-3.81440100	1.49630700	-2.95274300
H	-6.68290300	-2.13187100	-1.35351600
H	-9.15562900	-2.08809500	-1.32532100
H	-10.35445700	0.01323800	-0.76393600
H	-9.06598400	2.06211200	-0.21984400
H	-6.59774300	2.01573900	-0.21667500
C	-2.93466100	-0.95696500	1.34821900
C	-4.26678900	-0.71485900	0.95841800
C	-2.65920300	-1.40377800	2.64141600
C	-5.28549100	-0.93189100	1.89401900
C	-3.68161100	-1.62190700	3.55908300
H	-1.62456200	-1.57823600	2.92817800
C	-4.99862700	-1.38209900	3.18079700
H	-6.31901300	-0.74642600	1.61885100
H	-3.44946100	-1.96873800	4.56088900
H	-5.80734000	-1.53901900	3.88784200
H	-0.92102600	-0.35141500	0.98455500
H	-1.97828500	-0.03025000	-0.37886600

TS2

Ru	0.87074300	-0.43528900	1.04316000
Ru	2.05206000	1.32002400	-0.94136800
Ru	3.53103900	-1.10118200	-0.46810900
C	-0.32807000	-2.00557800	0.48860400
O	-1.01458000	-2.90461900	0.33008800
C	0.39086200	-0.85195300	2.79145700
O	0.10223600	-1.07084600	3.88263800
C	2.70089100	-0.49734400	1.68754200
O	3.36221900	-0.49316700	2.65879400
C	0.55556700	0.14132200	-1.25677800
O	-0.14853200	-0.22711700	-2.11708900
C	0.99207700	2.84273600	-1.02410900
O	0.30981300	3.76694100	-1.09282400
C	2.81240200	1.83367200	-2.54927600
O	3.16797900	2.09999400	-3.61481700
C	2.16432600	-2.35494500	-1.15302600
O	1.49446700	-3.13770500	-1.64801200
C	4.59719100	-2.54837000	0.30816100

O	5.32508700	-3.36194200	0.64719400
C	4.09620300	-0.84032400	-2.25904000
O	4.50529200	-0.75224300	-3.32862600
C	4.72617700	0.33671300	0.10994900
O	5.44768200	1.15049300	0.46281500
C	0.30069000	1.51704500	1.56838000
N	0.95412200	2.51344900	2.21693200
N	-0.93735900	2.03301700	1.34120200
C	0.14446200	3.61944300	2.39493300
H	0.49726100	4.51193100	2.88744700
C	-1.05143900	3.31606600	1.83936200
H	-1.96313000	3.88538900	1.74647400
C	2.34199600	2.46482200	2.65323300
H	2.48323800	1.67543100	3.39105400
H	2.59437600	3.42948000	3.09275500
H	2.99513100	2.28170100	1.79581400
C	-2.03843000	1.33874900	0.69082600
H	-1.63284800	0.77055200	-0.15149400
H	-2.69667200	2.10820900	0.27463100
C	-2.81642900	0.42623500	1.62093300
C	-3.67752800	-0.55583300	1.08411300
C	-2.71650100	0.57288000	3.00411100
C	-4.40411100	-1.36557000	1.96322400
C	-3.44472500	-0.24377700	3.86575200
H	-2.05272100	1.32662200	3.41870000
C	-4.28968800	-1.21606500	3.34377800
H	-5.06876400	-2.12724000	1.56769200
H	-3.34613400	-0.11861200	4.93957700
H	-4.86443400	-1.85772300	4.00441400
P	-3.70777900	-0.83148900	-0.75628000
C	-5.10176700	-2.03669800	-0.93443700
C	-6.45213100	-1.68071600	-1.01563600
C	-4.75394600	-3.39190200	-0.99304900
C	-7.43295700	-2.66132800	-1.14548900
H	-6.74326300	-0.63485600	-0.98323200
C	-5.73566800	-4.37330000	-1.11045700
H	-3.70652700	-3.68090500	-0.94758100
C	-7.07749800	-4.00825200	-1.18945300
H	-8.47749500	-2.37197400	-1.21143600
H	-5.45076600	-5.42017900	-1.14988900
H	-7.84411600	-4.77031500	-1.29088700
C	-4.46487100	0.75488600	-1.34297000
C	-5.32584800	1.54345600	-0.56844900
C	-4.11046200	1.19538200	-2.62287400

C	-5.82499100	2.74374100	-1.06889000
H	-5.59948300	1.21913900	0.43300600
C	-4.61411200	2.39362600	-3.12631900
H	-3.42876000	0.60024300	-3.22585300
C	-5.46980200	3.16984100	-2.34840800
H	-6.48936500	3.34841300	-0.45894500
H	-4.32916200	2.72338800	-4.12063500
H	-5.85563600	4.10806800	-2.73513700

IM3

Ru	0.40003100	-1.06256800	-0.07193400
Ru	1.03211900	1.86867400	0.12656700
Ru	3.20068800	0.10183800	-0.78903900
C	-0.09758300	-1.52905800	-1.88342800
O	-0.47859700	-1.87465100	-2.90441300
C	-0.43195100	-2.60356200	0.49875000
O	-0.84259700	-3.61655500	0.86171000
C	2.16830500	-1.82089800	-0.29802300
O	2.60888200	-2.91936300	-0.25581200
C	-0.07205700	1.56508200	-1.38793500
O	-0.59040500	1.73404000	-2.41079300
C	-0.28433800	2.89055000	0.92557600
O	-1.07707000	3.52483100	1.47256400
C	2.19914700	3.34166600	0.41973400
O	2.77657900	4.34096700	0.40513700
C	2.30657800	0.05994300	-2.53321200
O	1.85614000	0.06280900	-3.58448000
C	4.72589900	-1.05036200	-1.19388300
O	5.63009100	-1.70311700	-1.43241600
C	4.00334500	1.79156300	-1.28550200
O	4.53654600	2.74423100	-1.62444500
C	3.54614300	0.50167900	1.09094200
O	3.84705000	0.76411200	2.16613100
C	0.44814100	-0.55624700	2.04363900
N	1.29953100	-0.79786900	3.06736300
N	-0.57926900	0.12276900	2.62093800
C	0.83591000	-0.24899600	4.24908700
H	1.39070300	-0.32681000	5.17112100
C	-0.35085300	0.33903700	3.96527500
H	-1.04618500	0.88466700	4.58475800
C	2.42715400	-1.72162100	3.03989900
H	2.82883100	-1.79552700	2.03323400
H	2.09000300	-2.71054100	3.35963400
H	3.20218600	-1.36208800	3.71708500
C	-1.85300000	0.37875600	1.95525700

H	-1.62465600	0.68209700	0.93033100
H	-2.32613400	1.23293900	2.44995900
C	-2.77019700	-0.83438400	1.96587100
C	-3.60698400	-1.11270500	0.86478200
C	-2.80285900	-1.66908500	3.08389900
C	-4.45363000	-2.22571600	0.92807900
C	-3.64547500	-2.77543700	3.12895100
H	-2.15556000	-1.45910400	3.93077400
C	-4.47389200	-3.05365500	2.04730800
H	-5.10023800	-2.45794100	0.08782900
H	-3.65130300	-3.41487100	4.00595900
H	-5.13606300	-3.91352000	2.06944500
P	-3.43715100	-0.11632800	-0.69596100
C	-4.87021400	-0.72256400	-1.69523400
C	-6.18990800	-0.30012600	-1.49939800
C	-4.59911400	-1.66822900	-2.69035000
C	-7.21742700	-0.81899300	-2.28217400
H	-6.41566600	0.43793500	-0.73464500
C	-5.62900600	-2.19457100	-3.46761200
H	-3.57523200	-1.99318800	-2.85923300
C	-6.93910400	-1.76866600	-3.26475200
H	-8.23769700	-0.48260200	-2.12439200
H	-5.40640900	-2.92939500	-4.23515600
H	-7.74236700	-2.17191000	-3.87383900
C	-4.01851300	1.55512600	-0.15019900
C	-4.78285100	1.78294100	1.00076200
C	-3.64971900	2.64631000	-0.94718600
C	-5.17404800	3.07589400	1.34276500
H	-5.07445200	0.94673400	1.63193500
C	-4.05117000	3.93721100	-0.61045800
H	-3.04755800	2.48375100	-1.83780800
C	-4.81146700	4.15377700	0.53634100
H	-5.76538200	3.24148400	2.23846000
H	-3.76275700	4.77376000	-1.23953600
H	-5.11732700	5.16033100	0.80453800

IM3-a

Ru	-1.02122900	0.71497600	-1.39778800
Ru	-3.28913400	0.19666900	0.62726200
Ru	-1.56843700	-1.86055700	-0.45823000
C	-2.14361700	0.11377600	-2.84033900
O	-2.78247000	-0.21726600	-3.73225900
C	0.40022000	-0.10613200	-2.24977000
O	1.23746400	-0.53690500	-2.91657100
C	-3.83893900	1.34467000	-0.86980600

O	-4.36471800	2.04181800	-1.61628400
C	-0.91191700	2.51033600	-2.19803300
O	-0.75924700	3.35317800	-2.96334500
C	-2.94282500	1.78984400	1.67757000
O	-2.80161200	2.71161700	2.34124500
C	-2.30596500	-0.82270000	1.98397600
O	-1.86668100	-1.28227900	2.94319000
C	-3.45191400	-1.51517500	-0.76696100
O	-4.33193700	-1.94066500	-1.42396800
C	-1.08397400	-2.79140900	-1.98374300
O	-0.88434800	-3.35995200	-2.96453700
C	-5.06403900	-0.26700300	1.25541100
O	-6.11952300	-0.49569500	1.62682300
C	0.12898100	1.21222300	0.39355900
N	0.15077300	2.42840400	1.00351700
N	0.81943100	0.41355200	1.25574400
C	0.81098500	2.38172900	2.21440600
H	0.93361000	3.25621100	2.83409700
C	1.22716700	1.10734400	2.38081200
H	1.78835600	0.64167400	3.17494800
C	-0.38947100	3.67484400	0.48155500
H	-1.41916800	3.53758500	0.14965200
H	-0.36526100	4.41595600	1.28121000
H	0.21791400	4.03247900	-0.35266100
C	1.04951400	-1.02709900	1.10304300
C	2.33424700	-1.46565500	1.76574900
C	2.26039200	-2.22336600	2.93581700
C	3.41661600	-2.62836900	3.59760400
C	4.66002500	-2.26719900	3.08936500
C	4.74256600	-1.51001800	1.92230000
C	3.59039300	-1.09397500	1.24628000
H	1.28384900	-2.49367900	3.33053700
H	3.34467700	-3.21959200	4.50493000
H	5.56886000	-2.57329500	3.59820200
P	3.64340200	-0.11683300	-0.34153700
C	3.75621800	1.62187200	0.28498200
C	4.47252600	1.98635800	1.43238000
C	3.08441900	2.61029000	-0.44178500
C	4.51482300	3.31431500	1.84513300
H	4.99726000	1.22520700	2.00469700
C	3.13177000	3.94359400	-0.03140100
H	2.51712900	2.33581000	-1.33036800
C	3.84188100	4.29439600	1.11386200
H	5.07343400	3.58675700	2.73537900

H	2.61763700	4.70679500	-0.60823100
H	3.87684200	5.33119200	1.43464000
C	5.37683000	-0.45859700	-0.89409900
C	5.66931500	-1.77163800	-1.29248600
C	6.36986600	0.51770800	-1.01035400
C	6.93177000	-2.10491900	-1.76928600
H	4.90278600	-2.54090400	-1.22019600
C	7.63257700	0.18474500	-1.50248800
H	6.16435800	1.54332800	-0.71833800
C	7.91846400	-1.12425800	-1.87733400
H	7.14465200	-3.12839100	-2.06289300
H	8.39401300	0.95405900	-1.58938600
H	8.90304700	-1.38184000	-2.25534300
H	5.72002500	-1.24323100	1.53033600
C	-1.96723800	-3.48519900	0.41519300
O	-2.21146200	-4.47271300	0.94661600
H	0.20473600	-1.57209800	1.54301100
H	1.07359300	-1.23925400	0.02920200

TS3-a

Ru	0.90652900	0.86738500	1.24111600
Ru	3.31222000	0.55112400	-0.36008800
Ru	1.27056000	-1.61905500	-0.26574700
C	1.62472800	-0.06215600	2.78666800
O	1.96461300	-0.58401500	3.74669000
C	-0.56203300	1.38490100	2.29145600
O	-1.36189900	1.79994100	3.00826800
C	4.14728800	0.11112000	1.35693000
O	4.69712600	-0.09167000	2.33914500
C	2.08086800	2.32058800	1.43065500
O	2.60711700	3.28336500	1.80895300
C	4.35339700	2.15763800	-0.56107800
O	5.00035500	3.07792800	-0.77484700
C	2.26475600	0.90741500	-1.95899900
O	1.78502400	1.14258600	-2.97367900
C	2.46894000	-2.20119700	1.07520500
O	3.17009300	-2.69459400	1.84323400
C	-0.02340400	-2.83640800	0.31218100
O	-0.79964900	-3.58460400	0.70401800
C	4.29563200	-0.76603700	-1.29459600
O	4.97301600	-1.50591000	-1.85497500
C	-0.11080700	1.67185000	-0.45601900
N	-0.41097500	2.94081300	-0.80855900
N	-0.63731600	0.91145300	-1.44869700
C	-1.08332000	2.97896300	-2.01836900

H	-1.41623100	3.90710600	-2.45636100
C	-1.22081500	1.69593500	-2.42660700
H	-1.68617300	1.27047200	-3.30225300
C	-0.06982300	4.12823300	-0.04044500
H	0.96736100	4.41850500	-0.22554100
H	-0.73090100	4.94032900	-0.34440500
H	-0.20906600	3.93081900	1.02315600
C	-0.41298600	-0.52686600	-1.57213600
C	-1.64912900	-1.35207500	-1.81630000
C	-1.56214800	-2.27400100	-2.87043300
C	-2.61087800	-3.12480000	-3.19099900
C	-3.79366900	-3.05739200	-2.45980900
C	-3.89882700	-2.14929600	-1.41215800
C	-2.84352600	-1.29322300	-1.06367500
H	-0.64010800	-2.32157500	-3.44635700
H	-2.50728000	-3.82876900	-4.01075000
H	-4.63025800	-3.70556100	-2.70078500
P	-2.98768000	-0.16320300	0.41238700
C	-3.68881400	1.37411600	-0.35008900
C	-4.41022300	1.38774800	-1.55011400
C	-3.46734200	2.58304300	0.31801200
C	-4.89014700	2.58581700	-2.07357100
H	-4.59431000	0.45717500	-2.08117500
C	-3.94924800	3.78330400	-0.20341900
H	-2.90948700	2.58944400	1.25058500
C	-4.65694600	3.78630800	-1.40325300
H	-5.44725500	2.58274100	-3.00560800
H	-3.77011600	4.71365500	0.32785800
H	-5.03042500	4.72002800	-1.81283400
C	-4.47527300	-0.86806700	1.26483100
C	-4.27046900	-2.01686500	2.04209400
C	-5.75536600	-0.30800100	1.21580600
C	-5.32484300	-2.60733000	2.73103700
H	-3.27670200	-2.45491500	2.10517300
C	-6.80925100	-0.89205600	1.91874800
H	-5.93794600	0.58637600	0.62720600
C	-6.59900400	-2.04375500	2.67178800
H	-5.14930900	-3.50235000	3.32021800
H	-7.79791300	-0.44525700	1.87153700
H	-7.42190300	-2.49949300	3.21385900
H	-4.82401500	-2.10860100	-0.84570200
C	1.99242400	-2.72075400	-1.75099700
O	2.33096100	-3.45006100	-2.56297000
H	0.22455900	-0.64657200	-2.44666200

H	-0.05527100	-0.55561100	-0.09225300
IM4			
Ru	1.07431100	1.10514800	1.18024800
Ru	3.30550000	0.20986000	-0.44940200
Ru	1.01159000	-1.57385200	-0.02478900
C	1.97865500	0.42119700	2.75789400
O	2.39548300	0.01310500	3.74057900
C	-0.35412000	1.73869300	2.25736300
O	-1.14165900	2.15422800	2.97879300
C	4.15865700	-0.33160100	1.22484700
O	4.78892100	-0.62027500	2.13693300
C	2.15821600	2.67055600	1.10245400
O	2.76530200	3.64445500	1.16496300
C	4.43471000	1.74996000	-0.59216800
O	5.15620100	2.62810300	-0.73945700
C	2.26635900	0.67345900	-2.01987100
O	1.81593000	0.97299100	-3.03118800
C	2.16014000	-2.32365500	1.36695200
O	2.74837600	-2.84805000	2.19502200
C	-0.38788200	-2.74454300	0.45692400
O	-1.17056100	-3.50843700	0.79314100
C	4.30381400	-1.07473600	-1.43172100
O	4.95748900	-1.80825700	-2.02404100
C	-0.04514100	1.60613200	-0.56228700
N	-0.41084100	2.83492800	-1.00796300
N	-0.56472800	0.74723000	-1.47026500
C	-1.10974900	2.74820700	-2.19790700
H	-1.49647700	3.62277400	-2.69771800
C	-1.20667400	1.43270800	-2.48732400
H	-1.67827500	0.91714100	-3.30971600
C	-0.13904400	4.10858100	-0.36121500
H	0.85993000	4.47029600	-0.61611900
H	-0.87728800	4.83222600	-0.70933100
H	-0.22931300	4.00855900	0.72118700
C	-0.33130000	-0.70151000	-1.56535000
C	-1.62000600	-1.47075400	-1.76107900
C	-1.58058800	-2.47566800	-2.74219000
C	-2.65988400	-3.31078200	-2.99666600
C	-3.84100000	-3.14096500	-2.28069500
C	-3.90716400	-2.14804500	-1.30978100
C	-2.81753600	-1.31151600	-1.02136700
H	-0.66705400	-2.60223400	-3.31960900
H	-2.58073000	-4.07874200	-3.76036100
H	-4.70331200	-3.77107400	-2.47457000

P	-2.92640100	-0.10717100	0.40176900
C	-3.62856800	1.40466700	-0.40927200
C	-4.35932400	1.38219700	-1.60340700
C	-3.39649800	2.63452700	0.21491100
C	-4.83494600	2.56428100	-2.16536800
H	-4.54862300	0.43509800	-2.10261200
C	-3.87340500	3.81963200	-0.34422300
H	-2.83161800	2.66935800	1.14308000
C	-4.58828000	3.78610300	-1.53949100
H	-5.39708500	2.53274200	-3.09390600
H	-3.68613800	4.76655100	0.15403100
H	-4.95759500	4.70769500	-1.97930200
C	-4.41494900	-0.74143800	1.31239200
C	-4.20402400	-1.80605000	2.19962000
C	-5.70055900	-0.19990600	1.20928200
C	-5.25362900	-2.33241100	2.94598100
H	-3.20630900	-2.22556100	2.30912500
C	-6.75046700	-0.71889000	1.96636500
H	-5.88999900	0.63058000	0.53539100
C	-6.53203700	-1.78742700	2.83163000
H	-5.07175200	-3.16075500	3.62400400
H	-7.74222300	-0.28590500	1.87518000
H	-7.35136200	-2.19070200	3.41892200
H	-4.83072800	-2.02576900	-0.75201200
C	1.73153800	-2.66399500	-1.41645500
O	2.11559700	-3.32473000	-2.26862700
H	0.21236600	-0.81746800	-2.50659400
H	0.19400600	-0.46643300	1.14631200

Cartesian Coordinates for the Stationary Points Given in Fig. S3

TS3-b

Ru	-0.98613600	0.66921700	-1.50723700
Ru	-2.71974100	0.23989300	0.80562700
Ru	-1.63549200	-1.98653500	-0.52092500
C	-2.09681500	0.06062300	-2.95233400
O	-2.75795600	-0.28394700	-3.82119700
C	0.42591800	-0.40162100	-2.23150600
O	1.22820000	-0.95091700	-2.84490100
C	-2.92902100	1.47141200	-0.70618600
O	-3.75211900	2.20452200	-1.11008700
C	-0.56410500	2.36393500	-2.35171500
O	-0.28545700	3.24586500	-3.02906700
C	-2.55123500	1.64701300	2.04790100

O	-2.44640700	2.46508800	2.84588400
C	-1.69285300	-1.47567200	3.14461000
O	-2.27813700	-2.02335800	3.94328600
C	-3.44633000	-1.51349000	-0.72106500
O	-4.49283000	-1.61286800	-1.23070200
C	-0.98116500	-2.95634300	-1.99545000
O	-0.79587600	-3.54629800	-2.96804700
C	-4.40738000	-0.09801900	1.49882500
O	-5.50431900	-0.24065100	1.81771900
C	0.05979500	1.15538800	0.33964200
N	0.09748600	2.37683700	0.94080000
N	0.74310700	0.35264000	1.20651500
C	0.76410600	2.33192100	2.14559300
H	0.89749200	3.20917400	2.75924800
C	1.16437000	1.05248300	2.32202200
H	1.72993800	0.58967300	3.11465300
C	-0.46201400	3.61457100	0.41876500
H	-1.49127900	3.46270300	0.08994500
H	-0.44644900	4.35748800	1.21677900
H	0.13853800	3.98014800	-0.41628700
C	0.98895800	-1.08720400	1.04786400
C	2.27828700	-1.50050200	1.71751500
C	2.21138300	-2.26831900	2.88117200
C	3.37097700	-2.64335800	3.55521400
C	4.60923500	-2.23974800	3.06650000
C	4.68422600	-1.47040000	1.90660800
C	3.52931000	-1.08440700	1.21777000
H	1.23735600	-2.56885000	3.26207400
H	3.30597300	-3.24356900	4.45710100
H	5.52000700	-2.52128200	3.58580400
P	3.57897300	-0.09227400	-0.36240600
C	3.65899000	1.64671200	0.26712700
C	4.34684600	2.02417400	1.42740600
C	2.99570700	2.62506200	-0.48050500
C	4.36699400	3.35485400	1.83303000
H	4.86583100	1.27144600	2.01585300
C	3.02152300	3.96137900	-0.07807200
H	2.45483900	2.33935200	-1.38170500
C	3.70185000	4.32490300	1.08108900
H	4.90359900	3.63769900	2.73354700
H	2.51530900	4.71655100	-0.67236400
H	3.72066300	5.36374400	1.39654900
C	5.32309400	-0.39480100	-0.90452800
C	5.65054600	-1.69862000	-1.30565000

C	6.29108500	0.60734200	-1.01509800
C	6.92239000	-1.99753000	-1.78045500
H	4.90398100	-2.48753600	-1.23805600
C	7.56315300	0.30856300	-1.50460400
H	6.05880300	1.62670300	-0.72139200
C	7.88363800	-0.99136200	-1.88305400
H	7.16234500	-3.01407500	-2.07701900
H	8.30483900	1.09746700	-1.58686600
H	8.87539600	-1.22145400	-2.26005500
H	5.65806200	-1.16955700	1.53054500
C	-2.07820300	-3.57932200	0.36397900
O	-2.34948600	-4.54250800	0.92973900
H	0.14884900	-1.63765200	1.48686200
H	1.02067800	-1.29670400	-0.02397500

IM4-b

Ru	-0.97195800	0.66520100	-1.52907000
Ru	-2.64104500	0.22762500	0.79494400
Ru	-1.60045900	-2.00113600	-0.54566300
C	-2.06850900	0.04762900	-2.97682700
O	-2.72306400	-0.30252900	-3.84850300
C	0.45078700	-0.39866300	-2.23935500
O	1.26263400	-0.94004100	-2.84698000
C	-2.91585100	1.46287900	-0.71061800
O	-3.75589300	2.18417600	-1.09509100
C	-0.55829700	2.35978400	-2.37698000
O	-0.28122500	3.23664000	-3.06172700
C	-2.49814500	1.63117100	2.03643400
O	-2.42076900	2.45757300	2.83022000
C	-3.40807600	-1.53069700	-0.72159200
O	-4.47030700	-1.60829200	-1.20073900
C	-0.96699400	-2.94760200	-2.04783200
O	-0.80814800	-3.52110700	-3.03512700
C	-4.26901400	-0.17736600	1.56847300
O	-5.34100700	-0.36636600	1.94670200
C	0.05679800	1.16634100	0.33619000
N	0.10908700	2.39855900	0.91382900
N	0.72074800	0.37134600	1.22487700
C	0.77106900	2.36852300	2.12172200
H	0.91595500	3.25639900	2.71713100
C	1.15252800	1.08757400	2.32500500
H	1.70604000	0.63072900	3.12969200
C	-0.43822200	3.63291700	0.37115000
H	-1.46995500	3.48606800	0.04729000

H	-0.41386500	4.38893900	1.15653800
H	0.16504600	3.97810200	-0.47041400
C	0.95210200	-1.07575300	1.09182200
C	2.24867300	-1.49114700	1.74798600
C	2.19597800	-2.27377500	2.90219400
C	3.36270500	-2.65598500	3.55984700
C	4.59542200	-2.24429900	3.06503300
C	4.65707800	-1.46239900	1.91283700
C	3.49539900	-1.07073100	1.23892300
H	1.22826200	-2.58509900	3.28741000
H	3.30663900	-3.26852400	4.45398600
H	5.51187400	-2.53049100	3.57167300
P	3.53904100	-0.07619400	-0.34017400
C	3.64150800	1.66209000	0.28661200
C	4.32998200	2.03196100	1.44900500
C	2.99446300	2.64798700	-0.46522200
C	4.36611200	3.36265100	1.85320100
H	4.83648300	1.27317100	2.04051200
C	3.03562300	3.98423500	-0.06372700
H	2.45215300	2.36752600	-1.36749900
C	3.71605100	4.34018700	1.09779500
H	4.90281900	3.63962000	2.75548400
H	2.54038800	4.74535000	-0.65967700
H	3.74635400	5.37896500	1.41260200
C	5.27644800	-0.39204400	-0.89700000
C	5.58527300	-1.69376600	-1.31872700
C	6.25813100	0.59819000	-0.99341600
C	6.85250500	-2.00286200	-1.79945000
H	4.82773600	-2.47316900	-1.26268500
C	7.52549700	0.28952600	-1.48884500
H	6.04063100	1.61600200	-0.68352700
C	7.82757800	-1.00874500	-1.88742500
H	7.07806400	-3.01788500	-2.11209600
H	8.27777800	1.06948600	-1.55983200
H	8.81577700	-1.24686100	-2.26877000
H	5.62667900	-1.15699200	1.52967200
C	-2.02630400	-3.60813200	0.32013700
O	-2.28752200	-4.58711000	0.86330800
H	0.10794500	-1.61451000	1.54394700
H	0.97161700	-1.30002700	0.02116600

TS4-b

Ru	-2.82641500	0.83595500	0.24608400
Ru	-0.92880900	-1.34295300	0.61495200
Ru	-1.05629600	0.07870300	-1.82522000

C	-4.05275800	-0.40964100	-0.56624900
O	-4.78269100	-1.14219700	-1.05668300
C	-4.26765200	1.98757900	0.74886700
O	-5.22583400	2.55449800	1.02480100
C	-2.41770800	1.77551700	-1.60323400
O	-2.66790300	2.69915500	-2.26757900
C	-2.25751000	-2.69459800	0.58966300
O	-3.07916700	-3.49382100	0.65998600
C	-2.74807500	-0.21938400	1.91995400
O	-3.09851000	-0.52828000	2.97851700
C	0.26964100	-2.58259700	1.37021100
O	1.00662400	-3.34196900	1.81385600
C	-2.17734000	-0.65369000	-3.04028800
O	-2.90358200	-1.13873000	-3.79127200
C	-0.12188800	0.72176800	-3.34240200
O	0.35812400	1.13266600	-4.30130200
C	-0.17448100	-1.81796300	-1.39700500
O	0.29238100	-2.73071200	-1.93329300
C	-1.27487900	2.11139600	1.00929600
N	-1.28726500	3.44880800	1.22904900
N	-0.02779000	1.72197500	1.36391000
C	-0.07532800	3.88423000	1.72600000
H	0.10344000	4.91879900	1.97413500
C	0.72572600	2.79797500	1.80712800
H	1.74660500	2.69306600	2.13572700
C	-2.40512100	4.35084300	0.98761400
H	-2.84673900	4.14164200	0.01277500
H	-3.15721900	4.25340200	1.77271900
H	-2.02280600	5.37150800	0.98924300
C	0.53619400	0.40087200	1.07306500
H	0.87257700	0.44864000	0.03203600
H	-0.47705300	-0.47199700	1.87944700
C	1.68547800	0.05996600	1.99314200
C	1.48266100	0.16709800	3.37534000
C	2.47395100	-0.18470300	4.28176200
C	3.69252300	-0.66933800	3.81237900
C	3.90546000	-0.79009200	2.44326500
C	2.92004200	-0.42547300	1.51610100
H	0.52197900	0.52665200	3.74028100
H	2.29057600	-0.09241100	5.34766400
H	4.47513400	-0.95639400	4.50759400
H	4.85749600	-1.17290300	2.09013200
P	3.15577100	-0.69410200	-0.30907500
C	4.92709000	-1.21771700	-0.39279100

C	6.00903200	-0.33129400	-0.42132600
C	5.17495500	-2.59543700	-0.42128400
C	7.31366600	-0.81625900	-0.47116200
H	5.83496700	0.74091500	-0.40635100
C	6.48043000	-3.08003900	-0.45890900
H	4.33991400	-3.29256500	-0.41255300
C	7.55148000	-2.18985500	-0.48604900
H	8.14632200	-0.11986000	-0.49640200
H	6.65948400	-4.15061000	-0.47572200
H	8.56961700	-2.56485200	-0.52358800
C	3.22483500	1.05716100	-0.91363900
C	2.91509200	1.27596400	-2.26122800
C	3.53087900	2.15637700	-0.10172900
C	2.90743400	2.56626900	-2.78865700
H	2.67955000	0.42738200	-2.90024500
C	3.52007400	3.44680900	-0.62742400
H	3.77986200	1.99998300	0.94510800
C	3.20613100	3.65349700	-1.97000200
H	2.66266400	2.72165200	-3.83474600
H	3.75787400	4.29184200	0.01194400
H	3.19483700	4.65979800	-2.37705200

Cartesian Coordinates for the Stationary Points Given in Fig. S4

IM5			
Ru	-2.63044700	-0.98826300	0.87934400
Ru	-2.55957200	1.22974500	-0.98287800
Ru	-0.30823000	0.83852200	0.84080300
C	-3.51783700	0.04342000	2.27988100
O	-3.98888500	0.57060300	3.17643100
C	-2.60469800	-2.55531700	1.95395800
O	-2.62161200	-3.52229400	2.56695000
C	-3.74624200	2.05719300	0.33037300
O	-4.50495900	2.60920400	0.98912500
C	-4.25638900	-1.23813600	-0.07582700
O	-5.29595400	-1.42861900	-0.52836300
C	-4.00193000	0.85405700	-2.18283600
O	-4.81801100	0.68379700	-2.96909900
C	-1.21073000	0.33650400	-2.06375100
O	-0.48307400	-0.07825200	-2.84876300
C	-1.31001700	2.24402500	1.74578500
O	-1.79879100	3.08701200	2.34675300
C	0.91089300	0.73061200	2.28114700
O	1.56858000	0.73533400	3.21788300
C	-2.01380900	2.92064800	-1.65323400

O	-1.74386700	3.95340800	-2.07199400
C	-1.42545100	-2.07574000	-0.47876400
N	-1.75076900	-3.17104500	-1.21406800
N	-0.10507200	-1.90039200	-0.69006400
C	-0.64676800	-3.66003400	-1.88836000
H	-0.70837700	-4.52089100	-2.53563400
C	0.39067400	-2.86153500	-1.55228900
H	1.42940500	-2.87480300	-1.84673100
C	-3.07259100	-3.76676400	-1.33522400
H	-3.71385000	-3.15542600	-1.97388200
H	-2.96248400	-4.75250600	-1.78718400
H	-3.53011400	-3.88301700	-0.35127000
C	0.76298400	-0.83121400	-0.16519200
C	1.80866800	-1.47483500	0.71617400
C	1.38564500	-2.31302600	1.76144200
C	2.28408700	-2.88522800	2.64873300
C	3.64835900	-2.62278500	2.51803800
C	4.08975700	-1.82150700	1.47391600
C	3.19321100	-1.25627400	0.55067100
H	0.32045200	-2.49858000	1.87783400
H	1.92289500	-3.52758400	3.44651800
H	4.36240800	-3.04957600	3.21536800
P	3.81763500	-0.33937700	-0.94361300
C	3.99764400	1.39256100	-0.32286100
C	3.84974800	1.75361900	1.01913700
C	4.27257600	2.38946100	-1.26759100
C	3.94779300	3.08998500	1.40666600
H	3.66679000	0.98680900	1.76540400
C	4.39507600	3.71942900	-0.87839000
H	4.38315000	2.12182600	-2.31627800
C	4.22111100	4.07379700	0.45935700
H	3.82265700	3.35785300	2.45208200
H	4.61010200	4.48231700	-1.62051300
H	4.30097500	5.11353800	0.76177500
C	5.58368700	-0.90020900	-0.99680800
C	5.83575100	-2.13864100	-1.60168600
C	6.65907600	-0.16600800	-0.48783600
C	7.13097800	-2.64161200	-1.67919200
H	5.00890300	-2.71454100	-2.01269500
C	7.95831400	-0.66471700	-0.57590300
H	6.48550800	0.79703500	-0.01588800
C	8.19679900	-1.90273400	-1.16741300
H	7.30876900	-3.60561700	-2.14620500
H	8.78482100	-0.08442700	-0.17655900

H	9.20906400	-2.28950300	-1.23338800
H	5.15497600	-1.64239000	1.35971800
C	0.63576900	2.10186800	-0.25054000
O	1.17019600	2.85029900	-0.92889500
H	1.25670300	-0.42048100	-1.04988000
H	-1.08547200	-0.51454900	1.73437200
TS5			
Ru	-2.91989700	0.39146500	-0.89950000
Ru	-1.91328200	-0.82875400	1.61690100
Ru	-0.29594100	-1.02372400	-1.14688200
C	-3.99181700	-1.14094600	-1.46235300
O	-4.65933300	-1.98195400	-1.85392800
C	-4.09058000	1.47068000	-1.84907500
O	-4.88126000	2.12144400	-2.37875200
C	-2.74838300	-2.43537700	0.90976600
O	-3.26139400	-3.39969800	0.56933300
C	-3.67889500	0.40505200	0.86453000
O	-4.60424300	0.83328500	1.46076000
C	-2.85206700	-0.93815100	3.31884000
O	-3.38911700	-1.03795100	4.32062700
C	-1.09185900	0.90526400	2.07556200
O	-0.65881900	1.89784800	2.43270600
C	-1.13135200	-2.70629400	-1.61830000
O	-1.61074100	-3.66215600	-2.02684200
C	0.84999000	-1.23508400	-2.55408500
O	1.55496900	-1.41096500	-3.44497500
C	-0.26097700	-1.76122900	1.97584600
O	0.67230300	-2.33344500	2.32097800
C	-1.70255000	2.08847400	-0.50849700
N	-2.06072900	3.34593100	-0.15164700
N	-0.35057500	2.11104900	-0.56361400
C	-0.94944400	4.15057200	0.00952000
H	-1.03165200	5.18784700	0.29524400
C	0.12677800	3.37327400	-0.24597200
H	1.18271500	3.59209800	-0.21596000
C	-3.42082500	3.83570300	0.02627500
H	-4.05755300	3.02822000	0.38623500
H	-3.40439700	4.63139100	0.77242300
H	-3.81393600	4.23262800	-0.91232600
C	0.55928700	0.95339600	-0.68798100
C	1.71264600	1.31056300	-1.58163300
C	1.51156400	2.07387700	-2.73908700
C	2.56224500	2.37841800	-3.59781800
C	3.84784100	1.92585300	-3.31284300

C	4.06574400	1.15970100	-2.17031000
C	3.01686900	0.84185500	-1.30137600
H	0.50926600	2.42844300	-2.96806300
H	2.37407800	2.96940500	-4.48943800
H	4.67678600	2.16580100	-3.97118400
P	3.23506900	-0.28219000	0.16064700
C	5.03783900	-0.67719700	0.08184200
C	5.41656900	-1.72516400	-0.76809600
C	6.02210900	-0.01334900	0.81999500
C	6.75384600	-2.08952300	-0.89281700
H	4.65795200	-2.25317300	-1.34356500
C	7.35972500	-0.38845800	0.70548900
H	5.74744300	0.80064200	1.48465400
C	7.72826700	-1.42234400	-0.15179700
H	7.03394300	-2.89918100	-1.55958200
H	8.11602300	0.13280600	1.28460100
H	8.77127300	-1.71048900	-0.24006400
C	3.13467600	0.91043000	1.57525700
C	2.78110000	0.39974200	2.82997900
C	3.36164900	2.28536500	1.44125200
C	2.66651800	1.24455500	3.93254900
H	2.60002300	-0.66588500	2.94573500
C	3.23588000	3.13098000	2.54118100
H	3.64146800	2.69333300	0.47281200
C	2.88947800	2.61207800	3.78785100
H	2.39691600	0.83508300	4.90150500
H	3.41358800	4.19602100	2.42540300
H	2.79281800	3.27316200	4.64356800
H	5.06978600	0.80775700	-1.95216500
C	1.80835300	-3.35931800	-0.21019400
O	2.61486700	-4.05077000	0.17980300
H	-1.14884900	-0.31034100	-2.23082200
H	0.93810500	0.81088700	0.33066900

IM6

Ru	2.71868800	-0.38604500	-0.74357900
Ru	1.46248900	1.95571900	0.56956000
Ru	-0.35429300	-0.13975500	-0.59956400
C	2.90396700	1.14002400	-1.91661000
O	3.07113000	1.92646900	-2.73724200
C	3.33603200	-1.59757500	-2.05595200
O	3.71657100	-2.24749800	-2.92087800
C	0.78552900	2.91031500	-0.99207200
O	0.42249700	3.59028300	-1.84633200
C	4.37415100	-0.01513300	0.19975100

O	5.37000500	0.18804500	0.72739900
C	2.67007700	3.38922200	0.97015500
O	3.27437000	4.32130100	1.27306600
C	-0.71531200	0.85459000	-2.28545100
O	-0.99610600	1.31144300	-3.29323500
C	-0.74778500	-1.77798200	-1.33370000
O	-0.88916000	-2.82665700	-1.77881800
C	-0.09019200	2.11946900	1.61865000
O	-0.90853300	2.29404500	2.41816900
C	2.16513400	-2.05369400	0.54329900
N	2.80191200	-3.24846400	0.65648300
N	0.94834800	-2.26660400	1.10822500
C	1.98334600	-4.19948500	1.22627800
H	2.30777800	-5.21635300	1.38376200
C	0.80924000	-3.58249500	1.50604200
H	-0.09289500	-3.97052900	1.94818400
C	4.14894800	-3.55651000	0.19993400
H	4.74865500	-2.64816700	0.18252300
H	4.59988100	-4.26402300	0.89704500
H	4.12644400	-4.00191100	-0.79774000
C	-0.01198600	-1.15873900	1.26691600
C	-1.22874800	-1.46852500	2.11812000
C	-1.12558600	-2.10831600	3.36507800
C	-2.22618100	-2.22851600	4.20347100
C	-3.45994600	-1.68969400	3.83360100
C	-3.57748100	-1.02409600	2.62177400
C	-2.47105800	-0.91760700	1.77095000
H	-0.16251000	-2.48773900	3.69473800
H	-2.11761700	-2.72585200	5.16248900
H	-4.31682700	-1.77511600	4.49385500
P	-2.53012000	-0.09476500	0.13890300
C	-3.65354600	-1.14671000	-0.87583800
C	-4.00398200	-2.44103400	-0.48744500
C	-4.07781900	-0.65978700	-2.11929200
C	-4.77594300	-3.23863000	-1.33246700
H	-3.67482400	-2.83535600	0.46954800
C	-4.84427100	-1.45934200	-2.95981900
H	-3.81602300	0.35019200	-2.42819900
C	-5.19475600	-2.75144600	-2.56639900
H	-5.04762100	-4.24279000	-1.02234300
H	-5.17141700	-1.07388300	-3.92037100
H	-5.79463700	-3.37467400	-3.22214600
C	-3.49495200	1.46781300	0.22133500
C	-2.87554000	2.69429400	-0.02828100

C	-4.87735100	1.43231600	0.45198400
C	-3.61637400	3.87455900	-0.01168100
H	-1.81338800	2.73121600	-0.24776500
C	-5.61294000	2.61217900	0.47896900
H	-5.38698900	0.48154000	0.58166800
C	-4.98228500	3.83504100	0.25126500
H	-3.12276700	4.82084500	-0.20937200
H	-6.68179900	2.57561000	0.66381300
H	-5.56001500	4.75392300	0.26473000
H	-4.52983400	-0.58742600	2.33674900
H	0.52087200	-0.42969900	1.86713100
H	1.23562200	-0.66689000	-1.51637200
C	2.33165300	0.83677600	1.88874300
O	2.81697300	0.32368500	2.80263400

TS6

Ru	2.64586900	-0.62566300	-0.84666800
Ru	1.26291800	1.70221100	0.06282400
Ru	-0.46134600	-0.52416000	-0.75293800
C	2.67666500	0.33680300	-2.50505700
O	2.65370200	0.87590500	-3.51729600
C	3.45689300	-2.19237900	-1.62520800
O	4.03394100	-3.00844100	-2.19227100
C	-0.11576100	1.61145800	-1.29609300
O	-0.56110900	2.31873400	-2.12741500
C	4.07159500	0.36173000	-0.05789000
O	5.00388200	0.86068300	0.40425600
C	2.48436000	2.81614500	-0.71674400
O	3.21191700	3.52999800	-1.26185200
C	-0.94862800	-0.61360000	-2.62321000
O	-1.21687700	-0.65399000	-3.73306600
C	-0.74300100	-2.38749300	-0.42321200
O	-0.88481200	-3.50906800	-0.25405100
C	0.56823400	3.20503700	0.94696400
O	0.20535700	4.15687000	1.48464200
C	2.21777300	-1.62246900	1.01609500
N	2.84252900	-2.66472800	1.61509100
N	1.05493600	-1.48643700	1.69796500
C	2.06426300	-3.20340900	2.61858200
H	2.38347700	-4.05354300	3.20111200
C	0.93102000	-2.46002700	2.67180800
H	0.06846400	-2.54646700	3.31137000
C	4.14122700	-3.20127200	1.23915000
H	4.75846100	-2.39957000	0.83402700

H	4.62158800	-3.60937800	2.12936100
H	4.02966000	-3.99368100	0.49506900
C	0.12897500	-0.37378600	1.38063100
C	-1.03107200	-0.25071400	2.35995100
C	-0.80311600	-0.15395300	3.74336500
C	-1.84360900	0.11162200	4.62393300
C	-3.13904600	0.32315300	4.14428700
C	-3.37917900	0.26471700	2.77915300
C	-2.33348300	-0.03818000	1.89649300
H	0.20862700	-0.26505800	4.12617700
H	-1.64199200	0.18144600	5.68841400
H	-3.94730600	0.55103400	4.83149100
P	-2.56450500	-0.06681900	0.08408400
C	-3.77241000	-1.40505400	-0.28175800
C	-4.35086600	-2.19363500	0.71569900
C	-4.04749600	-1.69135000	-1.62690200
C	-5.20259100	-3.24318000	0.37194900
H	-4.13646000	-2.00520100	1.76256700
C	-4.90726200	-2.73046200	-1.96511700
H	-3.59547500	-1.09474200	-2.41573000
C	-5.48492000	-3.51066100	-0.96395000
H	-5.64314500	-3.85244500	1.15484700
H	-5.11846400	-2.93602200	-3.00970000
H	-6.14732600	-4.32914300	-1.22734700
C	-3.45866200	1.50064600	-0.26876200
C	-2.90016800	2.68494500	0.22777100
C	-4.63920600	1.55701000	-1.01214400
C	-3.50921700	3.90859900	-0.02172800
H	-1.99187800	2.64483500	0.82346000
C	-5.24471200	2.78752800	-1.26617600
H	-5.09852400	0.64938100	-1.38976800
C	-4.68211100	3.96155000	-0.77503300
H	-3.06919500	4.81991500	0.37125900
H	-6.16207100	2.82216400	-1.84526800
H	-5.15723200	4.91719700	-0.97342800
H	-4.37481900	0.45891400	2.38687800
H	0.73663800	0.50244500	1.69530400
H	1.09221500	-1.27654900	-1.35812500
C	3.13741700	1.90495600	2.73504000
O	3.64451500	2.91262700	2.82815100

IM7

Ru	2.82368100	-0.27895100	-0.67281000
Ru	1.15303700	1.77719800	0.42698000
Ru	-0.28238000	-0.42915000	-0.77299000

C	2.84085500	0.95599800	-2.14434400
O	2.81199600	1.65833500	-3.05112500
C	3.85019600	-1.61377100	-1.61163100
O	4.56032300	-2.26278000	-2.24049800
C	-0.11416100	1.80323000	-1.03553300
O	-0.58764700	2.57336200	-1.78829400
C	4.08366500	0.68216600	0.38026500
O	4.91346600	1.17546800	1.01113700
C	2.33122700	3.10398400	-0.02977600
O	3.03865100	3.94939300	-0.37741800
C	-0.66254800	-0.29903200	-2.66076100
O	-0.85575500	-0.19581700	-3.78233800
C	-0.44695800	-2.32850900	-0.68799700
O	-0.52347000	-3.46861300	-0.65658700
C	0.22274500	3.03813400	1.45336100
O	-0.30247600	3.84560200	2.08466700
C	2.38467700	-1.57728700	0.98625200
N	3.04442700	-2.65268100	1.47875100
N	1.18719400	-1.59609100	1.61565600
C	2.25644100	-3.35686100	2.36609500
H	2.60133100	-4.25580500	2.85287500
C	1.07847800	-2.68923600	2.45440900
H	0.19439000	-2.90542800	3.03118200
C	4.38831600	-3.06154000	1.10063100
H	4.98422600	-2.17722600	0.87421000
H	4.84124700	-3.59342400	1.93814100
H	4.35920000	-3.71987600	0.22888600
C	0.22212400	-0.49534000	1.39418600
C	-0.98067700	-0.54546400	2.32753000
C	-0.80961000	-0.59318000	3.72123700
C	-1.89407000	-0.48007800	4.58108300
C	-3.18029000	-0.28178100	4.07255300
C	-3.36718400	-0.20581200	2.70004000
C	-2.27619000	-0.35843800	1.83286600
H	0.19174800	-0.69659800	4.13199200
H	-1.73516100	-0.51831100	5.65425500
H	-4.02382600	-0.16921600	4.74569000
P	-2.44301200	-0.21921500	0.01754500
C	-3.56423800	-1.57595400	-0.52602000
C	-4.23945200	-2.40503100	0.37392800
C	-3.69432200	-1.81442300	-1.90143700
C	-5.04296400	-3.44262100	-0.09585300
H	-4.13469700	-2.26009300	1.44360200
C	-4.50807000	-2.84189900	-2.36726100

H	-3.15710200	-1.19758100	-2.61696500
C	-5.18378400	-3.65950700	-1.46311600
H	-5.55652500	-4.08357100	0.61389300
H	-4.60419700	-3.00969300	-3.43525900
H	-5.81141100	-4.46814600	-1.82414800
C	-3.40387200	1.32763100	-0.23168900
C	-3.09933300	2.43045000	0.57472500
C	-4.35891600	1.45801400	-1.24259100
C	-3.73932400	3.64791300	0.37090600
H	-2.36904200	2.33374700	1.37318900
C	-4.99553700	2.68111700	-1.44638100
H	-4.62077000	0.61073700	-1.86856300
C	-4.68570700	3.77635800	-0.64455700
H	-3.49632100	4.49606500	1.00336800
H	-5.73854900	2.77398600	-2.23219700
H	-5.18301200	4.72746400	-0.80668400
H	-4.35758100	-0.01893300	2.29200100
H	0.78703600	0.35591800	1.84719900
H	1.36108800	-0.97423100	-1.38363400

TS7

Ru	-2.75647100	0.18108200	-0.76581500
Ru	-0.93654800	-1.61961200	0.55561100
Ru	0.29691000	0.50372300	-0.78516900
C	-2.68405800	-1.12342900	-2.18645600
O	-2.63576800	-1.87046200	-3.05401500
C	-3.76910400	1.45401500	-1.77940700
O	-4.41441900	2.11972100	-2.45475300
C	-0.21021900	-2.33027600	-1.11635100
O	0.18196900	-2.97852900	-1.98592800
C	-4.14077300	-0.70586000	0.21095600
O	-5.02517600	-1.15203200	0.79267500
C	-2.36045100	-2.84629400	0.78997300
O	-3.18543200	-3.63467200	0.93469800
C	0.75359200	0.06778100	-2.65685900
O	1.05517100	-0.13174200	-3.74267600
C	0.46279400	2.33903700	-0.88467100
O	0.48241200	3.48899100	-0.89978100
C	0.19355700	-2.57951400	1.71930200
O	0.79695100	-3.19187200	2.48339400
C	-2.45614100	1.49198500	0.87814100
N	-3.14637300	2.53593300	1.38714800
N	-1.28647100	1.48685800	1.55297100
C	-2.40085800	3.20154400	2.34197800
H	-2.77856500	4.06756000	2.86286600

C	-1.21978300	2.54250500	2.44498400
H	-0.36131400	2.73466900	3.06753500
C	-4.47744600	2.95061500	0.97231400
H	-5.05244100	2.07457900	0.67218000
H	-4.97429800	3.42940900	1.81679300
H	-4.41808200	3.65864100	0.14204700
C	-0.26277100	0.48626600	1.22467900
C	0.81819100	0.39531300	2.28370000
C	0.52563600	0.31938600	3.65329300
C	1.52959900	0.08492600	4.58660600
C	2.84889400	-0.10804600	4.17633600
C	3.15724500	-0.04869600	2.82145400
C	2.15405400	0.22212200	1.88587600
H	-0.50535800	0.40951100	3.98639200
H	1.27625200	0.02481700	5.64071000
H	3.62607100	-0.31747200	4.90379000
P	2.41574700	0.30038100	0.08013900
C	3.55269000	1.71148700	-0.26605100
C	4.41161100	2.24625800	0.69942400
C	3.54923600	2.26362800	-1.55379700
C	5.25425200	3.30803000	0.37801100
H	4.42039900	1.85360100	1.71003100
C	4.40082500	3.31642100	-1.87524900
H	2.86847800	1.87969800	-2.30906900
C	5.25403700	3.84194400	-0.90794200
H	5.91028000	3.71943900	1.13863100
H	4.38584600	3.73239300	-2.87765500
H	5.90962700	4.67142600	-1.15376500
C	3.38364900	-1.18706000	-0.40187000
C	3.36176100	-2.34971200	0.37387100
C	4.04516700	-1.19495900	-1.63506000
C	3.99222100	-3.50588400	-0.08091500
H	2.85997600	-2.35648100	1.33558800
C	4.67439700	-2.35157200	-2.08476800
H	4.07396700	-0.29837500	-2.24870000
C	4.64621600	-3.51024000	-1.31005600
H	3.97075700	-4.40313400	0.52961400
H	5.18672400	-2.34647900	-3.04174200
H	5.13432400	-4.41273600	-1.66432400
H	4.17507200	-0.23256800	2.48611900
H	-1.23458200	-0.63157500	1.84268700
H	-1.36730800	0.98026200	-1.48374700

Cartesian Coordinates for the Stationary Points Given in Fig. S5

IM8

Ru	2. 80057000	-0. 02916600	-0. 71746600
Ru	0. 97685300	1. 37897300	0. 95099300
Ru	-0. 24304300	-0. 39959700	-0. 92855800
C	2. 65705200	1. 52334900	-1. 87293100
O	2. 56065000	2. 43765400	-2. 55739300
C	3. 91804400	-1. 04731500	-1. 90309200
O	4. 63535000	-1. 53851800	-2. 65146100
C	0. 02691600	2. 22037900	-0. 58441800
O	-0. 37735200	3. 03658900	-1. 28882800
C	4. 12094300	0. 72403200	0. 42951000
O	4. 96059600	1. 10346300	1. 11563300
C	2. 16255800	2. 89511200	0. 98775800
O	2. 90786700	3. 76094600	1. 06941600
C	-0. 57711700	0. 26130600	-2. 78489100
O	-0. 77238500	0. 56962200	-3. 86719200
C	-0. 45999200	-2. 17804500	-1. 33858300
O	-0. 51066200	-3. 29911600	-1. 58954400
C	-0. 18124700	1. 98404200	2. 32439700
O	-0. 81826600	2. 36341300	3. 19939400
C	2. 49310300	-1. 56500500	0. 67665100
N	3. 17958400	-2. 68300800	0. 99607600
N	1. 29710200	-1. 68518700	1. 28908000
C	2. 40239200	-3. 52847200	1. 76408400
H	2. 77017600	-4. 47584400	2. 12624600
C	1. 20887100	-2. 90806900	1. 93723100
H	0. 33069300	-3. 22777700	2. 47296200
C	4. 52371700	-2. 99888000	0. 54033400
H	4. 96984100	-3. 71169500	1. 23439000
H	4. 49565200	-3. 43958300	-0. 45944000
H	5. 12636800	-2. 09014000	0. 52578700
C	0. 24491300	-0. 68674200	1. 06929200
C	-0. 85506000	-0. 82984500	2. 08156200
C	-0. 62389700	-1. 06698800	3. 45034600
C	-1. 67730100	-1. 13510300	4. 35206300
C	-2. 99909300	-0. 96158800	3. 92918900
C	-3. 24851700	-0. 69795600	2. 58893400
C	-2. 18477500	-0. 62134000	1. 68428600
H	0. 39591600	-1. 18136800	3. 80784700
H	-1. 46769500	-1. 32278200	5. 40110200
H	-3. 81705700	-1. 02637300	4. 63896700
P	-2. 39602900	-0. 25011500	-0. 08490900
C	-3. 68291800	-1. 44434200	-0. 63848000
C	-4. 81104300	-1. 08006800	-1. 37694300

C	-3.48733400	-2.79020700	-0.29986600
C	-5.71990500	-2.05478700	-1.78779500
H	-4.99731400	-0.04063900	-1.62620800
C	-4.39698300	-3.75786200	-0.70977500
H	-2.62921600	-3.08171700	0.30174100
C	-5.51359100	-3.39142100	-1.46082900
H	-6.59410100	-1.76303300	-2.36122000
H	-4.23505700	-4.79687500	-0.44061200
H	-6.22305300	-4.14647100	-1.78463300
C	-3.15076000	1.41608700	-0.22231300
C	-3.40717500	2.20935300	0.89907100
C	-3.38215400	1.93823700	-1.50210900
C	-3.89772500	3.50478600	0.74018900
H	-3.22063500	1.82613300	1.89704700
C	-3.88713700	3.22482200	-1.65544400
H	-3.16118200	1.34102300	-2.38406300
C	-4.14275800	4.01133600	-0.53290100
H	-4.09134000	4.11440600	1.61728000
H	-4.06662700	3.61766900	-2.65112800
H	-4.52737600	5.01928200	-0.65222100
H	-4.26710500	-0.55469800	2.23436800
H	1.44800800	-0.79240600	-1.56332000
H	1.92596400	0.89293400	2.17240700

TS8

Ru	-2.84348700	0.03764700	-0.67020100
Ru	-0.94361400	-1.46253900	0.89099000
Ru	0.25970400	0.32859600	-0.91733700
C	-2.68199800	-1.54586100	-1.83913300
O	-2.55767600	-2.41868900	-2.56366700
C	-3.71111100	1.12266900	-1.96030800
O	-4.24442400	1.73572300	-2.76569200
C	0.21436700	-2.18772600	-0.49282800
O	0.69787700	-3.02940700	-1.13117100
C	-4.42862200	-0.51256800	0.26632400
O	-5.38617300	-0.80011800	0.82049000
C	-2.01061000	-3.04072400	0.83439700
O	-2.73394000	-3.93379900	0.85112700
C	0.63587000	-0.34671300	-2.75043300
O	0.86974300	-0.68607300	-3.81609900
C	0.40860700	2.12861300	-1.32694900
O	0.39866700	3.24574900	-1.59745100
C	-0.17556500	-1.94304200	2.55291100
O	0.30587000	-2.29496300	3.53869900
C	-2.46854800	1.58591100	0.67095700

N	-3.09028200	2.75126000	0.94735700
N	-1.27546200	1.63903900	1.30136400
C	-2.27858800	3.55940000	1.71738400
H	-2.59457100	4.53401600	2.05528200
C	-1.13128800	2.86773800	1.92860400
H	-0.24540000	3.14675600	2.47385200
C	-4.39654900	3.15090500	0.44799000
H	-4.83457200	3.86458100	1.14621100
H	-4.30288200	3.62040200	-0.53460500
H	-5.04575100	2.27773600	0.38118500
C	-0.24331400	0.60752000	1.10276600
C	0.86142000	0.75724700	2.10317500
C	0.64087500	0.99981600	3.47492500
C	1.69800300	1.06498200	4.37037100
C	3.01789300	0.88435900	3.94101200
C	3.25923800	0.62923200	2.59883500
C	2.19012600	0.56159300	1.69872000
H	-0.37716300	1.11381300	3.83869100
H	1.49435200	1.25210000	5.42072400
H	3.83947100	0.94224200	4.64722500
P	2.41090400	0.25115700	-0.07968300
C	3.62820900	1.53843200	-0.59046000
C	4.80740600	1.26365700	-1.28579200
C	3.33013900	2.86347200	-0.24336700
C	5.66218300	2.30346300	-1.65192200
H	5.07731400	0.24382700	-1.53696100
C	4.18588900	3.89647500	-0.60721300
H	2.43300700	3.08794000	0.32973600
C	5.35203000	3.61825300	-1.31982900
H	6.57544000	2.07809500	-2.19358300
H	3.94392200	4.91808600	-0.33162000
H	6.01899200	4.42516600	-1.60673600
C	3.26067900	-1.36107400	-0.26652600
C	3.45107400	-2.21547400	0.82257000
C	3.59888400	-1.79851900	-1.55362700
C	3.99691300	-3.48308000	0.62586600
H	3.16500500	-1.90385300	1.82240600
C	4.15617400	-3.05813100	-1.74315600
H	3.41907400	-1.15694800	-2.41342500
C	4.35485500	-3.90290800	-0.65207500
H	4.13992600	-4.14225500	1.47639700
H	4.42201700	-3.38430000	-2.74363000
H	4.78159400	-4.89001400	-0.80014000
H	4.27570300	0.48892100	2.23707900

H	-1.44945600	0.65625200	-1.51950000
H	-2.47747300	-0.84532700	1.21963600

IM9

Ru	-2.92954200	0.18553900	-0.78425100
Ru	-0.85130900	-1.66800500	0.64734500
Ru	0.25729600	0.34977100	-0.84535900
C	-2.94201800	-1.00356000	-2.35642400
O	-2.89381000	-1.68319200	-3.26635600
C	-3.48166900	1.75415800	-1.78970100
O	-3.77390500	2.67540500	-2.39197900
C	0.74482300	-2.43545700	1.23408200
O	1.68627500	-2.95791900	1.63982000
C	-4.66502300	-0.38196100	-0.09805100
O	-5.66448400	-0.74600100	0.30841500
C	-1.01992100	-3.00484200	-0.74837300
O	-1.12715000	-3.78073500	-1.59232000
C	0.64740200	-0.33839600	-2.65370400
O	0.95132800	-0.70040200	-3.69983100
C	0.45627200	2.17922600	-1.15865100
O	0.49795000	3.31980000	-1.31486200
C	-1.80894800	-2.16590000	2.25275300
O	-2.35021200	-2.48754300	3.21336800
C	-2.49731400	1.35783100	0.90400200
N	-3.15673100	2.41094500	1.43995300
N	-1.31552900	1.29267400	1.55560900
C	-2.38322900	3.02705900	2.40192000
H	-2.72989000	3.88946200	2.94988500
C	-1.22170200	2.33235000	2.46635800
H	-0.35130100	2.49310200	3.07961400
C	-4.45972300	2.92052900	1.03966900
H	-5.00565200	3.23548500	1.92995600
H	-4.34426200	3.77440900	0.36733600
H	-5.02749000	2.13760300	0.53932000
C	-0.24548800	0.35060900	1.17286800
C	0.84608800	0.31316800	2.20448900
C	0.60337200	0.21392800	3.58810000
C	1.64649200	0.04828900	4.48935800
C	2.96987200	-0.03323500	4.04645700
C	3.23260900	0.04458700	2.68415600
C	2.18279800	0.22112000	1.77942500
H	-0.42106200	0.23624800	3.95200200
H	1.42694200	-0.03332300	5.55008200
H	3.77955600	-0.16870700	4.75574800

P	2.38201700	0.27405800	-0.03896500
C	3.39126900	1.77283400	-0.38865800
C	3.86597000	1.95921500	-1.69366600
C	3.59809000	2.76706900	0.56865500
C	4.54946000	3.12230600	-2.02939300
H	3.69559900	1.19332900	-2.44835200
C	4.28191400	3.93427000	0.22704400
H	3.22285500	2.63776500	1.57955300
C	4.75860100	4.11228200	-1.06780500
H	4.91759900	3.25894600	-3.04141000
H	4.43926500	4.70286200	0.97734100
H	5.29183900	5.02037900	-1.33122600
C	3.53226200	-1.08071800	-0.52715900
C	4.91132200	-0.95631100	-0.31249000
C	3.03533100	-2.24015300	-1.12869400
C	5.77352300	-1.98594100	-0.67715500
H	5.31479500	-0.04696900	0.12531100
C	3.90128900	-3.26705100	-1.49823300
H	1.96695200	-2.34222500	-1.30388100
C	5.26920600	-3.14220800	-1.27055200
H	6.84024500	-1.88093300	-0.50559800
H	3.50410600	-4.16223000	-1.96651200
H	5.94360000	-3.94151800	-1.56195600
H	4.25428700	-0.03416000	2.32072500
H	-1.45321100	0.75327800	-1.40335100
H	-2.56576100	-1.18521000	0.18393800

TS9

Ru	-2.91055500	0.31325100	-0.89570900
Ru	-0.77889800	-1.73507300	0.46210600
Ru	0.22455600	0.50675400	-0.79661400
C	-2.86179600	-0.41199100	-2.71563700
O	-2.75366400	-0.84841800	-3.76048800
C	-3.79295800	1.94916900	-1.46111800
O	-4.25451400	2.90128500	-1.88566500
C	0.71542100	-2.55073700	1.21945400
O	1.61354000	-3.09830900	1.68605400
C	-4.44591900	-0.75262500	-0.26130500
O	-5.29231800	-1.40125600	0.13637400
C	-0.76834600	-2.98284200	-1.02710700
O	-0.77686400	-3.67679600	-1.94535900
C	0.63661200	0.05065500	-2.67427300
O	0.96233300	-0.19307900	-3.74716200
C	0.45588900	2.35766800	-0.87873200

O	0.55668100	3.50485600	-0.89548900
C	-1.97289200	-2.31738100	1.87060600
O	-2.64919500	-2.68750700	2.72217300
C	-2.58758200	1.11736600	1.03366600
N	-3.34766700	1.99440200	1.73281500
N	-1.40506700	1.06121500	1.68526100
C	-2.63249200	2.52504900	2.78587100
H	-3.06067400	3.24707500	3.46362100
C	-1.40651200	1.95006400	2.74784700
H	-0.55278000	2.09776400	3.38643100
C	-4.71675900	2.39177100	1.44064300
H	-5.23682300	2.56621300	2.38339900
H	-4.73613100	3.31055700	0.84954300
H	-5.22912300	1.59460000	0.90291000
C	-0.27829900	0.23836900	1.20957200
C	0.80736400	0.13610400	2.24096700
C	0.57320700	-0.10787600	3.60811400
C	1.62636700	-0.29630900	4.49380700
C	2.95073800	-0.26398400	4.04925600
C	3.20428200	-0.06735800	2.69704800
C	2.14470300	0.12955500	1.80903800
H	-0.44927300	-0.17777300	3.97098500
H	1.41342100	-0.48414800	5.54224100
H	3.76891900	-0.41010000	4.74656100
P	2.33237200	0.28393200	-0.00494100
C	3.42054300	1.74310100	-0.27936800
C	3.96881300	1.93090200	-1.55471300
C	3.62167800	2.71125100	0.70623100
C	4.71684200	3.06880900	-1.83464600
H	3.81335900	1.18234100	-2.32884600
C	4.37198900	3.85232400	0.42146700
H	3.19079900	2.58117200	1.69485400
C	4.91982100	4.03176400	-0.84516500
H	5.14230700	3.20488100	-2.82402200
H	4.52550200	4.60029800	1.19304600
H	5.50347600	4.92019100	-1.06533600
C	3.42513600	-1.09726700	-0.55856100
C	4.79862000	-1.06485400	-0.28011100
C	2.89792900	-2.18487600	-1.25850700
C	5.61955700	-2.11721000	-0.67305200
H	5.23407900	-0.20964200	0.22971400
C	3.72327000	-3.23468100	-1.65773300
H	1.83662800	-2.21090700	-1.48561500
C	5.08271800	-3.20478600	-1.36094000

H	6.68093800	-2.08420600	-0.44791100
H	3.29924100	-4.07284600	-2.20219800
H	5.72566100	-4.02289700	-1.67060400
H	4.22749900	-0.06549100	2.33061300
H	-1.53505000	1.19163800	-1.29489000
H	-2.00200300	-1.08041000	-0.71119000
2			
Ru	-1.06876100	-1.50145900	0.57159700
Ru	0.31210700	0.45617200	-0.95633100
Ru	-2.76970300	0.18142600	-0.91044500
C	-2.24725900	-1.40895300	2.05878100
O	-2.92501800	-1.32081500	2.98085100
C	0.29799500	-2.48661700	1.47147600
O	1.06802500	-3.12172200	2.03408200
C	-1.87969400	-3.06656900	-0.28556800
O	-2.39076300	-3.97416500	-0.76162700
C	0.60327300	2.31083100	-0.98680600
O	0.72179400	3.45185900	-0.98606300
C	0.82512400	0.08420400	-2.82601200
O	1.19020500	-0.13765000	-3.88707700
C	-4.16938200	-0.77785300	-0.04085700
O	-5.05170300	-1.32128400	0.45651200
C	-3.76661400	1.48355300	-1.91630000
O	-4.40991500	2.18695700	-2.55308900
C	-2.60861600	-1.05801300	-2.39084900
O	-2.47257600	-1.76501100	-3.28067600
H	-0.07650400	-1.34358400	-0.92483000
H	-1.34312400	1.00220600	-1.55703300
N	-1.30458200	1.43011800	1.40384000
N	-3.16510500	2.49772400	1.25448100
C	-0.27638000	0.43567100	1.06129900
C	-2.48663400	1.44366700	0.75076700
C	-2.39769300	3.17346800	2.18340200
H	-2.76191600	4.04619900	2.70284100
C	-1.21776300	2.50884400	2.26834100
H	-0.34721400	2.71020400	2.87059700
C	-4.50166200	2.90585500	0.85310200
H	-4.45757100	3.58935400	0.00145500
H	-4.98216900	3.41044600	1.69193900
H	-5.08399000	2.02261400	0.58872000
C	0.78273900	0.35278000	2.12243500
C	2.11894800	0.14114700	1.74499700
C	0.49278300	0.33436000	3.50108000
C	3.12404700	-0.08475700	2.69089800

C	1. 49197600	0. 12469300	4. 44130000
H	-0. 53426300	0. 45957200	3. 83397700
C	2. 81651100	-0. 08499900	4. 04462700
H	4. 14706000	-0. 25549500	2. 36440200
H	1. 23628600	0. 11052300	5. 49685600
H	3. 59225700	-0. 25204600	4. 78441800
P	2. 40417200	0. 14183900	-0. 05943500
C	3. 59035900	1. 50752300	-0. 38167600
C	4. 20386400	1. 57940700	-1. 63877300
C	3. 79704500	2. 52949200	0. 54700500
C	5. 02407000	2. 65709600	-1. 95506100
H	4. 04354000	0. 78909000	-2. 36914800
C	4. 61773700	3. 60993500	0. 22431800
H	3. 31740300	2. 48724500	1. 52078200
C	5. 23149500	3. 67451200	-1. 02281000
H	5. 50028000	2. 70499900	-2. 92936900
H	4. 77492300	4. 39972100	0. 95211400
H	5. 86890500	4. 51696400	-1. 27227400
C	3. 39034500	-1. 36165300	-0. 44785100
C	4. 75819100	-1. 40822500	-0. 14511600
C	2. 77713400	-2. 47738800	-1. 02515900
C	5. 49254800	-2. 56233600	-0. 39835300
H	5. 25289100	-0. 53790500	0. 27826100
C	3. 51726200	-3. 63065100	-1. 27996700
H	1. 72162700	-2. 44469500	-1. 27839600
C	4. 87234900	-3. 67559800	-0. 96423200
H	6. 55104900	-2. 58968300	-0. 15939100
H	3. 03281900	-4. 49054700	-1. 73189400
H	5. 44767400	-4. 57366500	-1. 16683300

Cartesian Coordinates for the Stationary Points Given in Fig. S7

TS5-1

Ru	-1. 05852000	0. 53481300	-1. 66394500
Ru	-2. 90985100	0. 33820100	0. 43651100
Ru	-1. 00663600	-1. 76094900	0. 22141800
C	-1. 81074100	-0. 60937500	-3. 03144500
O	-2. 19627700	-1. 30607800	-3. 85065600
C	0. 50875300	0. 90620500	-2. 70378700
O	1. 37273500	1. 18105300	-3. 40303400
C	-3. 74342400	-0. 62292300	-0. 86464400
O	-4. 44446300	-1. 16869300	-1. 60920600
C	-2. 16134700	1. 98045900	-2. 23220700
O	-2. 82135600	2. 80569500	-2. 68055500

C	-3.98731000	1.92590700	0.21588800
O	-4.75768200	2.75754100	0.03846100
C	-2.03250400	2.06998800	2.83622300
O	-2.30981500	2.67142800	3.75444800
C	-2.02510100	-2.89046000	-0.99168400
O	-2.57776300	-3.61535600	-1.68170000
C	0.49364600	-2.93760100	0.13213600
O	1.34275600	-3.70375700	0.07938900
C	-3.90183200	-0.37237700	1.89777500
O	-4.61896100	-0.83812800	2.66601200
C	-0.25272900	1.53305500	0.04132600
N	-0.03187900	2.86550400	0.21514900
N	0.24504800	0.96222900	1.16750000
C	0.56433300	3.12189000	1.43053000
H	0.83384200	4.12107500	1.73702900
C	0.73814200	1.91976900	2.03067600
H	1.17294400	1.65570400	2.98301000
C	-0.33730900	3.91385400	-0.74540800
H	-1.40785100	4.13394600	-0.74857000
H	0.20843500	4.81212400	-0.45600800
H	-0.01622900	3.61096900	-1.74363400
C	0.12180300	-0.44213100	1.59534000
C	1.44284800	-1.01720900	2.05477700
C	1.39839400	-1.76990700	3.24044100
C	2.51146600	-2.42747900	3.74627700
C	3.72969500	-2.32797500	3.07991300
C	3.80092600	-1.58142600	1.90939500
C	2.68133700	-0.92774000	1.37315200
H	0.45147100	-1.84318500	3.77127700
H	2.42938000	-3.00419400	4.66280500
H	4.61540200	-2.82396000	3.46417600
P	2.81853100	-0.05410200	-0.26864800
C	3.38837800	1.63767700	0.23601000
C	3.99643000	1.92685000	1.46330000
C	3.15748600	2.68449900	-0.66369100
C	4.35262900	3.23423000	1.78686500
H	4.18012500	1.12735500	2.17664000
C	3.51326500	3.99359100	-0.34264200
H	2.68772800	2.47758900	-1.62210700
C	4.10644900	4.27096400	0.88722700
H	4.82113400	3.44378400	2.74397100
H	3.32577300	4.79434800	-1.05220100
H	4.37976400	5.29031300	1.14293000
C	4.38394600	-0.77716000	-0.95329900

C	4.26250400	-1.99890400	-1.62983800
C	5.64053300	-0.16652700	-0.88947600
C	5.37253000	-2.60718900	-2.20797500
H	3.28742200	-2.47580400	-1.70815900
C	6.75104800	-0.76980200	-1.47923600
H	5.75778200	0.78475600	-0.37842000
C	6.62107200	-1.99096200	-2.13564300
H	5.26078700	-3.55647700	-2.72307000
H	7.71994200	-0.28245300	-1.42264900
H	7.48687800	-2.45858300	-2.59437800
H	4.75220500	-1.51136300	1.38999100
C	-1.86589000	-2.46340400	1.76851900
O	-2.31335100	-2.92299400	2.72011000
H	-0.49619100	-0.38006400	2.49718600
H	-0.12926000	-0.90740800	-1.10198000

IM5-1

Ru	-2.29037200	1.29010100	-0.94354700
Ru	-2.52173800	-0.70074500	1.11668500
Ru	-0.70968000	-1.22720200	-0.78108000
C	-3.62978100	0.45972500	-2.07851300
O	-4.39306300	0.02418500	-2.80931900
C	-1.91057700	2.59075300	-2.29030300
O	-1.74956300	3.38394900	-3.10148600
C	-3.88807700	-1.35767000	0.08108100
O	-4.79352800	-1.82206800	-0.46329900
C	-3.59591000	2.16077900	0.15235000
O	-4.37672700	2.76753500	0.73910500
C	-3.62345700	0.26290600	2.40515200
O	-4.38153300	0.72224800	3.13065100
C	-1.88939600	-2.09941300	-2.03868700
O	-2.58572400	-2.62530800	-2.77810100
C	0.71834500	-1.13130300	-2.06983000
O	1.41863400	-1.13359200	-2.97477900
C	-2.41934400	-2.33882000	2.07319600
O	-2.47203600	-3.35413100	2.60617200
C	-0.69479600	2.05900400	0.22522100
N	-0.35229900	3.33940400	0.50559300
N	0.21258400	1.30635900	0.88126000
C	0.74629400	3.38452800	1.34276800
H	1.17654700	4.31661800	1.67458200
C	1.09101100	2.10124400	1.59853500
H	1.87144000	1.69432800	2.22124800
C	-0.97924600	4.53976200	-0.02838400

H	-2.04684700	4.37191300	-0.16617600
H	-0.83687400	5.35061500	0.68669800
H	-0.52308700	4.81784700	-0.98141500
C	0.05805100	-0.15187500	1.01018100
C	1.24488600	-0.81599800	1.67807700
C	0.97664200	-1.59889400	2.81274600
C	1.95990200	-2.34624000	3.44724800
C	3.26559400	-2.31649100	2.96668800
C	3.55703100	-1.53286800	1.85627400
C	2.57539300	-0.77359000	1.20125000
H	-0.03814700	-1.62571700	3.20272800
H	1.70407100	-2.94497500	4.31601800
H	4.04878300	-2.89260400	3.44873800
P	3.02614700	0.21660100	-0.30900700
C	4.07797400	1.59342300	0.35731200
C	4.18751500	2.72377800	-0.46260300
C	4.74687500	1.58491800	1.58597100
C	4.96268000	3.81440100	-0.07414600
H	3.65671000	2.75064200	-1.41163300
C	5.50995000	2.68182900	1.98182400
H	4.66694700	0.72680600	2.24665800
C	5.62311200	3.79585500	1.15187900
H	5.04022200	4.68046500	-0.72425900
H	6.01954400	2.66390900	2.94056600
H	6.22032600	4.64789300	1.46186700
C	4.31208600	-0.90200300	-1.04541400
C	3.95628100	-2.23174300	-1.31677800
C	5.57642600	-0.45300500	-1.43639900
C	4.84576100	-3.09088000	-1.95217400
H	2.97971800	-2.60358500	-1.01062200
C	6.46662500	-1.31446700	-2.07822700
H	5.87600700	0.57227300	-1.23798900
C	6.10609800	-2.63329100	-2.33672700
H	4.55614000	-4.11928300	-2.14675600
H	7.44689400	-0.95091400	-2.37177400
H	6.80145300	-3.30326400	-2.83287900
H	4.57442600	-1.51683600	1.47471800
C	-0.18622400	-2.86907900	0.00991700
O	0.15592100	-3.87041800	0.44646400
H	-0.70838500	-0.20838300	1.84110200
H	-1.00670100	0.35724600	-1.69503300

TS6-1

Ru	-3.23509500	0.59332900	-0.41287600
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Ru	-1.88463400	-1.70584200	0.76986100
Ru	-0.21957900	-0.24947200	-1.16326000
C	-4.09911500	-0.75378100	-1.49691900
O	-4.63191300	-1.52117300	-2.15879500
C	-4.13857300	1.98150300	-1.40924500
O	-4.91996900	2.67528300	-1.89006100
C	-1.99345800	-2.68951500	-0.82651700
O	-2.19154200	-3.50215100	-1.62790200
C	-4.25754600	0.15004500	1.07068100
O	-5.03796900	0.07196700	1.92370600
C	-3.00319000	-2.24407800	2.24764800
O	-3.69978800	-2.77275300	2.99277000
C	-0.61898700	-0.98027300	-2.92865000
O	-0.91744400	-1.30926800	-3.98167200
C	0.61585600	1.23577900	-1.83122300
O	1.03484300	2.22480100	-2.24141500
C	-0.54467400	-2.85340900	1.33087400
O	0.31701800	-3.53786700	1.66923000
C	-2.08193600	2.03681900	0.70546300
N	-2.34485000	3.31478400	1.06949800
N	-0.77057200	1.86499800	0.99438700
C	-1.21017700	3.94044600	1.54498700
H	-1.21762300	4.96695100	1.87676400
C	-0.21235000	3.02157100	1.49826000
H	0.82447500	3.08696300	1.78912400
C	-3.63617300	3.97588300	0.95978700
H	-4.42933500	3.23482100	1.06058400
H	-3.72646400	4.70582300	1.76515400
H	-3.72694500	4.48819400	-0.00107600
C	-0.11949600	0.54378000	0.84991000
C	1.07048400	0.43012200	1.80696500
C	0.72987200	0.43151400	3.17555300
C	1.67439600	0.28461500	4.17842600
C	3.01723000	0.12196300	3.83678200
C	3.37638300	0.11064300	2.49883000
C	2.42593600	0.26765000	1.47053800
H	-0.31890600	0.54561700	3.44444500
H	1.36580100	0.28423800	5.21930100
H	3.77317400	-0.00557100	4.60504100
P	3.02057800	0.20606200	-0.28277100
C	4.04218800	1.74228500	-0.44618900
C	4.42318100	2.09187000	-1.74993500
C	4.40621400	2.58625600	0.60903600
C	5.18643900	3.23138000	-1.98880900

H	4.11702300	1.46660500	-2.58613300
C	5.15604700	3.73561100	0.36695500
H	4.10509400	2.35627000	1.62598100
C	5.55496200	4.05653600	-0.92826200
H	5.47971300	3.48125900	-3.00372200
H	5.43032000	4.37992600	1.19679500
H	6.14054300	4.95187300	-1.11300300
C	4.28798600	-1.14307000	-0.17712600
C	3.96395000	-2.33267600	0.49287700
C	5.49888600	-1.07606900	-0.87536700
C	4.82864000	-3.42345400	0.46508000
H	3.03745100	-2.40292500	1.05795700
C	6.36432100	-2.16776800	-0.89847400
H	5.77692300	-0.16714200	-1.40112300
C	6.03237500	-3.34500200	-0.23189300
H	4.56106500	-4.33281500	0.99454700
H	7.30366700	-2.09424200	-1.43823000
H	6.70790000	-4.19436500	-0.25233300
H	4.41979000	-0.03445800	2.23170400
C	1.30629100	-2.61809200	-1.11973600
O	1.54051600	-3.56998800	-1.68407800
H	-0.86023100	-0.07533600	1.40737800
H	-1.43940000	0.68232900	-1.44093400

TS6-2

Ru	-2.40876800	1.03559600	-1.11412600
Ru	-2.32565200	-0.77309800	1.17609200
Ru	-0.55081400	-1.34425000	-0.90272000
C	-3.73642000	0.05379100	-2.17102300
O	-4.50345900	-0.45760900	-2.84633300
C	-2.17523800	2.29299100	-2.53055700
O	-2.08520500	3.09424700	-3.34606400
C	-3.53041900	-1.80287600	-0.00832500
O	-4.32792100	-2.43083400	-0.54236300
C	-3.70436900	1.83301000	0.02595600
O	-4.47908600	2.45226700	0.61404100
C	-3.71612000	-0.04346500	2.25187000
O	-4.50814500	0.38265400	2.96077400
C	-1.67909200	-2.38195100	-2.16266200
O	-2.30454800	-2.96277500	-2.92062600
C	0.82063500	-1.18897100	-2.19144900
O	1.56625900	-1.12768100	-3.05907000
C	-2.05171700	-2.28348500	2.25875100
O	-1.98082600	-3.23925800	2.88942500

C	-0.91122100	1.96912400	-0.01342300
N	-0.66490700	3.26099200	0.28279200
N	-0.00904100	1.25743800	0.69615100
C	0.36842900	3.36431400	1.19944500
H	0.72456600	4.31774900	1.55707200
C	0.76973600	2.10334300	1.47724200
H	1.53061200	1.74518500	2.15044100
C	-1.33715900	4.41669100	-0.29286300
H	-2.37736200	4.17064800	-0.50482400
H	-1.30496800	5.23294000	0.42945300
H	-0.83687600	4.72807400	-1.21291000
C	-0.08176900	-0.19387500	0.77344500
C	1.05787300	-0.69185400	1.65195600
C	0.81779400	-1.28090900	2.89880300
C	1.82866600	-1.88667800	3.64102400
C	3.12891700	-1.90464100	3.15547800
C	3.40504600	-1.26126600	1.95230400
C	2.40640800	-0.62680700	1.20384700
H	-0.18288300	-1.25575000	3.30879300
H	1.58887000	-2.34642600	4.59505900
H	3.92508800	-2.39238800	3.70866300
P	2.88123800	0.31947200	-0.33523500
C	3.77299000	1.80447400	0.33872500
C	4.43619000	1.87343000	1.56884700
C	3.75418200	2.94071500	-0.48051300
C	5.06161500	3.05211700	1.96931900
H	4.45643800	1.01159100	2.22862600
C	4.39174300	4.11578600	-0.08728500
H	3.22753800	2.90565800	-1.43159300
C	5.04331000	4.17407300	1.14213000
H	5.56631100	3.09370600	2.92991400
H	4.37030600	4.98613800	-0.73593000
H	5.53275200	5.09057200	1.45735900
C	4.29794800	-0.70753200	-0.94966700
C	4.09453500	-2.07801600	-1.16786700
C	5.51644200	-0.14124600	-1.33680700
C	5.08697500	-2.86178100	-1.74687400
H	3.15593700	-2.54175600	-0.86820200
C	6.50890400	-0.92662700	-1.92254900
H	5.69808000	0.91857300	-1.18174600
C	6.29891800	-2.28679900	-2.12871700
H	4.91331900	-3.92256100	-1.90097000
H	7.45015800	-0.47023800	-2.21438200
H	7.07317200	-2.89691100	-2.58348700

H	4.42685100	-1.25023200	1.58265800
C	0.16906300	-2.90310900	-0.04346900
O	0.60803400	-3.84375300	0.43422900
H	-1.38702400	0.11635000	2.15562700
H	-1.01443300	0.13113300	-1.82586500