

Supporting Information

Mechanistic Insight into Water-Modulated Cycloisomerization of Enynyl Esters Using Au(I) Catalyst

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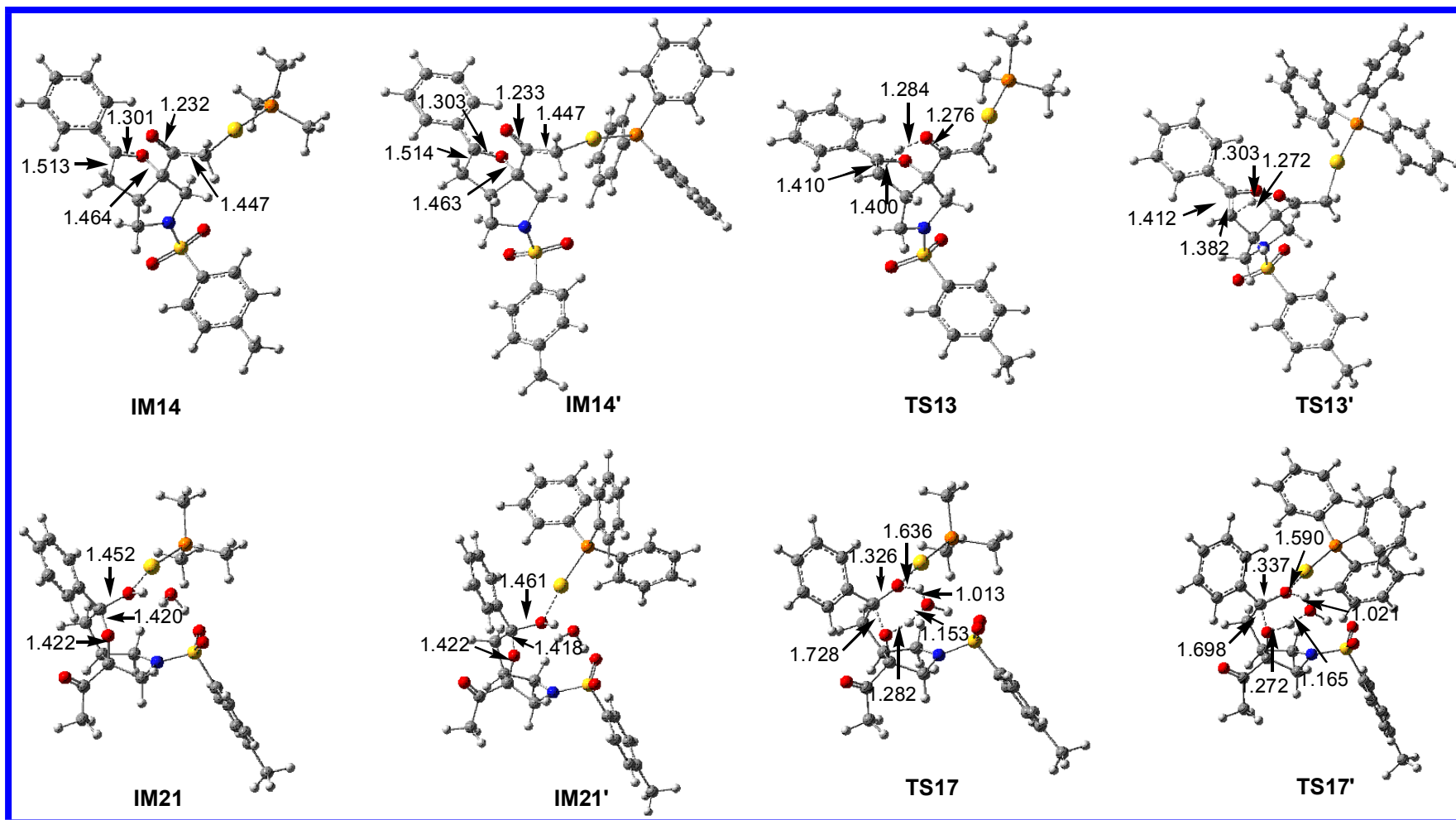


Fig. S1 Optimized geometries with selected structural parameters for several real structures using $\text{Me}_3\text{PAuSbF}_6$ catalyst, including **IM14** and **TS13** in Figure 2, and **IM21** and **TS17** in Figure 3, together with the corresponding model structures using real $\text{Ph}_3\text{PAuSbF}_6$ catalyst, involving **IM14'**, **TS13'**, **IM21'** and **TS17'**. The SbF_6^- anion has been omitted for clarity. The bond distances are given in Å.

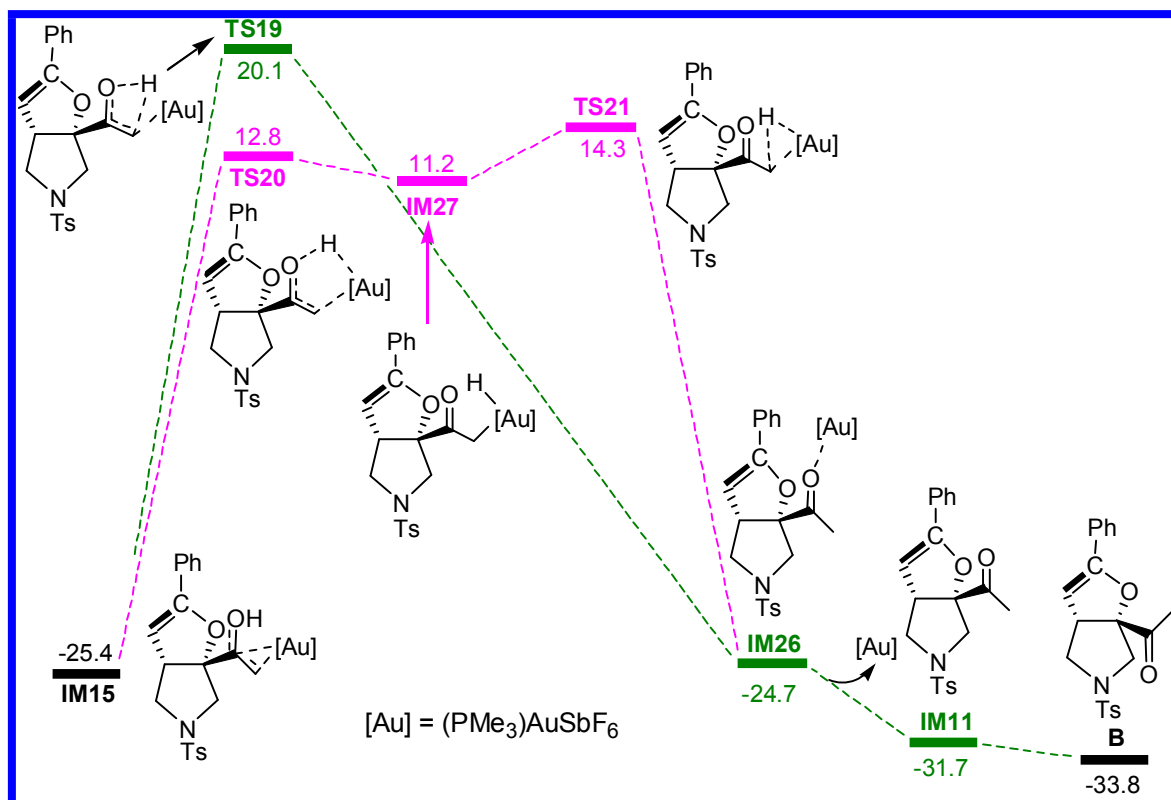


Fig. S2 Calculated free energy profiles in dry DCM solvent for the formation of the hydrogenation product **B** from **IM15** along other possible pathways proposed in this work. The relative free energies are given in kcal/mol.

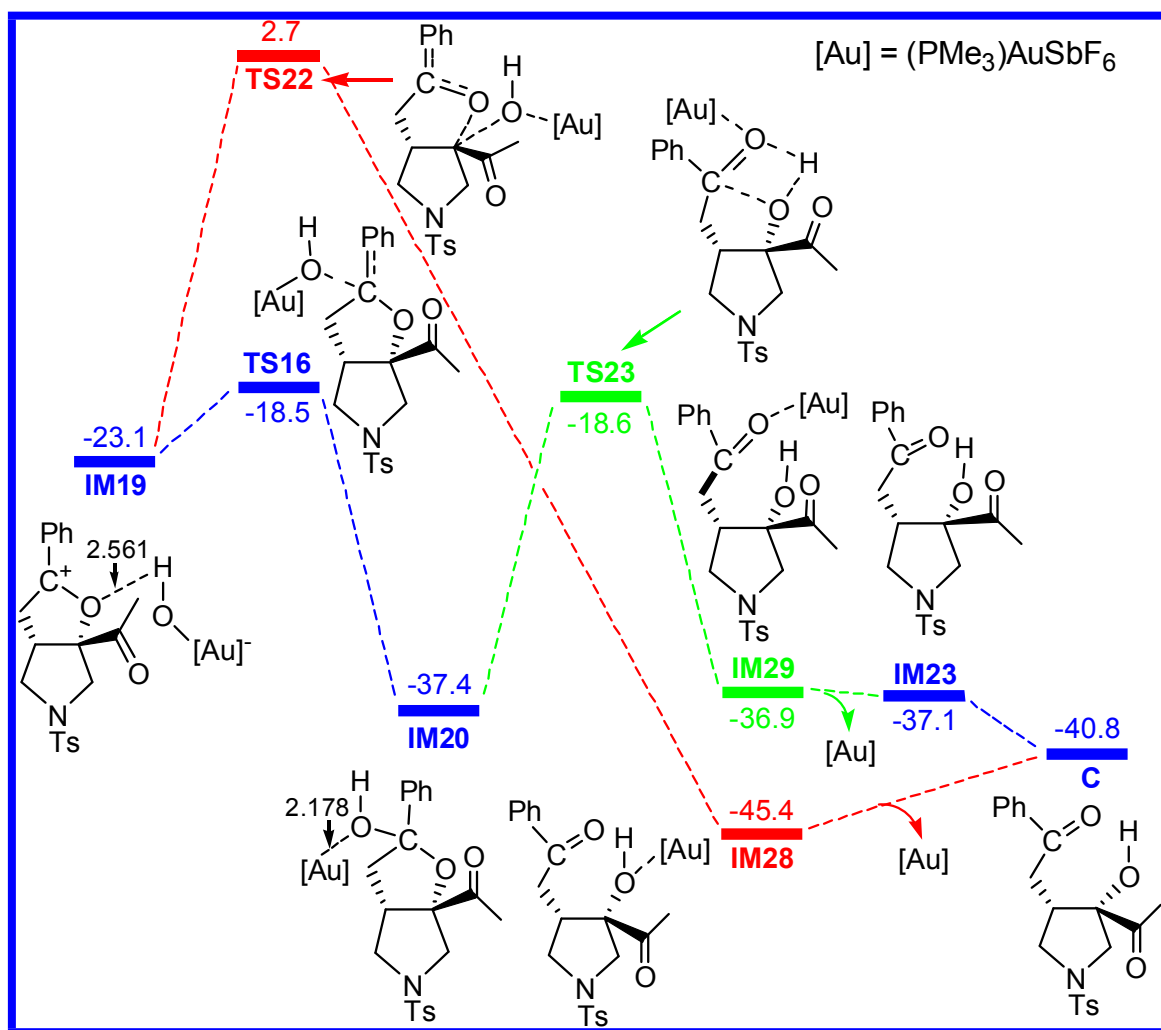


Fig. S3 Calculated free energy profiles in wet DCM solvent for the formation of the hydrolysis product **C** from **IM19** along other possible pathways proposed in this work. The relative free energies are given in kcal/mol.

Cartesian Coordinates for the Stationary Points Given in Fig. 1.

A				C	-3.04671300	1.20021400	0.97309800
SCF done: -1178.357795				C	-3.07869500	1.03628600	-1.45502900
C	-0.44071400	-1.28237300	1.73574800	C	-2.77326100	2.56578600	0.86749800
C	2.75945000	0.72170600	0.53037000	H	-3.17160200	0.73317500	1.94244100
C	0.32273400	-0.39720500	2.04342900	C	-2.80273500	2.40199900	-1.54284700
C	1.24719200	0.68410800	2.36256400	H	-3.23548800	0.44327200	-2.34825300
O	2.57849000	0.44308200	1.84625700	C	-2.63671800	3.18615400	-0.38703700
O	1.89062700	1.19017900	-0.17909800	H	-2.67523300	3.16100000	1.77055700
C	-1.38504300	-2.33072300	1.32423300	H	-2.72444400	2.86776700	-2.52065200
H	-2.18300200	-2.43756600	2.06510500	C	-2.30779200	4.65762400	-0.49385700
H	-0.86901700	-3.29801400	1.26717600	H	-1.22833400	4.80952300	-0.62855300
N	-2.02312600	-2.10150600	0.00853300	H	-2.80976100	5.11929500	-1.35085400
C	-1.28721700	-2.48119400	-1.22386900	H	-2.60571800	5.20173100	0.40803300
C	0.01119700	-1.73832500	-1.41697400	C	4.13773000	0.39779500	0.07168100
C	1.17328800	-2.34186500	-1.66870700	C	5.10010000	-0.17530000	0.92158800
H	-1.09993300	-3.56378300	-1.19259900	C	4.46771600	0.68034400	-1.26585000
H	-1.97097400	-2.30458500	-2.06010500	C	6.37810500	-0.46119700	0.43442000
H	-0.03527300	-0.65240100	-1.35241800	H	4.84275500	-0.39424600	1.95050500
H	1.25631000	-3.42628300	-1.72375500	C	5.74577300	0.39286600	-1.74815500
H	2.08488100	-1.77445100	-1.83230900	H	3.71311700	1.12449300	-1.90488600
S	-3.51185200	-1.32284600	-0.07349300	C	6.70269400	-0.17825100	-0.89855400
O	-4.12932300	-1.73605400	-1.36586600	H	7.11916200	-0.90443400	1.09156600
O	-4.16860100	-1.56027200	1.24444100	H	5.99709300	0.61270900	-2.78057900
C	-3.18361600	0.43718300	-0.19295900	H	7.69643900	-0.40192900	-1.27367000
				H	1.38795400	0.78300000	3.44211900

H	0.87218900	1.62855600	1.95665900
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(PMe₃)AuSbF₆

SCF done: -866.3320541

Au	1.07585800	-0.45033500	0.00038700
P	3.16760100	0.35188400	-0.00020300
Sb	-2.32213700	0.14918600	-0.00006700
F	-0.93076200	-1.31729800	0.00241700
F	-3.24221000	-0.79394500	-1.36847600
F	-3.24831900	-0.79372200	1.36426700
F	-3.50220600	1.63178000	-0.00323400
F	-1.14176700	0.93152700	-1.31695500
F	-1.14765700	0.93238300	1.32116200
C	3.44328000	1.59810700	-1.32575800
H	2.73529000	2.42297100	-1.20402300
H	4.46704900	1.98569600	-1.28102400
H	3.27011000	1.13993300	-2.30370000
C	4.47091000	-0.92495800	-0.24695800
H	5.46510600	-0.46483700	-0.23078600
H	4.40601200	-1.67557400	0.54606000
H	4.31820500	-1.42439700	-1.20806800
C	3.60538100	1.20409700	1.57108500
H	3.53904000	0.49871500	2.40436700
H	4.62204100	1.60879300	1.51700000
H	2.89819400	2.01844100	1.75324500

IM1

SCF done: -2044.717476

C	0.52488700	0.86110500	0.13661600
C	-1.86727600	3.35564000	-1.62751700
C	0.30478700	1.09625700	-1.05234700
C	-0.17643900	1.80454500	-2.26301600
O	-1.56167800	2.10289300	-2.09551300
O	-1.05707300	4.26119500	-1.60073000
Au	0.53033700	-1.21206500	-0.99878100
P	0.64646600	-3.51893000	-1.09447600
Sb	-2.87969900	-1.28935700	0.97183100
F	-2.30631200	-0.94024400	-0.85354400
F	-2.23445300	0.46360000	1.44158500
F	-4.60932200	-0.60777000	0.52666500
F	-3.39341000	-1.64196000	2.76824900
F	-1.08109000	-1.95180600	1.35003000
F	-3.33674400	-3.07243000	0.41800900
C	0.74746500	0.70535200	1.59270200
H	0.58591600	-0.33340700	1.88416300
H	-0.03122300	1.28775500	2.09765600
N	2.06214700	1.17495400	2.05353000
C	2.18220100	2.57737800	2.54160200
C	1.92626300	3.57687800	1.44309700
C	0.87393600	4.39624700	1.41360800
H	1.46978000	2.72024000	3.36438500
H	3.18526900	2.68738900	2.96508800

H	2.64669000	3.57856900	0.62532300
H	0.13663400	4.40325300	2.21465800
H	0.69785700	5.07853800	0.58778400
S	3.38149900	0.13372900	2.09212700
O	4.08852300	0.33239000	3.38738400
O	2.84296300	-1.19536800	1.67138200
C	4.50462900	0.70699100	0.81209300
C	4.27483500	0.36685000	-0.52874600
C	5.61967900	1.47353900	1.17128300
C	5.15311300	0.82696600	-1.51037800
H	3.43156800	-0.25968900	-0.79701300
C	6.48847600	1.92840500	0.17495900
H	5.80987400	1.68875500	2.21595600
C	6.26747000	1.62168700	-1.17818700
H	4.97858000	0.55961200	-2.54864600
H	7.35406400	2.52112200	0.45427600
C	7.19432500	2.13798500	-2.25455100
H	6.76980000	3.02207900	-2.74898500
H	8.16515800	2.42798800	-1.84156300
H	7.36647700	1.38459900	-3.03092200
C	-3.27484900	3.43609300	-1.18175900
C	-4.01163900	2.27892000	-0.86970400
C	-3.85120200	4.70828600	-1.00893700
C	-5.31784600	2.39825700	-0.38797300
H	-3.56036500	1.30216400	-0.97389100
C	-5.16307000	4.81936300	-0.54829100

H	-3.26131100	5.58906700	-1.23726800
C	-5.89588400	3.66430800	-0.23610300
H	-5.86010500	1.50029300	-0.11666000
H	-5.61264200	5.79927100	-0.42384300
H	-6.91216000	3.75381000	0.13529000
C	1.89608800	-4.22756000	-2.25099300
H	2.89126200	-3.86283000	-1.97932400
H	1.88708600	-5.32198100	-2.19970900
H	1.67603700	-3.91412700	-3.27587300
C	-0.95709100	-4.29830200	-1.54276800
H	-0.87712700	-5.38984300	-1.48859200
H	-1.73452800	-3.95227800	-0.85433200
H	-1.24036500	-4.00526200	-2.55814600
C	1.08000200	-4.16236000	0.57203800
H	0.29731000	-3.84523500	1.26601100
H	1.15374300	-5.25521900	0.55760200
H	2.02552000	-3.72261600	0.90234700
H	-0.08789600	1.18705300	-3.15702600
H	0.39403000	2.73048600	-2.38949500

TS1

SCF done: -2044.693569

C	0.13506500	1.27155700	-0.14336900
C	-2.10540000	2.61728100	-1.06792100
C	-0.04032000	0.62728000	-1.22254800
C	-0.84993600	1.05125900	-2.40919800

O	-2.07630800	1.73305100	-2.06296900	C	4.34382100	1.05581700	0.76820000
O	-1.09936500	2.94888400	-0.42492500	C	4.15760400	0.41770800	-0.46696600
Au	0.66769500	-1.34870200	-0.89048900	C	5.52848900	1.74745400	1.04299400
P	1.09312400	-3.55608600	-0.31060900	C	5.15898700	0.49918900	-1.43405100
Sb	-2.91416800	-1.49325100	0.71735800	H	3.24833400	-0.14039200	-0.66545000
F	-2.17757500	-1.60863900	-1.07774200	C	6.52222200	1.82026200	0.06115900
F	-3.06777700	0.40997500	0.46580300	H	5.67032900	2.20462900	2.01483100
F	-4.64593000	-1.81586500	-0.00689600	C	6.35474400	1.20395900	-1.18936900
F	-3.61705500	-1.38820600	2.48368000	H	5.01515500	0.00449400	-2.39043900
F	-1.12957200	-1.16956300	1.43034600	H	7.44198400	2.35616100	0.27418000
F	-2.53199000	-3.37636900	0.90173600	C	7.42729200	1.28694600	-2.25122500
C	0.49276400	1.45267000	1.27173800	H	7.07058700	1.83285100	-3.13390000
H	0.37923500	0.47209300	1.74726700	H	8.31893300	1.80016200	-1.87967600
H	-0.24802700	2.11382200	1.73358700	H	7.72996300	0.28892800	-2.59047400
N	1.84100700	1.98125600	1.54210900	C	-3.43937900	3.20360900	-0.83163600
C	2.05472800	3.45115900	1.60985900	C	-4.59281900	2.67115000	-1.43504300
C	2.27907000	4.09197700	0.26351100	C	-3.54408900	4.30976300	0.03040200
C	1.52885000	5.07799900	-0.22746000	C	-5.83741000	3.24850200	-1.17919700
H	1.18256300	3.89759100	2.10395600	H	-4.51091300	1.80218800	-2.07510200
H	2.91254300	3.62098200	2.27042100	C	-4.79016700	4.88690400	0.27619000
H	3.12659000	3.71217400	-0.30605400	H	-2.64821100	4.70200100	0.49727400
H	0.67035600	5.46685000	0.31565300	C	-5.93776600	4.35681400	-0.32819600
H	1.74028400	5.53242600	-1.19144900	H	-6.72859100	2.82916800	-1.63334300
S	3.07843700	0.94627400	2.03817700	H	-4.86973800	5.74139100	0.93982400
O	3.68606300	1.50413500	3.28010300	H	-6.90797100	4.80153800	-0.13099500
O	2.49458900	-0.42748200	1.99912000	C	2.73668100	-4.27392200	-0.74834400

H	3.52812500	-3.67437300	-0.28829800
H	2.81320300	-5.30695100	-0.39130100
H	2.87125200	-4.25698200	-1.83427900
C	-0.16709500	-4.70309500	-1.00789700
H	0.00147200	-5.72728800	-0.65693000
H	-1.14822600	-4.35752700	-0.66780800
H	-0.13793600	-4.68086500	-2.10112300
C	0.93089100	-3.73505900	1.51325100
H	-0.09366400	-3.46209700	1.77983500
H	1.13701100	-4.76481800	1.82543100
H	1.61538900	-3.04291900	2.01194100
H	-1.18306900	0.19635100	-2.99288100
H	-0.25292100	1.71999400	-3.04008400

IM2

SCF done: -2044.715803

C	-0.18243500	1.29172300	0.12060800
C	-1.96571000	2.58652800	-0.80579500
C	-0.12684700	0.49853300	-0.94307400
C	-0.99840000	0.77392400	-2.11154900
O	-1.89833400	1.97564400	-1.93243400
O	-1.13487700	2.39855400	0.15877400
Au	0.68912500	-1.39924700	-0.78784400
P	1.17530600	-3.60848900	-0.19788400
Sb	-3.14010200	-1.64512200	0.46809800
F	-2.23777800	-1.90687200	-1.23360900

F	-3.09547300	0.25591600	0.08425800
F	-4.81560700	-1.81360800	-0.42512500
F	-4.01016900	-1.33457400	2.13392800
F	-1.42600400	-1.45383200	1.35919000
F	-3.00302800	-3.53858000	0.76263800
C	0.47774200	1.17670000	1.46508100
H	0.55842700	0.11977800	1.71718300
H	-0.16699000	1.64406500	2.22147200
N	1.82950900	1.78087000	1.56461900
C	1.95278000	3.25670200	1.65369900
C	1.88700300	3.94560600	0.31347000
C	1.08922100	4.97780300	0.03659900
H	1.16604800	3.63646700	2.32050100
H	2.90787400	3.47752400	2.14441800
H	2.57403100	3.56517800	-0.44161300
H	0.39521200	5.37826100	0.77353200
H	1.10852500	5.47346200	-0.93019400
S	3.16177700	0.84674900	2.00586800
O	3.79987600	1.44509600	3.21635000
O	2.69695900	-0.57198900	2.01077500
C	4.33669300	1.06641800	0.66316300
C	4.02698800	0.61030000	-0.62654400
C	5.57818400	1.65023600	0.93589500
C	4.96841400	0.75718300	-1.64503400
H	3.06650500	0.14699200	-0.82893400
C	6.51055600	1.79034900	-0.09773700

H	5.80494300	1.97970300	1.94269500
C	6.22270200	1.35153600	-1.40002300
H	4.73017000	0.40145700	-2.64344100
H	7.47483000	2.24254900	0.11322300
C	7.22479500	1.51907100	-2.51941000
H	6.90871200	2.30332000	-3.21998100
H	8.21077600	1.79700700	-2.13531500
H	7.33494500	0.59506800	-3.09862100
C	-2.99956400	3.60042800	-0.62938400
C	-3.93674100	3.83087100	-1.65651500
C	-3.07427400	4.33223500	0.57310100
C	-4.93339200	4.78946200	-1.48028800
H	-3.88306000	3.25303900	-2.57076900
C	-4.07419900	5.28875400	0.73912500
H	-2.36102800	4.13848700	1.36438200
C	-5.00284600	5.51867400	-0.28549800
H	-5.65907600	4.96341600	-2.26679900
H	-4.13684000	5.84840700	1.66563100
H	-5.78325600	6.26023600	-0.15017400
C	2.77096400	-4.38316000	-0.71876800
H	3.60351100	-3.77771300	-0.34717400
H	2.85799000	-5.39982800	-0.31942400
H	2.82631200	-4.41948800	-1.81126300
C	-0.13843000	-4.78312100	-0.74262000
H	0.05552600	-5.79111500	-0.35881600
H	-1.10332300	-4.42913300	-0.36557600

H	-0.18364100	-4.81241200	-1.83549300
C	1.16166100	-3.72473300	1.64133600
H	0.18478700	-3.37461700	1.98882800
H	1.33079500	-4.75325900	1.97872400
H	1.92714800	-3.05984500	2.05217600
H	-1.69189700	-0.04956900	-2.28660600
H	-0.44381400	1.01092400	-3.02213900

TS2

SCF done: -2044.690845

C	-0.32198200	1.41088700	0.07698200
C	-2.05045500	2.75364000	-0.99214100
C	-0.15848900	0.58911400	-0.95122300
C	-0.72218300	0.48854000	-2.20274100
O	-1.92466400	2.29484700	-2.12638700
O	-1.24784300	2.46441700	0.05267600
Au	0.66617100	-1.36068300	-0.83283100
P	1.26697700	-3.53835400	-0.21371000
Sb	-3.00404900	-1.85707800	0.46348800
F	-2.12115300	-2.03051600	-1.26609200
F	-3.19233700	0.01786200	0.06508900
F	-4.66208700	-2.28846500	-0.36612600
F	-3.84191100	-1.66925600	2.16233400
F	-1.29052000	-1.44075200	1.29375000
F	-2.56709000	-3.70917900	0.76980400
C	0.31411100	1.29552100	1.44035400

H	0.32048400	0.24397300	1.72856000
H	-0.30936300	1.83307200	2.16525500
N	1.69805400	1.82244000	1.53362800
C	1.89279600	3.28560800	1.71966500
C	1.78071700	4.06412400	0.43407800
C	0.95360100	5.09378200	0.25273900
H	1.16031700	3.64792600	2.45397700
H	2.88217700	3.43278400	2.16804800
H	2.45018600	3.74899500	-0.36554100
H	0.27140600	5.42364300	1.03377300
H	0.92798200	5.65030100	-0.67998500
S	2.97428300	0.80284000	1.94460100
O	3.57753200	1.22814000	3.24221900
O	2.46357700	-0.59305100	1.77444200
C	4.21460100	1.12431000	0.68433700
C	3.93620000	0.86598100	-0.66613600
C	5.47652200	1.58035100	1.07856200
C	4.93080400	1.07864700	-1.62011600
H	2.95760900	0.50460900	-0.96373300
C	6.46261600	1.78983300	0.10846200
H	5.67601600	1.76151700	2.12782800
C	6.20839000	1.54591100	-1.25053800
H	4.71709100	0.87745200	-2.66596900
H	7.44221900	2.14427800	0.41385300
C	7.26991700	1.78554900	-2.29957800
H	7.01593500	2.64758000	-2.93015900

H	8.24467600	1.98369300	-1.84445200
H	7.37634100	0.92038700	-2.96433600
C	-3.09455700	3.74273900	-0.64659400
C	-3.95663500	4.18166700	-1.66860600
C	-3.25153700	4.23748900	0.66128700
C	-4.96057500	5.10802500	-1.38598600
H	-3.83045100	3.78453800	-2.66872600
C	-4.25896300	5.16348300	0.93804500
H	-2.59800200	3.88759600	1.45003900
C	-5.11269400	5.60055900	-0.08303600
H	-5.62596800	5.44169700	-2.17500500
H	-4.38386300	5.53801100	1.94841800
H	-5.89688000	6.31781500	0.13709900
C	2.99334800	-4.08646200	-0.56440100
H	3.68963400	-3.39183500	-0.08478300
H	3.16715200	-5.09725800	-0.17900000
H	3.17466700	-4.07558600	-1.64353400
C	0.15454600	-4.81612100	-0.93828600
H	0.42709900	-5.81449500	-0.57787200
H	-0.86932700	-4.58414600	-0.62764600
H	0.20870900	-4.79400300	-2.03043500
C	1.04107300	-3.70370600	1.60370500
H	-0.00868700	-3.49348600	1.82645500
H	1.30126800	-4.71316900	1.94027600
H	1.66132500	-2.96042600	2.11194900
H	-1.56930100	-0.18010600	-2.34854900

H	-0.20098800	0.84352300	-3.08886900
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IM3

SCF done: -2044.712786

C	-0.38341300	1.16316200	0.08271800
C	-0.06752700	3.07209900	-1.34885900
C	-0.80031100	0.30107900	-0.82119900
C	-1.33498700	-0.24912300	-1.92439800
O	0.52321800	2.43493900	-2.19484300
O	-0.52345900	2.53140800	-0.17153500
Au	-0.58524000	-1.97516400	-0.57664100
P	0.11410400	-4.06098200	0.22166600
Sb	-3.62388300	-1.99117600	1.73109800
F	-3.46838300	-1.16001500	-0.01326600
F	-4.15444200	-0.32489000	2.49053100
F	-5.41696800	-2.50765000	1.35988800
F	-3.61673500	-2.87095500	3.42452500
F	-1.75602400	-1.50396300	2.03260600
F	-2.94980000	-3.62556400	0.92414200
C	0.12970500	0.87609300	1.46934600
H	-0.09543700	-0.15404500	1.74191000
H	-0.42230800	1.51834200	2.16450100
N	1.57225300	1.19476200	1.66290600
C	1.93576900	2.28076700	2.62374500
C	1.49743900	3.63896400	2.15195500
C	0.75484500	4.47258300	2.88142500

H	1.51244700	2.06026700	3.61329400
H	3.02532500	2.25894400	2.73516400
H	1.85021200	3.93504900	1.16529000
H	0.38816600	4.19790900	3.86851300
H	0.49342200	5.46385400	2.52244400
S	2.72161300	-0.02312700	1.44286700
O	3.46964800	-0.26459700	2.71224700
O	1.99543400	-1.15814400	0.78612800
C	3.88706300	0.67810900	0.27639400
C	3.44838800	1.12297000	-0.97970400
C	5.24159300	0.72210800	0.62337600
C	4.38467400	1.62140600	-1.88479800
H	2.39825100	1.09740600	-1.24743500
C	6.16557700	1.22408900	-0.29863500
H	5.55798900	0.36762100	1.59696800
C	5.75525800	1.68080800	-1.56150900
H	4.04556000	1.97197300	-2.85487500
H	7.21738200	1.26008900	-0.03227800
C	6.75293800	2.23603100	-2.55194400
H	6.60619800	3.31383100	-2.69966300
H	7.78148500	2.08449900	-2.21165400
H	6.64757000	1.75924400	-3.53352800
C	-0.38093000	4.51905700	-1.43881300
C	0.07326800	5.21530600	-2.57405900
C	-1.11564000	5.19765800	-0.44883000
C	-0.20055900	6.57596100	-2.71633300

H	0.63200200	4.67477000	-3.32921600
C	-1.38849700	6.55975900	-0.59828300
H	-1.46542400	4.66035200	0.42346000
C	-0.93209500	7.24964600	-1.72880000
H	0.15041700	7.11021600	-3.59288000
H	-1.95955800	7.08127800	0.16254400
H	-1.14791400	8.30734100	-1.84131100
C	1.87005300	-4.40818800	-0.21381600
H	2.47778200	-3.56894500	0.13602100
H	2.21248400	-5.33823800	0.25322200
H	1.97453700	-4.48909000	-1.30019900
C	-0.86116000	-5.50490500	-0.36996300
H	-0.47786600	-6.43164800	0.07117000
H	-1.89996600	-5.34935100	-0.06969900
H	-0.80665400	-5.57292300	-1.46055800
C	0.04217000	-4.11703900	2.05699400
H	-0.98928100	-3.94959900	2.36863300
H	0.39673600	-5.08664000	2.42328000
H	0.66828000	-3.31680000	2.45970900
H	-2.40554200	-0.44472100	-1.96090800
H	-0.73941200	-0.38007900	-2.82640400

TS3

SCF done: -2044.700644

C	-0.37774100	1.40704700	0.11735200
C	-2.00822300	2.71124100	-0.75466100

C	-0.23598200	0.91552700	-1.10422400
C	0.22987200	0.10603100	-2.11021900
O	-1.65677300	2.19276100	-1.81458300
O	-1.30668900	2.40785900	0.35112600
Au	0.83768200	-1.68261600	-0.95495900
P	1.31134300	-3.61652400	0.23505400
Sb	-3.01370000	-1.72328300	0.29910400
F	-2.05340500	-1.69422700	-1.38537200
F	-3.26744600	0.17876500	0.11838900
F	-4.62758800	-2.12278300	-0.62662200
F	-3.90754400	-1.73495800	1.98230000
F	-1.34464800	-1.32867500	1.22232300
F	-2.53526200	-3.58407500	0.47211300
C	0.32742900	0.97209300	1.38219500
H	0.56692700	-0.08546200	1.32376400
H	-0.38512700	1.09093700	2.20753200
N	1.56207600	1.72339700	1.68692800
C	1.46403500	3.15340500	2.08998200
C	1.54066000	4.11977900	0.93349500
C	0.66256400	5.09822700	0.71225800
H	0.52256900	3.28397900	2.63799900
H	2.27355000	3.34595300	2.80262400
H	2.40282900	4.00262800	0.27792800
H	-0.20921000	5.23997000	1.34786600
H	0.78344900	5.79971100	-0.10856200
S	3.01765700	0.90746000	1.95444100

O	3.63477600	1.47280600	3.18885200
O	2.71371600	-0.55102700	1.83209300
C	4.10268700	1.35210600	0.59551900
C	3.99018000	0.69112300	-0.63589100
C	5.07601300	2.33831700	0.79117100
C	4.84358700	1.04579700	-1.68036600
H	3.25553100	-0.09604500	-0.76817600
C	5.92170700	2.68347100	-0.26803900
H	5.17848700	2.80955400	1.76133600
C	5.81868300	2.04978800	-1.51731300
H	4.75925900	0.53110900	-2.63326700
H	6.67797400	3.44752400	-0.11721600
C	6.73440800	2.42249400	-2.66057900
H	6.16463800	2.79745700	-3.51993500
H	7.44602600	3.19936300	-2.36642600
H	7.30884700	1.55527500	-3.00869600
C	-3.11426800	3.65698600	-0.58114300
C	-3.80670000	4.09292700	-1.72605300
C	-3.49632300	4.11550700	0.69342300
C	-4.86729100	4.98909300	-1.59562100
H	-3.50853800	3.71913600	-2.69863700
C	-4.55942100	5.01115300	0.81510700
H	-2.97646400	3.75755300	1.57358900
C	-5.24335600	5.44960000	-0.32659400
H	-5.40330200	5.32391700	-2.47695900
H	-4.86096400	5.35975800	1.79680700

H	-6.07188700	6.14326900	-0.22684800
C	3.08199000	-4.13147700	0.21922400
H	3.68173600	-3.32300500	0.64844500
H	3.22728700	-5.04355600	0.80867200
H	3.41169300	-4.30883800	-0.80894000
C	0.33529200	-5.06653700	-0.34557400
H	0.57388400	-5.95609400	0.24828700
H	-0.72580300	-4.82173100	-0.22813500
H	0.54126500	-5.26685600	-1.40111700
C	0.86929800	-3.43638100	2.00947500
H	-0.18825900	-3.16816900	2.06529400
H	1.05343500	-4.37159700	2.54957400
H	1.46330700	-2.62721800	2.44326000
H	-0.55264700	-0.44615000	-2.63726700
H	1.03236100	0.49694200	-2.73631900

IM4

SCF done: -2044.713483

C	-1.08466200	0.95009000	0.18373900
C	1.84536900	2.16839900	-1.93386000
C	-0.85380900	1.34677300	-0.95908800
C	-0.51298100	2.23304100	-2.09846500
O	1.82390900	1.04920500	-2.40845000
O	0.70910800	2.92726200	-1.81852400
Au	-0.13225700	-0.85079600	-1.05389300
P	0.82416300	-2.77473800	-1.93843400

Sb	2. 65492500	-0. 82059500	1. 68821900	H	-3. 96484000	2. 85434200	-0. 00916000
F	0. 87602900	-1. 63271100	1. 61584200	C	-6. 69041700	0. 12090900	-0. 42047900
F	1. 77790800	0. 82980700	1. 19902500	H	-6. 09197200	-0. 54192800	1. 54829000
F	2. 39154700	-0. 46194900	3. 53824300	C	-6. 49628200	1. 05441000	-1. 45544700
F	4. 37172400	0. 01007400	1. 67348400	H	-5. 34738200	2. 77254600	-2. 07530000
F	2. 85708500	-1. 19450700	-0. 21216400	H	-7. 46730200	-0. 63164300	-0. 51796500
F	3. 37352600	-2. 56289900	2. 01719300	C	-7. 36940700	1. 03017300	-2. 68924100
C	-1. 29515900	0. 79081800	1. 64410200	H	-8. 32619200	1. 53653100	-2. 50381000
H	-1. 21359900	1. 79282100	2. 07932000	H	-6. 88851200	1. 53783500	-3. 53112200
H	-0. 47663600	0. 18971300	2. 04369700	H	-7. 60044800	0. 00468000	-2. 99680800
N	-2. 56754300	0. 18761400	2. 06406400	C	3. 03909400	2. 84950800	-1. 39192700
C	-2. 60083900	-1. 25532700	2. 43113100	C	4. 07025000	2. 04106000	-0. 88126800
C	-2. 83418600	-2. 18094700	1. 26514500	C	3. 14502200	4. 25080400	-1. 33514100
C	-2. 00689100	-3. 17648100	0. 93980600	C	5. 19963700	2. 63370200	-0. 31446300
H	-1. 64672200	-1. 49370800	2. 91351500	H	3. 95250300	0. 96520600	-0. 88556900
H	-3. 38932700	-1. 37348200	3. 18081500	C	4. 29195100	4. 83582600	-0. 79517900
H	-3. 75333700	-2. 02362100	0. 70103500	H	2. 33882800	4. 86959300	-1. 71224400
H	-1. 07601900	-3. 33406300	1. 47868700	C	5. 31684700	4. 02884300	-0. 28170300
H	-2. 23626000	-3. 86119000	0. 12673200	H	5. 96828400	2. 00567400	0. 12099800
S	-3. 90483400	1. 17726700	2. 35012700	H	4. 38248100	5. 91665400	-0. 76183800
O	-4. 69950800	0. 52110000	3. 42586400	H	6. 19750000	4. 48807200	0. 15629400
O	-3. 37238600	2. 56483000	2. 46809700	C	-0. 31297400	-3. 72960800	-3. 03764600
C	-4. 91186000	1. 12814800	0. 86459000	H	-0. 63827500	-3. 09385800	-3. 86680600
C	-4. 71001100	2. 07902800	-0. 14247600	H	0. 18969800	-4. 61648400	-3. 43940800
C	-5. 91327000	0. 15621600	0. 73880900	H	-1. 19742400	-4. 04153200	-2. 47405800
C	-5. 49815600	2. 03194700	-1. 29542200	C	1. 41425800	-4. 00033400	-0. 69688400

H	1.89247300	-4.84285600	-1.20924200
H	2.13085000	-3.52449800	-0.02588500
H	0.57226500	-4.36845500	-0.10504500
C	2.28643900	-2.39289100	-2.98613300
H	3.02138300	-1.88471900	-2.35924800
H	2.71139600	-3.31392900	-3.40016900
H	1.99605200	-1.72000500	-3.79724800
H	-1.27543900	3.00980100	-2.19266900
H	-0.43544900	1.67369000	-3.03243900

TS4

SCF done: -2044.690717

C	0.96163900	0.51462800	-0.88422400
C	-1.31100200	2.91562000	0.54373100
C	0.70848100	1.70827700	-0.54990600
C	0.69252000	3.16989400	-0.53121600
O	-0.75128900	1.92238200	1.01259800
O	-0.63548100	3.67955000	-0.33930100
Au	0.24287100	-0.97838300	0.43073400
P	-0.47390100	-2.71622500	1.81385700
Sb	-3.47070700	-0.81577900	-0.92566200
F	-1.85872400	-1.74140700	-1.47541800
F	-2.55626500	0.85305900	-1.21760300
F	-4.13832800	-0.84166000	-2.70695600
F	-5.01408400	0.10539600	-0.27313400
F	-2.77934500	-0.81013500	0.90409900

F	-4.24415700	-2.52696400	-0.51774200
C	1.71225500	0.08012000	-2.15196000
H	1.52774200	0.81332600	-2.94140500
H	1.32245600	-0.88325600	-2.48259000
N	3.16316400	-0.10178500	-1.94172500
C	3.77440000	-1.42937900	-2.22929300
C	3.31448500	-2.48991900	-1.26661000
C	2.73619900	-3.63134300	-1.64396400
H	3.55109200	-1.72291400	-3.26394700
H	4.86071400	-1.30211400	-2.16628500
H	3.49343200	-2.28092400	-0.21268800
H	2.53988200	-3.85648700	-2.69030800
H	2.44415400	-4.39041000	-0.92363800
S	4.17085700	1.24504500	-1.87283300
O	5.22072900	1.15040900	-2.92736200
O	3.24680600	2.42016300	-1.82616500
C	5.01321400	1.08747000	-0.29619400
C	4.27721300	0.99122500	0.89445700
C	6.41171700	1.10885200	-0.27377900
C	4.95725700	0.91093000	2.10927900
H	3.19359500	0.96407900	0.87109500
C	7.07706200	1.02886200	0.95375800
H	6.96098700	1.18378400	-1.20449500
C	6.36557100	0.93180600	2.16048200
H	4.38983700	0.83058500	3.03189600
H	8.16237800	1.04165400	0.97236700

C	7.08596900	0.86648600	3.48757200
H	7.00041400	1.81773100	4.02919200
H	6.66457900	0.08832700	4.13408400
H	8.15145700	0.65691100	3.35510600
C	-2.67051800	3.36541300	0.85437700
C	-3.58601300	2.42708300	1.36406300
C	-3.06891000	4.69507400	0.61649800
C	-4.89805400	2.82106500	1.62869700
H	-3.27828200	1.39841500	1.49809400
C	-4.37623200	5.08399700	0.90745200
H	-2.36015300	5.40704000	0.20991200
C	-5.29096200	4.14710800	1.40965400
H	-5.61479100	2.08630700	1.97587800
H	-4.68698600	6.10865200	0.73302100
H	-6.31283600	4.44918000	1.61620300
C	0.90517900	-3.74011400	2.50271300
H	1.58353600	-3.10303200	3.07881600
H	0.51578300	-4.53206800	3.15260800
H	1.47114600	-4.19579700	1.68443600
C	-1.56997500	-3.93854300	0.98057400
H	-1.83963700	-4.73968200	1.67807400
H	-2.47439300	-3.44475700	0.61976000
H	-1.04961100	-4.36432000	0.11797800
C	-1.40682600	-2.16765400	3.30580000
H	-2.28853600	-1.62058800	2.96611000
H	-1.70798000	-3.03065400	3.91011100

H	-0.78353700	-1.49964000	3.90787800
H	1.04667500	3.52040500	-1.50406100
H	1.35281500	3.56595900	0.24799800

IM5

SCF done: -2044.7188413

C	0.92302200	0.46513400	-1.26859300
C	-1.32515600	2.98238600	-0.43333900
C	0.24952900	1.60927700	-1.22729300
C	0.27442500	2.89653400	-2.02226900
O	-0.77776200	1.83465200	-0.23458900
O	-0.81781300	3.67492700	-1.41778800
Au	0.45750500	-1.17545200	-0.10070700
P	-0.10597200	-3.12696400	1.10394200
Sb	-3.64903000	-0.81485800	-0.29223700
F	-2.30628800	-1.70167400	-1.35879600
F	-3.22885400	0.84204100	-1.18520700
F	-5.00004400	-1.23704300	-1.56287200
F	-4.90289600	0.10184200	0.83037700
F	-2.29484900	-0.38064200	1.04322000
F	-3.91215100	-2.47448800	0.65392900
C	1.97808400	0.34698200	-2.36067200
H	1.92655700	1.16906000	-3.08680500
H	1.80101300	-0.58244900	-2.91037300
N	3.37989300	0.23589900	-1.85961800
C	4.18634900	-0.95250900	-2.25184900

C	3.70765700	-2.21971600	-1.59749800
C	3.36966500	-3.31972900	-2.27212200
H	4.17673600	-1.05866500	-3.34593900
H	5.22396100	-0.74604400	-1.96844800
H	3.66429000	-2.20133800	-0.50942900
H	3.39696300	-3.35558900	-3.35956400
H	3.06029500	-4.23034700	-1.76655900
S	4.19797500	1.60524000	-1.33721100
O	5.50401900	1.70800900	-2.05415800
O	3.20776100	2.72283900	-1.41213800
C	4.59097200	1.29831200	0.38686700
C	3.56534000	1.06423200	1.31409300
C	5.92864500	1.34158300	0.79425400
C	3.89369000	0.86777700	2.65548700
H	2.53206800	1.01853600	0.98973700
C	6.23947700	1.14257600	2.14316900
H	6.70529700	1.52767500	0.06238600
C	5.23232000	0.90689100	3.09315500
H	3.10107900	0.68064700	3.37406500
H	7.27759000	1.17223200	2.45997400
C	5.56904900	0.72032800	4.55498600
H	5.38695500	1.64319700	5.12195400
H	4.95563200	-0.06480900	5.01063100
H	6.62112300	0.45283400	4.69306500
C	-2.40203200	3.50055800	0.36769200
C	-3.05726000	2.65859600	1.29104700

C	-2.82523900	4.83715900	0.18367600
C	-4.13768400	3.15646600	2.01703700
H	-2.74248400	1.63005400	1.40571500
C	-3.89366600	5.32353900	0.92979900
H	-2.31957200	5.47125800	-0.53510700
C	-4.55247700	4.48261400	1.84178600
H	-4.66810700	2.49768600	2.69364200
H	-4.22341300	6.34796700	0.79803900
H	-5.39707600	4.86233200	2.40753400
C	1.35026500	-4.09010500	1.72170700
H	1.93285600	-3.47129100	2.41159100
H	1.02910700	-5.00145200	2.23859300
H	1.99290300	-4.36309300	0.87894600
C	-1.06815800	-4.34384100	0.10463900
H	-1.26670900	-5.25256200	0.68381400
H	-2.01291500	-3.87478000	-0.17912900
H	-0.51680000	-4.60005700	-0.80467300
C	-1.15599200	-2.88937300	2.60276200
H	-2.13425500	-2.53050500	2.27736800
H	-1.27303800	-3.83540200	3.14346400
H	-0.70784800	-2.14155700	3.26287300
H	0.02473300	2.78121500	-3.07935700
H	1.20450000	3.45527800	-1.90212000

TS5

SCF done: -2044.684135

C	0.89504000	-0.24450100	-1.49455500	H	1.45547100	-5.15800500	-0.03715500
C	-0.21620500	2.95744100	-1.40251300	S	4.23610000	-0.11442700	-1.58264900
C	0.38922500	0.88731500	-2.08019000	O	5.58845200	-0.74058000	-1.59136500
C	0.80708300	1.55661500	-3.24239300	O	3.82313100	0.90244200	-2.59945500
O	-0.55855700	1.66062900	-1.37253400	C	4.01874100	0.64065100	0.02981500
O	0.69435700	3.33905800	-2.16342200	C	3.33012600	1.85322000	0.14647500
Au	0.28840000	-0.88030900	0.34828300	C	4.56407100	0.01569000	1.15888100
P	-0.38796700	-1.56664300	2.51488800	C	3.16607400	2.42667400	1.41001500
Sb	-3.57074900	-0.90517900	-0.55965700	H	2.94011100	2.34279000	-0.73731500
F	-2.22532600	-2.29239400	-0.42578900	C	4.38991000	0.60101200	2.41432000
F	-2.58579400	-0.16512600	-2.03434600	H	5.13301400	-0.90097900	1.05412800
F	-4.62699000	-1.98509300	-1.71713000	C	3.68836900	1.81253300	2.56154600
F	-4.82114500	0.53527900	-0.62378500	H	2.62953700	3.36632100	1.50111500
F	-2.49841300	0.18552800	0.66478700	H	4.81725800	0.12130500	3.28997400
F	-4.39966000	-1.64827500	1.00978500	C	3.53705600	2.45936600	3.91964900
C	1.81913600	-1.09229500	-2.34280600	H	4.35186900	3.17115400	4.10917100
H	1.98357100	-0.68228500	-3.34820000	H	2.59672200	3.01502000	3.99643100
H	1.32310800	-2.06191500	-2.47490400	H	3.56149900	1.71656700	4.72353200
N	3.12013400	-1.37336800	-1.70089100	C	-0.98140200	3.83539300	-0.51838900
C	3.55179500	-2.78958000	-1.53652800	C	-2.02605300	3.32048800	0.27702700
C	2.71837400	-3.52802000	-0.52516500	C	-0.67592700	5.21208000	-0.49874200
C	2.03352700	-4.64008200	-0.79692900	C	-2.75776600	4.19404700	1.08470400
H	3.50210400	-3.29466500	-2.51175800	H	-2.26126200	2.26218400	0.25792700
H	4.60478900	-2.76734300	-1.24257700	C	-1.40870300	6.06930900	0.31920900
H	2.70104800	-3.09894200	0.47599800	H	0.12335900	5.58936500	-1.12652600
H	2.02731400	-5.07903000	-1.79284600	C	-2.45127900	5.56059800	1.10889400

H	-3.57072200	3.80563800	1.68782800
H	-1.17845100	7.12903700	0.33796100
H	-3.02707000	6.23208600	1.73791700
C	0.98995600	-2.22212500	3.56451100
H	1.78914900	-1.47681900	3.62690300
H	0.63753500	-2.46373000	4.57360500
H	1.39888800	-3.12769800	3.10476600
C	-1.66970200	-2.89024600	2.57905400
H	-1.85578400	-3.18379000	3.61843300
H	-2.59621100	-2.53088900	2.12553200
H	-1.33066100	-3.75811200	2.00683000
C	-1.10471300	-0.19369300	3.51833800
H	-1.95250900	0.21448400	2.96256300
H	-1.43717800	-0.55390200	4.49810900
H	-0.35779800	0.59470300	3.65352700
H	0.10494500	2.07583500	-3.88332900
H	1.80841600	1.38117100	-3.62706400

IM6

SCF done: -2044.696425

C	-0.32138200	-0.69987100	-1.55311700
C	2.44658200	-2.93114200	-1.51367000
C	0.60545200	-1.54592200	-2.25747600
C	0.24917100	-2.20794700	-3.38599500
O	1.80985000	-1.70689400	-1.60669200
O	1.98856600	-3.95074200	-1.97714700

Au	-0.22192600	-0.57014100	0.46988800
P	0.11478100	-0.42222600	2.82048100
Sb	2.06857100	2.54253500	0.05340000
F	0.24266900	2.42446900	0.70787200
F	1.51702600	1.46353900	-1.46032000
F	1.61721700	4.14030900	-0.89035200
F	3.86184600	2.55981100	-0.58425400
F	2.43878500	0.88605500	1.01161500
F	2.51821000	3.49175400	1.65103100
C	-1.14473800	0.20938800	-2.37787800
H	-1.16683100	-0.06219200	-3.44399700
H	-0.54102500	1.13948000	-2.32491600
N	-2.47591000	0.54478700	-1.84698300
C	-2.95846700	1.96251500	-1.99669000
C	-1.88628400	2.92790200	-1.57813200
C	-1.36422400	3.85289300	-2.38794300
H	-3.28151800	2.15285200	-3.02869100
H	-3.83692800	2.06112500	-1.34770200
H	-1.50665900	2.82185800	-0.56503200
H	-1.70275400	3.97423500	-3.41586800
H	-0.56596400	4.50412300	-2.04548700
S	-3.65158200	-0.67237300	-2.01565000
O	-4.66075900	-0.24295300	-3.02821800
O	-2.86147000	-1.93134900	-2.19223400
C	-4.49173600	-0.73494000	-0.43782800
C	-3.98256900	-1.53827500	0.59037900

C	-5.68834700	-0.02585200	-0.27029300
C	-4.67145800	-1.60503900	1.80344300
H	-3.07638800	-2.11144400	0.43351200
C	-6.35706300	-0.09503800	0.95386200
H	-6.09489400	0.54893100	-1.09389700
C	-5.86271100	-0.88387300	2.00767900
H	-4.28887500	-2.23746900	2.59898100
H	-7.28099500	0.45916500	1.08771300
C	-6.61691400	-0.98608300	3.31358800
H	-7.40685200	-1.74666500	3.25219900
H	-5.95557500	-1.26843900	4.13873800
H	-7.09918800	-0.03777300	3.57262600
C	3.72802800	-2.80292400	-0.78609700
C	4.15699700	-1.58501500	-0.22445000
C	4.52944600	-3.95497300	-0.67140500
C	5.38503100	-1.52897200	0.44078400
H	3.53828400	-0.70028800	-0.29216700
C	5.75331900	-3.88888100	-0.00594400
H	4.18005600	-4.88292000	-1.10968600
C	6.18309800	-2.67472000	0.54887300
H	5.71461500	-0.58853600	0.86879700
H	6.37249200	-4.77583000	0.07891900
H	7.13773000	-2.62318100	1.06317900
C	-1.16104900	-1.28821500	3.84186300
H	-1.18992100	-2.34866200	3.57164300
H	-0.93607600	-1.19608100	4.91018100

H	-2.14402600	-0.85137600	3.64079700
C	0.16540400	1.28598700	3.50942800
H	0.30182400	1.24873300	4.59585900
H	0.98563100	1.84079300	3.05162600
H	-0.76457200	1.80805400	3.27075200
C	1.71455500	-1.17848200	3.33764900
H	2.51565100	-0.65936800	2.80591700
H	1.86194000	-1.08265100	4.41900800
H	1.73435700	-2.23671000	3.06015400
H	0.86309400	-2.99593500	-3.79935600
H	-0.72876100	-2.03718900	-3.81605700

IM7

SCF done: -2044.689727

C	0.84429700	-0.78190700	0.13457700
C	-0.00148700	1.62103500	1.66605400
C	0.94805800	0.59236700	-0.24489100
C	1.51772000	0.91792000	-1.43307100
O	0.11592300	1.54230200	0.30437000
O	0.60517800	0.87529100	2.41166100
Au	-0.98875800	-1.57417100	0.55036600
P	-3.12171900	-2.55832800	0.88169800
Sb	-3.06704300	0.95128100	-1.83651900
F	-2.17791800	-0.75127500	-2.10226400
F	-1.37177300	1.83803700	-2.07170100
F	-3.46274700	1.07731300	-3.69297700

F	-3.89278600	2.63249500	-1.45913300	H	5.71820500	3.28439500	-0.48844800
F	-2.68851300	0.76802200	0.06318000	H	8.95953600	0.45621200	-0.59688100
F	-4.69827300	-0.02295200	-1.49601700	C	8.44629600	3.14137000	-0.39637800
C	1.97848700	-1.74514300	-0.07688700	H	8.58869100	3.65352000	-1.35726600
H	1.89040400	-2.07316200	-1.12702900	H	8.09694700	3.89172900	0.32117200
H	1.79530000	-2.63683500	0.53071300	H	9.42599900	2.78407700	-0.06576800
N	3.36701400	-1.26733500	0.17567400	C	-0.90102700	2.71833800	2.07262800
C	3.93272200	-1.62804500	1.52207400	C	-1.68077300	3.42569900	1.13780900
C	3.05229400	-1.14814000	2.63864900	C	-0.98148600	3.03271700	3.44238800
C	2.57305300	-1.95035500	3.59120300	C	-2.53495100	4.43802800	1.57987800
H	4.08849700	-2.71411900	1.58786300	H	-1.63789800	3.16764700	0.08926100
H	4.91656800	-1.14742900	1.58506100	C	-1.82871500	4.05319000	3.87352200
H	2.80849300	-0.08964800	2.64477000	H	-0.37888000	2.47104700	4.14732200
H	2.78604000	-3.01785400	3.60648600	C	-2.60740100	4.75526900	2.94198000
H	1.95630600	-1.56202200	4.39613700	H	-3.15218300	4.96305700	0.85954500
S	4.47966000	-1.44578300	-1.11001800	H	-1.88829400	4.29920900	4.92867100
O	5.25660000	-2.71397900	-0.97988600	H	-3.27342400	5.54344100	3.27921500
O	3.67306200	-1.20012200	-2.34783300	C	-3.12444000	-4.02351800	2.00908200
C	5.61752100	-0.09106600	-0.83228700	H	-2.76141200	-3.72891500	2.99856700
C	5.15285200	1.22785600	-0.72895800	H	-4.13541300	-4.43502300	2.10470100
C	6.98729700	-0.37595500	-0.78557900	H	-2.45855400	-4.79605000	1.61226700
C	6.07459600	2.26257500	-0.57568500	C	-3.87191000	-3.16147200	-0.68872500
H	4.09017300	1.43786900	-0.75088800	H	-4.83019900	-3.65338800	-0.48851000
C	7.89699100	0.67446500	-0.63553400	H	-4.03019700	-2.30003600	-1.34098000
H	7.32446100	-1.40258300	-0.86267600	H	-3.19524600	-3.86255600	-1.18507400
C	7.45933100	2.00539300	-0.53228100	C	-4.38702300	-1.41595900	1.57781100

H	-4.54705800	-0.61160500	0.85713500
H	-5.32746600	-1.95034700	1.75177300
H	-4.03042300	-0.98374200	2.51683500
H	1.19251400	1.83125400	-1.92123300
H	2.16989000	0.23418700	-1.96463800

TS6

SCF done: -2044.69016

C	0.83251300	-0.80737300	0.25258100
C	-0.04165600	1.46528500	1.68942900
C	0.92228100	0.54314400	-0.22489700
C	1.48231600	0.83601300	-1.41922300
O	0.10561800	1.50252000	0.33659400
O	0.49266500	0.59594400	2.36230800
Au	-1.02656600	-1.64328900	0.48700400
P	-3.15831300	-2.66152300	0.60199700
Sb	-3.05210900	1.11069800	-1.77441200
F	-2.08441200	-0.52690100	-2.14866400
F	-1.40340900	2.09694000	-1.92804000
F	-3.43275800	1.34912000	-3.62366900
F	-3.96609700	2.71549500	-1.28945600
F	-2.68385200	0.79892600	0.11093900
F	-4.64524700	0.04466300	-1.53584900
C	1.99565700	-1.74881400	0.21350400
H	1.89647600	-2.26195500	-0.75998000
H	1.83093400	-2.52329200	0.97091300

N	3.38181100	-1.22018500	0.35904600
C	4.03196100	-1.45363800	1.69549400
C	3.23533600	-0.87111200	2.82584800
C	2.86184900	-1.57384400	3.89600600
H	4.19789600	-2.52880400	1.85250700
H	5.01672700	-0.97281500	1.64676700
H	2.97513700	0.18061900	2.74270200
H	3.09905000	-2.63102100	4.00068300
H	2.30968400	-1.11370000	4.70980500
S	4.43674700	-1.51261400	-0.95803700
O	5.23812500	-2.75270100	-0.73368000
O	3.57097000	-1.40882200	-2.17454300
C	5.56685800	-0.12540200	-0.87449400
C	5.08945300	1.19315700	-0.88402600
C	6.94115200	-0.39228400	-0.86411300
C	6.00373300	2.24581800	-0.87896600
H	4.02403900	1.39008600	-0.87999200
C	7.84260300	0.67575500	-0.86346300
H	7.28824200	-1.41844900	-0.85362200
C	7.39229300	2.00639800	-0.87411500
H	5.63811700	3.26813400	-0.87949600
H	8.90866100	0.47191500	-0.85300300
C	8.36931400	3.15876800	-0.89832900
H	8.45327300	3.58026200	-1.90883800
H	8.04828700	3.96986400	-0.23565600
H	9.37005600	2.84255600	-0.58951700

C	-0.86161200	2.57747000	2.19912600
C	-1.58052600	3.42066900	1.32986400
C	-0.93184900	2.76873100	3.59194500
C	-2.36065800	4.44922400	1.86176800
H	-1.54816100	3.25283700	0.26185400
C	-1.70571100	3.80531300	4.11265900
H	-0.37956500	2.10204900	4.24464600
C	-2.42096600	4.64565600	3.24721900
H	-2.93078700	5.08458400	1.19333900
H	-1.75764000	3.95720600	5.18571300
H	-3.02963200	5.44740400	3.65356200
C	-3.20781400	-4.22781300	1.58176900
H	-2.89692600	-4.02757200	2.61181900
H	-4.21889200	-4.64989700	1.58738700
H	-2.51698800	-4.95707400	1.14747200
C	-3.81548600	-3.10588000	-1.05951200
H	-4.79159300	-3.59465000	-0.96798000
H	-3.91948300	-2.18406600	-1.63527900
H	-3.11706100	-3.77102300	-1.57491200
C	-4.46129200	-1.58982400	1.33920000
H	-4.58867000	-0.72155800	0.68954400
H	-5.40766600	-2.13683700	1.41310500
H	-4.15386200	-1.25022800	2.33208300
H	1.16054900	1.73970300	-1.92691600
H	2.11461300	0.12369100	-1.93613800

IM8

SCF done: -2044.706446

C	0.62526900	-0.82573500	0.49463200
C	0.41867900	1.40804800	0.88206500
C	0.81899200	-0.02906400	-0.75725900
C	1.09812700	-0.32357900	-2.02094300
O	0.56845700	1.32845300	-0.40934600
O	0.55415500	0.29882200	1.51313400
Au	-1.29607600	-1.75700700	0.48336900
P	-3.40216600	-2.78999900	0.41839900
Sb	-3.14584200	1.48192800	-1.23704600
F	-2.38221600	-0.14603000	-1.94743100
F	-1.61426800	2.47062900	-1.86016500
F	-4.08523600	1.78478200	-2.86520900
F	-3.86644200	3.05695300	-0.43850200
F	-2.16985500	1.13343300	0.41532400
F	-4.59892100	0.41319200	-0.54434100
C	1.72535600	-1.79487000	0.89727400
H	1.65502200	-2.64275000	0.21202100
H	1.50742000	-2.17238300	1.90354300
N	3.13442900	-1.29842500	0.87189400
C	3.72971200	-0.76282100	2.13097300
C	3.79828000	0.74169500	2.17949900
C	3.50283500	1.47141000	3.25582300
H	3.15540000	-1.14914400	2.98257700
H	4.73876700	-1.18387100	2.22986700

H	4.16634500	1.22375000	1.27474800
H	3.14503000	1.01341500	4.17668900
H	3.62268200	2.55089700	3.26570700
S	4.22167500	-2.10889300	-0.16715300
O	5.11615900	-3.00731000	0.62579500
O	3.38196600	-2.66655300	-1.26816500
C	5.25917200	-0.79311100	-0.80531400
C	4.71532900	0.19487600	-1.63997400
C	6.62633100	-0.80863500	-0.50947500
C	5.55295700	1.18050800	-2.16022900
H	3.65701200	0.18806800	-1.87303600
C	7.45190100	0.18696000	-1.04198600
H	7.02934800	-1.59287900	0.11983600
C	6.93253200	1.19412200	-1.87082500
H	5.13543200	1.94697000	-2.80656400
H	8.51311000	0.17667500	-0.81375400
C	7.82483100	2.26888000	-2.44802000
H	7.51763300	3.26587200	-2.10806000
H	8.86856400	2.12228900	-2.15555900
H	7.78034500	2.27483000	-3.54395400
C	0.14876700	2.67364200	1.52327100
C	-0.27653600	3.76689900	0.73940800
C	0.26917000	2.79485600	2.92249100
C	-0.55446000	4.98232800	1.36346600
H	-0.44135900	3.63597200	-0.32360800
C	-0.00637800	4.01757100	3.53023900

H	0.58001000	1.94084900	3.51152000
C	-0.41414400	5.11091700	2.75169200
H	-0.90059700	5.82130600	0.77092200
H	0.08707000	4.12022300	4.60569300
H	-0.63617100	6.05917900	3.23036500
C	-3.38662600	-4.56967200	0.92064700
H	-3.02257000	-4.66027900	1.94875400
H	-4.39291100	-4.99859100	0.85572900
H	-2.71332400	-5.13109300	0.26559100
C	-4.17847000	-2.78040200	-1.25161900
H	-5.14558700	-3.29496000	-1.23132200
H	-4.31690000	-1.74015700	-1.55061900
H	-3.51682500	-3.26805500	-1.97291800
C	-4.66169200	-2.00762600	1.51409000
H	-4.81938400	-0.98366400	1.16434200
H	-5.60740100	-2.55948200	1.46815400
H	-4.30167200	-1.98777100	2.54698300
H	1.08275100	0.44963400	-2.77870700
H	1.31230700	-1.34548000	-2.30452600

TS7

SCF done: -2044.672067

C	-1.00594200	0.81981900	-0.96955500
C	0.42762400	2.35539000	-0.26664300
C	-0.80744300	0.64969200	0.44756200
C	-1.27680500	-0.20292300	1.40708100

O	0.16854400	1.62599600	0.79814300	C	-5.21232900	-0.22204700	0.31012700
O	-0.25060600	1.98809200	-1.30026100	C	-4.80689600	-1.50290700	0.70383900
Au	0.24350000	-1.35087300	-0.51762200	C	-5.87725200	0.62380000	1.20793300
P	1.13963400	-3.30808400	-1.26629500	C	-5.03993800	-1.92074700	2.01725600
Sb	3.77542000	-0.29800700	0.87093900	H	-4.34093300	-2.16522900	-0.01654600
F	2.36596300	-1.41805600	1.58113900	C	-6.09931000	0.19253300	2.51676100
F	3.35186200	1.03779700	2.18779600	H	-6.23826300	1.59044400	0.87626100
F	5.04450500	-1.13199100	2.01880300	C	-5.67802700	-1.08004600	2.94597500
F	5.10389000	0.82168500	0.09003700	H	-4.73184400	-2.91624900	2.32213100
F	2.44537700	0.50906900	-0.30833700	H	-6.61843400	0.84569000	3.21177300
F	4.05380900	-1.65272600	-0.48315800	C	-5.90051700	-1.52595200	4.37280100
C	-2.21200000	0.58391900	-1.81410700	H	-5.11286700	-1.13883500	5.03318200
H	-2.41638500	-0.48359900	-1.89933000	H	-6.85759100	-1.16240300	4.76182400
H	-1.98295300	0.93750100	-2.82921100	H	-5.89150500	-2.61696800	4.45769800
N	-3.48750100	1.22255800	-1.35178800	C	1.37349300	3.43745100	-0.27417800
C	-3.55043200	2.69870800	-1.22414800	C	2.28879100	3.57839700	0.79041600
C	-3.01804900	3.21893600	0.08875600	C	1.38795300	4.34670200	-1.35599300
C	-2.24251500	4.29782700	0.21493200	C	3.19875400	4.63523400	0.77005900
H	-3.00524900	3.14753500	-2.06638700	H	2.32587500	2.83732500	1.57880700
H	-4.60078000	2.98513800	-1.34364700	C	2.30032700	5.39751400	-1.35816800
H	-3.34340800	2.67431100	0.97469300	H	0.68977300	4.22237400	-2.17597400
H	-1.90593500	4.86690300	-0.64998600	C	3.20391900	5.54556400	-0.29433000
H	-1.93166200	4.66734900	1.18797700	H	3.91748500	4.73353000	1.57545000
S	-4.91826900	0.32244400	-1.37484600	H	2.31433200	6.09850800	-2.18548500
O	-6.02170200	1.26491500	-1.72151400	H	3.91805200	6.36238400	-0.30361800
O	-4.63380200	-0.90280200	-2.17904600	C	-0.14034100	-4.50682700	-1.84361800

H	-0.73109100	-4.06024700	-2.64896800
H	0.33167700	-5.42635300	-2.20788800
H	-0.81238200	-4.75124200	-1.01560300
C	2.11709000	-4.21370600	0.00112000
H	2.50233600	-5.15120400	-0.41545000
H	2.94450500	-3.57130000	0.30549100
H	1.49397100	-4.42132300	0.87473300
C	2.29287700	-3.10679100	-2.68614100
H	3.12254700	-2.47809200	-2.35208100
H	2.67589000	-4.08209700	-3.00762400
H	1.78045200	-2.61979000	-3.52036400
H	-0.85682200	-0.17830900	2.40243000
H	-2.13773800	-0.82299800	1.20287800

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SCF done: -2044.726029

C	-0.10755800	1.58974000	0.35713500
C	-1.77369300	2.60560500	-0.61361700
C	-0.07381800	1.24610200	-0.95560700
C	0.74647900	0.37979500	-1.78889400
O	-1.14961700	1.94480500	-1.55162500
O	-1.17917700	2.47265600	0.53534300
Au	0.70080000	-1.61353900	-1.03986800
P	0.59968200	-3.76798100	-0.10721100
Sb	-3.10365600	-1.29644800	0.62412400
F	-2.30817600	-1.88299000	-1.03655500

F	-3.09226600	0.51171500	-0.07019400
F	-4.84045200	-1.61378900	-0.08999300
F	-3.84132100	-0.67392400	2.26883500
F	-1.32659700	-0.94242100	1.32616500
F	-2.94038500	-3.09808200	1.28399300
C	0.64716800	1.17513400	1.56986200
H	0.81831700	0.09806400	1.52693900
H	0.01230900	1.35727200	2.44699800
N	1.95418400	1.85288900	1.74453900
C	1.96052300	3.31930300	1.97252000
C	1.87825600	4.12263500	0.69775200
C	1.01542800	5.11848800	0.48874800
H	1.12644500	3.57467300	2.64133300
H	2.88013900	3.56023900	2.51596900
H	2.61239500	3.86515600	-0.06547300
H	0.27525000	5.39913900	1.23601000
H	1.02711800	5.70318500	-0.42700500
S	3.32864100	0.94506200	2.13917100
O	4.04494200	1.67620700	3.22476600
O	2.86284800	-0.46247200	2.29958100
C	4.39497100	1.00368600	0.69695700
C	4.22310800	0.06540000	-0.33007300
C	5.41162100	1.96290900	0.62625700
C	5.05869000	0.11537500	-1.44649800
H	3.45310700	-0.69401300	-0.25193600
C	6.23940000	1.99931800	-0.50034100

H	5.56490600	2.65020100	1.44981000
C	6.07626900	1.08335100	-1.55312200
H	4.92329000	-0.61179200	-2.24202200
H	7.02997200	2.74137400	-0.55576100
C	6.97669900	1.11927000	-2.76687100
H	6.39695600	1.25113900	-3.68877600
H	7.69993500	1.93775600	-2.70528300
H	7.53886000	0.18292400	-2.87153600
C	-2.93591500	3.42285200	-0.83446900
C	-3.46145800	3.55771000	-2.13626100
C	-3.55416100	4.07296800	0.25401900
C	-4.59278100	4.34458200	-2.34201000
H	-2.99074400	3.04159200	-2.96473300
C	-4.68446000	4.85658400	0.03388700
H	-3.15864000	3.94577900	1.25477800
C	-5.20396000	4.99484100	-1.26105900
H	-5.00293300	4.44613000	-3.34041900
H	-5.16716900	5.35102400	0.86927100
H	-6.08757800	5.60218200	-1.42595100
C	2.08304900	-4.83611000	-0.39621200
H	2.97015200	-4.34614500	0.01727300
H	1.95826600	-5.81468800	0.08104400
H	2.23384900	-4.97697000	-1.47116600
C	-0.82869400	-4.78632200	-0.67464700
H	-0.80587500	-5.77818500	-0.20954200
H	-1.74646500	-4.26883100	-0.38785400

H	-0.80621300	-4.89028800	-1.76337300
C	0.41623600	-3.71417800	1.72668700
H	-0.53803000	-3.23429100	1.95531700
H	0.43071400	-4.72422200	2.15089600
H	1.22427200	-3.11699300	2.16031600
H	0.37161900	0.38661300	-2.81437600
H	1.78869900	0.71057700	-1.78149600

TS8

SCF done: -2044.704418

C	1.64483700	1.57803400	0.64111400
C	-0.05001300	2.85945900	0.26569400
C	0.77520500	0.87022400	-0.18923600
C	0.83295600	-0.41189200	-0.82190900
O	-0.31073800	1.67478900	-0.34955400
O	0.96787900	2.66621900	1.13490800
Au	-0.35042000	-1.78377800	0.33896700
P	-1.74949700	-3.24226000	1.51779000
Sb	-3.81744300	-0.16247700	-1.00175600
F	-2.73421100	-1.67461400	-1.53545500
F	-2.67332500	0.98774900	-2.04200500
F	-4.98997900	-0.44758600	-2.47485000
F	-4.82521600	1.36865700	-0.43574600
F	-2.63687200	0.11928300	0.51609100
F	-4.83188200	-1.35878700	0.11843000
C	3.02719400	1.32406100	1.11359600

H	3.20893300	0.25038700	1.22078800	H	6.83024000	-4.42853600	-2.21979100
H	3.18462200	1.79864900	2.09027800	H	6.22521400	-4.96014900	-0.64244600
N	3.96832200	1.87210100	0.08778100	C	-1.16702900	3.73687000	0.61097900
C	3.51509000	3.11466300	-0.58713100	C	-2.44569900	3.47423600	0.08659500
C	2.20350200	2.87205700	-1.28940600	C	-0.96009800	4.83436100	1.47043000
C	1.12233400	3.74285700	-1.22841100	C	-3.51726500	4.29490600	0.44433100
H	3.41717400	3.94655200	0.12700900	H	-2.60274400	2.63783300	-0.57864600
H	4.29342200	3.38839700	-1.30657200	C	-2.03641600	5.65287400	1.81080000
H	2.21413700	2.08093600	-2.03543700	H	0.02688000	5.03138900	1.87600200
H	1.24075300	4.70213000	-0.72941200	C	-3.31589800	5.38272200	1.30157800
H	0.37554700	3.71897000	-2.01654900	H	-4.50346700	4.05605200	0.06430900
S	5.61828700	1.53779000	0.28749200	H	-1.88249600	6.49500400	2.47717500
O	6.31727100	2.39901800	-0.70817500	H	-4.15151900	6.01719900	1.57865000
O	5.94588400	1.58232300	1.74271600	C	-0.90381400	-4.49347100	2.58569100
C	5.73529400	-0.17213100	-0.22759200	H	-0.29322500	-3.98320900	3.33705000
C	5.90466900	-1.17356300	0.73383000	H	-1.63666000	-5.13299700	3.09045900
C	5.68332400	-0.48663100	-1.59386100	H	-0.24625200	-5.11649600	1.97141900
C	5.99781900	-2.50696200	0.32042000	C	-2.86552200	-4.22981800	0.43354900
H	5.97800700	-0.90608400	1.78133000	H	-3.50856900	-4.88015300	1.03683400
C	5.77919500	-1.81963400	-1.98825600	H	-3.47855100	-3.53356600	-0.14283100
H	5.58608600	0.30317000	-2.32983400	H	-2.27649500	-4.83634600	-0.26035900
C	5.93211200	-2.85155500	-1.03923000	C	-2.90677800	-2.35717400	2.64702400
H	6.13070600	-3.28678900	1.06362700	H	-3.53686200	-1.70554100	2.03739500
H	5.74262500	-2.06730100	-3.04484900	H	-3.53544100	-3.06936000	3.19325700
C	6.02725800	-4.29219100	-1.48556600	H	-2.34424300	-1.74445300	3.35704100
H	5.09516000	-4.62138800	-1.96191700	H	0.32618600	-0.41721000	-1.78908300

H	1.85266000	-0.79267000	-0.88247700
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IM9

SCF done: -2044.761325

C	1.61331700	1.09399700	-0.10343600
C	0.19329300	2.68631400	-0.17858400
C	0.46156600	0.58261100	-0.94094800
C	0.25606200	-0.62985600	-1.57686500
O	-0.37511800	1.60091100	-1.03240000
O	0.88505800	1.94242700	0.80424100
Au	-0.73510900	-1.63880000	0.14843200
P	-1.92532000	-2.78860300	1.78520800
Sb	-4.13181800	-0.12489000	-1.02608500
F	-3.19231500	-1.78425100	-1.40098800
F	-2.97145600	0.74383800	-2.29155200
F	-5.43258300	-0.53002700	-2.35288400
F	-4.97843400	1.53937000	-0.60802600
F	-2.80789700	0.25553700	0.35006700
F	-5.11165700	-1.07613000	0.33523200
C	2.63819500	0.21829300	0.58033600
H	2.76091100	-0.73841500	0.05854600
H	2.35714400	0.01220200	1.61588800
N	3.87279600	1.04332700	0.49179500
C	3.65819600	2.37060900	-0.14533900
C	2.38010100	2.14983700	-0.97498500
C	1.34187300	3.29535900	-1.03030200

H	3.51684400	3.15039300	0.61172000
H	4.51484800	2.64446600	-0.76652100
H	2.62949400	1.74809400	-1.96133900
H	1.70167300	4.21365500	-0.55854400
H	1.00103200	3.53432300	-2.03972200
S	5.25697300	0.66749100	1.34971000
O	5.90502000	1.96551000	1.68833900
O	4.84324700	-0.33841100	2.36936600
C	6.32269400	-0.16886700	0.17666700
C	6.22346000	-1.55647300	0.01937200
C	7.25251500	0.57107100	-0.56705900
C	7.04275600	-2.19876500	-0.91278900
H	5.53540400	-2.12210600	0.63690800
C	8.06336100	-0.08612100	-1.49338100
H	7.35167500	1.63685200	-0.39752700
C	7.96886500	-1.47752800	-1.68619900
H	6.97213100	-3.27553900	-1.03230700
H	8.78892400	0.48457600	-2.06558700
C	8.85207400	-2.17416800	-2.69610600
H	8.61063000	-1.85878600	-3.71927000
H	9.91005300	-1.94026500	-2.52809600
H	8.73619200	-3.26076400	-2.64694900
C	-0.89754900	3.55696700	0.35524000
C	-2.23087300	3.36732700	-0.03667000
C	-0.57255500	4.56629700	1.27818400
C	-3.23477600	4.18058400	0.49936700

H	-2.48804600	2.58933400	-0.73957900
C	-1.57917200	5.37898800	1.80442700
H	0.45589600	4.70236900	1.59916900
C	-2.91207100	5.18661500	1.41555700
H	-4.26228300	3.99821200	0.20627100
H	-1.32614000	6.15398900	2.52076000
H	-3.69339300	5.81474000	1.83163800
C	-0.93574400	-3.88030300	2.89660700
H	-0.18852200	-3.28463200	3.42951200
H	-1.58601200	-4.37797600	3.62464300
H	-0.41566200	-4.63761600	2.30222700
C	-3.23480800	-3.86369900	1.06684500
H	-3.77532000	-4.38731800	1.86312500
H	-3.92461100	-3.22477100	0.51052100
H	-2.79585300	-4.59163200	0.37916800
C	-2.84465800	-1.64257900	2.89433100
H	-3.54334000	-1.07260300	2.27761300
H	-3.39385700	-2.20692700	3.65603200
H	-2.15338000	-0.94673100	3.37730600
H	-0.53757700	-0.66551900	-2.32031500
H	1.12282600	-1.26866500	-1.72568700

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SCF done: -1178.397963

C	-0.94731700	0.74974400	-0.45594300
C	-2.94576700	0.54281400	0.23987600

C	-1.58855700	2.10038000	-0.66570900
C	-1.10714400	3.23829000	-1.16002300
O	-2.86166800	1.94475000	-0.16091400
O	-2.09304000	-0.10877600	-0.68175900
C	0.28755200	0.27178100	-1.18633700
H	0.94746300	1.10998900	-1.44188700
H	0.03143000	-0.26490800	-2.10249100
N	0.92724200	-0.62470800	-0.18500900
C	0.17373500	-0.72500400	1.09631400
C	-0.70763600	0.53657900	1.07183000
C	-2.16386900	0.40982000	1.58147100
H	-0.42866300	-1.63987500	1.12036600
H	0.85946300	-0.74279000	1.94767900
H	-0.17395200	1.38684900	1.50572700
H	-2.36695700	-0.56293200	2.03927900
H	-2.45124000	1.19373000	2.28599100
S	2.21362600	-1.61155700	-0.55974000
O	2.14468600	-2.76256500	0.38471200
O	2.21220200	-1.76359000	-2.04292700
C	3.67647400	-0.66315400	-0.13378600
C	4.26175200	0.17573200	-1.09168400
C	4.22470300	-0.77049800	1.15036800
C	5.38332100	0.93173100	-0.74519800
H	3.85764800	0.20836900	-2.09676800
C	5.34741700	-0.00756900	1.48094100
H	3.79240700	-1.46179800	1.86437200

C	5.93910700	0.85963900	0.54543400	C	-6.74165200	0.44771200	0.44847700
H	5.84257800	1.57583800	-1.48936300	H	-5.22884400	1.97889200	0.62386500
H	5.77858200	-0.09592000	2.47367700	C	-5.93323600	-1.77922200	-0.05670100
C	7.14013900	1.69976000	0.91656400	H	-3.79344100	-1.97521200	-0.26840000
H	6.83741700	2.71382600	1.21117800	C	-6.99715100	-0.90555200	0.19869100
H	7.68837500	1.26468200	1.75801700	H	-7.56359900	1.13030300	0.63942800
H	7.83348700	1.80031000	0.07473800	H	-6.12631400	-2.82766900	-0.25993200
C	-4.36107500	0.05300800	0.19478200	H	-8.01739400	-1.27594200	0.19873500
C	-5.42820400	0.92836700	0.44665200	H	-1.71384200	4.13489400	-1.19860700
C	-4.61863400	-1.30391600	-0.05722200	H	-0.09450800	3.28601900	-1.54036900

Cartesian Coordinates for the Stationary Points Given in Scheme 3.

TS9

SCF done: -1178.352269

C	-0.95707300	1.56965100	-0.13231800	C	-0.80473100	1.11352500	1.33521300
C	-2.79851600	0.29332400	0.43674500	C	-2.27699100	0.84843900	1.66124900
C	-1.51881200	2.98635200	-0.23155100	H	-0.32840000	-1.04650500	1.48787700
C	-0.91976100	3.89534800	-1.04556700	H	0.96309900	0.02637900	2.06077500
O	-2.56542000	3.18655000	0.52666300	H	-0.40734700	1.93509700	1.93619800
O	-2.08381700	0.63828100	-0.59938100	H	-2.56162100	0.41081500	2.61490200
C	0.29424500	1.12169000	-0.85973600	H	-2.65854000	1.99286400	1.46907800
H	1.04024700	1.92515500	-0.83031900	S	1.68560800	-1.27368800	-0.67601300
H	0.10788300	0.84128600	-1.89706900	O	1.35500600	-2.49684700	0.11024200
N	0.72518600	-0.05970700	-0.07046000	O	1.56789400	-1.20281100	-2.16020000
C	0.17102300	-0.09006400	1.31032300	C	3.36881200	-0.81887800	-0.25403900
				C	4.10953100	-0.01357700	-1.12912800
				C	3.92609500	-1.26160100	0.95258000

C	5.40604100	0.36681800	-0.77664800
H	3.67914800	0.29076100	-2.07611900
C	5.22396800	-0.87124800	1.29069000
H	3.35568800	-1.91650100	1.60080100
C	5.98324200	-0.05242900	0.43585000
H	5.98137300	0.99091800	-1.45401500
H	5.65706600	-1.21315700	2.22612900
C	7.39930800	0.33801300	0.79394600
H	7.66711200	1.30969800	0.36639700
H	7.53764500	0.39347500	1.87861300
H	8.11970000	-0.39708400	0.41008900
C	-4.00968700	-0.46709100	0.20562100
C	-4.40335400	-0.78770800	-1.11400500
C	-4.80593300	-0.89821400	1.29027600
C	-5.56559800	-1.52254600	-1.33714200
H	-3.79349500	-0.45332900	-1.94423400
C	-5.96902500	-1.62938300	1.05772000
H	-4.51521500	-0.65841000	2.30651500
C	-6.35017200	-1.94403400	-0.25433300
H	-5.86318700	-1.76614100	-2.35110100
H	-6.57806100	-1.95561200	1.89363900
H	-7.25517700	-2.51578400	-0.43168900
H	-1.27787100	4.91829400	-1.06428200
H	-0.12104400	3.62502800	-1.72581000

IM10

SCF done: -1178.395317

C	-0.96406500	1.45965500	0.15067700
C	-2.82624600	0.17052200	0.55145300
C	-1.11550100	2.96133200	0.01743400
C	-1.45959200	3.81132900	0.98986100
O	-0.88458900	3.33197500	-1.28027100
O	-2.16308700	0.87061900	-0.42856100
C	0.26189800	0.91934800	-0.61597800
H	1.06422700	1.67178000	-0.63518000
H	0.00486000	0.64394700	-1.63760600
N	0.64503000	-0.26679900	0.17090600
C	0.38956100	-0.04771500	1.60835600
C	-0.86571500	0.87341400	1.60364900
C	-2.17648600	0.14811900	1.72691600
H	0.20915000	-1.00200400	2.10423800
H	1.24037700	0.45516400	2.09555400
H	-0.73584400	1.65483000	2.35863500
H	-2.51015300	-0.34307700	2.63065500
H	-1.06847200	4.28050800	-1.37619000
S	1.60626000	-1.49107000	-0.41733900
O	1.44887000	-2.63118000	0.52807700
O	1.31401400	-1.58820000	-1.87392600
C	3.29674300	-0.90496300	-0.25752000
C	3.87718200	-0.16991500	-1.29960800
C	4.01809100	-1.17169000	0.91377600
C	5.17777800	0.31783400	-1.15233300

H	3.32133300	-0.00445500	-2.21522200
C	5.31750300	-0.67678900	1.04557300
H	3.57044900	-1.77511900	1.69483900
C	5.91733200	0.07480000	0.01897300
H	5.62889700	0.88656800	-1.96009200
H	5.87781500	-0.88409600	1.95263800
C	7.33701500	0.57681500	0.15662600
H	7.50299300	1.47861700	-0.44152900
H	7.58076300	0.80964100	1.19852700
H	8.05721700	-0.17892200	-0.18521300
C	-4.11178100	-0.40779200	0.14299700
C	-4.62899600	-0.14898400	-1.14086000
C	-4.85042900	-1.22651400	1.02114700
C	-5.85519800	-0.69291800	-1.53282400
H	-4.06343500	0.47503200	-1.82165500
C	-6.07462200	-1.76561400	0.62621400
H	-4.46163100	-1.44733400	2.00953300
C	-6.58313400	-1.50099700	-0.65297000
H	-6.24046400	-0.48650000	-2.52637300
H	-6.63098100	-2.39610800	1.31257400
H	-7.53446500	-1.92430200	-0.95923000
H	-1.57776700	4.87356600	0.79308800
H	-1.65992400	3.47560900	1.99717000

TS10

SCF done: -1178.273446

C	-1.08629700	1.62087400	0.04074100
C	-2.78612000	0.15367500	0.48573600
C	-1.32252200	3.09975300	-0.11248100
C	-0.43326600	4.20090600	0.05485900
O	-2.48881900	3.54523100	-0.42433700
O	-2.18971800	0.89166300	-0.51418500
C	0.23170400	1.14234400	-0.62089500
H	0.93859400	1.97180000	-0.74781400
H	0.02918100	0.68510700	-1.58941900
N	0.75158400	0.14381500	0.32839900
C	0.39654900	0.50077900	1.71282500
C	-0.99067300	1.19013300	1.56436600
C	-2.18213100	0.28280400	1.67762400
H	0.35118200	-0.39690900	2.33034900
H	1.13189600	1.19776800	2.14051200
H	-1.04833700	2.05090300	2.24103000
H	-2.50083100	-0.17568000	2.60367200
H	-1.77012100	4.58966200	-0.53230700
S	1.50318000	-1.27435500	-0.12455500
O	1.29549100	-2.23348700	0.99649900
O	1.07561800	-1.54939000	-1.52467100
C	3.25590100	-0.89294800	-0.17580500
C	3.82920200	-0.42629000	-1.36562200
C	4.03822400	-1.06814800	0.97253600
C	5.18872500	-0.10788300	-1.39079100
H	3.22229100	-0.34091600	-2.25944600

C	5.39655400	-0.74581300	0.93054700
H	3.59127600	-1.47380300	1.87264000
C	5.99174200	-0.25415000	-0.24519000
H	5.63593900	0.24673600	-2.31469200
H	6.00599000	-0.88884800	1.81792000
C	7.45700500	0.11716800	-0.27504200
H	7.88956000	-0.03960700	-1.26855000
H	7.60152200	1.17591400	-0.01990600
H	8.03447100	-0.47269600	0.44404500
C	-3.96936500	-0.60851300	0.07578500
C	-4.60080500	-0.33180400	-1.15189300
C	-4.49711600	-1.61942100	0.90348800
C	-5.73984100	-1.04453200	-1.53526300
H	-4.19696900	0.44371800	-1.79105800
C	-5.63572900	-2.32657200	0.51695600
H	-4.00355000	-1.86239700	1.83854500
C	-6.26238200	-2.04134700	-0.70380600
H	-6.21887300	-0.82097200	-2.48315600
H	-6.02974700	-3.10595100	1.16135300
H	-7.14566500	-2.59565000	-1.00476400
H	-0.68686300	4.80062800	0.93280400
H	0.64035000	4.11595100	-0.09617500

IM11

SCF done: -1178.417202

C	-1.66065200	1.54818700	1.16187400
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C	-2.28763100	3.68397900	0.64642800
C	-0.50549800	1.33607700	2.16220900
C	-0.52190100	0.06212600	2.99623700
O	0.36597300	2.16686300	2.29305100
O	-1.36763300	2.70007800	0.36585100
C	-1.93654300	0.34993900	0.22795000
H	-1.58177700	-0.59599600	0.66258900
H	-1.46017600	0.49857900	-0.74113900
N	-3.40505200	0.35884300	0.09079100
C	-4.05954200	0.84304600	1.32071200
C	-3.02817100	1.85609200	1.89595700
C	-3.24108700	3.29277700	1.50724700
H	-5.01281200	1.31216200	1.07389400
H	-4.24031200	0.02104200	2.03199500
H	-2.95587700	1.72726800	2.98338700
H	-4.04620200	3.90589700	1.88813400
S	-4.21747100	-0.34653000	-1.18047300
O	-5.58190600	0.24968100	-1.18158100
O	-3.29368000	-0.28639400	-2.34654000
C	-4.39702100	-2.07760500	-0.73888500
C	-3.40057700	-2.99337800	-1.10317000
C	-5.52436800	-2.49906100	-0.02205800
C	-3.52761000	-4.33090900	-0.72236400
H	-2.55510800	-2.66146500	-1.69455900
C	-5.63663200	-3.84073000	0.35084400
H	-6.30674300	-1.78833900	0.21743000

C	-4.64337100	-4.77604300	0.01010500
H	-2.75675600	-5.04165500	-1.00565400
H	-6.51090800	-4.16895600	0.90515400
C	-4.78776700	-6.23287700	0.38785900
H	-5.42651800	-6.35739100	1.26803400
H	-5.24161100	-6.80850800	-0.43014400
H	-3.81608200	-6.68906100	0.60487800
C	-2.05425300	4.96615600	-0.02533800
C	-0.80918600	5.23261200	-0.62641900
C	-3.06169700	5.94997300	-0.07372100
C	-0.57779500	6.45928600	-1.25417600
H	-0.03256400	4.47869700	-0.58741600
C	-2.82456700	7.17418400	-0.69927400
H	-4.03403800	5.74672800	0.36256200
C	-1.58134800	7.43381500	-1.29203700
H	0.38657800	6.65414500	-1.71244500
H	-3.61012400	7.92233600	-0.73345900
H	-1.40025600	8.38514600	-1.78218800
H	-0.00429800	0.25312600	3.93815100
H	-1.53009600	-0.31427000	3.19292900
H	0.02647100	-0.72583900	2.46511100

B

SCF done: -1178.420157

H	-0.20806400	-1.40982300	0.78092200
C	-3.66806500	-1.12759600	0.18769400

C	-4.37252900	-3.30497700	-0.02011000
C	-2.19050900	-0.73505300	0.35865900
C	-1.22216600	-1.81185100	0.78954000
O	-1.84303500	0.40322300	0.10536000
O	-3.93389100	-2.35965500	0.88648500
C	-4.63701700	-0.02486000	0.66325800
H	-4.11885600	0.94143700	0.66234700
H	-5.03169300	-0.24172600	1.65595000
N	-5.71792700	-0.05416900	-0.33981600
C	-5.18351600	-0.40944200	-1.66518200
C	-4.02661000	-1.39656900	-1.32925600
C	-4.42184200	-2.84611600	-1.28082800
H	-5.96407000	-0.86892500	-2.27310700
H	-4.79359100	0.47746600	-2.18449900
H	-3.17863700	-1.20666600	-1.99873800
H	-4.75065700	-3.40524900	-2.14619200
S	-7.32801000	0.18624400	0.00146400
O	-8.09413000	-0.52052200	-1.06413200
O	-7.49728900	-0.10173600	1.45388000
C	-7.61910300	1.94294100	-0.22233700
C	-7.43194400	2.82004300	0.85436600
C	-8.02518400	2.42486500	-1.47222100
C	-7.63017100	4.18861700	0.66407400
H	-7.15385100	2.42899900	1.82606400
C	-8.22012400	3.79755400	-1.64625400
H	-8.20168300	1.73069100	-2.28542300

C	-8.02496800	4.69985200	-0.58620500
H	-7.48483100	4.86931800	1.49785200
H	-8.53570300	4.17277400	-2.61519100
C	-8.26458300	6.18117900	-0.77159100
H	-7.50647500	6.77754900	-0.25199300
H	-8.24889000	6.46008600	-1.82971500
H	-9.24229400	6.47632000	-0.36760200
C	-4.68977000	-4.61798600	0.55150200
C	-4.67974300	-4.80635200	1.94696600
C	-5.01120200	-5.71011200	-0.27997800
C	-4.98722900	-6.05466700	2.49478500
H	-4.43993600	-3.97062300	2.59250600
C	-5.31759900	-6.95390400	0.27140900
H	-5.01700600	-5.58551500	-1.35759100
C	-5.30682200	-7.13199700	1.66174600
H	-4.98014800	-6.18396400	3.57235900
H	-5.56396300	-7.78535300	-0.38118200
H	-5.54605800	-8.10067600	2.08862800
H	-1.48014000	-2.17178500	1.79061100
H	-1.29153800	-2.67934300	0.12359100

H₂O

SCF done: -76.4321031

H	0.75985700	-0.47575100	0.00000000
O	0.00000000	0.11897500	0.00000000
H	-0.75985700	-0.47605200	0.00000000

IM12

SCF done: -1254.805657

C	0.83591100	0.71106200	0.10023400
C	2.85222300	0.41349900	-0.54278500
C	1.45959100	2.08536800	0.06119100
C	0.96754300	3.28863200	0.35343800
O	2.73629900	1.86237200	-0.40730200
O	2.00317000	-0.07180800	0.48685100
C	-0.39969400	0.35667200	0.89768900
H	-1.07203900	1.22099200	0.97745000
H	-0.14297900	0.02576600	1.90562700
N	-1.01505600	-0.71878300	0.07350900
C	-0.24799600	-1.04270300	-1.16059800
C	0.61822600	0.21362300	-1.36132800
C	2.07956300	0.01408400	-1.83192900
H	0.36797200	-1.93726000	-1.01288800
H	-0.92269000	-1.22874500	-1.99986100
H	0.07885300	0.96257400	-1.94796800
H	2.29955300	-1.02527400	-2.09278200
H	2.36183600	0.65226100	-2.67230000
S	-2.30932900	-1.62284700	0.60192200
O	-2.30486600	-2.85690400	-0.23477200
O	-2.25612100	-1.64061300	2.09037500
C	-3.76033100	-0.66935000	0.14719100
C	-4.29117100	0.26030900	1.05009600

C	-4.35486500	-0.86686500	-1.10624900
C	-5.40509200	1.01719200	0.67680600
H	-3.85300200	0.36403500	2.03596900
C	-5.46853600	-0.10447100	-1.46274800
H	-3.96352200	-1.62604700	-1.77339700
C	-6.00600200	0.85425400	-0.58366400
H	-5.82202700	1.73346000	1.37850200
H	-5.93596600	-0.26332300	-2.43016700
C	-7.19710400	1.69201800	-0.99037500
H	-6.88506000	2.55764000	-1.59045700
H	-7.90398800	1.11546200	-1.59657400
H	-7.73340400	2.07600900	-0.11697300
C	4.27599500	-0.02965700	-0.39841100
C	4.55533000	-1.32262200	0.07306500
C	5.32983000	0.81825800	-0.77156300
C	5.87902200	-1.76095600	0.17090200
H	3.74064900	-1.97223200	0.37450500
C	6.65224300	0.37346700	-0.67512700
H	5.11334000	1.82118400	-1.12062000
C	6.92967000	-0.91529600	-0.20515500
H	6.08917600	-2.75795400	0.54415000
H	7.46383500	1.03470900	-0.96111200
H	7.95683700	-1.25711700	-0.12831100
H	1.56153500	4.18498400	0.22104100
H	-0.04734000	3.39062600	0.71638200
H	2.19601000	0.56294800	2.52142900

O	1.75945900	1.08942500	3.20704700
H	1.77741800	1.98345300	2.84136100

IM13

SCF done: -1254.80809

C	-1.36688500	1.76421300	-0.21382000
C	-2.34025200	-0.20972000	0.43275600
C	-2.41548300	2.87938400	-0.40594800
C	-3.72940700	2.51850700	-0.60523900
O	-1.93507500	4.05398500	-0.29908300
O	-1.96349000	0.46337700	-0.60489000
C	-0.06801900	1.89466700	-1.01270800
H	0.24304000	2.94067900	-0.99208500
H	-0.14629100	1.53580900	-2.03800600
N	0.92467800	1.09496000	-0.23256200
C	0.60225600	1.34261900	1.21128800
C	-0.94009700	1.54413200	1.26673400
C	-1.78656700	0.33427100	1.71612500
H	0.96495700	0.52426900	1.83505900
H	1.08536800	2.27938500	1.49380000
H	-1.16975900	2.43275600	1.85459100
H	-1.19208100	-0.44395300	2.20926500
H	-2.59575500	0.61567000	2.39872300
S	1.22250800	-0.50663900	-0.70098600
O	0.46949500	-1.46454000	0.18110000
O	1.04280000	-0.55140500	-2.18092500

C	2.95772000	-0.69995700	-0.30607000
C	3.90767000	0.09992500	-0.95772300
C	3.35227200	-1.68800000	0.60015100
C	5.26022300	-0.09076500	-0.68247100
H	3.58742100	0.85780200	-1.66296000
C	4.71438900	-1.86661100	0.86487100
H	2.60196000	-2.30454300	1.08023700
C	5.68597600	-1.07413900	0.23359700
H	5.99876600	0.52787000	-1.18361400
H	5.02444600	-2.63359300	1.56794700
C	7.15680000	-1.25872600	0.52947900
H	7.33312700	-2.14746800	1.14258000
H	7.73899700	-1.36392800	-0.39356700
H	7.56345000	-0.39451400	1.07063400
C	-3.15620700	-1.37654600	0.24845200
C	-3.58246200	-1.75556200	-1.04941200
C	-3.55034500	-2.15613100	1.36297100
C	-4.38120400	-2.88233700	-1.21844300
H	-3.27564100	-1.16192400	-1.90180800
C	-4.35023900	-3.28099700	1.18174200
H	-3.22717600	-1.87878900	2.36011500
C	-4.76729200	-3.64665000	-0.10676000
H	-4.70355700	-3.16995600	-2.21304800
H	-4.64925300	-3.87517300	2.03826400
H	-5.38956300	-4.52481400	-0.24401300
H	-4.47478500	3.30293000	-0.66817000

H	-4.05482900	1.49858800	-0.74372900
H	-0.54011800	4.39316900	0.61716800
O	0.30886900	4.46584900	1.12441200
H	0.64654000	5.34364700	0.91399100

TS11

SCF done: -1254.769914

C	-1.16460900	1.74968700	0.00654100
C	-2.80185300	0.16547200	0.44339200
C	-1.37174000	3.24431200	-0.36396700
C	-0.46322500	4.15635500	0.32669200
O	-2.13291900	3.48611500	-1.29375100
O	-2.40096500	1.01121000	-0.42294800
C	0.01079600	1.12129700	-0.78306000
H	0.77389000	1.90373500	-0.95644200
H	-0.30898000	0.63166200	-1.70284300
N	0.54233700	0.14990800	0.19836000
C	0.47169700	0.76909700	1.53941400
C	-0.96981200	1.32122000	1.49686100
C	-2.02129200	0.20661000	1.71713800
H	0.62973900	0.02355300	2.32007800
H	1.20234700	1.58563500	1.60474700
H	-1.12475800	2.15316500	2.18531100
H	-1.55058900	-0.77269300	1.87747200
H	-2.68950900	0.39540900	2.56581600
S	1.21128200	-1.32314000	-0.13798500

O	0.88338800	-2.21995400	1.01651100	H	-6.88670000	-3.02235000	-0.78088300
O	0.75275400	-1.68384000	-1.51160900	H	-0.60785500	5.18103100	-0.01999600
C	2.98741500	-1.07463000	-0.13796800	H	-0.54831600	4.10575600	1.41730000
C	3.54182000	0.21168300	-0.17944200	H	2.59956200	3.61419500	-0.23369200
C	3.80317500	-2.21720400	-0.10717800	O	1.93990300	2.98984200	0.09900100
C	4.93793400	0.33204200	-0.20507800	H	0.70464200	3.72815900	0.15542100
H	2.92807300	1.11964200	-0.16138900				
C	5.18846100	-2.06913700	-0.13939600				
H	3.35742400	-3.20397000	-0.04653900				
C	5.77874200	-0.79128800	-0.19453600				
H	5.37439300	1.32630700	-0.22750600				
H	5.82107200	-2.95190100	-0.11461800				
C	7.28258800	-0.64186500	-0.24926000				
H	7.77840300	-1.30729500	0.46702400				
H	7.66943200	-0.89386500	-1.24587000				
H	7.59000500	0.38463500	-0.02697600				
C	-3.91061200	-0.69539800	0.11430000				
C	-4.55869100	-0.56889100	-1.13889600				
C	-4.35190500	-1.67114000	1.03843700				
C	-5.62622500	-1.40422100	-1.45246500				
H	-4.21629000	0.18222200	-1.84096600				
C	-5.41957600	-2.50366700	0.71260200				
H	-3.85375200	-1.78137900	1.99511400				
C	-6.05626300	-2.37078700	-0.53003400				
H	-6.12322300	-1.30892000	-2.41102400				
H	-5.75410800	-3.25609600	1.41749700				

Cartesian Coordinates for the Stationary Points Given in Fig. 2.

TS12

SCF done: -2044.762738

C	1.22805500	1.41923000	-0.38389100	H	2.91166900	3.50255400	0.82633000
C	-0.08915800	3.17580200	-0.40917400	H	4.16865700	3.03156300	-0.33169200
C	0.32501500	0.86401900	-1.51615900	H	2.57937700	2.20887900	-1.92628800
C	0.53186800	-0.42629600	-2.09948700	H	1.46261100	4.62810800	-0.74103400
O	-0.51850100	1.71863100	-1.86113900	H	0.86796100	3.87616200	-2.23087100
O	0.27888200	2.19371600	0.39768000	S	4.51435700	0.97708700	1.78492800
Au	-0.34238900	-1.88925800	-0.75997700	O	5.06440400	2.25446900	2.31898000
P	-1.10567100	-3.59861200	0.64313400	O	3.94982900	-0.10292400	2.64189000
Sb	-3.94603200	-0.20878500	0.14129700	C	5.78581700	0.24019300	0.75835200
F	-3.34245500	-1.50691800	-1.15707500	C	5.72714200	-1.12807300	0.45790300
F	-3.73666800	1.20259100	-1.13102800	C	6.82858300	1.03514200	0.26698400
F	-5.76402400	-0.48414700	-0.35221400	C	6.70392100	-1.68871800	-0.36645300
F	-4.43765800	1.06457500	1.49547300	H	4.94463100	-1.74253800	0.88794900
F	-2.09085000	0.04354500	0.69278900	C	7.79848000	0.45763300	-0.55688400
F	-4.04949500	-1.64887800	1.42850400	H	6.89028300	2.07913200	0.55119200
C	2.09130700	0.55136500	0.50779000	C	7.74888700	-0.90630400	-0.89350900
H	2.35394800	-0.38813000	0.01161100	H	6.66437100	-2.74985200	-0.59389500
H	1.58018400	0.31132700	1.44313100	H	8.61223800	1.07056200	-0.93242500
N	3.29283500	1.40077200	0.72906600	C	8.78806100	-1.52075600	-1.80318900
C	3.20586200	2.73798900	0.09619300	H	8.41002500	-1.61011600	-2.83058100
C	2.12639200	2.53551500	-0.98695500	H	9.69748500	-0.91332800	-1.84003500
C	1.11540900	3.68720500	-1.18562400	H	9.06510700	-2.52734300	-1.47188000
				C	-1.30727900	3.89288800	-0.13435900
				C	-2.32766900	3.28035900	0.62581100
				C	-1.49663000	5.19657600	-0.65048400

C	-3.51340700	3.96902700	0.87540600
H	-2.20098000	2.26609600	0.97735100
C	-2.67892200	5.88026800	-0.38506800
H	-0.72456300	5.66688400	-1.25021100
C	-3.68623500	5.26627300	0.37749800
H	-4.30037100	3.46866500	1.42506700
H	-2.82530400	6.88187400	-0.77438600
H	-4.61297700	5.79776400	0.56858700
C	0.06943800	-5.02174400	0.76500500
H	1.03717200	-4.66987300	1.13562800
H	-0.31874300	-5.78861100	1.44481700
H	0.21801200	-5.46244000	-0.22577200
C	-2.71151100	-4.36044600	0.16272100
H	-2.95906000	-5.18541800	0.83994500
H	-3.48030700	-3.58872200	0.22295200
H	-2.65925400	-4.73003900	-0.86509700
C	-1.35733600	-3.04801600	2.38343500
H	-2.14731600	-2.29294300	2.38362400
H	-1.65898900	-3.89085200	3.01558300
H	-0.43444300	-2.61025100	2.77463200
H	0.04053200	-0.53860400	-3.06553000
H	1.57680400	-0.74356900	-2.10844100

IM14

SCF done: -2044.765932

C	1.16673900	1.36547300	-0.65152100
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C	-0.09384600	3.21750400	-0.48862600
C	0.28719400	0.73337900	-1.78586400
C	0.56213800	-0.60914100	-2.25055300
O	-0.56766700	1.51071700	-2.21421500
O	0.19845000	2.12050700	0.14629400
Au	-0.31062000	-1.99506500	-0.85448300
P	-1.09474300	-3.62062600	0.64336800
Sb	-3.88758900	-0.17201100	0.25015700
F	-3.37229900	-1.49143700	-1.06003800
F	-3.67239200	1.24006500	-1.02288600
F	-5.72951800	-0.37817700	-0.18695900
F	-4.29786000	1.12623000	1.61258400
F	-2.01193300	0.02733200	0.74536900
F	-4.00436900	-1.59684100	1.55077900
C	2.03576400	0.52861300	0.26654200
H	2.36471800	-0.38694700	-0.23403500
H	1.50078600	0.24583900	1.17551700
N	3.18090800	1.43038100	0.55724400
C	3.14219400	2.71964100	-0.16978100
C	2.04431500	2.50200900	-1.23697200
C	1.03537200	3.65921700	-1.39314100
H	2.89595900	3.54287000	0.51201700
H	4.11045200	2.94464800	-0.62902700
H	2.48118900	2.20366500	-2.19268900
H	1.43671200	4.62267300	-1.05590400
H	0.67644600	3.78175300	-2.41660900

S	4.32138400	1.09765500	1.72911500
O	4.79961900	2.41907100	2.22495500
O	3.71216900	0.05780000	2.60428900
C	5.68755700	0.33300800	0.85655000
C	5.68918300	-1.05401100	0.65281300
C	6.74347500	1.12496200	0.38823200
C	6.74214100	-1.63947500	-0.05200200
H	4.89249600	-1.66141600	1.06638800
C	7.78967700	0.52263400	-0.31542400
H	6.75491000	2.18775600	0.60004700
C	7.80336900	-0.86288500	-0.55406500
H	6.74903600	-2.71474300	-0.20351700
H	8.61353400	1.13358100	-0.67178300
C	8.92659400	-1.50559800	-1.33523200
H	8.64671900	-1.64262600	-2.38853200
H	9.83192200	-0.89112600	-1.31424600
H	9.17734800	-2.49398200	-0.93574800
C	-1.27537600	3.94037500	-0.14171100
C	-2.27410800	3.31847700	0.64694300
C	-1.46903800	5.26356200	-0.61609500
C	-3.43958900	4.01318000	0.96000400
H	-2.14423900	2.29535700	0.96991100
C	-2.63040700	5.95014200	-0.28660100
H	-0.71541200	5.74022400	-1.23370800
C	-3.61459100	5.32448900	0.50030400
H	-4.20937300	3.50709900	1.52806900

H	-2.78275700	6.96272100	-0.64312600
H	-4.52679700	5.86106000	0.74059300
C	0.02898100	-5.08451700	0.78110200
H	1.02320500	-4.75715700	1.10065900
H	-0.36155100	-5.80798600	1.50577800
H	0.12232400	-5.56966300	-0.19560600
C	-2.74350700	-4.34372900	0.25509400
H	-2.98933000	-5.13929300	0.96727200
H	-3.48528700	-3.54669000	0.32130400
H	-2.74476200	-4.74552100	-0.76202100
C	-1.25872300	-2.99963100	2.37123200
H	-2.01387300	-2.21040000	2.37392600
H	-1.57241400	-3.80538300	3.04447200
H	-0.30346300	-2.58949800	2.71172300
H	0.10961800	-0.79239800	-3.22579400
H	1.62230700	-0.87280200	-2.23385000

TS13

SCF done: -2044.727072

C	1.40975700	0.56494300	-0.94045900
C	0.47555100	2.63191100	-0.58490300
C	0.44310400	-0.17948800	-1.87273600
C	0.36651400	-1.59313900	-1.94382300
O	-0.23986600	0.59686100	-2.62115600
O	0.59217000	1.42551000	-0.03548000
Au	-1.04102400	-2.26418700	-0.42335300

P	-2.52344200	-3.28725100	1.06408300	C	7.23191600	-2.09365900	0.36491100
Sb	-3.73295900	0.76851900	-0.17796100	H	5.33662300	-1.94185700	1.39419900
F	-3.39873700	-0.72791000	-1.35494700	C	8.17262100	-0.01217700	-0.42496600
F	-2.52406000	1.86744900	-1.18891600	H	7.01038000	1.76422500	-0.00877500
F	-5.22803000	1.30308200	-1.22565700	C	8.27298900	-1.40814400	-0.28804600
F	-4.03160300	2.18414600	1.07869800	H	7.29857300	-3.17018300	0.49119700
F	-2.20532300	0.21289600	0.90140300	H	8.97249500	0.53510800	-0.91466400
F	-4.81642000	-0.41837500	0.89743300	C	9.48814500	-2.15112000	-0.79454600
C	2.43318500	-0.16542100	-0.08946500	H	9.22913200	-3.15946600	-1.13386700
H	2.79094500	-1.06699700	-0.60337000	H	9.96312200	-1.62302200	-1.62745100
H	2.04153900	-0.44682800	0.88883000	H	10.24184700	-2.25767900	-0.00268400
N	3.50658500	0.84594700	0.04765200	C	-0.27096000	3.63838500	0.13279000
C	3.48297100	1.90538800	-0.99590100	C	-1.16701400	3.27071300	1.15925900
C	2.18267600	1.60531000	-1.78889500	C	-0.10514100	5.00295000	-0.20091200
C	1.09757200	2.68194400	-1.84881700	C	-1.88984000	4.25516400	1.83078900
H	3.47050100	2.89132600	-0.52464000	H	-1.32774200	2.22472700	1.38270000
H	4.36346400	1.84550300	-1.64794500	C	-0.81855700	5.97889800	0.48813600
H	2.41809700	1.19927600	-2.77658700	H	0.59068800	5.29133900	-0.98089000
H	1.23671300	3.61613300	-2.38109700	C	-1.71350400	5.60468000	1.50256000
H	0.17156300	1.79485100	-2.41152400	H	-2.61463800	3.96136100	2.57940000
S	4.59856200	0.85697400	1.30927300	H	-0.68559000	7.02571500	0.23784000
O	5.00037000	2.27947200	1.49390700	H	-2.28019400	6.36661600	2.02795200
O	3.99029500	0.02749500	2.38669400	C	-1.98259400	-4.97607000	1.58798100
C	6.03824700	-0.02285800	0.70339700	H	-1.01853500	-4.91136700	2.10180900
C	6.12067400	-1.41244100	0.86525900	H	-2.72007400	-5.42723700	2.26146700
C	7.06808300	0.68496500	0.07050700	H	-1.86254100	-5.61420600	0.70704400

C	-4.20255200	-3.52985500	0.34821100
H	-4.84413500	-4.07313400	1.05109000
H	-4.62902800	-2.54401200	0.15124000
H	-4.13232300	-4.08551200	-0.59110200
C	-2.82048600	-2.38149000	2.63960600
H	-3.29435500	-1.42910900	2.39697400
H	-3.47643700	-2.96530300	3.29502900
H	-1.87058200	-2.18818200	3.14533000
H	-0.08159200	-1.95416100	-2.86939700
H	1.26611100	-2.12866300	-1.64386200

IM15

SCF done: -2044.762208

C	-0.10993500	1.50816500	1.14890400
C	1.21521700	3.37865700	0.94373600
C	0.29421700	0.33668200	2.03695800
C	-0.62137500	-0.56676400	2.59954900
O	1.54958400	0.23880300	2.36610200
O	1.07884900	2.04935500	0.56606600
Au	-0.46573400	-2.20158100	1.11096200
P	-0.35531700	-3.98131000	-0.38551600
Sb	3.08275600	-1.02989100	-0.76878300
F	2.69556100	-2.27666200	0.65476200
F	3.39936400	0.33650000	0.57957300
F	4.91825100	-1.52249500	-0.76077200
F	3.35462800	0.27576000	-2.13338700

F	1.19737900	-0.54650300	-0.71937100
F	2.63770900	-2.40783700	-2.03775400
C	-1.14708500	1.19465400	0.04682900
H	-1.68079800	0.25734200	0.25955900
H	-0.65023800	1.10479100	-0.91745300
N	-2.05149400	2.35788500	0.08770700
C	-2.15888600	2.90429500	1.45050900
C	-0.73812700	2.67412100	2.02963400
C	0.24445500	3.78221600	1.77666500
H	-2.42681900	3.96083400	1.41088100
H	-2.91462300	2.36659800	2.04594700
H	-0.80986600	2.40797200	3.09169400
H	0.13984700	4.77327400	2.19615000
H	2.15521800	0.66473100	1.69769000
S	-3.06131400	2.79040400	-1.16624200
O	-3.46932000	4.19623700	-0.89529800
O	-2.38268500	2.35399400	-2.41578900
C	-4.52686800	1.77055300	-0.97653500
C	-4.59365100	0.52695700	-1.61866700
C	-5.59011100	2.22039000	-0.18235000
C	-5.72310700	-0.27577400	-1.44051800
H	-3.78230900	0.21196700	-2.26476200
C	-6.71169700	1.40542600	-0.01377300
H	-5.54369500	3.20237700	0.27399300
C	-6.79729700	0.14722500	-0.63704000
H	-5.77894800	-1.23729700	-1.94250100

H	-7.53702500	1.75438800	0.59982500
C	-8.03218800	-0.71082300	-0.48049600
H	-7.79791400	-1.77485200	-0.58818400
H	-8.50257800	-0.56298700	0.49716600
H	-8.78238900	-0.46295400	-1.24354300
C	2.37098500	4.06990500	0.36737000
C	3.19200100	3.42711100	-0.58015000
C	2.66905400	5.39488300	0.74814300
C	4.28426800	4.10276500	-1.13200900
H	2.98644800	2.40967500	-0.88230700
C	3.76023500	6.06124000	0.19302000
H	2.04865900	5.90126200	1.48033000
C	4.57262900	5.41690500	-0.75078300
H	4.90717500	3.59479000	-1.86045000
H	3.97905000	7.08059500	0.49467400
H	5.42221000	5.93676900	-1.18202800
C	-1.71681500	-5.21607900	-0.20715200
H	-2.68398800	-4.72260400	-0.34241400
H	-1.61236500	-6.01402000	-0.95081800
H	-1.68890700	-5.65390100	0.79533200
C	1.20194500	-4.95351100	-0.27016100
H	1.19268400	-5.77314700	-0.99684100
H	2.03633600	-4.28169000	-0.47856500
H	1.31975100	-5.35654900	0.73948000
C	-0.42819600	-3.42209000	-2.13809200
H	0.44523900	-2.79358300	-2.33025700

H	-0.41072300	-4.28270400	-2.81609300
H	-1.33742900	-2.83943100	-2.31028000
H	-0.27367600	-1.07141600	3.49989000
H	-1.67014000	-0.28152300	2.59681000

IM16

SCF done: -2356.795349

C	3.39955400	0.94650300	-1.04691100
C	4.35612100	2.78056300	-2.03996600
C	1.99240000	0.50037500	-1.38602900
C	0.96695400	1.32491700	-1.63523600
O	1.93242500	-0.86451900	-1.41589500
O	3.45713200	2.38354000	-1.06872500
C	3.87751200	0.44030900	0.33548400
H	3.33169100	-0.46899200	0.62147900
H	3.74799000	1.20668400	1.09956700
N	5.30804900	0.16384100	0.11568300
C	5.54577400	-0.32068800	-1.25788400
C	4.47859700	0.44730700	-2.08712400
C	4.94849200	1.75264600	-2.66592000
H	6.56658500	-0.08638300	-1.56246200
H	5.38599200	-1.40687700	-1.33272000
H	4.04214800	-0.22090100	-2.83671100
H	5.69488000	1.82978900	-3.44479200
H	1.00610900	-1.14749000	-1.52112300
S	6.44714900	0.14265800	1.32712100

O	7.76937800	0.28686600	0.65676600	H	4.87096000	8.09369100	-2.61913200
O	5.95410800	1.07969600	2.37506200	H	-0.00130500	0.94715600	-1.94786300
C	6.39024600	-1.50903300	2.02861400	H	1.11656200	2.39462600	-1.60026100
C	5.51808000	-1.78193600	3.09091600	C	-3.19385800	-1.07038500	-0.08360100
C	7.20853400	-2.51667700	1.50207100	C	-3.81047500	-2.85342000	-1.38995100
C	5.45229600	-3.07760100	3.60757200	C	-1.74406100	-0.70478400	0.15980500
H	4.91986500	-0.98363200	3.51458200	C	-0.75294800	-1.58774600	0.33390400
C	7.13101700	-3.80761400	2.03024500	O	-1.60691000	0.65444200	0.17920200
H	7.90655900	-2.28286400	0.70668600	O	-3.31597100	-2.50286300	-0.14956800
C	6.25392900	-4.10986800	3.08702400	C	-4.13016900	-0.53024500	1.02476500
H	4.77717200	-3.28969500	4.43146300	H	-3.68097100	0.34274500	1.51727600
H	7.76560100	-4.58934100	1.62332600	H	-4.34336300	-1.30192600	1.76421200
C	6.19935400	-5.50168500	3.67509900	N	-5.35241500	-0.16704500	0.28380700
H	5.19223300	-5.74895600	4.02695500	C	-5.02150100	0.32369300	-1.06840500
H	6.49917300	-6.25815100	2.94281300	C	-3.77130200	-0.51831500	-1.44524100
H	6.87618300	-5.59292700	4.53546600	C	-4.06658100	-1.79756700	-2.17735700
C	4.49399300	4.23138600	-2.20399400	H	-5.86356700	0.15511200	-1.74084600
C	3.86555600	5.11310400	-1.30350100	H	-4.77592900	1.39664100	-1.05779800
C	5.25834000	4.76919800	-3.25950900	H	-3.04658700	0.11608700	-1.96668400
C	4.00262000	6.49577200	-1.45433000	H	-4.46966600	-1.83713900	-3.18030500
H	3.28210500	4.70854000	-0.48568900	H	-0.66013500	0.88844400	0.18534500
C	5.39247900	6.14958300	-3.40572000	S	-6.84361200	0.01421100	0.99868000
H	5.74193100	4.10558500	-3.96843300	O	-7.83903100	-0.00755800	-0.10916600
C	4.76499500	7.01980500	-2.50353500	O	-6.87225700	-0.93722800	2.14406500
H	3.51627200	7.16289300	-0.74970700	C	-6.85954900	1.67185300	1.68883500
H	5.98420300	6.54850700	-4.22345000	C	-6.39273400	1.88616800	2.99291100

C	-7.32361100	2.74203200	0.91356800
C	-6.37080300	3.18397700	3.50742200
H	-6.07418600	1.04363400	3.59566600
C	-7.29575000	4.03454400	1.44331100
H	-7.71763200	2.55593800	-0.07871300
C	-6.81916400	4.27732600	2.74356500
H	-6.00978500	3.35084700	4.51810700
H	-7.65633400	4.86483500	0.84336400
C	-6.82099800	5.67400800	3.32260300
H	-5.94616600	5.84530100	3.95907800
H	-6.82235400	6.43410200	2.53504700
H	-7.71176200	5.84249400	3.94278400
C	-3.95943700	-4.29530400	-1.61431000
C	-3.72339000	-5.20621000	-0.56656400
C	-4.34279400	-4.79490200	-2.87569000
C	-3.87022900	-6.58018300	-0.77637300
H	-3.43560700	-4.82986700	0.40725700
C	-4.48806200	-6.16674800	-3.08022000
H	-4.52382200	-4.10851200	-3.69599600
C	-4.25221500	-7.06619200	-2.03119100
H	-3.68940300	-7.27000100	0.04186300
H	-4.78465800	-6.53635600	-4.05664100
H	-4.36682000	-8.13329700	-2.19245400
H	0.25875100	-1.26901500	0.56264100
H	-0.96674700	-2.64669700	0.30787200

TS14

SCF done: -2356.749468

C	3.07322700	0.43631500	-0.92299300
C	4.01475900	2.12748200	-2.15011000
C	1.61801500	0.03394100	-1.03330500
C	0.54595300	0.94717200	-1.14155100
O	1.44787500	-1.24949200	-0.96156300
O	3.20122000	1.85565500	-1.06257400
C	3.71222500	-0.01494600	0.42358000
H	3.15760700	-0.86181400	0.84380900
H	3.73666800	0.80950600	1.13614600
N	5.07489900	-0.42276100	0.04699000
C	5.06572700	-1.01974800	-1.30102500
C	3.96840700	-0.21148500	-2.05643100
C	4.46025900	1.02035000	-2.76278700
H	6.04869900	-0.92022700	-1.76240600
H	4.79252700	-2.08164200	-1.24785600
H	3.39651900	-0.88234500	-2.70664300
H	5.12768700	0.99334100	-3.61315800
H	0.43004100	-1.48235400	-0.69163600
S	6.45526500	0.12595600	0.82419600
O	7.52434100	0.19633100	-0.21184500
O	6.04031100	1.29785300	1.64627700
C	6.90658700	-1.18401100	1.96143800
C	6.37854200	-1.18644900	3.25905000
C	7.78309300	-2.19229000	1.54427200

C	6.71496700	-2.22318600	4.13099000
H	5.73079300	-0.37909000	3.57994500
C	8.11016600	-3.22240900	2.42957100
H	8.21206500	-2.15756600	0.54978400
C	7.58244000	-3.25709400	3.73219200
H	6.30598000	-2.22706400	5.13704300
H	8.78989700	-4.00571000	2.10798700
C	7.96186000	-4.35903800	4.69500800
H	7.10659200	-4.67066700	5.30444700
H	8.34121700	-5.23921400	4.16683200
H	8.74802700	-4.02575400	5.38576700
C	4.22927500	3.55094700	-2.42525200
C	3.79898200	4.52732500	-1.50628100
C	4.87079100	3.96520300	-3.61020800
C	4.01022700	5.88395700	-1.76671900
H	3.31229100	4.21702600	-0.58994400
C	5.07988000	5.32022300	-3.86479200
H	5.19808700	3.22641700	-4.33400300
C	4.65010600	6.28575500	-2.94401800
H	3.67786300	6.62588500	-1.04786500
H	5.57487200	5.62518700	-4.78113200
H	4.81346300	7.33973400	-3.14438300
H	-0.20059400	0.61920700	-1.86982500
H	0.84654300	1.98266400	-1.26469200
C	-3.19897400	-0.92644000	-0.10933900
C	-3.84677700	-2.49935500	-1.65019900

C	-1.74313900	-0.67089700	0.29321000
C	-0.83064200	-1.70575100	0.42263600
O	-1.47466700	0.58876400	0.43699200
O	-3.42900200	-2.33020100	-0.34836000
C	-4.17384800	-0.43092100	0.98569100
H	-3.69773800	0.35370500	1.58707600
H	-4.49702600	-1.25171100	1.62571400
N	-5.30966000	0.10198400	0.20962900
C	-4.83945100	0.70861700	-1.05002500
C	-3.62548600	-0.18614500	-1.43325000
C	-3.95592500	-1.34589100	-2.32893400
H	-5.63556000	0.68434100	-1.79519100
H	-4.51691400	1.74865700	-0.89411400
H	-2.81813700	0.44623000	-1.81879400
H	-4.27801600	-1.24218000	-3.35631100
H	-0.28917100	0.82355000	-0.14599900
S	-6.87148700	0.17787800	0.76631000
O	-7.74096400	0.30629900	-0.43730400
O	-7.01679700	-0.92042700	1.76259300
C	-7.00224100	1.72445200	1.67077500
C	-6.69592700	1.75749800	3.03753500
C	-7.39864600	2.88943600	1.00191600
C	-6.76539700	2.97037800	3.72616300
H	-6.42741000	0.84162400	3.55093900
C	-7.46365100	4.09483000	1.70485900
H	-7.66907100	2.84210700	-0.04649400

C	-7.14802200	4.15639900	3.07377800
H	-6.52746100	2.99644000	4.78558600
H	-7.77128500	4.99846300	1.18676100
C	-7.25272300	5.45846600	3.83536100
H	-6.51277600	5.51220700	4.64088700
H	-7.10232600	6.32056800	3.17752400
H	-8.24404300	5.56759300	4.29598400
C	-4.08724200	-3.88967100	-2.05309800
C	-3.98468700	-4.93071400	-1.11035700
C	-4.42800700	-4.20963900	-3.38314900
C	-4.21810600	-6.25552800	-1.48968100
H	-3.73115500	-4.69166600	-0.08504800
C	-4.66014600	-5.53298900	-3.75714600
H	-4.50964600	-3.42126000	-4.12381500
C	-4.55600000	-6.56285800	-2.81184000
H	-4.13932500	-7.04670700	-0.75071400
H	-4.92288600	-5.76316800	-4.78487200
H	-4.73853500	-7.59191500	-3.10471500
H	-0.00454200	-1.52992900	1.11009300
H	-1.19215900	-2.72436000	0.35592100

Cartesian Coordinates for the Stationary Points Given in Fig. 3.

IM17

SCF done: -2121.198478

				H	5.71755400	1.89892600	-0.98889700
				H	4.11246200	0.83241300	-2.43565100
C	2.58752700	0.69105800	-0.84853600	H	3.16368100	3.60590400	-1.91286200
C	1.43309600	2.30471500	-1.63560200	H	2.78887900	2.62262200	-3.34546100
C	1.62984100	0.04871200	-1.82593000	S	5.69068000	0.40517000	1.58304700
C	1.46044600	-1.23807300	-2.17202700	O	6.40457100	1.69623300	1.79221700
O	0.94305700	1.08915100	-2.36134600	O	4.94048800	-0.30714500	2.65551200
O	1.75849300	1.77447800	-0.37108100	C	6.88590300	-0.75401900	0.91386800
Au	-2.62526200	-1.97848700	-0.67433800	C	6.66178800	-2.13053600	1.04108200
P	-4.80744600	-2.03436100	-1.27661900	C	8.03870300	-0.27417200	0.27802800
Sb	-3.16973500	0.77073800	1.96130700	C	7.58550800	-3.02695800	0.49783100
F	-3.61810800	0.69879400	0.07028700	H	5.79274800	-2.48738600	1.58151100
F	-2.90058100	2.65344300	1.79124800	C	8.95184900	-1.18330900	-0.25956700
F	-5.03745400	0.93875100	2.32966700	H	8.22491200	0.79261000	0.23492100
F	-2.66570700	0.80843000	3.79160000	C	8.73792400	-2.57099500	-0.16647300
F	-1.30927500	0.45984600	1.41942500	H	7.41742600	-4.09461000	0.60291000
F	-3.33920800	-1.15542200	2.01377100	H	9.84977400	-0.81258400	-0.74524000
C	3.29422300	-0.04395200	0.27122800	C	9.72323600	-3.54549500	-0.77087100
H	3.43821200	-1.10385400	0.02950300	H	9.55801300	-3.65618700	-1.85120900
H	2.73747900	0.02745900	1.20898400	H	10.75597100	-3.20669800	-0.63464200
N	4.60081100	0.66462400	0.34681800	H	9.63032500	-4.53910300	-0.32169200
C	4.70428200	1.81871300	-0.58663700	C	0.36254800	3.34729400	-1.59731500
C	3.66597700	1.46955600	-1.66710700	C	-0.67867200	3.24973100	-0.65889600
C	2.81973900	2.62529700	-2.25384100	C	0.37671700	4.41269600	-2.51215000
H	4.45797800	2.75730300	-0.07741200	C	-1.68733400	4.21774500	-0.63199200

H	-0.70260500	2.43192000	0.05090700
C	-0.63654000	5.37555400	-2.48648300
H	1.17345600	4.49340100	-3.24450500
C	-1.66703400	5.27963000	-1.54440200
H	-2.47717000	4.13071800	0.10411000
H	-0.61824600	6.19722800	-3.19544900
H	-2.45093300	6.03027700	-1.51986300
C	-5.38083400	-3.55474700	-2.14630100
H	-5.21919300	-4.42738000	-1.50655700
H	-6.44638600	-3.47815800	-2.38939300
H	-4.80883300	-3.69053800	-3.06890200
C	-5.24066000	-0.62963500	-2.38269200
H	-6.31416300	-0.62665300	-2.60149400
H	-4.96194500	0.29353100	-1.86738300
H	-4.67770900	-0.69802800	-3.31792800
C	-5.91363000	-1.85278100	0.18222000
H	-5.68537000	-0.91820700	0.69914300
H	-6.96093200	-1.85106100	-0.13991000
H	-5.74529600	-2.67628000	0.88130600
H	0.78541100	-1.51370400	-2.97478400
H	2.08981800	-2.00692100	-1.74000000
H	-0.70873700	-0.89536800	0.64120100
O	-0.60747700	-1.68657800	0.05618300
H	0.02310700	-1.43834100	-0.65687100

TS15

SCF done: -2121.179354

C	2.27873800	1.29124900	-1.01286500
C	1.37843900	3.31387600	-1.26166100
C	1.37065500	0.71611000	-2.14501100
C	1.33135100	-0.69345000	-2.38582500
O	0.72242600	1.60244400	-2.72377900
O	1.42993100	2.32047100	-0.41733800
Au	-2.09782700	-2.16266700	-0.78041200
P	-4.32859800	-2.47095200	-1.03936700
Sb	-2.65489500	0.72377500	1.83206200
F	-3.50147800	0.45805400	0.10603000
F	-2.76916600	2.62113500	1.53692700
F	-4.39510000	0.66311400	2.61991300
F	-1.79317200	1.01889200	3.50400100
F	-0.92516100	0.71841700	0.92642600
F	-2.49226700	-1.18435900	2.03218300
C	2.88768300	0.43350800	0.08691100
H	2.88558900	-0.62932200	-0.16665300
H	2.33204000	0.56429900	1.02237700
N	4.28189400	0.94980900	0.17369300
C	4.44723500	2.24977000	-0.51887100
C	3.40964500	2.13971800	-1.65269200
C	2.67045800	3.43883000	-2.04232200
H	4.22092800	3.09925800	0.14269600
H	5.47099500	2.36303600	-0.87744000
H	3.83853600	1.62825700	-2.51745300

H	3.20674800	4.34221200	-1.72405600
H	2.47653200	3.52107600	-3.11283400
S	5.32925500	0.44248800	1.38609400
O	6.49781500	1.36295100	1.27701900
O	4.55621100	0.27632900	2.64846100
C	5.82454500	-1.19180200	0.85127500
C	5.18021100	-2.31814000	1.37594700
C	6.86990200	-1.32641700	-0.07280100
C	5.57190800	-3.58923900	0.94504700
H	4.40309600	-2.19783200	2.12155700
C	7.25170500	-2.60209900	-0.48718600
H	7.38532000	-0.44540900	-0.43743600
C	6.60513900	-3.75206500	0.00684700
H	5.07437700	-4.46453800	1.35073800
H	8.06794800	-2.71135000	-1.19514300
C	7.00999400	-5.12753100	-0.47153100
H	6.53725000	-5.36469400	-1.43422400
H	8.09342700	-5.19836900	-0.61602600
H	6.71017300	-5.90293600	0.23990900
C	0.31378900	4.26624500	-1.15195300
C	-0.81240700	3.96660700	-0.34818300
C	0.38124200	5.49903500	-1.84640600
C	-1.84303600	4.89631800	-0.22987900
H	-0.88271600	3.01399100	0.16003800
C	-0.65482700	6.41834100	-1.72189100
H	1.23706100	5.72889200	-2.47218700

C	-1.76385200	6.11807100	-0.91231600
H	-2.69514000	4.64815300	0.38972700
H	-0.60687200	7.36471900	-2.24907400
H	-2.56946500	6.83940300	-0.81974100
C	-4.85826000	-4.08320800	-1.76987900
H	-4.50407900	-4.90484200	-1.13989400
H	-5.94980100	-4.13563600	-1.85142300
H	-4.41603300	-4.19653200	-2.76446900
C	-5.11224900	-1.19135100	-2.10923600
H	-6.19816500	-1.33050300	-2.15612400
H	-4.87867300	-0.21542400	-1.67589800
H	-4.69419400	-1.24162400	-3.11901500
C	-5.24205400	-2.35325600	0.55663300
H	-5.06156200	-1.37084500	0.99747400
H	-6.31659400	-2.49512200	0.39556200
H	-4.87131500	-3.11137900	1.25188200
H	0.88181100	-0.95164100	-3.34409100
H	2.26930300	-1.21835900	-2.19864900
H	-0.18010800	-0.99990300	0.21006200
O	-0.09468900	-1.73052200	-0.43110500
H	0.56698700	-1.17844900	-1.44392900

IM18

SCF done: -2121.198122

C	1.04170200	1.78740500	-0.92752400
C	-0.43140000	3.55224900	-1.06729100

C	1.36448200	1.29505400	-2.36578400	O	3.66510900	1.62754100	3.14994300
C	2.40465000	0.22596600	-2.52770700	O	2.72021900	-0.67206600	2.31038700
O	0.81308600	1.86119600	-3.28984700	C	4.79150000	0.43931000	1.07467100
O	-0.34900200	2.27652400	-0.99443400	C	4.84537500	-0.58804100	0.11843900
Au	0.02800800	-2.97545800	-0.51103900	C	5.89366500	1.27566200	1.29133400
P	-2.03282200	-3.90852100	-0.74864200	C	6.01134800	-0.74885400	-0.63396800
Sb	-2.96066100	0.30136500	1.22024800	H	3.99824800	-1.25031500	-0.03997800
F	-2.44074000	0.17308100	-0.64928100	C	7.05129700	1.09640000	0.52823900
F	-4.38918400	1.45894300	0.65497200	H	5.84637200	2.03687000	2.06110800
F	-4.08384700	-1.24197300	0.97496900	C	7.13020500	0.08438900	-0.44319500
F	-3.46938800	0.46543100	3.04603000	H	6.05669400	-1.54337800	-1.37315600
F	-1.79367300	1.83841700	1.35608700	H	7.90738100	1.74273900	0.69824700
F	-1.48119900	-0.84930400	1.65537800	C	8.39556300	-0.13085500	-1.24209300
C	1.16927900	0.82522500	0.26779400	H	8.17329700	-0.38715300	-2.28381500
H	1.45306000	-0.19790700	-0.00511300	H	9.02940500	0.76145500	-1.23871600
H	0.21570200	0.78017200	0.80032900	H	8.98790500	-0.95644500	-0.82538400
N	2.21386100	1.47735000	1.09292500	C	-1.71453100	4.17208700	-1.17389900
C	2.16668400	2.93457500	0.92581000	C	-2.88522900	3.37337100	-1.13936900
C	1.85787500	3.07356300	-0.58606300	C	-1.82065800	5.58487500	-1.26323600
C	0.91546300	4.21852400	-0.99787600	C	-4.13549000	3.98463100	-1.16764800
H	1.36503700	3.37354800	1.53840700	H	-2.80293800	2.29786100	-1.07399500
H	3.11108500	3.39851000	1.21560400	C	-3.07463500	6.17892500	-1.31745400
H	2.79168300	3.10008100	-1.15296900	H	-0.92928600	6.20231900	-1.28899800
H	0.91340400	5.06007200	-0.29831000	C	-4.23097000	5.37921500	-1.26117400
H	1.15703900	4.61248500	-1.99266300	H	-5.02202500	3.36879600	-1.08747800
S	3.30832400	0.67215700	2.06348900	H	-3.16301100	7.25695900	-1.38948500

H	-5.20781500	5.85136400	-1.28211000
C	-2.02805900	-5.56664400	-1.56839700
H	-1.41336800	-6.26074000	-0.98704700
H	-3.04580500	-5.96528300	-1.64814300
H	-1.59517000	-5.47970400	-2.56978100
C	-3.22727300	-2.91524100	-1.73996700
H	-4.19857700	-3.41988700	-1.79129600
H	-3.34915000	-1.93893100	-1.26761800
H	-2.83449200	-2.77318300	-2.75130600
C	-2.88114500	-4.18744400	0.86138200
H	-3.05583400	-3.21512700	1.32674700
H	-3.84302300	-4.69051600	0.71196200
H	-2.24624000	-4.79329300	1.51416500
H	2.56921500	0.05170800	-3.59161400
H	3.34466900	0.53862200	-2.05609300
H	2.02912400	-2.07624400	0.65302500
O	1.86946200	-2.12182600	-0.30385300
H	2.11374100	-0.70043700	-2.01287400

IM19

SCF done: -2121.202369

C	-1.72540000	0.31955000	1.86100300
C	-1.87825300	2.45963000	0.97669400
C	-0.50886100	-0.26582200	2.61400500
C	0.78399500	0.50882200	2.66034900
O	-0.76066000	-1.20502700	3.34729300

O	-1.29008800	1.32301400	0.86092100
Au	1.85621400	-2.17461000	0.23124900
P	3.95221000	-3.02014400	0.02400900
Sb	3.14564800	1.74138700	-0.71946900
F	3.61409200	0.43514200	0.62337500
F	2.18527900	2.74192900	0.62046200
F	4.75265100	2.70499600	-0.38394800
F	2.60406900	3.01362200	-2.05466200
F	1.46121100	0.81662700	-1.05254300
F	3.99661900	0.64001700	-2.04101600
C	-2.58986900	-0.75217700	1.16480900
H	-2.37236100	-1.71480400	1.62854800
H	-2.37652700	-0.82236500	0.10156600
N	-4.00493400	-0.37453700	1.45861500
C	-3.98756500	0.26309500	2.80416600
C	-2.69427800	1.11190300	2.80316200
C	-2.83592500	2.49832700	2.13061400
H	-4.90055200	0.83262000	2.97634400
H	-3.91109300	-0.53345700	3.55013400
H	-2.28193200	1.20759300	3.80989100
H	-3.84746800	2.69109300	1.75428500
H	-2.57719400	3.32418900	2.80177900
S	-4.91381300	0.37411700	0.23348700
O	-6.07210200	1.00912200	0.93231800
O	-4.02044400	1.22126900	-0.62662400
C	-5.46585200	-1.00501800	-0.75173700

C	-4.94750200	-1.18537200	-2.03795900
C	-6.43804600	-1.87217400	-0.23262300
C	-5.39785800	-2.26465400	-2.80446100
H	-4.21355600	-0.49029200	-2.42755600
C	-6.87591400	-2.94050500	-1.01229000
H	-6.84348800	-1.70540300	0.75842700
C	-6.35952200	-3.15851200	-2.30580400
H	-4.99708500	-2.41133000	-3.80231300
H	-7.62913400	-3.61530700	-0.61712500
C	-6.82476400	-4.33881600	-3.12660500
H	-6.53744900	-4.23442300	-4.17689700
H	-6.38483000	-5.27352400	-2.75448300
H	-7.91356600	-4.45337200	-3.08120600
C	-1.54050000	3.53077200	0.09276100
C	-0.46924300	3.38933400	-0.82485600
C	-2.25690000	4.75452900	0.16122300
C	-0.11444600	4.45951000	-1.64282400
H	0.08773800	2.46400600	-0.87313700
C	-1.90764700	5.80579900	-0.67577700
H	-3.08423700	4.86727200	0.85315400
C	-0.83357600	5.65973500	-1.57249400
H	0.73607800	4.34927700	-2.30347500
H	-2.45855300	6.73862500	-0.63454400
H	-0.55522100	6.49074900	-2.21258800
C	4.15207700	-4.85510700	0.13248800
H	3.55785400	-5.33454100	-0.65155200

H	5.20365100	-5.14018200	0.01422500
H	3.78950200	-5.20705800	1.10322900
C	5.11619900	-2.35542100	1.29104000
H	6.14017500	-2.69914100	1.10567300
H	5.07102100	-1.26388600	1.24529900
H	4.79927300	-2.67622700	2.28824000
C	4.73263700	-2.56452400	-1.58282200
H	4.66871400	-1.47981700	-1.71358700
H	5.78072000	-2.88351100	-1.61222200
H	4.18581200	-3.04007200	-2.40316000
H	0.72724200	1.22281900	3.49521300
H	1.59672400	-0.18612000	2.87187900
O	0.05399200	-1.23382500	0.39942100
H	0.22350800	-0.46664100	-0.17146400
H	1.01091000	1.05987500	1.75144200

C

SCF done: -1254.87717

C	-1.08897400	0.86609800	1.61920300
C	0.65573900	3.08655500	-0.26887100
C	-0.99328700	1.01058800	3.15663500
C	0.19206200	0.37807700	3.84591000
O	-1.86433900	1.60581900	3.76626400
O	0.78976900	2.01547000	-0.85632700
C	-2.29593200	-0.04541100	1.25910600
H	-3.10828200	0.07630000	1.98885100

H	-1.99242800	-1.09152900	1.21129200
N	-2.68910400	0.44530900	-0.07974200
C	-2.25813500	1.83941300	-0.34150100
C	-1.50422400	2.21717700	0.95865400
C	-0.41361400	3.29086300	0.80133500
H	-1.62830900	1.87299000	-1.23182800
H	-3.11694600	2.50573100	-0.49782400
H	-2.23738100	2.63432700	1.65739400
H	-0.90371300	4.25179600	0.59786200
H	0.09879400	3.43290200	1.76393500
S	-3.63157900	-0.41895600	-1.13890900
O	-3.34956300	0.13135100	-2.49497200
O	-3.45439400	-1.85505400	-0.78401600
C	-5.32671100	0.01838100	-0.73922200
C	-6.00755000	-0.68769600	0.26250000
C	-5.95460600	1.06661600	-1.42298500
C	-7.31169800	-0.31798100	0.59494400
H	-5.52698300	-1.52781500	0.75035800
C	-7.26127400	1.42398100	-1.07869300
H	-5.43248700	1.57052300	-2.22791300
C	-7.95675800	0.74639500	-0.06247100
H	-7.84166700	-0.86916000	1.36634500
H	-7.75166100	2.23161000	-1.61417800
C	-9.36125000	1.15228700	0.32315300
H	-9.98739500	0.27809400	0.53275200
H	-9.35852400	1.77368900	1.22892300

H	-9.84281800	1.73164300	-0.47073000
C	1.55601200	4.23033200	-0.60480400
C	2.49937500	4.04660100	-1.63602700
C	1.51249600	5.46672400	0.06986400
C	3.37242300	5.07506600	-1.98860000
H	2.52720900	3.09036100	-2.14507100
C	2.39191800	6.49404100	-0.28189600
H	0.80329000	5.63356100	0.87249000
C	3.32059600	6.30151300	-1.31181100
H	4.09216400	4.92434700	-2.78629700
H	2.35294200	7.44147800	0.24531600
H	4.00071900	7.10196000	-1.58494700
H	0.09959000	0.51294700	4.92416300
H	0.25667900	-0.68524000	3.59300200
O	0.12648900	0.32760200	1.15678000
H	0.28862100	0.64356000	0.24905700
H	1.12048300	0.82485100	3.47733500

TS16

SCF done: -2121.197597

C	1.01930900	3.52998400	0.74729600
C	-1.15970100	2.81975200	0.82106300
C	1.44018200	4.65189400	1.71076300
C	2.92819100	4.84736800	1.90989600
O	0.59843800	5.29478700	2.30073600
O	-0.38962700	3.77138000	0.39647500

Au	-1.78641100	-0.38292600	-1.49131200	C	3.61504200	-1.14695300	-1.05225900
P	-2.67425900	-2.46548000	-1.69898800	C	6.37363300	-0.63827300	-1.01236700
Sb	-0.05361100	-2.20197600	2.12587800	H	5.85979000	1.34794500	-1.70639000
F	-1.50201700	-1.01144900	1.57512100	C	4.51067300	-2.14019300	-0.65380300
F	-0.85966800	-2.34832100	3.84650800	H	2.55034200	-1.34782000	-1.06749100
F	-1.09866100	-3.67577900	1.45810600	C	5.89836900	-1.90424000	-0.62658800
F	1.38833300	-3.34830900	2.60635500	H	7.44179900	-0.44452800	-1.00792500
F	0.92282400	-0.63338100	2.68962600	H	4.12307000	-3.10955400	-0.35667100
F	0.69986200	-1.98696400	0.35431300	C	6.85029000	-2.99102000	-0.18306700
C	1.81719100	3.39337100	-0.55915700	H	7.89326500	-2.69436900	-0.32807000
H	2.59030000	4.15482100	-0.66261300	H	6.71263600	-3.22460800	0.88038100
H	1.12160000	3.45168800	-1.40634800	H	6.68135500	-3.91996900	-0.74028600
N	2.49020200	2.06247400	-0.42710500	C	-2.58075100	2.90456400	0.60328500
C	1.67352500	1.16301000	0.45155500	C	-3.14366500	4.01820500	-0.05886100
C	1.02990000	2.13479600	1.45195800	C	-3.41508800	1.86202200	1.06805500
C	-0.45621000	1.87462400	1.73022100	C	-4.52143000	4.09258000	-0.23987400
H	0.89495900	0.65103500	-0.11850300	H	-2.49607400	4.80822500	-0.41900100
H	2.30584500	0.42479900	0.94148300	C	-4.79399200	1.94795200	0.88006600
H	1.60369400	2.16721900	2.38002200	H	-2.98544300	0.98732900	1.54393400
H	-0.77023100	0.84800300	1.54658800	C	-5.34698000	3.05957300	0.23046000
H	-0.74174100	2.11817500	2.76390300	H	-4.95581600	4.94771600	-0.74549400
S	3.00771700	1.41023500	-1.91634300	H	-5.43588200	1.14932500	1.23448200
O	1.82850500	0.78959900	-2.60568700	H	-6.42096700	3.12132300	0.08712000
O	3.76468800	2.50799400	-2.58458300	C	-3.71422000	-2.72952100	-3.20419000
C	4.11941900	0.11221900	-1.41131500	H	-3.11726100	-2.53163100	-4.09981400
C	5.49422200	0.37434400	-1.40200600	H	-4.09077200	-3.75792100	-3.24097700

H	-4.55994000	-2.03497400	-3.19413400
C	-3.75321100	-2.96455600	-0.29004400
H	-4.15875600	-3.97001200	-0.44920000
H	-3.14489500	-2.96050500	0.61723200
H	-4.57642700	-2.25274300	-0.17934400
C	-1.39489500	-3.78807600	-1.78004100
H	-0.82867600	-3.76972200	-0.84663500
H	-1.86111100	-4.77179900	-1.90501000
H	-0.71609000	-3.59418100	-2.61551200
H	3.10790100	5.21634600	2.92096800
H	3.49953400	3.93391800	1.72417900
H	-0.15724300	1.43783000	-1.82870500
O	-0.93771900	1.46828900	-1.25014300
H	3.28419500	5.60842900	1.20492700

IM20

SCF done: -2121.228424

C	2.29484900	2.22982900	-0.80107900
C	0.11258600	2.39539000	0.09763200
C	2.94021500	3.47707200	-1.45367500
C	4.45638800	3.53113700	-1.55777700
O	2.25705000	4.40140700	-1.83957000
O	0.89040000	2.23074600	-1.06517400
Au	-0.65516800	-0.77546200	-0.60257600
P	-1.05915400	-2.85054300	-1.39036900
Sb	-3.79230100	-0.57618500	1.77422200

F	-3.47716100	-0.11268800	-0.07579000
F	-5.46464700	-1.36638600	1.32765600
F	-2.86867400	-2.23783300	1.41100700
F	-3.95309000	-1.02896900	3.61377300
F	-4.54901700	1.15979300	2.05478700
F	-2.03567600	0.23103700	2.17384300
C	2.91249900	0.89642700	-1.25192200
H	3.96197600	1.01309100	-1.55221700
H	2.35199100	0.47163400	-2.08542300
N	2.79248900	0.04454700	-0.05014100
C	2.66904800	0.81344300	1.21578500
C	2.43208400	2.28041300	0.75633500
C	1.09734100	2.92745400	1.15826800
H	1.83646600	0.42325100	1.80158600
H	3.58792600	0.74035800	1.81309800
H	3.27535400	2.90380700	1.06704900
H	0.77555600	2.68958200	2.17556100
H	1.16587100	4.01555700	1.06556500
S	3.00650400	-1.60231100	-0.09614800
O	2.24205600	-2.18080400	1.04511500
O	2.75624400	-2.00918200	-1.51195200
C	4.74550600	-1.88771300	0.23733100
C	5.66206000	-1.89787400	-0.82326000
C	5.17601300	-2.08342800	1.55709800
C	7.01900300	-2.08438700	-0.55108800
H	5.31101600	-1.78678800	-1.84257900

C	6.53712800	-2.26744200	1.81049700
H	4.45205500	-2.11483300	2.36296400
C	7.47891900	-2.27042500	0.76542500
H	7.73032000	-2.09660800	-1.37141400
H	6.87200100	-2.42156400	2.83182900
C	8.94490100	-2.50671000	1.04777000
H	9.57951100	-2.05906400	0.27647600
H	9.23905100	-2.08903700	2.01616100
H	9.17109400	-3.58114600	1.07461900
C	-1.10348500	3.26252800	-0.18786800
C	-0.99624900	4.31580500	-1.11377100
C	-2.31947000	3.06297300	0.48563600
C	-2.09203900	5.14893900	-1.35784900
H	-0.06218400	4.47128400	-1.63922900
C	-3.41385900	3.89631300	0.23345400
H	-2.45683000	2.26076900	1.19558000
C	-3.30391800	4.94218000	-0.68742400
H	-1.99926700	5.95550100	-2.07865000
H	-4.34586300	3.70118400	0.75223100
H	-4.15481600	5.58634300	-0.88591900
C	-0.08203900	-3.31172700	-2.87941600
H	0.97804600	-3.15298000	-2.66004500
H	-0.25918800	-4.35901300	-3.14846700
H	-0.36676100	-2.66968700	-3.71867700
C	-2.83096100	-3.10965100	-1.80601300
H	-3.01043400	-4.14537000	-2.11465700

H	-3.41784100	-2.87831500	-0.91427000
H	-3.13076100	-2.42899700	-2.60761300
C	-0.66307600	-4.10042100	-0.10264400
H	-1.32126100	-3.91488800	0.75061900
H	-0.81873700	-5.11581300	-0.48384300
H	0.37393900	-3.97333600	0.21987700
H	4.76510600	4.57645900	-1.60727400
H	4.96505400	3.02823600	-0.73060200
H	-0.92618600	1.01487600	1.24664000
O	-0.26766100	1.05461400	0.51321600
H	4.77328500	3.04055500	-2.48596700

IM21

SCF done: -2197.674808

C	2.42578300	2.77380200	-0.22048900
C	0.08372400	2.76508900	0.13493800
C	3.13466200	4.04822800	-0.73939800
C	4.59771200	4.25122400	-0.37276400
O	2.53707300	4.85890100	-1.41240100
O	1.13664700	2.69039800	-0.81467300
Au	-1.12166300	0.06341700	1.91859300
P	-1.63935900	-1.68361400	3.26175500
Sb	-3.35784400	2.36415800	4.21572300
F	-3.81132800	1.14967800	2.77786100
F	-5.10488800	2.18635000	4.95060600
F	-2.75968700	0.81594800	5.21598100

F	-2.79277600	3.52268300	5.61799600	H	6.70805200	-2.74911800	-1.73207000
F	-3.87621600	3.83765000	3.10627700	H	6.71512200	-2.72349600	2.57047100
F	-1.56032900	2.46081500	3.45056100	C	8.27777300	-3.37751200	0.42524000
C	3.20581300	1.47565700	-0.50762100	H	8.74305500	-3.31818700	-0.56294900
H	4.29132600	1.63716500	-0.51544600	H	8.92619900	-2.85568100	1.13800000
H	2.90170600	1.05084600	-1.46530500	H	8.25926200	-4.43503200	0.71953800
N	2.81590000	0.59209800	0.61011000	C	-1.05958900	3.59953600	-0.40859000
C	2.48584100	1.36161600	1.83988300	C	-0.96950200	4.25410700	-1.64666900
C	2.18966400	2.80167000	1.32751900	C	-2.22146900	3.73865600	0.36932000
C	0.73482800	3.28682200	1.42105500	C	-2.04603300	5.02056500	-2.10891100
H	1.62885300	0.91189300	2.34120000	H	-0.05464700	4.18581000	-2.22130600
H	3.33565900	1.36419100	2.53429000	C	-3.28791000	4.51421600	-0.09105400
H	2.86023800	3.50597000	1.82705200	H	-2.29182700	3.27081000	1.34084100
H	0.19768400	2.96634400	2.31547900	C	-3.20627700	5.14934900	-1.33666600
H	0.71338900	4.38030500	1.39242400	H	-1.97176900	5.52471900	-3.06776000
S	2.63300200	-1.04310300	0.43814900	H	-4.16523700	4.61955300	0.53711800
O	1.93997500	-1.52920100	1.66545300	H	-4.03584300	5.75010300	-1.69691000
O	2.06608100	-1.29282300	-0.93178000	C	-1.07208600	-3.26682500	2.50680100
C	4.27992000	-1.74351400	0.41612100	H	-0.00454600	-3.18611100	2.28205900
C	4.91540900	-2.01560500	-0.80080600	H	-1.25024800	-4.10694000	3.18761500
C	4.92224000	-2.00159800	1.63640500	H	-1.61115100	-3.44004200	1.57039900
C	6.21344500	-2.53451200	-0.78992600	C	-3.42817800	-1.89780100	3.61725200
H	4.39448300	-1.84219300	-1.73464600	H	-3.58647000	-2.79308100	4.22868100
C	6.21665800	-2.51995200	1.62756000	H	-3.77300700	-1.01155400	4.15094200
H	4.40671800	-1.81622000	2.57165200	H	-3.98679600	-1.98347800	2.68160500
C	6.88409500	-2.79339100	0.41747900	C	-0.81577500	-1.61249600	4.90497800

H	-1.16988900	-0.71643600	5.42046700
H	-1.06807000	-2.50181500	5.49382300
H	0.26838100	-1.56015100	4.77067500
H	4.80522500	5.32210600	-0.33743900
H	4.87954900	3.78448100	0.57463000
H	-0.42035600	0.91305000	-0.51879600
O	-0.36151600	1.40120700	0.35855900
H	5.22750700	3.81583600	-1.15823300
H	-0.14339500	0.35375200	-2.56889800
O	-0.32876700	-0.12949600	-1.75382700
H	0.48464100	-0.63715200	-1.55027300

TS17

SCF done: -2197.64189

C	2.38583700	2.63183100	-0.21067500
C	-0.17394800	2.59661700	0.28215500
C	3.09591800	3.91874400	-0.70313500
C	4.52660100	4.17171500	-0.24638000
O	2.53262800	4.70559700	-1.43205300
O	1.12943500	2.50191600	-0.84905000
Au	-1.08471800	0.04154300	2.02593700
P	-1.53464300	-1.60310000	3.51714000
Sb	-3.63340000	2.40228700	3.84647200
F	-3.82368200	1.10037000	2.41568400
F	-5.40797500	2.02507600	4.43261200
F	-2.96990400	0.95708500	4.96078500

F	-3.34033400	3.64714600	5.25762000
F	-4.22884200	3.76837000	2.65063100
F	-1.80024200	2.66225600	3.24724600
C	3.25089100	1.36759500	-0.41523900
H	4.31992900	1.58869500	-0.31148400
H	3.09091300	0.91855800	-1.39800700
N	2.80031300	0.47296000	0.66858500
C	2.37772800	1.24161400	1.87219800
C	2.09337700	2.67650200	1.33233300
C	0.65038500	3.18862900	1.43023500
H	1.49741300	0.77930600	2.31860900
H	3.18125900	1.25884500	2.61861900
H	2.76397400	3.37731400	1.83801800
H	0.15741000	2.95101300	2.37585800
H	0.65479300	4.27803900	1.32952300
S	2.63711600	-1.16187800	0.47462500
O	2.02318600	-1.67901400	1.72766400
O	1.98415500	-1.39240400	-0.86597300
C	4.28649000	-1.83268600	0.32109400
C	4.80901900	-2.14658700	-0.93885700
C	5.04000500	-2.03918700	1.48658100
C	6.10778600	-2.65565700	-1.02813900
H	4.20221700	-2.01181500	-1.82594900
C	6.33321400	-2.54817200	1.37730000
H	4.61170800	-1.82173400	2.45836000
C	6.88880400	-2.86387900	0.12141400

H	6.51579900	-2.90216600	-2.00324100
H	6.91903300	-2.71145200	2.27666500
C	8.28160500	-3.44083800	0.02141200
H	8.67549000	-3.36395500	-0.99617200
H	8.97659000	-2.92841500	0.69553500
H	8.28654400	-4.50344600	0.29793600
C	-1.17243700	3.52362600	-0.37458500
C	-0.79897000	4.57780200	-1.22791300
C	-2.52540900	3.36138300	-0.02537000
C	-1.77212300	5.44562800	-1.73148000
H	0.23942800	4.70354400	-1.50782300
C	-3.48877900	4.24978500	-0.51348200
H	-2.82500300	2.56949600	0.64652700
C	-3.11713100	5.28810700	-1.37292500
H	-1.47768300	6.24813100	-2.40109000
H	-4.51913400	4.13448100	-0.19699900
H	-3.86669600	5.97516400	-1.75369100
C	-0.81002400	-3.21706500	2.99720900
H	0.25908800	-3.08693700	2.80862000
H	-0.96757600	-3.97727900	3.77064700
H	-1.28439000	-3.54619200	2.06733800
C	-3.32856000	-1.92070700	3.76225400
H	-3.47598300	-2.74792000	4.46548500
H	-3.77819400	-1.00851900	4.15672800
H	-3.79815200	-2.16211700	2.80483400
C	-0.86208200	-1.29401200	5.20213500

H	-1.32476300	-0.37986300	5.58151800
H	-1.10020700	-2.13345300	5.86525200
H	0.22324900	-1.16666600	5.15334200
H	4.69264100	5.24960000	-0.20493400
H	4.76943700	3.72073600	0.71890200
H	-0.40127600	0.57370100	-1.01180600
O	-0.60920600	1.35042600	0.41253100
H	5.21756300	3.75896200	-0.99162700
H	0.81897800	1.42461700	-1.47157500
O	0.25952600	0.46167300	-1.77120400
H	0.82353400	-0.31630000	-1.51860900

IM22

SCF done: -2197.66926

C	2.11985600	2.56584100	-0.51897800
C	-0.87912800	2.79629200	0.31847800
C	2.89966500	3.87019400	-0.82044000
C	4.38504000	3.94479200	-0.50746500
O	2.30799800	4.84089600	-1.24768600
O	1.01896800	2.53571400	-1.38110200
Au	-1.47744100	-0.03386600	1.76814000
P	-1.63436000	-1.90275800	3.03538000
Sb	-1.43660700	2.31531200	4.85776600
F	-2.28534300	2.32010900	3.10839000
F	-2.93227500	3.22443300	5.60214200
F	-2.25046900	0.58937600	5.18263600

F	-0.54224600	2.24481200	6.53738500	H	6.81915300	-2.62364200	-1.16635500
F	-0.55321300	3.94283000	4.35743000	H	6.31799400	-2.24848800	3.09075100
F	0.04451500	1.34992500	4.03919700	C	8.18237800	-2.88847000	1.19552300
C	2.95044800	1.26291500	-0.59987200	H	8.77043700	-2.77543900	0.27995600
H	4.00991400	1.42310800	-0.36263000	H	8.65926300	-2.29420100	1.98247100
H	2.87601600	0.81033800	-1.59055400	H	8.24657800	-3.94133800	1.50083500
N	2.31455200	0.40700900	0.42695400	C	-1.68879200	3.75131600	-0.47319700
C	1.85827100	1.21032700	1.59250500	C	-1.12467100	4.87368100	-1.11410300
C	1.66861600	2.63651700	1.00238100	C	-3.07698000	3.51922900	-0.57393200
C	0.28533100	3.30695800	1.14497300	C	-1.94278500	5.74624700	-1.83431600
H	0.95089000	0.79260100	2.01805000	H	-0.05157300	5.02513800	-1.10567300
H	2.61755600	1.22188900	2.38484500	C	-3.88930500	4.40623600	-1.27983200
H	2.35447200	3.29728300	1.54533200	H	-3.50483800	2.65941100	-0.07246700
H	-0.03243000	3.25038300	2.19224600	C	-3.32324200	5.52141600	-1.91150200
H	0.41211900	4.36946200	0.93052500	H	-1.50172100	6.59841300	-2.34052900
S	2.35731100	-1.24341300	0.37549200	H	-4.95897700	4.23334600	-1.33432600
O	1.56682400	-1.72525900	1.54753700	H	-3.95496100	6.21076100	-2.46301400
O	1.98097200	-1.65088700	-1.01980700	C	-1.36173900	-3.44474400	2.06660500
C	4.05913200	-1.74645300	0.60521300	H	-0.37393500	-3.38430300	1.60150700
C	4.85996900	-2.03785800	-0.50593100	H	-1.40997200	-4.32331200	2.71980100
C	4.57794400	-1.82626300	1.90653500	H	-2.12063700	-3.53405100	1.28358400
C	6.19648200	-2.39507500	-0.30702000	C	-3.25583200	-2.10046000	3.88036600
H	4.43626300	-2.00291400	-1.50253000	H	-3.26331400	-3.01718000	4.48057900
C	5.91404600	-2.18459400	2.08497000	H	-3.40193600	-1.23204100	4.52808100
H	3.94089400	-1.62833600	2.76080800	H	-4.06219800	-2.14220300	3.14232100
C	6.74457000	-2.47373600	0.98481800	C	-0.36952000	-1.91957300	4.36427600

H	-0.51620500	-1.03136400	4.98052900
H	-0.46959200	-2.82432200	4.97398400
H	0.62070900	-1.88436600	3.90411500
H	4.69805200	4.98845800	-0.55389300
H	4.62590500	3.53099500	0.47721000
H	-0.75832600	0.12580900	-1.30780300
O	-1.30334800	1.61924000	0.38704700
H	4.95609800	3.37289000	-1.24866900
H	0.71350200	1.60929200	-1.57229100
O	-0.02778900	0.12802500	-1.94194200
H	0.54672800	-0.62150700	-1.69483900

IM23

SCF done: -1254.872969

C	2.19318300	2.53765100	-0.95234700
C	-0.66377300	2.80665600	0.58541500
C	2.85091500	3.89177500	-1.28188400
C	4.36420900	4.00189500	-1.24559500
O	2.16089200	4.86308700	-1.52116600
O	0.98309600	2.47606900	-1.67815000
C	3.04865600	1.28544500	-1.23281800
H	4.09821800	1.41773100	-0.93290800
H	3.00676000	0.98700400	-2.28101000
N	2.35774900	0.29351200	-0.38195500
C	1.88048100	0.90743200	0.89107900
C	1.93321200	2.43705700	0.59449600

C	0.72113200	3.27111800	1.05569300
H	0.87192900	0.56292600	1.11161100
H	2.54477800	0.65536600	1.72948100
H	2.81291300	2.84897400	1.10692000
H	0.67685400	3.22855500	2.15284200
H	0.89495800	4.31646900	0.79284200
S	2.55086700	-1.35578200	-0.56929700
O	1.44504800	-1.98998000	0.19622000
O	2.77218200	-1.57218500	-2.02642000
C	4.08270700	-1.76187700	0.27233000
C	5.29507600	-1.71887600	-0.42929100
C	4.05654500	-2.10705300	1.63066000
C	6.48593100	-2.00052600	0.24419400
H	5.29566200	-1.49266300	-1.48927700
C	5.25654300	-2.38456700	2.28941300
H	3.10749400	-2.17837200	2.14912800
C	6.48753500	-2.33519300	1.61049700
H	7.42587000	-1.97141900	-0.29901600
H	5.23736800	-2.65376700	3.34133400
C	7.77745500	-2.67239100	2.32333100
H	8.63378700	-2.17011600	1.86195700
H	7.74021500	-2.38245800	3.37857300
H	7.97491900	-3.75235000	2.28926000
C	-1.60950400	3.79149400	-0.02354300
C	-1.18306200	4.92717500	-0.73771100
C	-2.98921400	3.53848500	0.11182500

C	-2.12656700	5.79941700	-1.29002000	H	-4.22339900	6.24066400	-1.55147900
H	-0.12775800	5.09814300	-0.91610500	H	4.64057100	5.05239300	-1.34224500
C	-3.92604300	4.42014300	-0.42734400	H	4.78286400	3.59384600	-0.31944900
H	-3.30242000	2.64751600	0.64427500	O	-1.03326000	1.66066800	0.81631900
C	-3.49542200	5.55549600	-1.12789500	H	4.80614700	3.43702100	-2.07477400
H	-1.79170700	6.66410200	-1.85395300	H	0.62502300	1.58210100	-1.55930300
H	-4.98688700	4.22441100	-0.30740000				

Cartesian Coordinates for the Stationary Points Given in Fig. 4.

TS18

SCF done: -2121.192749

				H	3.03411000	0.63608000	2.86839700
				H	3.19353600	2.73743600	1.76041500
C	2.52550600	1.96443400	-0.18430000	H	0.34491800	2.23323000	2.17458300
C	0.41387900	2.80503300	0.17254100	H	1.09596100	3.85789800	1.89818400
C	3.54676600	2.96373800	-0.75901900	S	3.61111900	-1.66847300	1.02437500
C	5.00719200	2.57123400	-0.68185000	O	3.56548500	-1.93773700	2.48635800
O	3.16725900	4.02538200	-1.20446200	O	2.83942400	-2.47490700	0.03204300
O	1.22117400	2.33049500	-0.73038600	C	5.32046300	-1.69692500	0.48558600
Au	-0.89428200	-0.89094800	0.46525300	C	5.64034100	-2.15212300	-0.79812700
P	-1.30771600	-2.60408600	-0.97286200	C	6.32611800	-1.29067900	1.37458100
Sb	-4.68046400	0.20009300	0.45823500	C	6.97969000	-2.17545600	-1.20047000
F	-3.28200400	0.62968200	-0.80897000	H	4.85355700	-2.50003300	-1.45695500
F	-5.66609200	-0.60370900	-0.97407300	C	7.65673300	-1.32266000	0.95828500
F	-3.85118400	-1.52158700	0.78210100	H	6.06596100	-0.97692000	2.37904000
F	-6.03340900	-0.19762900	1.73903000	C	8.00587300	-1.76379300	-0.33369900
F	-5.46918700	1.92103000	0.12486200	H	7.23069400	-2.52912400	-2.19582600
F	-3.56813900	0.98516600	1.84092000	H	8.43823000	-1.01284400	1.64568000
C	2.77632200	0.47080100	-0.46557800	C	9.45482400	-1.82454200	-0.75939800
H	3.55701700	0.29237900	-1.20998800	H	9.55170800	-1.86558400	-1.84850900
H	1.84338500	0.00788700	-0.81280900	H	10.01557800	-0.95496100	-0.39969900
N	3.19404600	-0.04054500	0.85821800	H	9.94631500	-2.71787500	-0.35160300
C	2.46233600	0.68719900	1.94154200	C	-0.88263500	3.23138500	-0.23027600
C	2.38035200	2.12261700	1.36550900	C	-1.20620500	3.34320600	-1.60852600
C	1.01877200	2.82722000	1.53489600	C	-1.88163400	3.46899300	0.74868500
H	1.45776400	0.28321200	2.11151100	C	-2.49882200	3.67421100	-1.98781800

H	-0.43916000	3.16594200	-2.35265500
C	-3.17473900	3.78131300	0.35424600
H	-1.65726900	3.33297000	1.79846500
C	-3.48723100	3.87193800	-1.00996300
H	-2.75332500	3.74970400	-3.03868600
H	-3.95893500	3.88296600	1.09176300
H	-4.51189900	4.06246100	-1.30556000
C	0.12986700	-3.24604600	-1.93919400
H	0.96874100	-3.43118200	-1.26226100
H	-0.13676400	-4.16626700	-2.47129900
H	0.44053400	-2.49072500	-2.66887300
C	-2.59267100	-2.22580100	-2.24079700
H	-2.75834000	-3.09242300	-2.89087100
H	-3.52422200	-1.95566200	-1.73966200
H	-2.27338200	-1.36953100	-2.84101500
C	-1.97675100	-4.07598900	-0.08607600
H	-2.86974000	-3.75475500	0.45724200
H	-2.23526400	-4.87636000	-0.78855500
H	-1.23729500	-4.44401000	0.63151300
H	5.61241300	3.47119900	-0.55977800
H	5.21033700	1.85449700	0.11773400
H	-1.60343700	0.74159700	2.10740700
O	-0.67678400	0.59875900	1.84933900
H	5.29704000	2.10149300	-1.62968300

IM24

SCF done: -2121.220192

C	2.71428600	2.35497600	-0.66588000
C	0.52214600	2.85875600	-0.26182100
C	3.61414100	3.50881900	-1.16025400
C	5.09528100	3.44418400	-0.82220100
O	3.14036200	4.44161400	-1.77014100
O	1.41490700	2.52495100	-1.24281700
Au	-0.73925100	-1.19360100	0.69251100
P	-1.24276400	-2.67459500	-0.93314500
Sb	-4.38622200	-0.08579300	1.72395900
F	-3.45244800	0.08925400	0.03648800
F	-5.76479400	-1.07556700	0.85687300
F	-3.37344700	-1.70259200	2.04050300
F	-5.19785000	-0.22805100	3.43698200
F	-5.23473000	1.59826200	1.40069000
F	-2.87974800	0.88989900	2.53973300
C	3.22636900	0.94203300	-1.00048400
H	4.31641000	0.92904400	-1.14847000
H	2.73958800	0.55703100	-1.89637400
N	2.83703000	0.14911000	0.18855700
C	2.91011000	0.98189700	1.41461600
C	2.50523300	2.39353500	0.90202900
C	1.04464100	2.77726200	0.98434900
H	2.23347700	0.58967600	2.17398800
H	3.93282600	0.99954100	1.82437000
H	3.13991800	3.14648300	1.38473000

H	-0.02064700	1.10932100	1.72603200
H	0.57788600	3.17829400	1.87595200
S	2.97858700	-1.51542800	0.21389700
O	2.35955500	-1.96628800	1.49030200
O	2.50730600	-1.99298700	-1.12122000
C	4.73400500	-1.87049000	0.31292700
C	5.48208100	-2.02916800	-0.86152600
C	5.34719600	-1.96425800	1.57110200
C	6.85661200	-2.26303200	-0.76921100
H	4.98790800	-1.99405300	-1.82545500
C	6.72146000	-2.19812500	1.64373500
H	4.74993300	-1.88049100	2.47153600
C	7.49779900	-2.34973500	0.47939600
H	7.43759200	-2.39004700	-1.67757700
H	7.19735000	-2.27488700	2.61669700
C	8.97903600	-2.63507900	0.57329200
H	9.50034100	-2.35847700	-0.34821100
H	9.44047600	-2.08931600	1.40308500
H	9.16244500	-3.70395000	0.74625200
C	-0.79813900	3.26863200	-0.75059400
C	-0.88809600	3.95726300	-1.97830700
C	-1.97103400	2.98843800	-0.02589500
C	-2.13210300	4.37294500	-2.45458600
H	0.01899000	4.17224000	-2.53166200
C	-3.21558500	3.39355000	-0.51508700
H	-1.93328700	2.41371500	0.89092900

C	-3.29580200	4.09149100	-1.72583800
H	-2.19529900	4.91248500	-3.39428300
H	-4.11053300	3.12919100	0.03591700
H	-4.26328100	4.40340000	-2.10636900
C	-0.83570300	-2.05060000	-2.61658500
H	0.23965000	-1.85600500	-2.66554600
H	-1.11322300	-2.78695300	-3.37916700
H	-1.37732900	-1.11771900	-2.79718200
C	-3.04085300	-3.05685900	-0.94942800
H	-3.28620300	-3.75955000	-1.75285400
H	-3.33045900	-3.47545000	0.01818600
H	-3.59460300	-2.12327300	-1.07932400
C	-0.35999100	-4.28530700	-0.80393600
H	-0.58313300	-4.75109700	0.16025700
H	-0.66571800	-4.95821500	-1.61288500
H	0.71621100	-4.09977600	-0.86635900
H	5.48688900	4.46092400	-0.76063300
H	5.30430300	2.90552400	0.10638700
H	-1.29404300	0.57374100	2.49821600
O	-0.37739900	0.32881400	2.20827700
H	5.62748900	2.92824800	-1.63046500

IM25

SCF done: -2121.222937

C	-1.87061200	1.47937600	1.21967400
C	-2.26438900	3.66424400	0.64889700

C	-0.71868500	1.07507900	2.15096100	O	-6.13077100	0.20912800	-0.66497200
C	-0.94320000	-0.05281100	3.12592600	O	-4.04863900	0.08451700	-2.24596300
O	0.36550800	1.63971900	2.09354400	C	-4.56928800	-1.96009300	-0.65637700
O	-1.43435900	2.58532200	0.41671200	C	-3.42365900	-2.63513500	-1.10579400
Au	3.32737500	0.83281200	-0.09159200	C	-5.56747900	-2.63941000	0.05139000
P	5.17587900	-0.47008800	0.02449300	C	-3.27090600	-3.99077100	-0.81575400
Sb	0.91602900	-2.25486400	-0.20399600	H	-2.66197300	-2.11719100	-1.67583000
F	2.49515600	-1.96888000	-1.28129800	C	-5.40616100	-4.00225200	0.31884300
F	-0.04103800	-3.02150100	-1.66460100	H	-6.45704700	-2.10830500	0.36985700
F	1.63177100	-3.92869300	0.36249700	C	-4.25824800	-4.69579100	-0.10236100
F	-0.63920900	-2.42865500	0.91284000	H	-2.36932400	-4.49596700	-1.14675500
F	0.31006700	-0.47769300	-0.75741100	H	-6.18220300	-4.53477400	0.86078500
F	1.79787100	-1.37223100	1.27375200	C	-4.08483900	-6.16860900	0.19192000
C	-2.34183100	0.33097300	0.30051900	H	-4.88701100	-6.54654600	0.83314800
H	-2.07757600	-0.65272400	0.70637300	H	-4.08883600	-6.76052500	-0.73234300
H	-1.89622600	0.42917600	-0.68767500	H	-3.12952600	-6.36292300	0.69399500
N	-3.80123600	0.52137400	0.23973600	C	-1.92549300	4.88533100	-0.08936100
C	-4.31681900	1.04107900	1.51604700	C	-0.76603200	4.93941500	-0.88710700
C	-3.16178300	1.97043100	1.99255600	C	-2.75222100	6.02479600	-0.01206900
C	-3.24168900	3.39803500	1.52954600	C	-0.44254500	6.10705100	-1.58409900
H	-5.25189400	1.57822600	1.35525500	H	-0.12438400	4.06982400	-0.95915400
H	-4.49313700	0.23709500	2.24925000	C	-2.42393000	7.18728400	-0.70871300
H	-3.05731000	1.89650900	3.08256300	H	-3.65660300	5.99682600	0.58626800
H	-3.99785100	4.09269500	1.86850100	C	-1.26641000	7.23400200	-1.49791900
H	1.05360100	2.09382800	0.53369900	H	0.45312600	6.13351000	-2.19656300
S	-4.72589300	-0.19927400	-0.95204600	H	-3.07191200	8.05536100	-0.64169600

H	-1.01430700	8.13866500	-2.04196000	H	5.84724400	-2.53533300	1.14497900
C	6.69565900	0.36761500	0.64503600	H	4.66913600	-1.60685100	2.12259900
H	6.52162600	0.74439400	1.65725600	H	-0.35013100	0.12636700	4.02481500
H	7.53954200	-0.33089100	0.66053700	H	-1.99360400	-0.20353900	3.38372400
H	6.93983800	1.21477600	-0.00268300	H	-0.57685900	-0.97093600	2.65202700
C	5.62058700	-1.16721100	-1.61843100	O	1.47651200	1.91417200	-0.34873700
H	6.47843900	-1.84291700	-1.53040500	H	0.90080200	1.21787400	-0.73215300
H	4.75206000	-1.71559600	-1.99299600				
H	5.86143400	-0.36108600	-2.31726500				
C	4.93331000	-1.93213400	1.11322900				
H	4.10793600	-2.52995600	0.72253800				

Cartesian Coordinates for the Stationary Points Given in Fig. S2.

TS19

SCF done: -2044.678706

C	1.47113400	0.73672800	-1.13428200	F	-3.68735900	1.05428400	2.73196400
C	1.94418900	2.97013400	-1.28321000	F	-1.27427000	0.03634300	3.62359100
C	0.08321800	0.29436700	-1.56121200	F	-0.37742700	0.05316800	1.03650900
C	-0.46704700	-1.10158600	-1.57364200	F	-2.67841100	-1.17453500	1.62272500
O	-0.71075200	1.11428300	-2.04428800	C	2.24310300	-0.21927700	-0.20283100
O	1.32703100	2.01013200	-0.50921500	H	1.89908400	-1.25627700	-0.32387300
Au	-2.68322400	-1.30582200	-1.31642300	H	2.12442200	0.07639800	0.83782400
P	-4.89302900	-1.73530600	-0.63566500	N	3.63492800	-0.07108900	-0.65582700
Sb	-1.98717100	0.62152500	1.96149000	C	3.69592900	0.14936000	-2.11033300
F	-2.70448100	1.11470100	0.22844700	C	2.40307000	0.96531000	-2.40145700
F	-1.29420500	2.38423300	2.18513600	C	2.55443400	2.46253500	-2.36602900
				H	4.60171300	0.69878400	-2.36809900
				H	3.68681500	-0.80559600	-2.65886000

H	1.94241600	0.61301700	-3.33360400
H	3.08892300	3.02387800	-3.11980800
H	-1.55084200	-0.07905600	-2.06505400
S	4.96300600	-0.11503000	0.35345500
O	6.06657100	0.54290300	-0.40123700
O	4.50000500	0.33968300	1.69187500
C	5.38759800	-1.85195400	0.51020700
C	4.82896300	-2.60938200	1.54799400
C	6.27826500	-2.43498400	-0.39990000
C	5.14693600	-3.96533300	1.65227300
H	4.17900600	-2.13337200	2.27302800
C	6.58642800	-3.79218300	-0.28118200
H	6.73979300	-1.82530800	-1.16798900
C	6.02248800	-4.57977000	0.73864700
H	4.72150100	-4.55113100	2.46173900
H	7.28467700	-4.24376400	-0.97974600
C	6.34320600	-6.05334400	0.84711600
H	6.34296000	-6.38703200	1.89001100
H	5.60086100	-6.66042200	0.31100700
H	7.32363500	-6.28237100	0.41732200
C	1.79856100	4.33726200	-0.77785800
C	0.91593900	4.60416400	0.28823200
C	2.52755600	5.39838600	-1.35123900
C	0.76742600	5.91126600	0.76062900
H	0.35084400	3.79697400	0.73994600
C	2.37185100	6.69973300	-0.87501900

H	3.22421300	5.20094500	-2.15952200
C	1.49011000	6.96086600	0.18309300
H	0.08555500	6.10552800	1.58192700
H	2.94097100	7.50884100	-1.32180300
H	1.37271300	7.97382900	0.55520500
C	-6.08281300	-2.20821700	-1.96342900
H	-5.74161600	-3.12155000	-2.46013200
H	-7.08037800	-2.37754700	-1.54351900
H	-6.13832800	-1.40896900	-2.70855000
C	-5.62920600	-0.26373200	0.18624900
H	-6.65564200	-0.48293600	0.50058300
H	-5.02739300	0.00949600	1.05564300
H	-5.62932500	0.58409300	-0.50408600
C	-4.98044100	-3.08503300	0.61444300
H	-4.31364700	-2.81536100	1.43757000
H	-6.00473100	-3.19970200	0.98551000
H	-4.64540700	-4.02973000	0.17596100
H	-0.12131400	-1.65740800	-2.45109400
H	-0.26106700	-1.66604100	-0.66158300

IM26

SCF done: -2044.771266

C	-0.14423700	1.68681900	1.36336600
C	1.36774200	3.23964700	0.61279600
C	0.22292600	0.65134100	2.42234000
C	-0.76365200	0.32417500	3.50547000

O	1.30054200	0.04942400	2.40590600	C	-4.38263900	1.64246200	-0.87034800
O	0.98942700	1.91246400	0.51665100	C	-4.20029900	0.27359500	-1.12186600
Au	2.44419900	-0.68716300	0.67289200	C	-5.61089300	2.12984500	-0.41062400
P	3.42085700	-1.84820800	-1.00629400	C	-5.25237500	-0.60987500	-0.88092100
Sb	-0.90319200	-2.81542300	-0.06912200	H	-3.25946700	-0.10899900	-1.49731900
F	-0.07667600	-1.17059200	-0.70834900	C	-6.66052100	1.23190400	-0.19275500
F	-2.42996700	-2.41620400	-1.15550800	H	-5.73872400	3.19255000	-0.24016300
F	0.00086600	-3.71988200	-1.50807600	C	-6.49808000	-0.14646300	-0.41662400
F	-1.70894900	-4.41352800	0.56895800	H	-5.08936700	-1.66861400	-1.05460300
F	-1.64368500	-1.77143900	1.38123800	H	-7.61851200	1.60646200	0.15567800
F	0.66391400	-3.12072700	1.02238300	C	-7.63253200	-1.11543500	-0.17202200
C	-1.35426600	1.25339400	0.50368700	H	-7.93602500	-1.61320000	-1.10163700
H	-1.99159600	0.53276200	1.03059400	H	-7.33697400	-1.90311300	0.53163500
H	-1.00468400	0.79245700	-0.41806200	H	-8.51143600	-0.60879900	0.23816500
N	-2.04650500	2.52411000	0.25331200	C	2.53357900	3.61639000	-0.19204000
C	-1.95463400	3.41127700	1.42005700	C	2.91688100	2.83379500	-1.29878200
C	-0.52896300	3.09904000	1.97310100	C	3.27511800	4.77389800	0.11600800
C	0.57575600	3.95686300	1.42255200	C	4.01209500	3.20883800	-2.08187500
H	-2.07152900	4.45179300	1.11606800	H	2.33969500	1.95085300	-1.54694900
H	-2.72019800	3.17651000	2.17689500	C	4.36836400	5.14314800	-0.66887800
H	-0.54872000	3.10066600	3.06965700	H	3.00339600	5.37247600	0.97920600
H	0.66021100	5.01864700	1.60996300	C	4.74122400	4.36240900	-1.77098300
H	-0.23049300	0.08495900	4.42854200	H	4.28844800	2.60861400	-2.94333700
S	-3.00615800	2.76475800	-1.09610400	H	4.93264600	6.03586700	-0.41941300
O	-3.49982300	4.16722800	-0.98093500	H	5.59054100	4.65250800	-2.38106000
O	-2.23128000	2.27900200	-2.26947800	C	5.16882000	-1.38805300	-1.36518300

H	5.78500700	-1.56297700	-0.47828700
H	5.55852300	-1.98080700	-2.20011600
H	5.22127700	-0.32478200	-1.61753100
C	2.50561200	-1.66310500	-2.59032100
H	3.01184200	-2.22018700	-3.38652800
H	1.49802800	-2.06041900	-2.44697300
H	2.43161900	-0.60877800	-2.86888400
C	3.41091300	-3.65852400	-0.68609000
H	2.37029100	-3.96979400	-0.56551200
H	3.86410800	-4.19595100	-1.52631300
H	3.95569300	-3.88428200	0.23444900
H	-1.50302200	1.10793300	3.67690700
H	-1.28438000	-0.58163000	3.16724200

TS20

SCF done: -2044.693328

C	-2.34519700	-0.76296200	-0.39939100
C	-4.55031000	-1.34308400	-0.53639000
C	-1.21539800	-1.76137400	-0.62671600
C	-0.04709100	-1.35398200	-1.46988800
O	-1.24127000	-2.87227300	-0.09172500
O	-3.42826000	-1.41892100	0.26348500
Au	1.66007900	-2.22543600	-0.61358700
P	3.53255300	-3.19996700	0.59898700
Sb	2.85759400	1.16822400	0.15608600
F	1.76767500	-0.02099700	1.23633300

F	2.61314400	2.58836300	1.40168800
F	4.39088400	0.46456000	1.08040500
F	3.94205100	2.21404100	-0.99753000
F	1.26022400	1.60905600	-0.81746400
F	3.07219900	-0.37443100	-1.07442100
C	-1.83069400	0.41653400	0.47591400
H	-0.74712500	0.55945700	0.37783600
H	-2.07726900	0.24575900	1.52348200
N	-2.58540200	1.56177600	-0.05881300
C	-2.81414600	1.42846700	-1.50612600
C	-2.94623800	-0.11105600	-1.70582400
C	-4.34938900	-0.64965300	-1.66814600
H	-3.72334600	1.96120600	-1.79040400
H	-1.96645700	1.82512500	-2.08455200
H	-2.40678900	-0.41125200	-2.61146700
H	-5.07959600	-0.47567900	-2.44634200
H	0.37830000	-3.20454300	-0.35693700
S	-2.96338200	2.92751900	0.82482600
O	-4.25010800	3.44856200	0.28223800
O	-2.79130000	2.52941700	2.24980500
C	-1.70238700	4.13497600	0.41739400
C	-0.39567400	3.97387500	0.90191600
C	-2.03532300	5.23022700	-0.38721300
C	0.57947800	4.91080200	0.56154000
H	-0.13866700	3.13759700	1.54066100
C	-1.04768400	6.16477000	-0.71328400

H	-3.05376400	5.34651600	-0.73786700
C	0.26961400	6.02030500	-0.24847100
H	1.59091900	4.76769300	0.92535600
H	-1.30529800	7.01735000	-1.33463500
C	1.33714800	7.03193100	-0.59830400
H	2.21448100	6.54572500	-1.04136800
H	0.96676400	7.77581300	-1.31030600
H	1.68325200	7.56748400	0.29507900
C	-5.73117500	-2.03975000	-0.01767400
C	-5.61893000	-2.89225600	1.09744100
C	-6.99118800	-1.87559200	-0.62747700
C	-6.74060100	-3.56882400	1.58407900
H	-4.65324900	-3.01926700	1.57107600
C	-8.10696800	-2.55531900	-0.13936000
H	-7.09828500	-1.20431200	-1.47292300
C	-7.98629600	-3.40565000	0.96837900
H	-6.64116200	-4.22239100	2.44485700
H	-9.07218200	-2.41681000	-0.61587300
H	-8.85680900	-3.93009900	1.34929400
C	3.60450900	-5.04136200	0.66958000
H	3.68104600	-5.44777600	-0.34354200
H	4.46779100	-5.37346400	1.25627700
H	2.68901300	-5.42706500	1.12829200
C	3.52322800	-2.61894200	2.34644400
H	4.36904800	-3.03836800	2.90184600
H	3.59406000	-1.52824200	2.33823600

H	2.58691500	-2.90542900	2.83345200
C	5.16162500	-2.64490000	-0.05943400
H	5.20390800	-1.55588200	0.02659300
H	5.98203000	-3.08870700	0.51499200
H	5.26247100	-2.92236400	-1.11250400
H	-0.17715000	-1.78556400	-2.47009100
H	0.11362400	-0.27840900	-1.56135100

IM27

SCF done: -2044.696114

C	-2.14983300	-1.13944200	-0.35589300
C	-4.33990600	-1.75793400	-0.56202300
C	-1.00583400	-2.15441400	-0.52477700
C	0.16638700	-1.71427200	-1.37363200
O	-1.05400900	-3.25305300	-0.00405800
O	-3.25112300	-1.79576000	0.28092500
Au	2.00034000	-2.13247700	-0.45634600
P	4.08867200	-2.61710900	0.75848300
Sb	2.59927300	1.46913300	-0.06921600
F	1.77936900	0.23286100	1.18313400
F	2.24296500	2.95647100	1.06065200
F	4.27915200	1.07259700	0.77868600
F	3.46051800	2.49582200	-1.40963600
F	0.90874000	1.58412600	-0.96867000
F	2.92995900	-0.17747600	-1.15129700
C	-1.70842100	0.07333100	0.50746600

H	-0.62824000	0.24372500	0.45388400
H	-1.99910800	-0.07079100	1.54761900
N	-2.44688500	1.19995600	-0.09058200
C	-2.60718800	1.01302100	-1.54211700
C	-2.71055600	-0.53493000	-1.70292600
C	-4.10693300	-1.09203400	-1.70444300
H	-3.50738900	1.52397300	-1.88882900
H	-1.73411900	1.40681700	-2.07981100
H	-2.13461400	-0.85185100	-2.58072800
H	-4.80928600	-0.95451600	-2.51505300
H	1.22508500	-3.45064100	-0.16775400
S	-3.20460400	2.40287600	0.78039900
O	-4.54438600	2.64985300	0.17135300
O	-3.04761300	2.01508500	2.21108600
C	-2.22993100	3.87785100	0.47093500
C	-0.87182400	3.90833900	0.81923800
C	-2.84395300	4.99582100	-0.10207900
C	-0.13056000	5.06508000	0.58235800
H	-0.39108900	3.04570900	1.26311300
C	-2.08868600	6.15156900	-0.32764700
H	-3.89404100	4.95235800	-0.36449000
C	-0.72683000	6.20530500	0.00883900
H	0.92314600	5.07292800	0.83979700
H	-2.56466800	7.02054400	-0.77230100
C	0.08929900	7.45498500	-0.23229400
H	0.98429400	7.23712100	-0.82758600

H	-0.49128600	8.21637400	-0.76209200
H	0.43139800	7.89372000	0.71383800
C	-5.53014200	-2.46062100	-0.07273800
C	-5.43324500	-3.33642400	1.02566300
C	-6.78201400	-2.27959500	-0.69374700
C	-6.56214600	-4.02072700	1.48376900
H	-4.47256100	-3.47562200	1.50624800
C	-7.90530500	-2.96731100	-0.23413400
H	-6.87664400	-1.58584000	-1.52237100
C	-7.79997300	-3.84157600	0.85630800
H	-6.47480400	-4.69300600	2.33147800
H	-8.86479100	-2.81489200	-0.71812900
H	-8.67639600	-4.37157300	1.21569600
C	4.45145800	-4.40729500	1.00903800
H	4.55010200	-4.90352900	0.03867800
H	5.37891500	-4.54074700	1.57614100
H	3.62699700	-4.87649700	1.55458500
C	4.05127900	-1.85658200	2.43471500
H	4.97599000	-2.07153400	2.98106900
H	3.93897000	-0.77633400	2.31376300
H	3.19588100	-2.23738400	2.99984700
C	5.57468600	-1.89759000	-0.05840500
H	5.44238700	-0.81349000	-0.10640200
H	6.47962400	-2.12808600	0.51423200
H	5.67791100	-2.29087700	-1.07384100
H	0.15109200	-2.27780500	-2.31272700

H	0.20182500	-0.64409100	-1.59013600
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TS21

SCF done: -2044.689704

C	-2.04854700	-1.33316000	-0.28949900
C	-4.21392200	-1.99792900	-0.58728900
C	-0.88229300	-2.32329400	-0.36341300
C	0.30962400	-1.92865700	-1.21230100
O	-0.89468400	-3.38963900	0.22137100
O	-3.16503800	-1.99622600	0.30889200
Au	2.26737500	-2.10214500	-0.31098200
P	4.40975800	-2.19776100	0.81042200
Sb	2.49501900	1.62644700	-0.25680300
F	1.85062500	0.35641500	1.07148600
F	1.86821900	3.08840100	0.79188500
F	4.19667300	1.57113900	0.63667100
F	3.16201600	2.74855600	-1.63274200
F	0.79831000	1.41226200	-1.14435900
F	3.09636700	0.03479700	-1.24866500
C	-1.67084200	-0.08607600	0.56004200
H	-0.59391100	0.11126000	0.53976500
H	-1.99739200	-0.21118800	1.59206600
N	-2.40575700	1.01037900	-0.09367600
C	-2.48030100	0.78168900	-1.54794300
C	-2.55070000	-0.77274700	-1.67843000
C	-3.93498700	-1.35625100	-1.73301700

H	-3.36563500	1.26870100	-1.96035500
H	-1.58127500	1.17703900	-2.03525900
H	-1.92747800	-1.09827800	-2.52061400
H	-4.60016700	-1.24702700	-2.57839200
H	1.12217100	-3.23801500	-0.36794300
S	-3.40885700	2.07460200	0.72028900
O	-4.72317800	2.14108200	0.01533600
O	-3.31848400	1.68802900	2.15757900
C	-2.62606800	3.67163600	0.48709200
C	-1.24714400	3.82007300	0.68844700
C	-3.41945900	4.77040600	0.14037200
C	-0.66523600	5.07851200	0.54011500
H	-0.62380300	2.97036900	0.93361300
C	-2.82244600	6.02766100	0.00265900
H	-4.48104700	4.63400900	-0.02724300
C	-1.44298300	6.20245400	0.20055400
H	0.40596900	5.17658700	0.68105100
H	-3.43621900	6.88168000	-0.26797100
C	-0.79849400	7.56190200	0.05051700
H	-0.37962000	7.90918600	1.00363800
H	0.02660700	7.53350200	-0.67151100
H	-1.51913900	8.31155300	-0.29031000
C	-5.41345400	-2.71000400	-0.13696100
C	-5.35291700	-3.55924300	0.98468500
C	-6.63772000	-2.56508900	-0.81940900
C	-6.48991200	-4.25411400	1.40511200

H	-4.41432100	-3.66958600	1.51395100	C	4.34404500	-1.30396400	2.41806300
C	-7.76913100	-3.26307800	-0.39678900	H	5.30958500	-1.36009500	2.93217700
H	-6.70582700	-1.89065400	-1.66631400	H	4.09805600	-0.25963200	2.21179400
C	-7.69975000	-4.11141700	0.71674700	H	3.56408700	-1.73024200	3.05489600
H	-6.43080900	-4.90559900	2.27123500	C	5.76605600	-1.37333300	-0.12409900
H	-8.70751900	-3.13838800	-0.92769800	H	5.50517500	-0.31865500	-0.23988500
H	-8.58271800	-4.64939300	1.04698700	H	6.71184600	-1.45844000	0.42181700
C	5.01172800	-3.89839800	1.19231100	H	5.87468500	-1.82321400	-1.11486200
H	5.14858300	-4.46069600	0.26367200	H	0.27659100	-2.47465300	-2.15946500
H	5.96424800	-3.85820300	1.73173100	H	0.40472600	-0.85663200	-1.41727700
H	4.27184400	-4.42006600	1.80676300				

Cartesian Coordinates for the Stationary Points Given in Fig. S3.

TS22

SCF done: -2121.156132

C	-1.84327400	0.48844500	0.63214500	F	2.23162200	1.93208900	1.32620600
C	-0.24255100	2.90010500	0.01770900	F	4.79968600	1.18127100	1.98695700
C	-1.25173200	-0.54563500	1.56396600	F	4.31292000	2.25928600	-0.46966200
C	-0.04184800	-0.21988500	2.39425000	F	2.36266500	0.47584300	-0.90858000
O	-1.95664100	-1.52381400	1.76280500	F	4.82647900	-0.45275500	-0.24626700
O	-0.36871800	1.91406800	-0.70810800	C	-2.82493100	0.08218100	-0.41482400
Au	1.21108600	-2.27009700	-0.45988100	H	-3.21145200	-0.91926100	-0.21091500
P	2.95775400	-3.72200200	-0.49885700	H	-2.32611100	0.06035400	-1.39180400
Sb	3.60690300	0.80758600	0.55093600	N	-3.87279600	1.12748500	-0.31817700
F	2.86279300	-0.67392100	1.55035600	C	-3.31551400	2.38479000	0.22164600
				C	-2.18556300	1.87377100	1.14629300
				C	-1.04170700	2.88001600	1.31489100

H	-2.91180100	3.03050900	-0.56930600
H	-4.07870700	2.94557700	0.76380600
H	-2.60923100	1.66414200	2.14455500
H	-1.44382200	3.85988900	1.58795400
H	-0.34017900	2.59318200	2.10720100
S	-5.24067900	1.09295800	-1.29148600
O	-5.80129100	2.47157100	-1.19671100
O	-4.87609100	0.45638900	-2.58866500
C	-6.34061500	-0.03348400	-0.44153900
C	-6.40177200	-1.37452800	-0.83739300
C	-7.14275500	0.44443000	0.60359300
C	-7.25388100	-2.24786200	-0.15576100
H	-5.80740200	-1.71724000	-1.67606000
C	-7.99034300	-0.43999300	1.27037600
H	-7.11570300	1.49481800	0.86940000
C	-8.05323000	-1.79984300	0.90971200
H	-7.30439900	-3.28835200	-0.46138800
H	-8.61871300	-0.07175800	2.07580300
C	-8.95099500	-2.75535300	1.66162900
H	-9.21972000	-3.62021700	1.04722500
H	-8.45193100	-3.13587600	2.56311100
H	-9.87614100	-2.26633000	1.98449900
C	0.65369600	4.01709900	-0.32534100
C	1.70619100	3.77236900	-1.23147100
C	0.49902300	5.30283800	0.23231200
C	2.59024800	4.79627900	-1.56566600

H	1.84939900	2.77082100	-1.61532300
C	1.37228500	6.32987900	-0.12741500
H	-0.30392900	5.51231200	0.93035100
C	2.42008600	6.07634800	-1.02262200
H	3.42316000	4.58775900	-2.22659700
H	1.24357100	7.32123700	0.29375900
H	3.10932400	6.87218400	-1.28593700
C	2.55531500	-5.50372800	-0.76769700
H	2.03424600	-5.62253300	-1.72256000
H	3.46880600	-6.10879900	-0.77688600
H	1.89632300	-5.85650200	0.03136600
C	3.95508000	-3.67361700	1.04799000
H	4.82251300	-4.33840400	0.97125500
H	4.28421200	-2.64299400	1.19889100
H	3.33850400	-3.96911600	1.90149200
C	4.16981200	-3.29261200	-1.81820700
H	4.54013400	-2.28270800	-1.61655800
H	5.00846300	-3.99793600	-1.81629200
H	3.68262500	-3.30651100	-2.79739500
H	-0.38431100	0.18676900	3.35573500
H	0.50104400	-1.14259700	2.59981500
O	-0.24291700	-0.78639500	-0.49432500
H	0.27996300	-0.01746900	-0.77951300
H	0.64112400	0.48321300	1.92456400

IM28

SCF done: -2121.235702

C	-1.06133000	0.84878900	1.65099000	H	-0.75909300	4.32428400	0.91680000
C	0.65963100	3.13563200	-0.16692500	H	0.32284000	3.39368000	1.90846400
C	-0.45356700	0.81861500	3.07218200	S	-3.76295200	-0.14108100	-0.82282800
C	0.91544700	0.22912500	3.26215900	O	-3.36799700	0.44888000	-2.13377600
O	-1.11339100	1.29785500	3.97923200	O	-3.49938300	-1.57077200	-0.47731300
O	0.70616600	2.05834300	-0.76693400	C	-5.52412100	0.13431400	-0.62900600
Au	0.15360900	-1.84436900	0.09673100	C	-6.25622800	-0.64942700	0.27273600
P	0.90687700	-3.84439800	-0.63310500	C	-6.15189500	1.13136100	-1.38439500
Sb	3.73997400	-0.27445300	-0.02981200	C	-7.62182300	-0.40974600	0.43183800
F	2.86526400	-1.39858600	1.28837700	H	-5.76593400	-1.44558400	0.82071700
F	2.97984400	1.26018300	0.86692600	C	-7.52014200	1.35785200	-1.21296500
F	5.30980500	-0.19844000	1.04352200	H	-5.57943200	1.70038500	-2.10732800
F	4.51757900	0.86786400	-1.35357700	C	-8.27420700	0.60020500	-0.30024300
F	2.14528500	-0.38116200	-1.13098100	H	-8.19250500	-1.02000900	1.12557700
F	4.33186300	-1.88689600	-0.90378600	H	-8.01062200	2.12619300	-1.80293900
C	-2.44967000	0.18525900	1.59200700	C	-9.74871300	0.86696500	-0.10022000
H	-3.02685200	0.43916000	2.48681800	H	-10.30990100	-0.06428300	0.03283100
H	-2.38506000	-0.89931200	1.49003600	H	-9.92088700	1.48012400	0.79470100
N	-3.04089400	0.78748800	0.37065500	H	-10.17780300	1.40301100	-0.95234600
C	-2.41941900	2.10634400	0.05477000	C	1.59114400	4.22156500	-0.54933200
C	-1.42112500	2.30235600	1.22185700	C	2.78070600	3.85523800	-1.21648100
C	-0.29598300	3.33398700	1.00141500	C	1.35087300	5.58013400	-0.25816000
H	-1.92761500	2.06644300	-0.91954600	C	3.70245200	4.83447900	-1.58696400
H	-3.16859000	2.90602100	0.03916300	H	2.98937200	2.80911400	-1.40017500
H	-1.98258300	2.67786800	2.08465300	C	2.27148100	6.55548900	-0.64573800
				H	0.44414100	5.88597300	0.25222100

C	3.44816000	6.18388500	-1.30900700
H	4.62158300	4.54188200	-2.08245000
H	2.07425500	7.60045600	-0.43058500
H	4.16665800	6.94305700	-1.60147500
C	-0.34172300	-5.18348800	-0.83193300
H	-1.12768700	-4.85079300	-1.51623900
H	0.12878700	-6.09011400	-1.22830600
H	-0.80015900	-5.40578700	0.13614600
C	2.23092900	-4.52043400	0.45086800
H	2.62510800	-5.45496800	0.03655500
H	3.02776100	-3.77406300	0.50845700
H	1.84440900	-4.69866000	1.45807000
C	1.72401900	-3.64747100	-2.26958600
H	2.55464100	-2.94548200	-2.14846900
H	2.10595500	-4.61132200	-2.62444500
H	1.01824900	-3.24012400	-2.99854000
H	1.21343800	0.35061900	4.30432600
H	0.92267800	-0.83306500	2.99414500
O	-0.21739600	0.21179700	0.68993700
H	0.18704600	0.87814500	0.04176700
H	1.64482600	0.69099400	2.58892200

TS23

SCF done: -2121.192749

C	2.24640600	3.01862600	-0.52484300
C	-0.14921600	2.21756400	-0.34363000

C	2.41579000	4.54283000	-0.61703000
C	3.71781900	5.13672900	-0.11525000
O	1.52285000	5.23399800	-1.06023600
O	1.07199400	2.65137700	-1.31152300
Au	-0.96459500	-0.93172900	-0.30584100
P	-1.95173400	-2.90405500	0.17032000
Sb	-0.08048400	-0.68878000	3.73509700
F	-1.29639800	0.19185700	2.49639200
F	-1.02869200	0.07001600	5.19934300
F	-1.24050900	-2.23005300	3.69329800
F	1.14887800	-1.57271500	4.89096800
F	1.07243700	0.85000200	3.59061200
F	0.85408200	-1.45190400	2.20441400
C	3.43366200	2.16210300	-1.00508000
H	4.38056300	2.60609200	-0.66996000
H	3.47142600	2.04258300	-2.08872100
N	3.16461200	0.88122400	-0.33610800
C	2.55433500	1.08508500	1.00055000
C	1.93100300	2.51205600	0.92204800
C	0.40341000	2.59401000	1.02498600
H	1.81349200	0.31661000	1.20625700
H	3.31452200	1.04572700	1.78906200
H	2.39038400	3.15479700	1.67708000
H	0.00556900	1.92524100	1.78857800
H	0.09707500	3.61690600	1.26521900
S	3.41620900	-0.62202300	-1.03367800

O	2.14794400	-1.40284900	-0.97855100
O	4.08482500	-0.32704400	-2.33608200
C	4.57261000	-1.43336300	0.06192400
C	5.93544400	-1.42597900	-0.25881400
C	4.10366900	-2.06161900	1.22552300
C	6.83951700	-2.04946900	0.60387900
H	6.27116900	-0.95137100	-1.17352700
C	5.02643700	-2.67057400	2.07911500
H	3.04538100	-2.07025500	1.46499200
C	6.40209800	-2.67907200	1.78316600
H	7.89726500	-2.05054800	0.35804100
H	4.67051100	-3.14677100	2.98750800
C	7.38318600	-3.37368700	2.69968300
H	8.39044700	-2.95713800	2.59877900
H	7.08112800	-3.28648700	3.74851600
H	7.44682200	-4.44547500	2.46767900
C	-1.44151200	2.86635900	-0.75302400
C	-1.52755300	3.84560800	-1.75201500
C	-2.60246000	2.45168800	-0.07208400
C	-2.77310400	4.39208400	-2.08302600
H	-0.62753900	4.18972700	-2.24478700
C	-3.84071700	3.00538100	-0.40828400
H	-2.53124300	1.71241800	0.72088000
C	-3.92975300	3.97230800	-1.41780000
H	-2.83524500	5.14975700	-2.85754200
H	-4.73245100	2.68557600	0.12115400

H	-4.89282800	4.40052100	-1.67695500
C	-2.61780700	-3.80369600	-1.29628500
H	-1.80608000	-4.00463000	-2.00189300
H	-3.07467700	-4.75152900	-0.99044000
H	-3.36806800	-3.18564300	-1.79844100
C	-3.36883400	-2.72938000	1.33076100
H	-3.82625300	-3.70499700	1.52999400
H	-2.98418200	-2.31136100	2.26489700
H	-4.11734900	-2.05216900	0.91004200
C	-0.81158500	-4.08766000	0.99503200
H	-0.49009000	-3.64008400	1.93761800
H	-1.32134000	-5.03761400	1.19042400
H	0.06502300	-4.25847100	0.36424700
H	3.56470000	6.19737500	0.08798000
H	4.09817600	4.63415500	0.77850700
H	0.97283000	1.51463800	-1.41572900
O	0.00852000	0.90353300	-0.72577300
H	4.48390100	5.04246300	-0.89474500

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SCF done: -2121.224483

C	2.55292800	3.05718300	-1.07239400
C	-0.22051100	2.13270900	0.26070200
C	2.43496400	4.54631100	-1.45196700
C	3.66852700	5.42598900	-1.37898000
O	1.35517900	5.01180200	-1.76317200

O	1.59744000	2.36544400	-1.84986400	C	5.95672600	-1.55906000	0.22996500
Au	-1.02076500	-0.91200700	-0.19317800	C	3.76738500	-1.82531100	1.27465200
P	-1.95432100	-2.96598700	-0.10604300	C	6.52589500	-2.30938000	1.26017400
Sb	0.05202800	-0.96001100	3.55768800	H	6.56238800	-1.16708600	-0.57857000
F	-1.50677800	-0.24569700	2.64564900	C	4.35959800	-2.55225400	2.31043200
F	-0.64411600	-0.40058000	5.23471900	H	2.69803700	-1.65999800	1.27777400
F	-0.87391600	-2.65141600	3.62698800	C	5.74192200	-2.80888400	2.31815600
F	1.61582400	-1.70179200	4.37012100	H	7.59437600	-2.50332700	1.24956100
F	0.92687200	0.73127600	3.25616400	H	3.73125400	-2.89746500	3.12548900
F	0.75718800	-1.55653800	1.84265000	C	6.36875700	-3.62145000	3.42782700
C	3.95705700	2.42888400	-1.21697200	H	7.42459600	-3.36660700	3.56544400
H	4.75059900	3.09804700	-0.86982000	H	5.85076000	-3.46167100	4.37894600
H	4.17805800	2.12366800	-2.24075300	H	6.31732000	-4.69615500	3.20585600
N	3.89534700	1.24637700	-0.31185900	C	-1.56997300	2.67131200	-0.02677500
C	2.96295400	1.52985800	0.83123500	C	-1.71349400	3.81755100	-0.83396300
C	2.28756400	2.88443300	0.46264400	C	-2.70764900	2.02897200	0.50293100
C	0.81459900	3.05722700	0.86621300	C	-2.99298100	4.29262300	-1.13309400
H	2.22748300	0.73534800	0.94664900	H	-0.83482000	4.29579600	-1.25576400
H	3.52825200	1.61265800	1.76292800	C	-3.97921200	2.53529900	0.22184900
H	2.83591100	3.67989500	0.98462800	H	-2.58638800	1.18218200	1.17084400
H	0.72583800	2.86149600	1.94671600	C	-4.12398100	3.65813400	-0.60305300
H	0.50516200	4.09267800	0.70692300	H	-3.10638900	5.15891700	-1.77630600
S	3.86574500	-0.29228000	-1.02324500	H	-4.85410300	2.05927900	0.65236100
O	2.43405000	-0.70148700	-1.23939700	H	-5.11449000	4.04211600	-0.82589600
O	4.79245800	-0.22075800	-2.19078800	C	-2.69751500	-3.63761800	-1.65224200
C	4.57659100	-1.31779100	0.25175700	H	-1.93165900	-3.69257400	-2.43160700

H	-3.10977800	-4.63747800	-1.47704600
H	-3.49461500	-2.97204800	-1.99670800
C	-3.27370700	-3.03079300	1.17593200
H	-3.68153400	-4.04440000	1.25904200
H	-2.82463300	-2.73712100	2.12974900
H	-4.07754400	-2.33163900	0.92951800
C	-0.72053100	-4.20677600	0.46137000
H	-0.35835400	-3.88415000	1.44148300

H	-1.17853000	-5.19865500	0.54299500
H	0.12406600	-4.24432200	-0.23180700
H	3.37066400	6.46261400	-1.53991100
H	4.17891700	5.33474900	-0.41425200
H	1.67274100	1.40972000	-1.67564300
O	0.04812500	0.92801800	0.13562200
H	4.38923100	5.13389000	-2.15171200