

Supporting Information

Mechanisms and Origins of Switchable Regioselectivity of FeBr₃-Catalyzed

[1,2]-Aryl and [1,2]-Alkyl Shift of α -Aryl Aldehydes

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Table S1. Comparison of the relative free energies in toluene solvent of the doublet- and sextet-states for several mono-FeBr₃-involved species and the singlet-, triplet- and eleven-states for several bis-FeBr₃-involved species in the reaction under study. The free energies are given in kcal mol⁻¹.

mono-FeBr ₃ -catalyzed mechanism					bis-FeBr ₃ -catalyzed mechanism				
	1a	TS_{1a}	TS_{8a}	TS_{6a}		IM6a	TS_{10a}	TS_{14a}	TS_{12a}
<i>Quartet-state</i>	0.0	21.5	19.1	24.5	<i>Seven-state</i>	7.5	16.4	18.0	23.2
Doublet-sate	3.5	24.9	25.9	30.0	Triplet-sate	12.7	21.5		
Sextet-state	3.0	25.1	25.5	27.8	Eleven-state	11.6	17.5	22.4	24.2
					Singlet-state	57.7			

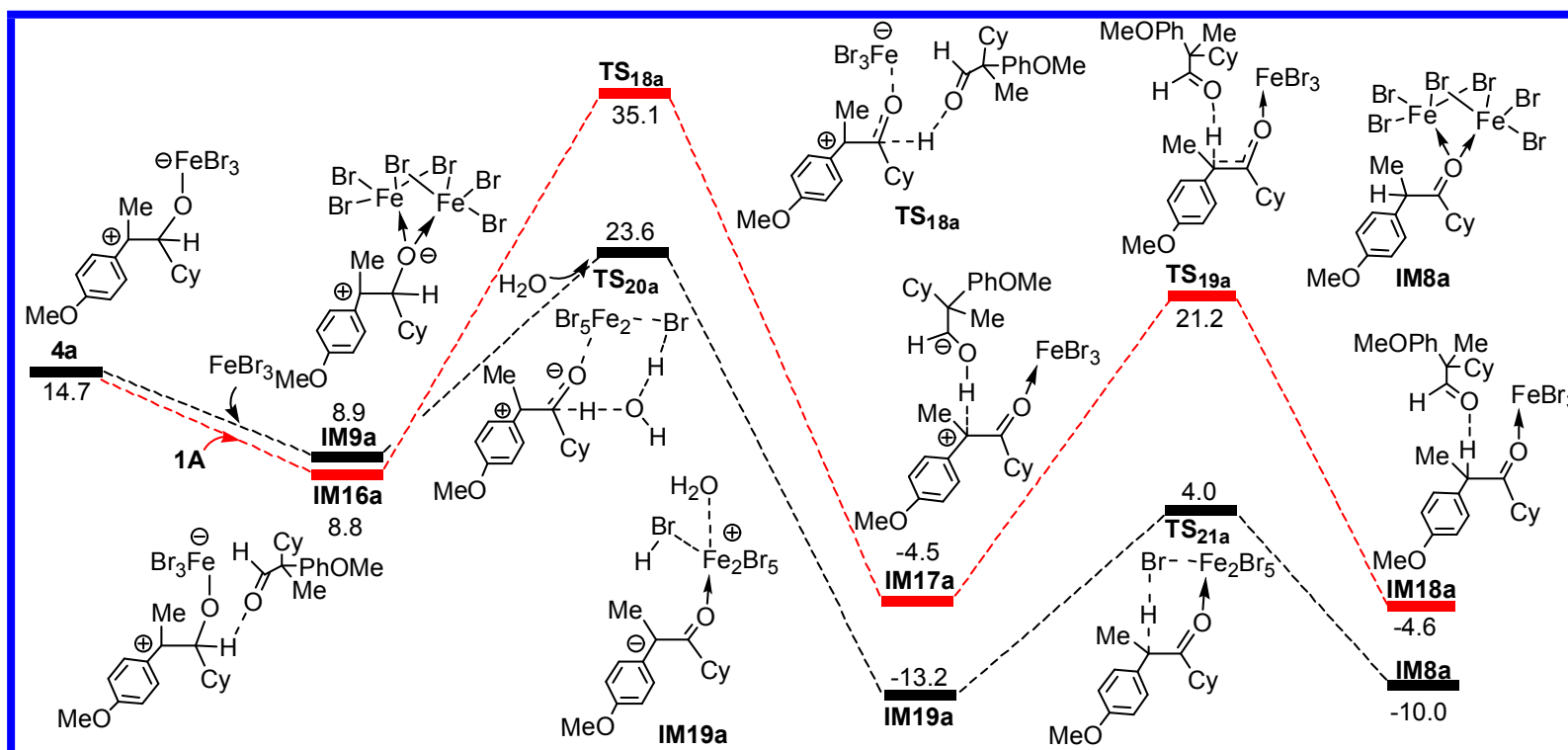


Fig. S1 Single-point solvation-corrected free energy profiles in toluene along other possible H-shift pathways for **1A** involved system and schematic structures for the species involved. The relative free energies are given in kcal mol⁻¹.

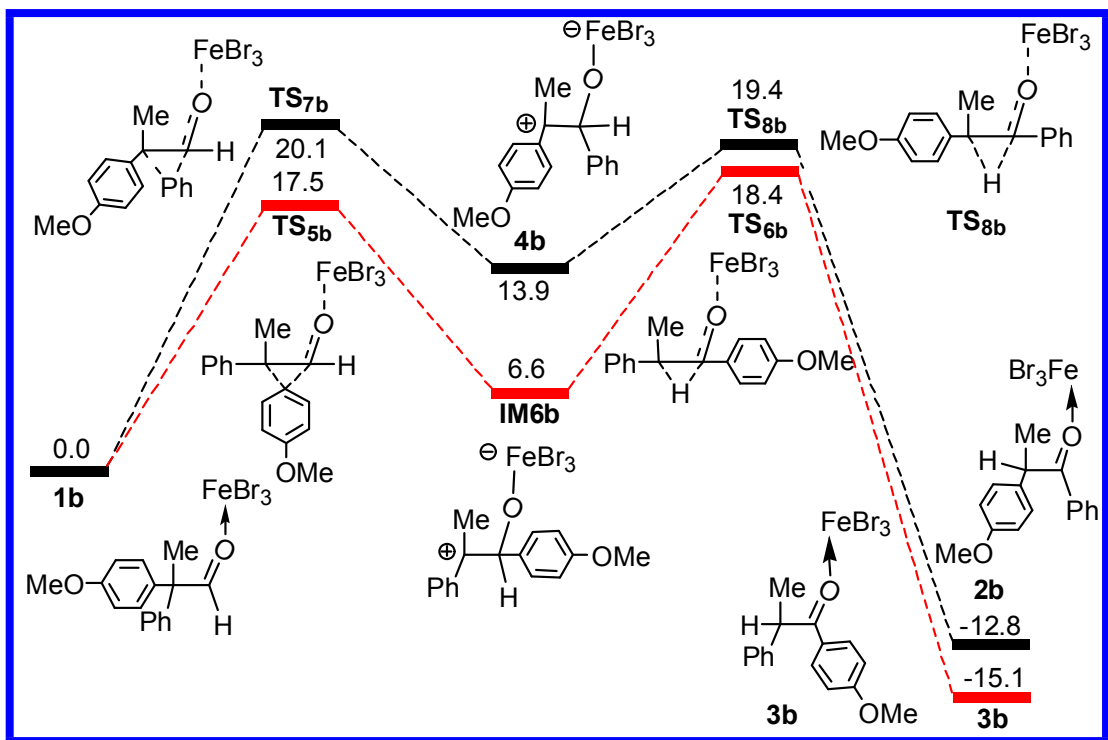


Fig. S2 Single-point solvation-corrected free energy profiles in toluene for the mono- FeBr_3 -catalyzed rearrangement of the 2-phenyl,2-*p*- $\text{C}_6\text{H}_4\text{OMe}$ -propylaldehyde precursor (**1b**) via two competitive aryl-shifts. The relative free energies are given in kcal mol^{-1} .

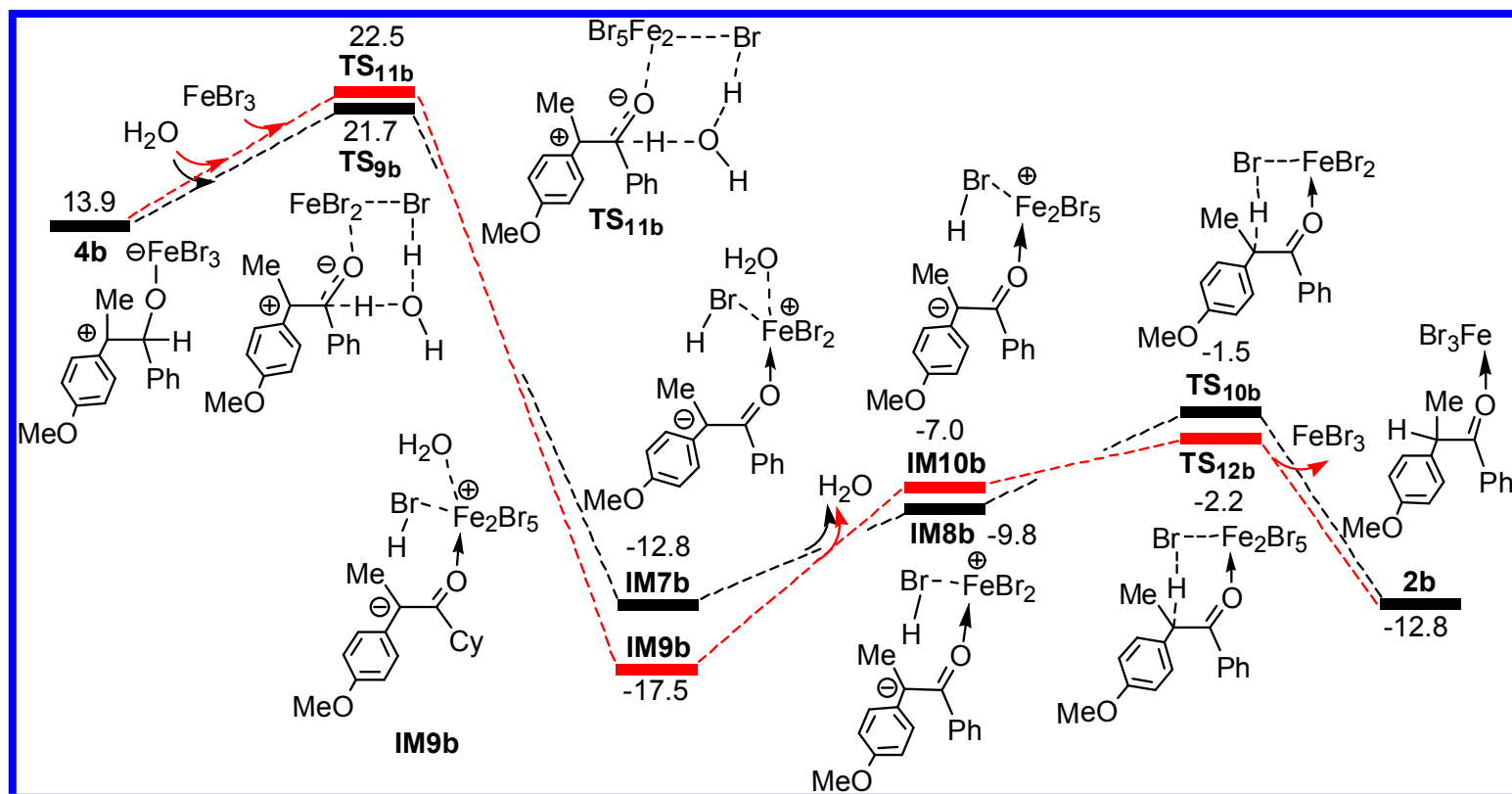


Fig. S3 Single-point solvation-corrected free energy profiles in toluene along possible H-shift pathways from **4b** and schematic structures for the species involved. The relative free energies are given in kcal mol⁻¹.

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

FeBr₃				C	-3.15735500	-1.43183100	-1.15760700
SCF done: -164.3475177				C	-3.06143800	-0.49045900	1.04719900
Fe	-0.39195300	-0.00055100	0.00002300	C	-3.93557100	-2.48831500	-0.68270500
Br	-2.72669200	-0.00011900	-0.00000800	H	-2.90862500	-1.42398000	-2.21180100
Br	1.50852700	1.59998900	-0.00000500	C	-3.82845500	-1.53721900	1.53599500
Br	1.50933000	-1.59946000	-0.00000500	H	-2.73507900	0.26774100	1.75162200
H₂O				C	-4.27725700	-2.54918100	0.67365600
SCF done: -76.4663367				H	-4.26222900	-3.25349800	-1.37643300
O	0.00000000	0.00000000	0.11884900	H	-4.09199200	-1.59553300	2.58666900
H	0.00000000	0.76007400	-0.47539600	O	-5.02356500	-3.52827500	1.24465900
H	0.00000000	-0.76007400	-0.47539600	C	-2.26959900	2.15065700	-0.28405300
1a				C	-1.18358600	3.25165900	-0.44924800
SCF done: -937.9462798				C	-3.61254100	2.62483300	-0.86480600
C	-1.82236400	0.75435200	-0.85042700	H	-2.42266600	2.01902500	0.79307000
C	-1.70592000	0.75711100	-2.38195300	C	-1.78741600	4.67553900	-0.45646900
H	-1.10311500	1.60072100	-2.72388900	H	-0.61162500	3.10424400	-1.37156800
H	-1.21909000	-0.14905400	-2.74672200	H	-0.46112600	3.16787900	0.37289400
H	-2.69276000	0.83470800	-2.84258100	C	-4.15396800	3.83644000	-0.06897700
C	-0.50202500	0.39507300	-0.22007800	H	-3.47158300	2.90599600	-1.91499800
H	-0.43254200	0.47113600	0.87670200	H	-4.34528000	1.81109200	-0.85623500
O	0.48096400	-0.00872200	-0.85247900	C	-3.02233300	4.75889200	0.44915000
Fe	2.34124900	-0.63175400	-0.26907200	H	-2.07415800	4.95130100	-1.47932500
Br	3.13532100	-2.71475700	-1.11187500	H	-1.02608500	5.39927900	-0.14731200
Br	3.70744700	1.55763400	-0.14075100	H	-4.75511000	3.48323800	0.77701300
Br	2.32800800	0.09564100	2.22447700	H	-4.83484400	4.40429400	-0.71320300
C	-2.71668500	-0.39946900	-0.31799700	H	-2.73562400	4.46639000	1.46782000
				H	-3.37965800	5.79159700	0.52069400
				C	-5.48235200	-4.59719900	0.42589600

H	-4.64596300	-5.15025800	-0.01861800
H	-6.04221400	-5.26030800	1.08616700
H	-6.14426100	-4.23783900	-0.37180000

TS1a

SCF done: -937.9103894

C	-1.32909700	0.38385400	-1.10525600
C	-2.56157400	-0.26022400	-0.66083800
C	-2.58233100	-1.04380800	0.51985600
C	-3.75098400	-0.17526200	-1.41081800
C	-3.73396900	-1.69321100	0.92575900
H	-1.67124700	-1.19011400	1.09068100
C	-4.91733200	-0.81179700	-1.00505100
H	-3.77834500	0.41819800	-2.31898300
C	-4.91565300	-1.58042700	0.17205200
H	-3.74381000	-2.31454900	1.81457200
H	-5.81456800	-0.71121800	-1.60338500
C	-0.98743400	0.46069100	-2.56290200
H	-0.20224900	1.19424400	-2.74723400
H	-0.58275600	-0.51986800	-2.84658700
H	-1.85275400	0.65734100	-3.19909800
C	-0.32149400	0.77776700	-0.18190700
H	-0.50852200	0.60286100	0.88096300
O	0.91921900	0.95302100	-0.54943700
Fe	2.46085600	-0.10590900	-0.11555900
Br	4.71344400	0.71896100	-0.27520300
Br	1.59725500	-1.51791100	1.96583300
Br	1.79617500	-2.53160700	-0.94046400
C	-1.36485400	2.42661600	-0.31484100
C	-2.38171200	2.49878800	0.83145900
C	-0.22093900	3.42800400	-0.19691500
H	-1.84876500	2.56279500	-1.28404400

C	-2.29567300	3.85970300	1.56499700
H	-2.23191400	1.69406800	1.55970000
H	-3.39133200	2.36060100	0.43233100
C	-0.80960300	4.86230200	-0.24700000
H	0.31745300	3.26990500	0.74239200
H	0.50933100	3.28551400	-0.99480400
C	-2.12205700	5.01203800	0.56832100
H	-1.45410000	3.85054200	2.26752400
H	-3.19963000	3.99645900	2.16803700
H	-0.98434800	5.14790700	-1.29042800
H	-0.04128100	5.54377400	0.13426600
H	-2.98510500	5.02074100	-0.11006900
H	-2.13716600	5.97353600	1.09168200
O	-5.98456300	-2.25164200	0.65175200
C	-7.20699500	-2.22044500	-0.08033300
H	-7.90504100	-2.84021300	0.48249400
H	-7.60381400	-1.20096700	-0.15299900
H	-7.07994600	-2.63701500	-1.08630300

TS2a

SCF done: -937.9242407

C	-1.69881100	-0.95840000	-0.24435500
C	-0.69758000	-1.61483400	-1.14954400
O	-1.16548300	0.28704600	-0.65056800
Fe	0.08918700	1.36742500	0.32564700
Br	0.20699700	0.85910200	2.70800200
Br	2.30488700	1.59929400	-1.06708700
Br	0.16147600	3.77558100	-0.65027600
C	-1.07974400	-1.67556600	-2.59568500
H	-1.85202300	-2.44835000	-2.70988200
H	-1.52122600	-0.72466000	-2.89764300
H	-0.26602100	-1.92050500	-3.27373700

C	0.57263000	-2.06860400	-0.66688800
C	0.80325000	-2.30372700	0.72319700
C	1.66725200	-2.30079000	-1.54349600
C	2.01857300	-2.74835100	1.18749200
H	0.01924600	-2.12557600	1.44552700
C	2.89699600	-2.73463500	-1.08739600
H	1.56690300	-2.10588000	-2.60307700
C	3.08619900	-2.96138400	0.29071700
H	2.18925200	-2.91557500	2.24478100
H	3.70734300	-2.87820700	-1.79097000
O	4.23461900	-3.37534300	0.84174500
C	5.38823700	-3.55660800	0.01575100
H	5.66644100	-2.62111600	-0.48058200
H	6.18603600	-3.86326900	0.69133400
H	5.21853400	-4.33975600	-0.73107300
H	-1.52215500	-1.14670900	0.81963900
C	-3.19604100	-1.12430800	-0.50781900
C	-3.65303000	-2.57395500	-0.19157500
C	-4.00083100	-0.11054600	0.32349500
H	-3.38938900	-0.90353800	-1.56442100
C	-5.13939300	-2.64957100	0.23083200
H	-3.02965600	-2.99211000	0.61046800
H	-3.48611600	-3.21128700	-1.06957000
C	-5.50176500	-0.15192000	-0.04730400
H	-3.86778300	-0.34196500	1.38871400
H	-3.59859400	0.89568100	0.17393000
C	-5.96806700	-1.56611700	-0.47039000
H	-5.22211500	-2.51562400	1.31671000
H	-5.53633000	-3.64761700	0.01525500
H	-5.70455100	0.55717500	-0.85813900
H	-6.08752900	0.19132100	0.81293700
H	-5.86290000	-1.68770100	-1.55686900

H	-7.03417100	-1.69472500	-0.25412900
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5a

SCF done: -937.9287261

C	-1.06993500	1.20832500	-0.72379000
C	-2.53749400	0.96024300	-0.52353900
C	-3.48300800	1.50778200	-1.40776900
C	-3.00308600	0.20929300	0.56130400
C	-4.84275900	1.31824500	-1.20605300
H	-3.16195100	2.09434500	-2.26218100
C	-4.36709200	0.00271700	0.76912300
H	-2.29117700	-0.24517700	1.24214400
C	-5.29814900	0.56151400	-0.11565100
H	-5.57506700	1.74215000	-1.88490000
H	-4.68685300	-0.59778100	1.61202900
C	-0.58553700	1.37925600	-2.14723800
H	0.50243500	1.33680500	-2.21067300
H	-1.00200700	0.59484200	-2.78458900
H	-0.91214400	2.34652500	-2.54127300
C	-0.27959400	1.74849600	0.41602400
H	-0.85192200	1.90692300	1.33173800
O	-0.21913100	0.31006000	0.11219700
Fe	1.29041200	-1.02459700	-0.23106400
Br	3.17097300	-0.29482800	-1.53768000
Br	1.44329200	-2.37320300	1.95465400
Br	0.08938900	-3.25754900	-0.69104100
C	0.98484000	2.56741400	0.33071000
C	0.61161100	4.07358600	0.21709400
C	1.89528900	2.33110500	1.55179300
H	1.54362200	2.26800800	-0.56168200
C	1.72248500	4.99633600	0.77104900
H	-0.32588300	4.26906000	0.75448200

H	0.41603300	4.30930100	-0.83540100
C	3.24937000	3.05678700	1.37547200
H	1.37877300	2.69488700	2.45021300
H	2.06574500	1.25962100	1.71013100
C	3.11027700	4.37358700	0.57348500
H	1.55832800	5.17368400	1.84144600
H	1.66057300	5.97652900	0.28635000
H	3.95527800	2.39150900	0.86758300
H	3.67004900	3.26295200	2.36603500
H	3.26397300	4.17718400	-0.49544700
H	3.89415900	5.07913000	0.86822200
O	-6.64706200	0.42812600	-0.01046100
C	-7.16954000	-0.34344300	1.06291500
H	-8.25381900	-0.32196600	0.94698800
H	-6.82146500	-1.38281600	1.01892800
H	-6.90179600	0.08617000	2.03641400

TS3a

SCF done: -937.8718511

C	-0.20441500	1.42429100	-1.37501500
C	-1.56613400	1.57170200	-0.78809000
C	-1.78124000	2.46048800	0.28143100
C	-2.66097900	0.86025300	-1.29433600
C	-3.04586200	2.63248300	0.82502200
H	-0.94706800	3.03481300	0.67512900
C	-3.93320700	1.00961700	-0.74595600
H	-2.52184500	0.14727000	-2.09990900
C	-4.13325000	1.90130700	0.31807800
H	-3.22184700	3.32388600	1.64218200
H	-4.75157700	0.42323500	-1.14463200
C	-0.05318000	1.59206000	-2.86875100
H	-0.31157400	2.62012400	-3.14320500

H	0.96894600	1.38379700	-3.19030900
H	-0.73282500	0.92434300	-3.40636100
C	0.95783700	1.46806400	-0.48985900
H	-0.16330000	0.65738500	1.74559900
O	0.61454600	0.18470300	-0.88644300
Fe	0.41476600	-1.85086900	-0.17876700
Br	2.66591500	-2.65643900	0.10214100
Br	-0.23593200	-0.65438900	2.37048200
Br	-1.62260700	-2.77882200	-1.06787900
C	2.34708600	2.01250200	-0.54464900
C	2.33065500	3.56524500	-0.50621300
C	3.25040700	1.44415000	0.57009500
H	2.77498300	1.68204200	-1.50684700
C	3.65850300	4.15126200	0.02766500
H	1.50084800	3.90925000	0.12356200
H	2.13075800	3.94443500	-1.51529700
C	4.72123400	1.86528200	0.34578400
H	2.88694600	1.82273600	1.53409500
H	3.17334800	0.35346600	0.60785400
C	4.84792500	3.25123600	-0.33201200
H	3.60683900	4.25327200	1.11901300
H	3.79936500	5.16303100	-0.36753600
H	5.22955800	1.11006600	-0.26373200
H	5.23444000	1.87423700	1.31371700
H	4.88799600	3.13388600	-1.42301300
H	5.79117700	3.72791900	-0.04486700
O	-5.32711700	2.12853300	0.92026800
C	-6.46361600	1.39356400	0.47912800
H	-6.31895800	0.31465400	0.61086800
H	-7.29370800	1.72582200	1.10334500
H	-6.69461100	1.60375700	-0.57227600

IM1a

SCF done: -937.9499742

C	1.54515000	-0.66386500	0.48375100
C	2.95788400	-0.74548000	0.17882300
C	3.55018300	0.01291400	-0.87032400
C	3.80715400	-1.64036800	0.87559300
C	4.88725700	-0.10900800	-1.18561000
H	2.92735200	0.65839300	-1.47899300
C	5.15926100	-1.75218500	0.58497200
H	3.40785600	-2.22898900	1.69400900
C	5.71357200	-0.98706000	-0.45548700
H	5.32577500	0.44941100	-2.00558700
H	5.77272800	-2.43004000	1.16567700
C	0.79687000	-1.89153500	0.92096700
H	0.11180700	-1.69065200	1.75208700
H	1.46199500	-2.70757400	1.20264000
C	0.77767100	0.54768400	0.34589600
O	-0.49396500	0.49508700	0.35756400
Fe	-2.11445400	-0.59620800	0.30627900
Br	-3.20365900	-1.35058800	2.31003700
Br	-3.88920400	1.19026800	-1.25548900
Br	-2.07769600	-1.87010600	-1.89100100
H	-3.42972600	-0.00675500	-2.02946400
H	0.19017800	-2.26323100	0.08058600
O	7.00734300	-1.02500400	-0.83570100
C	7.90204100	-1.90817400	-0.16184800
H	8.87059100	-1.77157100	-0.64268900
H	7.98462700	-1.65606100	0.90166900
H	7.58586500	-2.95206900	-0.26862700
C	1.37262500	1.94290600	0.34208100
C	0.93474100	2.76104200	-0.90931500
C	0.93316700	2.68144400	1.63368900

H	2.46152100	1.86592900	0.36962500
C	0.88896700	4.28117100	-0.63329600
H	-0.05064000	2.41723900	-1.23733800
H	1.63272900	2.55509800	-1.73058000
C	1.67248300	4.03154900	1.76673800
H	-0.15022000	2.83141900	1.58819300
H	1.12314900	2.05927300	2.51520100
C	1.94907200	4.69353900	0.39519000
H	-0.10312800	4.55886800	-0.25651000
H	1.02270400	4.82733100	-1.57315300
H	2.61754900	3.88655800	2.30298600
H	1.06526100	4.69909900	2.38871400
H	2.93914500	4.39362300	0.02645000
H	1.98264300	5.78288800	0.50188600

TS4a

SCF done: -937.9418823

C	1.14985100	-0.43525600	0.88451700
C	2.51656800	-0.58483300	0.42773100
C	2.95581100	-0.01118700	-0.80228500
C	3.45080800	-1.38803800	1.13018000
C	4.23727300	-0.19695100	-1.26874500
H	2.25734600	0.55911100	-1.40625800
C	4.74656700	-1.57569800	0.67437900
H	3.15971600	-1.85323300	2.06470700
C	5.15526700	-0.97863600	-0.53257100
H	4.56448700	0.23216600	-2.20950900
H	5.43218900	-2.18069400	1.25493300
C	0.65771300	-1.22186300	2.08889700
H	1.09787800	-0.82097600	3.01220200
H	-0.42757900	-1.15786100	2.18709900
H	0.92879100	-2.27811000	2.01714900

C	0.36310500	0.80834900	0.59913000
H	0.41874900	-1.31061300	-0.24326700
O	-0.87592800	0.76191300	0.55519700
Fe	-2.53965100	-0.40587000	-0.06878800
Br	-3.36632400	-1.60480000	1.86565300
Br	-3.52008200	0.85229100	-1.87758800
Br	-0.56257100	-2.10623500	-1.21662600
O	6.38303000	-1.09578700	-1.07161100
C	7.36572800	-1.88853500	-0.40441700
H	8.25841300	-1.83695200	-1.02722200
H	7.59000500	-1.48649500	0.58995100
H	7.04026900	-2.93096900	-0.31694500
C	1.02152500	2.17350400	0.49694400
C	0.52585800	2.97275100	-0.74429500
C	0.69082200	2.95510700	1.79894900
H	2.10594800	2.04548500	0.45640500
C	0.53478600	4.49874300	-0.50120500
H	-0.48465300	2.64562900	-1.00491800
H	1.17252300	2.73104000	-1.59697700
C	1.47400000	4.28602100	1.84632300
H	-0.38916800	3.13367000	1.81521600
H	0.92043600	2.35289800	2.68538300
C	1.67196000	4.90771200	0.44308600
H	-0.42343400	4.80994400	-0.06770300
H	0.61801200	5.01838300	-1.46138800
H	2.44901100	4.12622500	2.32115600
H	0.92685100	4.98254000	2.49171600
H	2.62736200	4.57349000	0.01682100
H	1.73928500	5.99782600	0.52117200

6a

SCF done: -937.9666997

C	0.58206600	0.96728600	0.28803500
O	-0.48303000	0.77614400	-0.32845100
C	1.05338700	-0.00447300	1.35669700
H	0.32504500	-0.82300800	1.37390000
C	1.03136900	0.67007500	2.74281300
H	0.00963300	0.95071900	3.01212000
H	1.40059900	-0.03531900	3.49223800
H	1.65547000	1.56712900	2.78499000
C	2.40321100	-0.58078300	0.92865200
C	2.43293400	-1.55277300	-0.08981400
C	3.61798500	-0.17935400	1.49131800
C	3.63124300	-2.10007100	-0.52283100
H	1.50363700	-1.89691600	-0.53770400
C	4.83352300	-0.72403400	1.06686500
H	3.63607900	0.55814400	2.28762600
C	4.84474000	-1.68869000	0.05219400
H	3.65394400	-2.85616800	-1.30043100
H	5.75327200	-0.39631100	1.53635300
Fe	-1.96903700	-0.58312200	-0.39773600
Br	-4.15975200	0.74830800	-0.59885100
Br	-1.41510000	-2.61812700	-1.53681700
Br	-3.04145700	-0.58309200	1.96642600
O	5.96384000	-2.28600700	-0.43817300
C	7.22195600	-1.92465900	0.11313200
H	7.27480700	-2.15579100	1.18452600
H	7.96496900	-2.51955800	-0.41942200
H	7.43758200	-0.85911000	-0.03683600
C	1.39317500	2.18964200	-0.05435500
C	1.83627900	2.16562000	-1.55167200
C	0.57665700	3.47510800	0.23674600
H	2.28585100	2.18925400	0.57871000
C	2.07246200	3.58763500	-2.10956500

H	1.06935000	1.65981300	-2.14590100
H	2.74947200	1.56644100	-1.62821300
C	1.46968000	4.72703500	0.07564300
H	-0.26883200	3.50437400	-0.45835300
H	0.14700400	3.44606800	1.24390300
C	2.55221800	4.54879800	-1.01483500
H	1.14292800	3.97582200	-2.54391100
H	2.79658500	3.53863400	-2.92959900
H	1.94680600	4.96829000	1.03247100
H	0.82660800	5.57936800	-0.17097500
H	3.47339600	4.15104500	-0.56901700
H	2.81779200	5.52087500	-1.44302800

3A

SCF done: -773.5947868

C	-2.03681400	0.00887500	0.07364700
C	-1.96762400	-1.10260500	-0.99273400
C	-3.52357800	0.30204300	0.44025500
C	-2.51822300	-2.44021900	-0.44402800
H	-2.54275700	-0.76843200	-1.86294000
C	-4.41907100	-0.95558900	0.33429200
H	-3.56688000	0.70941600	1.45766300
C	-3.62284100	-2.23456800	0.61848900
H	-2.91323800	-3.03064200	-1.27953600
H	-5.26840800	-0.86327200	1.02041400
H	-4.28586300	-3.10638000	0.64876000
H	-0.93642700	-1.23259300	-1.33785600
H	-1.70149900	-3.02965100	-0.01103600
H	-3.17270200	-2.15913700	1.61727900
H	-4.84641900	-1.02117800	-0.67437100
H	-3.90469400	1.07876800	-0.23101100
H	-1.50608200	-0.33587200	0.96949100

C	-1.37048400	1.29206100	-0.42012800
O	-1.68095300	1.78839300	-1.48971300
C	-0.29168000	1.92278600	0.47306100
C	0.96052700	1.05089100	0.42143700
C	1.52883800	0.51673200	1.58838600
C	1.58777400	0.77013500	-0.79785000
C	2.68126500	-0.25850600	1.54247400
H	1.06398300	0.71754800	2.55071100
C	2.74655500	-0.00751100	-0.86358300
H	1.16501900	1.16148000	-1.71944800
C	3.30033700	-0.52637600	0.31313300
H	3.12256800	-0.66800000	2.44537700
H	3.20095500	-0.20151500	-1.82798900
O	4.42575100	-1.29680500	0.36995100
H	-0.67119900	1.88504300	1.50349900
C	-0.01691800	3.38265800	0.08695000
H	-0.92493300	3.98622300	0.17923300
H	0.75519200	3.80886600	0.73388900
H	0.31823600	3.45309900	-0.95030200
C	5.09532700	-1.59682600	-0.84407200
H	5.44790600	-0.68779200	-1.34841000
H	5.95481500	-2.21096600	-0.57081700
H	4.45369000	-2.16159900	-1.53288600

TS5a

SCF done: -937.9124839

C	-1.51868100	-0.62849000	-0.92377300
C	-2.89916300	-0.65522000	-0.43754100
C	-3.28851100	-0.17825400	0.83790900
C	-3.90739500	-1.16860700	-1.27646400
C	-4.61101200	-0.19422700	1.23467800
H	-2.53573700	0.15070500	1.54711600

C	-5.24703800	-1.15729000	-0.90006600	H	-8.02696100	-0.56426700	-0.89604200
H	-3.65270400	-1.54108300	-2.26272700	C	-0.98250100	1.83303300	-0.20399700
C	-5.61023200	-0.67054800	0.36413200	C	-0.17981100	2.38958700	0.99991600
H	-4.90341800	0.14001700	2.22406100	C	-0.81638100	2.75009800	-1.43508600
H	-5.99252200	-1.53396200	-1.58937100	H	-2.04497800	1.81675100	0.05387600
C	-0.99269800	-1.75435400	-1.75112000	C	-0.07436800	3.93169500	0.97511400
H	-0.58076300	-1.35771000	-2.68644400	H	0.82988200	1.96546400	1.00451900
H	-0.13681700	-2.21209900	-1.24062200	H	-0.66003200	2.06059100	1.93065800
H	-1.73849100	-2.52634500	-1.93449200	C	-1.42899900	4.14416800	-1.16101100
C	-0.55716000	0.40338400	-0.58583800	H	0.25009800	2.83253000	-1.66316500
H	-0.63982900	-0.33206400	0.38986000	H	-1.28612600	2.29792000	-2.31658300
O	0.66266900	0.28538900	-1.10429700	C	-1.31054300	4.56401500	0.32404600
Fe	2.33678300	-0.09374400	-0.27312300	H	0.82006200	4.22948500	0.41484300
Br	4.13917600	1.47264800	0.00427400	H	0.06611100	4.30649900	1.99425500
Br	1.31023700	-1.53421900	1.76578200	H	-2.48356700	4.15434900	-1.46149800
Br	2.85933500	-2.65540100	-0.65086900	H	-0.92093500	4.87778700	-1.79712700
O	-6.87103100	-0.63320000	0.84482000	H	-2.20635300	4.24759100	0.87556000
C	-7.93322400	-1.13371400	0.03597000	H	-1.27544800	5.65569300	0.40455600
H	-7.79094100	-2.19571700	-0.19507200				
H	-8.83987100	-1.00995000	0.62812900				

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

TS6a

SCF done: -937.9066379

C	1.79547000	0.80026000	0.31482600	Br	-3.24605400	0.65528200	1.75120300
C	0.37251000	0.61268500	0.30601600	Br	-2.98420800	1.40800700	-1.22747400
H	-0.21106000	1.51646900	0.11792000	C	2.75250400	-0.31024600	0.31135100
O	-0.23651400	-0.52706700	0.09386300	C	4.08873000	-0.12427300	0.74857000
Fe	-2.12836000	-0.84026500	-0.12759900	C	2.39462900	-1.59430700	-0.15629700
Br	-2.95100300	-3.01875000	-0.73101000	C	5.00758300	-1.15412500	0.71841100
				H	4.41205800	0.83681300	1.13290300
				C	3.31786800	-2.63243400	-0.20658300

H	1.37961400	-1.76929800	-0.48490900
C	4.63289200	-2.42283900	0.23429200
H	6.02605600	-1.01256200	1.06345200
H	3.00251700	-3.59691500	-0.58525400
C	0.74806100	0.73962700	2.09179000
H	0.93633000	-0.29300900	2.37074300
H	1.47186100	1.42994600	2.52193200
H	-0.26661100	1.05219600	2.34740800
O	5.60400200	-3.35966000	0.23926200
C	5.29894800	-4.67113500	-0.23349700
H	4.99307200	-4.65355200	-1.28570300
H	6.22121200	-5.24340200	-0.13313900
H	4.51187800	-5.13814700	0.36913800
C	2.32835900	2.21541300	0.13169100
C	2.90934000	2.29837500	-1.32364300
C	1.36167900	3.39445700	0.35430000
H	3.16158600	2.35680100	0.83012400
C	3.02015600	3.75579100	-1.82703700
H	2.27232900	1.72252800	-2.00531900
H	3.88980600	1.81295800	-1.33598500
C	2.14686300	4.72768300	0.34620000
H	0.60797700	3.40912800	-0.44087000
H	0.81412300	3.30409200	1.29725700
C	3.31097500	4.72395900	-0.67516800
H	2.08664400	4.05228800	-2.32002700
H	3.80112000	3.81259700	-2.59267000
H	2.53667000	4.93213500	1.35023000
H	1.44718500	5.53840900	0.11728300
H	4.24501900	4.42309700	-0.18270200
H	3.48292900	5.73592600	-1.05572000

IM2a

SCF done: -937.9201298

C	1.87575400	0.81948400	0.47882800
C	0.37688900	0.65893500	0.73215800
H	-0.10308600	1.55224600	0.30389100
O	-0.18781500	-0.48672000	0.21854900
Fe	-0.86200400	-1.02457100	-1.44209600
Br	0.26058600	-2.98851300	-2.38889400
Br	-3.45734000	-0.70758100	-1.67201900
Br	-1.31932300	1.15945400	-2.87525000
C	2.76687000	-0.27797000	0.43116400
C	4.17536300	-0.11132300	0.18767900
C	2.30441400	-1.62529200	0.60752700
C	5.02511900	-1.18186200	0.11717700
H	4.59342500	0.87705800	0.04632700
C	3.15717700	-2.70556700	0.55053600
H	1.24342500	-1.78120900	0.75017800
C	4.52508300	-2.50030900	0.28436100
H	6.08460700	-1.05717900	-0.07690700
H	2.75197100	-3.70308700	0.66033500
C	0.13832400	0.70031800	2.27094800
H	0.59088500	-0.17874600	2.73749400
H	0.52554600	1.59999800	2.75558900
H	-0.94298200	0.65555700	2.42128500
O	5.42854600	-3.47128100	0.16485200
C	5.01440700	-4.84380500	0.25948000
H	4.27417900	-5.07819300	-0.51092000
H	5.91804400	-5.42956400	0.09699900
H	4.60726900	-5.05888900	1.25219000
C	2.36266600	2.20986100	0.18728800
C	2.23133800	2.38572500	-1.38167600
C	1.67658900	3.39311100	0.90541400

H	3.42358300	2.28543100	0.43769000
C	2.11623200	3.86979900	-1.78396400
H	1.36049100	1.83865600	-1.75685300
H	3.11189100	1.92346600	-1.84106700
C	2.43155600	4.70616500	0.59140700
H	0.63399200	3.48092500	0.58645500
H	1.66324900	3.23387000	1.98718800
C	2.95301500	4.76677200	-0.86641500
H	1.06605900	4.18174700	-1.74853400
H	2.43015100	3.97280100	-2.82828200
H	3.26961000	4.82281800	1.28851400
H	1.75375100	5.54473100	0.78363300
H	4.00022500	4.43870300	-0.90661100
H	2.94630600	5.80039400	-1.22675700

TS7a

SCF done: -937.9041559

C	1.81443300	-0.41276600	-0.90929600
C	0.63834900	-1.01024000	-1.54957200
O	-0.50726600	-0.36350000	-1.60982900
Fe	-1.96210600	-0.13495200	-0.37414900
Br	-3.11765100	1.99072900	-0.34140600
Br	-3.27169500	-2.38719300	-0.08764100
Br	-1.09243100	-1.32298900	1.82060900
H	1.45372700	-0.57914100	-2.39264800
C	3.01336700	-1.32207500	-0.67879800
C	4.40415800	-0.76896000	-1.11871900
C	3.02209600	-1.85502100	0.78675800
H	2.83877800	-2.21417700	-1.27972700
C	5.54411100	-1.31458600	-0.23717900
H	4.42249600	0.32288100	-1.12347800
H	4.57330200	-1.07899600	-2.15737300

C	4.03049300	-3.01670600	0.92082700
H	3.28208000	-1.05351600	1.48228800
H	2.01892100	-2.18540500	1.07382800
C	5.32395100	-2.79745500	0.09169500
H	5.60908700	-0.73908400	0.69586200
H	6.50105300	-1.17002000	-0.74989300
H	3.55158900	-3.95373600	0.61488200
H	4.27575500	-3.13206500	1.98216500
H	5.26353100	-3.35741100	-0.85087700
H	6.18779100	-3.20314700	0.62805900
C	1.83016600	0.99629400	-0.51723300
C	2.77954500	1.47000200	0.42920500
C	0.90540100	1.94815900	-1.01540000
C	2.76589900	2.77270700	0.88454800
H	3.51759500	0.80162400	0.84822800
C	0.90364700	3.26655600	-0.58659600
H	0.18080200	1.65344500	-1.75942900
C	1.82029400	3.68980500	0.38812700
H	3.47366900	3.11137300	1.63318900
H	0.16686600	3.94442800	-0.99812200
O	1.88081200	4.93382600	0.89849900
C	0.90658300	5.89551400	0.48681200
H	-0.10813500	5.55184900	0.71385700
H	1.12478400	6.79785300	1.05780500
H	0.99172100	6.11190400	-0.58406400
C	0.50701800	-2.51566900	-1.79989600
H	0.24537800	-3.00936500	-0.85887500
H	-0.32699600	-2.64589800	-2.49008700
H	1.38774900	-2.99974000	-2.22341800

IM3a

SCF done: -937.9609773

C	-1.78148300	0.73782500	1.39901000
C	-0.27362200	0.69747000	1.45191700
O	0.37383200	-0.09296800	0.74603700
Fe	2.34009100	-0.52322900	0.48944000
Br	3.45900100	-1.18638700	2.49795100
Br	2.52205900	-1.44237100	-1.89669500
Br	3.20816200	1.44085400	-0.96950500
C	-2.18459700	1.98967800	0.50920500
C	-1.69042800	1.91348900	-0.95645900
C	-3.70111700	2.24121700	0.55375100
H	-1.70522700	2.85656100	0.98555700
C	-2.53057000	2.80364600	-1.90489100
H	-1.73407900	0.88104600	-1.31409000
H	-0.63674600	2.21388600	-1.00215900
C	-4.04231700	3.62888800	-0.04276300
H	-4.20665600	1.44873400	-0.00851100
H	-4.07569400	2.17282900	1.58162800
C	-3.07471300	4.03924600	-1.17886100
H	-3.37391100	2.22500600	-2.30252500
H	-1.92399200	3.09314700	-2.76929200
H	-4.02160500	4.38789800	0.74812000
H	-5.07173700	3.60510000	-0.41810400
H	-2.23286800	4.61165100	-0.76746000
H	-3.58120400	4.70957800	-1.88140300
C	-2.47973300	-0.56848700	1.05702700
C	-3.55474000	-0.97255300	1.86974100
C	-2.14209000	-1.39489100	-0.02272000
C	-4.26747600	-2.13578700	1.61553000
H	-3.83856600	-0.36229300	2.72389300
C	-2.84682500	-2.57183300	-0.28999500
H	-1.30460500	-1.14721400	-0.66189700
C	-3.91845200	-2.94847800	0.52691500

H	-5.09349000	-2.44055000	2.24948100
H	-2.54441100	-3.18267000	-1.13204500
O	-4.67092200	-4.06991400	0.35598900
C	-4.34863700	-4.93975300	-0.72011700
H	-3.33186800	-5.34087200	-0.62451800
H	-5.06515300	-5.76053300	-0.66761900
H	-4.44690500	-4.43603200	-1.69007600
C	0.45148400	1.65652500	2.35594400
H	-0.21111200	2.38785500	2.81966400
H	0.94646900	1.07039300	3.14086300
H	1.24254400	2.16720700	1.79690800
H	-2.09713200	1.01956600	2.41181300

TS8a

SCF done: -937.9149435

C	-1.52556100	0.85688000	-0.40298700
C	-1.35037100	0.85841700	-1.88334500
H	-0.65223800	1.67696200	-2.11094700
H	-0.86746300	-0.04961200	-2.23652600
H	-2.28356900	1.04485300	-2.41866600
C	-0.79037700	-0.11666000	0.40787800
O	0.26370800	-0.75669600	-0.12300700
Fe	2.04962800	-0.13557500	-0.25225200
Br	2.23148900	2.00414900	-1.45006100
Br	3.26728700	-0.44654400	2.05067400
Br	3.75823300	-2.07356700	-0.53082000
H	-0.69676800	0.17479600	1.46376700
C	-2.16471500	-0.93599600	0.26306000
C	-3.21988600	-0.85561000	1.20048800
C	-2.21165700	-1.94962800	-0.71271900
C	-4.27533600	-1.74447300	1.15630600
H	-3.19984700	-0.10990700	1.98815600

C	-3.26796800	-2.84676400	-0.76928700	H	-0.66792800	-2.66918400	1.69692600
H	-1.37054400	-2.06314200	-1.38628800	H	0.33908500	-3.76409200	0.72802300
C	-4.31658000	-2.74481600	0.16302500	H	0.98514900	-3.03415400	2.20559800
H	-5.08086100	-1.70313300	1.88124700	C	0.63956500	-0.33674500	1.34463800
H	-3.26140200	-3.62959900	-1.51767000	O	-0.73394700	-0.11244200	1.55449900
O	-5.38990600	-3.55606500	0.20079500	Fe	-2.15988500	-0.04175400	0.49448100
C	-5.50214400	-4.60785200	-0.75894900	Br	-4.28489800	-1.02121000	0.09350300
H	-6.43822000	-5.11660400	-0.52979200	Br	-2.60713000	2.15365800	-0.40548200
H	-5.54208900	-4.21094200	-1.77943300	Br	-0.45179100	-1.55863000	-1.13731100
H	-4.67046800	-5.31542800	-0.67024000	H	1.05654600	-0.56769300	2.33891300
C	-2.25218100	1.99164800	0.25776400	C	1.33997800	0.93905000	0.88806700
C	-1.22345100	3.18315300	0.39224700	C	2.11850000	1.63963900	1.82644400
C	-3.54311900	2.46067500	-0.43422700	C	1.19704300	1.49964200	-0.38769000
H	-2.50073800	1.69657900	1.28105800	C	2.74942300	2.83228400	1.50311500
C	-1.95132800	4.54343700	0.45954600	H	2.22926700	1.24297100	2.83272300
H	-0.50257900	3.18821100	-0.42980300	C	1.82965600	2.69501500	-0.73181000
H	-0.63825000	3.01824000	1.30260700	H	0.58608900	1.01102900	-1.13598000
C	-4.27387000	3.51021400	0.43439500	C	2.61031100	3.37078400	0.21445100
H	-3.29294600	2.89453400	-1.40860700	H	3.35053000	3.36888700	2.22943700
H	-4.20139900	1.60669700	-0.63030900	H	1.69334400	3.09196800	-1.73035600
C	-3.29067300	4.43353600	1.19739600	O	3.26438700	4.54061300	-0.01277100
H	-2.12504100	4.92350800	-0.55463400	C	3.12838400	5.15492400	-1.28748800
H	-1.29285700	5.26883200	0.94867400	H	3.71372300	6.07413800	-1.24110800
H	-4.93342500	3.00340200	1.14851400	H	3.52259700	4.51562800	-2.08752800
H	-4.92517400	4.10733400	-0.21302800	H	2.08216300	5.40191500	-1.50556400
H	-3.10915500	4.03908100	2.20576800	C	2.30289600	-1.83242200	-0.00014900
H	-3.73575700	5.42405100	1.33610000	C	3.36781000	-1.74824900	1.14487100
				C	2.53986700	-3.12345400	-0.80771200
				H	2.47995600	-0.98146900	-0.66676700
				C	4.70913600	-2.40897200	0.74412200
				H	2.99535300	-2.22952100	2.05623300
				H	3.53384600	-0.69566300	1.39028800

IM4a

SCF done: -937.9388699

C	0.88208500	-1.66186600	0.55706300
C	0.34315900	-2.85776100	1.33417100

C	3.88548100	-3.04403700	-1.56498100
H	2.54961900	-3.98082600	-0.12391900
H	1.72656000	-3.30068100	-1.51670100
C	4.96722300	-2.28253800	-0.76139100
H	4.69971600	-3.47150500	1.01785100
H	5.52158100	-1.95263100	1.31995600
H	3.73397400	-2.55519600	-2.53418500
H	4.22680300	-4.06222800	-1.78350100
H	4.96172300	-1.21962200	-1.03456800
H	5.96439400	-2.65722000	-1.01525900

TS9a

SCF done: -937.9094338

C	-1.19483700	-1.56364900	-0.76302100
C	-0.33491300	-2.73123400	-1.08247900
H	0.13857100	-3.06000100	-0.14863200
H	-0.92340700	-3.57493200	-1.45714700
H	0.46490800	-2.45696100	-1.77193300
C	-0.75458200	-0.23548400	-1.26012500
O	0.57945000	-0.03763400	-1.38684800
Fe	1.88737700	-0.10773000	-0.03550500
Br	4.17763500	-1.07853600	-0.77410700
Br	3.60723600	1.79850300	0.21248700
Br	0.67953500	-1.07642100	1.93745700
H	-1.18427200	-0.57099300	-2.27734100
C	-1.57362900	0.99655200	-0.90254200
C	-2.51691800	1.51164100	-1.80566600
C	-1.35765300	1.68430300	0.29695900
C	-3.23449600	2.66539100	-1.51748300
H	-2.67888900	1.01701200	-2.76105000
C	-2.07356000	2.84181100	0.60159300
H	-0.63728600	1.30724200	1.01551300

C	-3.01673300	3.34149700	-0.30787300
H	-3.95686900	3.07120300	-2.21769000
H	-1.88470600	3.34355600	1.54287800
O	-3.76189000	4.46168600	-0.11333700
C	-3.55082400	5.21862000	1.07186000
H	-4.22822600	6.07092900	1.00668600
H	-3.78855700	4.63632700	1.97084700
H	-2.51780300	5.58095600	1.13899700
C	-2.56495800	-1.77352400	-0.23068900
C	-3.55768200	-2.09159800	-1.41754800
C	-2.65599400	-2.89743100	0.83132000
H	-2.89066600	-0.83297600	0.22307500
C	-4.80773000	-2.85256200	-0.92424200
H	-3.04878300	-2.67716500	-2.19154900
H	-3.83974600	-1.13617900	-1.87077600
C	-4.05032200	-2.86604900	1.49731000
H	-2.48754600	-3.86785700	0.35101900
H	-1.87218600	-2.76884700	1.58221100
C	-5.17415300	-2.46150900	0.51222200
H	-4.62835500	-3.93349800	-0.97050300
H	-5.63754200	-2.64815100	-1.60946300
H	-4.03404400	-2.17204000	2.34437100
H	-4.25496200	-3.85858800	1.91343500
H	-5.34191100	-1.37791300	0.55469600
H	-6.12033300	-2.92732100	0.80505100

IM5a

SCF done: -937.9689996

C	0.07250700	2.42951900	-1.46483000
C	-0.28558000	2.14848800	-2.94316300
H	-1.03939000	1.36005000	-3.01209900
H	-0.67399000	3.04970600	-3.42136800

H	0.59597800	1.82868200	-3.50818100	H	6.28515800	-0.74281600	1.86114300
C	0.75198700	1.18164400	-0.92354000	H	6.83695500	-0.86257700	0.16144500
O	0.04745900	0.14106100	-0.89221400	C	-1.15777700	2.79092300	-0.58331000
Fe	-0.63684700	-1.61250400	-0.28439900	C	-0.75087700	2.97151300	0.90527600
Br	-3.21398500	-1.55504000	-0.48811800	C	-1.89968900	4.04959600	-1.06590900
Br	0.72267700	-3.54179100	-0.76105200	H	-1.85058400	1.94284200	-0.65448800
Br	-1.55976900	-1.21816400	2.10832500	C	-1.75592200	3.83207700	1.70775000
H	0.77022400	3.27114400	-1.43812100	H	0.24246300	3.43715900	0.96149200
C	2.14937100	1.14266600	-0.50524300	H	-0.65927600	1.98453800	1.37283500
C	2.93392300	2.31147100	-0.34656600	C	-3.23859000	4.22603400	-0.30645500
C	2.75908700	-0.10335100	-0.23854200	H	-1.25420000	4.92374600	-0.90106800
C	4.24675000	2.23540800	0.07343000	H	-2.09857700	4.01364200	-2.14096500
H	2.50840100	3.28980800	-0.53366000	C	-3.17407400	3.69221300	1.14319700
C	4.07879800	-0.19234100	0.17253200	H	-1.45898900	4.88837800	1.66809800
H	2.19613000	-1.01971700	-0.37734800	H	-1.72662900	3.54569100	2.76430200
C	4.83477800	0.98252000	0.33886800	H	-4.03922800	3.71111900	-0.84965200
H	4.84930600	3.12670000	0.20938300	H	-3.50377400	5.28988400	-0.30272500
H	4.51064600	-1.16811100	0.35704100	H	-3.46382100	2.63430400	1.16792100
O	6.11901900	1.01476100	0.74015200	H	-3.89687000	4.22189300	1.77310700
C	6.78401400	-0.21316700	1.04218000				
H	7.79170300	0.06602100	1.34930100				

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

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IM6a SCF done: -1102.293735

C	2.12390000	0.11534100	1.02247100	H	4.85223500	0.01955500	1.54740600
C	3.28115300	-0.33310000	0.10763700	C	4.04512100	-1.32329600	-1.98639100
C	4.60680000	-0.34232100	0.55430900	H	2.00271600	-0.91920800	-1.54677700
C	3.02232300	-0.85180400	-1.17378400	C	5.37025600	-1.31033200	-1.52873300
C	5.64532400	-0.82421000	-0.24357300	H	6.65642000	-0.81557500	0.14528500
				H	3.83852000	-1.71891500	-2.97494000
				C	1.67415500	-1.07621600	1.88878500

H	0.82254300	-0.84245800	2.53216700
H	1.41100000	-1.93255400	1.26358900
H	2.50309200	-1.38336500	2.53185400
C	1.03457500	0.63318800	0.14005300
H	1.28839300	1.48261500	-0.50654800
O	-0.14126000	0.22436300	0.08973100
Fe	-1.65283300	-1.31158300	0.91758500
Br	-1.89230600	-2.40851200	3.01644700
Br	-2.75437600	-1.12616200	-1.58171400
Br	-0.60801100	-3.14988900	-0.79119600
Fe	-1.80669200	1.36656900	-0.84636600
Br	-2.96728400	1.10685500	1.34831700
Br	-0.80065000	3.82172600	-0.72858600
Br	-1.21003900	2.07834200	-3.22163600
C	2.52128500	1.36494500	1.93431900
C	3.26630700	2.51102700	1.18219100
C	1.33217700	1.94249300	2.73238900
H	3.21167000	0.93248600	2.67007700
C	3.05336000	3.89161500	1.84028700
H	2.96246100	2.56571700	0.13107000
H	4.33625600	2.28515800	1.15929200
C	1.82252700	2.91336800	3.83016700
H	0.65653300	2.47591400	2.05095300
H	0.73506200	1.15184900	3.19406000
C	3.02601000	3.77126000	3.36801700
H	2.11161000	4.33390700	1.49286800
H	3.84777900	4.57199400	1.51536200
H	2.09423900	2.34343200	4.72635900
H	0.98560800	3.55810600	4.11928200
H	3.96606000	3.31290200	3.70293300
H	2.98832000	4.76110100	3.83447900
O	6.30237000	-1.79286600	-2.39149400

C	7.66062900	-1.82666300	-1.97390100
H	7.79438300	-2.46046600	-1.08838100
H	8.21967400	-2.25216300	-2.80796800
H	8.04211100	-0.82043600	-1.75957300

TS10a

SCF done: -1102.279164

C	2.03873200	-1.04582200	-0.48550300
C	3.37326200	-0.61347900	-0.91087600
C	3.73204700	0.75703900	-0.91105400
C	4.33131300	-1.53768700	-1.37066400
C	4.98018000	1.17086400	-1.34133100
H	3.00866400	1.50974800	-0.61634400
C	5.59193300	-1.13548900	-1.79405100
H	4.10313800	-2.59868700	-1.37969300
C	5.92624400	0.22965000	-1.78445100
H	5.24554200	2.22214700	-1.36232700
H	6.30256700	-1.88068500	-2.12959000
C	1.31615100	-0.28111500	0.45493000
H	1.80825800	0.58273200	0.90000000
O	0.01052800	-0.29789000	0.61062100
Fe	-1.08274500	1.75547300	0.67448300
Br	0.78191200	2.98910200	1.96860000
Br	-3.05908400	0.29658100	1.44233600
Br	-1.90057200	4.21791800	1.08144500
Fe	-1.61217500	-0.95728800	-0.37586000
Br	-1.14153600	1.37360400	-1.84130300
Br	-2.55071200	-2.31347600	-2.33248100
Br	-2.02819000	-3.51853800	0.42499900
O	7.11281200	0.73249100	-2.18487800
C	8.11041000	-0.15775800	-2.68009100
H	7.75790300	-0.69704800	-3.56688800

H	8.95887600	0.47021500	-2.95152100	C	-5.38159000	1.00358200	-1.96261200
H	8.42087000	-0.87614200	-1.91238200	H	-3.62127500	2.03300900	-2.52760400
C	2.27429100	-1.67671700	1.61306900	C	-5.94618300	0.00592500	-1.13417600
C	3.34111600	-0.88427500	2.36257900	H	-5.57568200	-1.50198700	0.35607300
C	1.10688600	-2.16311200	2.45955700	H	-6.00010500	1.57566500	-2.64246900
H	2.70985600	-2.49505500	1.04110000	C	-0.98295300	0.49761200	0.29304100
C	2.78153500	-0.26562000	3.65001400	H	-1.38037000	-0.43419500	0.70967400
H	3.80479400	-0.12801300	1.71974900	O	0.37678700	0.27672900	0.00451800
H	4.15292600	-1.58266500	2.61051500	Fe	1.96100400	1.33209700	-0.59690400
C	1.66223400	-2.57006000	3.84516600	Br	2.17890600	3.70388500	-1.07668800
H	0.35205000	-1.38238500	2.59126600	Br	1.98954500	-2.62584800	-1.55667500
H	0.60356100	-3.00417800	1.97682800	Br	2.44382200	0.03949800	-2.89256000
C	2.23954100	-1.35403900	4.60703900	Fe	1.30251100	-1.44257900	0.63191600
H	1.98057400	0.43757500	3.39357300	Br	3.48139000	-0.01894000	1.02398400
H	3.55659200	0.32866900	4.14391000	Br	0.67836200	-1.75719100	3.18330600
H	2.43195700	-3.34099300	3.71545100	Br	-0.87968600	-3.12998300	0.97018000
H	0.85566900	-3.03782800	4.41859100	C	-1.06651000	1.50142900	-2.03864100
H	3.03721500	-1.69462100	5.27675000	H	-0.35617500	0.75675800	-2.43495700
H	1.46676900	-0.91350100	5.24556900	H	-1.69680900	1.83130500	-2.86174900
C	1.34671600	-2.16610100	-1.20706800	H	-0.43397700	2.33009100	-1.69400700
H	0.60615800	-2.67203300	-0.58371900	O	-7.23538500	-0.32809400	-1.12809000
H	0.82226500	-1.74099400	-2.07342100	C	-8.15442800	0.32549900	-2.01562800
H	2.04290600	-2.91141900	-1.59436100	H	-7.87215500	0.15999600	-3.05989600

IM7a

SCF done: -1102.293503

C	-1.78585000	0.85119200	-0.92235700	C	-1.16780000	1.56281400	1.46216200
C	-3.17166400	0.55532800	-0.99078800	C	-1.11081600	3.05008300	1.04155000
C	-3.77952500	-0.44677500	-0.16303400	C	-2.39504600	1.31665600	2.35256900
C	-4.02763300	1.24910500	-1.90064500	H	-0.28188400	1.33016900	2.06471400
C	-5.12226900	-0.71999100	-0.24255100	C	-1.57960100	3.99219300	2.18327100
H	-3.16738600	-1.05684400	0.48953900	H	-1.75353700	3.22496500	0.16955100
				H	-0.09420600	3.31201000	0.73424000

C	-2.22740200	2.06786600	3.70125800
H	-3.30174900	1.66460400	1.84054700
H	-2.53125700	0.24792700	2.55003800
C	-1.38099100	3.35467600	3.56252500
H	-2.64440700	4.22715900	2.05467700
H	-1.04443100	4.94436900	2.11327800
H	-1.75981500	1.39884000	4.43144200
H	-3.22089700	2.31288600	4.09392500
H	-0.31816800	3.12222600	3.70309200
H	-1.64336900	4.06327600	4.35516300

TS11a

SCF done: -1102.280833

C	-1.99667700	0.31244700	-0.79596200
C	-3.44069600	0.05437600	-0.90339600
C	-4.05259500	-1.17580800	-0.57004900
C	-4.26549400	1.09486300	-1.36988300
C	-5.42062700	-1.34147100	-0.67359400
H	-3.44452700	-2.02761000	-0.28173100
C	-5.64711700	0.94916600	-1.44342500
H	-3.83121500	2.05162900	-1.63962900
C	-6.23745200	-0.27493000	-1.09528700
H	-5.88851700	-2.29321000	-0.44719900
H	-6.24843000	1.78544000	-1.77715500
C	-1.17050000	-0.19112000	0.27017800
H	-1.35306400	-1.04304600	-0.62830300
O	0.14022200	0.12210400	0.25701700
Fe	1.09404800	1.89798500	0.69571800
Br	-0.12002700	3.76026200	1.64134700
Br	2.60319200	0.04467500	-2.49149600
Br	2.15380600	2.85812800	-1.51800400
Fe	1.77859000	-1.07752600	-0.31136500

Br	3.09581500	0.31609300	1.33518700
Br	2.36576500	-3.44258600	0.64122500
Br	0.40370700	-2.82615300	-1.58818400
C	-1.33014200	1.12925300	-1.86267300
H	-0.35687000	0.70947200	-2.12685500
H	-1.94615700	1.20969500	-2.75700800
H	-1.12162000	2.13214600	-1.46568700
O	-7.56004400	-0.53561200	-1.14636600
C	-8.45006700	0.48976900	-1.58456300
H	-8.23105400	0.79308600	-2.61479000
H	-9.44796300	0.05395000	-1.53964800
H	-8.40452000	1.36449500	-0.92565600
C	-1.73148400	-0.71715200	1.59758000
C	-1.23424100	-2.14423800	1.94918800
C	-1.38901700	0.25999300	2.74352700
H	-2.81990500	-0.73427000	1.50328200
C	-1.28161100	-2.42246600	3.46957300
H	-0.20991300	-2.28151100	1.59316300
H	-1.84778300	-2.87948800	1.41288700
C	-2.18366400	-0.11702300	4.01653800
H	-0.31220500	0.20711000	2.93869300
H	-1.60343500	1.29454200	2.46095700
C	-2.41451300	-1.64149500	4.14610500
H	-0.32626100	-2.13558200	3.92536600
H	-1.38964500	-3.49849100	3.63999800
H	-3.14781200	0.40424300	4.01690900
H	-1.63240300	0.25459500	4.88705800
H	-3.36977300	-1.91901300	3.68012000
H	-2.50062500	-1.92165800	5.20107900

IM8a

SCF done: -1102.324173

C	1.91103500	0.19477800	-1.65675200
C	1.55809400	-1.20851900	-2.17100700
H	1.72455400	-1.96646100	-1.39944000
H	0.52061000	-1.26903100	-2.50873400
H	2.21085100	-1.45810600	-3.01143400
C	0.93014000	0.71403700	-0.60945100
O	0.00763600	-0.02212900	-0.19491900
Fe	-0.36924300	-2.39542400	0.59888600
Br	1.69666200	-3.05250200	1.66059100
Br	-2.98310100	-1.04876900	-1.70847600
Br	-1.47946100	-3.63799000	-1.30456600
Fe	-2.26301700	0.44725500	0.19926000
Br	-2.22710200	-1.33879100	1.97511800
Br	-2.48422400	2.34552500	1.82548400
Br	-2.75838800	2.47973600	-1.17532700
H	1.76700700	0.90574700	-2.48500100
C	3.38161900	0.30175300	-1.25053900
C	4.28990500	1.02181900	-2.04346500
C	3.88072800	-0.38711800	-0.14006600
C	5.64259900	1.06528000	-1.73197400
H	3.93481300	1.55175100	-2.92401600
C	5.23784600	-0.35026200	0.18903100
H	3.21661400	-0.98259600	0.48003800
C	6.12842700	0.37982100	-0.60786000
H	6.34495900	1.61821800	-2.34688000
H	5.58221300	-0.89938300	1.05710900
O	7.46662800	0.48280500	-0.38378300
C	8.01923500	-0.20829100	0.72839900
H	9.08903300	0.00375700	0.71172000
H	7.59497400	0.14715600	1.67580300
H	7.86366200	-1.29129600	0.64821900
C	1.00442200	2.13145200	-0.08932800

C	1.70251400	2.12437300	1.31971100
C	1.63965800	3.19064700	-1.00768800
H	-0.03857200	2.41843800	0.07812600
C	2.25173200	3.52199200	1.68078200
H	2.51792400	1.39693200	1.33901300
H	0.96374000	1.79790500	2.05810000
C	1.37497900	4.60719700	-0.44210600
H	2.71562100	3.01254100	-1.08526900
H	1.23204000	3.12146100	-2.02265500
C	1.37247400	4.63878100	1.10645400
H	3.27272800	3.62965100	1.29402600
H	2.32539800	3.60443200	2.77052500
H	0.41595200	4.98076700	-0.81781200
H	2.14406500	5.28414400	-0.83044700
H	0.34943600	4.51467800	1.48300400
H	1.71165600	5.61699700	1.46282800

TS12a

SCF done: -1102.269

C	2.19791800	-0.35583500	-1.22210800
C	2.88758200	0.86892700	-0.75378200
C	3.84020200	1.50668200	-1.57922600
C	2.65502500	1.40641500	0.52302900
C	4.51440400	2.63624400	-1.15386200
H	4.04171200	1.13008400	-2.57754900
C	3.34563100	2.52965200	0.97015400
H	1.95014100	0.93102400	1.19056400
C	4.27390600	3.16052500	0.13015000
H	5.23287000	3.13867800	-1.79227400
H	3.14924200	2.90144100	1.96794400
C	0.86285800	0.19515300	-2.50343800
H	-0.04595200	-0.34085900	-2.78611100

H	0.67574500	1.22817700	-2.22083100
H	1.58330000	0.11200200	-3.31536800
C	0.87390600	-0.70193200	-0.84000000
H	0.53250200	-1.70384500	-1.10174300
O	0.11022300	-0.04809100	0.01773700
Fe	-0.45198300	-1.19994000	1.79729000
Br	1.57974900	-1.53442500	3.04308600
Br	-2.71105100	-1.30291900	-1.41014400
Br	-1.50211200	-3.22294400	0.58967100
Fe	-1.64062500	0.95682700	-0.29296400
Br	-2.29459800	0.52768000	2.20279300
Br	-0.58489500	3.44215000	-0.34770500
Br	-3.09443100	2.45242300	-1.78308300
C	3.06901500	-1.44674700	-1.84678200
C	4.01253300	-1.98531900	-0.71882400
C	2.36396600	-2.62963000	-2.53583900
H	3.69744900	-0.95939400	-2.60179900
C	4.57469400	-3.38591100	-1.05460200
H	3.46914300	-2.02720100	0.23221500
H	4.82769300	-1.26951800	-0.57776000
C	3.40130100	-3.48683500	-3.30131700
H	1.86356000	-3.25041700	-1.78347900
H	1.58668700	-2.29776500	-3.23272600
C	4.76149300	-3.56689000	-2.56520000
H	3.89467000	-4.16014500	-0.67936800
H	5.52137100	-3.52878100	-0.52360700
H	3.54785700	-3.07592800	-4.30701300
H	2.98584400	-4.49088600	-3.43710300
H	5.43852600	-2.78707800	-2.93780300
H	5.25105100	-4.52150500	-2.78282500
O	4.98444400	4.26283400	0.45429100
C	4.77355900	4.86421200	1.73036700

H	5.03838200	4.17804700	2.54312800
H	5.43168500	5.73268700	1.76068400
H	3.73387400	5.18969700	1.84980800

IM9a

SCF done: -1102.294078

C	2.11395500	-1.10500700	0.34407300
C	2.36863100	0.14974900	0.94862800
C	3.58289700	0.86983800	0.67472500
C	1.44937100	0.76233400	1.86264000
C	3.81985300	2.10699000	1.21161600
H	4.29438400	0.47461200	-0.03970700
C	1.71200900	1.97750300	2.45333000
H	0.55893100	0.23029900	2.16096500
C	2.88355800	2.68458600	2.10767200
H	4.70494400	2.67818200	0.95556100
H	1.00070800	2.38139500	3.16220100
C	0.39513400	-2.61560800	-0.92008900
H	-0.65059200	-2.91490400	-0.82446600
H	0.51959200	-2.12866200	-1.88904400
H	1.00804200	-3.51695200	-0.88392500
C	0.69315400	-1.63485500	0.22727400
H	0.57748700	-2.20080500	1.17892300
O	-0.28765300	-0.61755200	0.24210400
Fe	-2.05715800	-0.84329900	1.31858700
Br	-1.22410100	-1.81850600	3.40231500
Br	-2.60378200	-0.12830100	-2.51188600
Br	-3.71018800	-1.90628700	-0.30948200
Fe	-0.70425500	0.88331100	-0.95108300
Br	-2.35036700	1.70050000	1.03385400
Br	0.31661800	3.23550200	-1.43947400
Br	1.24569500	0.72559200	-2.87866000

C	3.28430900	-1.97363300	-0.03791700	H	0.85357200	0.09720300	2.19143500
C	3.26455300	-3.34843500	0.73320300	C	2.96623000	2.74291500	2.14654000
C	3.52136200	-2.20394800	-1.55877400	H	4.58156400	3.02306900	0.75864800
H	4.18049700	-1.46535400	0.32341700	H	1.28217000	2.15439500	3.38702100
C	4.12879900	-4.40511300	0.01389200	C	0.51954600	-2.46603500	-1.24850600
H	2.24873200	-3.72977500	0.85514500	H	-0.36297000	-2.98303900	-0.86611900
H	3.64995600	-3.16687200	1.74236500	H	0.24822100	-2.00942800	-2.20590200
C	4.94181600	-2.77784800	-1.76528400	H	1.31364100	-3.18935400	-1.41284000
H	2.77732300	-2.89312400	-1.95988700	C	0.88248400	-1.33834700	-0.30451900
H	3.40460600	-1.26592800	-2.10854500	H	1.39915400	-1.84082400	0.75064200
C	5.35768600	-3.77373300	-0.65201800	O	-0.16775500	-0.58974700	0.07027700
H	3.52974200	-4.91998100	-0.74728000	Fe	-1.70970400	-1.36235100	1.33283200
H	4.42803100	-5.17050900	0.73772100	Br	-0.21892300	-2.73155000	2.71870100
H	5.66755300	-1.95785100	-1.81674800	Br	-2.93539000	0.01432600	-2.10328800
H	4.96872100	-3.27223700	-2.74238900	Br	-3.50491000	-2.28983900	-0.20791700
H	5.95144500	-3.25836700	0.11417200	Fe	-0.97517300	1.09163000	-0.64547600
H	6.00863900	-4.55060200	-1.06509400	Br	-2.30623800	1.09787500	1.70759300
O	3.20280600	3.88843600	2.57262300	Br	-0.71518900	3.59696000	-1.08146600
C	2.28793800	4.58856000	3.43282700	Br	0.74602800	1.44962400	-2.71316800
H	2.14475700	4.04469000	4.37147600	C	3.43875400	-1.64405700	-0.55789000
H	2.75888200	5.54996800	3.63180200	C	3.59176000	-3.10736200	-0.01835300
H	1.32735400	4.73959700	2.93230300	C	3.59039400	-1.58363700	-2.09868500

TS13a

SCF done: -1102.277122

C	2.21738200	-0.89127200	-0.03083700	H	4.29260600	-1.10201500	-0.14688600
C	2.45972100	0.33247500	0.75607500	C	4.43759000	-3.97436500	-0.97312700
C	3.54063400	1.17427800	0.39671900	H	2.62311300	-3.58623200	0.15018900
C	1.65863900	0.73066300	1.84508100	H	4.07453200	-3.05380400	0.96357800
C	3.77691000	2.36256600	1.06208900	C	5.01888600	-2.01850500	-2.49983000
H	4.17056600	0.92960500	-0.45078600	H	2.85513500	-2.23423200	-2.57898800
C	1.91361000	1.90378000	2.54405300	H	3.38617500	-0.57198600	-2.46444900
				C	5.57267600	-3.15932800	-1.60703000
				H	3.80175800	-4.38716600	-1.76686400
				H	4.83453300	-4.83304500	-0.42199500

H	5.69340200	-1.15582600	-2.45414400
H	4.99916600	-2.33531500	-3.54812800
H	6.19659100	-2.74146500	-0.80627700
H	6.22909300	-3.81047300	-2.19278800
O	3.28292600	3.91275600	2.73733700
C	2.46646700	4.38628400	3.80824000
H	2.49571900	3.70175000	4.66375000
H	2.88995300	5.34759900	4.09897900
H	1.42939400	4.52604300	3.48372900

IM10a

SCF done: -1102.308873

C	-2.11942500	1.72150200	0.38234300
C	-1.95090700	0.64856000	1.44209900
C	-2.24564200	-0.70762900	1.19430900
C	-1.47130400	0.99120600	2.70878200
C	-2.05521600	-1.67624800	2.17872300
H	-2.68358200	-1.01208600	0.24877300
C	-1.28262800	0.03314300	3.70662100
H	-1.22531300	2.02650300	2.92934000
C	-1.56461200	-1.31302700	3.44362400
H	-2.28597200	-2.71824300	1.98852200
H	-0.90412700	0.34508800	4.67227000
C	-0.71239800	2.97495500	-1.42732400
H	-0.14849100	3.70290200	-0.82632100
H	-0.10642700	2.70973600	-2.29558600
H	-1.64782200	3.44558800	-1.72929800
C	-0.93236100	1.77257000	-0.56237900
H	-2.04277600	2.69282500	0.89530100
O	-0.05447300	0.88007900	-0.56637100
Fe	2.20018600	1.52820300	0.34668100
Br	1.66401000	3.59337000	1.46842200

Br	1.96420200	-1.17844800	-2.35562000
Br	3.63714400	1.25862300	-1.68140000
Fe	0.17989600	-1.23833100	-0.30191000
Br	1.93217700	-0.66382800	1.59052200
Br	0.13119800	-3.82029700	0.01419300
Br	-1.52384600	-2.33678600	-2.07546300
C	-3.52982100	1.72903000	-0.33631700
C	-4.16475700	3.14603000	-0.35666200
C	-3.59495600	1.09763400	-1.74053600
H	-4.15059900	1.10527600	0.31584900
C	-5.30677400	3.26902100	-1.39226200
H	-3.40294900	3.90644300	-0.56754300
H	-4.53984500	3.37086100	0.64953300
C	-5.06826100	0.85880100	-2.15458000
H	-3.11365300	1.76302200	-2.46838300
H	-3.05047600	0.14897600	-1.78550600
C	-6.02873900	1.92936500	-1.58228800
H	-4.89953100	3.59364800	-2.35840600
H	-6.00710700	4.05063400	-1.07960300
H	-5.38578400	-0.13530700	-1.82015200
H	-5.12780300	0.84751300	-3.24836300
H	-6.42792100	1.59908100	-0.61459900
H	-6.89452000	2.04888200	-2.24178300
O	-1.40939800	-2.32626800	4.33012500
C	-0.84065600	-2.03441900	5.60181300
H	-1.47604900	-1.35128500	6.17925300
H	-0.77279500	-2.98930300	6.12364200
H	0.16212800	-1.60304900	5.50027200

TS14a

SCF done: -1102.283915

C	1.38796500	0.55547800	0.81716100
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C	1.14549400	0.36661000	2.28361900
H	0.54805500	1.22402000	2.61448800
H	0.55984900	-0.52605100	2.49774000
H	2.07289200	0.36512900	2.86083600
C	0.73222100	-0.31838300	-0.15772100
O	-0.33684300	-1.11341900	0.20724900
Fe	-2.18317900	-0.47142800	0.77939800
Br	-2.05422100	1.92194400	1.06845300
Br	-4.10342800	-0.63387500	-0.86912100
Br	-2.60674500	-2.17695200	2.61871800
H	0.63845100	0.12141100	-1.15523600
C	2.13937600	-1.02025000	-0.04853600
C	3.10568100	-0.83475500	-1.07698900
C	2.37755400	-2.03008700	0.91319400
C	4.23578400	-1.61319500	-1.13344800
H	2.93166200	-0.10377200	-1.85927900
C	3.51465200	-2.81735000	0.86617300
H	1.64669700	-2.22669100	1.68771800
C	4.45371300	-2.62110100	-0.16353400
H	4.95824600	-1.50570800	-1.93464900
H	3.64978800	-3.59561600	1.60610800
O	5.57362800	-3.33370000	-0.31807600
C	5.83013100	-4.44353600	0.55161500
H	6.76356900	-4.87984500	0.19840200
H	5.94904500	-4.11094500	1.58819400
H	5.02676800	-5.18365100	0.48339400
C	2.17032000	1.76754300	0.35959500
C	1.34152400	3.08606900	0.55117000
C	3.54702000	1.91897400	1.04110600
H	2.34043500	1.66700800	-0.71639200
C	2.25978300	4.33112100	0.58263300
H	0.75062300	3.04765900	1.46807600

H	0.61763400	3.15792000	-0.26492000
C	4.39284000	2.98840800	0.31137200
H	3.39752200	2.20983000	2.08713100
H	4.07837800	0.96172500	1.05286200
C	3.52522600	4.13555900	-0.26044500
H	2.55094900	4.55097800	1.61736400
H	1.68935300	5.19858000	0.23526900
H	4.96358200	2.51773600	-0.49756600
H	5.13094600	3.38986200	1.01442900
H	3.23612900	3.91105100	-1.29540300
H	4.10684200	5.06189200	-0.30398800
Fe	-0.45655100	-3.01312000	-0.54281900
Br	-2.82150200	-3.25733900	-1.59210500
Br	-0.56260100	-4.26431000	1.75901600
Br	1.06541500	-3.98391000	-2.16472200

IM11a

SCF done: -1102.282997

C	1.79963100	-1.50879700	-0.80787900
C	1.96936100	0.33893400	0.98039000
C	2.50532200	1.43322500	0.28998300
C	2.09873700	0.28991600	2.37953200
C	3.15816100	2.46183800	0.97002800
H	2.38831900	1.50764500	-0.78663600
C	2.75219500	1.30365300	3.06295100
H	1.67870700	-0.54484300	2.93291100
C	3.28523600	2.40074400	2.36460700
H	3.54817900	3.30133300	0.40777700
H	2.85528600	1.27691200	4.14234000
C	0.92000800	-2.11294800	-1.82876500
H	0.10160600	-2.65271700	-1.33314500
H	0.41198800	-1.30707200	-2.37632600

H	1.44458900	-2.77606600	-2.51383400
C	1.18164400	-0.72773200	0.24408800
H	1.22743900	-1.67966900	0.92180300
O	-0.17488700	-0.47052300	0.06895500
Fe	-1.58631000	-1.31581600	1.38819500
Br	-0.07511200	-3.03647700	2.38953000
Br	-3.15104600	0.10737000	-1.84780800
Br	-3.36081500	-2.37114700	-0.13467100
Fe	-1.12314600	1.14784100	-0.51446900
Br	-2.31504700	1.00714400	2.00468800
Br	-0.93917300	3.68999100	-0.75274600
Br	0.28523500	1.76370000	-2.79593200
C	3.24531500	-1.83972900	-0.74392500
C	3.50669700	-3.39242900	-0.70241300
C	3.98594200	-1.17170900	-1.95409800
H	3.65714000	-1.38504400	0.16114200
C	4.09788500	-3.94587400	-2.00448900
H	2.59228600	-3.93115400	-0.43331500
H	4.20829600	-3.57109800	0.11987000
C	5.40993100	-1.73724200	-2.04664400
H	3.44448900	-1.35515800	-2.88877600
H	4.00586800	-0.08924600	-1.80278400
C	5.42200500	-3.25050200	-2.38158300
H	3.37300100	-3.83051700	-2.81963700
H	4.25485000	-5.02434700	-1.89821500
H	5.91556200	-1.55625100	-1.09017500
H	5.97084800	-1.17324700	-2.79876500
H	6.25366400	-3.72999500	-1.85364200
H	5.61109900	-3.39876900	-3.45007100
O	3.89962300	3.34007100	3.12497100
C	4.41301200	4.50424400	2.48743900
H	3.62004000	5.06468100	1.97798800

H	4.83516700	5.11827300	3.28347600
H	5.20162000	4.25340700	1.76723300

TS15a

SCF done: -1102.28292

C	1.89030700	-1.44812000	-0.80528300
C	1.92133300	0.47671700	0.91375300
C	2.44140000	1.59852000	0.25640300
C	1.97792500	0.42289200	2.31803100
C	3.00959900	2.65104300	0.97463600
H	2.37576700	1.67282300	-0.82438100
C	2.55088600	1.45907300	3.03812000
H	1.57183300	-0.43519300	2.84470900
C	3.06699200	2.58512900	2.37350300
H	3.38943300	3.51155700	0.43785500
H	2.60148300	1.42836300	4.12107500
C	1.05166900	-2.25653100	-1.73644800
H	0.35511800	-2.88374700	-1.16691800
H	0.42427500	-1.58440800	-2.33240200
H	1.65275100	-2.89408800	-2.38335800
C	1.22176100	-0.59798800	0.12284800
H	1.40172700	-1.66682200	0.71142700
O	-0.13791000	-0.48945700	-0.00284800
Fe	-1.45559100	-1.42446000	1.37764300
Br	0.22987700	-3.08090800	2.19755100
Br	-3.23936000	-0.05123100	-1.76664900
Br	-3.28258000	-2.52580200	-0.03683000
Fe	-1.21388100	1.08650500	-0.53218000
Br	-2.25863100	0.85005400	2.05374000
Br	-1.20406100	3.63027200	-0.75969100
Br	0.12522000	1.77369100	-2.81039600
C	3.37738700	-1.62086500	-0.76856200

C	3.82426400	-3.11787600	-0.61483000
C	3.98458500	-0.97020700	-2.05161200
H	3.76044900	-1.04777400	0.08007600
C	4.51157900	-3.67591300	-1.86856500
H	2.97444300	-3.74766600	-0.33178700
H	4.52202800	-3.16604400	0.22855000
C	5.47994100	-1.30884700	-2.13741700
H	3.46596900	-1.32789400	-2.94828100
H	3.83704400	0.11284400	-2.01218300
C	5.73451800	-2.83365100	-2.27978100
H	3.79416800	-3.71519100	-2.69759500
H	4.81294700	-4.71274000	-1.68607700
H	5.97130200	-0.92596200	-1.23456800
H	5.92298500	-0.76501900	-2.97780100
H	6.59606800	-3.11593300	-1.66427900
H	6.00437700	-3.07742500	-3.31285100
O	3.59542700	3.54610400	3.16971000
C	4.07696300	4.74244600	2.56747700
H	3.28228400	5.26227000	2.01913600
H	4.42063400	5.37184400	3.38882100
H	4.91614800	4.54228500	1.88986500

IM12a

SCF done: -1102.320666

C	1.74892800	-0.78172100	-1.35483000
C	1.73944400	1.40489400	0.11990600
C	2.87741100	1.97825800	-0.49016500
C	1.17871700	2.06996800	1.24468600
C	3.42469400	3.16294100	-0.02777100
H	3.32535300	1.50361900	-1.35234000
C	1.72558700	3.23764900	1.72452200
H	0.32205100	1.63618100	1.74609800

C	2.85228600	3.80324600	1.08929700
H	4.28575000	3.58501700	-0.53049500
H	1.31078200	3.74343700	2.58905900
C	1.44411500	-0.27267500	-2.79120100
H	0.36982500	-0.12646800	-2.92514500
H	1.94547000	0.66882600	-3.02506800
H	1.77118300	-1.02543700	-3.51275700
C	1.13538000	0.18293000	-0.35360800
H	1.13245000	-1.67911700	-1.24106700
O	-0.03086400	-0.12511700	0.09512600
Fe	-0.57830200	-1.92751400	1.24231700
Br	1.27084600	-2.38634900	2.69725600
Br	-2.80358900	-1.04597200	-1.93628900
Br	-1.46230600	-3.43214600	-0.65481200
Fe	-1.97583900	0.72342500	-0.21981700
Br	-2.62992900	-0.58355000	1.97017100
Br	-2.62434100	3.07261800	0.64004500
Br	-1.41112300	2.54668200	-2.10407100
C	3.23937100	-1.21031800	-1.08541400
C	3.29801200	-2.74430700	-0.84314700
C	4.27599800	-0.85871300	-2.17193600
H	3.56148700	-0.71969300	-0.15923600
C	4.72793900	-3.32456100	-0.97393800
H	2.64109500	-3.24513900	-1.56637400
H	2.88792600	-2.95762200	0.14961200
C	5.71148900	-1.08442200	-1.63658900
H	4.10255300	-1.49720800	-3.04702100
H	4.18312700	0.16914500	-2.53889900
C	5.79196500	-2.27014700	-0.64601500
H	4.89210000	-3.68627000	-1.99713900
H	4.83360500	-4.19766200	-0.32177000
H	6.06930400	-0.17162900	-1.14445000

H	6.38127300	-1.25747800	-2.48684100	H	4.24518300	5.88408500	0.01100400
H	5.63810100	-1.91400600	0.38029200	H	4.60966200	6.48443900	1.65151800
H	6.79423600	-2.71134800	-0.66702400	H	5.32849500	4.94976900	1.09204200
O	3.30689900	4.94533200	1.62592300				
C	4.44264700	5.59267800	1.04822000				

Cartesian Coordinates for the Stationary Points Given in Fig. 5.

TS16a				Br	0.67154700	-2.35056000	-1.17988100
SCF done: -936.293406				O	-6.29260400	-1.60331700	1.16826000
C	-1.37351800	0.08135200	-1.12440700	C	-7.55421800	-1.17630500	0.62948800
C	-2.67456600	-0.37676500	-0.55372500	H	-8.31888200	-1.61678200	1.28351400
C	-2.72318500	-1.21271200	0.59063700	H	-7.64648400	-0.07514500	0.64566700
C	-3.89353700	0.04896600	-1.12496700	H	-7.69553300	-1.54424500	-0.40273800
C	-3.94294900	-1.61140000	1.13192900	C	-0.81705200	2.20398700	0.20688300
H	-1.79664900	-1.58194700	1.04227700	C	0.08534900	2.76781800	1.32831000
C	-5.12658500	-0.33492000	-0.58444900	C	-0.82305300	3.15874800	-1.01954000
H	-3.87724600	0.71944900	-1.99097800	H	-1.84804600	2.12157300	0.60377800
C	-5.15746700	-1.17254200	0.55254000	C	-0.45883200	4.11726300	1.87477300
H	-3.98632300	-2.26563200	2.00697800	H	1.09140900	2.92579500	0.90107400
H	-6.04926600	0.03253400	-1.03882800	H	0.20294700	2.03120800	2.14367700
C	-1.20627200	0.26685900	-2.48447200	C	-0.69729400	4.65625700	-0.58923900
H	-0.29199500	0.73421600	-2.86175800	H	0.02929000	2.89660500	-1.67066900
H	-0.63759000	-1.00756600	-1.44307900	H	-1.74822600	3.01403700	-1.59748200
H	-1.90744900	-0.17000500	-3.20258200	C	-1.27964100	4.88769300	0.81131300
C	-0.38459000	0.74961400	-0.14830600	H	0.39749600	4.73372200	2.20240300
H	-0.40720400	0.16931900	0.80124800	H	-1.08425200	3.93858300	2.76801400
O	0.91629400	0.74256200	-0.71470900	H	-1.17176200	5.31380700	-1.33800700
Fe	2.06300400	-0.44831100	-0.04492900	H	0.37255300	4.93521300	-0.56568500
Br	4.06541500	0.78296800	-0.48414000	H	-2.32703200	4.52928100	0.82636000
Br	2.90743600	-1.84902100	1.67548000	H	-1.31684700	5.96604300	1.04486200

IM13a

SCF done: -936.317456

C	1.02939500	-0.52590300	0.39819500
C	2.51633100	-0.82908900	0.22411200
C	2.91671400	-1.75450000	-0.76844100
C	3.52299800	-0.21236300	0.99366500
C	4.26382100	-2.04359800	-0.98931900
H	2.15480500	-2.25535700	-1.37642200
C	4.88311300	-0.49882100	0.79284000
H	3.25734700	0.50806800	1.77511800
C	5.26116600	-1.41731500	-0.20795600
H	4.57082600	-2.75903200	-1.75773200
H	5.63214600	-0.00395000	1.41520800
C	0.67883200	-0.34927200	1.87629900
H	0.84738100	0.65078100	2.29019300
H	0.48451400	-1.42282600	0.04375200
H	1.14139500	-1.12164800	2.50313000
C	0.55964200	0.62040400	-0.57538700
H	0.70247800	0.19966400	-1.59440100
O	-0.81946300	0.89508200	-0.41069200
Fe	-2.24153400	-0.11166600	-0.22502100
Br	-4.51204500	-0.48489800	0.35282400
Br	-1.90018700	-1.60871500	-2.05970700
Br	-1.33675500	-0.66865900	2.25334100
O	6.54994800	-1.77099200	-0.49730200
C	7.59473800	-1.16426100	0.27467000
H	8.53380300	-1.58023200	-0.11603700
H	7.60218600	-0.06518800	0.15332100
H	7.50176500	-1.41326500	1.34800200
C	1.33242600	1.97447900	-0.54775000
C	0.95102400	2.84162900	-1.78988800

C	1.16970400	2.78966400	0.76533000
H	2.39459600	1.68170700	-0.64914900
C	-0.09555400	3.91807100	-1.45082000
H	0.58759200	2.19232800	-2.60646400
H	1.86417300	3.33382900	-2.17451000
C	1.49172300	4.27896700	0.53274000
H	0.13251600	2.69767600	1.13890500
H	1.83383900	2.38680600	1.55168300
C	0.46150000	4.93598400	-0.42203600
H	-0.99149800	3.41748600	-1.04193200
H	-0.42214800	4.43756700	-2.36875800
H	2.50914200	4.35659000	0.10436100
H	1.52314600	4.81764200	1.49607500
H	0.93901700	5.78423600	-0.94544500
H	-0.37388000	5.36277100	0.16205800

IM14a

SCF done: -1012.755498

C	-1.28981400	-0.10199200	-1.06318200
C	-2.53236500	-0.50088100	-0.46399000
C	-2.76328400	-0.40799300	0.95162900
C	-3.59958000	-1.00234400	-1.27412700
C	-3.98207400	-0.77001100	1.49735800
H	-1.95849500	-0.10068500	1.63166100
C	-4.82988600	-1.35568700	-0.73492900
H	-3.46306900	-1.09276300	-2.35466200
C	-5.03327800	-1.24103300	0.66524900
H	-4.15551900	-0.72134200	2.57582000
H	-5.62530000	-1.71698600	-1.38994600
C	-1.05179900	-0.28787700	-2.53545700
H	-1.68937500	0.42366300	-3.09741900
H	-0.00296500	-0.07417900	-2.77912600

H	-1.30568600	-1.30119800	-2.87728600
C	-0.36268200	0.85133800	-0.32436800
H	-0.39838600	0.63140700	0.76210700
O	0.96787100	0.77456600	-0.79316900
Fe	2.14551700	-0.45608500	-0.23828800
Br	0.47741600	-2.24760100	-0.38879900
Br	4.08144300	-1.66760600	-0.74902500
Br	2.85019700	0.63005400	1.81284400
O	-0.36153900	0.32696400	3.02262400
H	-0.25057800	1.27317000	3.23269700
H	0.54969500	0.06761200	2.75682600
O	-6.17777300	-1.56047100	1.30079800
C	-7.28372100	-2.07521100	0.52855000
H	-8.08412800	-2.26007200	1.25647100
H	-7.62181900	-1.33563200	-0.21725500
H	-7.00912800	-3.01942400	0.02863600
C	-0.85534500	2.35315600	-0.44565300
C	-0.14318200	3.17980500	0.66920100
C	-0.62392300	3.01577500	-1.81653000
H	-1.94401700	2.33354200	-0.24251700
C	-0.03245000	4.68458300	0.31787100
H	0.86500000	2.76139600	0.83715400
H	-0.70822800	3.05389300	1.61172100
C	-1.30081800	4.41352900	-1.86531400
H	0.46439200	3.10729400	-1.97887600
H	-1.00733900	2.40041300	-2.64711400
C	-1.24895300	5.14997200	-0.49872100
H	0.88809200	4.86457800	-0.26815500
H	0.07344900	5.27475700	1.24517300
H	-2.35239700	4.30720600	-2.18951700
H	-0.79820400	5.01913300	-2.64079000
H	-2.16915500	4.94058200	0.08027300

H	-1.22679500	6.24293500	-0.65363000
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TS17a

SCF done: -1012.731293

C	-0.94179100	-0.42586600	-0.77359400
C	-2.31269600	-0.78383400	-0.33975800
C	-2.72984300	-0.64791700	1.01493400
C	-3.26445600	-1.28222600	-1.26236200
C	-4.02258200	-0.96486500	1.41310900
H	-2.01421600	-0.33096400	1.77795900
C	-4.57336400	-1.59829300	-0.87947900
H	-2.99128400	-1.41500600	-2.31194000
C	-4.96391200	-1.44085800	0.46730200
H	-4.33216400	-0.87216200	2.45791800
H	-5.27564200	-1.96680700	-1.63045700
C	-0.58620700	-0.67873500	-2.23708400
H	-1.20850200	-0.02559900	-2.87674900
H	0.46694400	-0.43482800	-2.43262500
H	-0.76435900	-1.72424600	-2.52697200
C	-0.32305400	0.84963100	-0.19845800
H	-0.20517400	0.67982700	1.25047700
O	0.97741800	1.02761000	-0.44459800
Fe	2.41725400	-0.18860700	-0.22429200
Br	0.48385000	-2.00276400	0.19890900
Br	4.10940200	-0.97186100	-1.69249800
Br	3.09336800	0.15563500	2.19823000
O	0.07543200	0.63351600	2.42102400
H	0.02512300	1.56712100	2.72660200
H	1.09857600	0.39629500	2.43903600
O	-6.20003700	-1.72161100	0.95937900
C	-7.18400500	-2.24500000	0.05116300
H	-6.85431100	-3.20456900	-0.38545300

H	-8.08668100	-2.40703400	0.65563800
H	-7.40564900	-1.52589200	-0.75772500
C	-1.18178000	2.14659500	-0.21818000
C	-0.56649100	3.24767400	0.70454500
C	-1.35686800	2.70939600	-1.65601700
H	-2.18450100	1.87124200	0.15553400
C	-0.83447200	4.68638000	0.20069300
H	0.52315000	3.08561500	0.78402600
H	-1.00514300	3.14925800	1.71860800
C	-2.35376000	3.89653000	-1.67427800
H	-0.36354700	3.02009000	-2.02686200
H	-1.71662900	1.92560300	-2.34247800
C	-2.23964400	4.79381600	-0.41248900
H	-0.07932100	4.96460500	-0.55761200
H	-0.70890800	5.39770900	1.03550300
H	-3.38532800	3.51199600	-1.76722600
H	-2.16157600	4.49374500	-2.58390900
H	-2.98393700	4.48036200	0.34461000
H	-2.48016200	5.84141200	-0.66347100

IM15a

SCF done: -1012.791475

C	-1.89625100	-0.59015600	-0.19486200
C	-3.34604900	-0.62738900	-0.23390100
C	-4.16098200	0.06239300	0.72075900
C	-4.02559700	-1.41695600	-1.20947200
C	-5.54486600	-0.02232100	0.69019800
H	-3.68567400	0.61314000	1.53667600
C	-5.41614800	-1.48662800	-1.26925900
H	-3.44521400	-1.94669300	-1.96993100
C	-6.19259100	-0.78888600	-0.31319700
H	-6.16033000	0.47877000	1.44239300

H	-5.89154800	-2.07634700	-2.05590100
C	-1.10160800	-1.79990600	-0.60571200
H	-0.34897400	-1.56530400	-1.38167200
H	-0.53757300	-2.18563100	0.27242400
H	-1.73344700	-2.62737300	-0.95558200
C	-1.14038200	0.55267400	0.24272900
H	4.23178100	0.22848100	-1.39297200
O	0.13042700	0.43183000	0.45480100
Fe	1.64181500	-0.72971500	0.47784000
Br	1.97258900	-2.63223300	1.94917300
Br	2.63976200	-1.00020700	-1.81574000
Br	5.32091200	1.17876100	-0.84812300
O	3.02665600	0.54555400	1.49996800
H	3.40437300	-0.01429700	2.20885900
H	3.79627700	0.81705000	0.93592700
O	-7.54656700	-0.79454600	-0.26164500
C	-8.26476400	-1.56955000	-1.24080600
H	-9.32750700	-1.42518500	-1.00589300
H	-8.05841400	-1.20764100	-2.26321500
H	-8.00977900	-2.64091200	-1.16409200
C	-1.67785200	1.96881300	0.35436900
C	-1.49080400	2.54880100	1.79442900
C	-0.95484600	2.88427300	-0.67552300
H	-2.74803000	1.96433800	0.08966800
C	-1.35547700	4.09264300	1.79592200
H	-0.59438100	2.09472700	2.25009200
H	-2.35382600	2.24718300	2.41750100
C	-1.62479700	4.28082000	-0.72421400
H	0.10472200	2.96420000	-0.37667000
H	-0.96318500	2.42012600	-1.67702900
C	-2.17708600	4.72185400	0.65802700
H	-0.29323600	4.37588400	1.67401900

H	-1.66918100	4.48952900	2.77729700	H	-3.23311500	4.40638700	0.76218200
H	-2.44188200	4.27932900	-1.46802100	H	-2.17754800	5.82294000	0.73543300
H	-0.87927500	5.01306800	-1.08306900				

Cartesian Coordinates for the Stationary Points Given in Fig. 7.

1B

SCF done: -769.9609956

C	0.89450600	1.00393800	0.25168600
C	-0.51809100	0.40037300	0.17096000
C	-1.58066500	1.13248500	-0.36799800
C	-0.80975100	-0.85908500	0.72286200
C	-2.88820300	0.63615200	-0.38175000
H	-1.40412800	2.12251400	-0.78125900
C	-2.10242600	-1.36434100	0.72499900
H	-0.01077000	-1.45397800	1.15416300
C	-3.15439900	-0.62204200	0.16680300
H	-3.67809100	1.23748900	-0.81594300
H	-2.32494800	-2.33660800	1.15273800
C	1.99454800	-0.05933500	0.07253900
C	3.13319600	-0.09987300	0.88945400
C	1.91034400	-0.98107100	-0.98681000
C	4.14457800	-1.03685300	0.66621800
H	3.23891900	0.59668500	1.71312900
C	2.92299600	-1.91118400	-1.21574800
H	1.03180000	-0.98530600	-1.62499900
C	4.04657500	-1.94430800	-0.38780500
H	5.01199700	-1.05229400	1.32012600
H	2.83047100	-2.61344700	-2.03944900
H	4.83496000	-2.67087700	-0.56163300
C	1.02547900	1.81661900	1.55346600

H	1.96356000	2.37552000	1.58615500
H	0.21235200	2.54303000	1.61327100
H	0.96245800	1.15911100	2.42480200
C	1.09693200	1.94832100	-0.95116200
H	0.98217000	1.45400300	-1.94018900
O	1.37500100	3.12268600	-0.86902800
O	-4.38476600	-1.21017200	0.20967600
C	-5.48486300	-0.50434300	-0.34171400
H	-6.35536900	-1.14780300	-0.20515400
H	-5.65637200	0.44832700	0.17596800
H	-5.34541100	-0.30918600	-1.41291900

1b

SCF done: -934.3308346

C	-1.79194400	0.89417200	-0.86858200
C	-3.04772900	0.03946700	-0.61495500
C	-2.93034700	-1.33360600	-0.35850600
C	-4.34593500	0.57495000	-0.73542100
C	-4.05200200	-2.15281000	-0.20079900
H	-1.94877300	-1.79939000	-0.28640600
C	-5.46774400	-0.22615500	-0.59051400
H	-4.47629100	1.63476800	-0.93521800
C	-5.33137200	-1.59939900	-0.31562600
H	-3.91204600	-3.20627700	0.00741100
H	-6.46755300	0.18576700	-0.68353600

C	-1.89319800	2.31659500	-0.25351900
C	-1.38506600	3.44366700	-0.91959300
C	-2.42515700	2.48829700	1.04315100
C	-1.43634000	4.70592700	-0.32290500
H	-0.95497200	3.34898200	-1.91010800
C	-2.46404400	3.75192800	1.64143700
H	-2.83065300	1.63572500	1.57536700
C	-1.97219400	4.86457500	0.95965900
H	-1.05105400	5.56606200	-0.86270400
H	-2.88068000	3.86163700	2.63844900
H	-2.00419400	5.84669400	1.42202600
C	-1.46321000	0.88354100	-2.37310600
H	-0.50577700	1.36537500	-2.58591900
H	-1.40076400	-0.14915800	-2.72702700
H	-2.25635300	1.38554200	-2.93220000
C	-0.63689800	0.33659100	-0.06127100
H	-0.81654300	0.16742100	1.01475500
O	0.50149200	0.10602700	-0.54130600
O	-6.49342900	-2.29276600	-0.18069900
C	-6.41927900	-3.68186800	0.10508700
H	-7.45076400	-4.02851500	0.17951100
H	-5.91063600	-4.23263200	-0.69494300
H	-5.90429500	-3.86927700	1.05657500
Fe	2.23530000	-0.60087500	0.33750800
Br	4.09064700	1.09137200	-0.25927400
Br	1.55939600	-1.29155500	2.53755300
Br	3.57749400	-1.69785400	-1.53777600

IM1b

SCF done: -1098.689012

C	-1.99833300	1.26940200	0.26499100
C	-3.29669800	0.64285400	-0.26375400

C	-4.54994400	1.13925300	0.10441600
C	-3.24711500	-0.37349600	-1.23286900
C	-5.72489500	0.63725000	-0.45770500
H	-4.62160100	1.92968700	0.84512900
C	-4.40664300	-0.89038600	-1.79506200
H	-2.29018600	-0.76508700	-1.57328700
C	-5.65885800	-0.38787200	-1.41102200
H	-6.67730700	1.04926000	-0.14667800
H	-4.36733300	-1.67869200	-2.53902400
C	-1.57507700	2.41137600	-0.67437100
H	-0.62387900	2.87019200	-0.40169800
H	-1.49682300	2.03735500	-1.69805400
H	-2.34046400	3.19097100	-0.65801700
C	-0.96385300	0.18887700	0.41435800
H	-1.32230600	-0.74709200	0.86185400
O	0.25193400	0.25209400	0.13026300
Fe	1.87668100	1.60452900	-0.78014800
Br	1.99472900	3.86711200	-0.01083000
Br	1.20193100	-2.08279900	-2.24519000
Br	1.40076300	0.78087500	-3.17163800
Fe	1.49816100	-1.59329900	0.30021800
Br	3.58726100	-0.07389700	0.12942000
Br	1.65406200	-2.09454300	2.83922100
Br	-0.27366900	-3.48138700	0.93491900
O	-6.73537900	-0.95410300	-2.01723300
C	-8.03168900	-0.47741500	-1.68233900
H	-8.14647800	0.58572300	-1.92808200
H	-8.72982500	-1.06213600	-2.28237600
H	-8.25465900	-0.62896300	-0.61875800
C	-2.06688100	1.66874700	1.76843600
C	-1.39719900	2.80528000	2.25026100
C	-2.72567200	0.83201700	2.68952300

C	-1.42458200	3.11666200	3.60953300
H	-0.85513800	3.45779600	1.57665600
C	-2.74076700	1.14206600	4.04804800
H	-3.24796000	-0.05225500	2.33916300
C	-2.09272600	2.28781800	4.51220200
H	-0.91353000	4.00774000	3.96077400
H	-3.25867100	0.48662900	4.74149600
H	-2.10425000	2.53073500	5.57039900

TS1b

SCF done: -1098.668369

C	1.81699400	-1.40799600	0.26029000
C	3.22985500	-1.11606200	-0.07744900
C	3.56056300	0.01262800	-0.84600000
C	4.27079200	-1.99325600	0.29714800
C	4.87484400	0.26833500	-1.23286600
H	2.78288000	0.68883900	-1.18612000
C	5.57994500	-1.74142200	-0.06561300
H	4.05246800	-2.86679000	0.90362500
C	5.89676100	-0.60578100	-0.83816200
H	5.08547500	1.13773400	-1.84301900
H	6.38553300	-2.40422600	0.23129500
C	1.41837500	-0.90594400	2.02224400
C	0.49675000	-1.69747500	2.73256200
C	2.43479900	-0.21436800	2.71086500
C	0.59982600	-1.79266900	4.11682500
H	-0.31653200	-2.20623400	2.22663000
C	2.51874900	-0.30522400	4.09342300
H	3.14926100	0.38806700	2.15986500
C	1.60590200	-1.10061900	4.79684100
H	-0.11613400	-2.39746200	4.66364300
H	3.29164600	0.24071700	4.62458300

H	1.67693100	-1.17548900	5.87778400
C	1.31634800	-2.79191700	-0.05950500
H	0.32435400	-3.01499800	0.33030500
H	1.26997900	-2.86369800	-1.15310200
H	2.00834800	-3.56035300	0.29069400
C	0.93104900	-0.30065100	0.50131700
H	1.39703000	0.68395100	0.47404600
O	-0.38911900	-0.27620300	0.26999200
Fe	-1.88019900	-1.54964800	-0.39806300
Br	-2.41119200	-3.61282900	0.76580000
Br	-0.86283800	1.53435800	-2.67887100
Br	-1.26342800	-1.45508200	-2.92539400
Fe	-1.30378200	1.57686900	-0.08490700
Br	-3.60171200	0.35800600	-0.09215200
Br	-1.59875400	2.94275400	2.11274500
Br	0.74348100	3.36859900	0.22930300
O	7.20339500	-0.45437100	-1.14469400
C	7.60071100	0.67174100	-1.92467400
H	7.36066200	1.61307100	-1.41683900
H	8.68137000	0.58666400	-2.03861000
H	7.12795200	0.65796500	-2.91348300

IM2b

SCF done: -1098.686324

C	-1.00773000	1.78747100	1.90393700
C	-2.10493500	0.91384800	1.96066800
C	-1.93469600	-0.50871300	1.86097800
C	-3.45201200	1.40150600	2.09427600
C	-3.00198000	-1.37104300	1.88454100
H	-0.94148900	-0.92734100	1.77660500
C	-4.52220100	0.55019500	2.08699100
H	-3.63746300	2.46684900	2.14294000

C	-4.31497600	-0.85051700	1.96751900
H	-2.82508700	-2.43551800	1.80240900
H	-5.54175500	0.91380200	2.14516400
C	1.49923800	2.28475300	1.45897400
C	1.65806300	3.16417700	0.37855300
C	2.41818400	2.33106500	2.51533600
C	2.71192600	4.07661300	0.36368300
H	0.96136100	3.14591700	-0.45359300
C	3.47088300	3.24832400	2.50182300
H	2.32457500	1.63369500	3.34397000
C	3.61921200	4.12272000	1.42522000
H	2.82542500	4.74822400	-0.48178300
H	4.17986800	3.26679000	3.32402900
H	4.44219200	4.83097100	1.40733800
C	-1.11188600	3.22774800	2.25128600
H	-1.01294400	3.81171900	1.32473200
H	-2.03873100	3.50312700	2.75003700
H	-0.25993800	3.51657300	2.87488900
C	0.37549500	1.25612700	1.50300800
H	0.64120300	0.55615400	2.31646800
O	0.27373300	0.50991100	0.29747200
Fe	-0.66709200	1.02070000	-1.46430500
Br	-1.92026100	3.11960400	-1.52236600
Br	-0.26432200	-2.88846800	-0.79123900
Br	-2.28867800	-0.98312000	-1.97579300
Fe	1.48269100	-0.96121300	-0.25040900
Br	1.47529600	0.26082200	-2.65987400
Br	3.88224200	-1.88937400	-0.18635200
Br	2.05659100	-1.83645100	2.27607100
O	-5.41536600	-1.58920700	1.94406000
C	-5.32597900	-3.01209600	1.74087900
H	-4.79397200	-3.48759100	2.56997400

H	-6.35649700	-3.36206200	1.71327100
H	-4.82928500	-3.23212600	0.79218300

TS2b

SCF done: -1098.665795

C	-2.02149900	0.21731700	-0.87758200
C	-3.46415900	-0.07743700	-0.87496400
C	-4.03547500	-1.21463500	-0.25656700
C	-4.33003600	0.81680100	-1.53120500
C	-5.39775300	-1.43409900	-0.29247100
H	-3.40384300	-1.94965900	0.22810600
C	-5.70792000	0.62322200	-1.54172400
H	-3.93362800	1.70330100	-2.01318400
C	-6.25388200	-0.51140000	-0.92476000
H	-5.83368900	-2.31881300	0.15832800
H	-6.33951700	1.35180400	-2.03439600
C	-1.11704600	-0.18406700	0.16189100
H	-1.33437800	-1.06713800	-0.73602200
O	0.17608600	0.16365700	0.04999200
Fe	1.05871300	2.04372100	0.71022000
Br	-0.80196000	3.54113600	1.12686500
Br	3.19589200	-0.01989900	-2.09264200
Br	2.32048500	2.79021700	-1.45391600
Fe	1.80884800	-0.98001700	-0.13677600
Br	2.77185100	0.59065300	1.87338700
Br	2.60672400	-3.31974000	0.58419900
Br	0.38684700	-2.88919000	-1.50589900
C	-1.43772500	0.99645600	-2.02313700
H	-0.39391800	0.73188300	-2.18950600
H	-2.00967900	0.85955900	-2.94007400
H	-1.44354700	2.05783500	-1.74091500
O	-7.56818500	-0.81417900	-0.89037700

C	-8.49550800	0.06476500	-1.52426800
H	-8.29603000	0.14548400	-2.59904400
H	-9.47821300	-0.38080600	-1.37039400
H	-8.47250700	1.06215800	-1.07028300
C	-1.55273800	-0.67975200	1.51232000
C	-1.08974300	-1.90424200	2.01231800
C	-2.34098400	0.15397700	2.31770100
C	-1.42915600	-2.29883700	3.30603100
H	-0.47718800	-2.55266000	1.39384900
C	-2.66431600	-0.24231400	3.61498900
H	-2.67575600	1.11422000	1.93996600
C	-2.21465800	-1.46864500	4.10846400
H	-1.07301900	-3.25118100	3.68609400
H	-3.26334100	0.41226000	4.24045900
H	-2.47035400	-1.77422100	5.11856600

IM3b

SCF done: -1098.705607

C	-2.19581600	0.01601800	-0.71030600
C	-3.42849300	0.81599300	-0.29390200
C	-4.71211500	0.32923900	-0.59154300
C	-3.32114900	2.06969400	0.31422300
C	-5.84809300	1.06618100	-0.28670200
H	-4.82361100	-0.63791800	-1.07700000
C	-4.45508000	2.82134100	0.63137500
H	-2.34636400	2.48598900	0.55430000
C	-5.72804900	2.32142600	0.33096300
H	-6.84066300	0.69462600	-0.51884400
H	-4.32887900	3.78679800	1.10612500
C	-1.13936500	-0.09002300	0.37859500
H	-2.51794700	-1.02822300	-0.84736300
O	0.05887200	0.25293900	0.11084100

Fe	1.26016100	2.18608000	0.18155000
Br	0.09711800	3.70616800	1.61663500
Br	2.35012900	-0.33314800	-2.70897600
Br	1.81968800	2.60496000	-2.28280400
Fe	1.73137300	-1.07823200	-0.31297800
Br	3.17383800	0.69654900	0.99413400
Br	2.30877700	-3.08681300	1.20189500
Br	0.27229500	-3.18249900	-1.06790800
C	-1.62470900	0.50671300	-2.05064600
H	-0.79822000	-0.11851900	-2.39501400
H	-2.41759500	0.47942000	-2.80184300
H	-1.26954300	1.53746700	-1.97729400
O	-6.89769500	2.96486900	0.59230200
C	-6.84132900	4.24750300	1.20246600
H	-6.29722700	4.96703800	0.57818000
H	-7.87649200	4.57410400	1.30918200
H	-6.37210200	4.20281200	2.19323400
C	-1.43281200	-0.62452200	1.70726300
C	-0.44173100	-0.54019400	2.71131400
C	-2.66369900	-1.24876200	2.00905000
C	-0.67653900	-1.06266400	3.97631600
H	0.50220400	-0.05514100	2.49274900
C	-2.88489600	-1.78195800	3.27173200
H	-3.44231400	-1.31560400	1.26029400
C	-1.89534100	-1.68756900	4.25658600
H	0.08856000	-0.98586300	4.74162900
H	-3.82868600	-2.26955000	3.49297700
H	-2.07624800	-2.10083300	5.24450200

TS3b

SCF done: -1098.676303

C	-2.09345400	-1.30367600	0.60165500
C	-2.20772000	0.53383200	0.40760500
C	-1.70707000	1.31137700	1.47895400
C	-3.34585700	1.00730400	-0.30147500
C	-2.30705500	2.50511800	1.83564500
H	-0.80690300	1.00213600	1.99712500
C	-3.94584600	2.19348500	0.04427900
H	-3.74435500	0.42502100	-1.12538000
C	-3.43365900	2.95893200	1.11955400
H	-1.88543600	3.08979700	2.64331700
H	-4.80499600	2.57479100	-0.49599700
C	-1.62847300	-1.72798200	1.96886100
H	-1.34909300	-2.78493900	1.87783400
H	-0.74968400	-1.18412600	2.31000200
H	-2.42541600	-1.65924500	2.71274100
C	-1.22613900	-0.55328500	-0.28522200
H	-1.47808500	-0.57850500	-1.34664100
O	0.09790700	-0.39744600	-0.01892100
Fe	1.55521200	-1.95751000	0.18496900
Br	0.46297600	-3.99717100	-0.53633900
Br	2.18997800	1.45603500	1.91168400
Br	2.35629300	-1.49609200	2.57851000
Fe	1.25605600	1.08202600	-0.66476300
Br	3.14553000	-0.59449200	-1.33716100
Br	-0.00058200	1.52380800	-3.03862200
Br	1.04501000	3.61815500	-1.06345800
O	-4.08612400	4.09737600	1.37495600
C	-3.61786200	4.96430200	2.41547000
H	-2.59867800	5.30600900	2.20914100

H	-4.29796800	5.81511500	2.41308000
H	-3.65667400	4.46488100	3.38907600
C	-3.29255700	-1.99553200	0.05659900
C	-3.22685300	-2.63343500	-1.19390500
C	-4.47524300	-2.08852800	0.81181700
C	-4.32529700	-3.34594400	-1.67673100
H	-2.30307900	-2.62091100	-1.76199900
C	-5.57204800	-2.78790400	0.31935800
H	-4.54213900	-1.59204900	1.77519300
C	-5.49888100	-3.41927600	-0.92694100
H	-4.25569300	-3.85026600	-2.63531800
H	-6.48386600	-2.84414300	0.90596000
H	-6.35322500	-3.97164900	-1.30637700

IM4b

SCF done: -1098.68147

C	2.23479300	-0.60658800	-1.00103800
C	3.53582900	-1.20664300	-0.78878700
C	3.81437700	-1.95510100	0.38344200
C	4.54649400	-1.10804500	-1.77686400
C	5.04966000	-2.56455600	0.55661600
H	3.03987800	-2.11616900	1.12275600
C	5.78416300	-1.70626600	-1.58946200
H	4.36634100	-0.53895100	-2.68124800
C	6.03912000	-2.43580500	-0.42282700
H	5.23681200	-3.15538200	1.44716800
H	6.55203700	-1.60921000	-2.35005300
C	1.94672600	1.25100000	0.17942600
C	1.28474200	2.27993100	-0.51271400
C	3.09763900	1.56648800	0.93217300

C	1.72813200	3.59466000	-0.43046900
H	0.38450000	2.05898200	-1.07581900
C	3.54909300	2.86816900	1.01595100
H	3.62790400	0.78346600	1.46519500
C	2.86744900	3.89869700	0.33452500
H	1.17578100	4.37161600	-0.94408400
H	4.41834300	3.12896200	1.60958800
C	1.75196400	-0.33118100	-2.38753500
H	0.75647900	0.10790300	-2.38805600
H	2.43859200	0.31627700	-2.94178800
H	1.70793400	-1.28758900	-2.92083900
C	1.38271300	-0.19159200	0.15172300
O	0.01198600	-0.24487500	-0.06057400
Fe	-1.09364700	-1.88921700	-0.78864400
Br	0.59866100	-3.64669700	-0.94795200
Br	-2.67365700	1.58500900	-1.05003100
Br	-2.24783100	-0.85089700	-2.81860500
Fe	-1.34827700	0.52713400	1.14765600
Br	-2.75182100	-1.69616900	1.17445000
Br	-0.01178100	0.29820800	3.50764700
Br	-1.75827500	2.63256900	2.56638400
H	7.00467700	-2.91249400	-0.28283300
O	3.38620000	5.13344800	0.47963500
C	2.73426000	6.23804100	-0.14784400
H	3.32066900	7.11688600	0.11946100
H	2.72204900	6.12483100	-1.23786300
H	1.70984400	6.35500000	0.22243800
H	1.66328000	-0.68731400	1.08423400

TS4b

SCF done: -1098.666707

C	1.67380300	-1.17572400	-1.56220300
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C	3.06160200	-1.19985900	-2.05973700
C	3.86320800	-0.04579700	-2.17056500
C	3.60052000	-2.44297800	-2.44641600
C	5.16359100	-0.13957300	-2.65116900
H	3.46042500	0.92631100	-1.90901300
C	4.91745600	-2.53271600	-2.89138800
H	3.00411000	-3.34479600	-2.36375900
C	5.69932200	-1.38271100	-3.00211800
H	5.76120900	0.76051800	-2.75381000
H	5.32608200	-3.50136500	-3.16063300
C	1.21159000	-0.25965400	-0.55696100
H	1.21589300	0.29585800	-1.66732300
O	-0.09275200	-0.34404600	-0.19289300
Fe	-0.85664200	-1.65155300	1.34710500
Br	0.86104700	-3.33824900	1.66252400
Br	-3.58908300	-0.09364700	-1.27200100
Br	-2.89217700	-2.69554900	0.08002100
Fe	-1.50147200	1.05392100	-0.27404300
Br	-1.85667100	0.44106300	2.36403000
Br	-1.70044400	3.62315500	-0.26538900
Br	-0.37437500	2.09735800	-2.58063900
C	0.67223100	-2.11500200	-2.15606900
H	-0.31928700	-1.66149800	-2.18644600
H	0.96667100	-2.45609100	-3.14758800
H	0.58644200	-2.97597600	-1.47715000
C	2.12073400	0.47108000	0.38750500
C	1.91476200	1.82701000	0.66335500
C	3.11849300	-0.22454200	1.09357300
C	2.68912400	2.49370900	1.61076600
H	1.14973500	2.38598100	0.13329500
C	3.88662900	0.42716900	2.04489100
H	3.27073800	-1.28367100	0.91755400

C	3.68134700	1.79229700	2.31090900
H	2.50533500	3.54434000	1.79771100
H	4.64544300	-0.10242800	2.61063800
H	6.71931400	-1.45094900	-3.36764300
O	4.48634200	2.33438400	3.25594000
C	4.29259700	3.69789900	3.61779100
H	5.02159500	3.90407300	4.40190000
H	4.47420700	4.36861900	2.76914900
H	3.28191900	3.86860300	4.00698300

IM5b

SCF done: -1098.712845

C	1.88936700	-1.05031400	-1.49252700
C	3.06134400	-1.96287200	-1.12798800
C	4.18304400	-2.01485900	-1.96712400
C	3.00972100	-2.80954600	-0.01325800
C	5.23513300	-2.89058700	-1.69605200
H	4.23050800	-1.37076800	-2.84258900
C	4.06420300	-3.68220300	0.25982300
H	2.15184100	-2.79532100	0.65340200
C	5.17893900	-3.72596300	-0.57902800
H	6.09620200	-2.91920900	-2.35750300
H	4.00887800	-4.32808000	1.13104800
C	1.32499600	-0.26632200	-0.31250100
H	2.28034400	-0.26794600	-2.16076700
O	0.06486200	-0.34063500	-0.07342600
Fe	-1.20397600	-1.68574000	1.19905600
Br	0.18497700	-2.74829300	2.83436300
Br	-3.01626200	-0.29977900	-2.08544200
Br	-2.67486200	-2.86806600	-0.53454700
Fe	-1.45009500	1.10324400	-0.57764500
Br	-2.52056700	0.44997500	1.74023300

Br	-1.13287400	3.61511400	-0.03833700
Br	-0.11959300	2.27504300	-2.58255700
C	0.80901300	-1.82507700	-2.26637500
H	0.00953100	-1.16895600	-2.61625400
H	1.27037600	-2.30234500	-3.13433400
H	0.36449800	-2.60983600	-1.64993100
C	2.14184800	0.59228200	0.50988800
C	1.57644500	1.19481500	1.66041400
C	3.49924000	0.88114100	0.20391800
C	2.31094300	2.04227900	2.46864200
H	0.54810700	0.97824800	1.92413300
C	4.23448000	1.73434800	0.99468800
H	3.97248400	0.43072000	-0.65908500
C	3.65053200	2.32540200	2.13760600
H	1.84660300	2.47694600	3.34448600
H	5.26753100	1.97008900	0.76506300
H	5.99741800	-4.40673700	-0.36478300
O	4.45248600	3.13559200	2.84303200
C	3.94264300	3.78505600	4.01184100
H	4.76792900	4.38277200	4.39742700
H	3.10022500	4.43869800	3.76253400
H	3.63557100	3.05301500	4.76616000

3b

SCF done: -934.3556397

C	-1.27446000	-1.33631000	-1.49516700
C	0.04491300	-1.77131300	-2.15544800
H	0.77147000	-2.11609700	-1.41487100
H	-0.15341700	-2.60585500	-2.83303200
H	0.49312300	-0.95620200	-2.73109700
C	-1.10824900	-0.09551600	-0.61979500
O	0.02099800	0.19657600	-0.16303500

Fe	1.96159500	0.01162800	0.21833000	C	-6.64497700	3.18186500	0.36408000
Br	3.23544600	1.02550900	-1.79177900	H	-7.20448200	4.02568700	0.76759800
Br	2.70095900	2.38744000	0.93764800	H	-6.75660000	3.15842500	-0.72593100
Br	2.66414200	-1.99409100	1.33812800	H	-7.03021600	2.25018100	0.79374100
H	-1.98034400	-1.06821300	-2.28864900	C	-1.90507000	-2.47098600	-0.68083300
C	-2.23688300	0.77260800	-0.29165100	C	-3.04674500	-3.12820200	-1.15786300
C	-2.00014400	1.94903800	0.46150100	C	-1.32963300	-2.89839100	0.52406300
C	-3.55648700	0.49400300	-0.69625700	C	-3.60796300	-4.18892700	-0.44543200
C	-3.03273400	2.80292800	0.78608700	H	-3.49226200	-2.81889700	-2.10102900
H	-0.98739700	2.17563500	0.77501100	C	-1.89349600	-3.95696400	1.23740300
C	-4.60506700	1.34336900	-0.37003400	H	-0.42978400	-2.42203500	0.90277000
H	-3.77973400	-0.40835600	-1.25216600	C	-3.03446700	-4.60290000	0.75777600
C	-4.34849900	2.50869200	0.37383700	H	-4.48905200	-4.69233900	-0.83298500
H	-2.86087500	3.70889000	1.35686800	H	-1.43380300	-4.27783100	2.16736700
H	-5.60964300	1.09656100	-0.68999000	H	-3.46981300	-5.42740100	1.31454800
O	-5.28699900	3.40311500	0.74075600				

Cartesian	Coordinates	for	the	Stationary	Points	Given	in	Fig.	9.
				H	-6.44077000	0.26171600	-0.75236100		
				C	-1.89431300	2.30343200	-0.24103900		
				C	-1.42616700	3.43598100	-0.92277400		
				C	-2.40180100	2.46557300	1.06087200		
				C	-1.48889500	4.69778800	-0.32951800		
				H	-1.01879900	3.34599200	-1.92270800		
				C	-2.45458600	3.72519100	1.65497100		
				H	-2.77678000	1.60526800	1.60704700		
				C	-1.99909500	4.84704600	0.96032300		
				H	-1.13300700	5.56413800	-0.87892700		
				H	-2.85245100	3.82781100	2.65996500		
				H	-2.04073900	5.82922600	1.42127600		
1c									
SCF done: -1156.919522									
C	-1.77985400	0.88327500	-0.85003600						
C	-3.04089600	0.03684100	-0.61979300						
C	-2.93971400	-1.33725700	-0.36762200						
C	-4.31711400	0.60187000	-0.75532600						
C	-4.08070900	-2.12869100	-0.23412700						
H	-1.96499300	-1.81232000	-0.28414700						
C	-5.45870200	-0.18424000	-0.63467600						
H	-4.41774400	1.66387600	-0.95403200						
C	-5.34300300	-1.55219600	-0.36802800						
H	-3.98784900	-3.19064700	-0.03665900						

C	-1.42962500	0.87127200	-2.35099100
H	-0.46470700	1.34271200	-2.54626000
H	-1.37210300	-0.15978600	-2.70745700
H	-2.20607600	1.38628000	-2.92157900
C	-0.63163600	0.32551700	-0.02986700
H	-0.82153300	0.13760100	1.03842200
O	0.49435000	0.12964800	-0.48708500
Fe	2.26984900	-0.49404100	0.40114000
Br	4.08306300	1.02895800	-0.57731900
Br	1.55475200	-0.98038800	2.64266000
Br	3.44952600	-1.94406600	-1.35400000
C	-6.58765000	-2.37956100	-0.18307000
F	-7.55486200	-2.01954000	-1.05557500
F	-6.34922200	-3.69646200	-0.35582800
F	-7.10353400	-2.22649100	1.05779600

IM1c

SCF done: -1321.279568

C	-1.57252200	1.49708200	0.30101800
C	-2.97824400	0.95927800	-0.00598800
C	-4.11854400	1.66969400	0.39134600
C	-3.13930600	-0.19105500	-0.78959600
C	-5.38912700	1.23257200	0.02715400
H	-4.01375900	2.56811500	0.99072100
C	-4.40981800	-0.63808600	-1.14988200
H	-2.27238700	-0.74384100	-1.14505300
C	-5.53752800	0.07369100	-0.73954300
H	-6.26580900	1.79368800	0.33164600
H	-4.52150000	-1.52883700	-1.75818500
C	-1.16094900	2.45821300	-0.82737100
H	-0.14746700	2.84393000	-0.71405900
H	-1.22990000	1.94868300	-1.79161900

H	-1.84443900	3.31056800	-0.84509400
C	-0.62476500	0.34357300	0.49092800
H	-1.01444200	-0.50019100	1.07560600
O	0.55981300	0.26753300	0.10491600
Fe	2.25532900	1.36624800	-1.03917600
Br	2.53173100	3.70457400	-0.61815400
Br	1.23089500	-2.40346600	-2.02762300
Br	1.58473300	0.31070100	-3.29023200
Fe	1.67424600	-1.65688100	0.42236800
Br	3.86032000	-0.32277700	0.01064700
Br	1.89104500	-1.87409800	2.99172300
Br	-0.23316900	-3.29075200	1.33260100
C	-1.43899500	2.08776000	1.73385300
C	-0.62469200	3.20332800	1.98744100
C	-2.06084700	1.44183800	2.81957500
C	-0.47323100	3.68277500	3.28820500
H	-0.10735200	3.70913800	1.18133200
C	-1.89769900	1.91949100	4.11848900
H	-2.69280900	0.57631000	2.64731400
C	-1.10527600	3.04367400	4.35626500
H	0.14846400	4.55522500	3.46347200
H	-2.38951100	1.41135600	4.94211700
H	-0.97742000	3.41669500	5.36783000
C	-6.91422100	-0.43545100	-1.08000100
F	-6.92559900	-1.09261100	-2.25873700
F	-7.81229200	0.56964500	-1.16033100
F	-7.36643500	-1.29717700	-0.14131100

TS1c

SCF done: -1321.251417

C	1.78369000	-1.40542500	0.22276700
C	3.20604800	-1.12079800	-0.08582700

C	3.54429200	0.03122000	-0.81923100
C	4.22421600	-2.02685400	0.26816300
C	4.86788500	0.27197400	-1.18475800
H	2.77406300	0.72366300	-1.14123400
C	5.54410200	-1.77599700	-0.07986200
H	3.98635800	-2.91575100	0.84296900
C	5.86725000	-0.62470200	-0.80874100
H	5.11813100	1.15084800	-1.76785700
H	6.32533500	-2.47299800	0.20294500
C	1.36279100	-0.85444100	2.05934300
C	0.48981400	-1.70518900	2.76253900
C	2.41276500	-0.20153700	2.73634300
C	0.65985000	-1.87946800	4.13240000
H	-0.33784400	-2.19591600	2.26246200
C	2.56779400	-0.37703800	4.10454500
H	3.09081500	0.44730700	2.19158300
C	1.69487000	-1.22095000	4.80263000
H	-0.02337100	-2.52346200	4.67636000
H	3.36273100	0.14283900	4.62922700
H	1.82113100	-1.36134400	5.87193600
C	1.27601500	-2.77378400	-0.10272700
H	0.29574200	-3.00157600	0.31119200
H	1.18118800	-2.80569500	-1.19734900
H	1.98162300	-3.55529300	0.18571300
C	0.91358100	-0.30222700	0.57156500
H	1.39219500	0.67589300	0.50075100
O	-0.41519000	-0.25625300	0.32864600
Fe	-2.02798700	-1.48007300	-0.29795500
Br	-2.35964500	-3.60645400	0.82558500
Br	-0.72123400	1.36756500	-2.76044900
Br	-1.34648700	-1.59045700	-2.83807700
Fe	-1.18190100	1.59977900	-0.19794700

Br	-3.58907600	0.52582600	-0.18492600
Br	-1.47949000	3.08577400	1.92169300
Br	0.89836200	3.35457000	0.05304800
C	7.31294200	-0.33906900	-1.13822200
F	7.98597500	-1.47447100	-1.41651400
F	7.93589100	0.24787100	-0.09321500
F	7.43248000	0.48533300	-2.19600200

IM4c

SCF done: -1321.25769

C	-1.51196900	1.25791800	-0.19553400
C	-2.91999200	0.96715500	-0.36669600
C	-3.39254200	-0.37096600	-0.37458600
C	-3.85351700	2.01435300	-0.57206000
C	-4.73754800	-0.64068300	-0.58788800
H	-2.70343200	-1.20243700	-0.27461600
C	-5.20022300	1.73934400	-0.74776100
H	-3.52699600	3.04715300	-0.54426300
C	-5.64229000	0.41105500	-0.76187400
H	-5.08424800	-1.66705200	-0.62974800
H	-5.91044900	2.54646700	-0.88562400
C	-0.92021800	1.02583600	2.02379700
C	-0.17013000	2.12570600	2.46609600
C	-1.90944700	0.47760600	2.85819800
C	-0.38233100	2.64082200	3.74441400
H	0.60408100	2.56691500	1.84745000
C	-2.11961300	0.99977200	4.12998500
H	-2.49243300	-0.37528200	2.52305300
C	-1.35734700	2.08556300	4.57494200
H	0.21941600	3.47677200	4.08659200
H	-2.86751600	0.55449600	4.77859000
H	-1.52229100	2.49331400	5.56764500

C	-0.89867800	2.41286700	-0.87504500
H	-0.11730700	2.90917100	-0.29095300
H	-0.36924600	1.98542000	-1.74931500
H	-1.61165200	3.14345000	-1.25343700
C	-0.65480600	0.36398600	0.63871700
H	-1.09300600	-0.63588000	0.69740800
O	0.67767300	0.25740000	0.25732000
Fe	2.24366700	1.42278300	-0.22638000
Br	2.58498700	3.78015100	0.27505400
Br	1.65060700	-1.81411400	-2.52621600
Br	2.12105400	1.14114400	-2.87298700
Fe	1.54963600	-1.60454800	0.06205900
Br	3.87967700	-0.46445600	0.44793900
Br	1.37166800	-2.84321300	2.36742600
Br	-0.63317100	-3.29676400	0.13550900
C	-7.11835300	0.11287400	-0.91652000
F	-7.74515800	1.08011900	-1.61231000
F	-7.70871600	0.03083600	0.29280200
F	-7.31912000	-1.05665200	-1.54976500

TS2c

SCF done: -1321.250743

C	-1.67975700	0.38992100	-0.83827500
C	-3.13910400	0.17664500	-0.78922200
C	-3.73619100	-0.95882900	-0.20516700
C	-3.96668600	1.16325400	-1.35764400
C	-5.11678600	-1.09593500	-0.19049000
H	-3.12297800	-1.74755000	0.21490200
C	-5.35253100	1.03690600	-1.31172900
H	-3.53250700	2.05030400	-1.80474400
C	-5.92847000	-0.09454700	-0.73540000
H	-5.56737400	-1.97896900	0.24925400

H	-5.98278000	1.81466900	-1.72693000
C	-0.78450300	-0.07275000	0.18285500
H	-1.03182900	-1.00739500	-0.59618200
O	0.53126800	0.20117300	0.03117100
Fe	1.54039600	2.01699700	0.64219600
Br	-0.22790100	3.64666100	0.97234700
Br	3.48793500	-0.29046200	-2.12560800
Br	2.83100000	2.59598800	-1.55939400
Fe	2.06454600	-1.06953400	-0.12454900
Br	3.16081400	0.48190600	1.83281500
Br	2.63895100	-3.45242400	0.66730400
Br	0.42565200	-2.90505200	-1.39703600
C	-1.08192100	1.07614600	-2.02320900
H	-0.08368800	0.69004800	-2.23529600
H	-1.71650300	1.00777300	-2.90579100
H	-0.93850000	2.13192000	-1.74873500
C	-1.22741300	-0.44172000	1.57568800
C	-0.81514900	-1.65013600	2.15321300
C	-1.96113600	0.48180200	2.33322400
C	-1.14871100	-1.93851700	3.47599000
H	-0.24030000	-2.36702800	1.57537500
C	-2.28183600	0.19021100	3.65866500
H	-2.25329800	1.43208000	1.89946300
C	-1.88129500	-1.01919800	4.22983200
H	-0.82957300	-2.87793500	3.91614500
H	-2.83816100	0.91446500	4.24552400
H	-2.13331500	-1.24179900	5.26222700
C	-7.42655300	-0.28262300	-0.74336600
F	-8.07669500	0.88148100	-0.93583600
F	-7.80028400	-1.12564800	-1.72906900
F	-7.85806500	-0.81242800	0.41955000

TS3c

SCF done: -1321.254977

C	-2.08511700	-1.34604500	0.60176600
C	-2.28312000	0.52024200	0.47585200
C	-1.75182900	1.29713300	1.51966700
C	-3.40208900	0.97460300	-0.24597900
C	-2.34184300	2.51521500	1.83941100
H	-0.85740600	0.98312900	2.04397200
C	-3.97851100	2.19637400	0.07023000
H	-3.81756300	0.37175600	-1.04601400
C	-3.45167500	2.96264400	1.11733800
H	-1.93433200	3.12060900	2.64097500
H	-4.83699800	2.55581100	-0.48563900
C	-1.62272700	-1.76258400	1.97143800
H	-1.33314400	-2.81673600	1.88240600
H	-0.75046100	-1.20957100	2.31492600
H	-2.42460100	-1.69879800	2.70994900
C	-1.22446100	-0.60167700	-0.27492600
H	-1.51003700	-0.54427700	-1.32669500
O	0.07021400	-0.39336200	-0.01293300
Fe	1.59623500	-1.93429800	0.21815900
Br	0.48199600	-3.98481700	-0.42175600
Br	2.14407400	1.56066300	1.81349600
Br	2.38592500	-1.36067200	2.58481400
Fe	1.20495600	1.11112800	-0.72402300
Br	3.09310100	-0.57786900	-1.37948000
Br	-0.12311900	1.43169100	-3.07155200
Br	1.01757900	3.61230800	-1.25031200
C	-3.28164500	-2.03269200	0.04983900
C	-3.21959600	-2.63783500	-1.21784900
C	-4.45708800	-2.15593500	0.81303900
C	-4.31571100	-3.34693300	-1.71037300

H	-2.30035200	-2.60559100	-1.79260100
C	-5.55076200	-2.85233100	0.31099800
H	-4.52223400	-1.68474700	1.78895100
C	-5.48172900	-3.45013700	-0.95242700
H	-4.24981300	-3.82618700	-2.68184700
H	-6.45707800	-2.93265600	0.90298700
H	-6.33402600	-4.00080600	-1.33865900
C	-4.05427300	4.31542900	1.42455900
F	-5.38181700	4.32349600	1.18593600
F	-3.86248700	4.66046300	2.71222800
F	-3.49776300	5.27083000	0.65666200

IM2c

SCF done: -1321.275047

C	0.08957600	2.57682200	0.13554000
C	1.68736000	0.67124000	-0.15659500
C	1.81822400	-0.17964400	0.95021300
C	2.82680100	1.00770300	-0.89727700
C	3.06796100	-0.68093100	1.31041700
H	0.94205100	-0.46212000	1.52366000
C	4.07657300	0.50952900	-0.53803000
H	2.73984800	1.65699900	-1.76210200
C	4.19899400	-0.33404700	0.56855700
H	3.16278900	-1.33768600	2.16838000
H	4.95523900	0.77286200	-1.11625400
C	-0.02387900	2.50483200	1.64462900
H	-0.38387700	3.44408100	2.06521900
H	-0.69210600	1.70095300	1.95418300
H	0.96638500	2.29066900	2.06059500
C	0.30936000	1.21055300	-0.56478500
H	0.31885800	1.37572200	-1.64706300
O	-0.69633200	0.27056500	-0.24057000

Fe	-2.68497200	0.59957300	-0.05925900	C	4.14072100	0.38284500	-1.35593300
Br	-2.05930700	3.08941600	-0.44681100	H	2.96199700	2.08415900	-0.79719200
Br	-1.73633000	-2.42796300	1.51701400	C	4.23228600	-1.01082900	-1.36583900
Br	-3.45566100	0.01471200	2.24960200	H	3.27483300	-2.86557500	-0.82885000
Fe	-0.78510200	-1.57280900	-0.92969600	H	4.92023500	0.98002200	-1.81548800
Br	-3.30096800	-0.97805500	-1.89330500	C	-0.46026100	2.31864300	2.04453500
Br	0.48798200	-1.41336000	-3.27298400	H	-0.32733300	3.28208300	2.53716600
Br	0.33841900	-3.81570200	-1.35520900	H	-1.22185800	2.38484100	1.26691100
C	0.88586000	3.70426500	-0.43922400	H	-0.83192700	1.60861000	2.79622700
C	0.93216400	3.92941600	-1.83031400	C	0.79977500	0.88818600	0.41181600
C	1.63264900	4.55196400	0.39702600	H	0.85131500	2.08227600	0.01458500
C	1.70890000	4.95270800	-2.36194000	O	-0.40155700	0.40673000	0.02199100
H	0.32558300	3.32734400	-2.49894500	Fe	-1.44034500	1.16613000	-1.70147500
C	2.41773500	5.57241500	-0.13928600	Br	0.03869000	3.14480300	-1.95381800
H	1.62156500	4.41148000	1.47101900	Br	-3.83357600	-0.43164200	1.04575700
C	2.45989200	5.77635100	-1.51765500	Br	-3.72607400	1.96059900	-0.78595300
H	1.72122900	5.11456900	-3.43525200	Fe	-1.44973400	-1.23494400	0.40504600
H	2.99451700	6.20815600	0.52523100	Br	-1.80961700	-1.20811200	-2.37537100
H	3.06601000	6.57541100	-1.93348100	Br	-1.07128700	-3.75281500	0.70682600
C	5.53915700	-0.92223600	0.92649000	Br	-0.40251000	-1.67251200	2.86255200
F	6.55628800	-0.12403400	0.53385200	C	5.45737200	-1.68109500	-1.93446700
F	5.65923100	-1.11112400	2.25880300	F	5.16983500	-2.89114300	-2.45443500
F	5.72602600	-2.12290900	0.33772500	F	6.02866900	-0.93812700	-2.90483800
				F	6.39412700	-1.87151500	-0.97664800
				C	2.08876400	2.17278000	2.20089100
				C	3.01920900	1.19542900	2.60449600
				C	2.32351500	3.52367800	2.52375200
				C	4.15135300	1.56542800	3.32447400
				H	2.83598700	0.15061900	2.38239500
				C	3.47770800	3.88953600	3.20909200
				H	1.61956700	4.28807700	2.20991000
				C	4.38823200	2.91068900	3.61724800

TS4c
SCF done: -1321.251856

C	0.83746500	1.76929000	1.53834900
C	2.01717200	0.23395400	-0.19849400
C	2.10592100	-1.16358900	-0.23079100
C	3.03663300	1.00176500	-0.77765100
C	3.21263600	-1.78332800	-0.80609500
H	1.32670200	-1.77930700	0.20358900

H	4.85046400	0.80337700	3.65350400
H	3.66309500	4.93520700	3.43268100
H	5.27985900	3.19647500	4.16705300

IM3c

SCF done: -1321.294452

C	0.06967900	1.54022100	-2.51107600
C	1.80811200	0.06468800	-1.25101500
C	2.01832600	-1.18034400	-0.62391800
C	2.91718700	0.78995600	-1.72975500
C	3.30479000	-1.68429000	-0.47323300
H	1.17015700	-1.77159700	-0.29510600
C	4.20194300	0.29235200	-1.56029600
H	2.77894000	1.76022300	-2.18985700
C	4.39590800	-0.94432900	-0.93474500
H	3.46034000	-2.65074600	-0.00824100
H	5.05652000	0.85713600	-1.91548600
C	-1.37798800	1.42669300	-3.01592800
H	-1.53804500	2.18211000	-3.78940200
H	-1.57322500	0.44408900	-3.45353300
H	-2.09726100	1.61232500	-2.21555500
C	0.42589200	0.53849200	-1.42245300
H	0.74951800	1.35087000	-3.34734400
O	-0.47018800	0.08933300	-0.64966200

Fe	-2.24973600	-1.33602900	-1.07741500
Br	-1.82360300	-2.45902400	-3.14471000
Br	-2.60025000	1.24324700	1.94329000
Br	-4.20599200	0.15831100	-0.36550200
Fe	-0.44640400	-0.13843400	1.56952500
Br	-1.51887000	-2.48553300	1.08326700
Br	1.21490900	-1.02007700	3.34441200
Br	1.25028700	1.79430500	2.16568200
C	5.80255300	-1.45237100	-0.71662400
F	5.83686900	-2.79479200	-0.61588000
F	6.61705900	-1.09117400	-1.73002400
F	6.32393600	-0.94426000	0.41815500
C	0.36179700	2.95832800	-1.99247200
C	-0.24199000	3.43945300	-0.82302600
C	1.18894700	3.81394500	-2.73330700
C	-0.01594900	4.75091400	-0.40101100
H	-0.89847600	2.80083400	-0.24135000
C	1.41009600	5.12591400	-2.31237300
H	1.64582200	3.45969700	-3.65455700
C	0.81173200	5.59582500	-1.14176800
H	-0.48935500	5.10773600	0.50840000
H	2.04591700	5.77986100	-2.90178200
H	0.98650400	6.61513900	-0.81140000

Cartesian Coordinates for the Stationary Points Given in Scheme 3.

IM1d

SCF done: -984.1360688

C	2.41937600	-1.03070900	-0.38643500
C	3.52360800	-0.61642700	-1.36965300

C	3.21300500	0.16078000	-2.49341000
C	4.83257400	-1.09321000	-1.22012600
C	4.19264500	0.47484300	-3.43754500
H	2.19656100	0.51602400	-2.65324100
C	5.80905700	-0.78810400	-2.16741700

H	5.08967400	-1.69956000	-0.35718000
C	5.49415600	0.00137000	-3.27596000
H	3.93357200	1.08379900	-4.29827700
H	6.81869700	-1.16636600	-2.03734200
H	6.25765000	0.24242800	-4.00934800
C	2.87965400	-1.01612700	1.10110400
C	2.38227400	-1.95224000	2.02249600
C	3.73027700	0.00486500	1.56570400
C	2.76219800	-1.89157300	3.36294700
H	1.70319600	-2.73568100	1.70851100
C	4.09927700	0.06605200	2.90812400
H	4.12347800	0.74032800	0.87141200
C	3.61824800	-0.88404700	3.81064600
H	2.37832800	-2.63203900	4.05772700
H	4.76127700	0.85723000	3.24643000
H	3.90471400	-0.83681400	4.85687600
C	1.81732600	-2.37011700	-0.84459900
H	0.95909500	-2.68550700	-0.24959500
H	1.49790800	-2.29445700	-1.88596900
H	2.58099600	-3.14870000	-0.77734500
C	1.41332400	0.08001300	-0.26309600
H	1.83146900	1.09162000	-0.18152900
O	0.17398600	-0.03226300	-0.16705100
Fe	-1.61706500	-1.45971400	0.08732100
Br	-1.43754500	-3.57158700	1.19996800
Br	-2.93046700	0.46444300	-1.37057600
Br	-1.72426400	-2.07279500	-2.54916000
Fe	-1.13356900	1.68188600	0.35334500
Br	-2.06755400	0.26955900	2.19110600
Br	0.60242800	3.27671400	1.56413400
Br	-0.75785400	3.69872600	-1.15800700

TS3d

SCF done: -984.0976504

C	2.14414800	-1.42933200	-0.17503500
C	3.45873100	-1.41992600	-0.85896800
C	3.64061000	-0.63475500	-2.01304200
C	4.50970200	-2.25100800	-0.42652800
C	4.84334700	-0.68678400	-2.71772700
H	2.83090500	-0.01573000	-2.38553800
C	5.71322800	-2.28362300	-1.12123800
H	4.39305200	-2.84798800	0.47237200
C	5.88135200	-1.50460500	-2.27147100
H	4.96381600	-0.09044300	-3.61645000
H	6.52138300	-2.91731900	-0.76960700
H	6.81888100	-1.54003100	-2.81791400
C	2.18015400	-0.29980200	1.39854000
C	1.44586000	-0.75082500	2.51303700
C	3.38675400	0.40311500	1.58740600
C	1.91267800	-0.48302900	3.79559700
H	0.49807900	-1.26355600	2.39276700
C	3.83966500	0.67006900	2.87216000
H	3.95801500	0.74115900	0.72909600
C	3.10526100	0.22318000	3.97712600
H	1.33563600	-0.81532900	4.65225300
H	4.75876000	1.22875200	3.01566300
H	3.46189300	0.43126400	4.98141700
C	1.53311700	-2.76838900	0.10713100
H	0.66397800	-2.74153700	0.76126000
H	1.19438400	-3.15522600	-0.86310300
H	2.26607800	-3.47454200	0.50209500
C	1.40146200	-0.19263400	-0.06640500

H	1.86567500	0.66530200	-0.55653300
O	0.05974300	-0.11157000	-0.00923900
Fe	-1.67040900	-1.22574800	0.21011700
Br	-1.97754600	-2.98954000	1.83786100
Br	-2.76529100	0.27278100	-1.76803100
Br	-1.49071800	-2.47419400	-2.21911500
Fe	-0.92789200	1.69992300	-0.06412100
Br	-2.40046700	1.05924800	1.83848900
Br	0.82321100	3.46080400	0.91021900
Br	0.02712400	3.09402500	-2.02294500

IM2d

SCF done: -984.1106204

C	-1.87035600	1.44630100	-0.83308000
C	-3.18042300	1.23181700	-1.39030700
C	-3.75301700	-0.07017100	-1.42573700
C	-3.91632400	2.30754700	-1.95850300
C	-4.99303400	-0.27738700	-2.01394000
H	-3.20056300	-0.92590900	-1.05381400
C	-5.16835600	2.09380400	-2.51174700
H	-3.52237500	3.31599300	-1.91558800
C	-5.70580300	0.80046600	-2.54805100
H	-5.40174300	-1.28122000	-2.06210200
H	-5.72985900	2.92841900	-2.91827700
H	-6.68012900	0.63405400	-2.99786400
C	-1.86411900	1.33099800	1.50273300

C	-1.10435200	2.34707100	2.09959300
C	-3.10519700	0.97666600	2.05673800
C	-1.56781300	2.97124600	3.25744500
H	-0.13952800	2.63866400	1.69845200
C	-3.56526400	1.60706400	3.20878700
H	-3.69912800	0.19008500	1.59998800
C	-2.79708000	2.60833200	3.81107700
H	-0.96129900	3.74065600	3.72471400
H	-4.51518900	1.31071100	3.64279900
H	-3.15488500	3.10009400	4.71060500
C	-0.99551300	2.51860600	-1.34328000
H	-0.36011100	2.97158100	-0.57721200
H	-0.29639900	2.01692000	-2.04042000
H	-1.51217200	3.29046700	-1.91151600
C	-1.35314300	0.55549800	0.25747400
H	-1.89564600	-0.39271000	0.25555600
O	0.01610800	0.29272800	0.22196800
Fe	1.76826000	1.24791100	0.07494000
Br	2.29379300	3.56444000	0.59752900
Br	1.30335200	-1.99863800	-2.24833100
Br	2.23396900	0.85222300	-2.52685500
Fe	0.67625200	-1.66801200	0.25431700
Br	2.98821400	-0.78710700	1.11730100
Br	-0.14174100	-2.75408400	2.50317600
Br	-1.61982600	-3.15238100	-0.11444700

Cartesian Coordinates for the Stationary Points Given in Fig. S1.

SCF done: -1711.520047

IM16a

C	3.30571400	0.23264400	-0.46441200
C	3.43928100	1.61338300	-0.08314200

C	2.48618200	2.26550800	0.75315400	C	-2.79571400	2.21100800	2.86817200
C	4.55158200	2.37879700	-0.51767400	H	-2.29317100	1.81364100	3.75201100
				H	-2.22425000	3.08507100	2.54715400
C	2.65848200	3.57597200	1.14013700	H	-3.79658100	2.53553300	3.16185300
H	1.58789800	1.75495200	1.08230200	C	-1.43685700	0.79904000	1.31682200
C	4.73448100	3.69484200	-0.13122600	H	-1.37163300	0.02826600	0.52644600
H	5.29675100	1.92917700	-1.16296300	O	-0.42237200	1.29744700	1.77456900
C	3.78358800	4.30761800	0.70804800	C	3.01654500	-1.07536400	1.72344900
H	1.92856000	4.07200800	1.77024700	C	1.87157700	-1.58814400	2.63967900
H	5.60403600	4.23842300	-0.47935400	C	4.14609600	-2.11560800	1.67345700
C	4.37453100	-0.42241600	-1.29377800	H	3.41715800	-0.14476400	2.14650000
H	5.29411400	-0.47803900	-0.69509400	C	2.38879400	-2.46198600	3.80702500
H	4.07814400	-1.43453300	-1.56088900	H	1.16874300	-2.16852700	2.03394900
H	4.59819100	0.13770400	-2.20163200	H	1.31892700	-0.72324300	3.02386400
C	2.38907700	-0.69280600	0.33004700	C	4.80383400	-2.27423500	3.06753700
H	1.47070900	-0.14620700	0.57152100	H	3.71927700	-3.06695100	1.33945000
O	2.08838300	-1.85895600	-0.37659700	H	4.91614700	-1.85526300	0.94146000
Fe	0.87066200	-2.05239000	-1.68293100	C	3.80472900	-2.05132600	4.22673500
Br	0.13366700	-2.94244000	-3.75533800	H	2.39912700	-3.51677600	3.50470700
Br	-0.98152800	-2.83085800	-0.28091700	H	1.69596100	-2.39467800	4.65297600
Br	1.49250700	0.28604600	-2.51675500	H	5.64043300	-1.57157800	3.16631600
C	-2.85699800	1.15614300	1.75480900	H	5.23829100	-3.27828900	3.13724200
C	-3.54590100	1.67878500	0.47371000	H	3.79757700	-0.99228700	4.51727100
C	-4.02085000	2.99039200	0.36308000	H	4.12640800	-2.60764300	5.11409000
C	-3.68643000	0.85090400	-0.66039000	O	3.85729700	5.57708900	1.14303600
C	-4.62636400	3.46583800	-0.80428700	C	4.95519800	6.39471900	0.73644200
H	-3.93419000	3.67472100	1.19874800	H	4.79183900	7.36299100	1.20901300
C	-4.27735900	1.30913300	-1.82956700	H	5.90826800	5.97692400	1.07942600
H	-3.32958500	-0.17414500	-0.64435900	H	4.97558200	6.51769000	-0.35195600
C	-4.75721100	2.62378400	-1.91207400	C	-3.53917800	-0.17913900	2.23928700
H	-4.98627100	4.48769600	-0.83209900	C	-2.70119300	-0.95527700	3.29453600
H	-4.37597000	0.66263800	-2.69532500	C	-4.97716400	0.02670700	2.74615000

H	-3.60702800	-0.82410500	1.35567500
C	-3.57285600	-1.88806500	4.16698100
H	-2.15606300	-0.26389300	3.94683700
H	-1.94118500	-1.54996900	2.77346000
C	-5.70187600	-1.33114100	2.89876300
H	-4.95057700	0.54099700	3.71486800
H	-5.53659500	0.67640600	2.06510300
C	-4.74790000	-2.46015100	3.36375100
H	-3.96639700	-1.33266200	5.02855800
H	-2.95443900	-2.69327000	4.57896700
H	-6.16197400	-1.61172500	1.94407300
H	-6.52459000	-1.21550300	3.61455200
H	-4.35133700	-2.99853700	2.49364600
H	-5.29728200	-3.20097600	3.95526000
O	-5.32738100	2.97844200	-3.09953500
C	-5.81897700	4.30099400	-3.23836900
H	-5.02150900	5.04536400	-3.11472100
H	-6.21904500	4.36981500	-4.25118000
H	-6.62092400	4.51400100	-2.51929200

TS18a

SCF done: -1711.474913

C	-2.82022200	0.93363600	0.25966700
C	-3.74048400	-0.13227900	-0.24950100
C	-3.29332700	-1.12194500	-1.15149500
C	-5.08223200	-0.18770200	0.15157400
C	-4.13646500	-2.11864000	-1.60757700
H	-2.27680100	-1.09015900	-1.52650000
C	-5.94398100	-1.19434700	-0.29081100
H	-5.47947700	0.55346100	0.83496900
C	-5.47442900	-2.16873400	-1.17752300
H	-3.79055900	-2.86939800	-2.31017900

H	-6.97017000	-1.20002500	0.05613200
C	-3.47844200	2.05693100	1.05943200
H	-3.85248700	1.65196500	2.00764500
H	-2.75961700	2.84333300	1.29169100
H	-4.31491000	2.49888900	0.51588700
C	-1.50396400	0.47760900	0.93678000
H	-0.69244100	-0.35887300	-0.00668900
O	-0.57767900	1.40782600	1.07897800
Fe	-0.06325400	2.96010100	-0.05082700
Br	-0.52028200	5.19837600	0.73545800
Br	1.97248500	2.10333900	-1.24121300
Br	-2.14229400	2.01170800	-1.55104200
C	2.34668200	-1.51911700	-1.08278100
C	3.73093700	-1.08729900	-0.56563600
C	3.96209400	-0.77574800	0.78746600
C	4.83514900	-1.03934300	-1.42226900
C	5.22055000	-0.42207900	1.25341500
H	3.15320700	-0.80629000	1.51111100
C	6.11118700	-0.69094600	-0.97194400
H	4.72009600	-1.26544600	-2.47606700
C	6.31140800	-0.37370100	0.37455700
H	5.38145000	-0.17308500	2.29695900
H	6.92920500	-0.66133300	-1.68156500
C	2.19593100	-1.28199200	-2.61029900
H	1.15212900	-1.35784700	-2.91547100
H	2.55192000	-0.28469700	-2.87046500
H	2.76726600	-2.03041800	-3.16590200
C	1.26005700	-0.74423100	-0.38320000
H	1.47334200	-0.09765300	0.46803700
O	0.05156400	-0.93303600	-0.68859900
O	-6.21899500	-3.18601900	-1.68155900
C	-7.59141100	-3.26589900	-1.31864100

H	-8.14170700	-2.36946500	-1.62962400
H	-7.99022700	-4.13419200	-1.84435400
H	-7.71455900	-3.40937700	-0.23795600
C	-1.70138100	-0.43105700	2.19480700
C	-2.18747500	-1.88362600	1.91610400
C	-0.44037600	-0.46542800	3.07826500
H	-2.47917000	0.06758900	2.79490000
C	-1.81110600	-2.86427900	3.05288700
H	-1.76704900	-2.25066100	0.97348600
H	-3.27197900	-1.88573500	1.78050800
C	-0.76032300	-1.05086800	4.47236200
H	0.32384500	-1.08314600	2.58493300
H	-0.01509000	0.53444800	3.17320300
C	-1.82864500	-2.16956500	4.41892300
H	-0.80876200	-3.27731800	2.87794800
H	-2.49715200	-3.71853100	3.03839500
H	-1.10116400	-0.24733200	5.13559700
H	0.16606100	-1.43772400	4.91270400
H	-2.82727200	-1.74597300	4.58863500
H	-1.66528300	-2.89293600	5.22522100
C	2.15081600	-3.08180800	-0.78413300
C	2.21855100	-3.45775200	0.72054000
C	0.91979500	-3.75961900	-1.41525800
H	3.03678900	-3.50788900	-1.27290000
C	1.69346400	-4.88872500	1.00060700
H	1.62956800	-2.75108100	1.32015200
H	3.25086700	-3.36337000	1.06756200
C	1.10991300	-5.29806400	-1.42702700
H	0.02375000	-3.49830300	-0.84174000
H	0.74076900	-3.41428400	-2.43568900
C	1.90931900	-5.80917400	-0.20542100
H	0.62079000	-4.85409300	1.23086300

H	2.18348000	-5.29165200	1.89344800
H	1.61957100	-5.59810600	-2.35023900
H	0.12237100	-5.77299000	-1.45320100
H	2.98056900	-5.84301600	-0.44241400
H	1.61946500	-6.83772500	0.03483600
O	7.50451400	-0.01564700	0.92466300
C	8.63162600	0.09993000	0.06906500
H	8.46823200	0.85104600	-0.71391000
H	9.46004300	0.41692900	0.70411600
H	8.88433900	-0.85981800	-0.40014000

IM7a

SCF done: -1711.538725

C	-4.38726000	-1.20099100	-0.37178800
C	-5.81339600	-1.12009100	-0.62298700
C	-6.52700100	0.10976500	-0.62625500
C	-6.55802900	-2.28323700	-0.93431200
C	-7.87944200	0.16428900	-0.90257200
H	-5.99328900	1.03807000	-0.46225300
C	-7.92288200	-2.24367200	-1.19212600
H	-6.06195100	-3.24760400	-0.93561000
C	-8.59785700	-1.01332800	-1.17955200
H	-8.40977100	1.11040000	-0.92669900
H	-8.44985500	-3.16708600	-1.40001500
C	-3.54747700	-2.23084300	-1.07504100
H	-2.78788100	-1.72505100	-1.68692400
H	-2.98613400	-2.84919200	-0.36565600
H	-4.13725900	-2.86966500	-1.73228300
C	-3.66680500	-0.33907600	0.54414100
O	-2.40770700	-0.40183700	0.53899700
Fe	-0.52529200	0.13257000	0.02625500
Br	-0.25129700	-0.27464000	-2.40869100

Br	0.09140600	2.34723100	0.95459600	H	-2.82575200	1.94578300	3.85339500
Br	0.79906400	-1.75235100	1.31050700	H	-3.79435300	1.04577300	5.00777700
C	4.40965400	0.22953500	-0.28708700	H	-5.82477100	3.15419300	1.86872700
C	5.71757600	-0.58721200	-0.01315000	H	-4.31223000	3.92307800	2.31751400
C	5.69254700	-1.63048700	0.92852900	H	-5.88079600	1.78228500	3.77489600
C	6.92811100	-0.36460300	-0.70165700	H	-4.98979400	3.14040500	4.43636100
C	6.82266100	-2.39161600	1.21676300	O	-9.92075000	-0.85290100	-1.42710200
H	4.77593300	-1.86293700	1.45988200	C	-10.70257200	-2.00106500	-1.73535400
C	8.06180800	-1.11112700	-0.42216400	H	-10.70539400	-2.71933700	-0.90651000
H	7.00367800	0.41682900	-1.44759600	H	-11.71697300	-1.63606800	-1.89929300
C	8.02330800	-2.13259300	0.54182800	H	-10.34410100	-2.49767700	-2.64504500
H	6.75384900	-3.17870700	1.95758100	C	4.63264800	1.49741300	-1.18181000
H	8.99718200	-0.92180000	-0.93798500	C	3.30283800	2.01398600	-1.80133300
C	3.66785700	0.56288400	1.01611200	C	5.35658600	2.63825500	-0.44626500
H	2.77370200	1.16199300	0.83382900	H	5.27076300	1.19057200	-2.02098800
H	3.34534600	-0.32143300	1.56505200	C	3.38681000	3.50629100	-2.19820300
H	4.33667500	1.13281900	1.66455200	H	2.46476900	1.88661700	-1.11042400
C	3.79720600	-0.81695500	-1.15076900	H	3.06071800	1.41072000	-2.68585300
H	4.25026400	-0.95301200	-2.13680100	C	5.80506100	3.72702700	-1.44989200
O	2.88420100	-1.65243800	-0.91200800	H	4.66998800	3.07256800	0.28835700
H	2.28835200	-1.57427800	-0.05238200	H	6.21911500	2.26675400	0.11756300
C	-4.31596900	0.54855600	1.59418800	C	4.80766600	3.89728500	-2.62315600
C	-3.78269100	0.18385500	3.01619100	H	3.07901200	4.12795800	-1.34876700
C	-4.03910200	2.04325500	1.29671200	H	2.66826000	3.70972500	-2.99826800
H	-5.39644500	0.38570900	1.57987800	H	6.79944400	3.48268900	-1.84425500
C	-3.76824900	1.39727800	3.97022300	H	5.91558200	4.67435400	-0.91020600
H	-2.77174000	-0.22271000	2.92997100	H	5.11385900	3.26815100	-3.46984700
H	-4.41631500	-0.61010900	3.42994100	H	4.83229600	4.92894200	-2.99021800
C	-4.82246900	2.95434500	2.26753300	O	9.18301300	-2.80320000	0.73867400
H	-2.96250500	2.21789200	1.38786000	C	9.21034500	-3.85230000	1.70141000
H	-4.29513600	2.29342000	0.25971500	H	8.51450400	-4.65724700	1.43640200
C	-4.94088900	2.34406300	3.68554300	H	10.22981000	-4.23867500	1.69173600

H	8.97222600	-3.48062500	2.70516100	C	-4.04480300	4.08280900	-1.37689200
				H	-3.05822300	4.61115500	0.42978700
TS19a				C	-4.42179000	3.05123100	-2.24888000
SCF done: -1711.495818				H	-4.35371100	0.93590800	-2.61751600
C	2.14799900	1.09303300	-0.67660000	H	-4.29437500	5.11497300	-1.59156000
C	3.36242500	1.93886200	-0.42601200	C	-1.83371100	3.42999900	2.22172600
C	3.50272500	2.74453200	0.72020700	H	-1.24152900	3.16166900	3.10075800
C	4.40088000	1.98226600	-1.36696200	H	-1.23831300	4.12005800	1.62142200
C	4.62764200	3.53400800	0.92520700	H	-2.72889800	3.95013700	2.56400400
H	2.71510900	2.75827900	1.46911800	C	-0.99403300	1.58034000	0.80210100
C	5.53705500	2.77250300	-1.18076800	H	-1.02615200	0.61763300	0.28896400
H	4.33588300	1.37180400	-2.26299300	O	0.10813000	2.19813800	0.80043800
C	5.65649800	3.55532300	-0.02633500	C	2.69068400	-0.48963400	1.26851800
H	4.72883200	4.15076700	1.81236100	C	1.88252600	-0.41626400	2.59563900
H	6.31695400	2.76339100	-1.93318400	C	3.22210100	-1.92666300	1.06450800
C	1.42657900	1.34575800	-1.99499700	H	3.55718000	0.17159300	1.34565100
H	2.09247800	1.15397900	-2.84412700	C	2.41734800	-1.39203200	3.67069400
H	0.55799400	0.69571200	-2.11003200	H	0.83250700	-0.65081700	2.38790300
H	1.10260500	2.38990700	-2.08046600	H	1.91801300	0.61360700	2.97466100
C	1.86529100	-0.04051500	0.07377500	C	4.25312900	-2.28308400	2.16055800
H	0.91548000	1.66842800	0.28560500	H	2.37850700	-2.62567400	1.10417400
O	0.78256300	-0.76209500	-0.17006300	H	3.66938000	-2.03974300	0.07191000
Fe	0.39119200	-2.39527300	-1.07047000	C	3.92732900	-1.61540100	3.51865800
Br	1.89260600	-3.45464500	-2.63706100	H	1.90342500	-2.35717000	3.58136900
Br	-1.02948500	-3.84298800	0.63358600	H	2.17892100	-1.00981100	4.66978200
Br	-2.17686200	-2.21522300	-1.71231700	H	5.25648200	-1.98298700	1.83680200
C	-2.21050100	2.15772600	1.43894600	H	4.27935200	-3.37268700	2.27562200
C	-3.00776900	2.46653700	0.13706200	H	4.43905500	-0.64674700	3.59296800
C	-3.37967600	1.44529500	-0.76751800	H	4.31182400	-2.22610300	4.34291000
C	-3.33467300	3.78620300	-0.21494100	O	6.71686600	4.36450500	0.26103300
C	-4.07561200	1.72929100	-1.93229300	C	7.78835000	4.42146400	-0.66755600
H	-3.12415100	0.40933500	-0.58329100	H	7.45834800	4.79601600	-1.64518400

H	8.51676500	5.11543100	-0.24537600	H	2.37888800	4.55172000	1.28926700
H	8.26146300	3.44017700	-0.80165300	C	5.16630700	2.94260000	-0.87358900
C	-2.89832500	1.13388700	2.43123500	H	3.69000200	1.51533400	-1.46719600
C	-4.20421900	1.73780800	3.02089400	C	5.44654700	4.07631700	-0.09999500
C	-3.17610900	-0.29822100	1.93625600	H	4.66150500	5.53011900	1.26890100
H	-2.17022500	1.03949900	3.24995900	H	5.93074900	2.47388300	-1.48131500
C	-5.14837000	0.65933400	3.60106100	C	0.77134700	2.42370300	-1.47491000
H	-4.73131200	2.30280700	2.24282800	H	1.34268000	1.87542200	-2.22752000
H	-3.94706600	2.45262000	3.80996000	H	-0.23198000	1.99588500	-1.42287500
C	-3.50788200	-1.21696200	3.13583000	H	0.69604100	3.46577700	-1.79682000
H	-4.02108400	-0.28923200	1.24081200	C	1.56979300	0.95383700	0.44609500
H	-2.33327100	-0.73460500	1.39208900	H	0.84208100	2.91263700	0.62914400
C	-4.35167900	-0.49770500	4.21659200	O	1.43711900	-0.01297600	-0.32611400
H	-5.79971700	0.26727100	2.81040800	Fe	1.92719500	-1.80238400	-1.03189600
H	-5.81171100	1.11803000	4.34248100	Br	4.08412800	-1.82649400	-2.08766400
H	-2.57780500	-1.59342000	3.57639000	Br	1.10599200	-3.72072100	0.50688600
H	-4.04085000	-2.09502900	2.75743500	Br	-0.23473200	-2.74676600	-2.10753200
H	-3.69851900	-0.09903700	5.00429700	C	-3.85662700	0.72929700	1.06803600
H	-5.02164700	-1.20881100	4.71122400	C	-4.89116600	1.50436400	0.22903500
O	-5.10384900	3.22652500	-3.40589700	C	-4.50447000	2.53135900	-0.64937300
C	-5.45999000	4.54712400	-3.79739900	C	-6.26445100	1.28187200	0.38460700
H	-5.98312600	4.44502000	-4.74854600	C	-5.43904900	3.27879700	-1.35669500
H	-6.12814400	5.01712300	-3.06537500	H	-3.45263600	2.77006800	-0.78210300
H	-4.57299200	5.17687700	-3.93735600	C	-7.21930400	2.02608600	-0.31143000

IM18a

SCF done: -1711.538643

C	1.44685500	2.36140600	-0.10059300	H	-8.27061100	1.81431300	-0.15605500
C	2.85656500	2.96140800	-0.09129600	C	-3.78299600	1.37986000	2.46594300
C	3.15656900	4.09329000	0.68335100	H	-3.02357100	0.91263800	3.09712300
C	3.88074900	2.39779900	-0.86216900	H	-3.53245800	2.43973300	2.37854300
C	4.42892000	4.64976500	0.67882600	H	-4.75234600	1.29887800	2.96607800

C	-2.49942200	0.83406100	0.38351100
H	-2.42962500	0.34929000	-0.61101300
O	-1.52496400	1.39423300	0.85258900
C	1.91810100	0.74276700	1.89818300
C	0.78412400	-0.02904600	2.64369800
C	3.26007900	-0.01499400	2.05691200
H	2.03536000	1.73437400	2.34778600
C	1.31046300	-0.74701700	3.90871900
H	0.34075700	-0.76422600	1.96607200
H	-0.00765200	0.68123400	2.89722800
C	3.70756900	-0.00526800	3.53674900
H	3.12011500	-1.04518800	1.70974200
H	4.03330800	0.42975000	1.42401900
C	2.51250100	-0.01565300	4.51881600
H	1.60577000	-1.77266000	3.65548600
H	0.49827900	-0.83467100	4.63845800
H	4.33302900	0.87435600	3.72643100
H	4.34309900	-0.88066200	3.71163200
H	2.21932900	1.01362900	4.76454000
H	2.80747900	-0.48085500	5.46526900
O	6.65940800	4.68991500	-0.03460400
C	7.73022000	4.14978000	-0.79745400
H	7.50891200	4.16678900	-1.87188600
H	8.59222200	4.78756700	-0.59766500
H	7.96287300	3.12133900	-0.49442300
C	-4.20541700	-0.80722300	1.17264500
C	-4.61173100	-1.46548100	-0.18029100
C	-3.08916800	-1.64468300	1.83390900
H	-5.07197300	-0.85979200	1.84615900
C	-4.36611000	-2.99169700	-0.20201100
H	-4.07206700	-1.00420700	-1.01471100
H	-5.67023400	-1.26319600	-0.37050300

C	-3.60162200	-3.05284300	2.21304000
H	-2.24612600	-1.74073300	1.13737200
H	-2.69281000	-1.15019800	2.72573600
C	-4.61069900	-3.60935500	1.17951600
H	-3.33602200	-3.20332000	-0.51400200
H	-5.01283500	-3.45437600	-0.95574800
H	-4.06916600	-3.01971600	3.20477900
H	-2.74167200	-3.72644100	2.29897400
H	-5.63734500	-3.37940700	1.49499700
H	-4.54371200	-4.70162700	1.13433200
O	-7.64791400	3.81217300	-1.93287600
C	-9.04550200	3.59996800	-1.80915100
H	-9.51983800	4.31798200	-2.47978200
H	-9.32944800	2.58344200	-2.11058800
H	-9.39414200	3.78028300	-0.78401900

TS20a

SCF done: -1178.743904

C	-1.85476200	-0.44049200	-0.79021600
C	-1.31583700	-0.02604500	-2.15923800
H	-1.57608000	1.01637300	-2.36690200
H	-0.23147400	-0.10767300	-2.19202200
H	-1.73530800	-0.65633700	-2.94442700
C	-1.08091000	0.26253500	0.36980000
H	-1.27359700	-0.46337800	1.41046800
O	0.25644500	0.20533900	0.24394100
Fe	1.92809700	1.58939800	-0.06188000
Br	1.91053000	3.98712100	-0.23383700
Br	2.72666900	-2.23945100	-1.74334400
Br	2.60206200	0.70069600	-2.44594700
Fe	1.40666200	-1.56797400	0.32619200
Br	3.19853800	0.09170000	1.51301200

Br	1.14183100	-3.11591000	2.30160200
Br	-1.16198500	-2.50431400	-0.64729400
O	-1.38687200	-1.19607000	2.61181300
H	-0.72434400	-1.94545400	2.54268300
H	-1.03893000	-0.62126200	3.31424000
C	-1.69445400	1.57231100	0.94404400
C	-0.94967900	2.04736100	2.22418900
C	-1.80843100	2.72458800	-0.08942200
H	-2.72061900	1.30765000	1.21844900
C	-1.06163400	3.56821200	2.45906900
H	0.10757500	1.76317600	2.18212900
H	-1.38393500	1.52835000	3.09031200
C	-2.62424600	3.90392700	0.49682100
H	-0.80575300	3.05962500	-0.37099500
H	-2.30267300	2.37465200	-0.99779600
C	-2.43441000	4.08515300	2.02006900
H	-0.27760300	4.08588300	1.89590500
H	-0.87906800	3.78370100	3.51701600
H	-3.68715500	3.76121400	0.27113200
H	-2.31245400	4.81410700	-0.02776400
H	-3.21734500	3.54001700	2.56466000
H	-2.55406600	5.13924300	2.29036100
C	-3.34432500	-0.46591900	-0.64950000
C	-3.97691900	-0.92897100	0.52750200
C	-4.17249900	-0.02306300	-1.69295700
C	-5.35332700	-0.93092600	0.65279400
H	-3.38463200	-1.31522000	1.34948700
C	-5.56269600	-0.01456900	-1.57908700
H	-3.74186300	0.33327800	-2.62070500
C	-6.16557100	-0.47012900	-0.40084000
H	-5.83366400	-1.29446900	1.55486600
H	-6.15743200	0.34299400	-2.41059700

O	-7.49887700	-0.51120600	-0.17661400
C	-8.38081200	-0.07638700	-1.20734000
H	-8.26672300	-0.68361000	-2.11300900
H	-9.38811500	-0.20435800	-0.81064800
H	-8.21855700	0.97993600	-1.45297000

IM19a

SCF done: -1178.798284

C	-1.81360100	0.44071600	0.80746600
C	-3.09037600	1.06293200	0.55852900
C	-3.63864900	1.13245300	-0.75417500
C	-3.82322500	1.69985200	1.59322200
C	-4.82893000	1.77722000	-1.00848800
H	-3.07883800	0.71544200	-1.58184800
C	-5.03546400	2.32679600	1.35462200
H	-3.46014600	1.65745300	2.61344700
C	-5.55022700	2.37706200	0.04555800
H	-5.22741300	1.85169600	-2.01439500
H	-5.57509300	2.77113800	2.18181300
C	-0.90715400	0.98708300	1.87977100
H	-0.36065500	0.19305800	2.39301100
H	-0.16880000	1.66628800	1.43122800
H	-1.45444500	1.58055800	2.61180500
C	-1.29777200	-0.66929100	0.05697600
H	3.02040500	3.74480000	0.42092000
O	-0.00322600	-0.80938100	0.02951700
Fe	1.11615700	-2.43399200	0.94919000
Br	1.62957300	-3.86244600	-1.01862700
Br	2.61612100	4.40578200	1.65164200
Br	-0.11298200	-2.93477900	2.96823800
Fe	1.55031400	0.38787800	-0.77239000
Br	2.97311500	-0.53734700	1.13250700

Br	3.25359100	2.17888600	-1.80938500
Br	0.19732600	2.43224900	-1.65536500
O	1.77406800	-0.89247400	-2.39114000
H	2.56103500	-0.73964500	-2.93392000
H	1.76073700	-1.84974100	-2.14059600
O	-6.70595500	2.97084300	-0.30239300
C	-7.48905500	3.61821800	0.70160600
H	-8.35724600	4.02280500	0.18202900
H	-7.81955800	2.90613100	1.46589900
H	-6.93115200	4.43477900	1.17286900
C	-2.06439200	-1.82191600	-0.57103400
C	-3.46864500	-2.15702100	-0.00393700
C	-2.07016000	-1.79342400	-2.12596600
H	-1.41298100	-2.67029100	-0.32172900
C	-4.27952300	-3.03365300	-0.98567600
H	-4.03885500	-1.25536900	0.22481400
H	-3.32881300	-2.68719800	0.94479600
C	-2.37985200	-3.20767800	-2.67054600
H	-2.82868400	-1.08622100	-2.47814000
H	-1.10528700	-1.44498800	-2.50586400
C	-3.37056500	-3.98819300	-1.77097100
H	-4.82354900	-2.39326700	-1.69246900
H	-5.04093600	-3.59128000	-0.43012000
H	-1.44585900	-3.77191500	-2.76183700
H	-2.78782400	-3.10596400	-3.68277000
H	-2.81558700	-4.61503900	-1.06162900
H	-3.96831900	-4.67518300	-2.37904000

TS21a

SCF done: -1102.294043

C	-1.81251200	0.17536300	-1.33221700
C	-3.21165100	0.01813000	-1.01115200

C	-3.62160100	-0.26711100	0.32534300
C	-4.21625700	0.01936300	-2.01400000
C	-4.94394600	-0.48518500	0.63756100
H	-2.87295200	-0.37688400	1.10356700
C	-5.55054600	-0.18960700	-1.70712600
H	-3.94657500	0.21874300	-3.04496700
C	-5.93000600	-0.44192900	-0.37328600
H	-5.25222300	-0.72014900	1.65042300
H	-6.29034700	-0.15587100	-2.49751400
C	-1.34132100	0.24805100	-2.78204100
H	-1.57406100	1.22862400	-3.21775800
H	-0.26056100	0.10530500	-2.83867200
H	-1.82046100	-0.52160100	-3.39179300
C	-0.85550900	0.84870200	-0.41132900
H	-1.40525600	-1.38202800	-1.14569600
O	0.31279200	0.36844400	-0.31902700
Fe	2.33272500	1.35148900	-0.22635700
Br	2.18229900	3.61876200	-1.02319200
Br	2.89124200	-2.79397000	-0.34418000
Br	3.40614500	-0.28920600	-1.94131100
Fe	0.94482500	-1.55339500	0.84236400
Br	2.65705700	0.23692100	1.99708300
Br	-0.63733600	-1.86637300	2.64721700
Br	-0.82545000	-2.84834300	-1.08397700
O	-7.19093500	-0.66628000	0.03416100
C	-8.24793400	-0.68015500	-0.92694000
H	-9.15560600	-0.89100800	-0.36226000
H	-8.34337800	0.29178000	-1.42349500
H	-8.09106100	-1.46511800	-1.67477400
C	-1.13857200	2.16267800	0.28874300
C	-2.16527200	3.10678600	-0.38928900
C	-1.45719200	1.99726200	1.80669500

H	-0.16090400	2.65883500	0.25287800
C	-2.68965600	4.17565800	0.59831300
H	-3.01068700	2.54490600	-0.79516400
H	-1.66985500	3.59702200	-1.23538100
C	-1.24326000	3.35331500	2.51835600
H	-2.49666600	1.67464000	1.91677600
H	-0.82990300	1.22483000	2.25821200
C	-1.61822200	4.56209800	1.62692900
H	-3.57291700	3.79238800	1.12517600
H	-3.02447400	5.05354500	0.03602400
H	-0.19830000	3.43650800	2.83537600
H	-1.84826400	3.35393900	3.43210400
H	-0.72940400	4.92640700	1.09669000
H	-1.96503400	5.39419800	2.24822100

TS22a

SCF done: -1178.735162

C	-1.34437600	-1.50923200	-0.99106600
C	-2.17587700	0.61544700	0.44959800
C	-3.52584600	0.62800900	0.02540600
C	-1.77853800	1.62213800	1.37211600
C	-4.40306400	1.60472200	0.44940000
H	-3.87466500	-0.10771700	-0.68013300
C	-2.65338600	2.59949700	1.81396700
H	-0.75469500	1.63758700	1.73233900
C	-3.98074900	2.60903400	1.34517400
H	-5.42571700	1.63355600	0.08924800
H	-2.29763600	3.35524400	2.50331100
C	-0.88587800	-1.02072700	-2.35983400
H	-1.56114000	-0.22361900	-2.69488600
H	0.12212400	-0.61096900	-2.32697400
H	-0.91027700	-1.83152100	-3.09142300

C	-1.16435800	-0.39716500	0.07908000
H	-1.27089000	-1.03068400	1.31501500
O	0.11344900	0.08560000	0.11696700
Fe	0.90172900	1.95264800	-0.69317500
Br	-0.74487900	3.29401400	-1.83253800
Br	3.82703700	-1.08965400	-0.66649200
Br	2.63981100	1.05325700	-2.43056700
Fe	1.77863300	-0.71488200	0.86675400
Br	2.25384500	1.96692800	1.45237200
Br	1.85261600	-1.84633600	3.09623200
Br	0.22907200	-2.88867800	-0.38626700
O	-1.25348800	-1.50968000	2.50130000
H	-0.31737000	-1.79657800	2.72947500
H	-1.45597600	-0.77290800	3.10176400
O	-4.91192500	3.51404400	1.69118000
C	-4.54376900	4.60654800	2.53697500
H	-5.44150000	5.21594300	2.63659600
H	-4.23081600	4.25337600	3.52582800
H	-3.74347100	5.20122200	2.08416100
C	-2.58095900	-2.45763700	-1.06889900
C	-3.23134600	-2.85433700	0.27897100
C	-3.68596500	-2.12601600	-2.11112000
H	-2.13657000	-3.36952200	-1.48038100
C	-4.58537300	-3.57756800	0.07059100
H	-3.39648000	-1.97515000	0.90850300
H	-2.54055300	-3.50268400	0.82698700
C	-4.44395300	-3.43110700	-2.46124100
H	-4.40772900	-1.40392500	-1.71898200
H	-3.27407600	-1.68797500	-3.02242000
C	-4.60316000	-4.37276000	-1.24080300
H	-5.40056400	-2.84260300	0.05191900
H	-4.78631700	-4.23176700	0.92524900

H	-3.91556000	-3.95633300	-3.26524500
H	-5.42783400	-3.16341300	-2.86234500
H	-3.78925800	-5.10835000	-1.22354000
H	-5.52969300	-4.94947900	-1.32850900

IM20a

SCF done: -1178.794842

C	-1.66640600	1.03712100	0.64704200
C	-1.67827800	-0.38909300	-1.49823100
C	-2.53216800	0.42417900	-2.28149300
C	-1.33607000	-1.66527900	-1.99379800
C	-3.02409700	-0.02029300	-3.49187200
H	-2.77088600	1.42820000	-1.95199800
C	-1.84787600	-2.13341500	-3.19462000
H	-0.69225900	-2.30855000	-1.40503500
C	-2.69449900	-1.30954400	-3.95869900
H	-3.65783700	0.60590100	-4.11010400
H	-1.59028500	-3.13102900	-3.52791200
C	-0.73877000	1.81031500	1.52882500
H	-0.57168700	1.24620500	2.45966500
H	0.23593300	1.98696500	1.07201900
H	-1.18782000	2.76580900	1.81416700
C	-1.08220600	0.08206500	-0.25562300
H	4.94537900	3.34658200	-0.66407600
O	0.09731900	-0.38899300	0.07177400
Fe	0.56236100	-1.73589600	1.71445500
Br	0.97974800	-3.83198700	0.42318000
Br	5.23479200	4.61877300	-0.02175000
Br	-0.95699500	-1.43763900	3.57291700
Fe	2.02410100	0.07130500	-0.67436100
Br	2.82370800	-0.32430500	1.71269600
Br	4.25756900	0.98045100	-1.84870000

Br	1.41743300	2.13430800	-2.10913300
O	2.18659300	-1.70200000	-1.72758400
H	3.07726400	-1.87979400	-2.06351400
H	1.89871700	-2.48525300	-1.19531300
O	-3.23685900	-1.65583900	-5.14128200
C	-2.94145100	-2.93921700	-5.69370800
H	-3.48125900	-2.98391500	-6.63936200
H	-1.86774500	-3.05268700	-5.87972900
H	-3.28911400	-3.74366600	-5.03604300
C	-3.13515800	1.21147500	0.94085900
C	-3.69139600	2.59670700	0.44371300
C	-4.10195900	0.06701100	0.58077100
H	-3.14692300	1.26929200	2.04039700
C	-5.23257300	2.58372900	0.35341500
H	-3.26414100	2.86369700	-0.52882400
H	-3.36533500	3.37541000	1.14125100
C	-5.43223500	0.24937400	1.34797600
H	-4.29665400	0.04957300	-0.49444600
H	-3.65554900	-0.89965300	0.83419200
C	-5.84852000	1.73788700	1.47500300
H	-5.54535700	2.18052500	-0.61787900
H	-5.60285100	3.61412600	0.39115500
H	-5.34355100	-0.19358800	2.34602700
H	-6.21359200	-0.31582200	0.82810800
H	-5.52043900	2.14020700	2.44209100
H	-6.93957700	1.82820500	1.46584200

TS23a

SCF done: -1102.285818

C	-1.52874500	-1.41684700	-1.31841900
C	-2.08905300	0.85040600	-0.12694600
C	-3.29773700	1.16881000	-0.79246800

C	-1.72064700	1.62174100	1.00097500	O	-4.57957100	3.91669800	1.14985900
C	-4.09601600	2.20204800	-0.35239800	C	-4.26062400	4.74870000	2.26950000
H	-3.57470300	0.63797800	-1.69384400	H	-5.07763800	5.46580300	2.34296800
C	-2.53629600	2.63408400	1.47487300	H	-4.20315300	4.16218200	3.19273700
H	-0.81166400	1.37905900	1.53964000	H	-3.31725200	5.28027200	2.10731500
C	-3.72770700	2.94331600	0.79268000	C	-2.84028500	-2.18780300	-1.24619900
H	-5.00563200	2.47824300	-0.87389400	C	-3.61653000	-2.14491200	0.09744100
H	-2.24106800	3.17834100	2.36290300	C	-3.80803100	-1.95188300	-2.44945400
C	-0.62828400	-1.74421100	-2.48965100	H	-2.51173600	-3.22860400	-1.39046700
H	-0.91778500	-1.12899200	-3.35461600	C	-5.08612900	-2.59385500	-0.07086900
H	0.41738300	-1.51433200	-2.27854000	H	-3.59179600	-1.14596300	0.53586300
H	-0.72163500	-2.79260800	-2.78378800	H	-3.10767200	-2.80540100	0.80858600
C	-1.16332800	-0.16218300	-0.60423800	C	-4.81567600	-3.12058000	-2.54398600
H	-0.75497400	-2.36080900	-0.24616800	H	-4.34989000	-1.01371300	-2.30123900
O	0.08953200	0.01680000	-0.39374400	H	-3.25337000	-1.85432800	-3.38714200
Fe	1.44119700	1.66252200	-0.81893100	C	-5.22352200	-3.67032000	-1.15460600
Br	0.27748000	3.59488500	-1.63681400	H	-5.71143900	-1.73188200	-0.33714800
Br	3.33522500	-1.80488500	-0.34768700	H	-5.46579800	-2.95895900	0.88876500
Br	3.04865600	0.40704900	-2.39106700	H	-4.38705400	-3.92701300	-3.14986000
Fe	1.47664100	-0.95451000	1.24061300	H	-5.70100600	-2.76571400	-3.08383800
Br	2.54807300	1.31570600	1.47431000	H	-4.58928100	-4.52585700	-0.88891600
Br	0.30732100	-0.78766200	3.36730100	H	-6.24817100	-4.05428700	-1.18949400
Br	0.13506000	-3.23105800	0.71253200				

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

TS5b

SCF done: -934.3023133

C	1.60476000	0.98481300	0.64457900	H	0.83274300	-0.08105200	2.34129200
C	1.42358700	0.80495100	2.11824400	H	2.36502800	0.80266500	2.67289800
H	0.85143800	1.67788700	2.46169300	C	0.81153000	0.15621400	-0.26591100
				O	-0.27552500	-0.46468400	0.22526400
				Fe	-2.00847400	-0.25267900	-0.52810800

Br	-1.91884900	1.45153700	-2.30533700
Br	-3.31574200	-2.49476400	-0.78354300
Br	-3.86751100	-0.28345500	1.30458900
H	0.71765600	0.55225000	-1.28215200
C	2.13782800	-0.75418800	-0.23660500
C	3.20462900	-0.57166500	-1.14377500
C	2.10991300	-1.91376100	0.55871600
C	4.19491500	-1.52510400	-1.26311600
H	3.24708800	0.32180300	-1.75869000
C	3.10439000	-2.87579500	0.45095500
H	1.25716900	-2.08252100	1.20628400
C	4.15838200	-2.68606800	-0.46173500
H	5.01112400	-1.40981100	-1.96785400
H	3.04238900	-3.77462200	1.05202900
O	5.17178100	-3.55282600	-0.65019200
C	5.20087400	-4.76383400	0.10557900
H	6.09609800	-5.29306400	-0.22029200
H	5.26772200	-4.55978500	1.18011200
H	4.31787300	-5.37944400	-0.09856500
C	2.40015300	2.11488400	0.14958800
C	3.58820400	2.51482500	0.79621700
C	1.92869600	2.87293400	-0.94429100
C	4.29498100	3.62451600	0.34985800
H	3.97022100	1.93630600	1.63105900
C	2.63303900	3.99723800	-1.37225800
H	0.98899200	2.61611200	-1.42414600
C	3.81728400	4.36957800	-0.73467300
H	5.21672500	3.91371600	0.84511500
H	2.24939300	4.58387000	-2.20091400
H	4.36645100	5.24210400	-1.07588500

IM6b

SCF done: -1098.665795

C	-0.56790000	-1.74436200	-0.27235200
C	0.37898300	-2.81477500	-0.81113200
H	1.37610500	-2.41293200	-0.99065600
H	0.45791800	-3.65544600	-0.11998300
H	-0.00216800	-3.18351600	-1.77039500
C	-0.61729300	-0.52660900	-1.26007800
O	0.63017800	0.07727000	-1.42367100
Fe	2.06175900	0.38867900	-0.39506800
Br	4.08675000	-0.85936200	-0.82981200
Br	2.93694600	2.19253400	0.91414700
Br	0.44747900	-1.01955600	1.46461000
H	-0.88906300	-1.01626500	-2.21136600
C	-1.65978400	0.55681100	-1.02328600
C	-2.88367500	0.50710200	-1.71382600
C	-1.42024400	1.64777600	-0.17683900
C	-3.85357500	1.47841100	-1.52597200
H	-3.08239000	-0.31537200	-2.39553500
C	-2.38402600	2.63387000	0.02329400
H	-0.47142100	1.74059300	0.33933200
C	-3.61232200	2.55225900	-0.64998800
H	-4.80460500	1.43714700	-2.04610000
H	-2.16500900	3.45991200	0.68886100
O	-4.61820000	3.45422100	-0.53372600
C	-4.43319200	4.57671400	0.32177800
H	-5.35556100	5.15485200	0.25884100
H	-4.26935800	4.26598100	1.36069400
H	-3.59177400	5.19757800	-0.00812600
C	-1.92499300	-2.26069900	0.15507700
C	-2.40372400	-3.48087500	-0.35209700
C	-2.76321800	-1.53107400	1.01761000

C	-3.67601100	-3.94862800	-0.01790800
H	-1.79124200	-4.07938600	-1.01550000
C	-4.02704600	-2.00348500	1.35824200
H	-2.41506400	-0.59639800	1.43983800
C	-4.49226400	-3.21404500	0.83949000
H	-4.02058600	-4.89408600	-0.42618400
H	-4.64854400	-1.42483500	2.03495800
H	-5.47818900	-3.58229600	1.10715700

TS6b

SCF done: -934.298136

C	-1.61176400	-1.84070900	-0.80549300
C	-0.76917200	-3.06677500	-0.78419600
H	-0.26793100	-3.09291500	0.19764700
H	-1.33348300	-3.98361800	-0.94753700
H	0.04260200	-2.96834500	-1.50840700
C	-0.90906400	-0.59964700	-1.14597700
O	0.41565600	-0.65171400	-1.29661500
Fe	1.74816900	-0.41727100	0.05919100
Br	4.11023000	-1.03219400	-0.82375000
Br	3.11658600	1.78562400	-0.03503900
Br	0.88500500	-1.30813200	2.18967900
H	-1.41051900	-0.95504000	-2.17401100
C	-1.47839700	0.75749800	-0.80143300
C	-1.49249600	1.77479500	-1.76878700
C	-1.87292900	1.05698500	0.50522900
C	-1.92043200	3.05315800	-1.44355900
H	-1.15279400	1.56410300	-2.77924500
C	-2.29337100	2.34352600	0.84660600
H	-1.82812700	0.29282700	1.27483900
C	-2.32379000	3.34775200	-0.13002100
H	-1.93806400	3.84767300	-2.18180100

H	-2.57854500	2.55019800	1.87089000
O	-2.72098300	4.62823200	0.08964300
C	-3.07497000	5.01085200	1.41261400
H	-3.32821100	6.07032800	1.35982300
H	-3.94476900	4.44918100	1.77602400
H	-2.23841200	4.87205400	2.10808600
C	-3.05765300	-1.94013300	-0.59556200
C	-3.99177900	-1.02959400	-1.13905200
C	-3.53748400	-2.99057400	0.21738200
C	-5.34793200	-1.17242800	-0.87925100
H	-3.65696300	-0.22770700	-1.78592800
C	-4.89504700	-3.10232400	0.50541500
H	-2.84282700	-3.69335800	0.66256800
C	-5.80475300	-2.20134300	-0.04831200
H	-6.05319900	-0.47841700	-1.32528500
H	-5.24035400	-3.90028700	1.15487000
H	-6.86572300	-2.30140500	0.15950300

TS7b

SCF done: -934.2980945

C	-1.29405400	0.88807300	-0.88198300
C	-2.53839100	0.14835700	-0.62321900
C	-2.54208800	-0.94069800	0.26803400
C	-3.73341200	0.44392900	-1.31714900
C	-3.68638600	-1.70946700	0.46756500
H	-1.62841800	-1.23216300	0.77615500
C	-4.87827200	-0.30184100	-1.11505900
H	-3.76676200	1.28412100	-2.00351000
C	-4.86567100	-1.39138800	-0.22054600
H	-3.64123300	-2.55615800	1.14119400
H	-5.80174200	-0.07341900	-1.63615200
C	-1.20067000	2.50722000	0.18608900

C	-0.52598000	3.62536300	-0.32642300
C	-2.29973100	2.67332500	1.04158300
C	-0.96200800	4.90393200	0.00947100
H	0.36751200	3.48383800	-0.92326200
C	-2.71749400	3.95494500	1.38743500
H	-2.82821900	1.80632600	1.42424200
C	-2.05722200	5.07057700	0.86252700
H	-0.43498100	5.77035800	-0.37778200
H	-3.56028500	4.08464100	2.05920700
H	-2.39060300	6.06979800	1.12637100
C	-0.91561100	1.18652000	-2.30548600
H	0.00515900	1.76290500	-2.36734200
H	-0.73076800	0.21621600	-2.78263500
H	-1.71522500	1.68242800	-2.86008600
C	-0.29746100	1.03992800	0.15128800
H	-0.52727200	0.58651000	1.12035600
O	0.97381700	1.23203600	-0.13894200
Fe	2.40102900	-0.03600600	-0.00140200
Br	4.72757900	0.54999400	-0.15061700
Br	1.45025300	-1.75227600	1.80459700
Br	1.44245000	-2.17800000	-1.24803900
O	-6.03184000	-2.06334900	-0.10386900
C	-6.09149900	-3.18985700	0.76852600
H	-5.88214100	-2.90281500	1.80557300
H	-7.11155700	-3.56722700	0.69588500
H	-5.39022900	-3.97237300	0.45687200

4b

SCF done: -934.3085039

C	-1.16002100	0.94546000	-1.01094900
C	-2.34945600	0.21681200	-0.75370900
C	-2.53167600	-0.48432300	0.47684800

C	-3.38970100	0.09778200	-1.73016400
C	-3.65776100	-1.24407000	0.72159900
H	-1.73844500	-0.49681200	1.21437000
C	-4.52363400	-0.63365400	-1.48447800
H	-3.30422400	0.61949900	-2.67541000
C	-4.67132600	-1.32250500	-0.25531600
H	-3.73520700	-1.79441900	1.65066800
H	-5.32217500	-0.70946000	-2.21406100
C	-0.62349600	2.88096600	0.29130900
C	0.25648500	3.88334000	-0.13175400
C	-1.83583500	3.23282400	0.90010700
C	-0.07001500	5.22514900	0.06790300
H	1.20264100	3.58962900	-0.57267800
C	-2.15927200	4.57498900	1.09642000
H	-2.52432400	2.45986000	1.23252300
C	-1.27811300	5.57434300	0.67628800
H	0.62483800	5.99913800	-0.24506200
H	-3.09568800	4.84037700	1.57860200
H	-1.52932700	6.61991600	0.82886100
C	-0.72271800	1.28509800	-2.39104200
H	-0.00781100	2.10664100	-2.38472600
H	-0.18671900	0.40214900	-2.76905700
H	-1.54446500	1.48825200	-3.07924500
C	-0.21989400	1.39638700	0.08730700
H	-0.43688700	0.87336600	1.02755800
O	1.08966800	1.25497500	-0.29654500
Fe	2.24106300	-0.20520100	-0.03456400
Br	4.64611000	-0.16679700	-0.20426700
Br	1.00166200	-1.62599900	1.89986300
Br	0.89979200	-2.28520800	-1.10268400
O	-5.79871700	-2.02432400	-0.12372000
C	-6.03432100	-2.77433700	1.07605100

H	-6.07201800	-2.11397400	1.94811800
H	-7.00286500	-3.25175600	0.93405600
H	-5.26276200	-3.53779800	1.21582300

TS8b

SCF done: -934.2964041

C	-1.50651600	-0.65461200	-0.90505600
C	-2.89566700	-0.61692500	-0.45174500
C	-3.34618000	0.16898600	0.64029800
C	-3.85871400	-1.38530800	-1.13752400
C	-4.67357100	0.17840300	1.01311500
H	-2.64002400	0.74859700	1.22197400
C	-5.20620900	-1.35178700	-0.79443000
H	-3.56502700	-1.99197000	-1.98625500
C	-5.62477600	-0.57260400	0.29346200
H	-5.01091100	0.75652300	1.86638900
H	-5.91313900	-1.93734100	-1.36881100
C	-0.90271500	1.80454800	-0.30826400
C	-1.75876300	2.52265800	-1.15237000
C	-0.30785200	2.44632500	0.78496900
C	-2.02356500	3.86830800	-0.89827600
H	-2.21297300	2.03118500	-2.00776200
C	-0.58260000	3.78976900	1.04126900

H	0.37087000	1.89786900	1.43204700
C	-1.44005800	4.50227000	0.20059700
H	-2.68180200	4.42196000	-1.56125500
H	-0.11933600	4.27965400	1.89215900
H	-1.64774100	5.54983800	0.39730000
C	-0.97194100	-1.85510200	-1.62102700
H	-0.74025400	-1.57513800	-2.65701600
H	-0.01075300	-2.14629300	-1.18753300
H	-1.64885800	-2.70652800	-1.59369000
C	-0.52245600	0.38240400	-0.65427200
H	-0.60111100	-0.31510700	0.35620300
O	0.68750100	0.23362200	-1.18685900
Fe	2.39453000	0.02839800	-0.35329300
Br	4.22887500	1.57025700	-0.27231700
Br	1.41741600	-1.15839200	1.87674500
Br	2.91365400	-2.56892700	-0.41807700
O	-6.89627000	-0.48111100	0.73346600
C	-7.91242700	-1.23204500	0.07179600
H	-8.83864000	-1.00627700	0.60004600
H	-8.00936500	-0.93176200	-0.97796500
H	-7.71259300	-2.30816700	0.12939800

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

TS9b

SCF done: -1010.769433

C	-0.88753600	-0.25350400	-0.87128400
C	-2.26152300	-0.68508000	-0.45653900
C	-2.56578400	-0.97999700	0.89083000

C	-3.29923600	-0.79993600	-1.39100600
C	-3.84246500	-1.34401900	1.27952800
H	-1.78610800	-0.94394700	1.64331100
C	-4.59418400	-1.16162000	-1.01393900
H	-3.11817500	-0.59094500	-2.43847300

C	-4.87543000	-1.43597200	0.32858600
H	-4.06897400	-1.57796800	2.31434100
H	-5.36518400	-1.22671200	-1.77197400
C	-0.65309900	-0.11236600	-2.37427500
H	-1.25618900	0.72304600	-2.74836800
H	0.39464300	0.11172500	-2.57594800
H	-0.92873300	-1.02143700	-2.91087500
C	-0.26554400	0.97473300	-0.14499300
H	-0.31178900	0.80646900	1.26785900
O	1.04337900	1.10386300	-0.26248900
Fe	2.54781300	-0.12229000	-0.07270400
Br	0.42805000	-1.90863200	-0.31920600
Br	4.28878200	-0.61444000	-1.64544900
Br	2.86987500	-0.05732500	2.46538200
O	-0.15055300	0.73460100	2.48417000
H	-0.17963200	1.64560800	2.82240500
H	0.81189700	0.41730100	2.60368800
O	-6.08994000	-1.79774300	0.81084700
C	-7.17094000	-1.93727700	-0.10362200
H	-6.96282700	-2.70774500	-0.85583300
H	-8.03112400	-2.23970000	0.49436000
H	-7.39540600	-0.98923200	-0.60783500
C	-0.97189800	4.64336800	-0.82464700
C	-0.33671600	3.40795900	-0.73436500
C	-1.02864800	2.27688400	-0.25681100
C	-2.36798500	2.43001200	0.15168400
C	-2.99567900	3.67192700	0.06223900
C	-2.30472400	4.78167800	-0.42798800
H	-0.42534100	5.49984300	-1.20852700
H	0.69773900	3.29591400	-1.03735400
H	-2.92005700	1.58682800	0.54753200
H	-4.02863900	3.77152600	0.38272600

H	-2.79870200	5.74636600	-0.49676800
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IM7b

SCF done: -1010.822681

C	1.86042600	-0.31986600	0.59277200
C	3.28990100	-0.43772000	0.40736000
C	3.95238600	0.13241100	-0.71919300
C	4.09060800	-1.19531200	1.29875600
C	5.30362700	-0.04072800	-0.92734000
H	3.37649400	0.68179000	-1.45394000
C	5.45621100	-1.35473400	1.11169600
H	3.64121200	-1.63652900	2.18104200
C	6.07760200	-0.78064500	-0.01039700
H	5.79532900	0.37274900	-1.80126200
H	6.02788200	-1.92240100	1.83565500
C	1.08196300	-1.43490800	1.23130000
H	0.26677900	-1.06372700	1.86044800
H	0.63180000	-2.06465400	0.44644200
H	1.71017100	-2.09784000	1.82624600
C	1.08549900	0.78321800	0.07662800
H	-4.71769400	0.35171200	1.01368000
O	-0.16027100	0.63408100	-0.14894900
Fe	-1.65818500	-0.62900000	-0.27055100
Br	-1.44827800	-2.65895100	-1.67019500
Br	-2.96002700	-0.68160100	1.88691100
Br	-5.70360500	1.06995100	0.12532900
O	-2.89570400	0.37707100	-1.69594700
H	-3.05472500	-0.27246200	-2.39867800
H	-3.76991400	0.67161600	-1.37462000
O	7.39142900	-0.88283700	-0.30052600
C	8.23489600	-1.63928200	0.56564000
H	9.23214600	-1.58533000	0.12900800

H	8.25574300	-1.21174600	1.57476500
H	7.91556000	-2.68645300	0.61717600
C	1.00540500	2.96219900	-1.11554300
C	1.62328300	2.14949000	-0.14756100
C	2.65438000	2.68862600	0.64325000
C	3.06736300	4.00513900	0.45508000
C	2.46696200	4.79516600	-0.52840600
C	1.43595400	4.27070800	-1.31331400
H	0.19178700	2.55133200	-1.70328800
H	3.11317300	2.08542300	1.41834700
H	3.85327800	4.41733700	1.08057000
H	2.79520000	5.81976700	-0.67670700
H	0.96301800	4.88539600	-2.07309800

IM8b

SCF done: -934.3399199

C	1.79513700	-0.55557100	1.07072300
C	3.12307300	-0.36764100	0.53471900
C	3.35127000	0.37310900	-0.66326600
C	4.25553300	-0.98465700	1.12534800
C	4.60866800	0.48820700	-1.21360000
H	2.51200700	0.82271000	-1.17953600
C	5.52920100	-0.85530500	0.59218900
H	4.14315000	-1.54684200	2.04513800
C	5.71859800	-0.11861200	-0.59029100
H	4.76920800	1.02965500	-2.13955100
H	6.36520900	-1.32585700	1.09503800
C	1.43752300	-1.82341100	1.79541200
H	0.66524400	-1.65238100	2.54897200
H	1.03580900	-2.55199600	1.07553500
H	2.30156600	-2.29122000	2.26836600
C	0.70995100	0.36479100	0.83537100

H	-4.24876700	0.99768900	-0.29232400
O	-0.49266700	-0.07236200	0.89103000
Fe	-1.79217600	-1.36375300	0.26716200
Br	-0.90964100	-3.03442200	-1.22044200
Br	-4.06407100	-1.05301700	1.06010400
Br	-4.11977800	2.19757400	-1.13485800
O	6.90555800	0.05987600	-1.20385600
C	8.07051300	-0.55159900	-0.65225400
H	8.88985800	-0.28139400	-1.31820700
H	8.27930700	-0.17278900	0.35484400
H	7.96925900	-1.64231200	-0.62158600
C	-0.13023000	2.52965400	-0.05219500
C	0.87597500	1.82207500	0.63238700
C	1.95491500	2.53486800	1.19191900
C	2.03159900	3.91700500	1.04971100
C	1.04075800	4.60602900	0.34441000
C	-0.03937700	3.90956000	-0.20494500
H	-0.97842800	1.99419200	-0.46307800
H	2.71600700	2.00879400	1.75665700
H	2.85962700	4.45901000	1.49627000
H	1.10557800	5.68433900	0.23204900
H	-0.81767200	4.44013500	-0.74417500

TS10b

SCF done: -934.3277818

C	1.08206600	-0.33850300	0.96297600
C	2.42856100	-0.51057500	0.45923600
C	2.86659700	0.13977800	-0.73411600
C	3.33523500	-1.41852100	1.06554700
C	4.12022900	-0.08101000	-1.25546800
H	2.19188600	0.80960300	-1.25568400
C	4.60400600	-1.64078500	0.55291600

H	3.04403500	-1.94264700	1.96832300
C	5.01094400	-0.97263900	-0.61689200
H	4.44630100	0.40759000	-2.16715500
H	5.26899100	-2.32935900	1.05968800
C	0.58696300	-1.15901300	2.14289200
H	1.04889300	-0.80587500	3.07523700
H	-0.49544700	-1.07101800	2.25594300
H	0.82649900	-2.21882400	2.02662100
C	0.30561600	0.92594700	0.73317600
H	0.34958500	-1.17633200	-0.19161400
O	-0.93200400	0.87145500	0.61028100
Fe	-2.58081000	-0.26661300	-0.07914700
Br	-3.45801700	-1.51799200	1.79892500
Br	-3.49162400	1.10265800	-1.84826800
Br	-0.60316800	-1.94451500	-1.21725700
O	6.21288700	-1.11690800	-1.20609000
C	7.16151800	-2.02366300	-0.64355600
H	8.03669000	-1.97403700	-1.29095800
H	7.44151900	-1.72438100	0.37274800
H	6.77180600	-3.04753100	-0.63298200
C	0.94084400	2.26698400	0.70929900
C	2.16958400	2.53602200	1.33920600
C	2.67658000	3.83265900	1.35495900
C	1.97379200	4.86646400	0.73046300
C	0.75083300	4.60768200	0.10337700
C	0.22678000	3.31940500	0.10364500
H	2.71642600	1.73993900	1.83182600
H	3.61770800	4.03807900	1.85557700
H	2.37664300	5.87509800	0.73707400
H	0.20435200	5.41168600	-0.37953300
H	-0.72868000	3.10505200	-0.36371100

TS11b

SCF done: -1175.129322

C	-1.79233200	-0.25024700	-0.81316200
C	-1.51603400	1.53413300	1.14064200
C	-2.74002200	2.19443100	0.89350700
C	-0.69696600	2.01024600	2.19714200
C	-3.10247200	3.30507700	1.64822000
H	-3.39065000	1.86054300	0.09784000
C	-1.07638100	3.10857900	2.95551200
H	0.24741100	1.51480200	2.40306200
C	-2.28222300	3.76393100	2.68319500
H	-4.03156700	3.81957600	1.42371200
H	-0.42861000	3.46198600	3.75141000
C	-1.29760400	0.42298600	-2.09079100
H	-1.62237500	1.47068600	-2.09408000
H	-0.21024000	0.40786500	-2.14044800
H	-1.68586400	-0.07724400	-2.97854500
C	-1.03423500	0.32299700	0.41220600
H	-1.27181300	-0.50293200	1.45154500
O	0.31356400	0.22978100	0.31640200
Fe	1.83477000	1.75773000	-0.14058900
Br	0.90073600	3.93428100	-0.54373100
Br	2.99619900	-2.06860500	-1.56201000
Br	2.76485100	0.82135100	-2.39532400
Fe	1.48869100	-1.41446600	0.43872500
Br	3.17830900	0.47347400	1.57292500
Br	1.24474700	-3.10564200	2.25109600
Br	-0.96233500	-2.26844900	-0.95253300
O	-1.34730600	-1.26674400	2.53602500
H	-0.63446700	-1.97123500	2.48975900
H	-1.12012900	-0.69954700	3.29167700
H	-2.57848000	4.62697100	3.27132600

C	-3.27489400	-0.43488000	-0.69541500
C	-3.86888000	-1.03980800	0.43500100
C	-4.13435300	-0.01203400	-1.72198100
C	-5.23968400	-1.18693900	0.53868300
H	-3.25242700	-1.42235200	1.23918400
C	-5.51972800	-0.14915900	-1.62910100
H	-3.73494500	0.45097900	-2.61578500
C	-6.08513400	-0.73869400	-0.49243500
H	-5.68807200	-1.65696600	1.40744400
H	-6.13918700	0.20094800	-2.44563600
O	-7.41096100	-0.92427100	-0.29142300
C	-8.32009400	-0.51572000	-1.30851600
H	-8.13802200	-1.05254600	-2.24706800
H	-9.31433100	-0.76461800	-0.93685500
H	-8.26008700	0.56437600	-1.48914600

IM9b

SCF done: -1175.190836

C	2.02178600	-0.33783300	-1.15971200
C	1.79603100	1.57875900	0.53598800
C	2.79493300	2.41776000	-0.00359000
C	1.23076900	1.90283200	1.78740600
C	3.22189400	3.53912300	0.69772400
H	3.20385500	2.20610100	-0.98456600
C	1.67852500	3.01566100	2.49104400
H	0.47433800	1.25744600	2.21920000
C	2.67123400	3.83656500	1.94841400
H	3.97600400	4.18948600	0.26575900
H	1.25187900	3.24232500	3.46268900
C	1.22868800	-1.04286300	-2.22367400
H	0.66076300	-1.86967000	-1.77406100
H	0.49514700	-0.37354400	-2.68327600

H	1.86274000	-1.47519000	-2.99685200
C	1.27321200	0.43070400	-0.21614700
H	-3.42276100	-2.92231100	-1.04084300
O	0.00322300	0.12764600	-0.05608500
Fe	-0.58421000	-1.65299700	1.16500900
Br	1.24077200	-1.86171800	2.75463100
Br	-4.71623800	-2.37598700	-1.54017000
Br	-1.28489000	-3.45044800	-0.39687100
Fe	-1.65340500	1.26980500	-0.18140000
Br	-2.58604000	-0.13079600	1.84320800
Br	-0.82025300	2.80652300	-2.25658200
Br	-2.08568900	3.75806200	0.38086100
O	-3.20675100	0.66093500	-1.40954600
H	-3.76735200	-0.12858000	-1.27495400
H	-3.19197700	0.88218800	-2.35026700
H	3.01047000	4.71106500	2.49555600
C	3.44809600	-0.51487400	-1.05880600
C	4.24034700	-0.80517500	-2.20121900
C	4.11391300	-0.49432400	0.20527200
C	5.60468700	-1.02213700	-2.11115100
H	3.78204900	-0.81570800	-3.18359800
C	5.46462200	-0.73735900	0.30612600
H	3.53485300	-0.35430700	1.11005800
C	6.23205100	-0.99588100	-0.84986500
H	6.17466100	-1.21144900	-3.01235900
H	5.96062700	-0.75876100	1.27025100
O	7.54276500	-1.21217700	-0.64368100
C	8.38578200	-1.52319100	-1.75388800
H	8.40969200	-0.69962300	-2.47616800
H	9.38136900	-1.66848300	-1.33545000
H	8.06015900	-2.44310700	-2.25167000

IM10b

SCF done: -1098.674016

C	1.99957100	0.01911000	-1.06866600
C	1.29397300	1.51870600	0.89883900
C	2.11452100	2.62677700	0.59856200
C	0.59734100	1.49448900	2.12616700
C	2.24093700	3.67196700	1.50653400
H	2.61737000	2.68137500	-0.35962700
C	0.74331800	2.53653800	3.03580900
H	-0.02763400	0.64355700	2.37458100
C	1.56204900	3.62743200	2.72796600
H	2.85760300	4.52966500	1.25700900
H	0.21838300	2.49721000	3.98477100
C	1.42466300	-0.65922400	-2.28077400
H	1.02850200	-1.64463800	-1.99895100
H	0.58287900	-0.09748300	-2.69664400
H	2.17206200	-0.82686300	-3.05538600
C	1.06566000	0.44291100	-0.07639200
H	-2.32268000	-1.98388400	-1.85226800
O	-0.12435400	-0.11845700	-0.08082000
Fe	-0.44065400	-2.17392100	0.77111500
Br	1.47337000	-2.44752600	2.22815400
Br	-3.00680000	-0.67216900	-2.23062900
Br	-1.07496200	-3.58331700	-1.19265600
Fe	-1.96114000	0.71134200	-0.08065900
Br	-2.60887900	-1.10914600	1.71538900
Br	-1.38548800	2.87634400	-1.57360200
Br	-3.53058100	2.61062800	0.59427100
H	1.66470700	4.44487500	3.43529800
C	3.42454900	0.15894000	-0.90708800
C	4.28318600	0.28175500	-2.03161400
C	4.04137700	0.10659000	0.38028100

C	5.65597300	0.39595700	-1.89570700
H	3.85766500	0.33896800	-3.02706000
C	5.40787200	0.18750700	0.52140400
H	3.42871800	-0.06833400	1.25646600
C	6.23470700	0.34668400	-0.61183900
H	6.27033900	0.52162700	-2.77870800
H	5.87766800	0.11166500	1.49585200
O	7.55285400	0.43257300	-0.36474100
C	8.46423200	0.56748300	-1.45672800
H	8.27610100	1.48991200	-2.01722500
H	9.45624600	0.61049000	-1.00805700
H	8.40403600	-0.29422400	-2.13036200

TS12b

SCF done: -1098.689088

C	-1.84234800	0.11012900	-1.15123800
C	-3.27432300	0.04687700	-0.91104200
C	-3.78636900	-0.16901000	0.40460200
C	-4.20784800	0.06240000	-1.97835500
C	-5.13342200	-0.31973400	0.63151000
H	-3.09879100	-0.25065200	1.23986700
C	-5.56864500	-0.07368100	-1.75880500
H	-3.85821900	0.20881100	-2.99382100
C	-6.04693700	-0.26844300	-0.44701900
H	-5.52189700	-0.49958600	1.62783500
H	-6.25141200	-0.03143500	-2.59837400
C	-1.32140200	1.82669100	0.72980600
C	-2.34707000	2.73194000	0.38080900
C	-0.59743900	2.02784300	1.92552800
C	-2.63563000	3.81048300	1.20737900
H	-2.88709700	2.60987600	-0.55053200
C	-0.91415400	3.09243600	2.76013000

H	0.18528400	1.33143400	2.20286400
C	-1.92661900	3.98717200	2.40010300
H	-3.40681400	4.51860500	0.92187800
H	-0.36780800	3.22786000	3.68768100
H	-2.16059300	4.82719400	3.04738700
C	-1.29698800	0.12649000	-2.57733100
H	-1.48441000	1.10022800	-3.04776900
H	-0.21861300	-0.03820700	-2.57106300
H	-1.75871100	-0.65190600	-3.18851900
C	-0.92496400	0.73260800	-0.16134100
H	-1.52458000	-1.31502500	-0.86660000
O	0.28173700	0.31955300	-0.13511600
Fe	2.19353700	1.47676500	-0.33131400
Br	1.62205900	3.71035100	-1.00148800
Br	2.77287700	-2.59946100	-0.82634200
Br	3.11355700	0.01485000	-2.29228300
Fe	1.10096800	-1.52061900	0.84017400
Br	3.02149000	0.27851100	1.71232100
Br	-0.08382500	-1.83580900	2.92456800
Br	-1.02045200	-2.86923200	-0.68203300
O	-7.33901900	-0.42473000	-0.11927100
C	-8.33335300	-0.42888500	-1.14673800
H	-9.28247900	-0.58492400	-0.63510700
H	-8.35626200	0.52916600	-1.67738700
H	-8.16111700	-1.24405600	-1.85757700