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Supporting Information

An Efficient Route to Regioselective Functionalization of Benzo[*b*]thiophenes via Palladium-Catalyzed Decarboxylative Heck Coupling Reactions: Insights from Experiment and Computation

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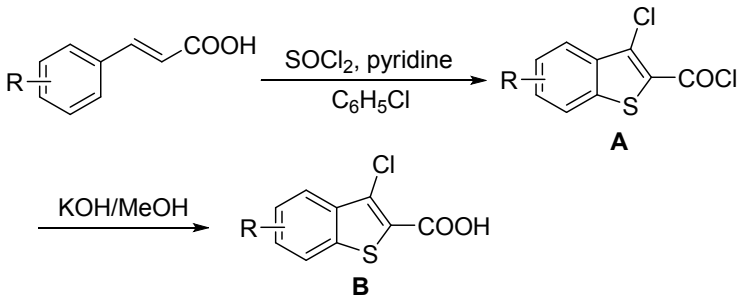
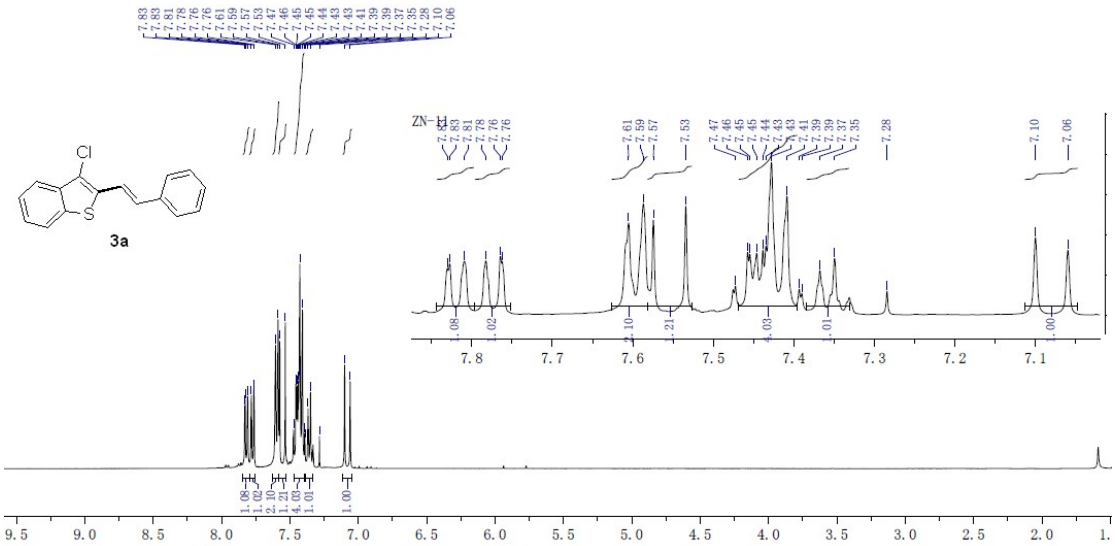
General Procedure for Preparation of 3-chlorobenzo[*b*]thiophene-2-carboxylic acids:[1]



To a solution of chlorobenzene (30 mL) was added cinnamic acid (50 mmol), pyridine (0.4mL, 5 mmol), thionyl chloride (15 mL, 77 mol), the mixture was heated at relux for 3 days. Excess thionyl chloride was removed under reduced pressure and the remaining material was suspended in hot hexane then filtered. The hot filtrate was treated with charcoal, allowed to cool, then the precipitate collected by filtration to give **A**. Hydrolysis of **A** in the presence of KOH and methanol, then acidified the mixture with HCl gave the product **B**.

Reference：

1. Higa,T. *J. Org. Chem.* **1975**, *40*, 3037–3045.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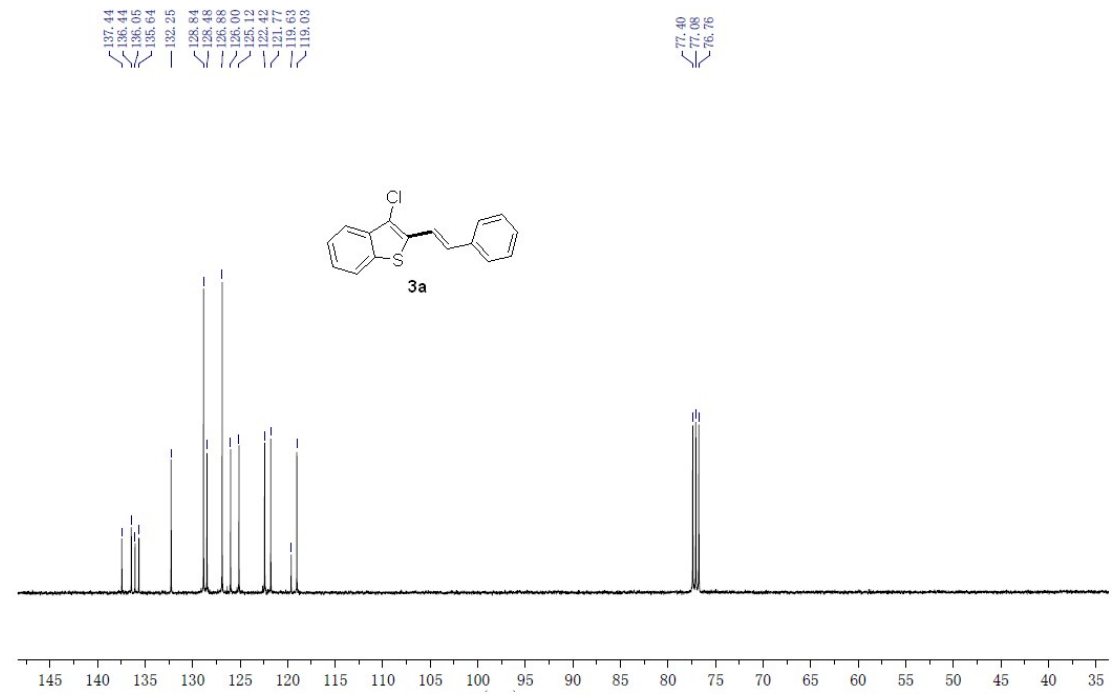
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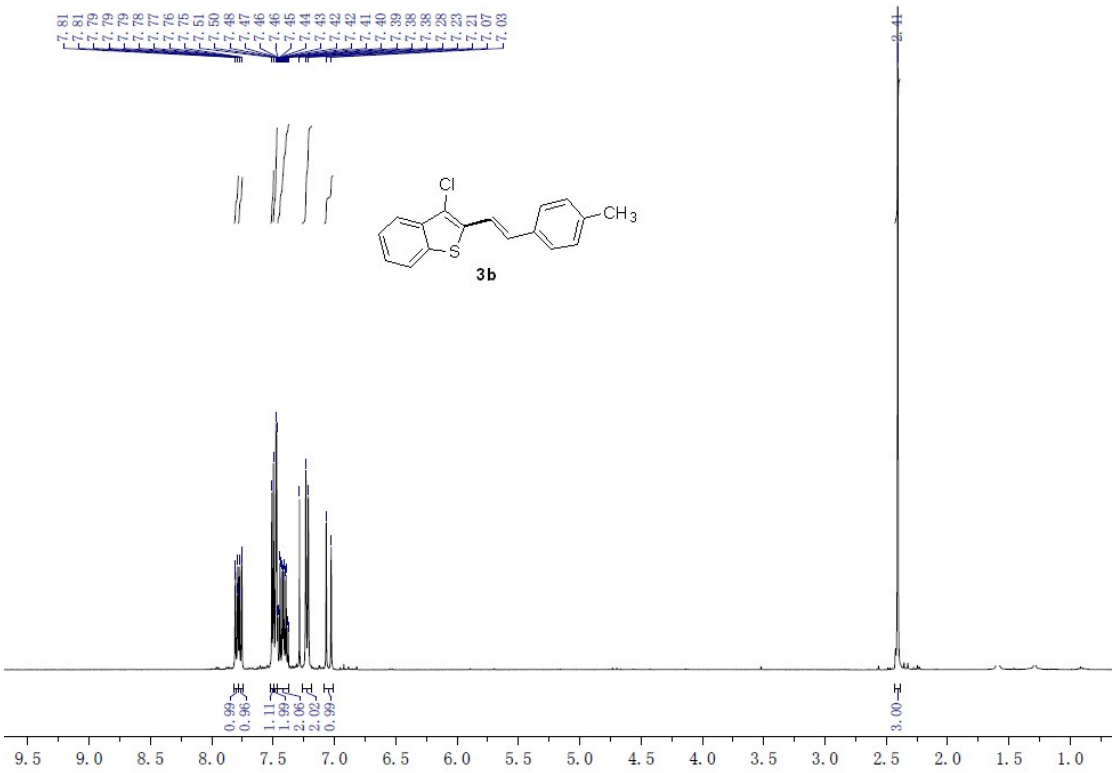
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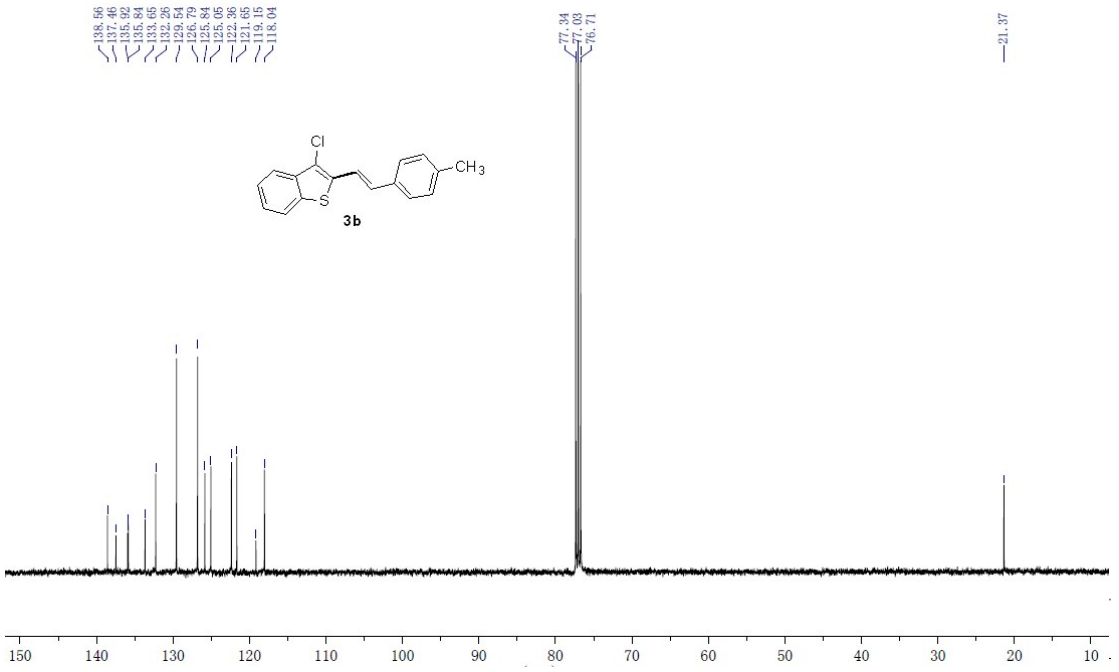
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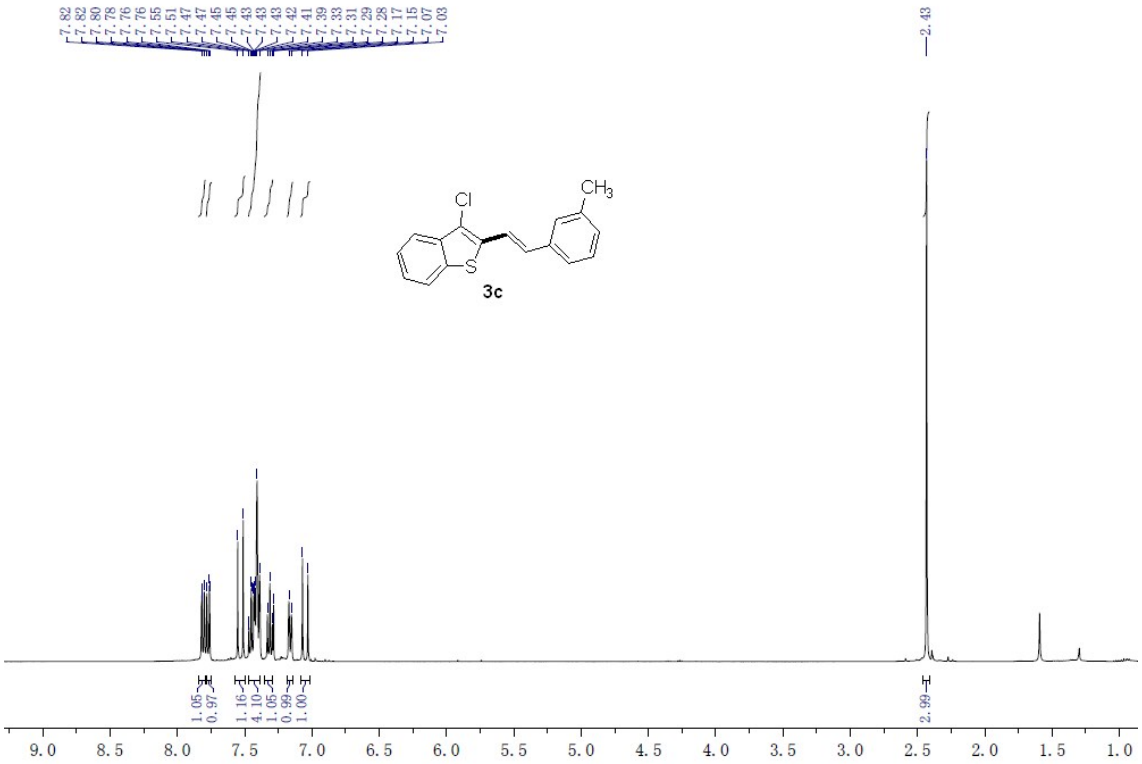
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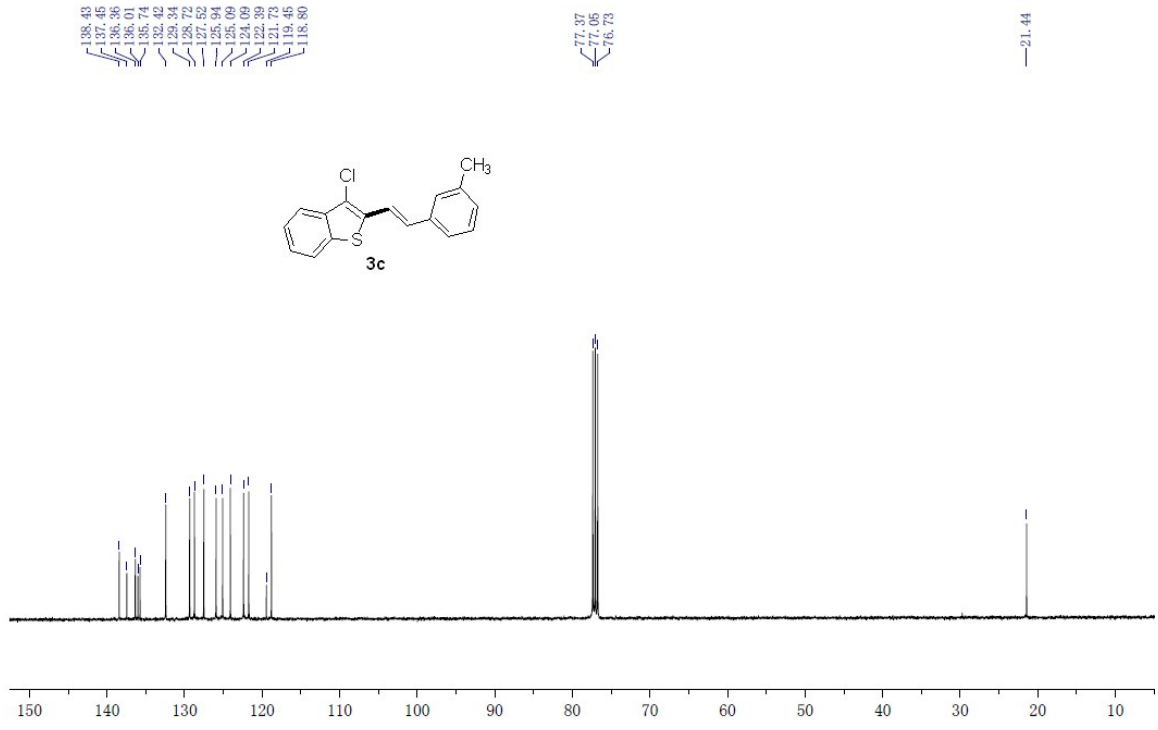
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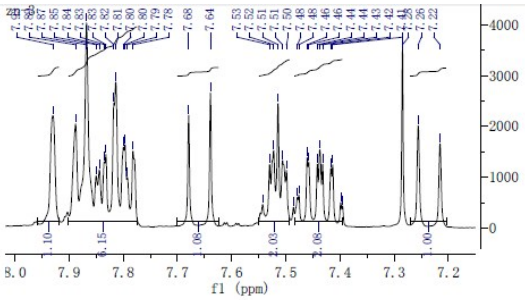
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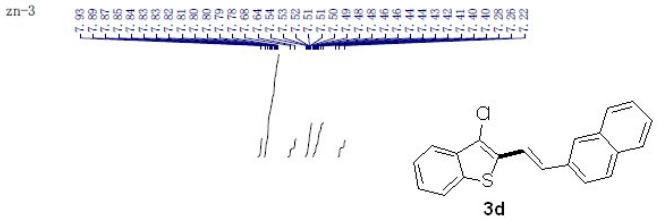
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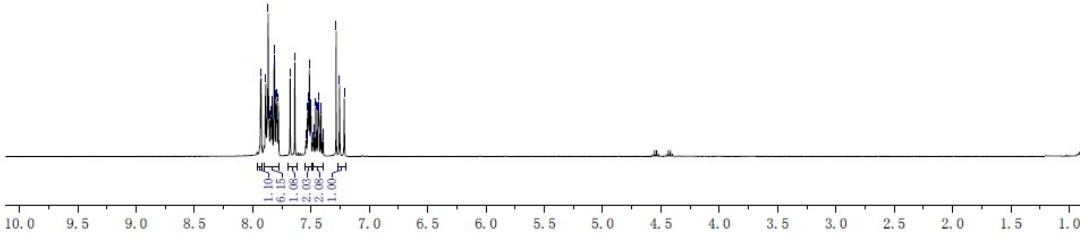
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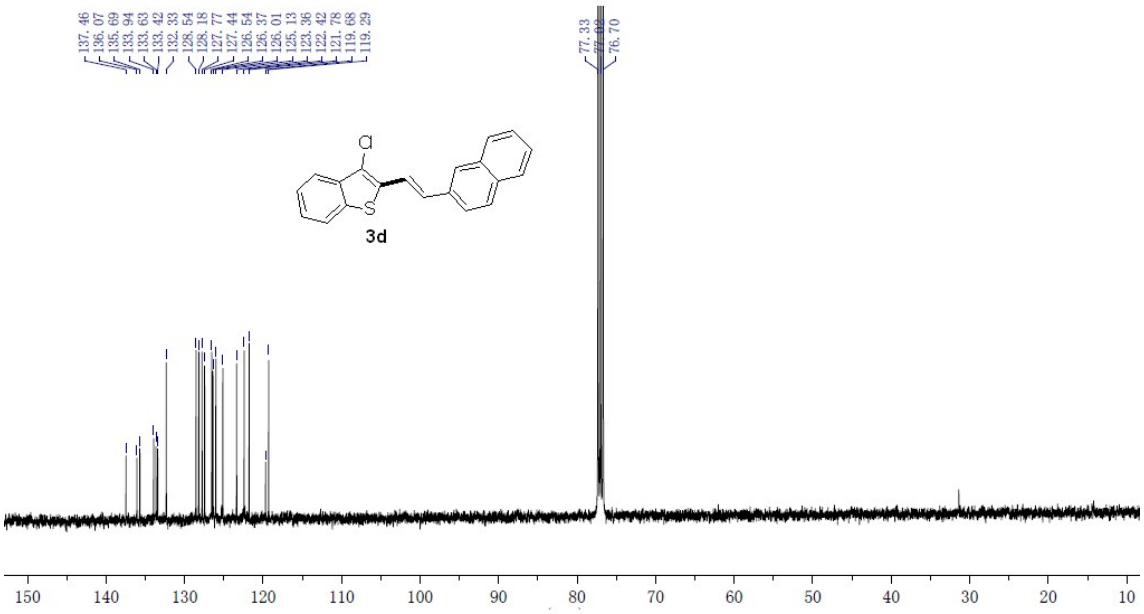
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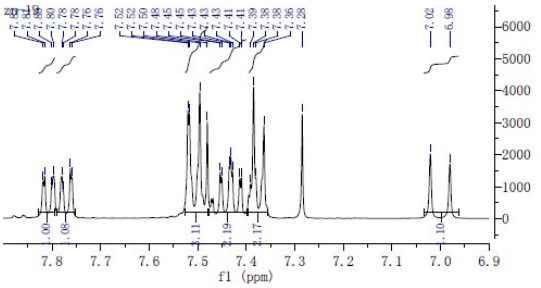
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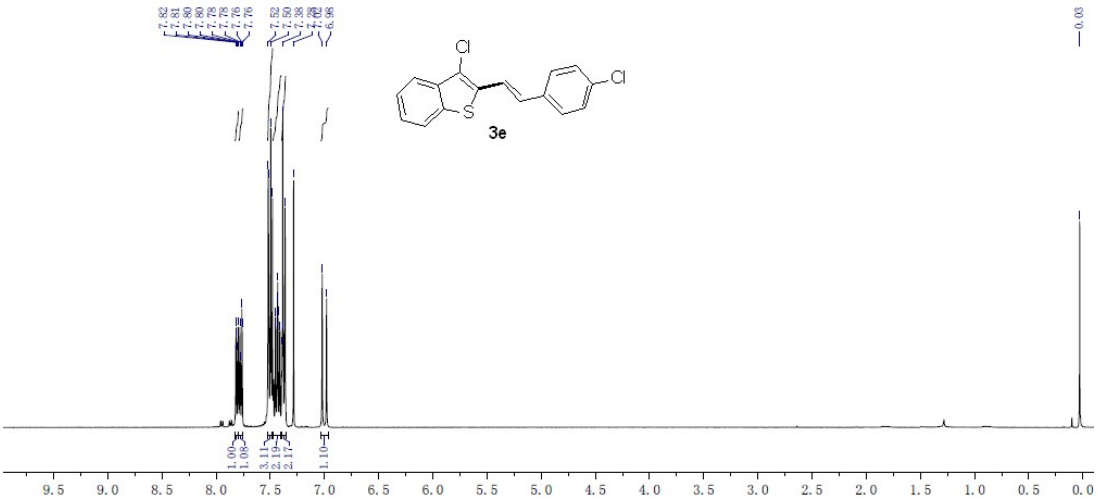
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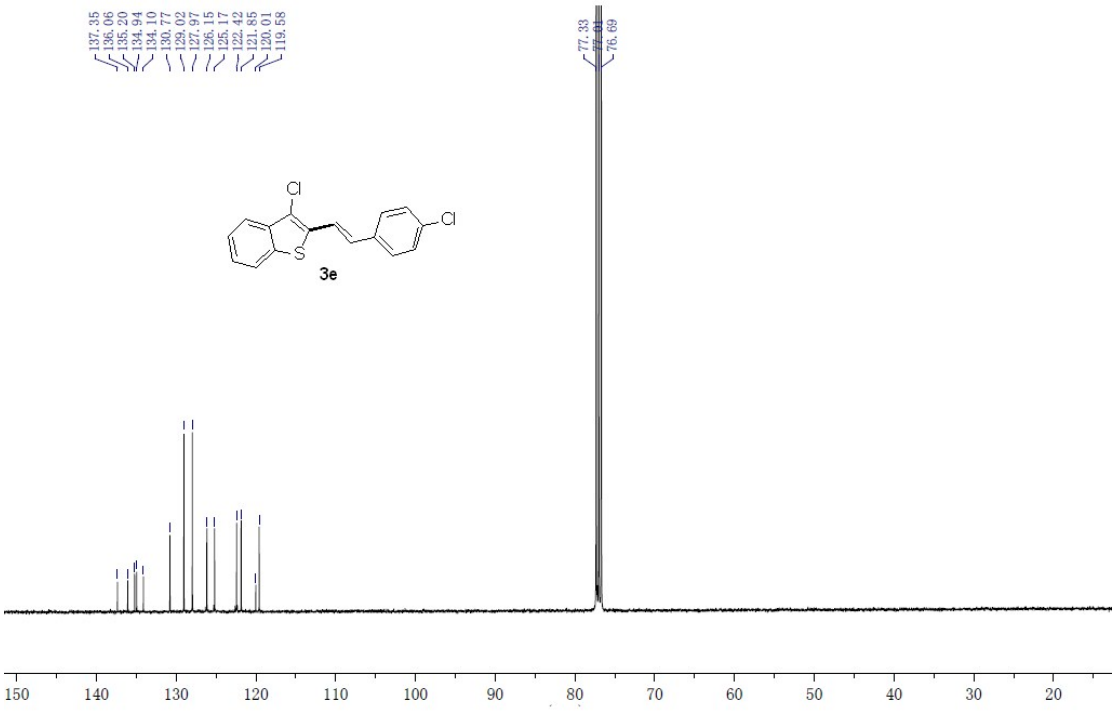
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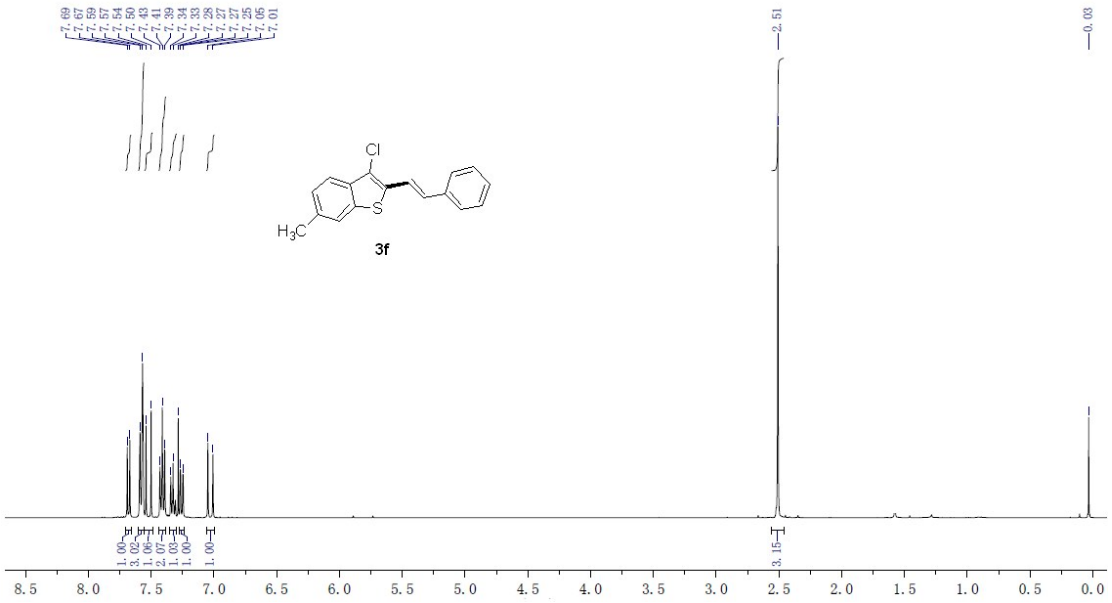
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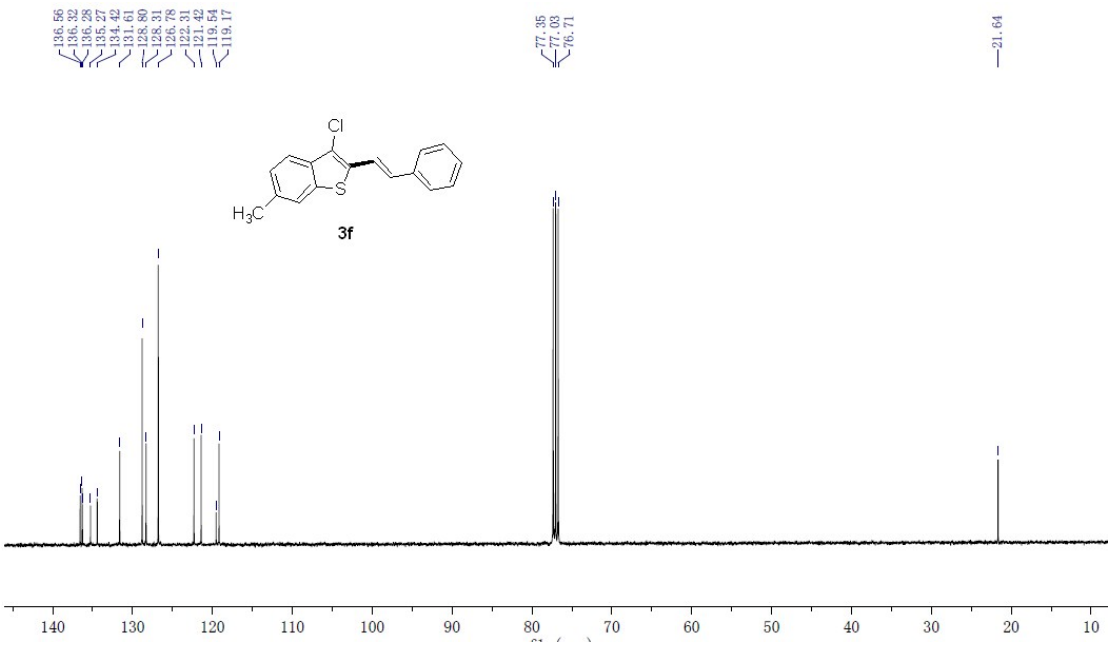
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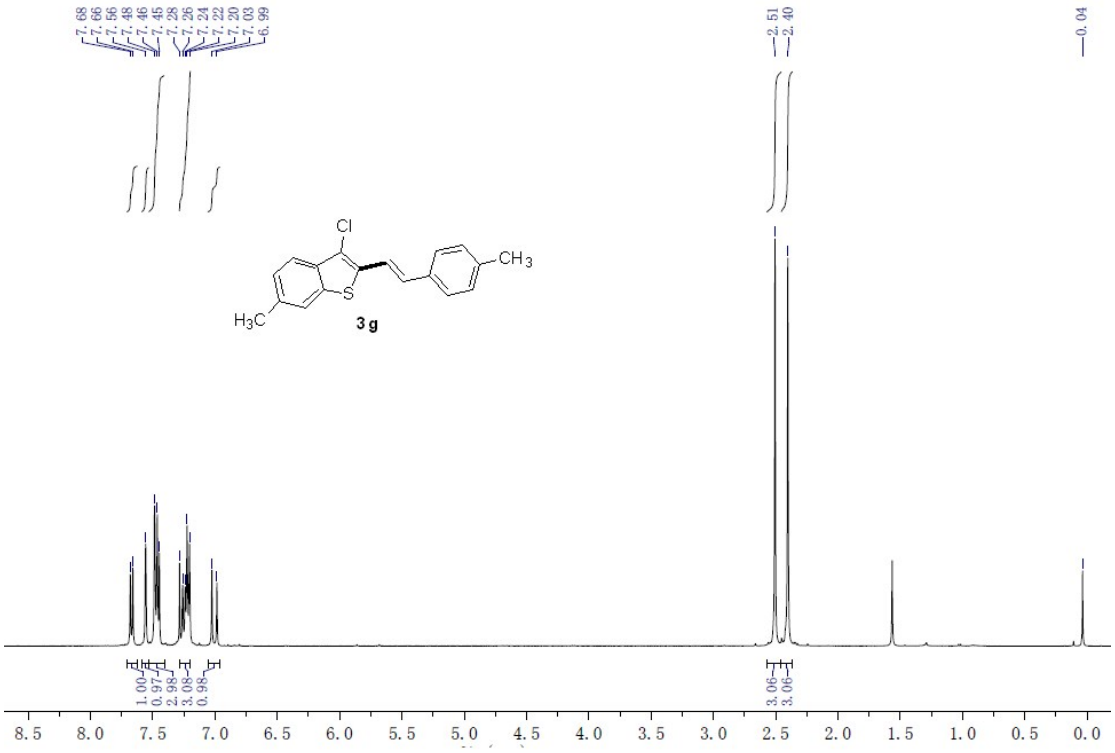
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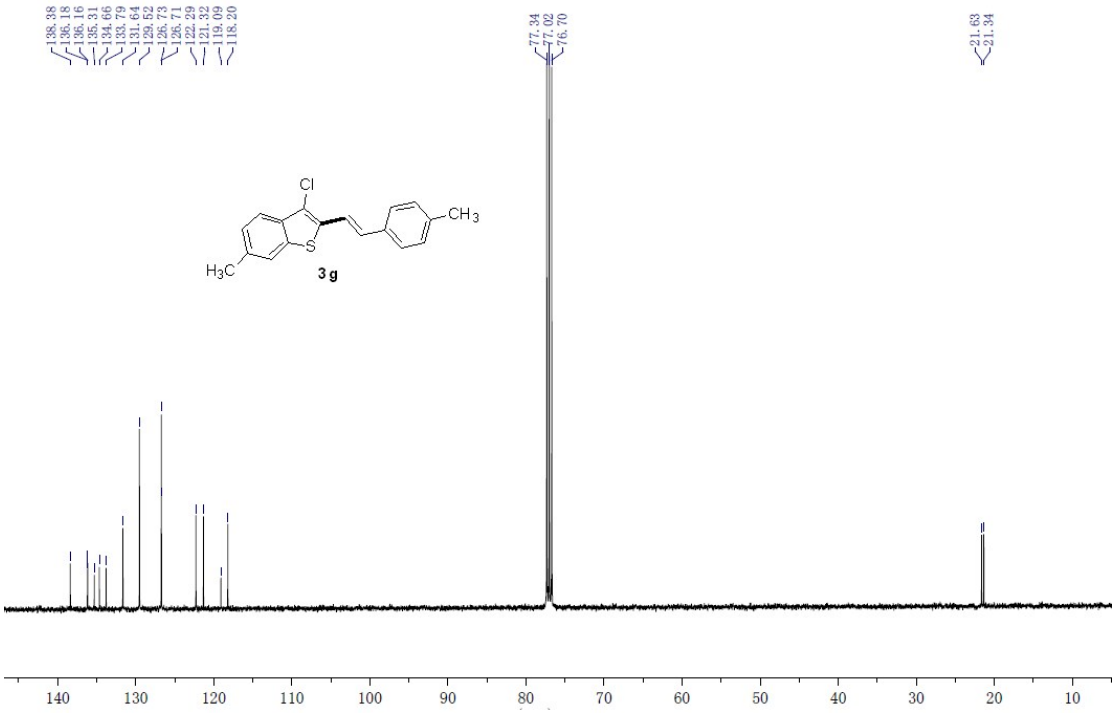
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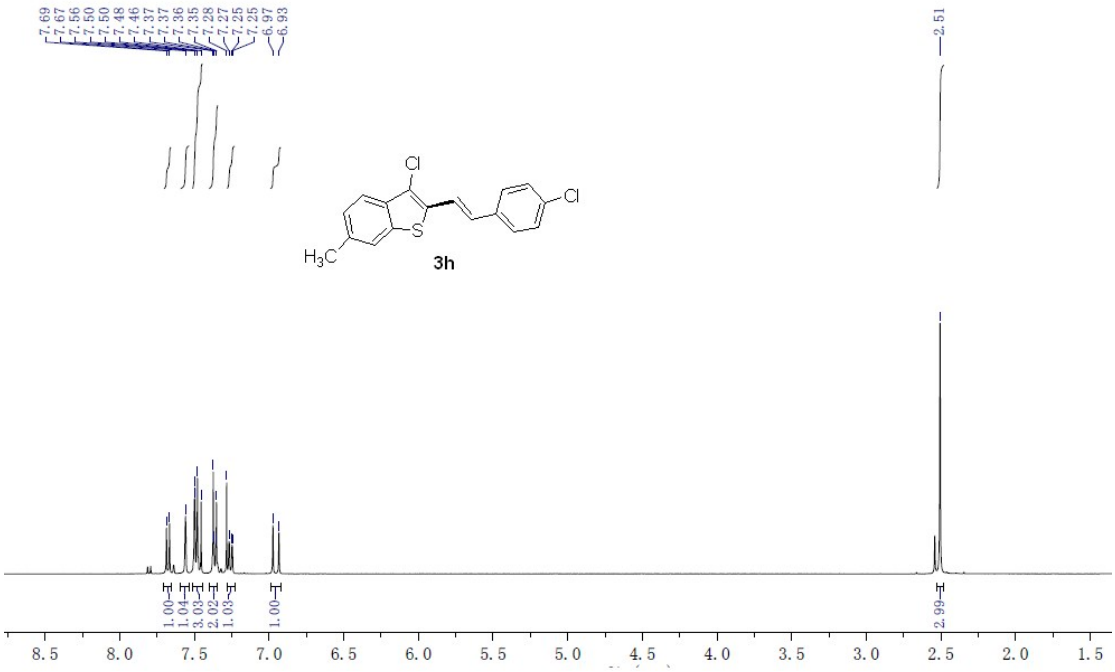
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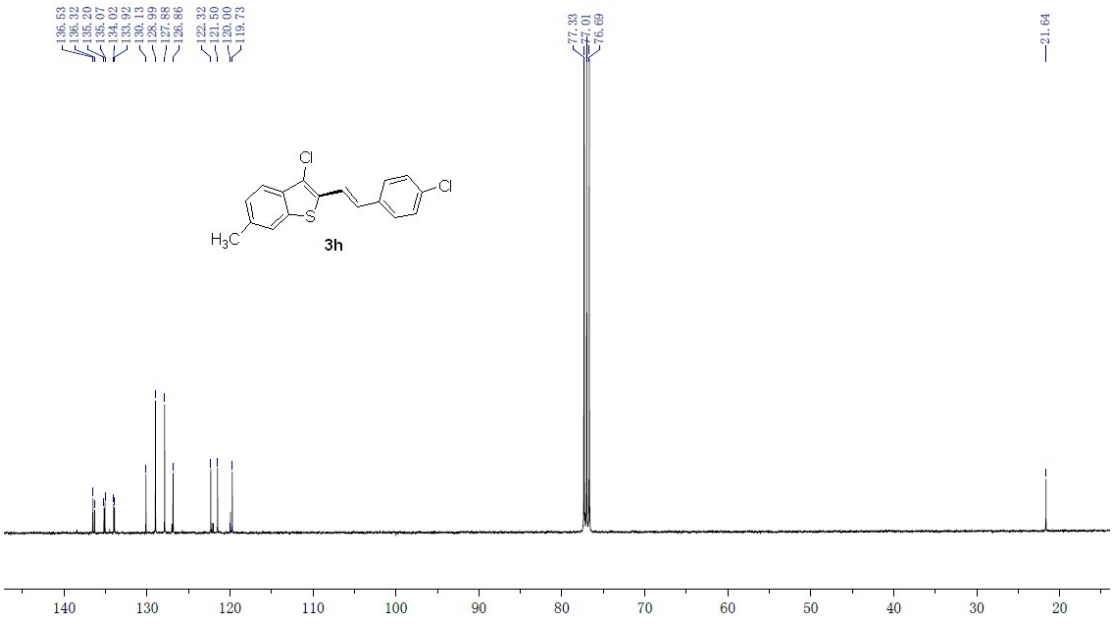
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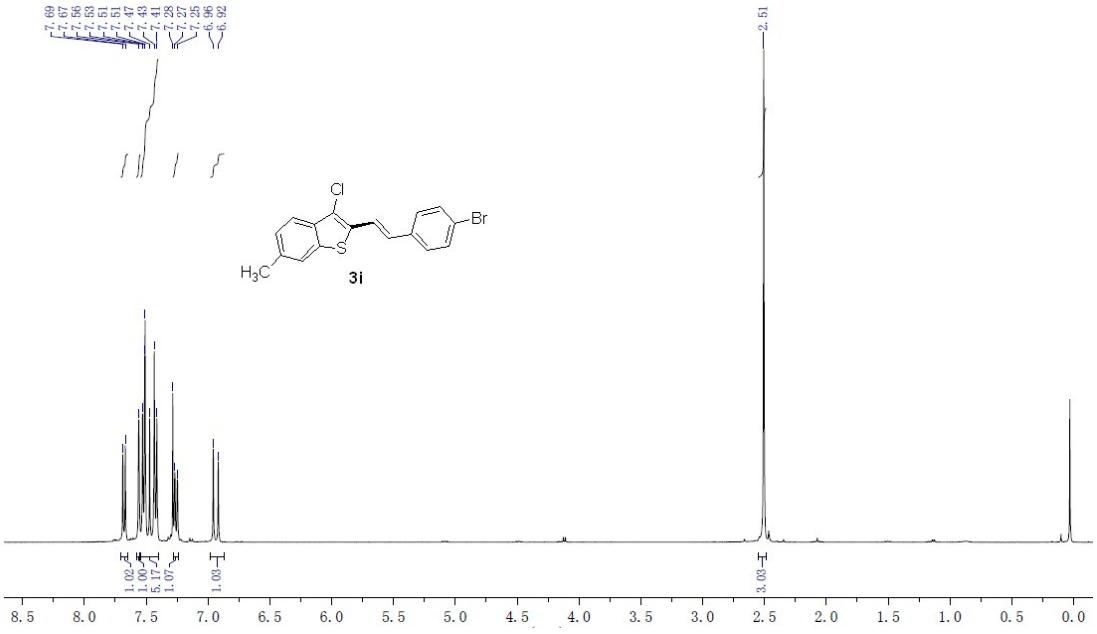
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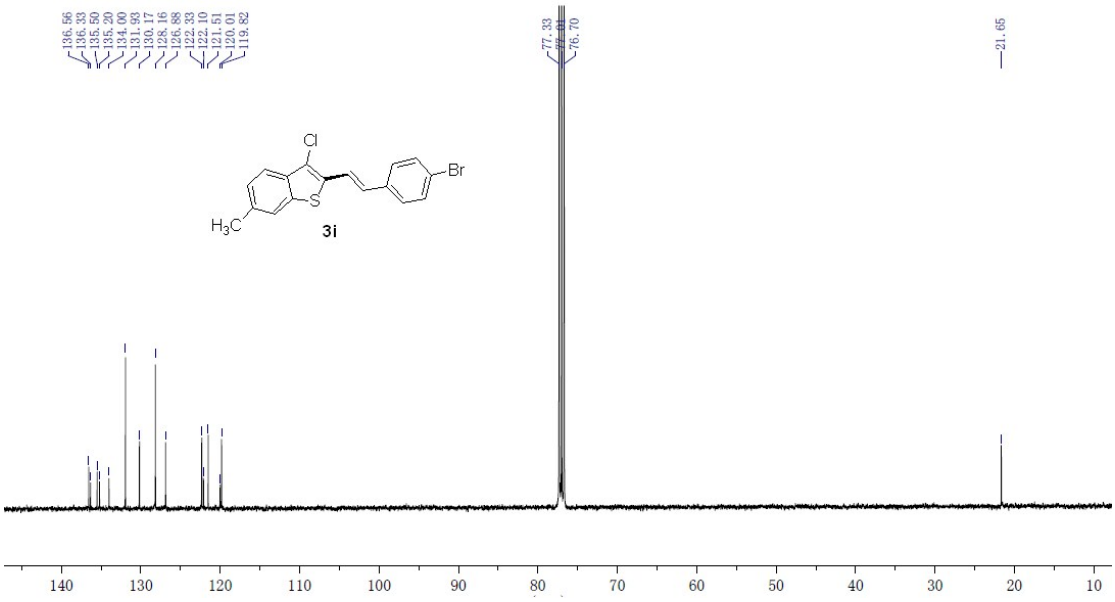
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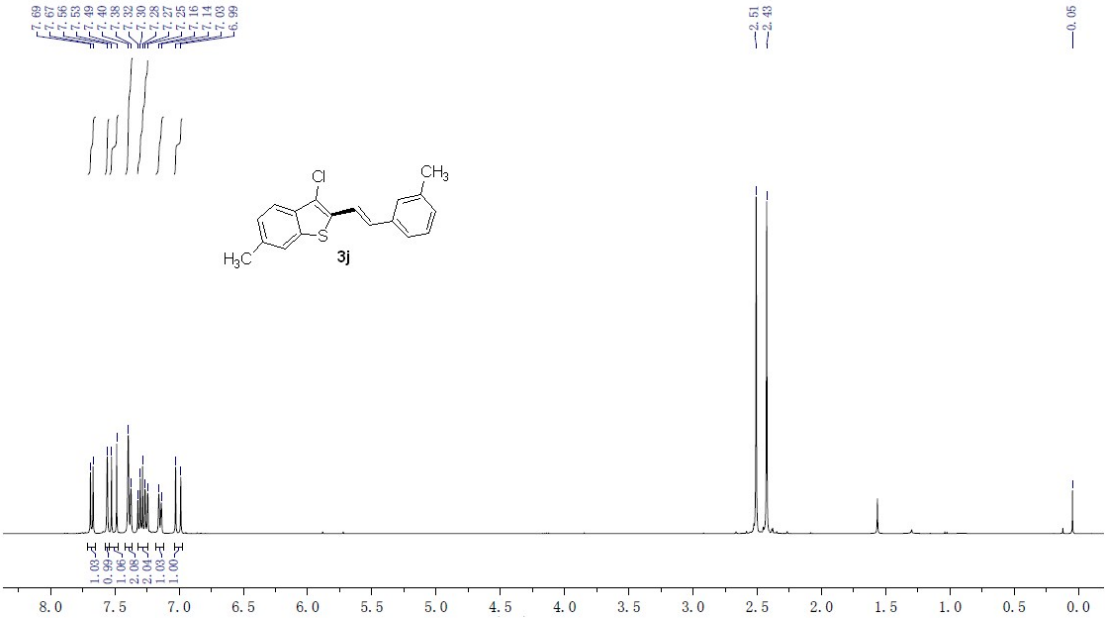
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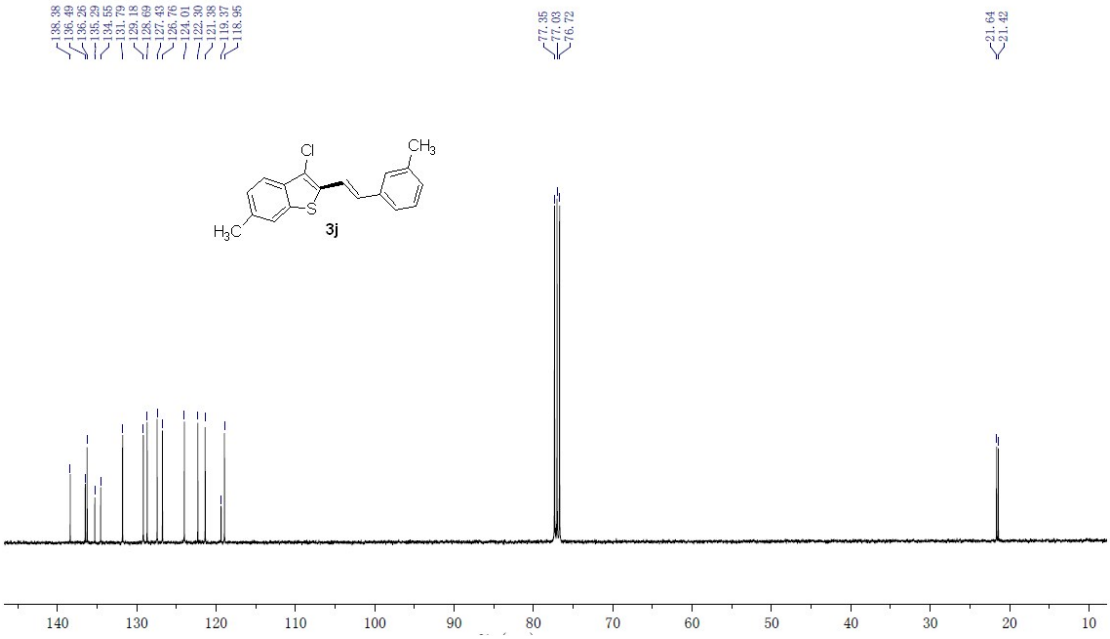
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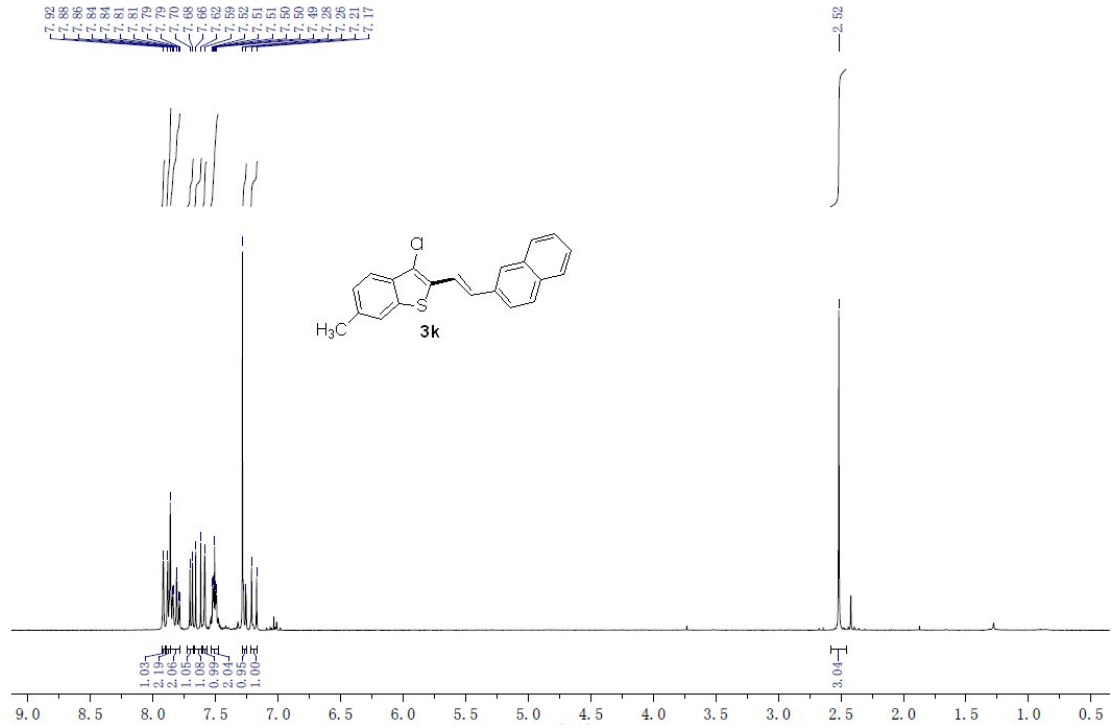
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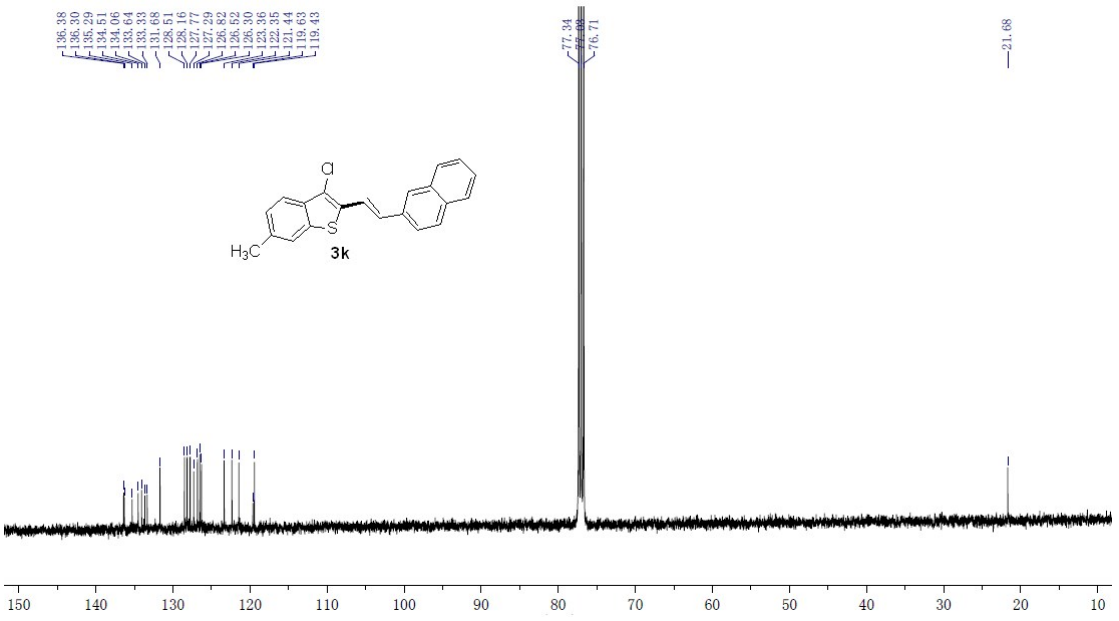
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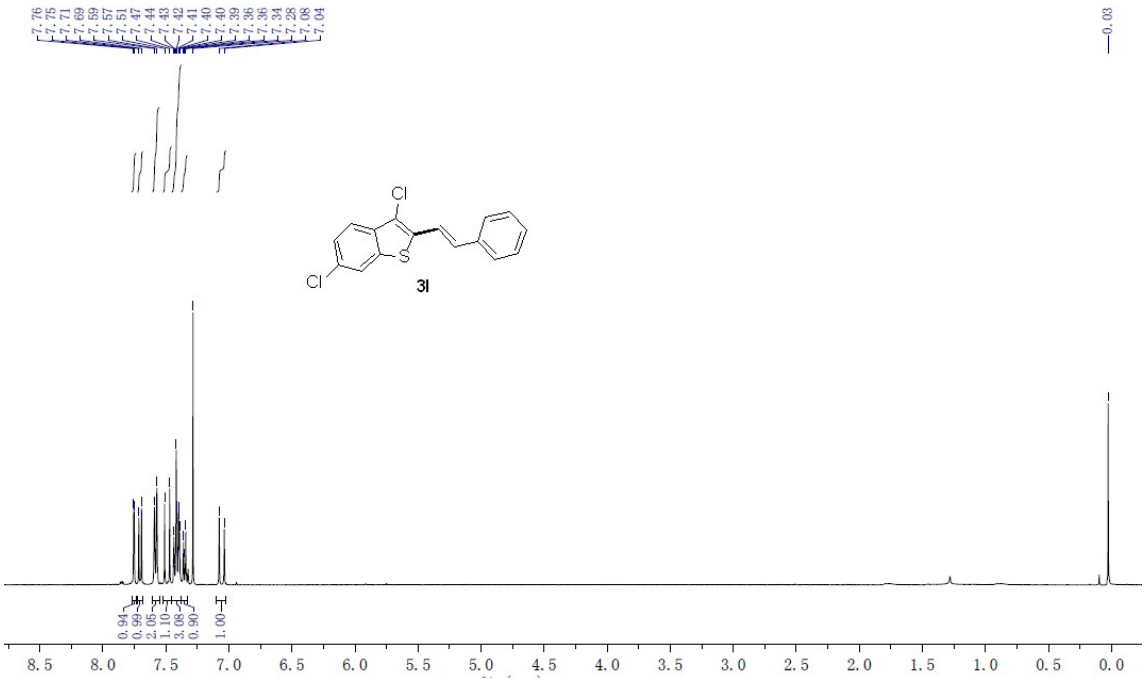
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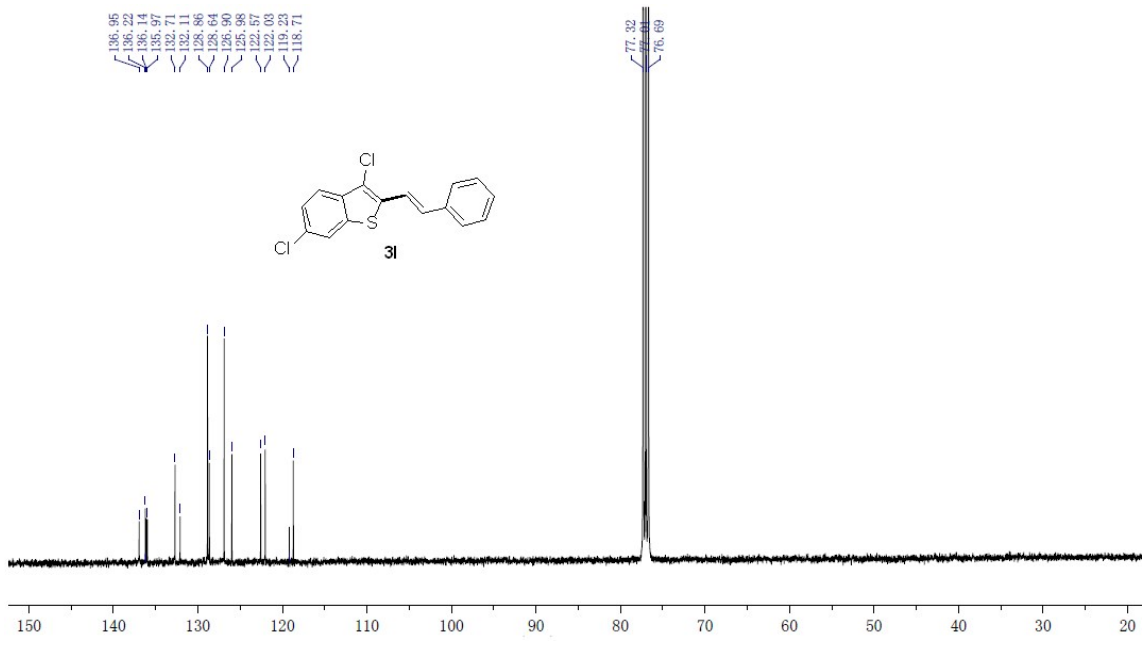
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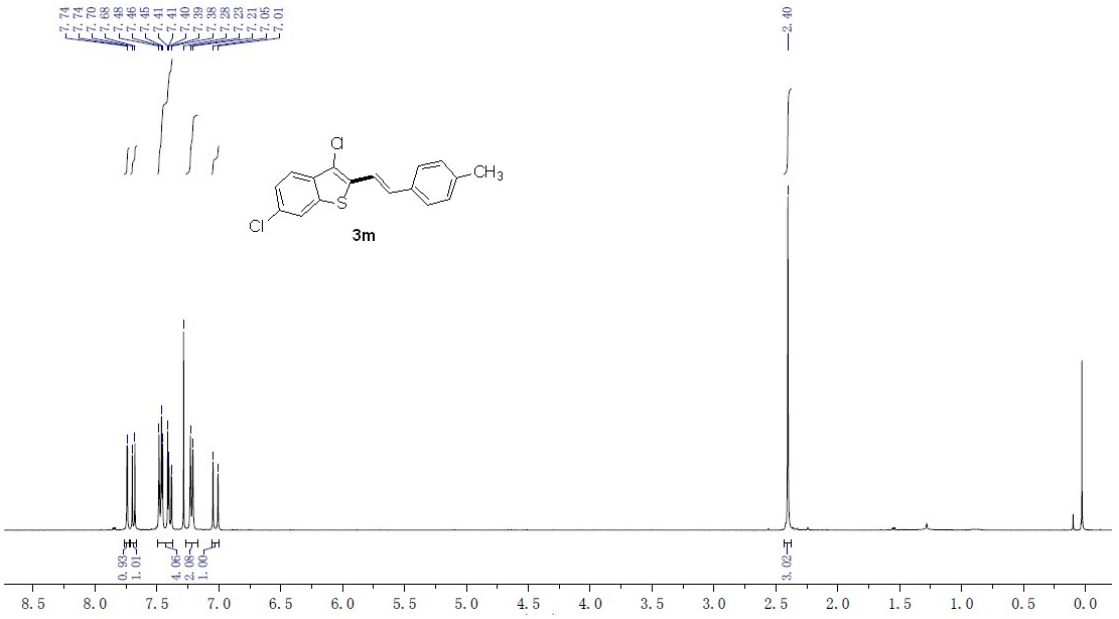
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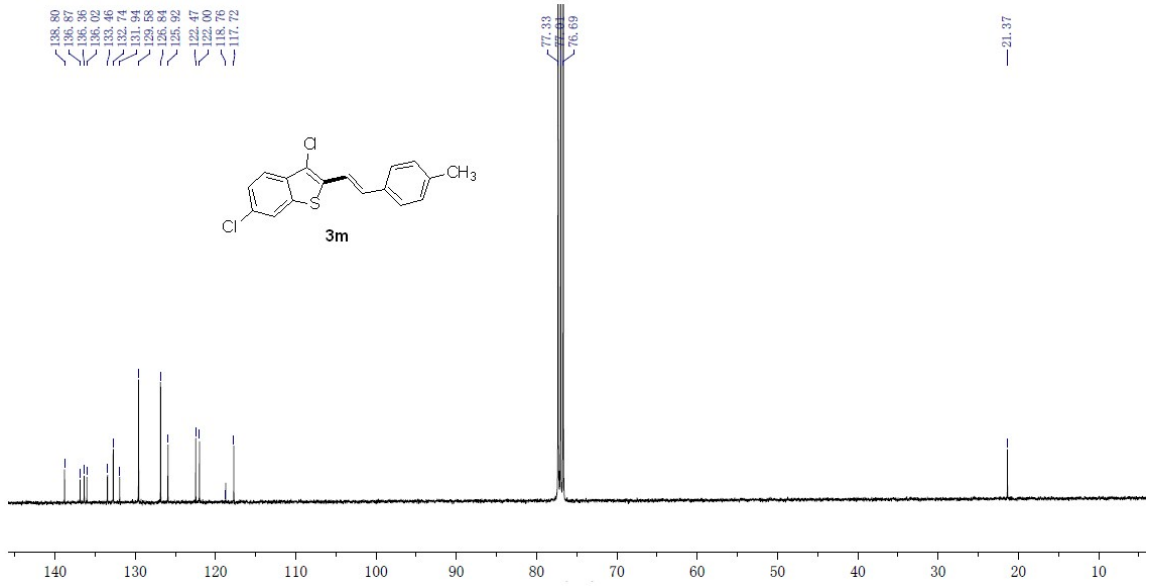
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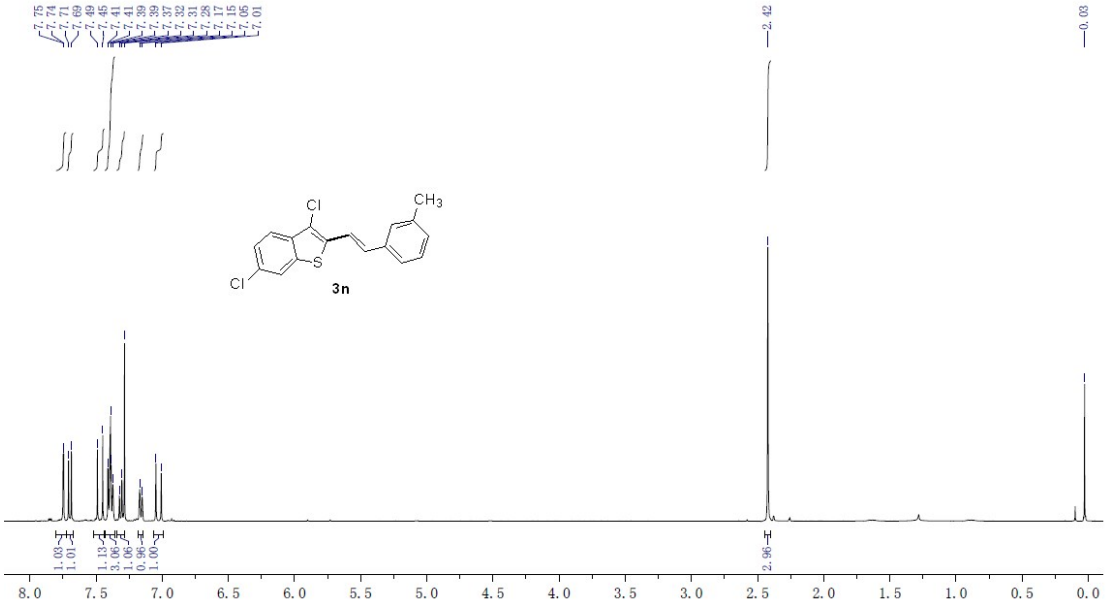
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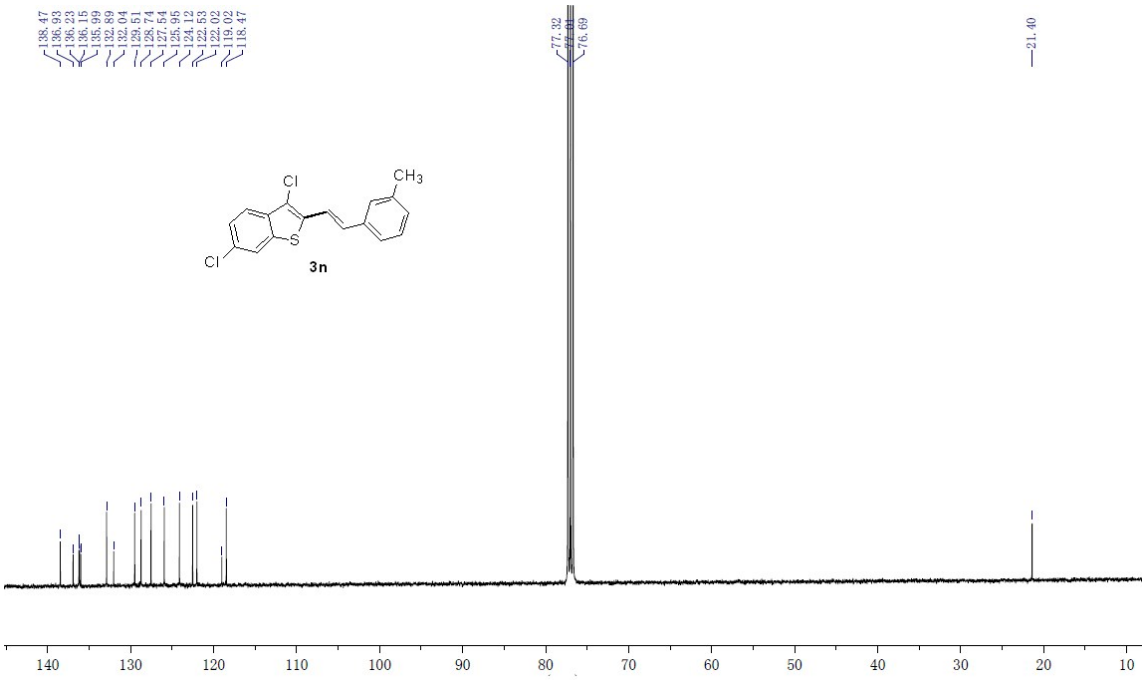
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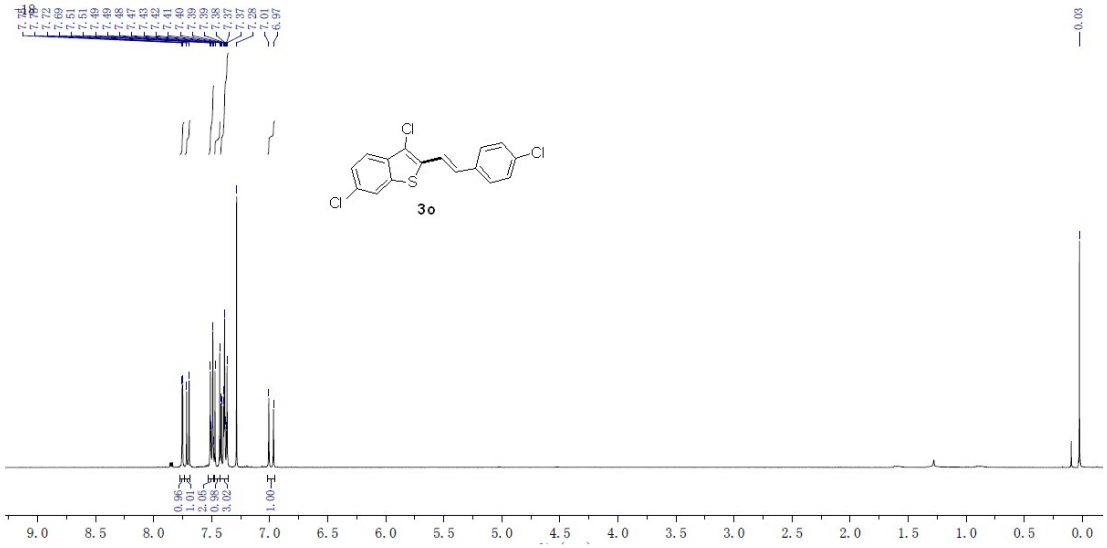
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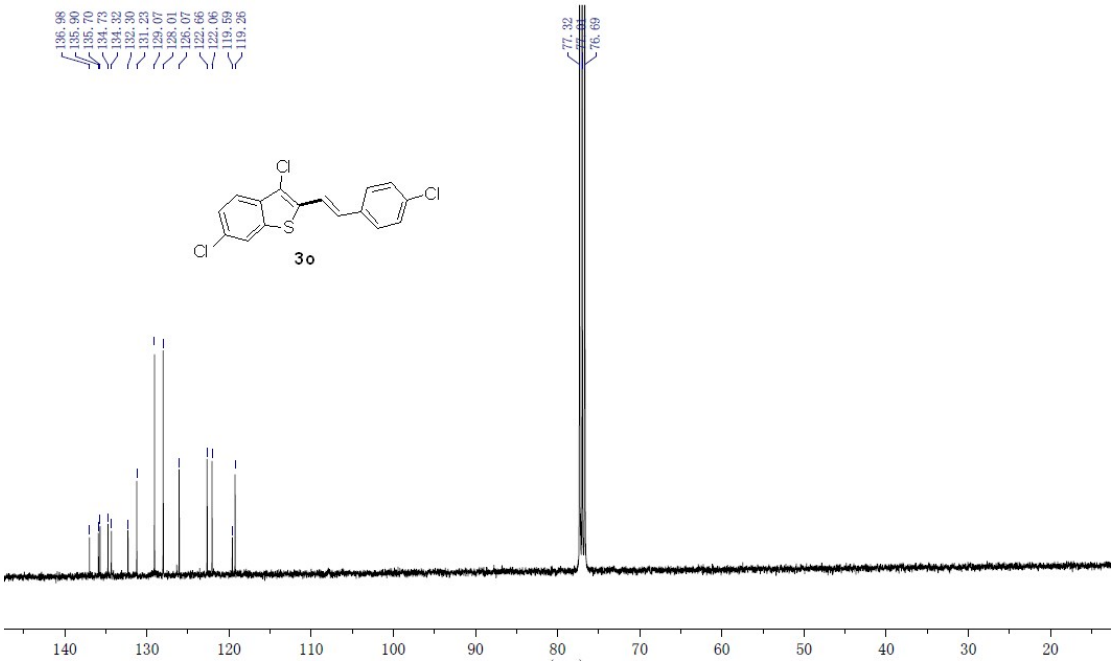
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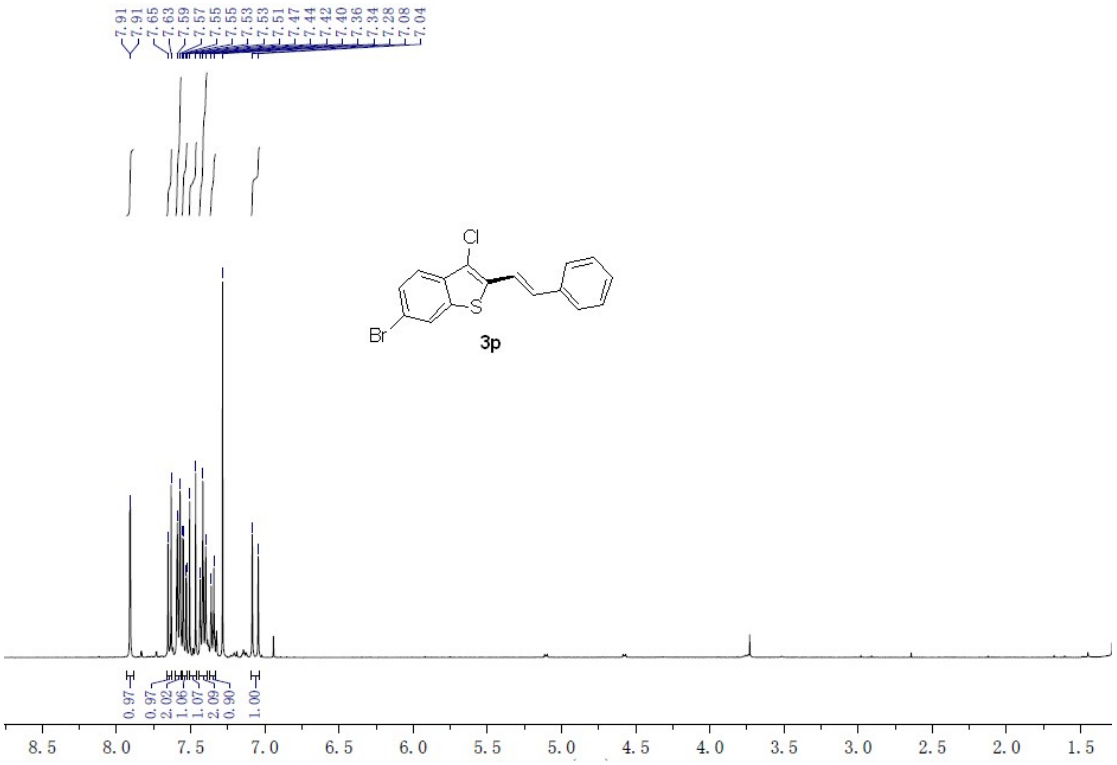
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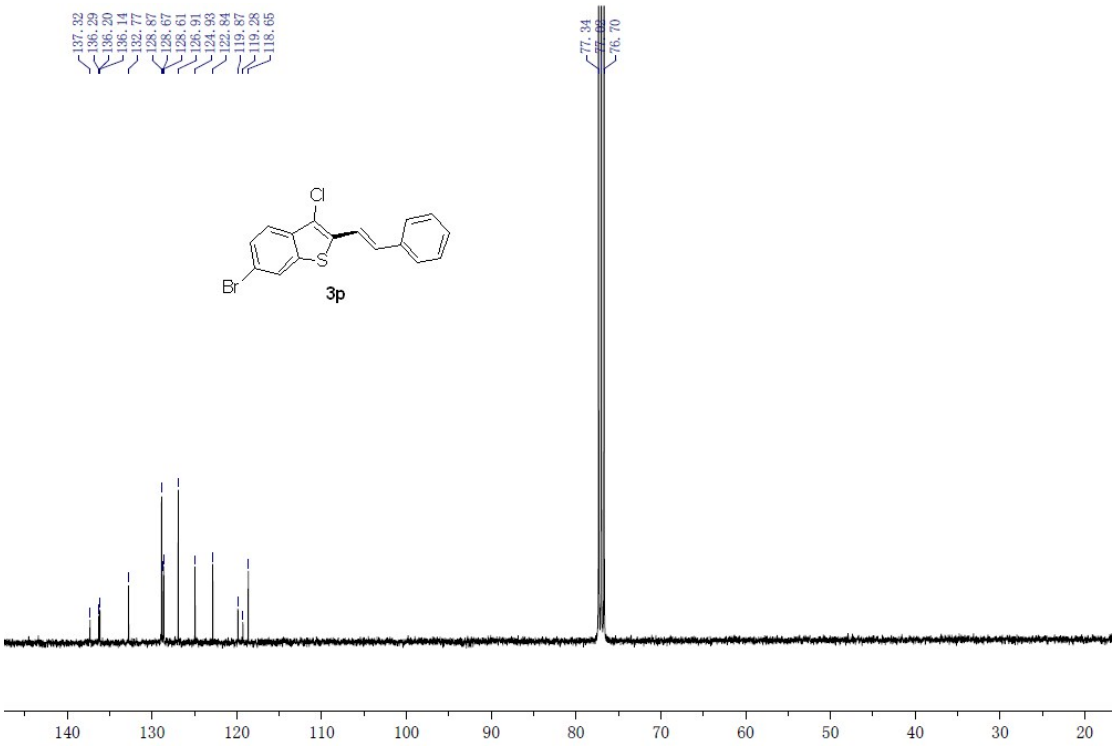
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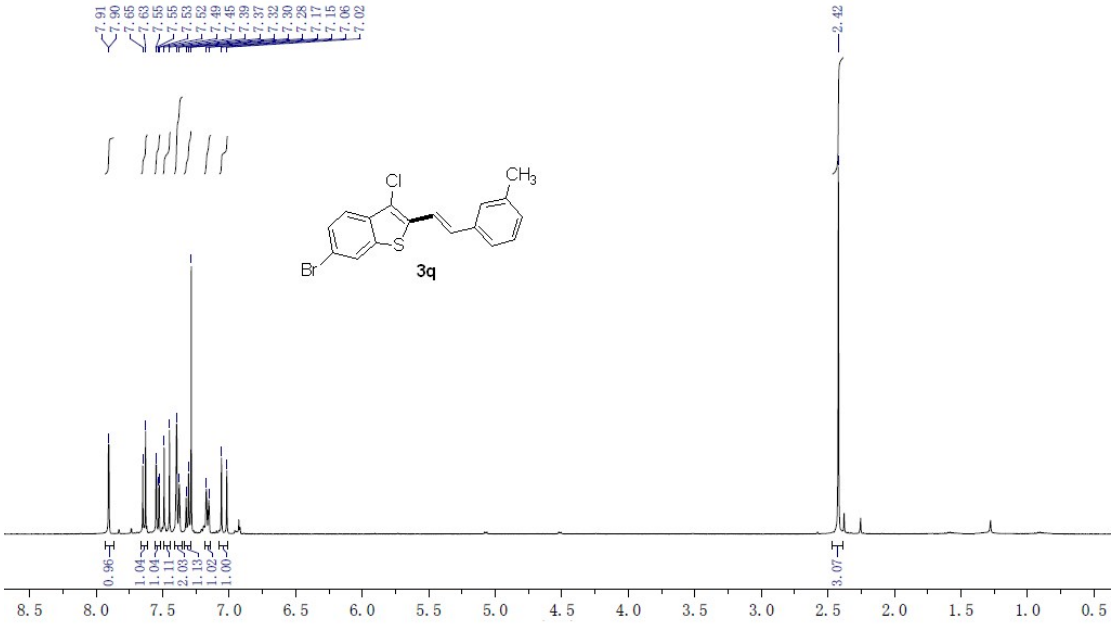
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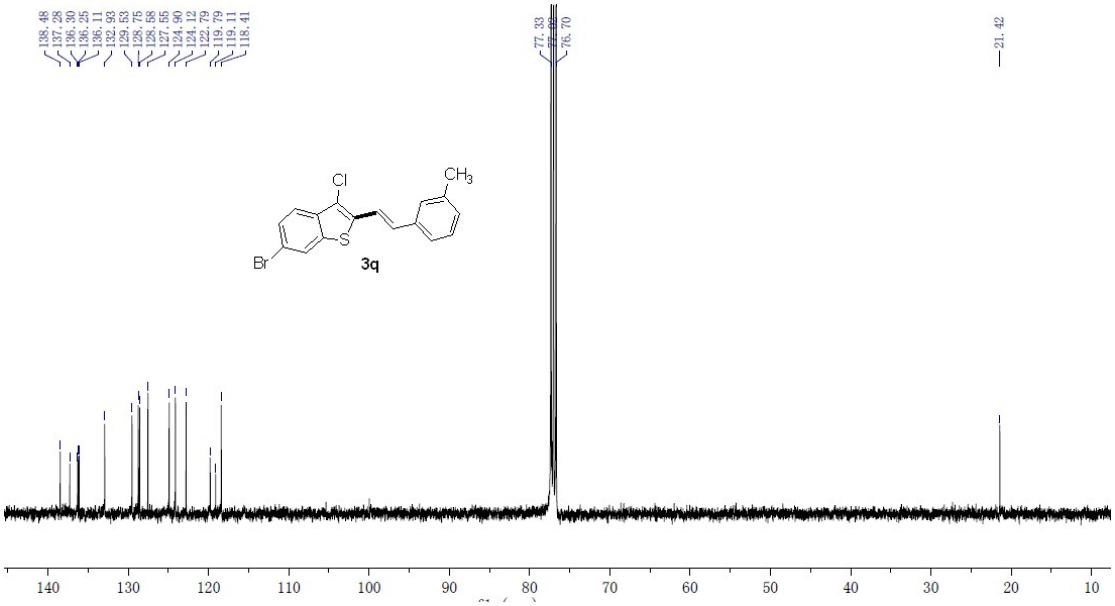
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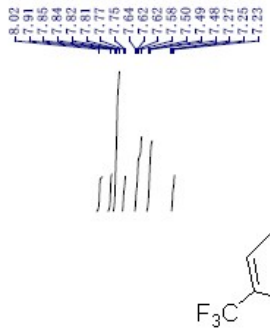
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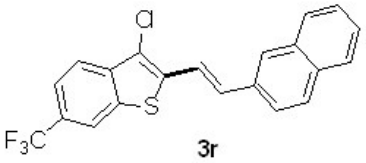
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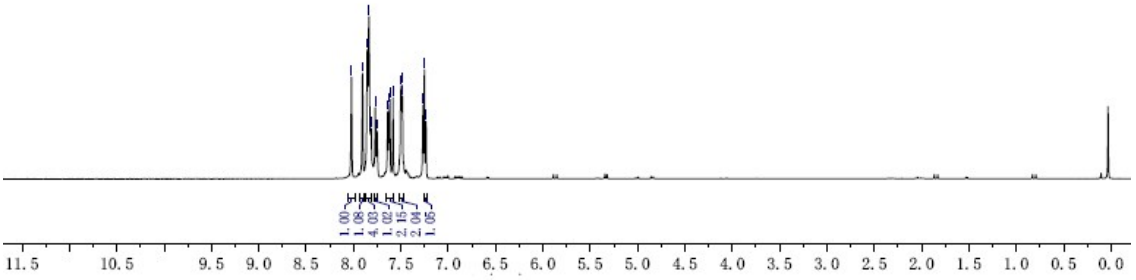
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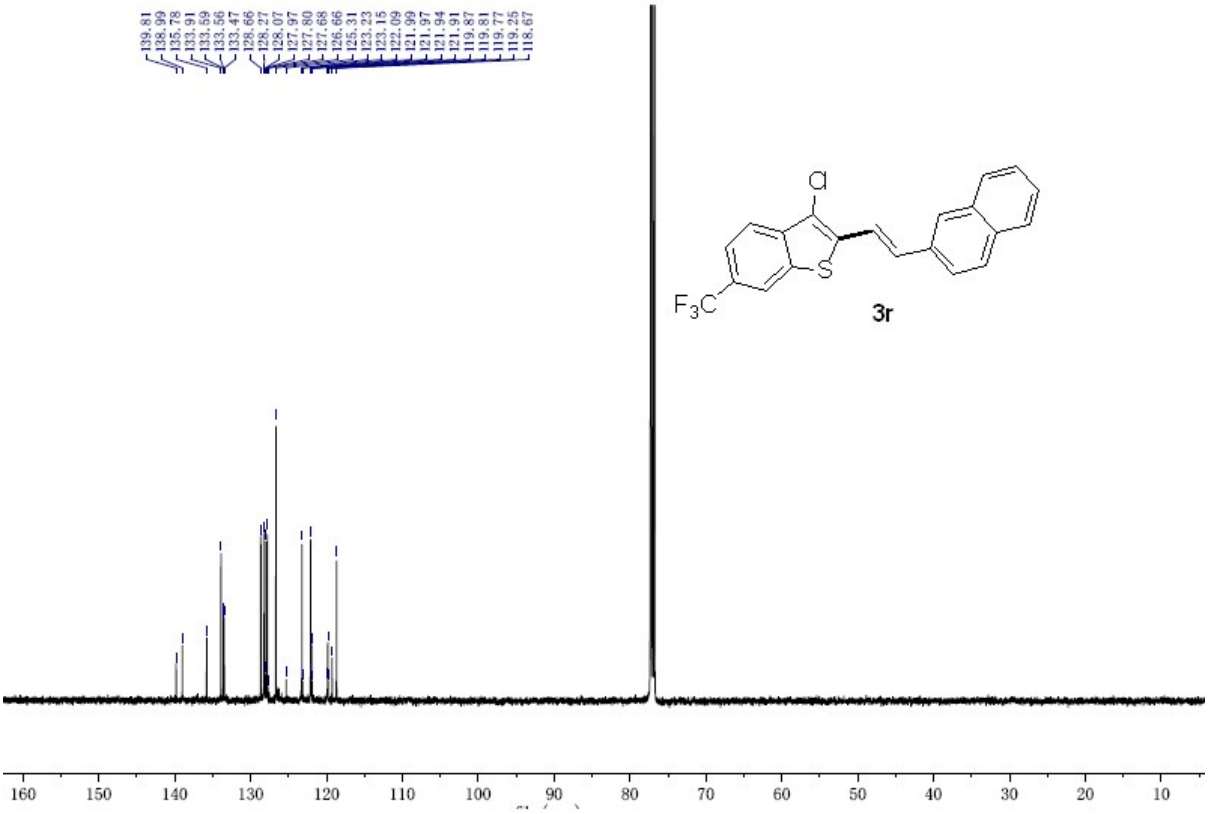
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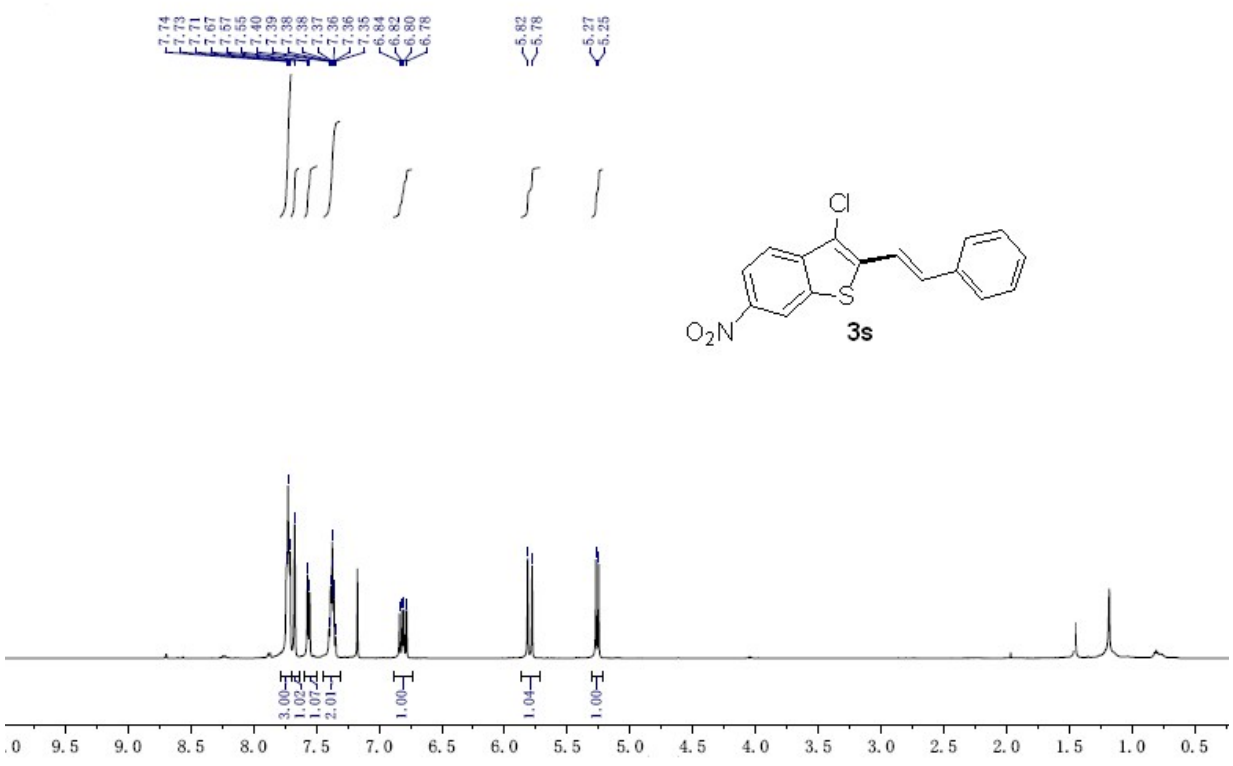
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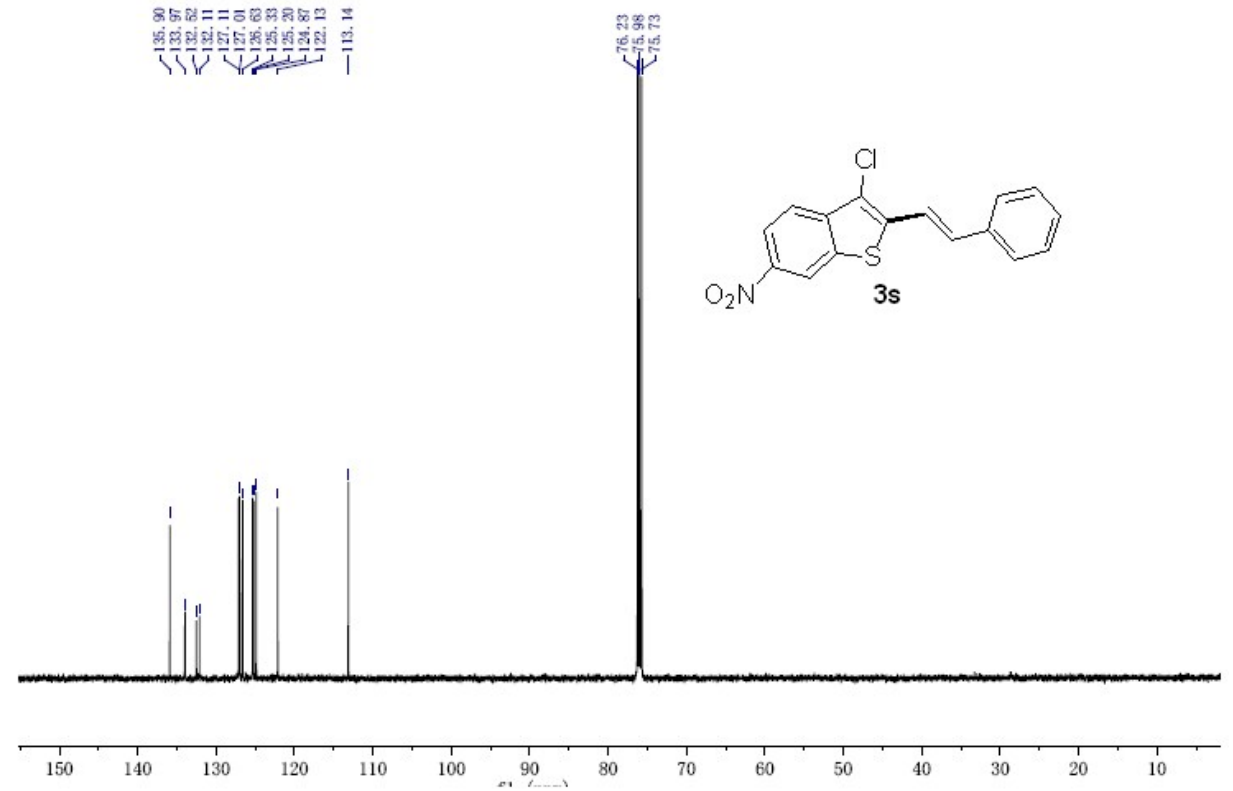
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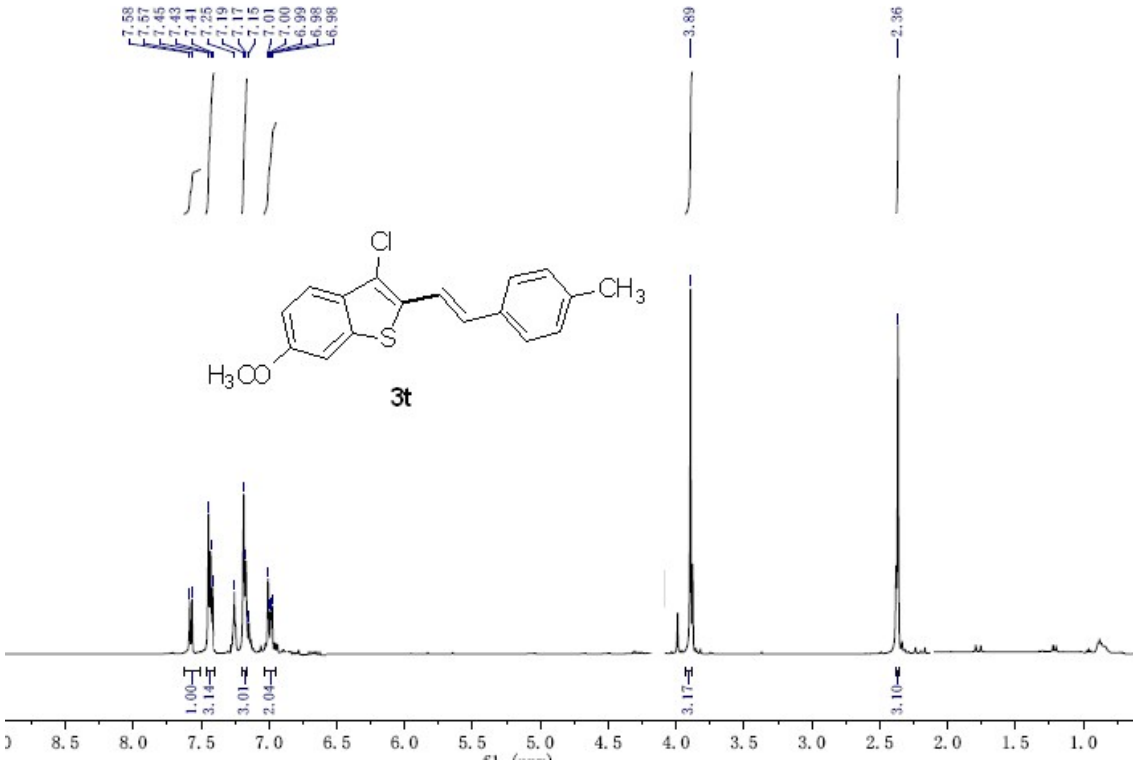
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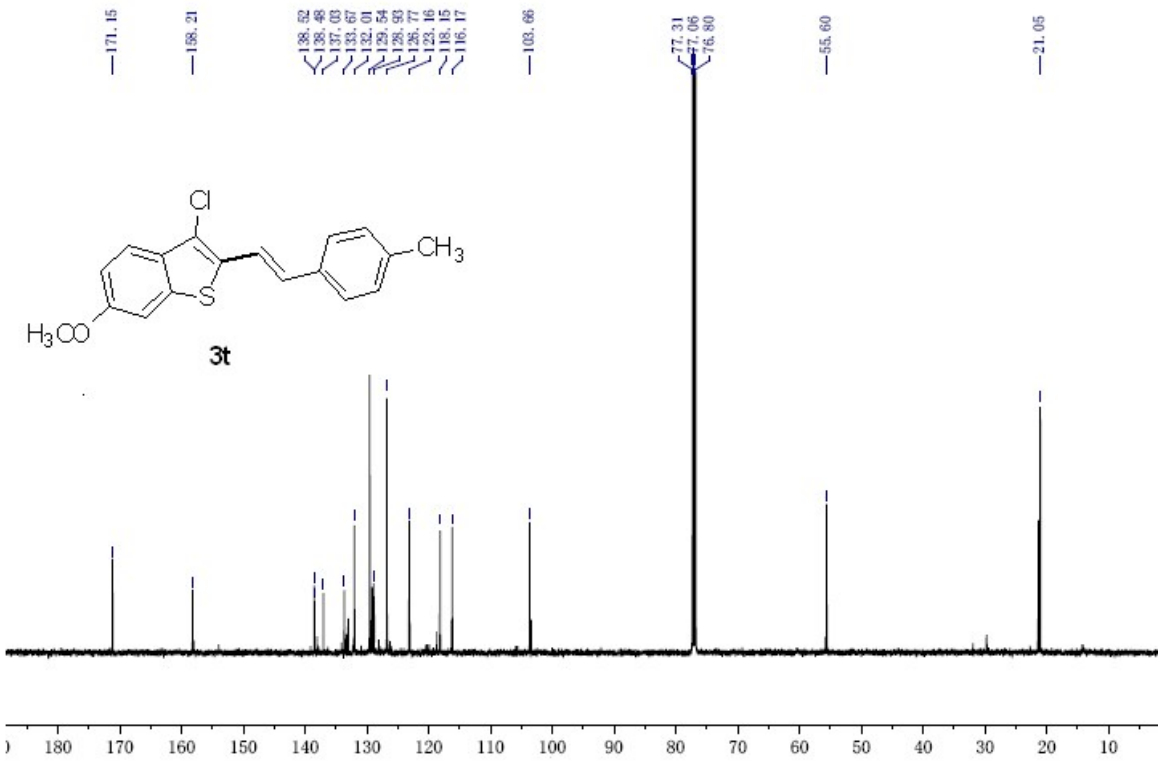
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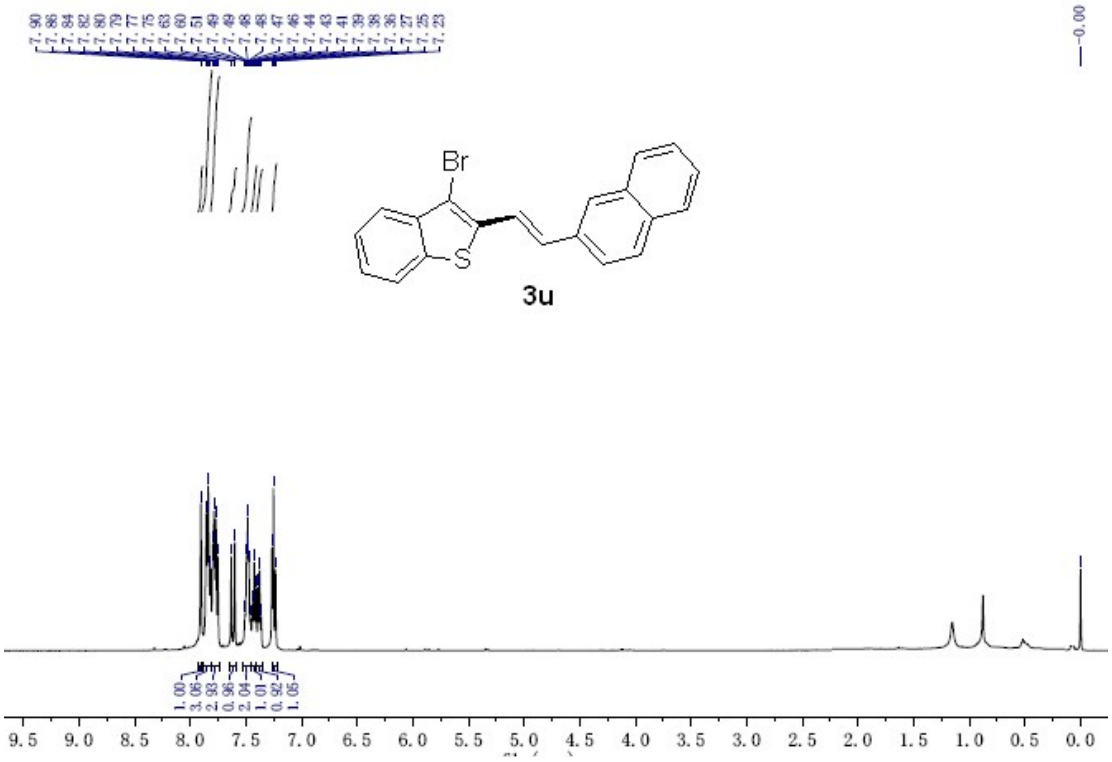
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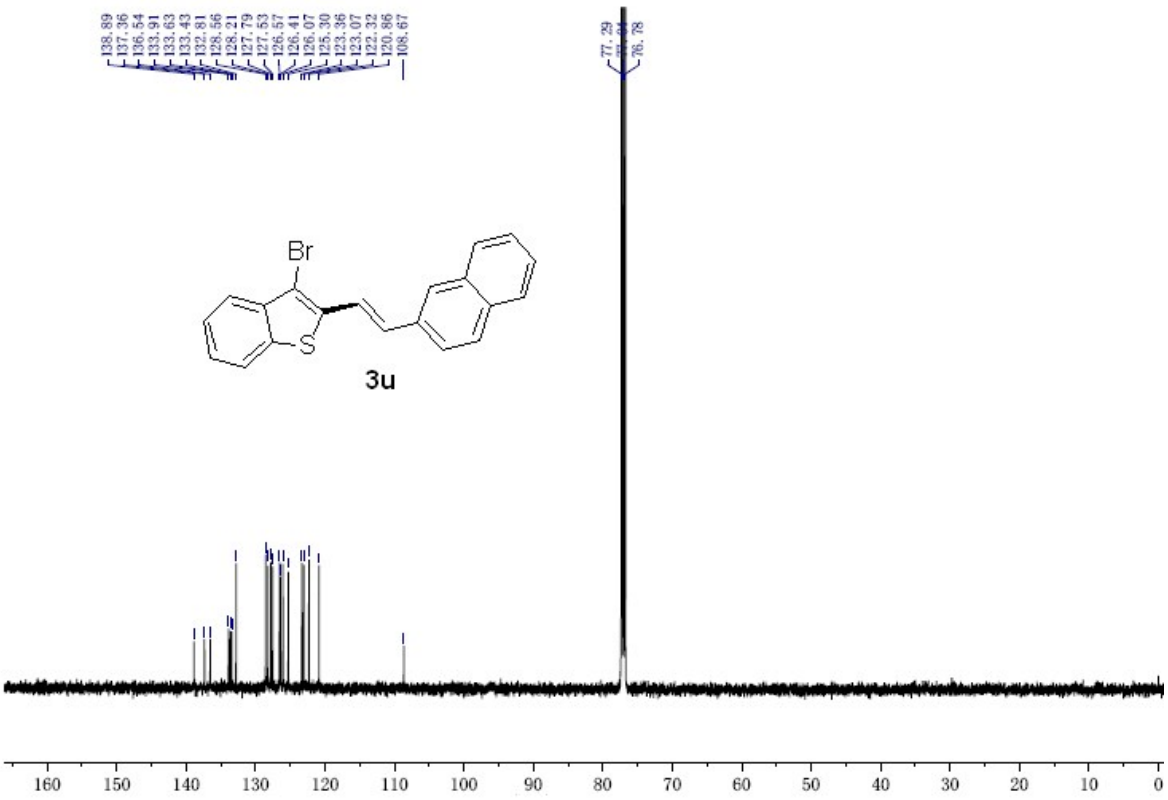
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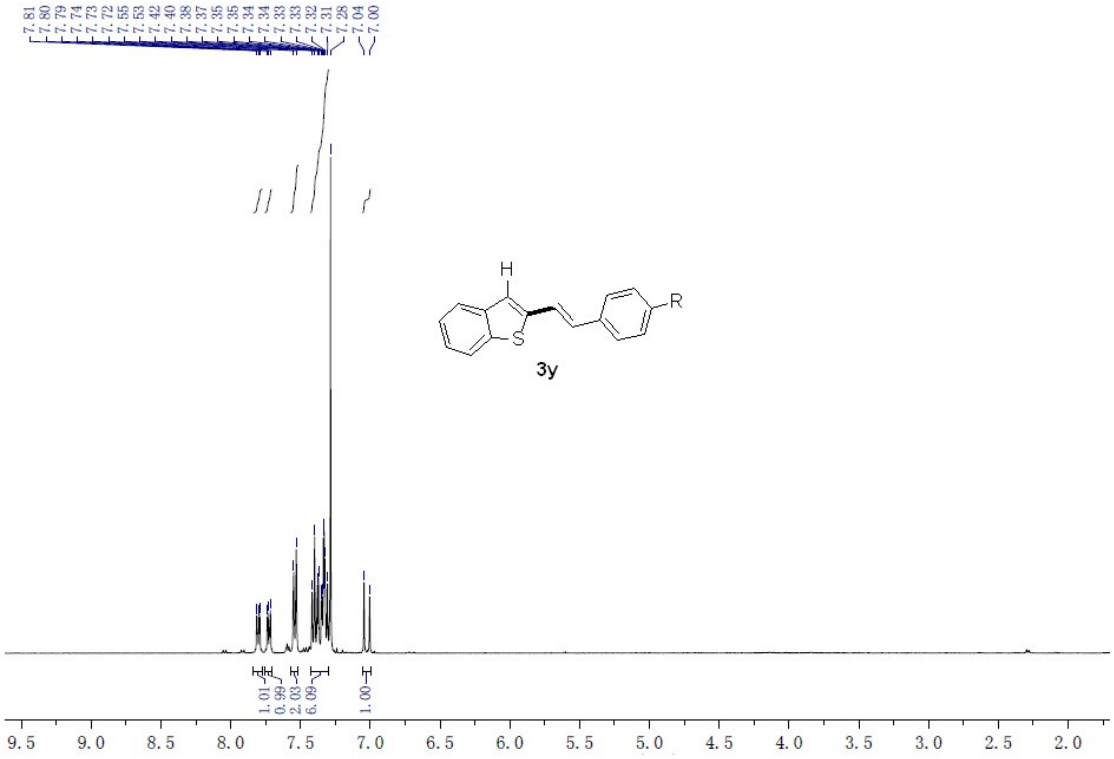
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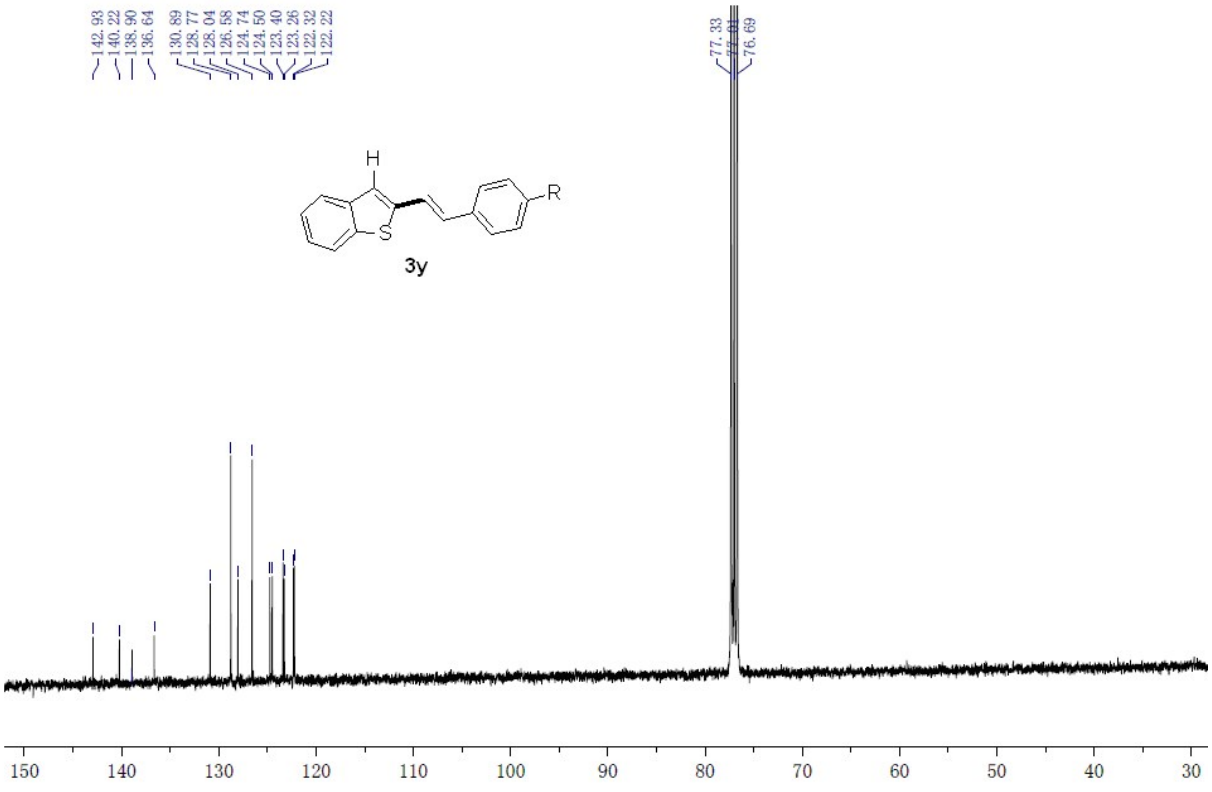
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Computational Section

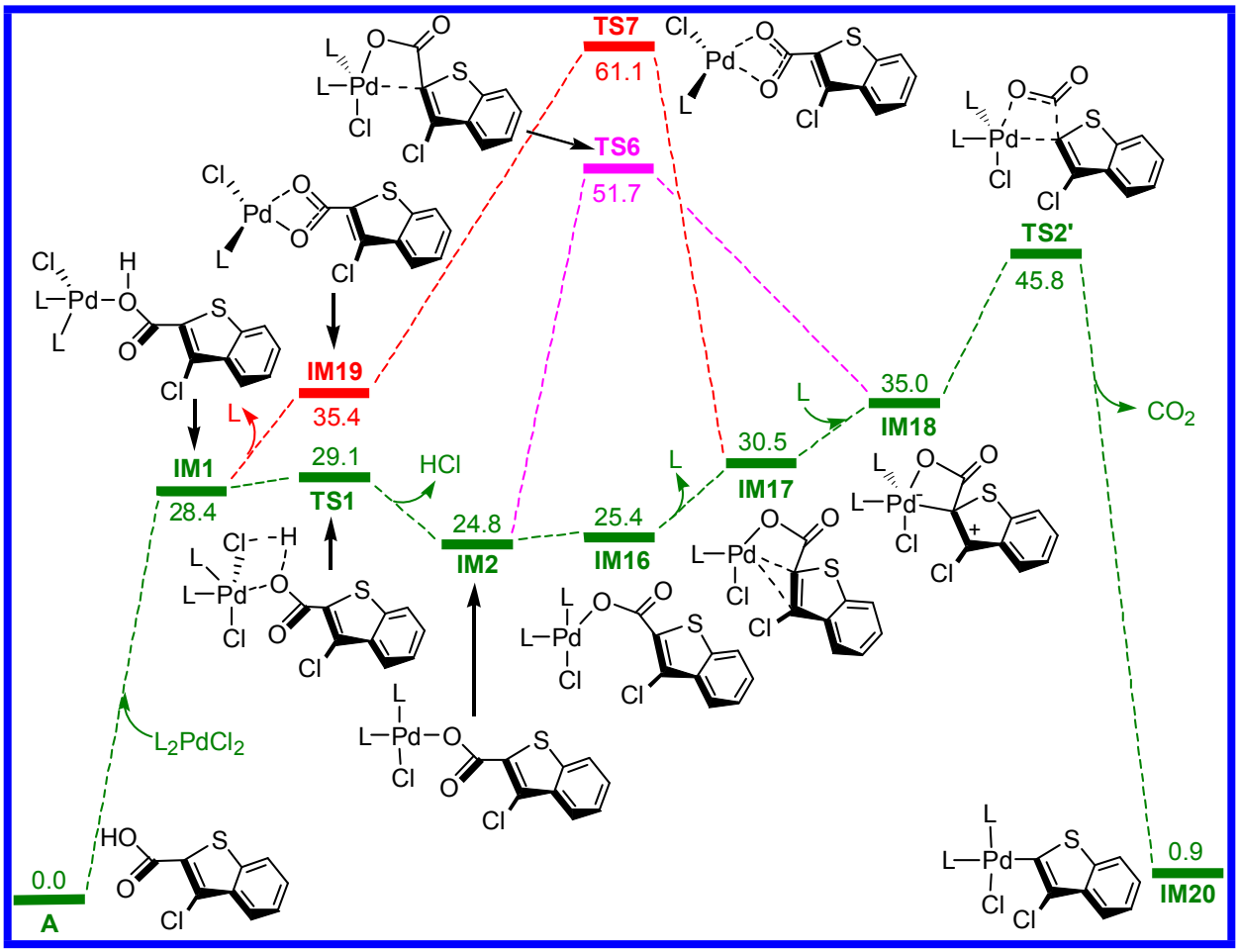

Figure S1. Calculated free energy profiles in DMF solution along various possible pathways for the metalation-depronation followed by the decarboxylation in the Cl-substituted system as well as schematic structures of intermediates and transition states involved (L =DMSO). The relative free energies are given in kcal/mol.

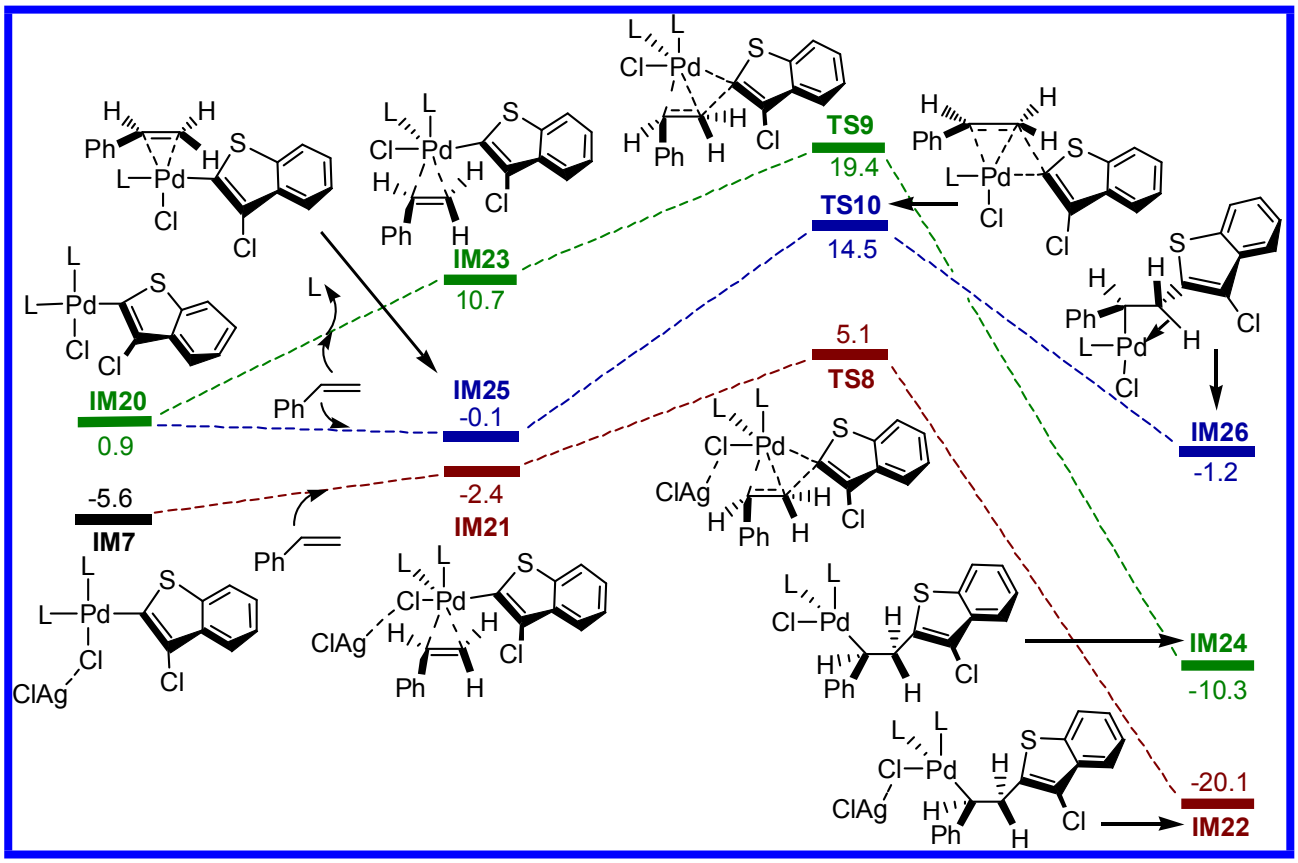

Figure S2. Calculated free energy profiles in DMF solution along various possible pathways for the olefin insertion in the Cl-substituted system as well as schematic structures of intermediates and transition states involved (L =DMSO). The relative free energies are given in kcal/mol.

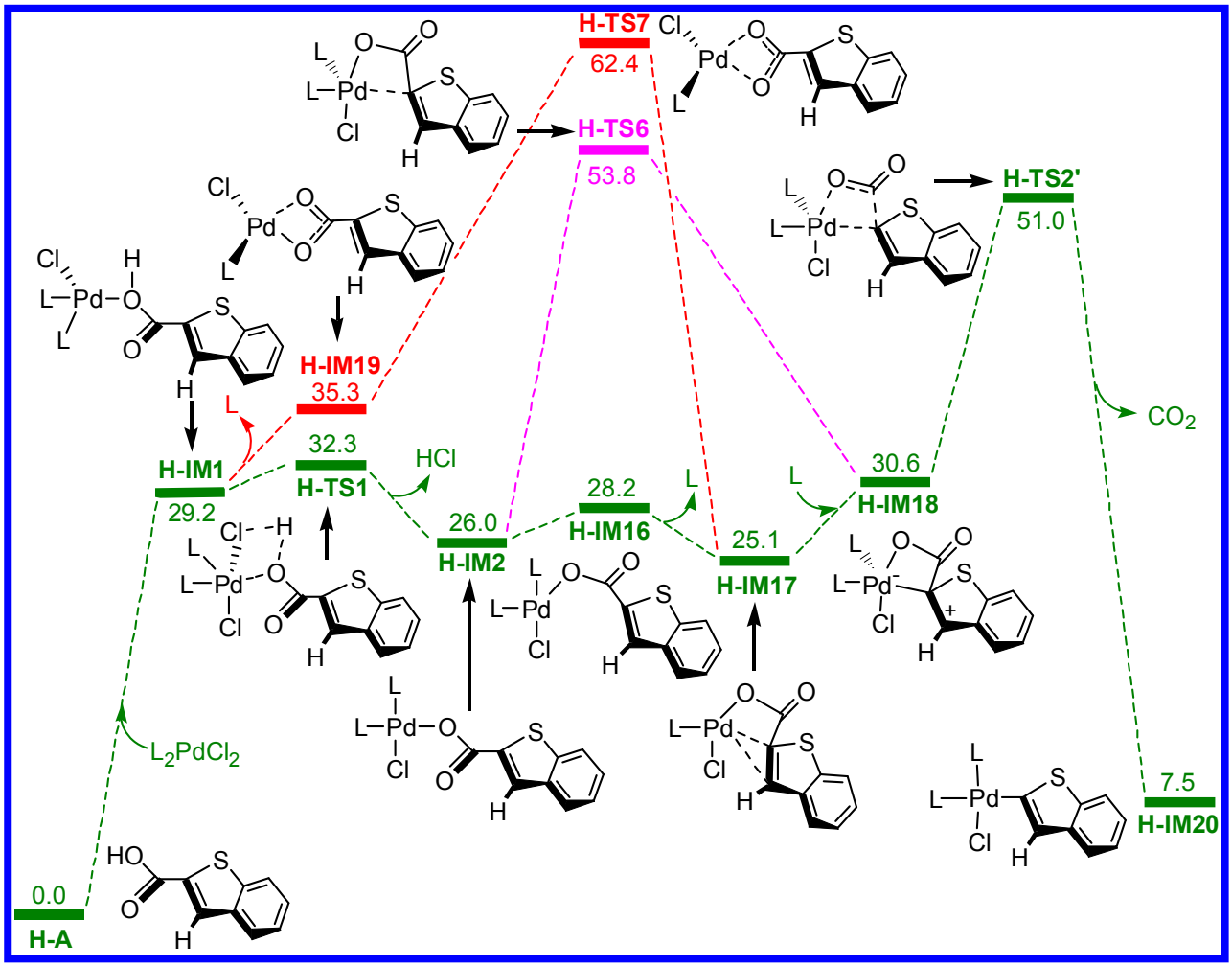

Figure S3. Calculated free energy profiles in DMF solution along various possible pathways for the metalation-depronation followed by the decarboxylation in the H-substituted system as well as schematic structures of intermediates and transition states involved (L =DMSO). The relative free energies are given in kcal/mol.

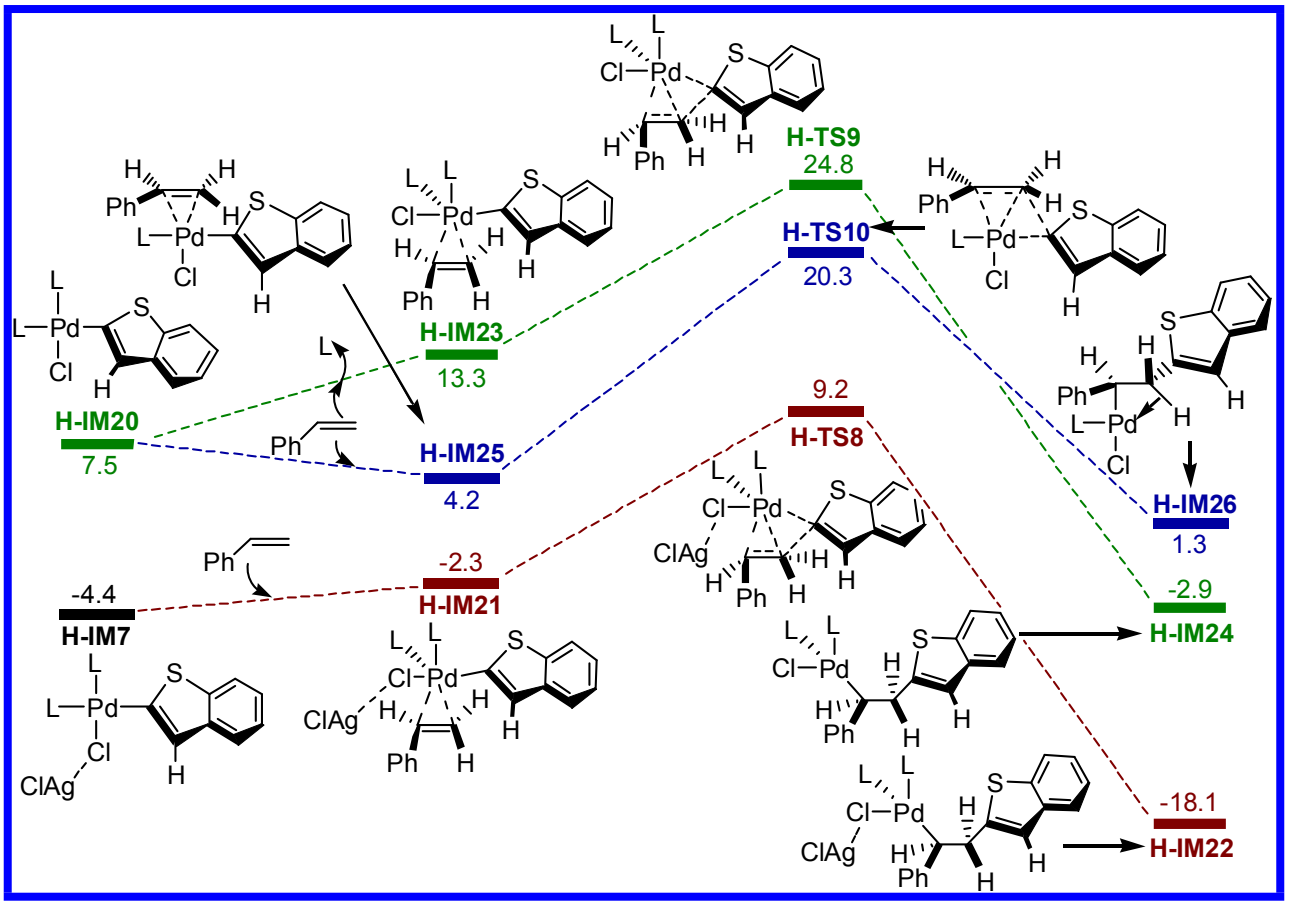

Figure S4. Calculated free energy profiles in DMF solution along various possible pathways for the olefin insertion in the H-substituted system as well as schematic structures of intermediates and transition states involved (L =DMSO). The relative free energies are given in kcal/mol.

Cartesian Coordinates for the Stationary Points Given in Figure 1.

A

C	-1.29021400	-0.94208200	0.00020200
C	-1.06790100	0.44568400	0.00015400
C	-2.16400100	1.31888400	0.00024700
C	-3.44112800	0.79352200	0.00038700
C	-3.64640500	-0.59477400	0.00044200
C	-2.57625500	-1.47446100	0.00035100
C	0.33084200	0.75330400	-0.00000400
H	-1.99374900	2.39253800	0.00020100
H	-4.29855800	1.46127100	0.00045100
H	-4.66007100	-0.98791400	0.00055400
H	-2.73240300	-2.55029400	0.00039300
Cl	0.86637300	2.42878100	-0.00005700
S	0.23599800	-1.86456600	0.00005900
C	1.16095700	-0.32466800	-0.00008600
C	2.62655200	-0.35091900	-0.00030600
O	3.09390500	-1.61487500	-0.00038400
H	4.05984800	-1.54126100	-0.00070200
O	3.34683700	0.61768700	-0.00076500

IM1

C	-4.21386400	-1.17703800	0.41624600
C	-4.60812600	0.07416600	-0.08810700
C	-5.96266000	0.30926700	-0.37135300
C	-6.87765800	-0.69951300	-0.14870100
C	-6.46649100	-1.94545500	0.35366900
C	-5.13619800	-2.19689200	0.63976100
C	-3.48696100	0.94654300	-0.23743500
H	-6.27103000	1.27590400	-0.76256600
H	-7.92910700	-0.53043300	-0.36580000
H	-7.20522500	-2.72581500	0.51939300
H	-4.81399700	-3.15985500	1.02726600
Cl	-3.73164000	2.58046100	-0.84154000
S	-2.46444400	-1.27703600	0.70739800
C	-2.28155100	0.41724700	0.12922100
C	-0.97773800	1.07225600	0.06614600
O	0.05792700	0.45525100	0.68847200
Pd	1.85404000	0.03968500	-0.37202400
O	3.01038400	1.06348800	1.03218900
O	3.57474400	-0.49917100	-1.25660600
S	2.98855600	2.70103000	0.96723800

S	4.20080900	-1.92499800	-0.69279700
C	1.39622000	3.19316500	1.79758100
H	1.44877600	4.27095700	1.96870400
H	0.56080000	2.91456200	1.14956600
H	1.38136000	2.64102700	2.73893400
C	2.55310500	3.12984700	-0.79248800
H	1.52586900	2.80219000	-0.99182800
H	2.66317300	4.21354000	-0.88874000
H	3.27803000	2.60149700	-1.41613000
C	4.28438300	-1.75304500	1.15942000
H	4.82733700	-0.82614500	1.34879300
H	3.26121600	-1.72203100	1.56365400
H	4.84050900	-2.62613100	1.51133500
C	2.83826800	-3.18821500	-0.82382200
H	2.43462700	-3.08457400	-1.83290700
H	3.32114700	-4.15695400	-0.66940200
H	2.07509800	-2.96678200	-0.06326800
Cl	0.80634700	-1.99317300	1.90665800
O	-0.76789600	2.14158300	-0.46433000
Cl	0.59282900	-0.97913300	-2.07832400
H	0.00308200	-0.45227300	1.19255100

TS1

C	4.40694200	-1.32215600	-0.05881600
C	4.69585100	0.05319300	-0.01302500
C	6.02200000	0.48494000	-0.15500300
C	7.01777400	-0.45538100	-0.33052100
C	6.71383800	-1.82542400	-0.36977200
C	5.40998400	-2.27180300	-0.23459000
C	3.50836000	0.82399000	0.19009000
H	6.24672300	1.54828400	-0.12214800
H	8.05001300	-0.13282500	-0.43904000
H	7.51311800	-2.54901200	-0.50983500
H	5.17098800	-3.33160900	-0.26729800
Cl	3.58942200	2.58794400	0.23814400
S	2.66600400	-1.65234200	0.12632900
C	2.35799400	0.10663200	0.28975100
C	0.99209600	0.60289300	0.51512000
O	0.03717700	-0.17294900	0.03946300
Pd	-1.97702400	-0.00584600	0.45194300
O	-2.28991500	1.27727800	-1.17255500
O	-3.98592800	-0.08347100	0.66519800
S	-2.26150600	2.89765800	-0.90042800

S	-4.68996800	-1.27158000	-0.24251100
C	-0.50406900	3.36604400	-1.28494800
H	-0.44145800	4.45602700	-1.23920100
H	0.15072300	2.88512000	-0.55223000
H	-0.32460000	3.00393400	-2.29840100
C	-2.22648100	3.11126000	0.94736700
H	-1.35372100	2.56895000	1.33138300
H	-2.15954000	4.18698800	1.13466400
H	-3.16749400	2.70395400	1.32324500
C	-4.08623500	-1.03089500	-1.98891900
H	-4.29279500	0.00954600	-2.24085400
H	-3.01045900	-1.24619400	-2.03372300
H	-4.67094400	-1.72258800	-2.60126800
C	-3.78591000	-2.85265800	0.15244500
H	-3.72161600	-2.89887800	1.24124700
H	-4.40174100	-3.65555900	-0.26145400
H	-2.78578300	-2.81641500	-0.29701600
Cl	-0.55283300	-2.11205900	-1.78560400
O	0.75401800	1.65223000	1.08748300
Cl	-1.65777000	-1.38221500	2.32290100
H	0.01358900	-1.04152000	-0.78594600

IM2

C	4.46188400	-1.39553700	-0.41286700
C	4.67374100	-0.10727900	0.10842900
C	5.98238200	0.37668300	0.23470400
C	7.03809800	-0.42715300	-0.15198300
C	6.81112700	-1.71265000	-0.66639100
C	5.52407600	-2.20702200	-0.80121000
C	3.43111300	0.52614500	0.44234000
H	6.14755600	1.37372600	0.63604200
H	8.05696300	-0.06018900	-0.05598300
H	7.65609300	-2.32946300	-0.96320200
H	5.34340900	-3.20193900	-1.20098500
Cl	3.44277700	2.17242100	1.09567300
S	2.73005300	-1.80226900	-0.50420800
C	2.31355400	-0.20647200	0.20169300
C	0.88094300	0.12833000	0.41336700
O	0.09028800	-0.70920400	-0.16291000
Pd	-1.86034400	-0.25992500	-0.01972200
O	-1.58133900	1.25442700	-1.40632800
O	-3.84652700	0.35016600	0.05964200
S	-1.76645000	2.82657500	-0.94616900

S	-5.07132700	-0.61918900	-0.44466200
C	-0.00478700	3.42564000	-0.89736800
H	-0.02771500	4.48348500	-0.62308900
H	0.53488200	2.80777500	-0.16993100
H	0.37676800	3.29337800	-1.91080000
C	-2.10047200	2.79326700	0.88249800
H	-1.29671900	2.19769500	1.33171600
H	-2.10153100	3.83391500	1.21916000
H	-3.08022100	2.32668200	1.00120000
C	-4.26609800	-1.96975800	-1.43388200
H	-3.75864400	-1.46956300	-2.26157800
H	-3.55333300	-2.48697600	-0.78153600
H	-5.06723400	-2.62081100	-1.79444600
C	-5.53785000	-1.58436000	1.07544500
H	-5.99204700	-0.86467200	1.75762100
H	-6.26252700	-2.34242200	0.76672600
H	-4.61425600	-2.00698100	1.48742500
Cl	-2.15530900	-2.13947500	1.39497500
O	0.56316600	1.12235600	1.06957100

IM3

C	-1.02376300	2.29752000	-1.13320300
C	-1.61759200	2.52130500	0.11880600
C	-2.24325500	3.74752400	0.37038300
C	-2.26490300	4.70689500	-0.62516200
C	-1.66990100	4.46409700	-1.87075800
C	-1.04235800	3.25679200	-2.13821300
C	-1.49007200	1.37426400	0.96972400
H	-2.70682000	3.92336000	1.33818500
H	-2.75453000	5.65989100	-0.44275800
H	-1.70563100	5.22961700	-2.64185900
H	-0.58785500	3.06128500	-3.10619300
Cl	-2.13697500	1.37704300	2.61092900
S	-0.25906100	0.68116700	-1.22943200
C	-0.83167700	0.31889800	0.43962000
C	-0.65958700	-1.05102500	0.99816200
O	-1.67913100	-1.69627100	1.32281700
Pd	2.18791300	-0.69618600	0.36031300
O	3.92990100	0.03358200	-0.38448600
S	3.99877900	1.68329900	-0.43172500
C	5.23563100	2.03950800	0.90621700
H	5.58200000	3.06904900	0.78772300
H	4.68836000	1.89466800	1.83950900

H	6.04009300	1.30862500	0.79214700
C	5.12862500	1.82048000	-1.89628900
H	4.53761000	1.53385900	-2.76648000
H	5.47524200	2.85343700	-1.97366300
H	5.94817800	1.11639000	-1.73545800
Cl	2.18581100	0.91875500	2.08729000
O	0.49938500	-1.57789400	1.05952200
O	2.29787800	-1.99556800	-1.25868400
S	1.61086300	-3.48128600	-1.33851400
C	-0.24525100	-3.24723400	-1.37351400
H	-0.64748600	-4.07432100	-1.96204200
H	-0.64565300	-3.22992100	-0.35827000
H	-0.40988500	-2.29597900	-1.88909900
C	1.82902000	-4.23666000	0.34493900
H	2.90602600	-4.33529300	0.48898300
H	1.37187600	-3.56831100	1.07896500
H	1.34658800	-5.21699500	0.31504200
Ag	-3.47320400	-1.12193800	0.18609700
Cl	-5.13498800	-0.55989100	-1.38460600

IM4

C	2.98594000	2.21030600	-0.71750900
C	2.35158400	2.54243900	0.49189000
C	3.09815700	3.13940400	1.51499400
C	4.44358800	3.38943700	1.30827200
C	5.05930200	3.05728300	0.09331200
C	4.33613800	2.46666600	-0.93261900
C	0.96812500	2.16420900	0.46684300
H	2.61143800	3.39962200	2.45219600
H	5.02984400	3.85519500	2.09625200
H	6.11597300	3.26910500	-0.05024000
H	4.80775700	2.21143400	-1.87860600
Cl	-0.08522400	2.45838700	1.86056300
S	1.86987800	1.40248300	-1.86262500
C	0.54870700	1.54486300	-0.65838600
C	-0.82270200	1.02313800	-0.92999400
O	-1.00932100	-0.23509700	-0.96882100
Pd	0.40649200	-1.56212800	-0.33151000
O	0.16921200	-0.92744800	1.63589100
O	1.63292400	-3.01107300	0.42708400
S	-1.11375800	-1.47401400	2.50946100
S	3.21961100	-2.63915900	0.64666300
C	-1.41283000	-3.18840800	1.86145400

H	-2.26540100	-3.60010800	2.40739100
H	-1.61311100	-3.11668300	0.78740800
H	-0.49784700	-3.75330200	2.04766500
C	-2.58662700	-0.61653400	1.76586200
H	-2.61559500	-0.84964100	0.69803400
H	-3.48554500	-0.96848200	2.27811400
H	-2.42777400	0.45163400	1.93648500
C	3.94939800	-2.59304600	-1.06324200
H	3.98492000	-3.62645500	-1.41015900
H	3.28665000	-2.00042500	-1.70406800
H	4.95325300	-2.17130300	-0.96327100
C	3.24561000	-0.81655000	1.01726700
H	2.54489900	-0.66323800	1.84225000
H	4.27085100	-0.54438300	1.28408100
H	2.90553900	-0.29334300	0.11866100
Cl	0.85006200	-2.21812500	-2.54226500
O	-1.73145200	1.86234300	-1.06999500
Ag	-3.74319300	1.07766200	-0.74340400
Cl	-5.67444600	0.08504000	0.21400500

IM5

C	-3.47251200	-1.14221200	-0.89284800
C	-3.45054200	-0.47729300	0.34010800
C	-4.61715400	0.11823400	0.82435700
C	-5.76951900	0.04624500	0.06281300
C	-5.77008700	-0.61040700	-1.17371200
C	-4.62078200	-1.21043900	-1.66817700
C	-2.13279400	-0.47689900	0.93313900
H	-4.59848700	0.64430100	1.77543100
H	-6.68210700	0.51316300	0.42255000
H	-6.68431300	-0.64937500	-1.76036500
H	-4.61904500	-1.71783600	-2.62891000
Cl	-1.99398000	-0.23930400	2.69529300
S	-1.87732300	-1.85178200	-1.32605100
C	-1.17597800	-1.16864700	0.15552100
C	0.26550100	-1.39092400	0.48801300
O	0.75552500	-0.35028100	1.05928000
Pd	-0.62345800	0.97257600	0.15931300
O	0.76831400	2.46194100	-0.12326000
S	2.25624000	1.73410900	-0.32354400
C	3.13801900	3.07179100	-1.23952000
H	2.67190300	3.12997300	-2.22332000
H	3.00525300	4.00181600	-0.68262300

H	4.18198500	2.75611600	-1.30850200
C	3.00408200	1.95742800	1.35699800
H	2.44713800	1.28208500	2.00880100
H	4.05128400	1.65426400	1.27658300
H	2.85877200	3.00345900	1.63728500
Cl	-2.19640400	2.25839200	-0.98655900
O	0.89597100	-2.38728100	0.11446900
Ag	3.01655700	-1.65370800	-0.07987200
Cl	4.92320600	-0.24530800	-0.48649100

IM6

C	-3.76413500	-0.10546900	-0.97058800
C	-3.58564600	0.11840000	0.41114800
C	-4.52864700	0.87952200	1.12912500
C	-5.61717300	1.39031200	0.46203900
C	-5.78149000	1.16239600	-0.91896000
C	-4.86292200	0.42754400	-1.64488800
C	-2.39578100	-0.48284200	0.88038100
H	-4.37431000	1.05986300	2.18976400
H	-6.35398600	1.98204300	0.99786100
H	-6.64938400	1.57796900	-1.42570000
H	-4.99186900	0.26037500	-2.71105500
Cl	-2.07068000	-0.51383500	2.59571200
S	-2.48065800	-1.08403200	-1.68479700
C	-1.57103100	-1.10208600	-0.08178800
C	-0.71596000	-2.36208100	0.20859900
O	-0.02369700	-2.30230800	1.27403200
Pd	-0.01217600	0.37450600	-0.59156300
O	1.58871500	1.54730100	-1.16053900
S	1.71757000	3.13515500	-0.71035200
C	2.29257500	3.12970600	1.06179600
H	2.77617000	4.09708800	1.22540900
H	1.39515700	3.01609900	1.67034000
H	2.97686100	2.27970400	1.18546900
C	3.38437400	3.38290500	-1.48655200
H	3.24497500	3.25101900	-2.56010900
H	3.73207500	4.39172100	-1.25309300
H	4.04262600	2.61449000	-1.07092900
Cl	-0.90899400	2.14142700	0.72200700
O	-0.78519700	-3.27785600	-0.60072300
O	0.54658600	-0.96435700	-2.07540100
S	1.93219300	-1.78735500	-2.36972500
C	2.28142400	-2.94252000	-0.95276000

H	3.05252600	-3.62218600	-1.32553900
H	2.64059000	-2.36439900	-0.09513600
H	1.33861700	-3.46201800	-0.74256600
C	3.34939100	-0.60644900	-2.13757300
H	3.22772200	0.17061400	-2.89312400
H	3.31922600	-0.19203400	-1.12350900
H	4.25265200	-1.19815800	-2.31102600
Ag	1.54621400	-0.86205600	1.62977600
Cl	3.80506200	0.01055900	1.49607500

TS2

C	-3.90963700	0.95587100	0.53425800
C	-3.70187200	-0.40891900	0.23588900
C	-4.72403600	-1.34586900	0.48606200
C	-5.91181600	-0.90831500	1.02476100
C	-6.10342600	0.45569300	1.32138100
C	-5.11439400	1.39249300	1.08401300
C	-2.41032500	-0.61697400	-0.29790700
H	-4.55834200	-2.39527400	0.25652100
H	-6.71013500	-1.61746700	1.22493100
H	-7.05097700	0.77915300	1.74591400
H	-5.26894100	2.44373200	1.31213000
Cl	-1.95606900	-2.25552200	-0.78348500
S	-2.51602300	1.95729500	0.11760700
C	-1.57784800	0.49643900	-0.48904400
C	-1.06028500	0.61686400	-2.19141300
O	-0.25636500	-0.28391200	-2.46265300
Pd	0.26657500	0.66326100	0.47026900
O	2.20284600	0.83461800	1.29119000
S	2.50083100	0.18589900	2.78093500
C	2.98878800	-1.57677600	2.44490600
H	3.59952600	-1.90029000	3.29247000
H	2.05595100	-2.13764400	2.37643800
H	3.51834500	-1.60541400	1.48421100
C	4.20852500	0.87904900	2.98281700
H	4.09724900	1.96116100	3.06256300
H	4.64563000	0.46300000	3.89346800
H	4.77802200	0.59942900	2.09269400
Cl	-0.35816000	-1.00962200	2.03606700
O	-1.59060900	1.53239300	-2.75515500
O	0.57433400	2.34627200	-0.71795700
S	1.87160600	2.62705100	-1.67964300
C	2.68031400	0.98864300	-2.01470400

H	3.63275200	1.20849100	-2.50505700
H	2.82131600	0.46169600	-1.06351900
H	2.00681100	0.44843000	-2.68437900
C	3.11309300	3.31550300	-0.47922600
H	2.71184300	4.27459000	-0.14910900
H	3.17758400	2.60168100	0.34592900
H	4.05962100	3.44574600	-1.00991600
Ag	0.97098600	-1.70716300	-1.10373200
Cl	3.28941500	-2.41282300	-0.87780600

IM7

C	-4.13075900	-0.79090600	-0.53614100
C	-3.75672900	0.44502700	0.01899500
C	-4.75129900	1.36616300	0.36520600
C	-6.07926400	1.03871700	0.14882900
C	-6.43493500	-0.19612400	-0.40763000
C	-5.46164700	-1.12261300	-0.75533300
C	-2.32814200	0.53364100	0.13523300
H	-4.47250400	2.32580900	0.79489900
H	-6.85657100	1.75148300	0.41339100
H	-7.48351000	-0.43267000	-0.57128200
H	-5.72961500	-2.08325500	-1.18847300
Cl	-1.58868000	2.03250000	0.82248100
S	-2.69356400	-1.80862800	-0.89505600
C	-1.60048000	-0.52241800	-0.28342500
Pd	0.32167200	-0.89297100	-0.30368600
O	2.42345200	-1.37059600	-0.03762700
S	3.68183800	-1.33483100	-1.07383700
C	3.00454000	-2.02301700	-2.65890400
H	2.76418000	-3.06795000	-2.45746900
H	2.11236400	-1.44998100	-2.92641700
H	3.79070300	-1.93878000	-3.41353800
C	3.94341500	0.43833100	-1.57289900
H	4.01793800	1.01072400	-0.63867100
H	4.88076600	0.45787700	-2.13539900
H	3.08920900	0.76775500	-2.17035300
Cl	0.45369500	0.49881300	-2.29739300
O	-0.05171200	-2.14596000	1.31564200
S	0.49644500	-1.80680200	2.82666700
C	0.88469800	0.00655900	2.86003000
H	1.25447000	0.23157400	3.86441100
H	1.64307600	0.23054200	2.10002600
H	-0.05327100	0.53351300	2.66530700

C	2.23837600	-2.46126500	2.82770400
H	2.15376400	-3.54854900	2.82202000
H	2.71450700	-2.08611400	1.91543000
H	2.71661800	-2.10841800	3.74514400
Ag	1.09397900	1.98002300	-0.21273200
Cl	2.97897800	2.43845800	1.26023000

IM8

C	-3.99656600	1.58680900	0.45320200
C	-4.00498400	0.32479800	-0.16509800
C	-5.23116300	-0.28025900	-0.46097900
C	-6.40414800	0.38088200	-0.13796700
C	-6.37625700	1.63904600	0.47632200
C	-5.16948500	2.25478100	0.77825600
C	-2.66461000	-0.14150800	-0.39388700
H	-5.24892200	-1.25834100	-0.93679100
H	-7.36067900	-0.08425600	-0.36287900
H	-7.30921300	2.14042500	0.72180000
H	-5.14038500	3.23016200	1.25772900
Cl	-2.37622200	-1.74542900	-1.14617600
S	-2.31652200	2.15815800	0.74824800
C	-1.65523600	0.66059300	0.00110400
Pd	0.29029500	0.33151800	-0.05311200
O	2.34300000	-0.16664000	-0.41334700
S	3.59753900	-0.33865600	0.61246900
C	3.23230800	0.82833700	2.01194700
H	3.27905100	1.83431900	1.58462000
H	2.23615100	0.59775200	2.40374600
H	4.01097400	0.68638400	2.76592200
C	3.35084000	-1.97559700	1.46448600
H	3.20381500	-2.71572800	0.66483200
H	4.26567300	-2.16596200	2.03199400
H	2.46513700	-1.91243400	2.10191900
Cl	0.00260600	-0.87103400	2.05205600
Ag	0.20656500	-2.62933300	0.08148800
Cl	1.78259900	-4.09787200	-0.99840900
C	1.66259700	3.77430100	-0.14180300
C	1.75076500	2.75557800	-1.09989800
C	3.00594700	2.42420400	-1.62684600
C	4.14465600	3.08404800	-1.18622200
C	4.04888300	4.07996000	-0.21426000
C	2.80425300	4.42754100	0.30585100
H	0.68450400	4.03664400	0.26198400

H	3.08890900	1.64415100	-2.37864200
H	5.11377400	2.82319300	-1.60462400
H	4.94410800	4.59530000	0.12591500
H	2.72229000	5.21195800	1.05408400
C	0.51706200	2.06399400	-1.48615900
H	-0.39776700	2.63767600	-1.32138600
C	0.39855100	0.86407900	-2.16999400
H	1.26933900	0.29965400	-2.50159300
H	-0.56234800	0.58315300	-2.59541800

TS3

C	4.23690500	-0.98662700	-0.18956800
C	3.83159800	0.31792800	-0.51947000
C	4.79051600	1.33635000	-0.58422200
C	6.11373000	1.03218000	-0.31728700
C	6.49867000	-0.27306400	0.01553900
C	5.56264200	-1.29530800	0.08534400
C	2.41808100	0.38044900	-0.74406800
H	4.48523400	2.34954000	-0.83535200
H	6.86442400	1.81683700	-0.36399800
H	7.54351800	-0.49018500	0.22332700
H	5.85521900	-2.30921100	0.34607400
Cl	1.64909100	1.91300000	-1.22041600
S	2.84570200	-2.11871900	-0.15851600
C	1.71424800	-0.77094400	-0.58733200
C	0.49303000	-1.20653200	-2.17867300
Pd	-0.16512600	-1.17633900	0.04604000
O	-1.98699400	-2.15978000	0.62857800
S	-3.27757600	-1.65795400	1.48693100
C	-3.49005800	0.16367700	1.19606800
H	-4.38478900	0.46081700	1.74968100
H	-2.60530400	0.70025000	1.55446800
H	-3.62733600	0.31131600	0.12165400
C	-2.68142800	-1.59975500	3.24862800
H	-1.75313500	-1.01971500	3.27623100
H	-3.48007300	-1.15198300	3.84583100
H	-2.50597200	-2.63544400	3.54215000
Cl	0.46584000	-0.27030400	2.32842100
C	-0.83403100	-1.63815700	-1.92100800
H	0.63775500	-0.22864900	-2.63630600
H	1.21301300	-1.96661100	-2.47170000
C	-2.03604700	-0.82958100	-2.14362600
C	-3.27034600	-1.49005100	-2.24012900

C	-2.01134200	0.57110800	-2.21094500
C	-4.44489400	-0.77154700	-2.41388700
H	-3.29527800	-2.57604400	-2.16600000
C	-3.18997600	1.29007900	-2.36380200
H	-1.07707400	1.11848900	-2.09257600
C	-4.40777400	0.62133300	-2.47274900
H	-5.39370500	-1.29677300	-2.49662100
H	-3.14703400	2.37585400	-2.35578000
H	-5.32899400	1.18629800	-2.59365300
H	-1.00410300	-2.71671200	-1.87009000
Ag	-0.40628700	1.76203300	1.13807100
Cl	-1.83612200	3.41399400	0.14960400

IM9

C	-4.69014700	-0.99670100	0.33592200
C	-4.91989800	0.31421900	-0.11315700
C	-6.23228000	0.73544100	-0.35204800
C	-7.27191100	-0.15243800	-0.13974800
C	-7.02409400	-1.45701500	0.30776800
C	-5.72988900	-1.89270400	0.55078900
C	-3.68606300	1.03279100	-0.25789500
H	-6.41667500	1.74855600	-0.70167700
H	-8.29496700	0.16495000	-0.32417000
H	-7.85545400	-2.13938600	0.46551600
H	-5.53215600	-2.90444900	0.89566000
Cl	-3.66478100	2.71608400	-0.81637600
S	-2.94417900	-1.32392200	0.57057900
C	-2.56120000	0.35257700	0.05490900
C	-1.15088100	0.80722000	0.00711100
Pd	0.53845300	-0.85309000	0.24634700
O	1.50800400	-1.50986700	2.03943200
S	3.13048700	-1.60054800	2.17982100
C	3.83271200	-0.28849200	1.06554300
H	4.92105900	-0.38161300	1.11022500
H	3.45327000	-0.45291300	0.04967600
H	3.50178100	0.67830900	1.45636900
C	3.59647600	-3.10014800	1.18436100
H	3.12388800	-3.01748900	0.19861600
H	4.68762000	-3.13030300	1.12768500
H	3.20957200	-3.95848100	1.73496400
Cl	1.44158800	-2.43890000	-1.58869400
C	-0.37035000	0.67064900	1.26601800
H	-0.62735600	0.16495100	-0.83052500

H	-1.07665300	1.80365500	-0.44763200
C	0.69004100	1.59729600	1.65318200
C	1.13794200	1.58131100	2.98599600
C	1.34797600	2.42312300	0.72763200
C	2.21300300	2.36486300	3.37915300
H	0.63753200	0.93200700	3.70213900
C	2.43377700	3.19370400	1.12113400
H	1.06261800	2.43919200	-0.32368000
C	2.86702200	3.17038500	2.44554700
H	2.54465000	2.34913000	4.41474400
H	2.94767600	3.79384500	0.37455800
H	3.71434600	3.77975300	2.75150700
H	-0.90118300	0.20599500	2.10380900
Ag	2.13477600	-0.14712000	-2.21969100
Cl	2.80311900	2.12370100	-2.44313100

TS4

C	-4.55278900	-1.35027200	0.12678200
C	-4.52100100	0.05398100	0.16496500
C	-5.68012900	0.77552200	-0.14382600
C	-6.83145600	0.08499400	-0.47625200
C	-6.84646300	-1.31604200	-0.50479600
C	-5.70787600	-2.04851300	-0.20213400
C	-3.22166700	0.52807400	0.53082100
H	-5.65899300	1.86252900	-0.11972200
H	-7.73642800	0.63556200	-0.71951800
H	-7.76223600	-1.83886900	-0.76907600
H	-5.71565800	-3.13503900	-0.22567400
Cl	-2.84261100	2.25147100	0.58565200
S	-2.96846900	-2.06854800	0.54866300
C	-2.28248800	-0.42077100	0.77416300
C	-0.88382700	-0.20951400	1.12871300
Pd	0.49609700	-0.48493200	-0.64785500
O	1.56159000	-2.33390200	-1.07498200
S	3.16721500	-2.42215000	-1.32285800
C	3.90274400	-0.83697500	-0.67942100
H	4.96787700	-0.86136200	-0.92541400
H	3.38878600	-0.00094700	-1.16523800
H	3.75149200	-0.83483100	0.40308200
C	3.34311700	-2.08543300	-3.14611600
H	2.83831400	-1.13875000	-3.36064600
H	4.41049200	-2.05875500	-3.37963300
H	2.85163800	-2.91880300	-3.64961700

Cl	1.28813200	0.82555300	-2.68129500
C	0.03893600	-1.27693800	1.27375900
H	-0.37815600	0.74192700	-0.16392500
H	-0.70256700	0.70814500	1.69684700
C	1.29512800	-1.19956500	2.02558600
C	2.03077700	-2.37834900	2.21769600
C	1.81806100	0.01312100	2.49944000
C	3.26024600	-2.34591300	2.86417000
H	1.63283700	-3.31744700	1.83540200
C	3.05209300	0.04233100	3.13437000
H	1.29339900	0.95664700	2.34691400
C	3.77619800	-1.13452600	3.32167200
H	3.81677300	-3.26842100	3.01344400
H	3.44325700	0.99722200	3.47790900
H	4.73920200	-1.10835000	3.82639900
H	-0.31399100	-2.28967000	1.05936400
Ag	1.34428200	2.33906700	-0.66281500
Cl	1.40871300	3.41656700	1.46635900

IM10

C	-4.59845000	-1.19186900	0.15303600
C	-4.55016000	0.21034900	0.23871500
C	-5.70276700	0.95455700	-0.04056700
C	-6.86277500	0.28853200	-0.39246600
C	-6.89321800	-1.11029100	-0.47074700
C	-5.76156100	-1.86514500	-0.19757500
C	-3.24584100	0.65651200	0.61915900
H	-5.67018600	2.03974700	0.02227200
H	-7.76264700	0.85694300	-0.61250700
H	-7.81564300	-1.61353400	-0.74954000
H	-5.78127300	-2.95013100	-0.25851700
Cl	-2.85506400	2.37501200	0.74528900
S	-3.02318400	-1.94415500	0.54947800
C	-2.31578100	-0.31235600	0.83015500
C	-0.93384500	-0.12682900	1.21235800
Pd	0.37016900	-0.41375900	-0.63324800
O	1.23379300	-2.42910200	-0.80419000
S	2.81729700	-2.73539400	-1.01214500
C	3.75394200	-1.16101700	-0.66419000
H	4.80544600	-1.37796500	-0.87201200
H	3.36064700	-0.37445600	-1.31512900
H	3.60699200	-0.92793400	0.39357900
C	3.00045200	-2.75235100	-2.86515700

H	2.58336600	-1.81647300	-3.24629200
H	4.06212100	-2.86732700	-3.09765900
H	2.42627700	-3.61188800	-3.21277200
Cl	1.30852100	0.47194600	-2.76764100
C	-0.02004900	-1.15671100	1.41539000
H	-0.26866300	0.99733400	-0.56847400
H	-0.70939500	0.86959700	1.59692700
C	1.26339500	-1.03627600	2.11237500
C	1.98300900	-2.20845600	2.38557700
C	1.82008500	0.20105300	2.46993500
C	3.22831000	-2.14718400	2.99961300
H	1.55717600	-3.16842900	2.09663100
C	3.07063000	0.25946900	3.06924200
H	1.30792800	1.13755300	2.25097200
C	3.77759900	-0.91204500	3.33867500
H	3.77184800	-3.06475200	3.21350400
H	3.49044100	1.23206400	3.31449900
H	4.75489700	-0.86165700	3.81308000
H	-0.34850500	-2.18151200	1.22470200
Ag	1.60678200	2.19656500	-0.89082300
Cl	1.98352200	3.52028400	1.05528500

P

C	-3.01774200	-0.97809200	0.05675400
C	-2.74828800	0.39944300	-0.01478200
C	-3.82023000	1.30094600	-0.04818900
C	-5.11381400	0.81378200	-0.00795100
C	-5.36292400	-0.56354300	0.06568800
C	-4.31576300	-1.47246400	0.09916700
C	-1.34088200	0.65809700	-0.04688900
H	-3.62129100	2.36828400	-0.10479900
H	-5.94962200	1.50842200	-0.03324500
H	-6.38760100	-0.92540400	0.09652900
H	-4.50126000	-2.54225500	0.15586400
Cl	-0.76497600	2.33553200	-0.16417800
S	-1.51296700	-1.93556600	0.08433300
C	-0.51659200	-0.42692500	-0.00416100
C	0.91097300	-0.62171500	-0.02365500
C	1.87492600	0.31769600	0.05178100
C	3.31006800	0.06287500	0.02241700
C	3.86739700	-1.19522100	-0.25421700
C	4.18325600	1.12908000	0.27981200
C	5.24143000	-1.37724000	-0.25712400

H	3.22069000	-2.03964000	-0.48367200
C	5.55986800	0.94730900	0.27740500
H	3.76370600	2.11249300	0.48802500
C	6.09506300	-0.30837000	0.01098300
H	5.65353900	-2.35990300	-0.47524600
H	6.21677400	1.78913800	0.48347700
H	7.17247000	-0.45503100	0.00594100
H	1.21219100	-1.66822900	-0.09337700
H	1.59198800	1.36320200	0.15997700

Cartesian Coordinates for the Stationary Points Given in Figure 2.

IM11

C	-4.34341600	-1.99772000	0.60172200
C	-4.62213900	-0.86628400	-0.18398400
C	-5.95392600	-0.47974200	-0.38795900
C	-6.96424200	-1.22466200	0.18817600
C	-6.66906900	-2.35385900	0.96750900
C	-5.35958400	-2.75108400	1.18212500
C	-3.41932800	-0.26419300	-0.67615600
H	-6.17199800	0.39655900	-0.99345900
H	-8.00056700	-0.93450300	0.03648800
H	-7.47996800	-2.92555400	1.41214500
H	-5.12738700	-3.62428300	1.78633300
Cl	-3.52136800	1.19414300	-1.66628300
S	-2.59289500	-2.29874500	0.74197300
C	-2.26174800	-0.87653700	-0.30296700
C	-0.86404900	-0.50986400	-0.59545900
O	0.03006100	-1.18614900	0.03385900
Pd	1.96338100	-0.44190800	-0.12644800
O	1.26582800	1.24729300	0.77251100
O	2.29255800	-2.16060600	-1.17398500
S	2.27629300	2.05204800	1.82187500
S	3.52389100	-3.22179300	-0.94249200
C	0.98478900	2.85522800	2.88369700
H	1.51398900	3.45316200	3.62989300
H	0.34277700	3.46955100	2.23858900
H	0.43907500	2.03577400	3.35349600
C	2.82034100	3.51263700	0.81282200
H	1.92158700	4.04045200	0.46878800
H	3.44335200	4.13068900	1.46466900
H	3.40544800	3.08374700	-0.00268100
C	4.92142500	-2.49549300	-1.92817900
H	4.60789900	-2.55560300	-2.97110000

H	5.05485700	-1.45881600	-1.60785700
H	5.80364300	-3.11498500	-1.74745200
C	4.16897100	-2.95974000	0.78018000
H	3.34153700	-3.22787300	1.44239200
H	5.01087200	-3.64712200	0.89885800
H	4.46314000	-1.91046300	0.88010200
Cl	0.76113600	-3.91255300	1.29319400
O	-0.61307200	0.40516400	-1.40048900
Cl	4.19137200	0.41383400	-0.17376300
H	0.33464000	-2.81743900	0.68432300
Ag	-0.60941600	2.47915000	-0.67262100
Cl	-0.50900200	4.71237100	0.22981000

IM12

C	4.83880300	0.87260200	0.59227600
C	4.81505600	-0.42434600	0.05131400
C	6.01231300	-1.14261400	-0.06341200
C	7.19164400	-0.55644500	0.35545900
C	7.19804800	0.74020700	0.89004800
C	6.02390300	1.46611100	1.01420800
C	3.48584300	-0.81578500	-0.32127900
H	5.99586800	-2.14660600	-0.48021500
H	8.12588500	-1.10505500	0.26880400
H	8.13670000	1.18339800	1.21365600
H	6.02568200	2.47069500	1.42966300
Cl	3.20082700	-2.42028100	-0.99170200
S	3.20723600	1.59127300	0.65918400
C	2.51937900	0.11007600	-0.09035100
C	1.06264500	0.05603400	-0.34018500
O	0.39463900	0.96538700	0.25833400
Pd	-1.61215700	1.17643900	-0.16792300
O	-1.96509700	-0.52604700	0.89303800
O	-1.05073000	2.70901500	-1.38614300
S	-3.46246900	-0.75342100	1.59076900
S	-0.83340400	4.20233100	-0.74494700
C	-3.00874800	-2.18618900	2.67777100
H	-3.91354100	-2.47638700	3.21757700
H	-2.63069400	-2.99359800	2.03629500
H	-2.24652700	-1.80931200	3.36083600
C	-4.44553800	-1.65095100	0.29204700
H	-3.90276300	-2.56437100	0.01880100
H	-5.41838400	-1.86317400	0.74396300
H	-4.54355500	-0.94109200	-0.53132800

C	-2.54320600	4.81257800	-0.34071700
H	-3.04323100	4.96631700	-1.29783700
H	-3.06435000	4.03797800	0.23068400
H	-2.42571700	5.75337400	0.20348400
C	-0.21154000	3.92264400	0.98308400
H	0.72366400	3.36740300	0.88558700
H	-0.06168400	4.90657000	1.43458700
H	-0.95346100	3.32131400	1.51801700
Cl	-3.90970800	1.67445800	-0.46833500
O	0.61886900	-0.82497200	-1.09793400
Ag	-0.81683500	-2.39192900	-0.60872100
Cl	-2.14102000	-4.32808900	-0.04221200

IM13

C	-5.17863700	-1.18989600	-0.25654400
C	-5.23877700	0.20898000	-0.13792000
C	-6.48722500	0.84324600	-0.08037700
C	-7.63421700	0.07598900	-0.14166600
C	-7.55858400	-1.32009200	-0.26171500
C	-6.33367300	-1.96471400	-0.32029800
C	-3.92787200	0.78775900	-0.08879200
H	-6.53532600	1.92547500	0.01203100
H	-8.60766700	0.55765900	-0.09671200
H	-8.47357300	-1.90571200	-0.30883700
H	-6.27112300	-3.04609400	-0.41328600
Cl	-3.76155600	2.53663400	0.06383300
S	-3.50016700	-1.78417900	-0.30593200
C	-2.89764800	-0.09718500	-0.16286300
C	-1.43449800	0.12241300	-0.13180300
O	-1.01063500	1.29006000	-0.05654300
Pd	1.26282100	-1.05402800	-0.32910200
O	3.29037000	-1.25182600	-0.35358500
S	4.12321200	-0.99402800	-1.76456300
C	4.48181000	0.83316600	-1.76637500
H	5.44450300	0.97282900	-2.26537300
H	3.66259900	1.30009800	-2.31442400
H	4.47851100	1.16676300	-0.71982200
C	5.75581900	-1.57311600	-1.10688000
H	5.63561200	-2.63367500	-0.88473300
H	6.51691800	-1.41176700	-1.87349200
H	5.95788600	-0.99885900	-0.19906300
Cl	1.21781500	0.08678600	-2.41595700
O	-0.75850600	-0.96401000	-0.15478600

O	1.28768900	-2.20321600	1.37726800
S	1.64471100	-1.57799100	2.84711000
C	0.62232500	-0.03741700	3.01722900
H	0.74623100	0.31300600	4.04500900
H	0.97789800	0.70896100	2.29687900
H	-0.40805500	-0.33874900	2.82076200
C	3.33056500	-0.80918300	2.70763900
H	4.02266600	-1.63478200	2.53627900
H	3.33742700	-0.08625600	1.88368100
H	3.52124000	-0.32148200	3.66774700
Ag	1.11588600	1.86858500	0.03386000
Cl	3.23233200	2.40868500	1.10613100

Cartesian Coordinates for the Stationary Points Given in Figure 3.

H-A

C	-1.08389700	-0.63590500	0.00017100
C	-0.97109000	0.77042000	0.00012000
C	-2.14238000	1.54452100	0.00022800
C	-3.37294700	0.91617000	0.00038800
C	-3.46096300	-0.48456600	0.00044200
C	-2.32141000	-1.27255500	0.00033500
C	0.39085400	1.20377700	-0.00005800
H	-2.06865200	2.62999200	0.00018200
H	-4.28330000	1.51027700	0.00047300
H	-4.43897800	-0.95985100	0.00058200
H	-2.39041100	-2.35724500	0.00039000
S	0.51236400	-1.43159800	0.00006200
C	1.28579800	0.18363000	-0.00016400
C	2.73876700	0.35659000	-0.00040700
O	3.40005800	-0.81447000	-0.00049300
H	4.34301000	-0.59200900	-0.00065200
O	3.29362100	1.43214000	-0.00052700
H	0.71469100	2.24056300	-0.00014100

H-IM1

C	-4.54045100	-0.58185900	0.37037100
C	-4.74389900	0.60624200	-0.36207800
C	-6.04218200	0.92880600	-0.79221900
C	-7.08714600	0.08049500	-0.48747400
C	-6.86237100	-1.09791300	0.24382500
C	-5.59283500	-1.44118700	0.67718000
C	-3.53356200	1.33240000	-0.55484500

H	-6.20954300	1.84231700	-1.35902300
H	-8.09502100	0.32264200	-0.81493800
H	-7.69945700	-1.75270500	0.47399200
H	-5.41941600	-2.35391000	1.24139000
S	-2.83369400	-0.81304900	0.82077200
C	-2.44404700	0.73678800	0.00421100
C	-1.10708600	1.31126000	-0.07593000
O	-0.10926200	0.70794300	0.61653900
Pd	1.63331000	0.02990600	-0.39797600
O	2.88218100	1.04898900	0.92630300
O	3.29243600	-0.74115900	-1.22584700
S	2.99953400	2.67193400	0.73268200
S	3.78702900	-2.16232300	-0.53337600
C	1.44280400	3.36781900	1.48039000
H	1.59168600	4.44682100	1.56698900
H	0.59598300	3.11313800	0.83699800
H	1.35955600	2.89863200	2.46242400
C	2.62861600	2.98793100	-1.06521600
H	1.58313300	2.72166200	-1.26040900
H	2.82209500	4.04875000	-1.24691300
H	3.31930100	2.35635900	-1.62885300
C	3.88886900	-1.83221700	1.29542100
H	4.55562100	-0.97696100	1.41045700
H	2.87692400	-1.62693500	1.67775600
H	4.31521200	-2.73864500	1.73401500
C	2.31708400	-3.30696400	-0.55506000
H	1.91093600	-3.24758500	-1.56686700
H	2.71798100	-4.29913700	-0.33050200
H	1.58600000	-2.96362800	0.19198600
Cl	0.41440800	-1.69029600	2.04782100
O	-0.84852500	2.32829300	-0.68764300
Cl	0.28178400	-1.00008700	-2.02425200
H	-0.24735900	-0.14948100	1.18290700
H	-3.45444300	2.27240200	-1.09268600

H-TS1

C	4.77151700	-0.75914300	-0.25847800
C	4.91883100	0.52653700	0.30163900
C	6.21266700	1.02945900	0.51602200
C	7.30631200	0.25842700	0.17451900
C	7.13605700	-1.01860200	-0.38346500
C	5.87171700	-1.53898400	-0.60514600
C	3.66106900	1.14303000	0.57561000

H	6.33992200	2.01925100	0.94989600
H	8.31048200	0.64160600	0.33799900
H	8.01014100	-1.61000400	-0.64561300
H	5.73893900	-2.52769600	-1.03691000
S	3.05988700	-1.21439300	-0.44652600
C	2.59127900	0.37283600	0.24331200
C	1.19714100	0.78033000	0.44262500
O	0.26955000	-0.07100700	0.04205900
Pd	-1.75120800	0.04747200	0.45462300
O	-2.08277100	1.21205800	-1.24892300
O	-3.75710700	-0.06470600	0.67504200
S	-2.24818500	2.83204300	-1.01651100
S	-4.42758800	-1.34492000	-0.12889000
C	-0.54779300	3.47334900	-1.40440800
H	-0.58443200	4.56320200	-1.33229100
H	0.14942400	3.03213000	-0.68485600
H	-0.34097600	3.15367800	-2.42668500
C	-2.23079600	3.09737500	0.82667200
H	-1.29670300	2.67358200	1.21676200
H	-2.29559500	4.17831300	0.98372300
H	-3.11237900	2.58768700	1.22149400
C	-3.85207400	-1.21794100	-1.89625500
H	-4.14108500	-0.22550400	-2.24276600
H	-2.76365200	-1.35816200	-1.93545400
H	-4.38552700	-2.00627300	-2.43450800
C	-3.46649500	-2.86152400	0.37229000
H	-3.38642600	-2.82299600	1.46062900
H	-4.06322500	-3.71153200	0.03028300
H	-2.47360900	-2.82898400	-0.09473900
Cl	-0.30645200	-2.16851400	-1.60302900
O	0.90420700	1.85622300	0.94503500
Cl	-1.41054500	-1.16179200	2.43378000
H	0.26934700	-0.99027600	-0.68189400
H	3.53643400	2.12836400	1.01499000

H-IM2

C	4.80504900	-0.86977200	-0.44885500
C	4.86394800	0.17296100	0.49889200
C	6.12062400	0.63195500	0.92191500
C	7.26749400	0.05922100	0.40411800
C	7.18649900	-0.97582800	-0.53929900
C	5.95756700	-1.44876800	-0.97252900
C	3.56307500	0.62044800	0.89493100

H	6.18087300	1.43434100	1.65487600
H	8.24291000	0.41235300	0.73033700
H	8.09937900	-1.41422800	-0.93607700
H	5.89242100	-2.25227100	-1.70242300
S	3.12225500	-1.30665900	-0.84506200
C	2.54832100	-0.04272700	0.28794600
C	1.10224600	0.21188200	0.48879900
O	0.34012400	-0.57853200	-0.18363400
Pd	-1.62328200	-0.21445400	-0.03425000
O	-1.37231100	1.42721400	-1.27343700
O	-3.62980100	0.33402200	0.04589400
S	-1.67149100	2.92763900	-0.66062400
S	-4.83638900	-0.64945500	-0.47387300
C	0.05172700	3.61183200	-0.51377500
H	-0.02637600	4.61564100	-0.08813300
H	0.61544100	2.91910300	0.12246100
H	0.44389900	3.64665600	-1.53102000
C	-2.01504100	2.68997600	1.15349000
H	-1.18187800	2.09353400	1.54639100
H	-2.06942100	3.69065600	1.59229600
H	-2.97124300	2.16539700	1.21765600
C	-4.01499500	-1.96158300	-1.50051100
H	-3.52520800	-1.43407900	-2.32166700
H	-3.28651300	-2.48041200	-0.86685600
H	-4.80848200	-2.61792100	-1.86819500
C	-5.27025100	-1.65449600	1.02956700
H	-5.73109800	-0.95723700	1.73034500
H	-5.98310400	-2.42067000	0.71364900
H	-4.33412900	-2.06741600	1.42244100
Cl	-1.86998400	-2.18937500	1.25783900
O	0.74980100	1.13305400	1.23678700
H	3.37313600	1.40975200	1.61609300

H-IM3

C	-4.69888500	0.62897300	0.04150800
C	-4.81098000	-0.75491900	-0.21228000
C	-6.05294200	-1.38154600	-0.02248300
C	-7.13376700	-0.63501400	0.40510200
C	-7.00078000	0.74057300	0.65136300
C	-5.78646300	1.38353700	0.47297600
C	-3.57578400	-1.32838100	-0.64623900
H	-6.15198200	-2.44804900	-0.21472900
H	-8.09860500	-1.11403400	0.55253000

H	-7.86342300	1.31171600	0.98634900
H	-5.68284900	2.44881300	0.66370700
S	-3.04825000	1.22821600	-0.26102300
C	-2.55855500	-0.43229400	-0.72531000
C	-1.17155000	-0.69315800	-1.12427000
O	-0.35676300	0.30001200	-1.13882400
Pd	0.68635600	0.93333400	0.58371600
O	0.68787700	2.78763600	-0.22196700
S	1.95181100	3.11184200	-1.23081900
C	3.49320900	2.58396100	-0.32744900
H	3.44559300	3.05861500	0.65476000
H	3.50369900	1.49124100	-0.24112200
H	4.33176000	2.95067700	-0.92528000
C	1.91850400	1.81030500	-2.57549200
H	0.86945500	1.51645900	-2.66848900
H	2.29365400	2.29393000	-3.47961900
H	2.54029100	0.95912400	-2.27385500
Cl	1.77233900	1.73726500	2.52553100
O	-0.84631100	-1.85539800	-1.46103600
O	0.69029200	-0.98138100	1.29696400
S	2.08418300	-1.38047100	2.10994800
C	2.17007400	-3.17185200	1.63616300
H	2.69004000	-3.19403000	0.67375400
H	2.73856400	-3.69889800	2.40654900
H	1.13897300	-3.52773500	1.56065400
C	1.39380000	-1.55354400	3.82204800
H	2.15156200	-2.02200200	4.45463500
H	1.18039900	-0.53093200	4.13988500
H	0.48266700	-2.15148600	3.74557700
Ag	1.36612100	-1.71285500	-1.51128600
Cl	3.69941600	-1.24339200	-1.07666000
H	-3.43442000	-2.37591700	-0.89588000

H-IM4

C	-3.30505800	2.12994700	0.29631700
C	-2.65352300	2.80170900	-0.75610100
C	-3.42303200	3.55894200	-1.65173200
C	-4.79428800	3.62673000	-1.48351700
C	-5.42196500	2.94826600	-0.42873900
C	-4.68386000	2.19535400	0.47226700
C	-1.23491800	2.59489900	-0.73582400
H	-2.93422900	4.08743100	-2.46763800
H	-5.39421700	4.21489100	-2.17342100

H	-6.50090600	3.01654100	-0.31246700
H	-5.16703800	1.67591800	1.29698900
S	-2.15535600	1.20781500	1.30932400
C	-0.80941400	1.77445800	0.25506800
C	0.60405500	1.39195500	0.49054900
O	0.91901900	0.20997000	0.85432300
Pd	-0.23513200	-1.41793300	0.41604700
O	0.17641400	-1.15754100	-1.61289400
O	-1.23754000	-3.11548800	-0.13583200
S	1.52105500	-1.91010200	-2.20106900
S	-2.81972700	-2.94472600	-0.54892200
C	1.64796300	-3.50602700	-1.25591700
H	2.51066700	-4.04285500	-1.65843500
H	1.76924000	-3.27154400	-0.19370600
H	0.71349500	-4.04376300	-1.42187700
C	2.93058500	-0.99658000	-1.40676000
H	2.72903400	-0.93964500	-0.33272100
H	3.85805500	-1.53180600	-1.62440800
H	2.94905300	-0.00464100	-1.86210400
C	-3.70065200	-2.51730100	1.03067400
H	-3.72436100	-3.42975200	1.62742400
H	-3.12382100	-1.74168500	1.54585600
H	-4.70706300	-2.19531000	0.74856800
C	-2.95137700	-1.30162400	-1.42112500
H	-2.12567700	-1.27716900	-2.13730300
H	-3.92749400	-1.28423200	-1.91212400
H	-2.84691300	-0.50213700	-0.68025700
Cl	-0.74647200	-1.75826300	2.68192000
O	1.45493800	2.28941100	0.30052500
Ag	3.52233200	1.62961800	0.35742400
Cl	5.64435300	0.65228500	-0.06821800
H	-0.54061900	3.04127700	-1.44167800

H-IM5

C	-3.66419200	-1.20109200	-0.51608700
C	-3.55865200	-0.46434700	0.67419700
C	-4.69789000	0.15652200	1.19661500
C	-5.90067000	0.03254800	0.52507700
C	-5.98214800	-0.70339700	-0.66345800
C	-4.86467100	-1.32736400	-1.20033600
C	-2.21542600	-0.43234100	1.19402700
H	-4.62223400	0.74438800	2.10847400
H	-6.79055500	0.51752500	0.91683100

H	-6.93597500	-0.78663100	-1.17829000
H	-4.92756700	-1.89523100	-2.12444800
S	-2.09288600	-1.92266300	-1.00964400
C	-1.31953900	-1.15997100	0.39030200
C	0.13368100	-1.35079600	0.67565300
O	0.62156100	-0.31629200	1.26668700
Pd	-0.72056200	1.00425700	0.31416000
O	0.69721700	2.45577100	-0.06821500
S	2.15369500	1.67541300	-0.27901600
C	3.06571800	2.93747800	-1.26985400
H	2.56851300	2.98480000	-2.23893900
H	2.99975100	3.89162800	-0.74267600
H	4.08831500	2.56198000	-1.36043300
C	2.95456100	1.93060200	1.37271800
H	2.39642200	1.29127800	2.05918700
H	3.99056400	1.59547000	1.27287500
H	2.84673300	2.98886000	1.62243700
Cl	-2.30944700	2.25870800	-0.83413200
O	0.77279500	-2.33127100	0.27002500
Ag	2.88154300	-1.65874900	-0.00171000
Cl	4.81969300	-0.31720000	-0.47936000
H	-1.98501500	-0.15107000	2.22083800

H-IM6

C	3.79872000	-0.11454600	0.22606200
C	3.14377900	0.59815000	-0.79071500
C	3.62685500	1.85628500	-1.16387100
C	4.74057300	2.36941300	-0.51757400
C	5.37584300	1.64474900	0.49762200
C	4.91091500	0.39323900	0.88213500
C	1.99671400	-0.11582700	-1.32040300
H	3.11613500	2.41453400	-1.94630600
H	5.12615700	3.34543300	-0.80100100
H	6.24846400	2.06473400	0.99201800
H	5.40638400	-0.17170300	1.66755500
S	3.02308800	-1.71152900	0.51275400
C	1.81277400	-1.36009200	-0.71739900
C	0.80691400	-2.45200100	-1.05825100
O	-0.02433800	-2.12837700	-1.96634400
Pd	0.22948000	0.63416200	-0.15685000
O	-1.29068500	1.65251300	0.80233600
S	-2.07894000	2.90914100	0.07011700
C	-3.46808100	2.14592100	-0.91018100

H	-4.22558800	2.92670100	-1.02304400
H	-3.03539300	1.85644100	-1.86819600
H	-3.82129900	1.27098100	-0.34943100
C	-3.07648800	3.36500400	1.56546000
H	-2.36440500	3.71001700	2.31598800
H	-3.77693400	4.15668700	1.29037300
H	-3.58942400	2.45466400	1.88840000
Cl	-0.42928500	1.56802300	-2.25310400
O	0.89284300	-3.48767900	-0.39796800
O	0.93141500	0.14256200	1.71838300
S	0.19089500	-0.75206100	2.88169600
C	-0.48072300	-2.30588500	2.11757200
H	-0.78024300	-2.93034300	2.96394200
H	-1.34867900	-2.04621100	1.50002200
H	0.31503100	-2.78449900	1.53606700
C	-1.42846600	0.07294000	3.28870700
H	-1.18560500	1.10431700	3.54741000
H	-2.09986200	0.00658200	2.42493100
H	-1.81606300	-0.47434500	4.15260700
Ag	-1.87020900	-1.47195900	-1.04580400
Cl	-3.64031500	-0.98678400	0.55302700
H	1.56770800	0.08047500	-2.30141300

H-TS2

C	-4.29092000	0.54425800	0.28025000
C	-3.96645600	-0.83091000	0.33177400
C	-4.96955200	-1.77270200	0.63565400
C	-6.25090200	-1.33365300	0.88938900
C	-6.55561600	0.03914200	0.83387900
C	-5.59003100	0.98378500	0.52852500
C	-2.60350100	-1.06859500	0.04078100
H	-4.71868200	-2.83067800	0.67002900
H	-7.03472400	-2.04721400	1.12912000
H	-7.57370700	0.36548100	1.03432900
H	-5.83679700	2.04143700	0.48369300
S	-2.89363800	1.54713100	-0.14251900
C	-1.83494000	0.05025800	-0.27114500
C	-1.12916600	-0.29706100	-1.96857300
O	-0.65887200	-1.42816400	-1.98637300
Pd	0.03615300	0.40851600	0.51679800
O	1.95365500	0.90362300	1.27082000
S	2.47091400	0.17033400	2.65144300
C	3.51698900	-1.26414100	2.08664800

H	4.28457700	-1.41626600	2.85058200
H	2.84175600	-2.11767600	2.01453200
H	3.92693800	-1.01318900	1.09770500
C	3.85356800	1.34804700	3.02723400
H	3.38731600	2.31531000	3.21926200
H	4.39214200	0.98833500	3.90675300
H	4.49392100	1.38294600	2.14191600
Cl	0.17620200	-1.80083400	1.46886600
O	-1.27190400	0.66567500	-2.67230000
O	-0.13864200	2.33890200	-0.21018500
S	0.88117900	2.98732800	-1.32278100
C	1.75090600	1.59903400	-2.19605900
H	2.50033700	2.06875600	-2.83953700
H	2.22449200	0.94279300	-1.45557800
H	0.98883800	1.08998100	-2.79007300
C	2.30681700	3.57832700	-0.28313000
H	1.91454300	4.38721100	0.33458500
H	2.63297400	2.72844700	0.32382700
H	3.08052300	3.94203000	-0.96406400
Ag	1.46443900	-1.73536900	-1.06503100
Cl	3.84375000	-1.29127300	-1.39074000
H	-2.16767300	-2.06298800	-0.00683000

H-IM7

C	-3.73797200	0.99757500	-0.19903300
C	-3.47145300	-0.30240000	-0.66091300
C	-4.54045400	-1.18232400	-0.88065600
C	-5.83306900	-0.75443600	-0.63544700
C	-6.07935700	0.54508000	-0.16932100
C	-5.03631000	1.43120400	0.05318600
C	-2.06158400	-0.53949100	-0.85422100
H	-4.34460500	-2.19061600	-1.24106700
H	-6.66734100	-1.43084500	-0.80474600
H	-7.10209000	0.86364900	0.01850300
H	-5.22534700	2.44040400	0.41144000
S	-2.23808700	1.95188000	-0.00611000
C	-1.24241800	0.54082400	-0.56193400
Pd	0.75192600	0.60481700	-0.74502800
O	2.92503900	0.48517500	-0.76029300
S	3.84375100	0.95180100	0.51767100
C	4.15565600	2.76098300	0.22304700
H	4.75461800	2.81244100	-0.68701900
H	3.18289900	3.24787600	0.09797400

H	4.71706600	3.13093600	1.08493100
C	2.73600700	1.03371300	2.00945200
H	2.33983200	0.02312700	2.17717100
H	3.38093000	1.33862700	2.83874300
H	1.93657900	1.75423600	1.80986200
Cl	0.76724600	2.91394600	-0.17909600
O	0.53991300	-1.40330900	-1.40463600
S	1.70434800	-2.52566400	-1.63658100
C	2.75905500	-2.57157100	-0.10786500
H	3.36484400	-3.47826000	-0.18057200
H	3.35863200	-1.66117300	-0.09520400
H	2.07204200	-2.61644100	0.74890800
C	2.88452900	-1.73598100	-2.83474500
H	2.31660800	-1.58491100	-3.75389400
H	3.21832100	-0.79135900	-2.39391400
H	3.70311600	-2.44295100	-2.99354200
Ag	-0.78470200	-0.89922100	1.21481200
Cl	0.70793200	-1.94811100	2.79674200
H	-1.66731600	-1.43439100	-1.33203900

H-IM8

C	-4.24797900	0.79876800	0.46348900
C	-4.10073300	-0.25488200	-0.45726800
C	-5.25566600	-0.86966200	-0.95823000
C	-6.50153600	-0.43071000	-0.54147300
C	-6.62143600	0.61950400	0.37660800
C	-5.49255500	1.24400800	0.88949300
C	-2.71993700	-0.54669800	-0.76123500
H	-5.16399500	-1.68779400	-1.67021900
H	-7.39798400	-0.90767500	-0.93058700
H	-7.60755500	0.95052100	0.69345800
H	-5.57953200	2.05797700	1.60514600
S	-2.64686300	1.43122800	0.98119400
C	-1.83890900	0.23551200	-0.09612300
Pd	0.12884600	0.20581100	-0.15340400
O	2.26255800	0.04493500	-0.55422800
S	3.56135200	0.09437800	0.42172200
C	3.04362300	1.13327800	1.87188200
H	2.94623400	2.15322300	1.49127200
H	2.09084100	0.74530600	2.24557300
H	3.83586200	1.06816800	2.62226100
C	3.63932900	-1.58098700	1.23576200
H	3.58484800	-2.31128700	0.41936000

H	4.59830000	-1.63403600	1.75793800
H	2.78995200	-1.68458000	1.91659300
Cl	0.08049400	-1.03588000	1.98528100
Ag	0.66703600	-2.69149900	0.14930000
Cl	1.98724300	-3.98037100	-1.35054200
C	0.68601200	3.87340000	-0.06708200
C	1.03692900	2.92388200	-1.03607900
C	2.35931500	2.87770300	-1.49701400
C	3.30717900	3.75273600	-0.98401000
C	2.95205200	4.68150700	-0.00508600
C	1.63770000	4.74217300	0.45170700
H	-0.34426700	3.90620100	0.28766500
H	2.64419600	2.14732200	-2.24973000
H	4.32980300	3.71505900	-1.35236300
H	3.69810200	5.36678700	0.39056900
H	1.35331500	5.47040500	1.20703900
C	-0.00749500	2.00338200	-1.49858700
H	-1.02703900	2.35955000	-1.33726500
C	0.14412300	0.84233600	-2.24093600
H	1.11645800	0.49590600	-2.58695000
H	-0.73322000	0.39053100	-2.69858600
H	-2.41585300	-1.33284900	-1.45002200

H-TS3

C	3.97773600	-0.68022200	-0.82085200
C	3.49186000	0.62231500	-0.59997900
C	4.39923000	1.63674000	-0.26034600
C	5.74487500	1.33441900	-0.15132900
C	6.20682400	0.03060400	-0.37841800
C	5.32799300	-0.99013600	-0.71379300
C	2.06978200	0.72448100	-0.76509900
H	4.03132300	2.64483000	-0.07805600
H	6.45321100	2.11483200	0.11537900
H	7.26833800	-0.18731800	-0.28833900
H	5.68444300	-2.00289600	-0.88359400
S	2.64415700	-1.80951400	-1.21918900
C	1.45438800	-0.46057800	-1.04701700
C	0.08856000	-0.27603500	-2.62223300
Pd	-0.39826700	-1.08801200	-0.50361300
O	-2.32908400	-1.95580400	-0.13398000
S	-3.41458700	-1.51515500	1.00081400
C	-2.95706300	0.18240400	1.60699900
H	-3.71460000	0.46056700	2.34459300

H	-1.95691600	0.14304100	2.05091600
H	-2.97996200	0.85798600	0.74827900
C	-2.90294500	-2.48848800	2.50293500
H	-1.83298400	-2.31671000	2.66236300
H	-3.51805500	-2.14703300	3.33965200
H	-3.10600400	-3.53386500	2.26800500
Cl	0.46510600	-1.60590100	1.85461600
C	-1.27428500	-0.55409200	-2.36407300
H	0.38674300	0.75998600	-2.75183100
H	0.65758800	-0.99146900	-3.21011800
C	-2.28855300	0.47357800	-2.09770600
C	-3.63948200	0.15084700	-2.28825300
C	-1.96140200	1.74614200	-1.60708200
C	-4.63503500	1.07956600	-2.01214900
H	-3.90002500	-0.84340100	-2.64816200
C	-2.95830300	2.66750700	-1.31531700
H	-0.92932200	2.01730400	-1.38752300
C	-4.29713000	2.34019500	-1.52382300
H	-5.67808800	0.81789100	-2.17450200
H	-2.67604300	3.63106400	-0.89844900
H	-5.07623900	3.06481000	-1.29929800
H	-1.66372300	-1.52376400	-2.68495800
Ag	0.44471300	0.90234700	1.69191200
Cl	-0.21170100	3.17085600	1.22922200
H	1.53843400	1.67378700	-0.69221500

H-IM9

C	-4.78792900	-0.76676200	-0.49159800
C	-4.90547400	0.13659900	0.58099800
C	-6.18352500	0.56887600	0.95830000
C	-7.29167800	0.10420800	0.27153400
C	-7.14901200	-0.79431700	-0.79369400
C	-5.89472900	-1.24012300	-1.18542500
C	-3.63224700	0.49105000	1.14367800
H	-6.29314700	1.26757700	1.78520000
H	-8.28468400	0.43954100	0.56038100
H	-8.03086400	-1.14658000	-1.32325400
H	-5.77996800	-1.93702600	-2.01174900
S	-3.07670900	-1.18972000	-0.80413200
C	-2.57979100	-0.11455100	0.54886500
C	-1.14294500	0.06023300	0.87237900
Pd	0.55652700	-0.39910300	-0.73375600
O	1.61141700	-2.22884900	-1.10736800

S	3.23957400	-2.31055900	-1.15369600
C	3.85098700	-0.85313000	-0.17367300
H	4.93454900	-0.80304200	-0.31104200
H	3.34605100	0.04023600	-0.55892500
H	3.59312200	-1.04524800	0.87175100
C	3.68238700	-1.71335600	-2.85988100
H	3.22952900	-0.72728400	-3.00535200
H	4.77321200	-1.69005600	-2.92519200
H	3.26479600	-2.44831300	-3.54920500
Cl	1.64015100	1.17258800	-2.51873500
C	-0.30177600	-1.15619800	0.96450900
H	-0.70766200	0.74469200	0.00499000
H	-1.00692800	0.76410900	1.70565300
C	0.80072600	-1.29854100	1.91536700
C	1.37282100	-2.57124400	2.08739700
C	1.36405700	-0.20481000	2.59446400
C	2.48665100	-2.74329800	2.89668200
H	0.93848800	-3.41935700	1.56094500
C	2.48132400	-0.38280000	3.39981600
H	0.95355000	0.79950000	2.48060900
C	3.04894800	-1.64712600	3.55145700
H	2.91675100	-3.73437900	3.02235400
H	2.90836600	0.47705200	3.91035100
H	3.92055000	-1.78116600	4.18795100
H	-0.78630800	-2.09735800	0.68385400
Ag	1.38298100	2.47132400	-0.42127600
Cl	0.84296400	3.29220400	1.75356000
H	-3.51265700	1.18913900	1.96857200

H-TS4

C	-4.59577000	-1.22997000	-0.29152300
C	-4.64154000	0.00065700	0.39235800
C	-5.87326300	0.66017200	0.51086300
C	-7.00632600	0.09184900	-0.04300800
C	-6.93530700	-1.13367700	-0.71891100
C	-5.72929600	-1.80752300	-0.84971900
C	-3.35789200	0.40141400	0.88466900
H	-5.92516500	1.61147100	1.03626200
H	-7.96355500	0.59934000	0.04634200
H	-7.83707700	-1.56445300	-1.14732000
H	-5.67204100	-2.75861300	-1.37306300
S	-2.93962600	-1.90527700	-0.32244400
C	-2.36156100	-0.47967600	0.60990700

C	-0.97084400	-0.32802700	1.00579400
Pd	0.55636800	-0.29769100	-0.72193700
O	1.79463300	-1.98846700	-1.31129700
S	3.41730700	-1.94801400	-1.41136500
C	3.98021300	-0.47949500	-0.41261600
H	5.05665700	-0.37950900	-0.57710300
H	3.42916900	0.40181500	-0.75846800
H	3.76490200	-0.71193700	0.63408000
C	3.73068600	-1.26315900	-3.11513100
H	3.18563800	-0.31830500	-3.20251600
H	4.81048600	-1.14203400	-3.23332600
H	3.34166900	-2.00967000	-3.80873800
Cl	1.48586300	1.40347600	-2.40554100
C	-0.02632000	-1.38002300	1.01946500
H	-0.48356800	0.78289200	-0.25101800
H	-0.80873200	0.53128800	1.66627500
C	1.17845000	-1.40360000	1.86039100
C	1.94264600	-2.57942600	1.88330700
C	1.61596100	-0.29650800	2.60598600
C	3.11705600	-2.64967500	2.62234500
H	1.61083400	-3.43482000	1.29685000
C	2.79164300	-0.37225000	3.34156000
H	1.05245800	0.63741100	2.60523800
C	3.54759700	-1.54393000	3.35236600
H	3.69554400	-3.57073200	2.63248700
H	3.11652000	0.49344300	3.91366200
H	4.46420800	-1.59636800	3.93527100
H	-0.34674500	-2.35523800	0.64124300
Ag	0.84192500	2.60805200	-0.28599100
Cl	-0.01042200	3.11941800	1.90267200
H	-3.17383800	1.32764000	1.42597500

H-IM10

C	4.80667000	0.37393300	0.24735600
C	4.66942100	-1.00767000	0.48705700
C	5.79047500	-1.83416500	0.32259600
C	6.99510400	-1.27851300	-0.06936800
C	7.10687600	0.09935900	-0.30063700
C	6.01388900	0.93957300	-0.14367700
C	3.34002600	-1.36419900	0.87919400
H	5.70194400	-2.90347000	0.50317300
H	7.86602700	-1.91579000	-0.19956600
H	8.06209800	0.51740600	-0.60872100

H	6.09778400	2.00850600	-0.32270700
S	3.26826500	1.24485900	0.51086200
C	2.47792400	-0.31465300	0.94881400
C	1.08047900	-0.37691900	1.32157000
Pd	-0.12651700	0.21973000	-0.51938000
O	-0.24350900	2.41848200	-0.65192900
S	-1.61075500	3.23808200	-0.96936200
C	-3.03590200	2.07785900	-0.65538600
H	-3.94578800	2.62250200	-0.92230300
H	-2.89788800	1.18387800	-1.27041600
H	-3.01809200	1.84605000	0.41313600
C	-1.68045300	3.27004100	-2.83015800
H	-1.59895900	2.23885400	-3.18515700
H	-2.62052300	3.74543400	-3.12134900
H	-0.82395800	3.86638700	-3.14693000
Cl	-1.16680900	-0.27166500	-2.73376700
C	0.28398100	0.73238000	1.59247400
H	-0.02186400	-1.32282000	-0.40507800
H	0.74774800	-1.36523500	1.64299100
C	-1.02813200	0.73890800	2.24371200
C	-1.53263900	1.97016900	2.68822100
C	-1.82308900	-0.40865000	2.38877900
C	-2.79433300	2.05398500	3.26568200
H	-0.92043900	2.86469500	2.57474700
C	-3.09081200	-0.31816300	2.94508800
H	-1.49149700	-1.38201500	2.02808100
C	-3.57981700	0.91010800	3.38834000
H	-3.16655600	3.01393900	3.61647400
H	-3.69659200	-1.21900700	3.00840900
H	-4.57285600	0.97544200	3.82675200
H	0.75114900	1.71567500	1.49896200
Ag	-2.06518500	-1.93531200	-1.02324100
Cl	-2.90189700	-3.37013600	0.68597000
H	3.02963600	-2.38292700	1.09932000

H-P

C	3.13876200	-0.59753800	-0.07983600
C	2.74044400	0.74139100	0.11170700
C	3.73512300	1.72557100	0.22020500
C	5.06769000	1.36494700	0.13505900
C	5.43812800	0.02665500	-0.05755600
C	4.47585300	-0.96665200	-0.16695300
C	1.31976300	0.89105700	0.17976400

H	3.44872700	2.76475900	0.37053700
H	5.83881900	2.12693400	0.21969600
H	6.49086100	-0.23787200	-0.12092400
H	4.75756800	-2.00611100	-0.31605000
S	1.72481600	-1.68127400	-0.18455800
C	0.62330400	-0.27076900	0.03791500
C	-0.79935100	-0.51510300	0.04566200
C	-1.73519000	0.44768000	-0.05332300
C	-3.17961100	0.26435400	-0.01413500
C	-3.78757600	-0.95943600	0.30549300
C	-4.00801200	1.35710900	-0.30457500
C	-5.16814800	-1.08335800	0.31771200
H	-3.17154600	-1.81979800	0.55977800
C	-5.39115500	1.23372200	-0.29140100
H	-3.54900300	2.31479600	-0.54778900
C	-5.97759400	0.01118300	0.01776200
H	-5.62006800	-2.04021900	0.56931600
H	-6.01278600	2.09552000	-0.52323100
H	-7.06013800	-0.08959500	0.03147900
H	-1.10636400	-1.55881000	0.12880900
H	-1.40123900	1.47833500	-0.19404500
H	0.83352600	1.84757100	0.35435800

Cartesian Coordinates for the Stationary Points Given in Scheme 1.

IM14

Pd	-0.33815100	0.72516600	-1.02250500
O	-1.51928800	1.48462600	0.71904100
O	0.72790700	2.48217800	-0.81851900
S	-2.75844200	0.81618100	1.52074800
S	1.99335500	2.56284000	0.21959100
C	-2.20235900	-0.90876500	1.95652000
H	-2.98312800	-1.35976000	2.57405600
H	-2.03215600	-1.46344800	1.02968400
H	-1.27448600	-0.79058800	2.52224800
C	-4.01101600	0.40372500	0.20886000
H	-3.50939900	-0.18008300	-0.56883200
H	-4.82176400	-0.15044100	0.68854200
H	-4.36604700	1.36113500	-0.17498900
C	1.45064000	1.71400800	1.79095500
H	0.36318200	1.85007700	1.80848700
H	1.73069200	0.65338300	1.74971400
H	1.94600700	2.23525200	2.61301100
C	3.21146000	1.31776300	-0.41957300

H	3.52890000	1.67904100	-1.39870000
H	4.04474500	1.28278200	0.28721700
H	2.71374800	0.34423000	-0.47650600
Cl	-1.45310400	-1.41127600	-1.53985500
H	0.61676600	0.35420500	-2.15045600
Ag	0.65465800	-1.82430600	-0.16933600
Cl	2.43598900	-1.78814800	1.43517200

TS5

Pd	0.32649200	-0.66240300	0.16373400
O	0.76500100	1.23410800	1.11379300
O	2.55876700	0.22852400	-1.09926100
S	0.40482200	2.67903700	0.43579800
S	3.88220800	-0.18367400	-0.27628600
C	-0.18023200	2.27763800	-1.28305600
H	-0.05657600	3.18256600	-1.88526000
H	0.45090800	1.45295000	-1.63601500
H	-1.23914700	2.00886200	-1.19050900
C	2.11566000	3.25196900	-0.02148600
H	2.54958600	2.44816700	-0.62789800
H	2.03315100	4.19930200	-0.55961300
H	2.64854700	3.38835200	0.92145200
C	3.31976400	-0.51517000	1.47599500
H	2.85455200	0.41050200	1.82520300
H	2.57134500	-1.31613400	1.44770700
H	4.20205200	-0.78836100	2.06116300
C	4.17526800	-1.95308200	-0.77967200
H	4.46986100	-1.93109500	-1.82948200
H	4.97290900	-2.36359900	-0.15559700
H	3.23284800	-2.49331800	-0.65106300
Cl	-1.03315400	-2.64824900	0.03063700
H	0.91181600	-1.29335200	-1.05700000
Ag	-2.55483700	-0.61000700	-0.04499400
Cl	-3.45558400	1.60360500	-0.09529900

IM15

Pd	-0.52479900	0.08286500	-0.99583800
O	-0.72605500	2.20271900	-0.73629900
O	-1.72929300	0.25220900	1.76078200
S	0.57379000	3.05793200	-0.20939700
S	-3.33719200	0.05760200	1.33767900
C	2.00710100	2.29388000	-1.11345100

H	2.88824200	2.31225900	-0.46633300
H	1.69920000	1.25447100	-1.30518900
H	2.14659300	2.85631900	-2.03708300
C	0.90606600	2.38225200	1.49077900
H	1.11854400	1.30998200	1.40849100
H	1.77731100	2.90956200	1.88825300
H	0.00969200	2.59044200	2.07737700
C	-3.50906200	0.94544700	-0.29213700
H	-2.99841400	1.90559900	-0.16778300
H	-2.99235100	0.36043700	-1.06498500
H	-4.58450000	1.05724600	-0.45475600
C	-3.41432700	-1.72414700	0.82198800
H	-3.30056900	-2.30308100	1.73937000
H	-4.40437500	-1.87359300	0.38309500
H	-2.59868700	-1.92636600	0.11342600
Cl	-0.43255100	-2.36856900	-1.05678000
H	-1.15202500	0.12557100	0.91026600
Ag	1.58343100	-1.36951200	0.17203800
Cl	3.37545500	-0.15473200	1.23367200

Cartesian Coordinates for the Stationary Points Given in Figure S1.

IM16

C	-3.02935400	0.01399400	0.77565100
C	-2.81620000	1.09809900	-0.09366600
C	-3.75794600	1.36655600	-1.09496100
C	-4.87483300	0.55656100	-1.20546600
C	-5.07360100	-0.51973700	-0.32890400
C	-4.15437900	-0.79816500	0.67229700
C	-1.56841100	1.74860700	0.18957200
H	-3.59840800	2.20405500	-1.77019800
H	-5.61047000	0.75798900	-1.98026900
H	-5.95954500	-1.14176300	-0.43082500
H	-4.30316600	-1.62938300	1.35797900
Cl	-1.04004100	3.12500100	-0.79802600
S	-1.67301200	-0.19571300	1.92256500
C	-0.82456200	1.20604200	1.18004600
C	0.52251300	1.64841100	1.68435000
O	1.47134700	0.76172300	1.66448700
Pd	1.38186200	-0.72999400	0.29831200
O	1.36513500	0.69617500	-1.23693800
O	1.47465500	-2.15625300	-1.17514400
S	2.73503600	1.55286700	-1.51659000
S	0.05187300	-2.68099800	-1.79817600

C	4.09839400	0.40058500	-1.00217400
H	5.04886900	0.91520000	-1.16644300
H	3.94081400	0.14239100	0.05063600
H	4.00492700	-0.48409300	-1.63513500
C	2.87309300	2.79870800	-0.13929700
H	2.92686700	2.27446000	0.81847300
H	3.75943700	3.39783400	-0.36350600
H	1.96285600	3.40078000	-0.17488800
C	-0.85157200	-3.50380700	-0.39500700
H	-0.31901000	-4.43086700	-0.18024600
H	-0.81824000	-2.83920900	0.47515500
H	-1.86808900	-3.69250200	-0.75227300
C	-1.02352300	-1.16814100	-1.95011000
H	-0.43313400	-0.41916800	-2.48291100
H	-1.92237900	-1.46237100	-2.49949600
H	-1.26284200	-0.81762100	-0.94406700
Cl	1.40184000	-2.37787500	1.97195300
O	0.66326900	2.79810800	2.06261000

IM17

C	2.97053500	0.25075900	-0.69053700
C	2.42716700	-0.09030900	0.55382200
C	3.10239500	-0.98963600	1.37946300
C	4.29649400	-1.53460700	0.94076000
C	4.81777600	-1.19654300	-0.31286400
C	4.15861200	-0.30236600	-1.14558200
C	1.15176000	0.55632000	0.77814300
H	2.67075400	-1.26372200	2.33883400
H	4.82867700	-2.24238900	1.57031200
H	5.75325800	-1.64060100	-0.64386600
H	4.56091300	-0.04002600	-2.12029100
Cl	0.58088700	0.76002300	2.46643000
S	1.95475800	1.43801300	-1.58882900
C	0.75933100	1.41374900	-0.26968000
C	-0.41384400	2.37481700	-0.22546500
O	-1.47995300	1.65127200	-0.00722800
Pd	-0.65100800	-0.23515600	-0.21220400
O	-2.45742400	-1.17972900	-0.57269200
S	-3.76698900	-0.18266800	-0.42441100
C	-5.05567000	-1.51218800	-0.47663700
H	-5.01564600	-1.92875700	-1.48356300
H	-4.76871800	-2.26287200	0.26303900
H	-6.03004700	-1.06492200	-0.26852800

C	-3.80571600	0.18476200	1.39850300
H	-3.04398300	0.95136200	1.55635100
H	-4.80386900	0.55163600	1.65006400
H	-3.55824600	-0.74856400	1.91191200
Cl	0.35875100	-2.33577100	-0.50006900
O	-0.32235900	3.56341600	-0.39617300

IM18

C	-2.99979400	-0.87767100	-0.73882000
C	-2.77357600	0.28661700	0.00941100
C	-3.52548900	1.43499300	-0.25031400
C	-4.47621700	1.40316000	-1.25428200
C	-4.68104100	0.23799600	-2.00372400
C	-3.94409000	-0.91136700	-1.75683200
C	-1.71140400	0.10391700	0.96893900
H	-3.34488400	2.33700500	0.33004300
H	-5.06397600	2.29124600	-1.47056900
H	-5.42862000	0.23191500	-2.79317700
H	-4.10098600	-1.81501300	-2.33992400
Cl	-1.70265000	1.16724500	2.41700800
S	-1.93848200	-2.24095600	-0.25029800
C	-1.14999700	-1.19278700	0.95753200
C	-0.18461200	-1.71714900	2.00539700
O	0.83329600	-0.89981300	1.99595900
Pd	0.42353400	0.08014600	0.25231900
O	2.43140000	0.93259400	0.22014000
S	2.65419000	2.54044900	0.42252500
C	2.64067700	3.21085100	-1.31455400
H	3.56786200	2.86738200	-1.77635300
H	1.75854700	2.79536900	-1.81500900
H	2.62205200	4.30159400	-1.24571600
C	1.01179200	3.19002200	0.99949000
H	0.80314300	2.68273300	1.94462700
H	1.12435100	4.26816100	1.14424900
H	0.26376800	2.93864400	0.23780200
Cl	-0.17440000	1.20832600	-1.77667600
O	-0.36712300	-2.70589100	2.67086200
O	1.19694900	-2.04394500	-0.81507500
S	2.70823700	-2.42796800	-1.18648200
C	3.69307700	-2.01796500	0.34491100
H	4.75239300	-2.16326700	0.11610200
H	3.45709000	-0.98677400	0.62738700
H	3.35645300	-2.71677800	1.11247600

C	3.27573300	-0.99521800	-2.23982500
H	2.65259800	-1.02128000	-3.13517600
H	3.08508300	-0.08688700	-1.65887800
H	4.33276400	-1.13584000	-2.48116600

TS6

C	-3.41185800	-0.79593700	0.52630600
C	-3.15017000	0.27680000	-0.34812100
C	-4.01377300	0.51658200	-1.42738200
C	-5.10747100	-0.30641000	-1.60731800
C	-5.35566900	-1.37255600	-0.72799800
C	-4.51258900	-1.62695400	0.34109400
C	-1.98398500	0.98850500	0.06190800
H	-3.81375500	1.34486400	-2.10279100
H	-5.78488700	-0.12924600	-2.43878500
H	-6.22082600	-2.01088200	-0.89062700
H	-4.69999700	-2.45501200	1.02003000
Cl	-1.52673900	2.48299900	-0.79642300
S	-2.18761800	-0.92545000	1.80826800
C	-1.30813700	0.49868800	1.14723500
C	-0.17334500	1.03261400	2.04642500
O	0.56571100	0.09450200	2.45137900
Pd	0.86564900	-0.32340900	-0.04427400
O	2.22418300	1.15158600	0.50478800
O	2.43311200	-0.94085000	-1.26103100
S	2.59444200	2.41742000	-0.48001000
S	3.53238900	-1.91582700	-0.50563100
C	1.48191500	3.79297300	0.12563800
H	1.02527700	4.27400700	-0.74221400
H	0.74610400	3.32472700	0.80075100
H	2.12785100	4.48401400	0.66845900
C	1.82139500	2.02309400	-2.12145200
H	0.74896200	1.86843100	-1.97215900
H	2.02581100	2.87208300	-2.77901100
H	2.30991400	1.11144900	-2.47060000
C	3.26890200	-1.67786200	1.32078800
H	3.43541300	-0.61713900	1.52312600
H	2.23494700	-1.94574600	1.56661200
H	4.00158900	-2.31681100	1.82182100
C	2.81108000	-3.61752000	-0.69380200
H	2.91748200	-3.87906700	-1.74704000
H	3.39874400	-4.28533300	-0.05856300
H	1.75328700	-3.56609700	-0.41152800

Cl	-0.35507600	-2.20317500	-0.74659000
O	-0.13051800	2.24916100	2.23716300

IM19

C	-4.37494600	-0.91939200	0.13539000
C	-4.25129600	0.47702700	0.02094700
C	-5.40500800	1.27347200	0.00735300
C	-6.64060400	0.66529300	0.11110900
C	-6.74683500	-0.72964000	0.22905700
C	-5.61951800	-1.53365000	0.24164900
C	-2.87743700	0.87084800	-0.06641800
H	-5.31098600	2.35298500	-0.08403200
H	-7.54216400	1.27219400	0.10216300
H	-7.72966100	-1.18727200	0.31179600
H	-5.69988200	-2.61384700	0.33168700
Cl	-2.45010200	2.57077500	-0.21431000
S	-2.79569700	-1.74311600	0.12720000
C	-1.98121000	-0.15195600	-0.02741800
C	-0.52618300	-0.14800300	-0.09353500
O	0.09931900	-1.26457200	-0.08079800
Pd	1.89544300	-0.26823900	-0.21460600
O	3.25415900	1.23589200	-0.39970000
S	4.71683600	1.35030100	0.33337100
C	4.60230000	0.34984800	1.89280200
H	3.82433500	0.82615500	2.49232600
H	4.33477100	-0.67706800	1.61992600
H	5.57548700	0.42132000	2.38554400
C	5.85416200	0.27905000	-0.67291500
H	5.88238900	0.73597000	-1.66307200
H	6.83617600	0.32073600	-0.19433000
H	5.42973000	-0.72857200	-0.70464200
Cl	3.40327100	-2.09063200	-0.23386800
O	0.15486800	0.92138400	-0.16246900

TS7

C	3.49318000	-1.25916300	-0.23600700
C	4.09131400	-0.05217500	0.16525700
C	5.42918000	-0.05404600	0.58175000
C	6.13035800	-1.24479100	0.58902000
C	5.51802900	-2.44137200	0.18706500
C	4.19651000	-2.45996700	-0.22858400
C	3.16969400	1.04325700	0.07898500

H	5.89487100	0.87848000	0.89212600
H	7.16884400	-1.25556700	0.90996700
H	6.08744800	-3.36758100	0.20163900
H	3.71799200	-3.38517700	-0.54012200
Cl	3.68668200	2.66382900	0.53787300
S	1.79584900	-1.03053700	-0.72907200
C	1.92522700	0.72621500	-0.36402100
C	0.73932300	1.59346600	-0.55172400
O	-0.28598700	0.96426000	-1.10748300
Pd	-1.79491100	0.07276800	-0.18242800
O	-3.41571100	0.94197300	0.63836100
S	-4.99263400	0.58511100	0.31076500
C	-4.98898700	-0.35028200	-1.29056900
H	-4.58462600	0.33469000	-2.03827100
H	-4.35603100	-1.23379500	-1.16260500
H	-6.02943000	-0.60264700	-1.51161900
C	-5.44734600	-0.76617300	1.50217500
H	-5.34187200	-0.32531900	2.49447300
H	-6.48882000	-1.02833800	1.29786700
H	-4.75223300	-1.59624400	1.35739200
Cl	-2.46723500	-2.09998300	0.41910900
O	0.71780100	2.76449100	-0.24150500

TS2’

C	3.40532000	0.82444000	-0.64795000
C	3.38607400	-0.45687300	-0.05183800
C	4.53943600	-1.26303100	-0.07790200
C	5.67446400	-0.78156700	-0.68947200
C	5.68325900	0.49849700	-1.27844800
C	4.56186900	1.30609400	-1.26245100
C	2.11454600	-0.71713400	0.50912400
H	4.51647200	-2.24802500	0.38213500
H	6.57424600	-1.39025500	-0.71904100
H	6.59200400	0.85753800	-1.75603800
H	4.57355800	2.29275300	-1.71840100
Cl	1.79146700	-2.25186100	1.33017100
S	1.85418700	1.66918800	-0.51717000
C	1.16198500	0.28707000	0.43098300
C	0.62323100	0.81741300	2.14892400
O	-0.53638200	0.38565200	2.22768400
Pd	-0.77826400	-0.18433200	0.20446100
O	-2.87676400	-0.64258800	0.34294800
S	-3.44038000	-2.15786800	0.10360500

C	-3.69015100	-2.25540100	-1.73937000
H	-4.53009900	-1.59552200	-1.96262000
H	-2.76155100	-1.91097300	-2.21103100
H	-3.93562700	-3.29256600	-1.98268200
C	-1.95717600	-3.26833000	0.25601000
H	-1.58506600	-3.13145700	1.27352200
H	-2.30726300	-4.29210700	0.09726900
H	-1.21649200	-2.94774800	-0.48535600
Cl	-0.48296600	-0.95760000	-2.04417500
O	1.46120300	1.40158800	2.75095300
O	-0.92288800	2.49049200	0.02785800
S	-2.35396700	3.11161200	-0.30219900
C	-3.45102700	2.49309500	1.08017900
H	-4.47457400	2.82302200	0.88230200
H	-3.36371500	1.40186600	1.11580100
H	-3.06151900	2.94687800	1.99288300
C	-3.04680200	2.01602400	-1.65230600
H	-2.33983800	2.08495400	-2.48089100
H	-3.08084100	0.99420300	-1.26051100
H	-4.03302500	2.39770600	-1.93067700

IM20

C	3.22974500	-0.92784100	-0.93325700
C	3.16279900	-0.64316600	0.44302100
C	4.34501400	-0.63686500	1.19233300
C	5.54834900	-0.91073500	0.56266200
C	5.59619300	-1.19309700	-0.80829500
C	4.43426000	-1.20547300	-1.56766300
C	1.80765100	-0.38372300	0.85177600
H	4.30313400	-0.42445100	2.25856600
H	6.46868900	-0.91042900	1.14222900
H	6.55096800	-1.40811000	-1.28264200
H	4.46114300	-1.43011200	-2.63157800
Cl	1.44797700	0.00137700	2.56075600
S	1.59665100	-0.88363400	-1.68211100
C	0.84451100	-0.44857700	-0.09676900
Pd	-1.07956100	-0.09766500	-0.06398500
O	-0.77244300	1.88380600	-0.66949700
O	-3.16508300	0.40924100	-0.11732000
S	0.41889900	2.65905600	0.14568600
S	-4.23604700	-0.73806200	0.33134300
C	-0.26573700	4.38108200	0.03526000
H	0.49231200	5.08710700	0.38182700

H	-0.54579400	4.54670600	-1.00775900
H	-1.14582100	4.39673200	0.67866400
C	1.74710700	2.82779400	-1.14390000
H	1.25507600	3.14222900	-2.06794200
H	2.47798100	3.55775500	-0.78726100
H	2.19247400	1.83676200	-1.25906000
C	-4.36959100	-1.81263900	-1.18397700
H	-4.39132000	-1.13733800	-2.04346300
H	-3.46821300	-2.42896500	-1.17465900
H	-5.27763100	-2.41512400	-1.09992200
C	-5.78582400	0.25019900	0.06165000
H	-5.79933400	1.01740900	0.83624700
H	-5.70408500	0.70418900	-0.92866300
H	-6.65027900	-0.41225000	0.14681700
Cl	-1.46551900	-2.35157800	0.54987400

Cartesian Coordinates for the Stationary Points Given in Figure S2.

IM21

C	4.24498800	-0.03507400	-0.78487000
C	3.62491600	-1.27597400	-1.00918100
C	4.41946200	-2.40518800	-1.23790700
C	5.79807000	-2.27086500	-1.23956300
C	6.40048800	-1.02623200	-1.01731400
C	5.62785500	0.10423300	-0.78979800
C	2.19138200	-1.15400600	-0.95402400
H	3.94669400	-3.36913600	-1.41345800
H	6.42134900	-3.14340900	-1.41927800
H	7.48448000	-0.94205100	-1.02579800
H	6.08911400	1.07521200	-0.62356800
Cl	1.16590400	-2.59240800	-1.20055200
S	3.03204700	1.26915600	-0.53588200
C	1.68425500	0.07331300	-0.69554900
C	-0.06366400	0.83746500	-2.44903700
Pd	-0.13269900	0.70520200	-0.19647500
O	0.52899300	3.29426200	-0.82702200
O	0.37549700	0.26108300	1.80315900
S	0.62074100	4.43671200	0.29203200
S	1.10272300	-1.19686800	2.08917100
C	0.69563800	3.51937400	1.91942700
H	0.67990600	4.26072300	2.72314800
H	-0.15555600	2.83288000	1.96535600
H	1.63672200	2.96492500	1.91119100
C	-1.14058800	5.03725500	0.45216400

H	-1.77242100	4.14782300	0.54544400
H	-1.21105900	5.69168500	1.32467200
H	-1.36072200	5.58478900	-0.46538600
C	0.23100700	-1.67190900	3.65679200
H	0.05789900	-0.74371700	4.20726700
H	-0.69752900	-2.16203400	3.33855300
H	0.87757400	-2.36778600	4.19745800
C	2.70696200	-0.60823500	2.81341600
H	3.25408300	-0.13517000	1.99362700
H	2.46435600	0.11715600	3.59430300
H	3.24885700	-1.47259200	3.20442300
Cl	-2.31550700	1.56222700	0.84780200
C	-1.37596100	1.09210400	-2.11287400
H	0.61872200	1.67151200	-2.59442000
H	0.23239400	-0.13236500	-2.84408800
Ag	-2.42992600	-0.96411200	0.94447000
Cl	-2.05654700	-3.27164600	1.53241100
H	-1.65364100	2.13415900	-1.94516700
C	-2.48604600	0.13447300	-2.16173900
C	-2.29519400	-1.25094200	-2.04361300
C	-3.78951700	0.62962300	-2.28046300
C	-3.38598500	-2.11206600	-2.03742700
H	-1.29312500	-1.65713000	-1.91232100
C	-4.87659000	-0.23510400	-2.30406700
H	-3.94253600	1.70593000	-2.33909800
C	-4.67807800	-1.60687000	-2.17470200
H	-3.22270800	-3.17707100	-1.89393800
H	-5.88283100	0.16475000	-2.40304100
H	-5.52932300	-2.28303500	-2.16462500

TS8

C	4.04603500	0.22112700	-0.86024200
C	3.49560200	-1.03666900	-1.16433200
C	4.33907600	-2.15099800	-1.25663900
C	5.69866500	-1.98529500	-1.05053500
C	6.23389200	-0.72422800	-0.75719600
C	5.41157300	0.39021100	-0.66110700
C	2.06857200	-0.95692300	-1.28864300
H	3.91741600	-3.12786300	-1.48316700
H	6.36002600	-2.84555700	-1.11765800
H	7.30468000	-0.61549200	-0.60283300
H	5.82160200	1.37151100	-0.43271500
Cl	1.13721800	-2.40417100	-1.73165100

S	2.78537600	1.49008600	-0.73890000
C	1.48604100	0.25133700	-1.04952400
C	0.04675000	0.80910000	-2.37879700
Pd	-0.24344300	0.68667500	-0.09955200
O	0.39089200	3.30438400	-0.68112100
O	0.57196300	0.04234600	1.80964700
S	0.53322000	4.35492500	0.52291200
S	1.33027400	-1.41569500	1.82705000
C	0.77939100	3.31474800	2.05690300
H	0.83533800	3.99345700	2.91240300
H	-0.05468800	2.61065800	2.13658100
H	1.71995300	2.77923200	1.90980100
C	-1.22830500	4.86832700	0.86903700
H	-1.82339400	3.95174200	0.94235200
H	-1.24604800	5.45068400	1.79383000
H	-1.54012800	5.47708700	0.01907200
C	0.62046100	-2.15150100	3.37565700
H	0.50390400	-1.32642400	4.08286500
H	-0.33604300	-2.59591600	3.07420000
H	1.31363800	-2.91773300	3.73179000
C	2.99860300	-0.92384600	2.48074300
H	3.49291200	-0.37050800	1.67731900
H	2.83000600	-0.29162900	3.35629400
H	3.55684700	-1.83105000	2.72534200
Cl	-2.33560200	1.37717900	1.18520200
C	-1.25042000	1.16700400	-1.91474300
H	0.67971700	1.63468700	-2.69634500
H	0.14904100	-0.12265000	-2.93358000
Ag	-2.31600400	-1.14477300	0.99048100
Cl	-1.81647100	-3.48929300	1.22804300
H	-1.43010400	2.23648700	-1.78551900
C	-2.44945600	0.32884000	-2.02492700
C	-2.40866000	-1.07464300	-2.06747500
C	-3.69818600	0.96427200	-2.01347900
C	-3.58658700	-1.81309900	-2.08277400
H	-1.45456400	-1.59914600	-2.05246500
C	-4.87235600	0.22573800	-2.04912400
H	-3.73564200	2.05046800	-1.95190600
C	-4.82079800	-1.16539800	-2.07503300
H	-3.53361700	-2.89888200	-2.07640300
H	-5.83237000	0.73623000	-2.03958500
H	-5.73950800	-1.74681100	-2.08184400

IM22

C	-2.22959000	-0.40453000	2.76041300
C	-2.76682600	-1.17275200	1.71538500
C	-4.12736200	-1.05707900	1.41194600
C	-4.90992100	-0.18876700	2.15393500
C	-4.36063500	0.55979900	3.20236100
C	-3.01223200	0.45956800	3.51711700
C	-1.74134000	-1.94970700	1.07585000
H	-4.54801700	-1.62318600	0.58472200
H	-5.96330700	-0.08052900	1.91021100
H	-4.99531900	1.23157200	3.77535300
H	-2.57651300	1.04189000	4.32577800
Cl	-2.16291100	-3.06505500	-0.25557700
S	-0.46294600	-0.64375000	2.91621900
C	-0.47532800	-1.79036300	1.52028500
C	0.80723700	-2.36233300	1.02070800
Pd	1.34940400	0.34565700	-0.08996300
O	2.25605500	1.38020600	1.55644700
O	0.72828400	2.37543000	-1.00233800
S	3.33538500	2.56598900	1.23387700
S	-0.87769600	2.18398000	-1.23259800
C	2.26769500	4.07673500	1.02218600
H	2.91276600	4.89969200	0.70316500
H	1.50342600	3.80833800	0.28214800
H	1.84128200	4.27318800	2.00730500
C	3.84491200	2.31145900	-0.53979300
H	2.93823100	2.30102100	-1.15460100
H	4.52457000	3.12792400	-0.80022600
H	4.35727700	1.34590900	-0.56735200
C	-1.42840700	3.83392400	-1.87267400
H	-1.05076000	4.60388900	-1.19465600
H	-1.00629000	3.93948000	-2.87245400
H	-2.52040400	3.79734100	-1.90821500
C	-1.57243100	2.30905400	0.49176000
H	-1.02190500	1.56502200	1.07799500
H	-1.38274200	3.31916600	0.86619200
H	-2.63678800	2.05948900	0.42097600
Cl	0.49353900	-0.95948400	-2.01287000
C	1.91849100	-1.32798200	0.94473900
H	1.13762400	-3.17542500	1.69167800
H	0.61287800	-2.81905100	0.04321000
Ag	-2.02298700	-0.57198900	-1.94246400
Cl	-3.98935500	0.86463400	-1.75703200
H	2.08320100	-0.86633500	1.92910300
C	3.21448000	-1.72172700	0.35648700

C	4.39337500	-1.19413100	0.91195800
C	3.32933100	-2.56566100	-0.75875600
C	5.63755000	-1.48760000	0.36950400
H	4.30999900	-0.54778000	1.78658200
C	4.57470800	-2.86051700	-1.29760100
H	2.43248100	-2.96452000	-1.22744500
C	5.73291100	-2.32266800	-0.74153600
H	6.53768000	-1.07573300	0.82177900
H	4.64132400	-3.51392800	-2.16460200
H	6.70518600	-2.55870500	-1.16790000

IM23

C	3.78421100	0.39299500	-0.83089300
C	3.51146800	-0.83425100	-0.20091100
C	4.57498600	-1.66766300	0.16083200
C	5.87247600	-1.26627900	-0.11310000
C	6.12832700	-0.04308200	-0.74467100
C	5.08390000	0.79597300	-1.10956400
C	2.09590500	-1.00949300	-0.03209200
H	4.37110200	-2.61916200	0.64778000
H	6.70361200	-1.91057600	0.16423800
H	7.15369700	0.25283300	-0.95350800
H	5.27456400	1.74724800	-1.60139000
Cl	1.46260900	-2.47443200	0.80646000
S	2.27103700	1.29075500	-1.20378000
C	1.28293100	-0.02772900	-0.47585400
C	-0.59366700	-0.23876800	-2.32425000
Pd	-0.64707300	0.27489100	-0.13980300
O	-0.73301100	2.64144800	-1.79048000
O	0.02202900	0.78562500	1.80718300
S	-0.97105400	4.03353700	-1.04465200
S	-0.59236600	-0.31568600	2.85895500
C	-0.48493500	3.72476400	0.73488500
H	-0.65557300	4.64833500	1.29519300
H	-1.07763400	2.88407000	1.10988300
H	0.57518000	3.45975200	0.71723300
C	-2.81831000	4.08509500	-0.76404200
H	-3.10245600	3.12560400	-0.31424300
H	-3.04816300	4.93733200	-0.11883100
H	-3.26966900	4.21117900	-1.74941500
C	-1.57470400	0.79479700	3.97552200
H	-0.93641200	1.64859100	4.21795300
H	-2.43276500	1.09100200	3.36606400

H	-1.87232500	0.22837300	4.86137700
C	0.90759600	-0.57051000	3.92267600
H	1.59794400	-1.15714600	3.31166000
H	1.31538000	0.41851400	4.14444700
H	0.61226800	-1.11412900	4.82328100
Cl	-2.93875700	0.75845300	0.74458800
C	-1.84875600	-0.58265200	-1.86742000
H	-0.42239600	0.74869800	-2.74661400
H	0.16429400	-0.99668900	-2.50852900
C	-2.29847100	-1.93491600	-1.51728800
C	-3.65885100	-2.14638000	-1.26700300
C	-1.41928600	-3.02298400	-1.43744200
C	-4.13319400	-3.41576900	-0.96274000
H	-4.33702700	-1.29567600	-1.29746500
C	-1.89212400	-4.28783800	-1.12355000
H	-0.35340600	-2.87391000	-1.59986700
C	-3.25153200	-4.48970000	-0.89055200
H	-5.19372500	-3.56579400	-0.77440600
H	-1.19667000	-5.12150500	-1.05906500
H	-3.62115100	-5.48366800	-0.64839100
H	-2.63062700	0.17544000	-1.92151100

TS9

C	3.60526300	0.39774700	-1.04394600
C	3.34681900	-0.95021700	-0.73727900
C	4.41992700	-1.82718300	-0.53581300
C	5.71396200	-1.34610500	-0.64436500
C	5.95652300	-0.00176900	-0.95383800
C	4.90334600	0.87977600	-1.15745000
C	1.93754500	-1.19183600	-0.67469100
H	4.22441700	-2.87156500	-0.30147700
H	6.55238300	-2.02114200	-0.48995100
H	6.97978500	0.35676600	-1.03651100
H	5.08661900	1.92450300	-1.39846400
Cl	1.32721000	-2.82942900	-0.28026300
S	2.09240800	1.33657400	-1.25169500
C	1.10346800	-0.13816800	-0.88208600
C	-0.48142100	-0.36570500	-2.09462600
Pd	-0.61997700	0.19930100	0.11214200
O	-0.67468000	2.59500200	-1.63350200
O	0.62558000	0.45567300	1.88779600
S	-0.87505500	3.94807300	-0.80629600
S	0.30187200	-0.82315600	2.84894500

C	-0.17516500	3.61038100	0.89543400
H	-0.28380900	4.52524400	1.48452400
H	-0.71582900	2.76448200	1.33346300
H	0.87684600	3.35732000	0.74223500
C	-2.68001400	3.91709800	-0.32427600
H	-2.87831000	2.94806400	0.15043400
H	-2.87244500	4.75397400	0.35231300
H	-3.23959700	4.03265600	-1.25408100
C	-0.54911700	-0.01252300	4.28834100
H	0.07047200	0.83585100	4.59012300
H	-1.50923100	0.31918600	3.87956700
H	-0.66949600	-0.75098100	5.08473500
C	1.98189900	-1.08801800	3.59297000
H	2.61236900	-1.45070300	2.77824500
H	2.33366500	-0.11685900	3.94950400
H	1.90487200	-1.82540100	4.39528600
Cl	-2.58905700	0.71758600	1.48852900
C	-1.80555300	-0.18344000	-1.58927300
H	-0.10212500	0.42930100	-2.73178000
H	-0.17923100	-1.37451700	-2.37259900
H	-2.24590600	0.80049900	-1.76520900
C	-2.75109400	-1.28092400	-1.35259300
C	-4.11076900	-0.97142000	-1.22137700
C	-2.35855400	-2.62330500	-1.26491500
C	-5.05305200	-1.97093600	-1.02659500
H	-4.41476700	0.07328100	-1.26118600
C	-3.30143500	-3.62199000	-1.06541100
H	-1.30526800	-2.88804000	-1.33959700
C	-4.65190500	-3.30160700	-0.94989300
H	-6.10446200	-1.71062700	-0.92906500
H	-2.98047100	-4.65939700	-1.00148000
H	-5.38901100	-4.08681200	-0.79759300

IM24

C	3.33609800	-0.38312700	-1.55795400
C	3.68405800	-1.11061400	-0.40728400
C	4.96650500	-0.96055600	0.13169300
C	5.86073700	-0.09726200	-0.47944900
C	5.49888600	0.61791700	-1.62873700
C	4.23280000	0.47864300	-2.17976700
C	2.57768600	-1.89616000	0.06129400
H	5.24000200	-1.52010100	1.02350500
H	6.85774600	0.02546500	-0.06290600

H	6.21660000	1.28840300	-2.09554500
H	3.94404900	1.03073900	-3.07138600
Cl	2.75107800	-2.91715700	1.50283000
S	1.64239300	-0.68008400	-2.03871900
C	1.41948500	-1.78780500	-0.62736600
C	0.08541200	-2.39010200	-0.35085800
Pd	-0.82589400	0.39313700	0.11784500
O	-1.80133000	1.06883100	-1.67993800
O	-0.45538300	2.50864900	0.79578900
S	-3.19469700	1.89623900	-1.49240400
S	0.77159200	2.66492900	1.86090100
C	-2.63300600	3.61685000	-1.05283100
H	-3.51464500	4.18446700	-0.74314600
H	-1.87776000	3.52136500	-0.26304200
H	-2.20428500	4.03248000	-1.96590900
C	-3.86832300	1.40646300	0.17619300
H	-3.05337900	1.49721900	0.90524200
H	-4.70766900	2.07436900	0.39092800
H	-4.19640200	0.36719800	0.08283400
C	1.26805800	4.41322700	1.45430800
H	1.43437500	4.46137500	0.37554800
H	0.42900100	5.04586300	1.74617200
H	2.16627500	4.67004600	2.02087800
C	2.22171200	1.82359400	1.03756400
H	2.09632300	0.75741600	1.24156700
H	2.15492100	2.04186800	-0.03306000
H	3.13761900	2.21762900	1.48752100
Cl	-0.03181900	-0.41955900	2.25728200
C	-1.07420200	-1.46655500	-0.69139300
H	-0.02238300	-3.32431700	-0.93090000
H	0.06714500	-2.66643600	0.71015900
C	-2.43188000	-1.92045300	-0.31143700
C	-2.73693700	-2.38140200	0.97981600
C	-3.47567100	-1.83532700	-1.24619400
C	-4.03729700	-2.73103900	1.31752800
H	-1.95074100	-2.41113800	1.73253900
C	-4.77778400	-2.18887100	-0.90677300
H	-3.24908700	-1.47888700	-2.25122600
C	-5.06546900	-2.63528000	0.38035400
H	-4.25378400	-3.07573400	2.32657800
H	-5.56841000	-2.12015700	-1.65178100
H	-6.08207000	-2.91228500	0.65084200
H	-1.05985900	-1.21698500	-1.76365400

IM25

C	3.59506000	0.95219800	-0.88904000
C	3.81521900	0.05840800	0.17259100
C	5.12014800	-0.13647700	0.63648800
C	6.16149800	0.55399900	0.03833400
C	5.92364600	1.43911600	-1.01985000
C	4.63512900	1.64503900	-1.49430300
C	2.58071600	-0.52831000	0.62172000
H	5.29908600	-0.82869800	1.45608300
H	7.17794300	0.40522100	0.39495000
H	6.75488500	1.96966900	-1.47813700
H	4.44262000	2.32854700	-2.31790700
Cl	2.57527400	-1.70527800	1.96755100
S	1.85129500	1.03292600	-1.31904100
C	1.45602900	-0.15349900	-0.02125400
Pd	-0.42637800	-0.66830500	0.25136500
O	-2.45960800	-1.24326800	0.72141600
S	-3.68348900	-1.33287900	-0.35094100
C	-3.19835700	-0.31565700	-1.83363600
H	-3.15802000	0.72445800	-1.49806500
H	-2.22573000	-0.67141000	-2.19349000
H	-3.99220000	-0.45410300	-2.57304600
C	-3.49676100	-3.03079900	-1.09074300
H	-3.67589000	-3.72929800	-0.27246500
H	-4.25574400	-3.13541000	-1.87043100
H	-2.47257900	-3.11144700	-1.47026400
Cl	-0.18312900	-2.12449300	-1.62740900
C	-1.83754100	2.75894800	-0.17646500
C	-1.90669400	1.89441800	0.92383300
C	-3.15025000	1.65692300	1.52190900
C	-4.29636800	2.25788700	1.01734400
C	-4.21934800	3.10361600	-0.08853600
C	-2.98549000	3.35512900	-0.68419600
H	-0.86754900	2.94011100	-0.64056100
H	-3.21709300	0.99469800	2.38164900
H	-5.25652700	2.07069500	1.49268600
H	-5.11941200	3.57368900	-0.47790700
H	-2.91737300	4.02026800	-1.54165500
C	-0.65946200	1.27170700	1.38651400
H	0.24361800	1.81991000	1.11224100
C	-0.51886200	0.21097000	2.26117700
H	-1.38253400	-0.28362600	2.70259000
H	0.45150700	-0.00144700	2.70558300

TS10

C	-3.95408900	0.12503900	-0.63421200
C	-3.49989000	-0.60278000	0.48080200
C	-4.42792100	-1.05128600	1.42950200
C	-5.76930900	-0.76839900	1.24537500
C	-6.20402300	-0.04118100	0.12889500
C	-5.29986300	0.41454800	-0.81964000
C	-2.08125800	-0.77117300	0.43757600
H	-4.08293200	-1.60856300	2.29747500
H	-6.49614600	-1.11238900	1.97699000
H	-7.26309000	0.17091000	0.00356600
H	-5.63107400	0.98308300	-1.68508300
S	-2.60212200	0.60039500	-1.70630100
C	-1.41485100	-0.21686300	-0.61269300
C	-0.17181500	-1.41735100	-1.59457400
Pd	0.44026900	0.59778200	-0.58073100
O	2.40184300	1.43270000	-0.77866000
S	3.35322300	1.74872400	0.51012800
C	2.63043600	0.80956900	1.94669600
H	3.19345300	1.11260600	2.83406200
H	1.56684300	1.07012100	2.01531200
H	2.78267700	-0.25189300	1.73093500
C	2.86020500	3.47311500	1.01175600
H	1.77284500	3.47338600	1.15138900
H	3.41728500	3.72193900	1.91896900
H	3.15689100	4.11416600	0.18063800
Cl	-0.39858100	2.35899200	0.88836100
C	1.19668200	-1.03654800	-1.69976000
H	-0.41253700	-2.27833500	-0.97264300
H	-0.77036400	-1.34248000	-2.49947900
C	2.28875700	-1.63681500	-0.92376100
C	3.61031800	-1.33103100	-1.28255700
C	2.07555000	-2.47452600	0.18179400
C	4.68226400	-1.83700500	-0.55937900
H	3.78325600	-0.66719700	-2.12726500
C	3.14952100	-2.98067400	0.90295900
H	1.06198800	-2.71589700	0.49670800
C	4.45695700	-2.66264100	0.53938700
H	5.69866600	-1.58598700	-0.85428700
H	2.96346900	-3.62866200	1.75650000
H	5.29478300	-3.06143000	1.10640400
H	1.50691300	-0.54261100	-2.62415200
Cl	-1.23634200	-1.67429800	1.71791200

IM26

C	4.00931600	-1.06319600	-0.60139700
C	4.39710900	0.16302400	-0.03666100
C	5.75318800	0.50571700	-0.00752800
C	6.68059000	-0.37581300	-0.53408600
C	6.27690000	-1.59593100	-1.09236900
C	4.93667500	-1.95146400	-1.13213200
C	3.25643300	0.89133900	0.43787800
H	6.05861400	1.45527200	0.42597900
H	7.73658200	-0.11869000	-0.51517700
H	7.02202400	-2.27501900	-1.49926900
H	4.61784100	-2.89717100	-1.56307800
Cl	3.44277100	2.48575800	1.19981300
S	2.23487900	-1.29872000	-0.53118100
C	2.05381200	0.29971100	0.26443200
C	0.70838100	0.80398100	0.62802900
Pd	-1.15882200	-0.67902700	0.44818900
O	-2.35684400	-1.01559600	-1.28622800
S	-3.95648500	-1.31835800	-1.16657600
C	-4.50825100	-0.39234100	0.34733300
H	-5.58377800	-0.55600500	0.45629800
H	-3.93300100	-0.77446200	1.20095900
H	-4.28748500	0.65880500	0.14415700
C	-4.06956100	-3.05849100	-0.51983700
H	-3.46521400	-3.11692100	0.39485900
H	-5.12819800	-3.26688200	-0.34269500
H	-3.67371500	-3.69446300	-1.31279600
Cl	-2.02986200	-2.21441700	2.16614000
C	-0.27350000	0.90633100	-0.48522000
H	0.27494000	0.07262700	1.44039600
H	0.80274300	1.72536200	1.21757100
C	-1.32127000	1.92742200	-0.50457900
C	-2.02900300	2.14975800	-1.69808300
C	-1.71153200	2.63537900	0.64464800
C	-3.08578200	3.04723800	-1.74125800
H	-1.74382000	1.58798600	-2.58565300
C	-2.77011000	3.53300100	0.59817400
H	-1.19026600	2.47637800	1.58754200
C	-3.46084700	3.74385600	-0.59326600
H	-3.61774900	3.20995200	-2.67592100
H	-3.05582000	4.07423600	1.49707500
H	-4.28455900	4.45289700	-0.62840700
H	0.08238700	0.58944200	-1.47028400

Cartesian Coordinates for the Stationary Points Given in Figure S3.

H-IM16

C	3.38612300	-0.12934400	0.43181200
C	3.34573800	-1.25805700	-0.41214600
C	4.43384900	-1.50113500	-1.26399600
C	5.51415800	-0.63685800	-1.25811000
C	5.53403000	0.47870500	-0.40866300
C	4.47224600	0.74108500	0.44399600
C	2.14122200	-2.01677100	-0.24604900
H	4.42032300	-2.37121300	-1.91767100
H	6.36006900	-0.82550700	-1.91480900
H	6.39449500	1.14380400	-0.41405700
H	4.48797800	1.60049400	1.11061100
S	1.90735500	0.00666000	1.42571300
C	1.27657400	-1.49989600	0.66010000
C	-0.04620800	-2.09227300	1.01604100
O	-0.95364600	-1.31035000	1.52427400
Pd	-1.36080100	0.35277800	0.44538200
O	-1.44488800	-0.87543300	-1.24346500
O	-1.90598600	1.91231100	-0.78518500
S	-2.82988700	-1.72201300	-1.48296300
S	-0.67778200	2.72853000	-1.50593000
C	-4.17015600	-0.45291800	-1.27122100
H	-5.12861000	-0.97074200	-1.36030800
H	-4.04018100	0.01385500	-0.28907400
H	-4.03409800	0.28446400	-2.06286400
C	-3.14991400	-2.72758200	0.05101000
H	-3.31402000	-2.05103400	0.89230700
H	-4.02259100	-3.34297000	-0.18424800
H	-2.24316400	-3.31714100	0.23496600
C	0.18116200	3.64989100	-0.13898800
H	-0.47620100	4.47473100	0.13769000
H	0.30688300	2.96600700	0.70831200
H	1.12608800	4.01263800	-0.55275000
C	0.63683100	1.45579000	-1.86329200
H	0.12268700	0.61711000	-2.33987800
H	1.36053000	1.92704800	-2.53328700
H	1.09143900	1.14536100	-0.91620800
Cl	-1.25657000	1.74434100	2.33908300
O	-0.20690100	-3.29256400	0.81626600
H	1.90936700	-2.93487000	-0.77790000

H-IM17

C	3.00105400	0.46217900	-0.54603800
C	2.56306900	-0.00194700	0.70270600
C	3.35011600	-0.92056700	1.40225800
C	4.54274700	-1.35116700	0.84713300
C	4.95752700	-0.87997800	-0.40357400
C	4.18872200	0.02883000	-1.11811200
C	1.28639200	0.55417500	1.08923200
H	3.00546700	-1.30362400	2.36020500
H	5.15813000	-2.07041600	1.38088600
H	5.89506400	-1.23282100	-0.82632600
H	4.50870600	0.39207000	-2.09117300
S	1.85484100	1.64594200	-1.26865100
C	0.77929700	1.45141000	0.13310000
C	-0.43944800	2.32798400	0.32340300
O	-1.43451700	1.54508600	0.65860000
Pd	-0.58732300	-0.28232500	0.21457200
O	-2.42118600	-1.21618400	-0.09767000
S	-3.59253200	-0.14741400	-0.54233500
C	-4.89648100	-1.39208300	-0.96806500
H	-4.55050800	-1.89600400	-1.87097800
H	-4.94960500	-2.09237600	-0.13132800
H	-5.83994200	-0.86900400	-1.13886100
C	-4.26703600	0.43342300	1.08799200
H	-3.52290900	1.13661200	1.46701500
H	-5.22792400	0.92069100	0.90488100
H	-4.35990700	-0.44989600	1.72500300
Cl	0.45937800	-2.30276800	-0.34344400
O	-0.44809800	3.52289300	0.15736700
H	0.92856300	0.53441900	2.11808200

H-IM18

C	3.22424600	-0.66136500	0.49638500
C	2.94790200	0.24286500	-0.54202900
C	3.77029000	1.36056300	-0.71646100
C	4.83533600	1.55887700	0.14400200
C	5.08661700	0.65384500	1.18274700
C	4.28375300	-0.46233600	1.37205500
C	1.78448700	-0.13311000	-1.30306300
H	3.55584700	2.06799900	-1.51502700
H	5.47786600	2.42678100	0.02087900
H	5.92347800	0.82779600	1.85497400
H	4.47767700	-1.16139800	2.18141000

S	2.05548500	-2.02233900	0.55067300
C	1.19258100	-1.32237600	-0.83405700
C	0.08327600	-2.03531200	-1.57162600
O	-0.80665100	-1.12710400	-1.88032400
Pd	-0.28170000	0.25627500	-0.47692300
O	-2.32636300	0.94509700	-0.44225400
S	-2.80539000	2.50628800	-0.44979100
C	-2.63474900	3.05240100	1.32170700
H	-3.44969600	2.57092300	1.86457800
H	-1.65083800	2.71629600	1.67058700
H	-2.74568400	4.13977300	1.34187500
C	-1.39248000	3.44700800	-1.20435000
H	-1.27882600	3.04263800	-2.21215900
H	-1.68197100	4.50079000	-1.23296900
H	-0.50191200	3.26441200	-0.59126000
Cl	0.55905500	1.78710200	1.16478800
O	0.04963400	-3.22258400	-1.79914700
O	-1.01084800	-1.72852000	1.09882800
S	-2.45734100	-2.39783500	1.24061900
C	-3.24688000	-2.30870600	-0.45185400
H	-4.26218600	-2.70370000	-0.35682600
H	-3.22201000	-1.26756900	-0.78420800
H	-2.63353800	-2.93123500	-1.10629600
C	-3.46534300	-1.03537500	2.02647700
H	-3.07903300	-0.91840300	3.03995400
H	-3.26853800	-0.14498900	1.42105800
H	-4.52004900	-1.32283300	2.03172400
H	1.56921000	0.26850900	-2.29167200

H-TS6

C	-3.41338600	-0.54195900	0.36585000
C	-2.87059400	0.39786000	-0.53131900
C	-3.46613400	0.55779800	-1.78946300
C	-4.57165100	-0.20472000	-2.12323600
C	-5.09707900	-1.13278300	-1.21452200
C	-4.52313600	-1.30986200	0.03659600
C	-1.74326000	1.08701000	0.02594400
H	-3.05442700	1.27971300	-2.49416200
H	-5.03752200	-0.08507300	-3.09844600
H	-5.96461000	-1.72628800	-1.49340000
H	-4.92671700	-2.03386600	0.73989600
S	-2.48840100	-0.59590200	1.89528500
C	-1.39220900	0.67004300	1.28674100

C	-0.23511300	1.16936300	2.15084100
O	0.57955800	0.24372000	2.43256100
Pd	0.73635400	-0.22751800	0.02177600
O	1.91201700	1.46303900	0.22822300
O	2.23098000	-0.82057800	-1.32662200
S	1.90769100	2.70609300	-0.84324900
S	3.52636200	-1.57262100	-0.63586500
C	0.53645300	3.83402600	-0.24678400
H	-0.26292400	3.85705600	-0.99149400
H	0.20823600	3.41530200	0.72319500
H	0.98067300	4.82270700	-0.12173800
C	1.15560500	2.00793500	-2.39036000
H	0.17286100	1.59240500	-2.14517000
H	1.09519200	2.82077100	-3.11846700
H	1.82747400	1.21180200	-2.71760900
C	3.46328600	-1.14341700	1.17322200
H	3.53767800	-0.05576200	1.24114800
H	2.50368300	-1.48055500	1.58214000
H	4.31750600	-1.64227600	1.63988700
C	2.99546500	-3.34942600	-0.52778200
H	3.01675600	-3.73848100	-1.54623700
H	3.72004000	-3.86462600	0.10801100
H	1.97572000	-3.36193700	-0.12472200
Cl	-0.29846900	-2.32126500	-0.14968200
O	-0.19669800	2.37887800	2.39785700
H	-1.27466100	1.94363100	-0.44919700

H-IM19

C	4.62660400	0.50025900	0.09575600
C	4.35958200	-0.87848200	-0.03560000
C	5.43761300	-1.77662000	-0.09008600
C	6.72928900	-1.29313500	-0.01518400
C	6.97212700	0.08326400	0.11464000
C	5.92702500	0.99116800	0.17189300
C	2.95931300	-1.15633200	-0.09870800
H	5.24481400	-2.84265700	-0.19133800
H	7.56841800	-1.98289300	-0.05722700
H	7.99628000	0.44424500	0.17069500
H	6.11498500	2.05726700	0.27194600
S	3.12970000	1.46901700	0.14405600
C	2.18640200	-0.04227100	-0.01968000
C	0.73529700	0.00735800	-0.06311400
O	0.11610000	1.12334800	0.01322700

Pd	-1.68476800	0.15314200	-0.16910600
O	-3.05429800	-1.32974900	-0.43630400
S	-4.57364500	-1.42229000	0.17465800
C	-4.54148800	-0.51424600	1.79390100
H	-3.81764400	-1.04660600	2.41368300
H	-4.23136400	0.51838500	1.60174400
H	-5.54676800	-0.58692300	2.21707000
C	-5.59096300	-0.25744900	-0.85611800
H	-5.57302300	-0.67336100	-1.86440700
H	-6.60390300	-0.27101500	-0.44515400
H	-5.11932900	0.72976700	-0.81508700
Cl	-3.15382700	2.00766900	-0.09199500
O	0.04474200	-1.05636000	-0.18210200
H	2.52788900	-2.14774400	-0.20331700

H-TS7

C	3.89519700	-0.71131200	-0.22192800
C	4.33056800	0.49888500	0.35754500
C	5.64217700	0.57863500	0.85004500
C	6.47328900	-0.52205500	0.75836900
C	6.01846600	-1.71633700	0.17983600
C	4.72826600	-1.82220900	-0.31557800
C	3.30940700	1.50185100	0.35913900
H	5.99174300	1.50623300	1.29899100
H	7.49028700	-0.46443600	1.13865100
H	6.68630000	-2.57248500	0.11970100
H	4.37316700	-2.74755200	-0.76247800
S	2.20460700	-0.60180500	-0.78306600
C	2.14201500	1.09183800	-0.19342400
C	0.91221400	1.90547900	-0.29716400
O	-0.07265500	1.31690100	-0.95646200
Pd	-1.52233500	0.19910600	-0.19413500
O	-3.20812300	0.88669100	0.66819000
S	-4.75437000	0.36892700	0.42097600
C	-4.76640100	-0.43651600	-1.25023900
H	-4.48000600	0.34418500	-1.95744700
H	-4.04390000	-1.25876700	-1.23554100
H	-5.79029500	-0.77345200	-1.43134100
C	-4.97087000	-1.10331600	1.53494800
H	-4.86543800	-0.71520600	2.54902200
H	-5.98210300	-1.48164000	1.36348700
H	-4.18860400	-1.82964400	1.29718600
Cl	-2.03293100	-2.07862500	0.11195400

O	0.84147400	3.02183300	0.17659900
H	3.42074700	2.50348900	0.76432300

H-TS2’

C	3.60459200	0.26079000	-0.60306500
C	3.46746800	-0.78632000	0.33974200
C	4.58077700	-1.59170600	0.65015100
C	5.78409000	-1.34930600	0.02580100
C	5.90387300	-0.30267500	-0.90865200
C	4.82836400	0.50661800	-1.22664200
C	2.15350600	-0.85327500	0.86355600
H	4.47718600	-2.39410500	1.37786700
H	6.65086500	-1.96357600	0.25566800
H	6.86376100	-0.12690100	-1.38918800
H	4.93009500	1.31449900	-1.94676400
S	2.09564300	1.15857000	-0.84277500
C	1.28723500	0.12526800	0.39805800
C	0.77628200	1.09978200	1.94320500
O	-0.34059900	0.62137700	2.19223900
Pd	-0.67232200	-0.27087400	0.30262400
O	-2.79617300	-0.55340100	0.56465700
S	-3.50679200	-2.02302300	0.52648500
C	-3.88641200	-2.29003200	-1.27679000
H	-4.65936700	-1.56240700	-1.52945000
H	-2.95977500	-2.11117400	-1.83318900
H	-4.26278300	-3.31038800	-1.38716000
C	-2.13109400	-3.26124500	0.71304900
H	-1.70663400	-3.09067000	1.70432600
H	-2.58665000	-4.25318700	0.64539100
H	-1.39501800	-3.07163800	-0.07794400
Cl	-0.53969000	-1.38641600	-1.81577600
O	1.58609000	1.87923600	2.31484300
O	-0.58675400	2.35359100	-0.30794700
S	-1.98868900	3.02955000	-0.65718100
C	-3.05212000	2.69082800	0.84416000
H	-4.06419200	3.04921100	0.63682400
H	-3.02305800	1.61446000	1.04522100
H	-2.59708800	3.25394500	1.66064800
C	-2.82410300	1.81742600	-1.81302300
H	-2.17180300	1.74149100	-2.68462300
H	-2.88471500	0.85549600	-1.29370900
H	-3.80557000	2.21966500	-2.07907500
H	1.83846100	-1.58032200	1.61052300

H-IM20

C	-3.33839400	-0.91738900	0.63942400
C	-3.19511400	-0.68959400	-0.74492000
C	-4.34891200	-0.68774200	-1.54185100
C	-5.58802900	-0.90688300	-0.96251000
C	-5.70572200	-1.13108500	0.41530000
C	-4.57892400	-1.14055700	1.22635800
C	-1.82531600	-0.46587500	-1.13375600
H	-4.26002200	-0.52062400	-2.61423400
H	-6.48089300	-0.90775200	-1.58405400
H	-6.68608600	-1.30234800	0.85424900
H	-4.66196500	-1.31980000	2.29619600
S	-1.74291700	-0.87863100	1.46023700
C	-0.92907800	-0.51515400	-0.11392000
Pd	0.97948100	-0.11623500	-0.08056400
O	0.55502700	1.85042800	0.51695300
O	3.05883500	0.47567800	0.02809700
S	-0.56956600	2.60719500	-0.40357800
S	4.17734000	-0.64308900	-0.36380000
C	0.03009000	4.34709600	-0.14564600
H	-0.69726000	5.04255400	-0.57055700
H	0.15742900	4.48269400	0.93097400
H	0.99047600	4.41262500	-0.65757200
C	-2.05711000	2.68837000	0.71416000
H	-1.66777800	2.83084300	1.72588500
H	-2.68326400	3.52065100	0.38240100
H	-2.57961400	1.73330000	0.62565800
C	4.27154200	-1.70823400	1.16094900
H	4.25326700	-1.02950400	2.01781200
H	3.38007400	-2.33758400	1.12274200
H	5.18988500	-2.29896200	1.11264300
C	5.69235600	0.38051600	-0.03106500
H	5.72281200	1.14564700	-0.80730100
H	5.55861100	0.83602000	0.95292800
H	6.57477500	-0.26206700	-0.07603900
Cl	1.47312200	-2.34648700	-0.71669500
H	-1.52259900	-0.28584300	-2.16327700

Cartesian Coordinates for the Stationary Points Given in Figure S4.

H-IM21

C	-3.43488600	-1.95715600	0.22438400

C	-3.34529000	-0.61720000	0.64581200
C	-4.46317600	-0.02404600	1.24843700
C	-5.61893000	-0.76680000	1.42446900
C	-5.68242000	-2.10302900	1.00770400
C	-4.58989100	-2.71011900	0.40377100
C	-2.06439200	-0.02781200	0.35574100
H	-4.41218300	1.01789500	1.56048600
H	-6.48896200	-0.30847200	1.88926800
H	-6.59879600	-2.67037700	1.15349400
H	-4.63657900	-3.74520200	0.07313200
S	-1.90461700	-2.50658000	-0.53491100
C	-1.19773500	-0.86723000	-0.25825500
C	-0.04457700	-0.35579600	-2.84124500
Pd	0.64001800	-0.43722400	-0.81114100
O	1.11773200	-2.78415200	-0.32728200
O	1.37782900	-0.30453200	1.28467300
S	2.55985400	-3.50007400	-0.37079900
S	0.27395300	-0.22217200	2.49900500
C	3.69983700	-2.43482200	0.65390200
H	4.71261400	-2.82633600	0.52435200
H	3.59967500	-1.39767800	0.32087500
H	3.36588400	-2.54574900	1.68668500
C	3.23793400	-3.07969000	-2.05625900
H	3.23956000	-1.99029100	-2.16191700
H	4.24217500	-3.50362100	-2.13617100
H	2.55772500	-3.54982600	-2.76859600
C	1.38574300	0.31183900	3.88236900
H	2.31579000	-0.25339600	3.77561400
H	1.53294300	1.38554500	3.72385000
H	0.87844500	0.10817300	4.82879900
C	0.10551100	-2.03192900	2.90030400
H	-0.08978400	-2.52117000	1.94025100
H	1.05515000	-2.37509300	3.31934500
H	-0.72121900	-2.15845300	3.60300500
Cl	3.01629400	0.45349900	-1.40418900
C	-0.08186600	0.97637600	-2.42224400
H	0.82564100	-0.71493700	-3.39018900
H	-0.95915700	-0.93532200	-2.96047000
Ag	2.08254800	2.02341000	0.37960200
Cl	0.83337800	3.29518900	2.02083200
H	-1.81966000	1.01037200	0.58400000
H	0.83791600	1.55309700	-2.53851700
C	-1.26047100	1.77541300	-2.08098300
C	-1.06592500	2.96000400	-1.35912900

C	-2.56495800	1.39050400	-2.41405600
C	-2.14794800	3.72341800	-0.94311600
H	-0.05412100	3.25722600	-1.07764800
C	-3.64591100	2.16686900	-2.01976800
H	-2.73441200	0.47125000	-2.97293000
C	-3.44106300	3.32807700	-1.27592400
H	-1.97525300	4.61930400	-0.35233900
H	-4.65520400	1.86018700	-2.28424100
H	-4.29224500	3.92666700	-0.95924400

H-TS8

C	3.95331500	0.03317300	-1.20454500
C	3.28670000	-1.20274400	-1.32921600
C	4.04559800	-2.38192900	-1.34503300
C	5.42473700	-2.30857700	-1.24261300
C	6.06978700	-1.06936600	-1.13305500
C	5.33934300	0.11191600	-1.11653200
C	1.85846500	-1.06242300	-1.35752800
H	3.54231800	-3.34347700	-1.42984800
H	6.01558100	-3.22150000	-1.24923500
H	7.15390700	-1.02960400	-1.05897800
H	5.83675800	1.07497500	-1.02484500
S	2.78995500	1.39482100	-1.10507600
C	1.41384600	0.21539000	-1.20052400
C	-0.10916800	0.86305200	-2.45165100
Pd	-0.24409500	0.69202000	-0.15432000
O	0.19404500	3.32262600	-0.69581700
O	0.77374100	0.14644100	1.69990600
S	0.37408700	4.32635100	0.54173400
S	1.50696300	-1.32181200	1.73638500
C	0.76056500	3.24287000	2.01477700
H	0.88369200	3.89865400	2.88127000
H	-0.05354100	2.52353500	2.14880000
H	1.68799900	2.71849900	1.77442300
C	-1.38009900	4.74916800	1.02319000
H	-1.92941800	3.80462300	1.10030300
H	-1.35969800	5.29556200	1.96970100
H	-1.77505200	5.37378600	0.22074500
C	0.92865200	-1.95061400	3.38241200
H	0.90708500	-1.09178600	4.05753100
H	-0.06224800	-2.37455300	3.20115700
H	1.62386400	-2.72776800	3.70929500
C	3.23313100	-0.83129400	2.22346300

H	3.65598800	-0.30564100	1.36279400
H	3.15688300	-0.17615800	3.09500100
H	3.80232000	-1.74038200	2.43425400
Cl	-2.32757100	1.17794400	1.25335600
C	-1.39917900	1.07580700	-1.90249000
H	0.46494400	1.74420700	-2.72578500
H	0.04589100	-0.01358600	-3.07503700
Ag	-2.07302900	-1.32534600	0.94078300
Cl	-1.15180500	-3.56060700	0.98859800
H	1.18157400	-1.91336600	-1.42539400
H	-1.68785700	2.11332200	-1.72006500
C	-2.49447200	0.09992400	-1.99008700
C	-3.81474000	0.55637800	-1.90046000
C	-2.26773300	-1.28136500	-2.09975200
C	-4.87864400	-0.33547800	-1.93552400
H	-3.99534100	1.62325400	-1.78223400
C	-3.33157600	-2.17547000	-2.11359800
H	-1.25081500	-1.66957900	-2.13980700
C	-4.64055800	-1.70376100	-2.03556400
H	-5.89781800	0.03741500	-1.86828400
H	-3.13097100	-3.24293000	-2.15894000
H	-5.47210600	-2.40410000	-2.04357300

H-IM22

C	-2.38930600	-1.06316400	2.55228000
C	-2.79450300	-1.67636500	1.35302600
C	-4.14658900	-1.61411400	0.99199200
C	-5.04322100	-0.95481700	1.81553100
C	-4.61684700	-0.35436400	3.00655100
C	-3.28248000	-0.40249400	3.38817300
C	-1.69112500	-2.25939100	0.63417400
H	-4.47717800	-2.05057700	0.05192600
H	-6.08882200	-0.89236300	1.52552100
H	-5.33708300	0.15749600	3.64065300
H	-2.94393100	0.06111100	4.31201700
S	-0.62191700	-1.21299600	2.79188400
C	-0.48296800	-2.10050500	1.22630400
C	0.85771300	-2.54052100	0.74454400
Pd	1.24680400	0.29451100	-0.06062700
O	2.06258300	1.19772400	1.71189500
O	0.49785300	2.37888600	-0.72810800
S	3.04930500	2.49177500	1.56380000
S	-1.09524700	2.12209300	-0.97337400

C	1.87685300	3.93680600	1.49983900
H	2.46733400	4.83509000	1.30054500
H	1.15070900	3.70655400	0.70962600
H	1.41598600	3.98383900	2.48796200
C	3.61249700	2.48863200	-0.21191000
H	2.72087400	2.48158300	-0.84871000
H	4.22922300	3.38016800	-0.35714700
H	4.20148500	1.57523700	-0.33631500
C	-1.74959400	3.79988600	-1.41232300
H	-1.43367100	4.50318500	-0.63730000
H	-1.32318200	4.05641800	-2.38245700
H	-2.83609400	3.69740300	-1.47528700
C	-1.80221800	1.98439300	0.74593900
H	-1.23873500	1.18421700	1.23961600
H	-1.65427500	2.94069700	1.25576000
H	-2.85685600	1.71092600	0.62824700
Cl	0.48922000	-0.87561900	-2.12702900
C	1.90653000	-1.44353300	0.79621300
H	1.21981800	-3.38256900	1.36163000
H	0.72544300	-2.92888600	-0.27160900
Ag	-2.00227600	-0.57895600	-1.96421500
Cl	-4.12224400	0.58424500	-1.76342000
H	-1.80542500	-2.79939300	-0.30586500
H	2.02500300	-1.07405900	1.82524100
C	3.22606000	-1.69030200	0.18114300
C	4.36829600	-1.11864400	0.77024700
C	3.39519900	-2.43777600	-0.99417900
C	5.62508300	-1.27511600	0.20082400
H	4.24725500	-0.55025600	1.69319900
C	4.65315700	-2.59581600	-1.56062300
H	2.52747600	-2.87197700	-1.48527300
C	5.77256400	-2.01365800	-0.97125200
H	6.49603500	-0.83153800	0.67962400
H	4.75999700	-3.17574000	-2.47459100
H	6.75561400	-2.14139900	-1.41867900

H-IM23

C	-2.79309500	-2.22353900	0.28378300
C	-2.94288100	-0.94007900	0.84315900
C	-4.16177900	-0.61226100	1.45306300
C	-5.17790100	-1.55244000	1.50727200
C	-5.00150400	-2.82897900	0.95826300
C	-3.80589100	-3.17410600	0.34233500

C	-1.77544200	-0.11997800	0.66157700
H	-4.30067200	0.38482400	1.87000600
H	-6.12438700	-1.29786300	1.97961900
H	-5.80855500	-3.55632000	1.01084600
H	-3.66529600	-4.16244400	-0.09009800
S	-1.17477400	-2.41990100	-0.46306100
C	-0.76693900	-0.72335900	-0.01298300
C	0.37399300	0.15709400	-2.54366100
Pd	0.96429900	0.08347200	-0.50056100
O	1.86300000	-2.09694900	-0.25781400
O	1.40826900	0.22867100	1.67792700
S	3.40962600	-2.52449700	-0.13239700
S	1.12765700	1.76855900	2.10891500
C	4.18758000	-1.31548500	1.05981600
H	5.22533600	-1.62736000	1.20596700
H	4.09635000	-0.31068300	0.63370000
H	3.60376400	-1.40254300	1.97770000
C	4.20140100	-1.89972100	-1.70303300
H	3.96727900	-0.83268100	-1.79224400
H	5.27675300	-2.08598800	-1.63814800
H	3.75295000	-2.48206300	-2.50962000
C	2.83532200	2.38313000	2.51541300
H	3.29300700	1.63881100	3.17265800
H	3.34475800	2.43147900	1.54886100
H	2.75306200	3.36478500	2.98850100
C	0.48714800	1.52732500	3.83813000
H	-0.48181300	1.03799300	3.72536000
H	1.19177600	0.86956400	4.35256200
H	0.39194000	2.50070400	4.32508300
Cl	3.09529100	1.39492900	-0.93912900
C	0.02981300	1.41592200	-2.03910600
H	1.32498700	0.03640400	-3.06125600
H	-0.38174100	-0.59994300	-2.74931300
H	-1.74095800	0.92694000	0.96498100
H	0.80297200	2.18582600	-2.07660000
C	-1.31308800	1.91718600	-1.73034100
C	-1.41941000	3.14236600	-1.05973600
C	-2.48663900	1.22444000	-2.05031000
C	-2.65915300	3.64640900	-0.68764300
H	-0.50641500	3.68888500	-0.82033900
C	-3.72639900	1.72895700	-1.68267800
H	-2.42850000	0.26967500	-2.57050300
C	-3.81737100	2.93631800	-0.99375500
H	-2.72397700	4.59731200	-0.16303300

H	-4.62697000	1.16909900	-1.92392700
H	-4.79024200	3.32656600	-0.70338500

H-TS9

C	3.57818200	-0.10293900	-1.09739900
C	3.18273900	-1.35445300	-0.58136200
C	4.17725600	-2.27114600	-0.20544400
C	5.51256600	-1.93434800	-0.35218900
C	5.88311300	-0.68984100	-0.87814600
C	4.91754000	0.23341400	-1.25735300
C	1.75638200	-1.49476900	-0.51021400
H	3.88992900	-3.24284500	0.19385200
H	6.28301000	-2.64510000	-0.06163500
H	6.93622000	-0.44345200	-0.99187500
H	5.20089400	1.20044800	-1.66678200
S	2.15938600	0.91685500	-1.48999900
C	1.05857600	-0.39202800	-0.91139000
C	-0.59895500	-0.60024800	-2.11894300
Pd	-0.62793600	0.18394400	0.03001300
O	-0.84015700	2.27488300	-1.86969600
O	0.69174800	0.89810600	1.62356300
S	-1.05875600	3.73499400	-1.25558300
S	0.74343300	-0.29922100	2.72603000
C	-0.29347100	3.67102200	0.44913000
H	-0.44233000	4.64817600	0.91735800
H	-0.76616600	2.85690300	1.00944000
H	0.76734900	3.46017100	0.29596400
C	-2.84433600	3.72960800	-0.70619300
H	-2.99603600	2.83774900	-0.08491700
H	-3.03906000	4.65451000	-0.15664900
H	-3.43891300	3.68918900	-1.62039000
C	-0.14113700	0.48981000	4.15577400
H	0.33313300	1.45829200	4.33294300
H	-1.16602100	0.61378100	3.79304800
H	-0.08357300	-0.17350400	5.02196400
C	2.49953000	-0.13494100	3.30894600
H	3.12085600	-0.47636500	2.47734100
H	2.67093300	0.92540200	3.51018900
H	2.64157500	-0.75653700	4.19609700
Cl	-2.55885700	0.78577500	1.44237600
C	-1.87235400	-0.59170000	-1.48270400
H	-0.35718200	0.25413900	-2.74597900
H	-0.18721000	-1.55196600	-2.44322800

H	1.26548000	-2.39549000	-0.14412200
H	-2.50018600	0.28349400	-1.66291100
C	-2.56258500	-1.81245800	-1.04266500
C	-3.91020300	-1.73420000	-0.67043000
C	-1.92489500	-3.05921900	-0.97918100
C	-4.60164100	-2.86558200	-0.26016300
H	-4.40089400	-0.76303400	-0.68626500
C	-2.61488400	-4.18964500	-0.56410600
H	-0.87619600	-3.14855600	-1.26082100
C	-3.95744200	-4.09836500	-0.20537200
H	-5.64804400	-2.78391100	0.02470900
H	-2.10434500	-5.14955300	-0.52511200
H	-4.49920900	-4.98533400	0.11512600

H-IM24

C	3.17566900	-1.66390200	-1.12285700
C	3.15503000	-1.59378200	0.28491300
C	4.29668500	-1.11959600	0.94780700
C	5.40917600	-0.73564600	0.21491400
C	5.40992300	-0.82507900	-1.18452700
C	4.29285300	-1.29475800	-1.86397800
C	1.89020700	-1.97850600	0.84243100
H	4.29384100	-1.05510800	2.03490500
H	6.29580700	-0.37100500	0.72932100
H	6.29353600	-0.52844800	-1.74505300
H	4.28649400	-1.36164000	-2.94940400
S	1.60204600	-2.22121800	-1.75981900
C	0.95344500	-2.31280700	-0.07420000
C	-0.49664100	-2.59281700	0.13521900
Pd	-0.66618200	0.33698100	0.35722300
O	-0.85698200	1.04516500	-1.66925600
O	0.34616300	2.30663400	0.96930700
S	-1.86286500	2.31192300	-1.89801300
S	1.84508400	1.71149700	1.17857400
C	-0.80465300	3.79286900	-1.50274800
H	-1.45892600	4.66729200	-1.45238100
H	-0.29621400	3.57167400	-0.55518500
H	-0.09813400	3.88555200	-2.32969100
C	-2.96222200	2.36759000	-0.39391300
H	-2.32391000	2.37598300	0.49710000
H	-3.58212100	3.26479100	-0.48198000
H	-3.56950900	1.45843500	-0.42332400
C	2.72572400	3.19546600	1.87715300

H	2.46296000	4.05534400	1.25578300
H	2.35076400	3.31974600	2.89362000
H	3.79968600	2.99359500	1.87269800
C	2.54269400	1.78239100	-0.54945200
H	1.89430700	1.13451300	-1.14727100
H	2.48126100	2.81956100	-0.89159100
H	3.57037900	1.40674000	-0.52602700
Cl	-0.59277100	-0.38970700	2.65460000
C	-1.35560700	-1.44235500	-0.37708100
H	-0.79014700	-3.52020100	-0.38632600
H	-0.65369700	-2.75468800	1.20753200
H	1.64727800	-1.91417000	1.90076700
H	-1.15659300	-1.28156200	-1.44704500
C	-2.81617200	-1.49012600	-0.14359200
C	-3.68753000	-1.17215800	-1.19827600
C	-3.37734600	-1.79422700	1.10667700
C	-5.06573900	-1.14614800	-1.01235100
H	-3.26496500	-0.95406200	-2.17985700
C	-4.75307800	-1.76951500	1.28987700
H	-2.71798000	-1.99618400	1.94820600
C	-5.60497300	-1.44235600	0.23626300
H	-5.72032400	-0.90475400	-1.84788200
H	-5.16654300	-1.99961400	2.26964700
H	-6.68211500	-1.42474900	0.38705600

H-IM25

C	3.84910000	0.50093400	-0.66687100
C	3.94201400	-0.22391000	0.53564900
C	5.20625700	-0.39873200	1.11289200
C	6.32385200	0.14062200	0.49695300
C	6.20625800	0.85753900	-0.69958400
C	4.96458800	1.04182600	-1.29365000
C	2.66189300	-0.68683700	1.01256700
H	5.30036400	-0.95833300	2.04203300
H	7.30497100	0.00460800	0.94653100
H	7.09412000	1.27304700	-1.17065400
H	4.86684200	1.59326900	-2.22599900
S	2.14602500	0.58906300	-1.23084400
C	1.62037800	-0.35272100	0.21556200
Pd	-0.30280700	-0.69599600	0.46832200
O	-2.39136100	-1.07874000	0.99700300
S	-3.62167500	-1.32050700	-0.04019500
C	-3.11237200	-0.57607200	-1.66929900

H	-3.09989300	0.50734400	-1.52222000
H	-2.12476300	-0.97368200	-1.92956400
H	-3.88017900	-0.86055400	-2.39414400
C	-3.48213900	-3.12346100	-0.48388500
H	-3.69347700	-3.66956400	0.43635600
H	-4.23576300	-3.33390400	-1.24719600
H	-2.45749300	-3.29719400	-0.82896400
Cl	-0.13380300	-2.41372100	-1.18925500
C	-1.42627000	2.69358700	-0.57642400
C	-1.60795300	2.01441000	0.63531000
C	-2.89508200	1.93751100	1.18255300
C	-3.97237600	2.51378200	0.52199800
C	-3.78308500	3.17504100	-0.69113200
C	-2.50550100	3.26606600	-1.23857600
H	-0.42429500	2.74887600	-1.00232900
H	-3.05026800	1.42044500	2.12606700
H	-4.96677800	2.45199600	0.95841800
H	-4.62916900	3.62867900	-1.20222300
H	-2.34942800	3.78547100	-2.18099700
C	-0.42852200	1.40180800	1.26142200
H	0.52233100	1.83863600	0.95038400
C	-0.39695800	0.49289500	2.30340500
H	-1.30665200	0.13583500	2.78299200
H	0.54282300	0.31321300	2.82078600
H	2.54729900	-1.27181700	1.92252300

H-TS10

C	-4.01699400	-0.04826900	-0.38787300
C	-3.48162500	-0.73639700	0.71989100
C	-4.35511900	-1.16340600	1.73152500
C	-5.70886600	-0.90154200	1.62263000
C	-6.21804800	-0.21529800	0.51136100
C	-5.37607200	0.21792400	-0.50302500
C	-2.06367700	-0.91085100	0.62937700
H	-3.95830500	-1.69069800	2.59717500
H	-6.38713500	-1.22905100	2.40700400
H	-7.28508200	-0.01707200	0.44296300
H	-5.76686700	0.75350000	-1.36477400
S	-2.73484900	0.40516900	-1.54856400
C	-1.49393600	-0.36357200	-0.48192000
C	-0.24934000	-1.57579400	-1.52785600
Pd	0.36243500	0.45981400	-0.55111100
O	2.32723600	1.28193700	-0.88200200

S	3.31449700	1.77273800	0.31955400
C	2.67273100	0.99011600	1.88219800
H	3.26904300	1.39405400	2.70516000
H	1.60908200	1.24599600	1.96705200
H	2.83158700	-0.08669700	1.77606600
C	2.78961500	3.53100900	0.63733900
H	1.70725100	3.51956200	0.81246700
H	3.36550100	3.89569300	1.49212500
H	3.04416300	4.07970400	-0.27037700
Cl	-0.42985400	2.30603500	0.84390600
C	1.12945800	-1.23893000	-1.55422800
H	-0.55869500	-2.43529600	-0.93986600
H	-0.81335800	-1.44896000	-2.44826100
C	2.13057500	-1.83202800	-0.65812900
C	3.49134300	-1.65787800	-0.94799200
C	1.78287500	-2.52242100	0.51245200
C	4.47095000	-2.15785000	-0.09963100
H	3.76849500	-1.10258300	-1.84220500
C	2.76256900	-3.02043200	1.36116400
H	0.73315700	-2.65533700	0.77161000
C	4.11172100	-2.83997400	1.06030600
H	5.52090700	-2.01282200	-0.34396300
H	2.47249500	-3.55190300	2.26475400
H	4.87733100	-3.23214600	1.72538400
H	1.52570000	-0.78252500	-2.46427400
H	-1.48098500	-1.42592100	1.39131400

H-IM26

C	4.36937200	-0.41150700	-0.52100000
C	4.60148700	0.64572600	0.37854900
C	5.92388600	1.03361300	0.63228000
C	6.96288400	0.37291000	0.00011900
C	6.70695200	-0.67781800	-0.89032400
C	5.40656100	-1.07952300	-1.16038400
C	3.38340000	1.18075500	0.91927400
H	6.12270100	1.84954000	1.32452700
H	7.99001100	0.67035300	0.19699000
H	7.53588200	-1.18700000	-1.37596500
H	5.20367300	-1.89537500	-1.84959800
S	2.62057000	-0.74754900	-0.69831700
C	2.26367900	0.57728000	0.46012300
C	0.85669100	0.88759000	0.81823400
Pd	-0.86864800	-0.67702400	0.34835200

O	-2.10809500	-0.81988100	-1.38599000
S	-3.69843600	-1.16135800	-1.24378500
C	-4.20436300	-0.47413500	0.40945900
H	-5.26316500	-0.71133700	0.54596900
H	-3.56577000	-0.93691100	1.17483600
H	-4.04832300	0.60670100	0.34434400
C	-3.75599400	-2.97886200	-0.84834500
H	-3.10421000	-3.15402700	0.01858800
H	-4.80128800	-3.23319300	-0.65296600
H	-3.39051400	-3.48520800	-1.74272400
Cl	-1.62659200	-2.50243500	1.82259100
C	-0.09534300	1.10085300	-0.30250800
H	0.47157900	-0.02206400	1.47168000
H	0.83207700	1.68694200	1.57110500
C	-1.23064600	2.01925200	-0.19980300
C	-1.90532800	2.40112800	-1.37114800
C	-1.74560100	2.45023800	1.03480500
C	-3.05592400	3.17422400	-1.31098200
H	-1.52043700	2.06129200	-2.33079300
C	-2.89752300	3.22340500	1.09248300
H	-1.25493000	2.15913700	1.96243100
C	-3.55971000	3.58719600	-0.07856300
H	-3.56298600	3.45926300	-2.23004500
H	-3.28137500	3.54524200	2.05785000
H	-4.45938700	4.19615800	-0.03162400
H	0.31543300	0.98368600	-1.31001500
H	3.35465200	1.99890100	1.63514800