

Supporting Information for

Intramolecular alkyne–dithiolium cycloaddition: a joint experimental and DTF mechanistic study

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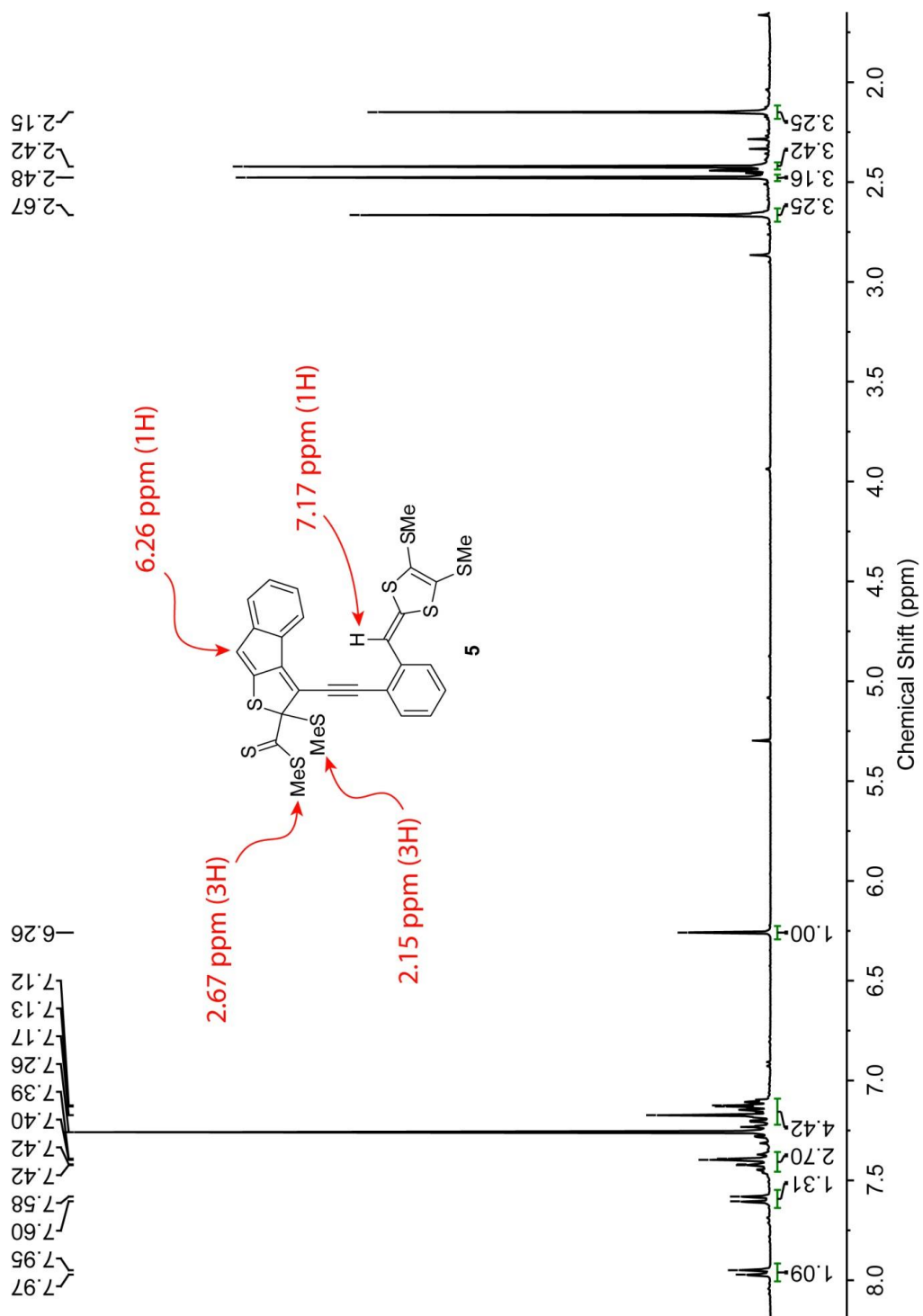
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1. NMR Spectra for New Compounds

Fig. S-1 ^1H NMR (300 MHz, CDCl_3) spectrum of compound **5**.

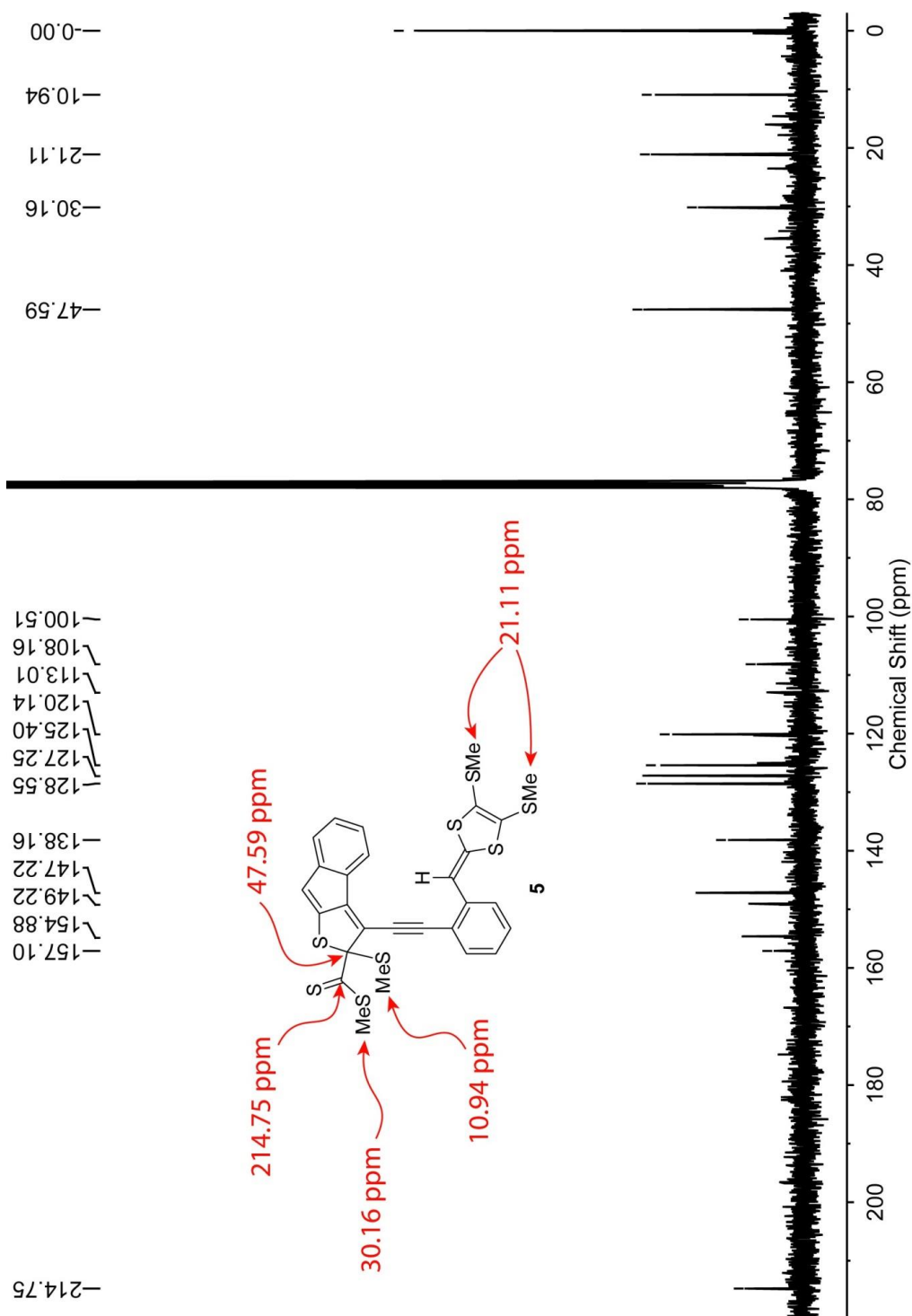


Fig. S-2 ^{13}C NMR (75 MHz, CDCl_3) spectrum of compound 5.

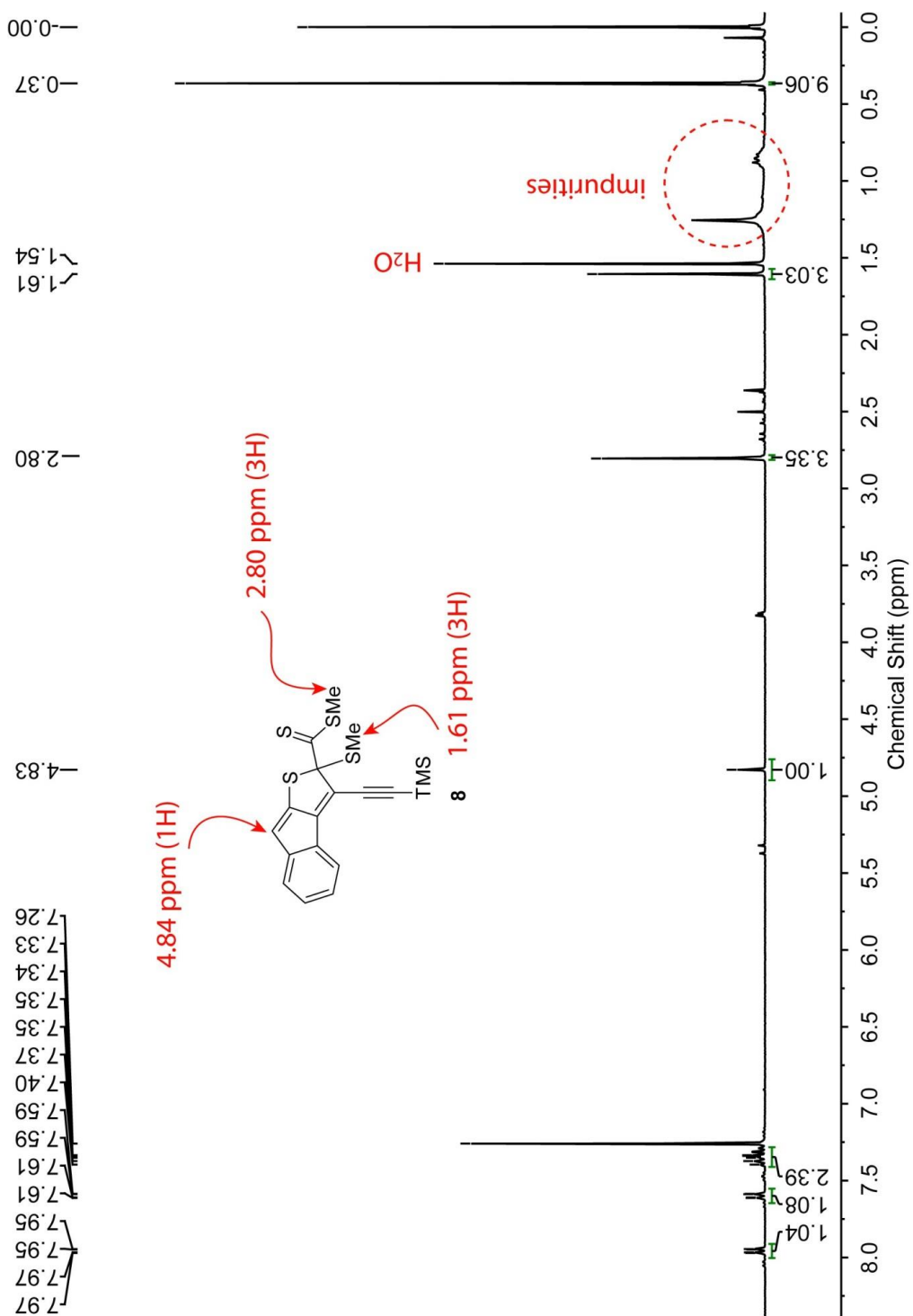


Fig. S-3 ^1H NMR (300 MHz, CDCl_3) spectrum of compound **8**.

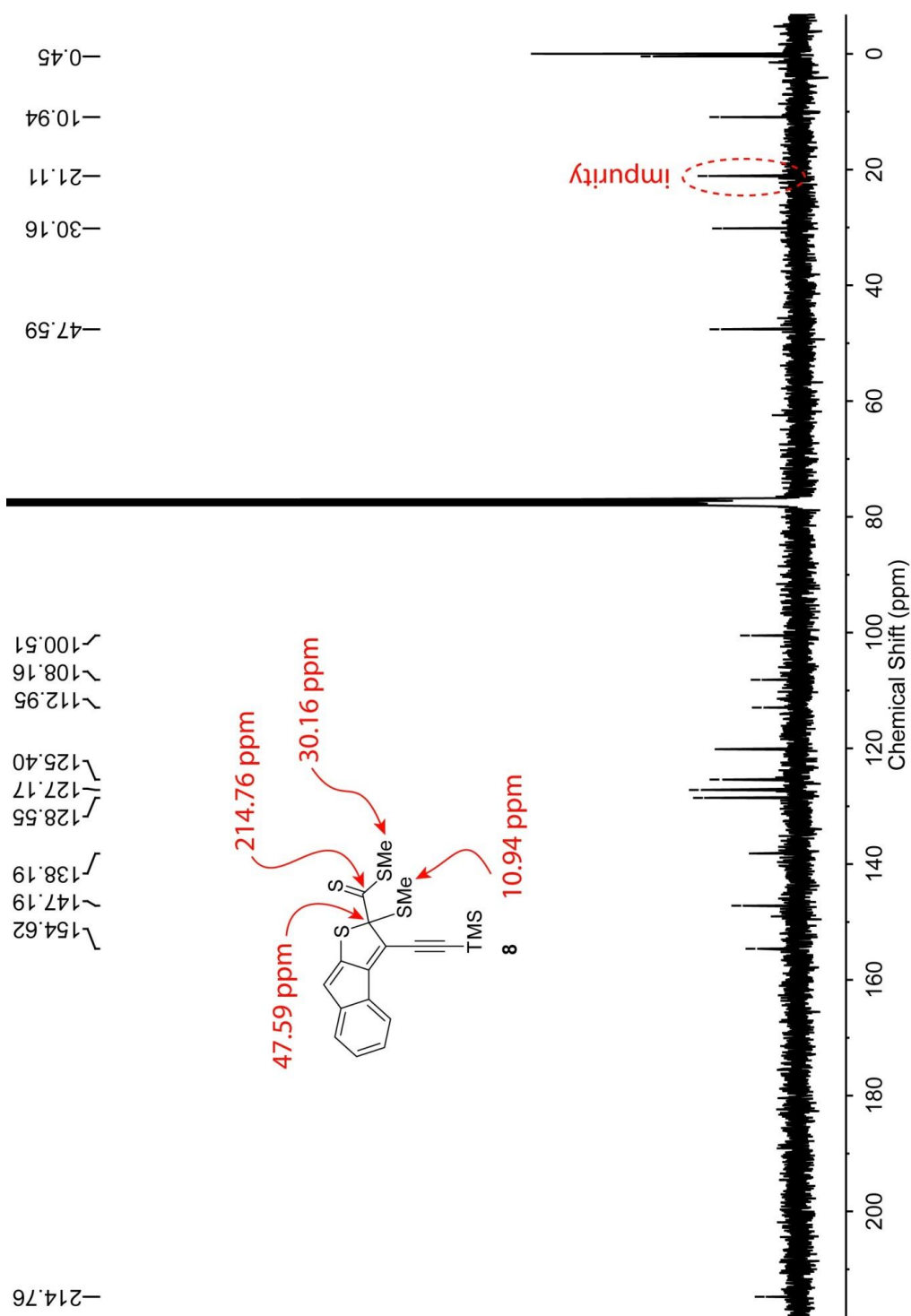


Fig. S-4 ^{13}C NMR (75 MHz, CDCl_3) spectrum of compound **8**.

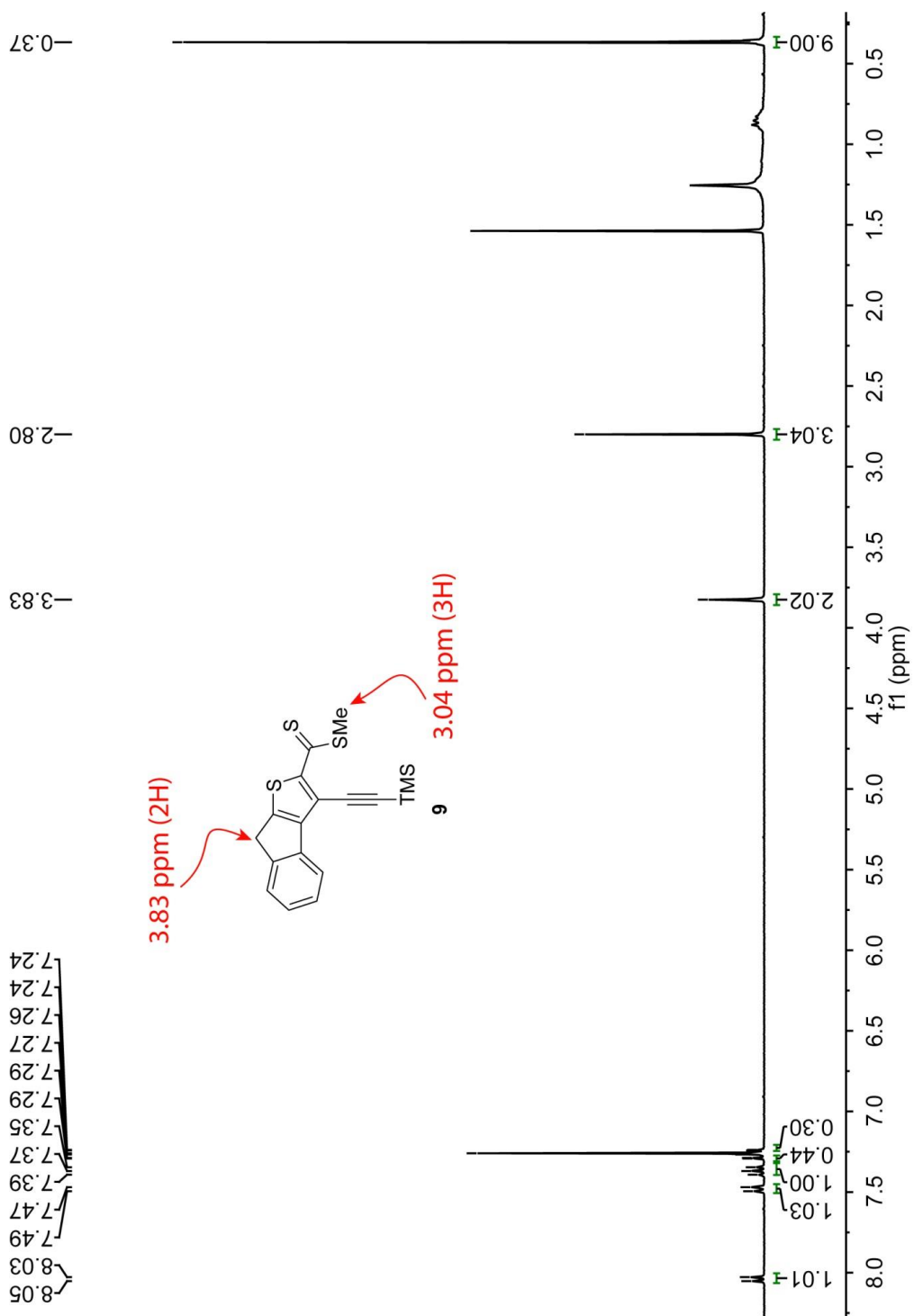


Fig. S-5 ^1H NMR (300 MHz, CDCl_3) spectrum of compound **9**.

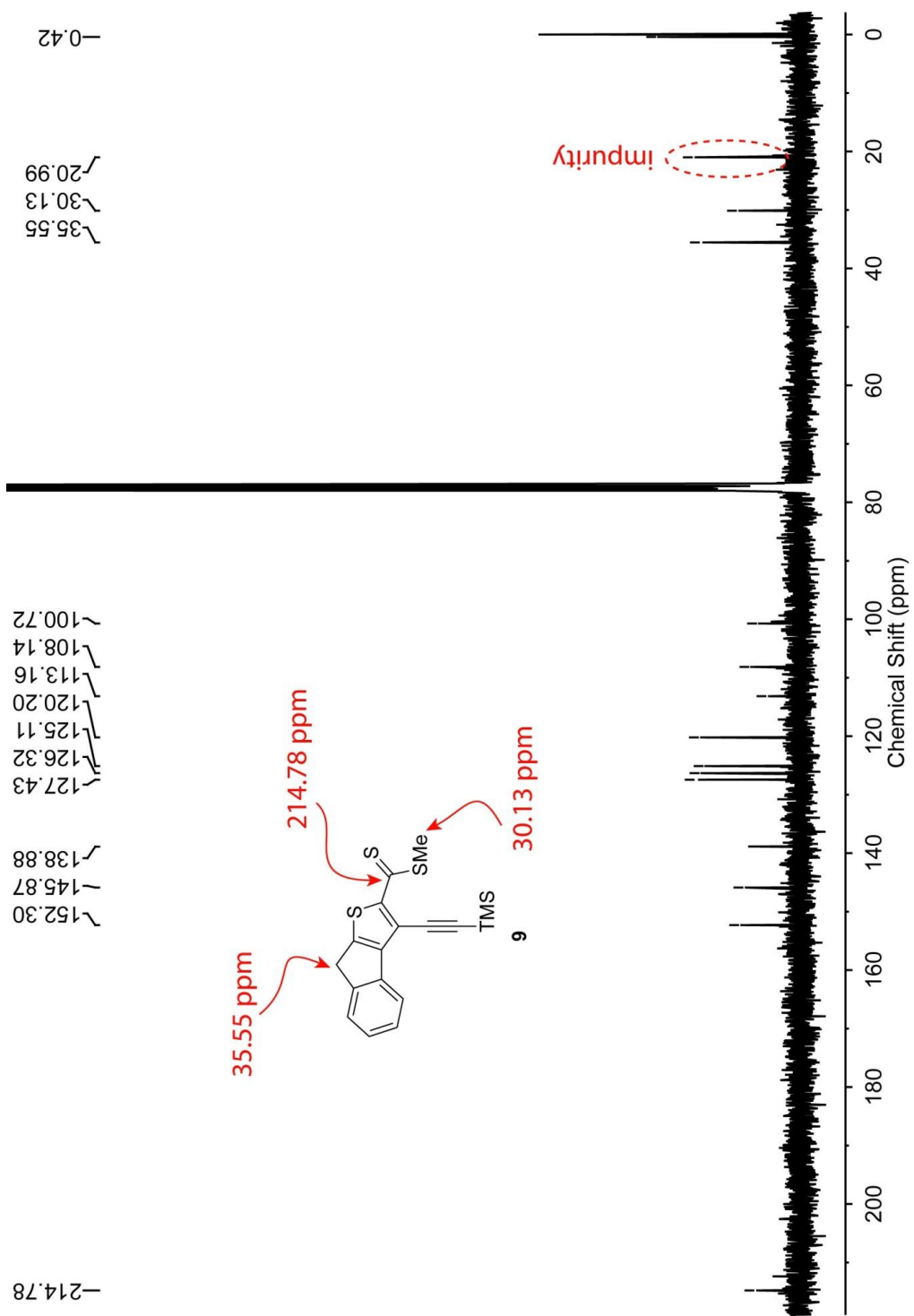


Fig. S-6 ^{13}C NMR (75 MHz, CDCl_3) spectrum of compound 9.

2. Results of DFT Calculations

Table S-1 Optimized geometries and energies for stationary points involved in the cycloaddition of compounds **10** and **11** (B3LYP/6-31+G(d), charge = +1, spin multiplicity = 1)

10			10-TS1				
H	-1.78405500	-2.17562000	1.49598200	H	-3.03811800	-2.38556300	0.00001000
C	-2.12668000	-1.35786000	0.86575500	C	-2.87935000	-1.31039700	0.00000300
C	-3.04046800	0.74844500	-0.72333200	C	-2.49433900	1.48611000	-0.00001000
C	-1.33268900	-0.21600300	0.72111700	C	-1.58852600	-0.78381000	-0.00001100
C	-3.36350400	-1.45499300	0.22239400	C	-3.97051600	-0.43811300	0.00000800
C	-3.81741000	-0.39972600	-0.57224300	C	-3.77914100	0.95215000	0.00000400
C	-1.79346400	0.85822400	-0.08104900	C	-1.39862800	0.60672000	-0.00002100
H	-3.96999400	-2.34667600	0.34963100	H	-4.97885100	-0.84150700	0.00001600
H	-4.78014600	-0.46623300	-1.07033300	H	-4.63791200	1.61651500	0.00001100
H	-3.39305500	1.57541100	-1.33161400	H	-2.33907000	2.56046200	-0.00000900
C	-0.00235400	-0.11374700	1.44171300	C	-0.31003800	-1.59157100	-0.00000900
H	0.07591200	-0.91367400	2.19192500	H	-0.24850400	-2.24422200	-0.87901200
H	0.07949500	0.83472200	1.98762900	H	-0.24849000	-2.24423300	0.87898300
C	1.19587700	-0.23564100	0.53160900	C	0.85083700	-0.58811900	-0.00000900
S	2.73319400	0.34641100	0.96886500	S	1.87553400	-0.52388800	1.46368200
S	1.11482400	-1.01358300	-0.97744800	S	1.87560000	-0.52393000	-1.46365100
C	3.55957400	-0.19373500	-0.45720300	C	2.98594700	0.55454800	0.68725100
H	4.62084400	0.01114500	-0.55024600	H	3.70693400	1.09958000	1.28862200
C	2.79507000	-0.83578600	-1.37149600	C	2.98597600	0.55453100	-0.68719900
C	-1.01204000	2.04661900	-0.23340400	C	-0.00229900	1.02568300	-0.00003800
H	3.14639100	-1.22887500	-2.31965200	H	3.70698900	1.09954800	-1.28855200
C	-0.35338200	3.05630500	-0.36554200	C	0.73365200	2.05200700	-0.00004800
H	0.18514800	3.97195300	-0.48590800	H	1.25741800	2.98607400	-0.00009000
E(RB3LYP) = -1258.76053293 a.u. Zero imaginary frequency			E(RB3LYP) = -1258.71570334 a.u. One imaginary frequency (-286.95 cm ⁻¹)				
10-IM1			10-TS2				
H	-3.22190000	-2.26413900	0.00024300	H	-3.16996900	-2.29439800	-0.02340100
C	-2.91807000	-1.22147300	0.00009400	C	-2.90189900	-1.24174900	-0.01703500
C	-2.21494100	1.55272600	-0.00031800	C	-2.27196900	1.53675700	-0.01987000
C	-1.57902300	-0.85870700	-0.00002000	C	-1.57414600	-0.83774900	-0.08576000
C	-3.88297200	-0.20515600	0.00005200	C	-3.89799900	-0.26116500	0.05834600
C	-3.54097500	1.16825900	-0.00011500	C	-3.58858200	1.11636400	0.05656000
C	-1.22431900	0.53305900	-0.00028700	C	-1.25482300	0.55427400	-0.08052000
H	-4.93460200	-0.47979500	0.00018000	H	-4.93897100	-0.56699400	0.11627600
H	-4.32947400	1.91392400	-0.00001700	H	-4.39142600	1.84462900	0.11377000
H	-1.93140300	2.60086100	-0.00036700	H	-2.02221100	2.59354900	-0.02482200
C	-0.35300800	-1.74631800	-0.00017300	C	-0.33791300	-1.70731900	-0.22619200
H	-0.32992700	-2.39985800	-0.88031400	H	-0.32041900	-2.20830600	-1.20281100
H	-0.32972500	-2.40005400	0.87980200	H	-0.28220900	-2.49303200	0.53441300
C	0.80200900	-0.73748000	-0.00024100	C	0.14900400	0.70889300	-0.16433700
S	1.88910700	-0.60187800	1.49484100	C	0.80081700	-0.68876600	-0.11632200
S	1.88993300	-0.60225100	-1.49436100	S	2.10724900	-0.55453500	-1.39655800
C	2.39418600	0.98528000	0.74544900	S	1.71183100	-0.63229400	1.54858300
H	3.07720900	1.61086700	1.31095200	C	2.45653400	0.80201200	0.93848300
C	2.39457200	0.98510700	-0.74512800	H	2.99551500	1.46288000	1.61301400
C	0.16626100	0.63043100	-0.00018900	C	2.44804500	1.02733400	-0.52423200
H	3.07802500	1.61045300	-1.31039300	H	3.24039200	1.64308500	-0.94400800
C	1.19646700	1.64162800	-0.00033200	C	1.10664300	1.69738000	-0.22822800
H	1.01603400	2.70964900	-0.00051600	H	0.98175600	2.77026100	-0.16018300

E(RB3LYP) = -1258.77575296 a.u. Zero imaginary frequency				E(RB3LYP) = -1258.76614232 a.u. One imaginary frequency (-300.68 cm ⁻¹)			
10-IM2				10-TS3			
H	-3.14932700	-2.31241100	-0.09272600	H	3.16651700	-2.31104100	0.03138200
C	-2.90652000	-1.25413400	-0.05143400	C	2.91940900	-1.25301900	0.01662300
C	-2.32109700	1.52417200	0.04434400	C	2.31924600	1.52251300	-0.02350800
C	-1.59179900	-0.81399700	-0.16889800	C	1.60832900	-0.82385100	-0.16257500
C	-3.91964400	-0.30390600	0.11456300	C	3.92418300	-0.29140300	0.17147600
C	-3.63034700	1.07305300	0.15986700	C	3.62779100	1.08310700	0.14965300
C	-1.29562600	0.57410400	-0.11230800	C	1.30560300	0.56240000	-0.17679500
H	-4.95022600	-0.63402400	0.20834500	H	4.95253800	-0.61219900	0.31062400
H	-4.43894700	1.78598500	0.28899600	H	4.42863300	1.80589800	0.27237400
H	-2.09468700	2.58574500	0.08158200	H	2.08872300	2.58387100	-0.03714000
C	-0.34553000	-1.65021600	-0.41472400	C	0.36737700	-1.67399500	-0.39510200
H	-0.32940200	-2.04318800	-1.44086400	H	0.24535900	-2.48995700	0.32416900
H	-0.25454600	-2.51279800	0.25329700	H	0.37819400	-2.13550100	-1.39333300
C	0.12718100	0.76046700	-0.24226000	C	-0.73881700	-0.63754200	-0.33697600
C	0.77235500	-0.62371500	-0.24607200	S	-2.22861900	-0.58398100	-1.30366900
S	2.20329400	-0.46883500	-1.35539000	S	-1.66238000	-0.53260200	1.68143500
S	1.64742400	-0.67955900	1.55585900	C	-0.12007900	0.72836300	-0.35552800
C	2.62401900	0.55513300	1.04836100	C	-2.43302100	1.04893300	-0.44105300
H	3.34903000	0.99340500	1.73319800	H	-3.26939700	1.63723500	-0.81699200
C	2.43740200	1.08786200	-0.36594500	C	-2.62167400	0.62154800	1.03221300
H	3.26581700	1.70776700	-0.70675300	H	-3.37147800	1.12562500	1.64158000
C	1.05984700	1.73678900	-0.31285600	C	-1.06328400	1.69479100	-0.46721600
H	0.92936100	2.81016500	-0.24840600	H	-0.93347900	2.77033600	-0.44419700
E(RB3LYP) = -1258.77021841 a.u. Zero imaginary frequency				E(RB3LYP) = -1258.76965218 a.u. One imaginary frequency (-167.83 cm ⁻¹)			
10-IM3				10-TS4			
H	3.59656400	-2.15339000	0.38991200	H	3.37420900	-2.26407500	0.26330200
C	3.22788900	-1.13959300	0.26067900	C	3.06920100	-1.22759100	0.14824800
C	2.31794300	1.54002600	-0.06456800	C	2.32527500	1.50774400	-0.13119400
C	1.88797800	-0.88748100	0.00209700	C	1.74471100	-0.88639600	-0.06266900
C	4.10513600	-0.05040400	0.36108400	C	4.02454100	-0.19798500	0.21239500
C	3.65680900	1.27337400	0.20253100	C	3.65536100	1.15156300	0.07484200
C	1.43378600	0.45266400	-0.16629200	C	1.36586900	0.48314300	-0.20236400
H	5.15571900	-0.23277900	0.56831600	H	5.06833400	-0.45068700	0.37410800
H	4.36488500	2.09175200	0.28891500	H	4.41779500	1.92245700	0.13117500
H	1.96995500	2.56141200	-0.18985300	H	2.04122500	2.55065500	-0.23793100
C	0.73453200	-1.86873400	-0.14139700	C	0.52085500	-1.79132700	-0.16779400
H	0.55549500	-2.42210400	0.79061900	H	0.38437100	-2.41310400	0.72561400
H	0.90933900	-2.61205500	-0.92996300	H	0.57438700	-2.46913300	-1.03085800
C	-0.38714000	-0.92176200	-0.47606300	C	-0.54914900	-0.75375000	-0.34293300
S	-2.09980900	-1.06812200	-0.53052800	S	-2.32936300	-0.89757000	-0.87068100
S	-2.74822600	0.04931400	1.39056700	S	-2.10177200	-0.26865100	1.49803800
C	0.02226300	0.39960000	-0.43691400	C	-0.06096000	0.52756300	-0.40659600
C	-2.31496100	0.70224500	-1.11334400	C	-2.46164300	0.94422300	-0.81984600
H	-2.84692200	0.88320400	-2.04422800	H	-3.18033300	1.40386600	-1.48978200
C	-2.38107200	1.36804200	0.21276400	C	-2.22286000	1.30486200	0.60777400
H	-2.84043100	2.33664000	0.38889300	H	-2.72032600	2.12235300	1.12035900
C	-1.04948300	1.38077900	-0.63502000	C	-1.10399300	1.55072600	-0.43900200
H	-0.81813500	2.35569500	-1.05657300	H	-0.90474400	2.58054500	-0.71885800
E(RB3LYP) = -1258.75032319 a.u. Zero imaginary frequency				E(RB3LYP) = -1258.69173135 a.u. One imaginary frequency (-575.23 cm ⁻¹)			

10-TS5				10-P			
H	-3.62074900	2.10639300	0.54535500	H	3.96432000	2.01405400	0.56773900
C	-3.24926700	1.10315600	0.35626300	C	3.57830800	1.01319700	0.39476600
C	-2.33231300	-1.54955700	-0.12438600	C	2.60650500	-1.61539900	-0.05270500
C	-1.91559000	0.87442200	0.04931800	C	2.23161100	0.79641400	0.12897300
C	-4.11688700	0.00382900	0.42541500	C	4.43749000	-0.09251400	0.43449900
C	-3.66470600	-1.30780800	0.18974800	C	3.95768900	-1.39183400	0.21355400
C	-1.45690000	-0.45125400	-0.19578800	C	1.74766600	-0.51229800	-0.09191900
H	-5.16285700	0.16802500	0.66821400	H	5.49298000	0.05984800	0.63982400
H	-4.36494500	-2.13481900	0.25434000	H	4.64477700	-2.23163500	0.25052300
H	-1.98015600	-2.56048100	-0.30828500	H	2.23794400	-2.62319600	-0.22223800
C	-0.77731600	1.87715600	-0.07429600	C	1.11032900	1.82555900	0.03059300
H	-0.58788100	2.40420700	0.87052400	H	1.25859800	2.55765600	-0.77693200
H	-0.97005000	2.64412700	-0.83605300	H	0.96516600	2.41011100	0.95049500
C	0.35579000	0.96603900	-0.46255800	C	-0.07545600	0.95753700	-0.25110200
S	2.03088100	1.15221500	-0.53637600	S	-4.26714700	-0.25629700	0.90466200
S	2.89187600	-0.20248800	1.43809600	S	-1.70265200	1.28684500	-0.46078000
C	-0.05207700	-0.38400600	-0.49698800	C	-2.05071700	-0.51087700	-0.80136600
C	2.28439400	-0.60520300	-1.13618500	C	0.30842800	-0.42958200	-0.33742100
H	2.79588400	-0.72404900	-2.09290700	C	-0.75126700	-1.23813900	-0.62451800
C	2.50840200	-1.29899800	0.14049500	H	-0.71370900	-2.31680300	-0.74503900
H	2.80602400	-2.34144900	0.22007900	C	-3.21528700	-1.07841700	-0.00409600
C	1.00000000	-1.30332400	-0.77121400	H	-2.33785800	-0.53848200	-1.87020200
H	0.81943000	-2.30431600	-1.14772700	H	-3.30721500	-2.16219400	-0.13183900
E(RB3LYP) = -1258.74672585 a.u. One imaginary frequency (-433.79 cm ⁻¹)				E(RB3LYP) = -1258.79366799 a.u. Zero imaginary frequency			
11				11-TS1			
H	2.66763100	-2.16480500	-1.26387900	H	-3.32073100	-2.28384100	-0.00049400
C	2.72383700	-1.22513400	-0.71899900	C	-3.17009900	-1.20633500	-0.00028000
C	2.90250100	1.20113600	0.65649300	C	-2.81453600	1.54696400	0.00030300
C	1.61696200	-0.37339000	-0.69209300	C	-1.86505800	-0.69658700	-0.00027700
C	3.90991000	-0.87683600	-0.06546800	C	-4.28033000	-0.36471000	-0.00002400
C	3.99582800	0.33690000	0.62084100	C	-4.09955700	1.02193900	0.00027400
C	1.70157500	0.86201000	0.00287300	C	-1.67532400	0.70405000	0.00001600
H	4.76227400	-1.54867000	-0.10031100	H	-5.27936800	-0.79031700	-0.00004600
H	4.91645400	0.61455700	1.12552600	H	-4.95612800	1.68922500	0.00048200
H	2.96591200	2.14878900	1.18196700	H	-2.65961900	2.62109700	0.00052300
C	0.34435800	-0.74231100	-1.43142200	C	-0.76201300	-1.76908400	-0.00070600
H	0.51582100	-1.64711800	-2.03193900	H	-0.91376400	-2.41324200	-0.87578200
H	0.05369300	0.04798700	-2.13507900	H	-0.91403500	-2.41419200	0.87362100
C	-0.83121600	-1.02141600	-0.52630600	C	0.68264800	-1.35030900	-0.00022400
C	0.58820900	1.74825500	0.03742600	C	-0.40427100	1.35208400	0.00000100
C	-0.36797100	2.50843100	0.06939700	C	0.58022900	2.07747400	-0.00004400
S	-2.43859700	-0.76986500	-1.01941100	S	1.57326300	-1.15746900	1.43478500
S	-0.64193200	-1.67633600	1.03200500	S	1.57410800	-1.15719300	-1.43466100
C	-3.18289400	-1.36616800	0.42895500	C	3.07846700	-0.76211100	0.67819000
H	-4.26554500	-1.35743300	0.49665500	H	3.93329800	-0.54091300	1.30808700
C	-2.33464100	-1.79432300	1.39321100	C	3.07886600	-0.76198300	-0.67711000
H	-2.62890300	-2.18504000	2.36150800	H	3.93406900	-0.54067100	-1.30646100
C	-1.43432700	3.35969000	0.10044000	C	1.69192000	2.86912500	-0.00014000
H	-3.19934700	4.80883100	0.15083900	H	3.52001300	4.23957300	-0.00034200
C	-2.38205000	4.12017600	0.12685300	C	2.67544500	3.58412800	-0.00023900
E(RB3LYP) = -1334.92095557 a.u. Zero imaginary frequency				E(RB3LYP) = -1334.89024157 a.u. One imaginary frequency (-243.00 cm ⁻¹)			

11-IM1				11-TS2			
H	-3.61345600	-2.20191300	-0.00001900	H	-3.65911700	-2.13208600	-0.00014100
C	-3.26611700	-1.17222000	-0.00001900	C	-3.26474300	-1.11950000	-0.00011500
C	-2.39215700	1.51995300	-0.00000800	C	-2.27307000	1.53544400	-0.00003300
C	-1.90386200	-0.88017800	-0.00002800	C	-1.89216000	-0.88784000	-0.00038800
C	-4.18360100	-0.11791500	-0.00000200	C	-4.13381500	-0.02384300	0.00017300
C	-3.74997400	1.21854400	0.00000500	C	-3.64230300	1.29306300	0.00020000
C	-1.47371400	0.45731900	-0.00002300	C	-1.40010800	0.43411600	-0.00032600
H	-5.24778900	-0.33489200	0.00000700	H	-5.20669300	-0.19301900	0.00038300
H	-4.47993700	2.02228300	0.00002000	H	-4.33787300	2.12671500	0.00043200
H	-2.05354600	2.55170900	-0.00000300	H	-1.88869100	2.55099800	0.00003700
C	-0.75766700	-1.85917000	0.00000100	C	-0.78399300	-1.91989700	-0.00092000
H	-0.77981800	-2.51502900	-0.87770200	H	-0.83178600	-2.57281700	-0.88014900
H	-0.77981900	-2.51497600	0.87774200	H	-0.83193200	-2.57424600	0.87722300
C	0.52577100	-0.98946900	-0.00000400	C	0.50754900	-1.07917500	-0.00026900
S	1.57712400	-1.19301400	1.47452100	S	1.59261400	-1.24578000	-1.47504300
S	1.57722600	-1.19321200	-1.47442800	S	1.59110900	-1.24544600	1.47566200
C	2.91639900	-0.41178100	0.68330200	C	2.72558400	-0.18381700	-0.69205600
H	3.73958100	-0.04028100	1.28528500	H	3.47522500	0.33639400	-1.28070400
C	2.91645600	-0.41189800	-0.68323700	C	0.05216700	0.43838300	-0.00039200
C	-0.01404400	0.54829300	-0.00004400	C	2.72479800	-0.18351300	0.69349300
H	3.73968200	-0.04049600	-1.28521900	H	3.47385100	0.33685000	1.28275100
C	0.76614100	1.58422400	-0.00006300	C	0.94911300	1.40035800	-0.00018100
C	1.40924500	2.74765100	-0.00006900	C	1.39949000	2.66821700	-0.00030400
H	2.44406300	4.80136900	-0.00005600	C	1.81572600	3.81938100	-0.00041700
C	1.96736100	3.84195300	-0.00006800	H	2.16204500	4.83257900	-0.00053100
E(RB3LYP) = -1334.89083741 a.u. Zero imaginary frequency				E(RB3LYP) = -1334.89105285 a.u. One imaginary frequency (-104.18 cm ⁻¹)			
11-IM2				11-TS3			
H	-3.64090400	-2.14759900	0.00011600	H	-3.61413100	-2.16959300	-0.05852500
C	-3.19422000	-1.15770200	0.00002000	C	-3.18946300	-1.17014300	-0.03534400
C	-2.11161300	1.49448800	-0.00017600	C	-2.15187000	1.48957600	0.01081600
C	-1.81865000	-0.98517600	-0.00019100	C	-1.81690400	-0.97013900	-0.07974100
C	-4.00796200	-0.01567500	0.00007400	C	-4.02680000	-0.04917400	0.03941500
C	-3.47820000	1.29631600	-0.00003000	C	-3.51636100	1.26765300	0.06173100
C	-1.27363900	0.34497200	-0.00025700	C	-1.29321200	0.36225700	-0.05220200
H	-5.08760100	-0.14137300	0.00020300	H	-5.10275200	-0.19598800	0.07892900
H	-4.15573000	2.14412700	0.00002400	H	-4.20408100	2.10547000	0.11860500
H	-1.67821900	2.48918800	-0.00022400	H	-1.74039500	2.49355000	0.02704000
C	-0.72796600	-2.03519500	-0.00045900	C	-0.71878700	-2.00944500	-0.20344700
H	-0.79492200	-2.68560400	-0.88065800	H	-0.77139800	-2.52244300	-1.17227000
H	-0.79480700	-2.68608700	0.87937400	H	-0.78217000	-2.78281200	0.56936700
C	0.11504200	0.24738800	-0.00027200	C	0.10920800	0.30101500	-0.11236900
C	0.55689500	-1.19656500	-0.00023800	C	0.55726800	-1.16656500	-0.09396400
S	1.65398800	-1.22031600	-1.49474500	S	1.82687600	-1.18849200	-1.42556800
S	1.65292500	-1.22033100	1.49507500	S	1.50187500	-1.26299200	1.53108100
C	2.38175600	0.26650400	0.74130100	C	2.39107000	0.11138500	0.91209400
H	3.13368100	0.80852500	1.30590200	H	3.01165400	0.70408600	1.57859500
C	2.38226800	0.26649700	-0.74047600	C	2.43221700	0.29739900	-0.54657800
H	3.13460900	0.80850600	-1.30453200	H	3.27622200	0.82201000	-0.98706100
C	1.26922100	1.11715400	-0.00005600	C	1.20927600	1.16487700	-0.14214100
C	1.25231000	2.54366200	-0.00007200	C	1.24961600	2.57467900	-0.06509800
H	1.29052100	4.82249600	-0.00007700	H	1.37086600	4.85044400	0.03865000
C	1.26855200	3.75302700	-0.00007200	C	1.31410600	3.78312700	-0.00676100
E(RB3LYP) = -1334.91909149 a.u. Zero imaginary frequency				E(RB3LYP) = -1334.91528419 a.u. One imaginary frequency (-305.91 cm ⁻¹)			

11-IM3				11-TS4			
H	3.80330000	-2.29716600	-0.16005400	H	3.67171700	-2.31051600	-0.13266800
C	3.37480500	-1.30964500	-0.01338000	C	3.27301400	-1.30258600	-0.05760400
C	2.30533700	1.30178900	0.38755900	C	2.28089000	1.36002000	0.16360300
C	2.01953600	-1.07791900	-0.19779900	C	1.92029200	-1.05110600	-0.20317800
C	4.18782800	-0.23650300	0.37816600	C	4.13249500	-0.21828100	0.19375100
C	3.66001400	1.05194300	0.57853000	C	3.64052000	1.09396900	0.30324100
C	1.48378100	0.22901600	-0.00243300	C	1.41718600	0.28062800	-0.09132800
H	5.25020200	-0.40398000	0.53091800	H	5.19732200	-0.39954700	0.30719600
H	4.32052000	1.85845900	0.88167200	H	4.33135400	1.90847700	0.49855800
H	1.89444200	2.29562800	0.53072200	H	1.89828700	2.37217200	0.24354200
C	0.92645000	-2.05448400	-0.60065700	C	0.78210400	-2.03107400	-0.46998000
H	0.79677800	-2.84993900	0.14580700	H	0.71721700	-2.81332800	0.29643800
H	1.13133100	-2.54339800	-1.56192600	H	0.88163100	-2.53436200	-1.44163500
C	-0.25707000	-1.12655800	-0.66693700	C	-0.37916800	-1.08176400	-0.45365500
S	-1.94976900	-1.38162000	-0.73532300	S	-2.15504700	-1.30490600	-0.96838000
S	-2.62383700	-0.85846700	1.44378200	S	-1.92279000	-1.09154300	1.47279700
C	0.07381500	0.16134700	-0.27624500	C	-0.01255800	0.22687200	-0.28345000
C	-2.30754700	0.45608400	-0.80667400	C	-2.46294500	0.46816700	-0.58168400
H	-2.86671400	0.85205900	-1.65164000	H	-3.22973800	0.98013400	-1.15318200
C	-2.39621600	0.72851700	0.64294200	C	-2.22250200	0.58792900	0.87976000
H	-2.88028200	1.59890900	1.07659400	H	-2.76622500	1.26298400	1.53338600
C	-1.05737400	1.09799500	-0.20401700	C	-1.14319200	1.15106100	-0.12230200
C	-0.87311900	2.50810500	-0.39800900	C	-1.03133200	2.57632500	-0.24104700
H	-0.63128300	4.75305900	-0.70644600	H	-0.88880700	4.84272900	-0.42543800
C	-0.74700500	3.69994000	-0.55787800	C	-0.95603200	3.77891400	-0.33560500
E(RB3LYP) = -1334.88247660 a.u. Zero imaginary frequency				E(RB3LYP) = -1334.83310375 a.u. One imaginary frequency (-575.17 cm ⁻¹)			
11-TS5				11-P			
H	3.81390900	-2.29977000	-0.09632700	H	-4.12807600	-2.26816900	0.29921800
C	3.38551600	-1.30913000	0.02762300	C	-3.70778600	-1.26667000	0.26694900
C	2.31740800	1.31100700	0.36957500	C	-2.64655400	1.36618900	0.18876000
C	2.03354300	-1.07800000	-0.17881200	C	-2.35173800	-1.06210000	0.04961200
C	4.19594400	-0.23069400	0.41063200	C	-4.53261200	-0.14723800	0.44419300
C	3.66878700	1.06259200	0.58149600	C	-4.00832400	1.15276500	0.40514600
C	1.49801100	0.23263800	-0.01184000	C	-1.82155800	0.24911900	0.01250800
H	5.25598300	-0.39764700	0.57949900	H	-5.59569400	-0.29028100	0.61425100
H	4.32730500	1.87292000	0.87866000	H	-4.66962700	2.00234700	0.54564000
H	1.90593400	2.30748600	0.49101500	H	-2.24156900	2.37262700	0.16058300
C	0.94548700	-2.06154900	-0.57981800	C	-1.25914500	-2.10132600	-0.17089400
H	0.80986300	-2.85111100	0.17158700	H	-1.41784800	-2.71681400	-1.06814300
H	1.15768300	-2.55888000	-1.53531500	H	-1.14473600	-2.80259900	0.66793100
C	-0.24109600	-1.13928800	-0.66828400	C	-0.04547900	-1.23683200	-0.32287900
S	-1.91482900	-1.40218500	-0.75949100	S	4.26427700	-0.40547600	0.89682800
S	-2.70337500	-0.82023700	1.47376400	S	1.57811800	-1.59928600	-0.56445100
C	0.09090400	0.16728500	-0.29778000	C	1.99965300	0.20890500	-0.63648200
C	-2.28457800	0.43547500	-0.81935600	C	-0.38550100	0.14481500	-0.22171600
H	-2.82978800	0.81804300	-1.68208800	C	0.71046700	0.97433000	-0.37916200
C	-2.46077100	0.69659700	0.61542800	C	3.17359400	0.59542100	0.25103000
H	-2.86355000	1.61690300	1.02863000	H	2.30737300	0.38808600	-1.68204900
C	-1.02410100	1.09086000	-0.26381000	H	3.24698400	1.67851500	0.38713000
C	-0.86581300	2.50228600	-0.41450500	C	0.71077200	2.37472300	-0.35782200
H	-0.66642300	4.76043200	-0.65788400	H	0.74872700	4.66078500	-0.33740700
C	-0.76251600	3.70164900	-0.53823800	C	0.73356900	3.58985000	-0.34677400
E(RB3LYP) = -1334.89108447 a.u. One imaginary frequency (-304.10 cm ⁻¹)				E(RB3LYP) = -1334.94945032 a.u. Zero imaginary frequency			