Synthesis

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Supporting Information

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Supporting Information

Dienylation of Unfunctionalized Arenes with 1,6-Diynes via Rhodium-Catalyzed Directing Group-Free C-H Bond Activation

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I. Computational Studies

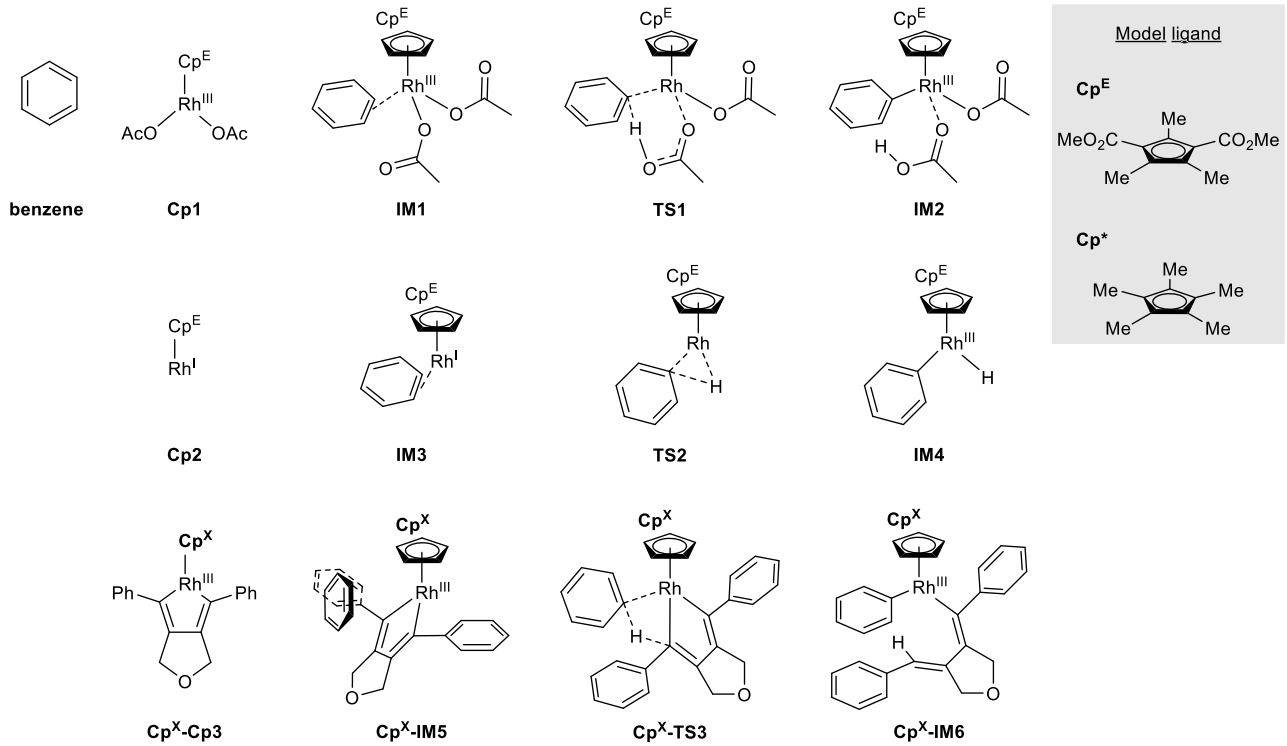


Table S1. The Gibbs-free energies.

	G (hartree) (M06/6-31g* & LANL2DZ)	imaginary frequency
benzene	-231.982758	
Cp1	-1332.698089	
Cp2	-875.990270	
Cp^{E}-Cp3	-1644.708940	
Cp*-Cp3	-1267.782603	
IM1	-1564.649855	
TS1	-1564.634724	-1621.53
IM2	-1564.666181	
IM3	-1107.995672	
TS2	-1107.962681	-589.68
IM4	-1107.965514	
Cp^{E}-IM5	-1876.678678	

Cp^E-TS3	-1876.666788	-784.60
Cp^E-IM6	-1876.685236	
Cp*-IM5	-1499.759345	
Cp*-TS3	-1499.733636	-777.86
Cp*-IM6	-1499.754397	

benzene

Sum of electronic and zero-point Energies= -231.955287

Sum of electronic and thermal Free Energies= -231.982758

C	-0.78644300	1.14787300	-0.00016600
C	-1.38750100	-0.10699400	0.00013400
C	1.38747000	0.10709900	0.00001000
C	0.78637800	-1.14795200	-0.00004100
C	-0.60100200	-1.25504700	0.00001200
H	-2.47319800	-0.19096000	0.00030400
H	2.47320700	0.19072900	-0.00016800
H	-1.07096700	-2.23737400	-0.00022400
H	1.40213500	-2.04609100	-0.00010400
H	-1.40192700	2.04622500	-0.00057200
C	0.60109500	1.25502100	0.00013900
H	1.07077000	2.23747400	0.00023800

Cp1

Sum of electronic and zero-point Energies= -1332.638997

Sum of electronic and thermal Free Energies= -1332.698089

Rh	-0.10473900	0.46306700	0.28406400
O	-0.79285800	1.93498500	-1.18215200
C	-1.21206400	2.66486900	-0.23728500
C	-1.73507500	4.03904600	-0.50057800
O	-1.15305500	2.21993700	0.95189800
C	0.79835700	-1.49996300	0.08146900
C	0.48927000	-1.24585000	1.47145200
C	-0.93813200	-1.08045600	1.56537300
C	-1.49323600	-1.20857200	0.24032700
C	-0.41161200	-1.46039000	-0.68742600
C	2.41231000	1.52306900	-0.53157500
O	1.55688000	1.66207100	0.43881200
H	-0.91471300	4.75754200	-0.38214600
H	-2.11522400	4.11552500	-1.52335100
H	-2.51584900	4.29508800	0.22211400
C	2.12832700	-1.78822400	-0.51720100
C	-2.93584700	-1.04053300	-0.03951400
O	-3.73253900	-0.60159200	0.75832900
O	2.26906700	-2.37737300	-1.56087300
O	3.13167900	-1.38094600	0.26669500
O	-3.26627400	-1.45551300	-1.26863700
C	4.41985500	-1.46018900	-0.34203100
H	4.44169000	-0.79483000	-1.21293500
H	5.12994100	-1.12895800	0.41857500
H	4.63988400	-2.48559300	-0.65606800
C	-4.64358900	-1.29872500	-1.60419300
H	-4.93202200	-0.24349800	-1.55541500
H	-4.74610000	-1.67793300	-2.62230800
H	-5.27344800	-1.86985800	-0.91416400
C	3.62893600	2.40764600	-0.35970800
H	4.25281100	2.00290400	0.44834400
H	4.21103600	2.42879800	-1.28563000
H	3.34005000	3.42263400	-0.06767400
O	2.31256500	0.74687300	-1.47696500
C	-0.48350600	-1.52611200	-2.16925100
H	-0.61209000	-2.56770100	-2.49392400
H	-1.32920900	-0.94149200	-2.53903000
H	0.44761500	-1.15123900	-2.60327700
C	1.46065600	-1.18351100	2.59788000
H	1.98017800	-2.14337000	2.71370600
H	2.22152600	-0.42013800	2.40528300
H	0.96139200	-0.94543600	3.54213500
C	-1.70479900	-0.75342400	2.79567400
H	-2.24968800	0.18855800	2.66867100
H	-2.45831400	-1.52704600	2.98928800
H	-1.04903200	-0.67160600	3.66761700

Cp2

Sum of electronic and zero-point Energies= -875.940414

Sum of electronic and thermal Free Energies= -875.990270

Rh	-0.00065000	0.63919900	1.35949700
C	-1.12731300	-0.33372600	-0.40584400
C	-0.88635700	1.05208700	-0.59257200
C	0.56835800	1.26341900	-0.66267600
C	1.21723200	0.01104900	-0.52302000
C	0.17531100	-0.92078300	-0.10166300
C	-2.40207700	-1.04031100	-0.35397600
C	2.65674600	-0.18819900	-0.64256800
O	3.45407500	0.65197300	-1.01512800
O	-2.56854400	-2.19453400	-0.01029200
O	-3.42734500	-0.26420000	-0.78221000
O	3.03620200	-1.44733300	-0.32533100
C	-4.69682100	-0.90041600	-0.76364100
H	-4.96821500	-1.20271100	0.25435700
H	-5.40784400	-0.16295100	-1.14318600
H	-4.69574700	-1.79225100	-1.40021200
C	4.42986200	-1.69298100	-0.44192900
H	4.99935500	-1.03830000	0.22760900
H	4.57428200	-2.73937300	-0.16352600
H	4.77247400	-1.52032400	-1.46834600
C	0.38639500	-2.33293400	0.32238800
H	0.60425200	-2.95895000	-0.55565000
H	1.25180900	-2.41291700	0.98751000
H	-0.51283900	-2.73029300	0.79844300
C	-1.87899900	2.13720400	-0.82832200
H	-1.44644500	3.12200500	-0.61784900
H	-2.20621000	2.13368900	-1.87851500
H	-2.77453300	2.00202000	-0.21547200
C	1.19495600	2.57908600	-0.96583900
H	1.11652200	2.79925600	-2.04166600
H	0.68730300	3.39240900	-0.43165000
H	2.25620900	2.57650800	-0.70753000

Cp^E-Cp3

Sum of electronic and zero-point Energies= -1644.642623

Sum of electronic and thermal Free Energies= -1644.708940

Rh	0.02934800	-0.05404700	-0.27661800
C	-0.75689600	-1.02442100	1.49136400
C	-1.08967000	-1.97131300	0.46220500
C	0.69942200	-0.96331200	1.57643300
C	0.13503800	-2.41703400	-0.13916000
C	1.23144500	-1.86728700	0.60104600
C	-1.35652400	1.48013200	-0.27437000
C	1.29992900	1.56270900	-0.19743700
C	-0.79583000	2.69489000	-0.12921300
C	0.65763200	2.73950300	-0.09400800
C	-1.27285400	4.11986100	-0.16854500
C	1.05068500	4.18893400	-0.12131900
O	-0.13995000	4.89604300	0.19369200
C	-2.77554600	1.19703900	-0.47329600
C	-3.20102900	0.32966500	-1.49236600
C	-3.75525000	1.77983100	0.34687900
C	-4.55131600	0.09231600	-1.71254000
C	-5.10659000	1.52978900	0.13544400
C	-5.51236100	0.69421300	-0.90148300
C	2.74025800	1.35053800	-0.31404200
C	3.26861100	0.58396900	-1.36550800
C	3.63478900	1.89995200	0.61771300
C	4.63862000	0.39901800	-1.49539100
C	5.00492900	1.69928000	0.49576300
C	5.51375100	0.95179000	-0.56205200
C	2.66904700	-2.13690700	0.46282600
C	-2.43525600	-2.39735100	0.04346600
O	3.49754600	-1.87032800	1.30619900
O	-2.70653000	-2.99134500	-0.97963400
O	-3.36061500	-2.08334500	0.96660900
O	2.97683000	-2.75031700	-0.69640700
C	4.35044600	-3.09882400	-0.83097600
C	-4.68636200	-2.50377600	0.66477800
C	0.25094900	-3.31469200	-1.32143900
C	1.45462100	-0.21752300	2.61662900
C	-1.66087600	-0.34450800	2.45720200
H	-1.63210700	4.39361300	-1.17930100
H	-2.07830800	4.35500100	0.53948000
H	1.81469500	4.47056300	0.61512700
H	1.42990600	4.48134700	-1.11930500
H	-2.45401700	-0.15499700	-2.12380200
H	-3.43758200	2.42663200	1.16588800
H	-4.85390800	-0.57482700	-2.51920100
H	-5.84838600	1.99358100	0.78460300
H	-6.57115400	0.50427800	-1.07131800
H	2.58498800	0.14176900	-2.09372100

H	3.23466900	2.47761500	1.45219700
H	5.02775500	-0.17841800	-2.33410700
H	5.68049700	2.12817500	1.23452400
H	6.58741200	0.79972700	-0.65916900
H	4.45752500	-3.51145400	-1.83660300
H	4.98538900	-2.21581200	-0.70169100
H	4.63265600	-3.84612000	-0.08029200
H	-4.73441900	-3.59612700	0.59113400
H	-5.30529400	-2.14688100	1.49099700
H	-5.02460600	-2.06342700	-0.27873400
H	0.83949400	-2.82889800	-2.11022000
H	0.80243500	-4.22463400	-1.05174000
H	-0.73464900	-3.57930900	-1.70733400
H	1.56889100	-0.84596900	3.51228000
H	2.46131900	0.03445700	2.27220900
H	0.92832800	0.70050700	2.90351700
H	-2.62628700	-0.09766700	2.00862300
H	-1.85599600	-1.01013900	3.31111200
H	-1.20099600	0.57497100	2.83734300

Cp*-Cp3

Sum of electronic and zero-point Energies= -1267.721895

Sum of electronic and thermal Free Energies= -1267.782603

Rh	-0.00431900	-0.51455600	-0.28088400
C	1.21913200	-2.06323200	0.91514300
C	0.13557900	-1.38262300	1.61784100
C	0.62791900	-2.78422500	-0.12680900
C	-1.13497000	-1.90372300	1.10574300
C	-0.82993400	-2.69643200	-0.00517200
C	1.33434100	1.07226100	-0.22456600
C	-1.33757900	1.07316100	-0.20015700
C	0.72769000	2.25878300	-0.01667400
C	-0.72635100	2.26012500	-0.00891000
C	1.15823700	3.69511900	0.05309400
C	-1.15402700	3.69760800	0.05624900
O	0.00211300	4.43947800	-0.30703500
C	2.77401500	0.87825600	-0.35805000
C	3.68249600	1.52855900	0.49361200
C	3.29745400	0.00219100	-1.32395500
C	5.05198500	1.30981500	0.38484600
C	4.66402100	-0.20823900	-1.44015900
C	5.55019700	0.43961600	-0.58022000
C	-2.77668900	0.87696000	-0.34076800
C	-3.69606900	1.56153500	0.47110000
C	-3.29007900	-0.03408400	-1.27934900
C	-5.06366300	1.33939400	0.35359300
C	-4.65555500	-0.25158100	-1.40284500
C	-5.55174300	0.42997100	-0.58042800
C	-2.46937000	-1.63363600	1.70574900
C	1.31547400	-3.55521600	-1.19883900
C	2.65685500	-1.99259300	1.29362100
C	0.29852200	-0.56079600	2.84767500
C	-1.78532700	-3.39868400	-0.90662700
H	1.48450800	3.97423900	1.07574100
H	1.97168200	3.95760000	-0.63693400
H	-1.96843400	3.95864200	-0.63345100
H	-1.47920000	3.97969300	1.07847000
H	3.29505800	2.19297800	1.26745000
H	2.60149900	-0.51564300	-1.98762500
H	5.73496000	1.81873200	1.06428700
H	5.04447300	-0.88504900	-2.20485800
H	6.62183400	0.26573300	-0.66249700
H	-3.31964600	2.25474300	1.22462700
H	-2.58795100	-0.57358200	-1.91869700
H	-5.75427700	1.87602800	1.00331100
H	-5.02579300	-0.95818300	-2.14542900
H	-6.62242300	0.25299000	-0.66808600
H	-3.27986400	-1.71303900	0.97073300
H	-2.67475100	-2.34682500	2.51807200

H	-2.52213000	-0.62392100	2.13091100
H	1.15547600	-4.63723700	-1.07832700
H	0.92921000	-3.28483600	-2.19202800
H	2.39603700	-3.37216900	-1.20311700
H	2.97775900	-0.96623800	1.51452300
H	2.84393500	-2.60006000	2.19199500
H	3.31144300	-2.36321700	0.49667300
H	-0.51842100	0.16395100	2.94873700
H	0.30592200	-1.19507400	3.74797200
H	1.23975300	0.00205200	2.82101300
H	-1.50037800	-3.28366700	-1.96193800
H	-1.81342000	-4.47916800	-0.69853200
H	-2.80478800	-3.01001100	-0.79536500

IM1

Sum of electronic and zero-point Energies= -1564.583363

Sum of electronic and thermal Free Energies= -1564.649855

Rh	-0.03209000	-0.21409200	0.03854400
O	-0.17905500	0.74503900	1.89541600
C	0.39148200	0.37312300	3.00504300
C	-1.23266700	-2.01578000	1.20353300
C	0.72100500	1.55503600	3.89268700
O	0.66935200	-0.77414100	3.33573300
C	-2.49336900	-1.40589200	1.33118800
C	1.07385900	0.81065700	-1.49661700
C	0.32763000	-0.24853900	-2.13551600
C	-1.06006500	0.05097200	-1.95265900
C	-1.16838100	1.24434800	-1.14434300
C	0.16047300	1.74733800	-0.88768000
C	2.56609900	-0.86133000	1.10425800
O	1.50871000	-1.45793800	0.64114000
C	-2.12534500	-3.46297100	-0.52517000
C	-3.38050600	-2.87824700	-0.35227200
C	-3.56366500	-1.83721400	0.55829100
H	-2.61502800	-0.60334300	2.05773200
H	-1.99222200	-4.26078400	-1.25483400
H	-4.53761100	-1.36126100	0.65494800
H	-4.22366700	-3.22536900	-0.94920800
H	1.59058500	2.06449500	3.45533200
H	-0.10502200	2.27472100	3.91900000
H	0.96910700	1.22026200	4.90400700
H	-0.45466500	-1.81817200	1.95086400
C	-1.05273600	-3.02986800	0.24358800
H	-0.06511800	-3.47633000	0.13894300
C	2.55084400	1.01864400	-1.54585000
C	-2.45966200	1.78355600	-0.67039500
O	-3.53331900	1.25418000	-0.86264400
O	3.06410700	2.10981800	-1.49904300
O	3.21406400	-0.12126100	-1.75002700
O	-2.31118400	2.93085100	0.00003600
C	4.63135800	-0.00370600	-1.63214800
H	4.87702400	0.35702600	-0.62685400
H	5.02693600	-1.00895700	-1.79103200
H	5.02769400	0.69141000	-2.37959700
C	-3.51344500	3.47341200	0.53836100
H	-3.96260300	2.77306900	1.25073900
H	-3.22316400	4.39660800	1.04270200
H	-4.23491200	3.67934900	-0.25945100
C	3.52606900	-1.82090500	1.76740000
H	3.58827500	-2.76815400	1.22111200
H	4.51625100	-1.36414100	1.86081100
H	3.13414500	-2.03574400	2.76948200
O	2.79283900	0.34498400	1.04675100

C	0.88930800	-1.41665600	-2.87032100
H	1.42031100	-1.09950100	-3.77760400
H	1.60659700	-1.95093600	-2.23851300
H	0.09821900	-2.11556200	-3.16235300
C	-2.19349300	-0.68839200	-2.55400700
H	-2.99571300	-0.85809200	-1.83072500
H	-2.62694800	-0.06997900	-3.35333000
H	-1.88012900	-1.64357100	-2.98560800
C	0.54203200	2.92925600	-0.07657900
H	0.20468200	3.84802700	-0.57323500
H	0.05150100	2.86852200	0.90198800
H	1.62448000	2.96722200	0.05654600

TS1

Sum of electronic and zero-point Energies= -1564.571208

Sum of electronic and thermal Free Energies= -1564.634724

Rh	0.06339900	-0.11124500	0.01080600
O	0.14172300	-0.30114800	2.12475900
C	0.11600800	-1.45593500	2.64319000
C	-1.52313100	-1.64322700	-0.10465100
C	0.61739100	-1.56979500	4.05419500
O	-0.26915400	-2.49708800	2.04743000
C	-2.78281600	-1.20431100	0.34301100
C	1.29669000	1.54401800	-0.71749900
C	0.63564400	0.90423300	-1.84433600
C	-0.77004500	1.09068800	-1.67790800
C	-0.98300600	1.76562600	-0.41565000
C	0.30222900	2.07977500	0.16288200
C	2.51955400	-1.66279200	0.24213300
O	1.35280600	-1.71388400	-0.33082900
C	-2.61593500	-2.76570500	-1.96044200
C	-3.85207900	-2.30354800	-1.50875800
C	-3.94026200	-1.52271200	-0.35492000
H	-2.83569500	-0.61683500	1.26316300
H	-2.56197800	-3.38212000	-2.85701600
H	-4.91079800	-1.17169100	-0.00599300
H	-4.75777900	-2.55786200	-2.05811900
H	1.71400900	-1.54992800	4.01367900
H	0.29354600	-0.70892000	4.64707300
H	0.28968600	-2.50576700	4.51383900
H	-0.77855800	-2.04895900	0.87427000
C	-1.45838800	-2.42729200	-1.26975900
H	-0.47989600	-2.76723800	-1.61195200
C	2.74934700	1.63715300	-0.43858000
C	-2.33525100	2.10699700	0.07401600
O	-3.29084600	2.26493400	-0.65213100
O	3.22449500	2.34729200	0.41524500
O	3.46866100	0.87253500	-1.27029900
O	-2.40196400	2.19654700	1.41089400
C	4.84941000	0.76468900	-0.92603300
H	4.93309400	0.25563000	0.04119400
H	5.30809200	0.17043600	-1.71955600
H	5.31425300	1.75413100	-0.86771600
C	-3.69894500	2.48852400	1.92394900
H	-4.40638900	1.69961500	1.64235200
H	-3.58696600	2.53283100	3.00854000
H	-4.06556700	3.44352400	1.53271700
C	3.43403400	-2.77724900	-0.22521900
H	4.32080400	-2.83139000	0.41331700
H	2.91167700	-3.73972900	-0.23247500
H	3.74823100	-2.56847300	-1.25750200
O	2.90003000	-0.80982900	1.03636500

C	0.58149600	2.75839200	1.45424700
H	1.13303800	3.68830100	1.27275100
H	-0.34096400	2.96600200	1.99849400
H	1.22905800	2.12301500	2.07075900
C	1.29251700	0.19754500	-2.97829200
H	1.99150300	0.86179300	-3.50052300
H	1.86632100	-0.66056100	-2.60784000
H	0.55234700	-0.16488800	-3.69933600
C	-1.83231700	0.68354500	-2.63435300
H	-2.71006500	0.27961900	-2.11947200
H	-2.17384200	1.56428100	-3.19472100
H	-1.46900600	-0.06538700	-3.34499300

IM2

Sum of electronic and zero-point Energies= -1564.600568

Sum of electronic and thermal Free Energies= -1564.666181

Rh	-0.00047200	-0.09607300	-0.07050100
O	-0.51821500	-0.57371500	2.01476700
C	-0.54417500	-1.69888900	2.51788100
C	-1.62783100	-1.17097000	-0.61913500
C	-0.92281400	-1.90970100	3.94634800
O	-0.24909700	-2.80446500	1.88483600
C	-2.86861200	-0.89252000	-0.04608500
C	1.61532400	1.54913100	-0.48564800
C	0.98374800	0.96747200	-1.67632900
C	-0.39885500	1.35309700	-1.67883400
C	-0.66051400	1.95286400	-0.40259400
C	0.60580400	2.11069700	0.31477500
C	2.26578600	-1.90249600	0.33611100
O	1.08971500	-1.92513900	-0.25175800
C	-2.67843100	-2.75822700	-2.10242600
C	-3.92029800	-2.47143800	-1.54252600
C	-4.01218500	-1.54241200	-0.51095400
H	-2.95009100	-0.16538300	0.76448800
H	-2.59853300	-3.49032600	-2.90610100
H	-4.98019500	-1.31493400	-0.06458200
H	-4.81488200	-2.97345600	-1.90792600
H	-0.04093700	-2.24722600	4.50369700
H	-1.29652300	-0.98088400	4.38163300
H	-1.67776300	-2.69989200	4.01936600
H	0.09672600	-2.58913700	0.96963600
C	-1.53143000	-2.11340300	-1.64202800
H	-0.55838800	-2.34499100	-2.07695500
C	3.02942600	1.43309700	-0.07786200
C	-1.99350100	2.44766300	-0.00749600
O	-2.88610200	2.70104400	-0.78477400
O	3.53464100	2.00953400	0.85839000
O	3.72045800	0.62199400	-0.89782600
O	-2.12004600	2.56880000	1.32475000
C	5.04032600	0.32366900	-0.45393200
H	4.98638700	-0.22268600	0.49504400
H	5.48400400	-0.29935900	-1.23434800
H	5.62377200	1.23994400	-0.31657300
C	-3.39826500	3.01865500	1.76201800
H	-4.17836700	2.31231200	1.45599000
H	-3.33871900	3.07518600	2.85051600
H	-3.63053300	4.00127700	1.33733200
C	3.17786000	-3.01115200	-0.13603000
H	3.50096900	-2.79106500	-1.16282400
H	4.05809500	-3.08319500	0.50955400
H	2.64984600	-3.97072800	-0.16622800
O	2.62026300	-1.07926000	1.16738900

C	0.74671200	2.67277900	1.68400700
H	0.26706100	3.65732100	1.74668600
H	0.23165200	2.02135700	2.40211900
H	1.79999600	2.75051300	1.95700707
C	1.66775600	0.26330200	-2.79724400
H	2.39275300	0.92727300	-3.28605700
H	2.22103600	-0.60834600	-2.43406700
H	0.94513900	-0.07379100	-3.54789300
C	-1.37618200	1.15833900	-2.78440400
H	-2.37279400	0.91480000	-2.40451300
H	-1.46866000	2.09024200	-3.35919200
H	-1.06060600	0.36075400	-3.46514300

IM3

Sum of electronic and zero-point Energies= -1107.939973

Sum of electronic and thermal Free Energies= -1107.995672

Rh	0.06278200	0.41050700	-0.73531700
C	0.08894800	2.47603300	-1.44707000
C	-0.12392100	3.45911500	-0.43498600
C	0.62337000	-1.55144100	0.38366100
C	0.72994600	-0.38993800	1.19722100
C	-0.61589000	0.17895400	1.35693700
C	-1.52730800	-0.62826100	0.62885400
C	-0.72968600	-1.56906700	-0.13156300
C	2.44687600	2.35849200	-0.73875400
C	2.19781400	3.28523700	0.24013300
C	0.89966700	3.84087300	0.39394000
H	-1.10959000	3.91349600	-0.33875900
H	3.45329500	1.96562200	-0.88192100
H	0.72607700	4.59544800	1.16038900
H	3.00511800	3.62035000	0.89041200
H	-0.62818100	2.41494800	-2.27193200
C	1.40077900	1.91158900	-1.60117600
H	1.67480500	1.42553100	-2.54273200
C	1.69082400	-2.46484400	-0.02819500
C	-2.97058200	-0.38930800	0.57284700
O	-3.57219500	0.44991000	1.21359900
O	1.63333400	-3.27911800	-0.92771400
O	2.79011400	-2.33806400	0.75026600
O	-3.60447000	-1.23970600	-0.26378700
C	3.86131500	-3.20682400	0.40846900
H	4.20050300	-3.02492900	-0.61755500
H	4.66206600	-2.98870900	1.11869100
H	3.55335200	-4.25503600	0.49080600
C	-5.01133900	-1.05782000	-0.34123900
H	-5.25560800	-0.05353800	-0.70531900
H	-5.37299100	-1.81457600	-1.04091300
H	-5.47623000	-1.19264600	0.64171500
C	-1.24431300	-2.52710400	-1.15034300
H	-1.83762500	-3.31356400	-0.66278000
H	-1.91905900	-2.02069600	-1.84885200
H	-0.41846800	-2.99733000	-1.68734000
C	-0.91459800	1.30457100	2.27991200
H	-0.80871000	0.96830100	3.32292400
H	-0.20866200	2.13194400	2.12951500
H	-1.93463900	1.66755600	2.13732600
C	1.90792300	0.12957000	1.94101000
H	1.96967200	-0.35097900	2.92919600
H	2.84203400	-0.07897500	1.41423700
H	1.82443600	1.21185200	2.09529700

TS2

Sum of electronic and zero-point Energies= -1107.906545

Sum of electronic and thermal Free Energies= -1107.962681

Rh	-0.07064900	-0.74929400	0.24268300
C	1.74103600	-1.48224000	-0.28185400
C	2.74213200	-0.78425600	-0.96147500
C	-2.00073000	0.36553600	-0.20033200
C	-1.81553900	0.41592400	1.20521900
C	-0.64373100	1.22305900	1.49152100
C	-0.05257600	1.58563700	0.27069600
C	-0.81143600	0.94853700	-0.80984600
C	3.40988200	-3.00292000	0.59475500
C	4.40905400	-2.28312900	-0.05372100
C	4.06991700	-1.18295600	-0.83895300
H	2.48492700	0.08727600	-1.56445500
H	3.66421800	-3.88016400	1.18866000
H	4.84972700	-0.62520300	-1.35781800
H	5.44933900	-2.59175000	0.03506700
H	0.25805900	-1.78275900	-0.96511200
C	2.07625900	-2.62636000	0.45412100
H	1.28826100	-3.22893800	0.91478600
C	-3.11239000	-0.23575700	-0.95235500
C	1.20412600	2.33953300	0.19415000
O	1.76048600	2.84763200	1.14475400
O	-3.15539000	-0.39108700	-2.15394300
O	-4.14169700	-0.57366900	-0.14722600
O	1.69354300	2.41148500	-1.05958000
C	-5.24969500	-1.16191600	-0.81752400
H	-4.94989200	-2.08326300	-1.32901200
H	-5.98775100	-1.37823100	-0.04216700
H	-5.66504300	-0.47130900	-1.55948000
C	2.96337000	3.04488200	-1.16498600
H	3.71561000	2.48708900	-0.59405800
H	3.21164000	3.04152500	-2.22867200
H	2.92093500	4.07036200	-0.78308700
C	-0.13646900	1.55487900	2.85171300
H	-0.23861800	2.63057700	3.04608500
H	-0.68259800	1.01521900	3.63222100
H	0.93259300	1.33417500	2.94295500
C	-2.68445200	-0.18622500	2.25682600
H	-2.13015000	-0.33754400	3.18973400
H	-3.54287600	0.46411000	2.47703100
H	-3.08756800	-1.14957200	1.93395700
C	-0.59805900	1.15110400	-2.27146500
H	-1.24399900	0.48485700	-2.84587100
H	-0.83607700	2.19089500	-2.54075300
H	0.44872600	0.98600200	-2.54173800

IM4

Sum of electronic and zero-point Energies= -1107.909347

Sum of electronic and thermal Free Energies= -1107.965514

Rh	-0.08896500	-0.79663200	0.21726000
C	1.75548600	-1.41536300	-0.25425700
C	2.75420300	-0.67018100	-0.88488100
C	-1.98625500	0.35191700	-0.17787500
C	-1.82975700	0.42151700	1.22289700
C	-0.61497900	1.16133700	1.50881700
C	-0.01707000	1.52658900	0.28937200
C	-0.78707100	0.92618800	-0.79710200
C	3.43414500	-2.99782000	0.49147100
C	4.42741900	-2.23523800	-0.11330700
C	4.08251100	-1.07944800	-0.81221600
H	2.49748200	0.24245500	-1.42488500
H	3.69240200	-3.91773100	1.01553800
H	4.85746200	-0.48824900	-1.30103500
H	5.46805700	-2.55144800	-0.05918800
H	-0.30727600	-1.96265200	-0.84112000
C	2.09770400	-2.61020800	0.38930300
H	1.31826600	-3.25110000	0.81038200
C	-3.10875400	-0.23223300	-0.94076000
C	1.24980600	2.26781700	0.22201800
O	1.87350700	2.65005000	1.18859500
O	-3.10591200	-0.47578900	-2.12608000
O	-4.19041600	-0.43156100	-0.16320800
O	1.65459300	2.49099100	-1.04260300
C	-5.31135700	-0.99363900	-0.83803000
H	-5.05556000	-1.96804800	-1.26804400
H	-6.09169600	-1.10101100	-0.08187800
H	-5.64707300	-0.33283200	-1.64436600
C	2.92295300	3.12861700	-1.15444500
H	3.70227500	2.50710800	-0.69667400
H	3.10517600	3.24508700	-2.22477700
H	2.91289900	4.10391700	-0.65665800
C	-2.71377300	-0.15295800	2.27693200
H	-2.13031400	-0.46248900	3.15204700
H	-3.45350600	0.58718700	2.61553800
H	-3.26746500	-1.01819600	1.90529600
C	-0.09925200	1.46065600	2.87357100
H	-0.08455300	2.54405500	3.04833200
H	-0.71644700	0.99574500	3.64926400
H	0.93753200	1.12602100	2.98999600
C	-0.58668800	1.14701100	-2.25712200
H	-1.22415300	0.47369800	-2.83295700
H	-0.84001300	2.18573300	-2.51664200
H	0.46010400	0.99427600	-2.53483100

Cp^E-IM5

Sum of electronic and zero-point Energies= -1876.602864

Sum of electronic and thermal Free Energies= -1876.678678

Rh	-0.45504900	0.55766600	-0.48264600
C	0.26162500	1.51321300	1.35492300
C	-0.01852000	2.62968300	0.50911200
C	-0.99758800	0.81343100	1.58366200
C	-1.42159400	2.60942300	0.17962200
C	-2.03544100	1.55232600	0.91141900
C	1.29884400	-0.30656400	-1.13914200
C	-1.17006500	-1.35102000	-0.84667600
C	1.06278700	-1.50375500	-1.69959200
C	-0.27344600	-2.07222500	-1.53625200
C	1.84889500	-2.48063300	-2.52403200
H	1.94189800	-2.14485200	-3.57333600
H	2.86028400	-2.68095900	-2.14424800
C	-0.27530800	-3.39026900	-2.25380300
H	-0.72483600	-4.21253100	-1.68098000
H	-0.80316900	-3.32778900	-3.22353100
O	1.10241000	-3.69288700	-2.45694000
C	2.58944000	0.37613900	-1.09077000
C	2.78583100	1.63010100	-1.68861300
C	3.66429200	-0.21542400	-0.40671300
C	4.02291500	2.25960100	-1.62388500
H	1.95780100	2.10436400	-2.21769700
C	4.89518200	0.42617900	-0.33040400
H	3.51097700	-1.18046800	0.08089500
C	5.08065800	1.66572700	-0.93745200
H	4.16422700	3.21805500	-2.12391500
H	5.71453000	-0.04622500	0.21027900
H	6.04720200	2.16441100	-0.88246500
C	-2.55996200	-1.73469200	-0.60085200
C	-3.61882600	-1.05657600	-1.22404400
C	-2.86662900	-2.81495400	0.23996100
C	-4.93231800	-1.46954800	-1.04090300
H	-3.39399500	-0.20933800	-1.87535500
C	-4.18426800	-3.21227900	0.43944800
H	-2.04966000	-3.34557500	0.73216000
C	-5.22193600	-2.54530000	-0.20368800
H	-5.73777400	-0.95409100	-1.56440900
H	-4.40086300	-4.05200800	1.09828400
H	-6.25263000	-2.86296600	-0.05555400
C	-3.45952600	1.22131800	1.04792000
C	0.92981200	3.65794700	0.04695900
O	-3.90111400	0.43500100	1.85696000
O	0.80704400	4.34167700	-0.94802100
O	1.95706600	3.79555800	0.90260400
O	-4.24336300	1.92688700	0.20892700
C	-5.63908300	1.70885800	0.38378300
H	-6.13362700	2.29861900	-0.39118700
H	-5.87878800	0.64520900	0.27771700
H	-5.95813300	2.04182500	1.37820500
C	2.90258100	4.80125500	0.55863400
H	2.42141400	5.78494000	0.52357200
H	3.66386700	4.77362600	1.34087700
H	3.35269500	4.59017000	-0.41681200
C	-2.10461100	3.54884000	-0.75154400
H	-2.66953600	2.99083500	-1.50850200
H	-2.84150300	4.15315700	-0.20651600
H	-1.38238000	4.20374100	-1.24263900
C	-1.18416900	-0.31626100	2.53044600
H	-1.51613900	0.06789500	3.50615900
H	-1.96320900	-1.00320200	2.18516800
H	-0.24575500	-0.86337600	2.67604800
C	1.55012100	1.15617500	2.00355000
H	2.40865900	1.46752700	1.40172100
H	1.62712100	1.66088700	2.97805500
H	1.62438700	0.07409100	2.16745800
C	3.42595200	-2.85952000	3.02017900
C	2.09315600	-2.56288600	2.74328900
C	1.52165800	-2.96738700	1.53951400
C	2.27719100	-3.69171600	0.61988700
C	3.60816400	-3.99197200	0.89956400
C	4.18502400	-3.57141500	2.09593700
H	3.87157200	-2.53845100	3.96063100
H	1.49801100	-2.01670400	3.47667900
H	0.48704300	-2.71037700	1.30138300
H	1.83038800	-4.00927100	-0.32368100
H	4.19870600	-4.55645900	0.17866200
H	5.22704700	-3.80450500	2.31102600

Cp^E-TS3

Sum of electronic and zero-point Energies= -1876.593342

Sum of electronic and thermal Free Energies= -1876.666788

Rh	-0.00807800	-0.23761200	0.19087500
C	-1.08021100	-2.31448000	-0.33010800
C	-0.85586300	-1.46530600	-1.47971600
C	0.18860500	-2.64916900	0.19431700
C	0.55333800	-1.30513000	-1.68784300
C	1.20061600	-2.03881200	-0.62794600
C	-1.59371200	1.19334700	0.31837900
C	1.03851300	1.45122700	-0.30997400
C	-1.16351900	2.36268000	-0.21533600
C	0.23489400	2.52560800	-0.49436900
C	-1.82552900	3.66645600	-0.54412700
H	-2.26778000	3.63492000	-1.55973700
H	-2.61212500	3.96559700	0.16038000
C	0.43370100	3.97084700	-0.87244900
H	1.27225800	4.46209900	-0.35976800
H	0.59083500	4.08807200	-1.96238600
O	-0.77224300	4.61399800	-0.48616200
C	-2.98142000	0.79826600	0.54667200
C	-3.93897000	1.00474300	-0.46016600
C	-3.40050200	0.20448100	1.74737500
C	-5.26678700	0.64075100	-0.26554800
H	-3.61578700	1.43152600	-1.41128100
C	-4.72682700	-0.15935200	1.93786200
H	-2.67344500	0.04289400	2.54363600
C	-5.66692800	0.05529700	0.93215400
H	-5.99479900	0.81348900	-1.05819400
H	-5.03148400	-0.61013500	2.88130900
H	-6.70628100	-0.23153800	1.08249600
C	2.48827700	1.45520100	-0.49335200
C	3.07527100	2.16631600	-1.55350600
C	3.33660300	0.76312600	0.38669600
C	4.45497100	2.19883500	-1.71723900
H	2.42955900	2.67339900	-2.27115600
C	4.71594400	0.82615900	0.24181400
H	2.89871700	0.17998400	1.19712400
C	5.28249300	1.53864000	-0.81339800
H	4.88613800	2.74648600	-2.55416000
H	5.35354000	0.30409600	0.95505600
H	6.36426100	1.57437700	-0.93358600
C	2.63616600	-2.27506200	-0.43485900
C	-1.88565200	-0.89067800	-2.37028600
O	3.13278600	-2.76848500	0.55711900
O	-1.79071500	0.14252100	-2.99752000
O	-2.96974800	-1.68512000	-2.43407100
O	3.36187400	-1.91773500	-1.51178200
C	4.75577700	-2.17227500	-1.41211300
H	5.20239500	-1.74291400	-2.31200900
H	5.17582100	-1.69833300	-0.51886800
H	4.94671200	-3.25087100	-1.36448000
C	-4.00679500	-1.22528700	-3.29174900
H	-3.63777500	-1.10980700	-4.31670000
H	-4.78910300	-1.98587900	-3.24861400
H	-4.39594200	-0.26105300	-2.94511900
C	1.18385300	-0.65621000	-2.87388700
H	2.11242000	-0.14341600	-2.60736100
H	1.44726600	-1.42257300	-3.61678900
H	0.49086700	0.05659900	-3.33026800
C	0.45626500	-3.52552200	1.36973900
H	0.98778800	-4.43245500	1.05241500
H	1.10667800	-3.03301800	2.10087700
H	-0.47367500	-3.83272700	1.86231100
C	-2.40298600	-2.78205800	0.17933700
H	-3.16888700	-2.00228800	0.09555500
H	-2.76236700	-3.64783800	-0.39432000
H	-2.34428600	-3.08021500	1.23374000
C	0.23481900	-0.81214300	4.50832900
C	-0.21139900	-0.75787400	3.19280900
C	0.22038800	0.25806700	2.32818100
C	1.05197300	1.26295500	2.83927200
C	1.48475800	1.21803600	4.16150100
C	1.08936600	0.17503600	4.99306600
H	-0.09220500	-1.62190800	5.15921900
H	-0.89965700	-1.52112800	2.82762400
H	-0.72179800	0.79848000	1.46184300
H	1.36081600	2.08599800	2.19726500
H	2.13723900	2.00273800	4.54170800
H	1.43500800	0.13813600	6.02500500

Cp^E-IM6

Sum of electronic and zero-point Energies= -1876.613480

Sum of electronic and thermal Free Energies= -1876.685236

Rh	0.05558500	-0.35892500	-0.06886300
C	-1.06668900	-0.16830900	-2.21246700
C	-0.78972500	1.16295700	-1.70893400
C	0.17569700	-0.79686400	-2.43778900
C	0.61258500	1.35364700	-1.62380500
C	1.22194800	0.12134100	-2.05916100
C	-1.50375700	-0.16426400	1.43313200
C	1.10122900	0.55593700	1.32358000
C	-1.08216700	1.08074200	2.04008600
C	0.26764700	1.36273800	2.12110900
C	-1.82544500	2.17737500	2.72768900
H	-2.22991300	2.88764000	1.98078200
H	-2.65791900	1.82457600	3.35309000
C	0.43593600	2.56541800	3.01165500
H	1.14238000	2.42384800	3.84282000
H	0.76991100	3.44612600	2.42725600
O	-0.85380000	2.79703800	3.54975000
C	-2.89811100	-0.41648700	1.02683700
C	-3.78556400	0.60720000	0.67049200
C	-3.36557600	-1.73970600	0.98452900
C	-5.09458300	0.32089600	0.29544500
H	-3.43991900	1.64152400	0.67745100
C	-4.66827900	-2.02505700	0.60193300
H	-2.68247800	-2.54781900	1.25141600
C	-5.54241600	-0.99532000	0.25738800
H	-5.76930200	1.13469600	0.03003300
H	-5.00810600	-3.05942500	0.57862900
H	-6.56613600	-1.21890800	-0.03772200
C	2.55756100	0.61578300	1.33739000
C	3.26331500	1.74474800	1.79462400
C	3.29921400	-0.48887300	0.87876300
C	4.65089100	1.76582300	1.79414100
H	2.72001500	2.63030300	2.11883700
C	4.68548200	-0.48080400	0.91714900
H	2.76263400	-1.35948900	0.50314300
C	5.36534600	0.64775700	1.37004400
H	5.17841500	2.65530200	2.13410100
H	5.23727200	-1.35619200	0.57786400
H	6.45421900	0.65922400	1.38762200
C	2.64425800	-0.16628700	-2.24851300
C	-1.77635300	2.19727700	-1.37105200
O	3.10871200	-1.24724600	-2.54985200
O	-1.65078000	3.05964300	-0.52009700
O	-2.87520800	2.10775100	-2.14317600
O	3.41870400	0.92843400	-2.07111700
C	4.80260900	0.72942100	-2.31391700
H	5.29211300	1.66833000	-2.04293200
H	5.19461400	-0.09175000	-1.70400500
H	4.97983800	0.49625200	-3.37065500
C	-3.86337600	3.10195300	-1.91420600
H	-3.46737900	4.09884100	-2.13844200
H	-4.69168900	2.86037900	-2.58377800
H	-4.20232900	3.09111500	-0.87137700
C	1.29771800	2.63097200	-1.26439200
H	2.15718300	2.46005600	-0.60771100
H	1.69819600	3.10825900	-2.16940500
H	0.59942900	3.31960300	-0.77964500
C	0.39662600	-2.12977200	-3.06802500
H	0.93350900	-2.00888200	-4.01814100
H	1.01667300	-2.78269000	-2.44440100
H	-0.55309000	-2.63466800	-3.27998500
C	-2.41371900	-0.73583700	-2.51642100
H	-3.15508500	-0.44484300	-1.76253100
H	-2.78610600	-0.37855200	-3.48689300
H	-2.38639300	-1.83206500	-2.54999600
C	-0.34901500	-4.63617000	0.32452000
C	-0.38519900	-3.31322700	-0.11255200
C	0.22783100	-2.28404400	0.61543400
C	0.84198700	-2.63481900	1.82715100
C	0.88078300	-3.95806900	2.26605500
C	0.29054700	-4.96776100	1.51489800
H	-0.83317000	-5.41055400	-0.27082300
H	-0.92331000	-3.08550900	-1.03264900
H	-1.11709000	-0.98750500	2.04848800
H	1.30220500	-1.86725400	2.45085400
H	1.37406200	-4.19419100	3.20915000
H	0.31898700	-6.00101800	1.85746600

Cp*-IM5

Sum of electronic and zero-point Energies= -1499.692579

Sum of electronic and thermal Free Energies= -1499.759345

Rh	-0.11037000	-0.45774500	-0.16082600
C	-1.43196800	-1.79635500	-1.53974400
C	-0.56041200	-0.83582200	-2.20009600
C	-0.60411200	-2.70194000	-0.86255300
C	0.81066400	-1.31541400	-2.06066600
C	0.78832900	-2.41445800	-1.18698100
C	-1.52800400	1.04387300	0.13209400
C	1.12242500	1.21477000	-0.18357100
C	-0.99121800	2.28338300	0.07890900
C	0.43901100	2.37752700	-0.08156500
C	-1.49493200	3.68411500	0.29021800
H	-1.92600700	4.10988800	-0.63887600
H	-2.25119700	3.78188100	1.08094300
C	0.79466900	3.83163700	0.06130300
H	1.67087300	4.02232300	0.69781700
H	0.98749700	4.30975600	-0.92133300
O	-0.34315400	4.42431400	0.67092600
C	-2.95354200	0.79135600	0.32898200
C	-3.91581200	1.57260800	-0.33655300
C	-3.42428000	-0.23952900	1.15987300
C	-5.27645900	1.33582800	-0.17647400
H	-3.57689200	2.36054600	-1.01041400
C	-4.78236000	-0.46911700	1.33044500
H	-2.70012400	-0.87302200	1.67347500
C	-5.71891200	0.31382000	0.65829000
H	-5.99689500	1.95196200	-0.71350700
H	-5.11543600	-1.27009200	1.98989700
H	-6.78406100	0.12594600	0.78219700
C	2.57481700	1.11449400	-0.29901700
C	3.32900100	2.11915500	-0.93217800
C	3.27206100	-0.00697200	0.18018000
C	4.70771100	2.00958100	-1.06876500
H	2.81495300	2.98214800	-1.35589900
C	4.65047600	-0.11281000	0.05513100
H	2.70388900	-0.80829500	0.65146800
C	5.37929500	0.89471800	-0.57436300
H	5.26180800	2.79924600	-1.57525700
H	5.15953200	-0.99466900	0.44545300
H	6.45905100	0.80839400	-0.68512100
C	1.96904700	-0.76513800	-2.81695300
H	2.92913600	-0.96927600	-2.32850900
H	1.99943700	-1.20686100	-3.82472900
H	1.89325700	0.32242800	-2.93679500
C	-1.04796300	-3.85819900	-0.03387100
H	-1.09025800	-4.78067200	-0.63289000
H	-0.35605600	-4.05197700	0.79641000
H	-2.04820700	-3.69833400	0.38938700
C	-2.91506700	-1.84311400	-1.66322000
H	-3.36702600	-0.84306800	-1.66237100
H	-3.20171500	-2.33466200	-2.60570800
H	-3.38034100	-2.40362800	-0.84335800
C	1.06388000	-2.34818600	2.75478400
C	-0.02082500	-1.52287800	2.42899800
C	0.09600400	-0.13521600	2.55876100
C	1.30552200	0.42041700	2.99976900
C	2.37147800	-0.40049100	3.32530100
C	2.25002500	-1.78949600	3.20456300
H	0.96234400	-3.43149800	2.68395300
H	-0.97792800	-1.96974100	2.16050800
H	-0.76490300	0.51024600	2.39687800
H	1.39431100	1.50214500	3.08605400
H	3.30922600	0.03426900	3.66721700
H	3.08837700	-2.43223400	3.46987700
C	-1.00552800	0.22166200	-3.15108700
H	-0.31248000	1.07194700	-3.14842100
H	-1.06092500	-0.16777600	-4.17968700
H	-1.99713100	0.60488100	-2.88115700
C	1.94760600	-3.24673800	-0.75416600
H	1.94337300	-3.42198900	0.33119400
H	1.93705200	-4.23348500	-1.24228500
H	2.90158500	-2.76511500	-1.00131800

Cp*-TS3

Sum of electronic and zero-point Energies= -1499.668650

Sum of electronic and thermal Free Energies= -1499.733636

Rh	-0.00672300	-0.40835300	-0.32864200
C	-1.30222000	-1.53973300	-1.92734700
C	-0.52515700	-0.45803800	-2.48600600
C	-0.39698700	-2.49807900	-1.41121300
C	0.86190600	-0.79362400	-2.34159500
C	0.94479700	-2.04083000	-1.63869000
C	-1.37499700	1.12694600	0.35952700
C	1.34146200	1.09371300	0.11220000
C	-0.69327800	2.28902000	0.51717400
C	0.74096300	2.26475900	0.44114700
C	-1.08627500	3.69155200	0.87651000
H	-1.37977400	4.27175000	-0.02148500
H	-1.90955500	3.75545300	1.59988000
C	1.21655300	3.63148100	0.86544100
H	2.03345500	3.61740900	1.60057100
H	1.55733600	4.23596100	0.00128100
O	0.08203200	4.24324400	1.46091700
C	-2.82786700	0.99755700	0.29545000
C	-3.57582500	1.87546600	-0.50720300
C	-3.52135400	-0.00094300	0.99774000
C	-4.95862200	1.76147300	-0.60103400
H	-3.05017600	2.64526800	-1.07428700
C	-4.90192600	-0.11217700	0.90512700
H	-2.96296000	-0.68568800	1.63660600
C	-5.62876200	0.76521100	0.10252200
H	-5.51503500	2.45354400	-1.23192200
H	-5.41809400	-0.88881400	1.46822700
H	-6.71089500	0.67289200	0.02753100
C	2.79237000	0.92701900	0.03660700
C	3.61029900	1.94214200	-0.48857400
C	3.41432500	-0.25808400	0.46187700
C	4.98629300	1.77775300	-0.58978900
H	3.14707700	2.85826900	-0.85587200
C	4.79118600	-0.41757600	0.37273800
H	2.79169900	-1.05735100	0.86413200
C	5.58457200	0.59678100	-0.15919200
H	5.59506300	2.57498600	-1.01449000
H	5.24870200	-1.34531800	0.71519000
H	6.66237900	0.46572400	-0.24081600
C	1.99895000	-0.05069200	-2.95395900
H	2.93434900	-0.19161700	-2.39802800
H	2.16631400	-0.39834700	-3.98433600
H	1.80288300	1.02843600	-2.99538900
C	-0.73443000	-3.81773300	-0.80709900
H	-0.52864500	-4.62998900	-1.52077700
H	-0.13821000	-4.02046300	0.09258600
H	-1.79396100	-3.88892800	-0.53160800
C	-2.78865700	-1.64101900	-1.96136500
H	-3.26793900	-0.66024800	-1.84184800
H	-3.13513100	-2.06310200	-2.91682100
H	-3.17363700	-2.28257800	-1.15812200
C	-0.55639200	-2.84534300	3.28498000
C	-0.76705400	-2.13391400	2.10823000
C	-0.02542400	-0.98095700	1.81394500
C	0.88315900	-0.51823700	2.77527100
C	1.08574600	-1.22052300	3.96033300
C	0.37836600	-2.39199000	4.21222500
H	-1.13170900	-3.74912300	3.48364800
H	-1.52191200	-2.48132600	1.40078400
H	-0.74951200	0.07694200	1.20761300
H	1.43822200	0.40080200	2.59468600
H	1.80327000	-0.84866400	4.69081400
H	0.54170700	-2.94225900	5.13775100
C	-1.06644200	0.73510400	-3.19840100
H	-0.44367900	1.62160100	-3.01679000
H	-1.11060300	0.57475700	-4.28650200
H	-2.08261200	0.97375600	-2.85799900
C	2.17358300	-2.83855200	-1.36264500
H	2.12286700	-3.32487700	-0.37780600
H	2.31327200	-3.63337700	-2.11210700
H	3.07454800	-2.21313400	-1.37233700

Cp*-IM6

Sum of electronic and zero-point Energies= -1499.688528

Sum of electronic and thermal Free Energies= -1499.754397

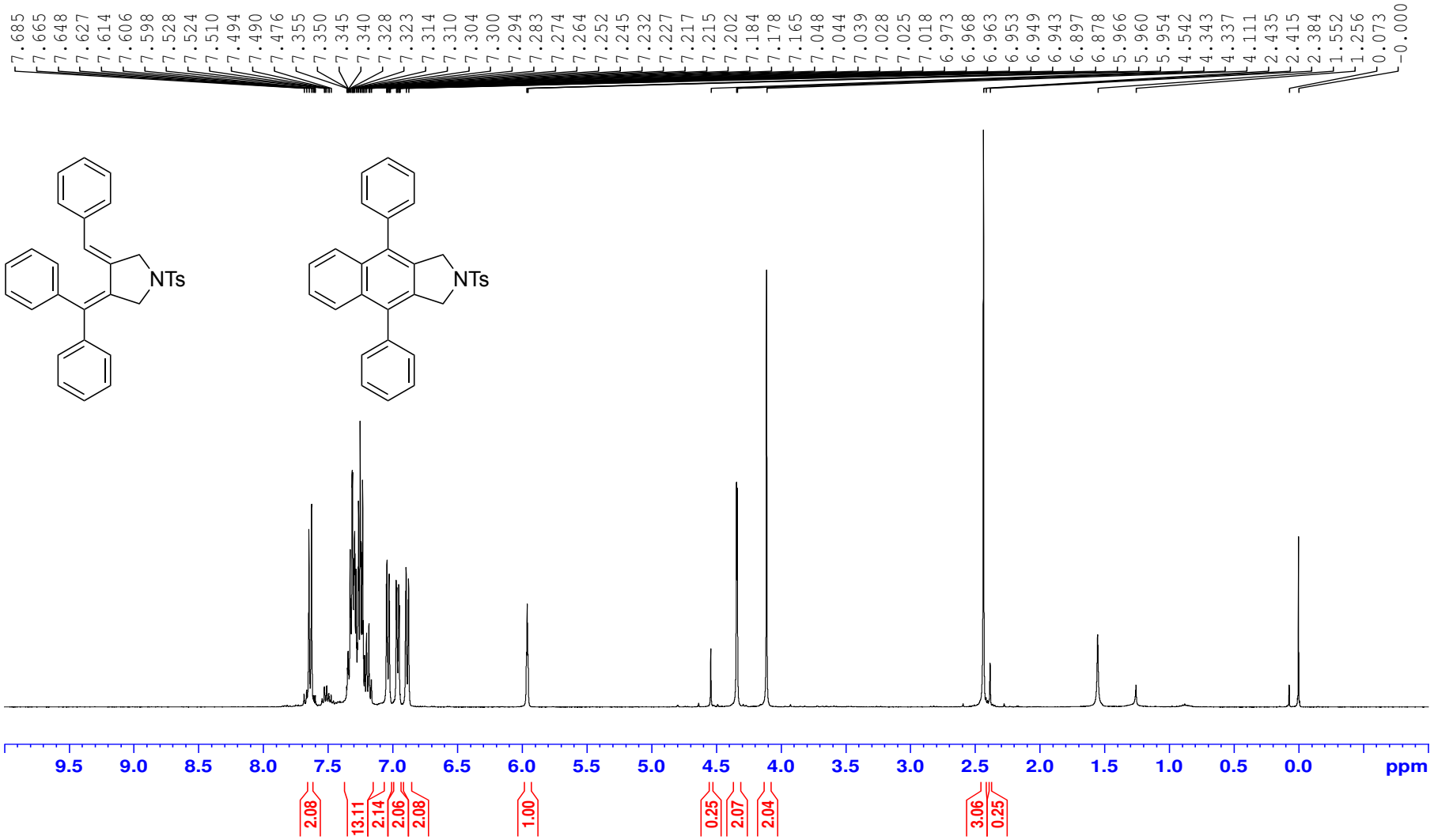
Rh	0.10094800	-0.41881100	-0.36599900
C	-1.20910000	-0.94261600	-2.24502500
C	-0.59095100	0.37134500	-2.42998100
C	-0.18776600	-1.89715700	-2.13619300
C	0.80264800	0.20751700	-2.43746900
C	1.08018400	-1.19113000	-2.13977500
C	-1.54408900	0.96507700	0.93484200
C	1.35808400	0.93302000	0.54226100
C	-0.76116900	2.08071200	0.97945900
C	0.68148700	2.04110400	0.96826100
C	-1.14415200	3.51947600	1.15579100
H	-1.27848500	4.02898000	0.17699900
H	-2.05748300	3.66988100	1.74591000
C	1.12291100	3.42347200	1.40577500
H	1.86623700	3.43303300	2.21472200
H	1.54247000	3.99783700	0.55440100
O	-0.05138400	4.06934100	1.86147300
C	-2.98248900	0.86648500	0.75476600
C	-3.75411000	1.89292600	0.18563700
C	-3.63293000	-0.32474000	1.12091700
C	-5.12467800	1.73947600	0.00943700
H	-3.27115500	2.81405200	-0.14189800
C	-4.99993400	-0.47550900	0.94234400
H	-3.03905900	-1.13694100	1.54531300
C	-5.75445400	0.55723200	0.38711400
H	-5.70352600	2.54821800	-0.43435500
H	-5.48299700	-1.40583100	1.23751500
H	-6.82696900	0.43781500	0.24417600
C	2.82373300	0.83976700	0.49732700
C	3.64509200	1.97215000	0.34175200
C	3.46539400	-0.41034700	0.55708600
C	5.02791000	1.86202400	0.26219000
H	3.19550500	2.95654400	0.23692400
C	4.84820100	-0.51992700	0.50034200
H	2.85047500	-1.30387300	0.65066400
C	5.63977800	0.61583400	0.35037700
H	5.63060900	2.75924800	0.12741500
H	5.31076800	-1.50421200	0.56304100
H	6.72367100	0.52926400	0.29433700
C	1.82254400	1.26123400	-2.70005000
H	2.78488600	1.02308600	-2.23008500
H	1.99823100	1.37176700	-3.78022200
H	1.50475900	2.23966700	-2.31363600
C	-0.31324700	-3.37996700	-2.08768100
H	0.04954700	-3.82214400	-3.02797400
H	0.27653500	-3.81537700	-1.27066500
H	-1.35312800	-3.70198400	-1.95557200
C	-2.67926900	-1.18085700	-2.25520800
H	-3.21717300	-0.41908500	-1.67381800
H	-3.07790400	-1.14952400	-3.28062100
H	-2.93818300	-2.15680100	-1.82610300
C	-0.71784200	-3.79843100	2.20261800
C	-0.62491600	-2.87637100	1.16085200
C	0.24481400	-1.77412400	1.21407300
C	0.98521500	-1.61882400	2.39582400
C	0.90034600	-2.53911400	3.44018000
C	0.05569700	-3.63973900	3.34748500
H	-1.40527500	-4.64075400	2.11747800
H	-1.27076700	-3.01507100	0.29146700
H	-1.06082500	0.03314700	1.29231700
H	1.63865100	-0.75645400	2.52380800
H	1.49757500	-2.38384000	4.33910500
H	-0.01087500	-4.35735100	4.16415900
C	-1.33704200	1.64245600	-2.64835800
H	-0.75553200	2.51050900	-2.30879200
H	-1.56656800	1.79669500	-3.71377000
H	-2.29261800	1.64650700	-2.10669500
C	2.40803100	-1.85786900	-2.22851300
H	2.44664400	-2.74977900	-1.58926000
H	2.61378200	-2.17946900	-3.26178400
H	3.22301800	-1.19351800	-1.91709000

II. ^{1}H and ^{13}C NMR NMR Spectra

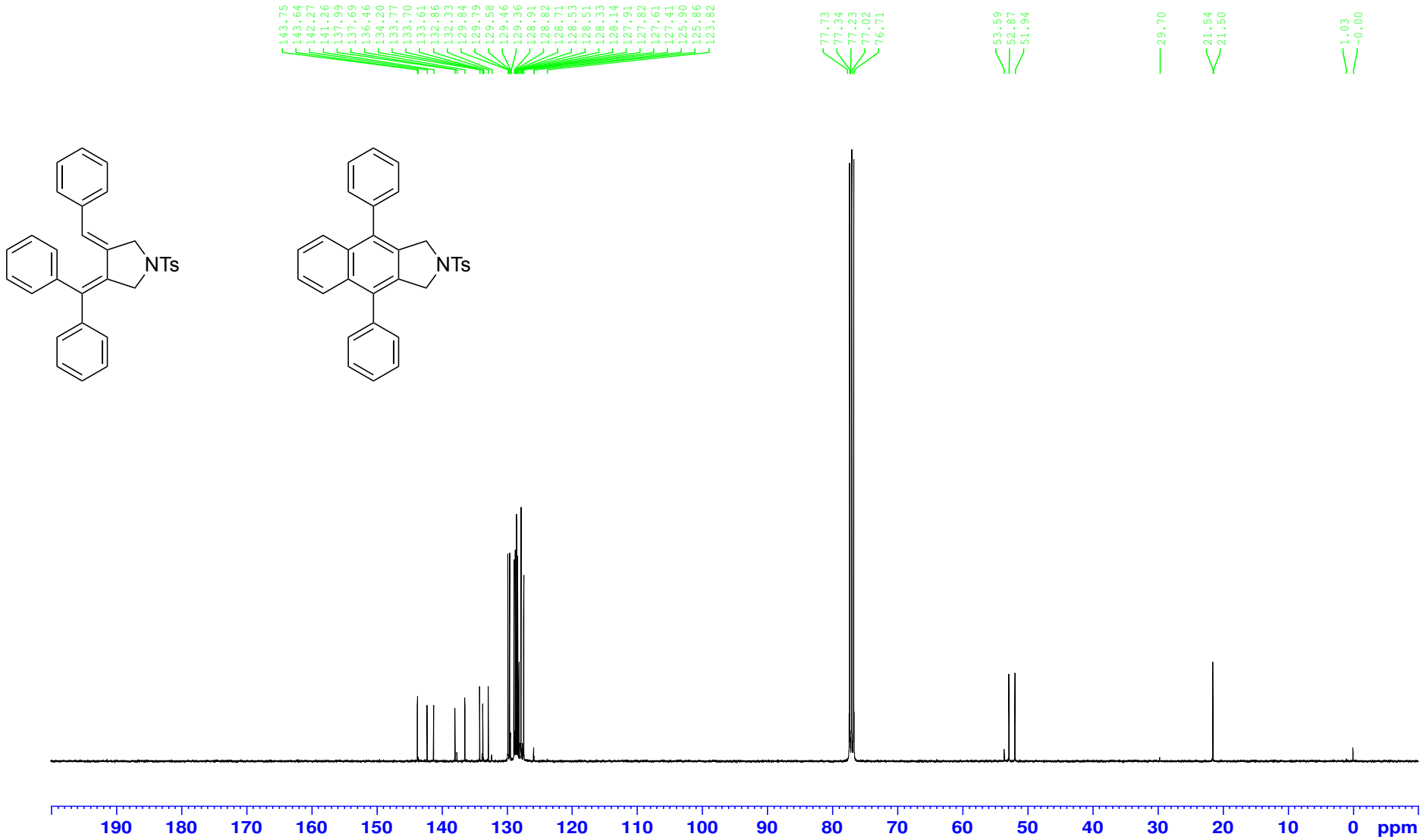
(4*Z*)-3-(Diphenylmethylidene)-1-(4-methylbenzenesulfonyl)-4-(phenylmethylidene)pyrrolidine (4aa)

2-(4-Methylbenzenesulfonyl)-4,9-diphenyl-1*H*,2*H*,3*H*-benzo[*f*]isoindole (5aa)

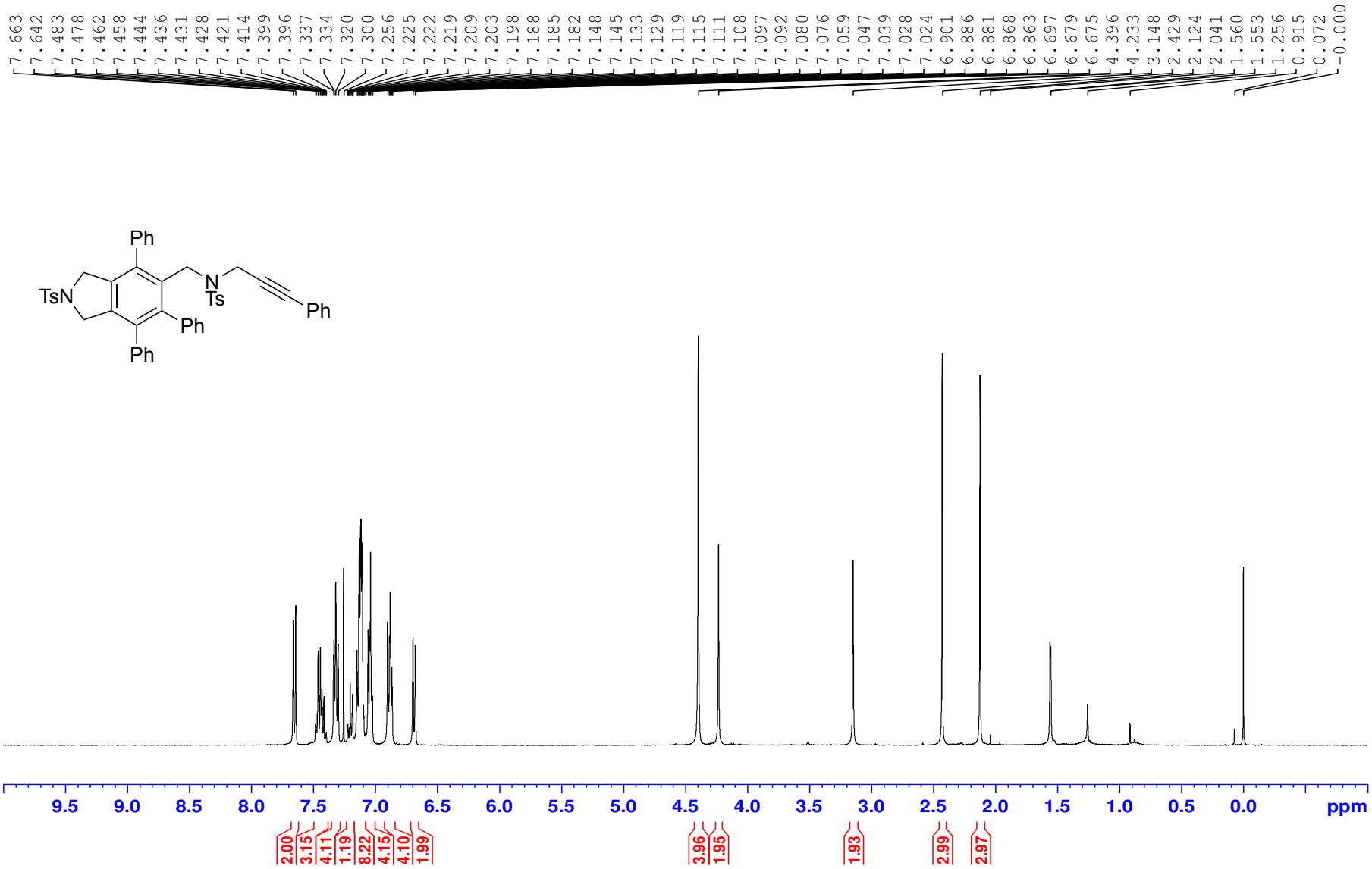
4aa/5aa = 96:4



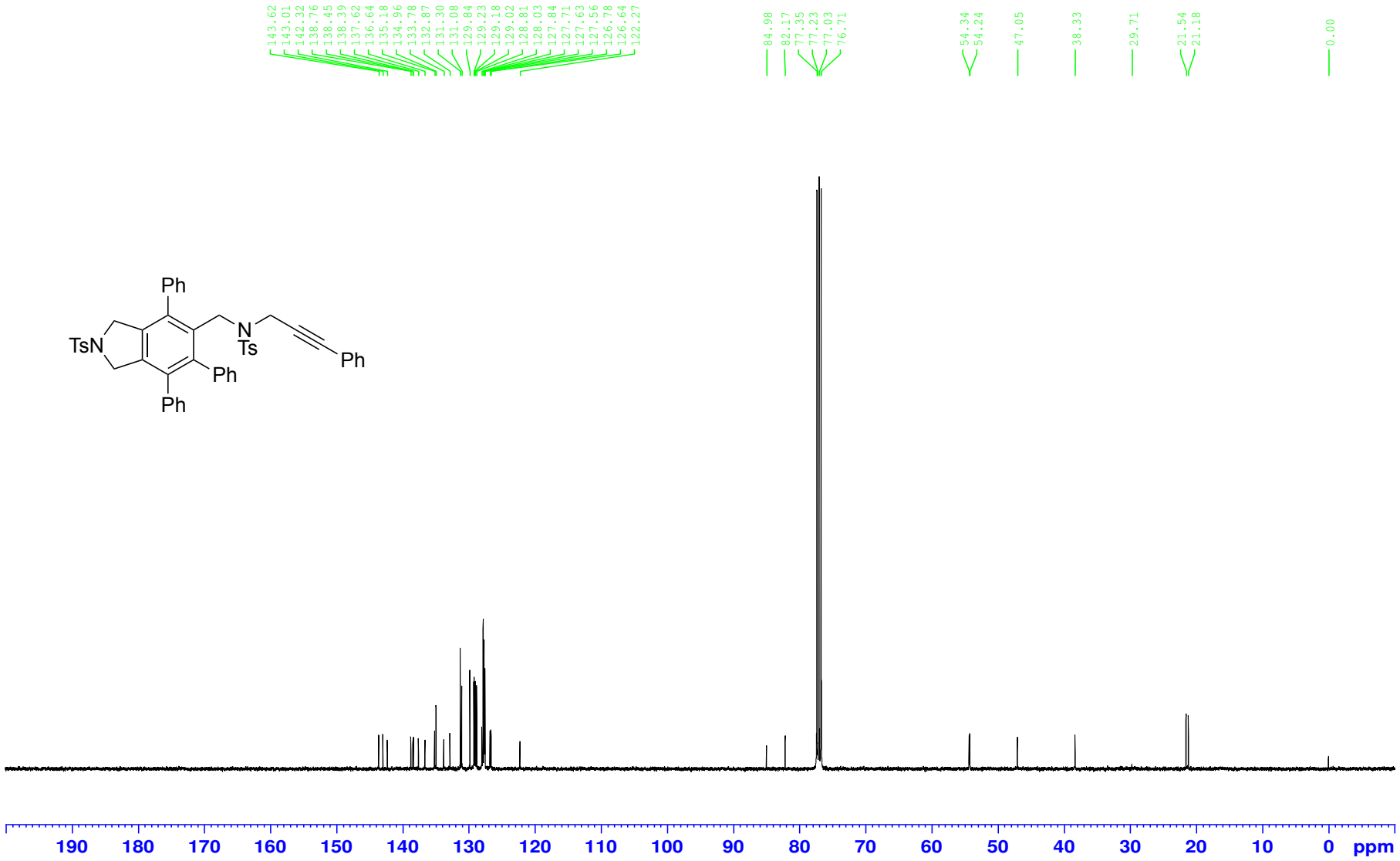
(4*Z*)-3-(Diphenylmethylidene)-1-(4-methylbenzenesulfonyl)-4-(phenylmethylidene)pyrrolidine (4aa)
2-(4-Methylbenzenesulfonyl)-4,9-diphenyl-1*H*,2*H*,3*H*-benzo[*f*]isoindole (5aa)
4aa/5aa = 96:4



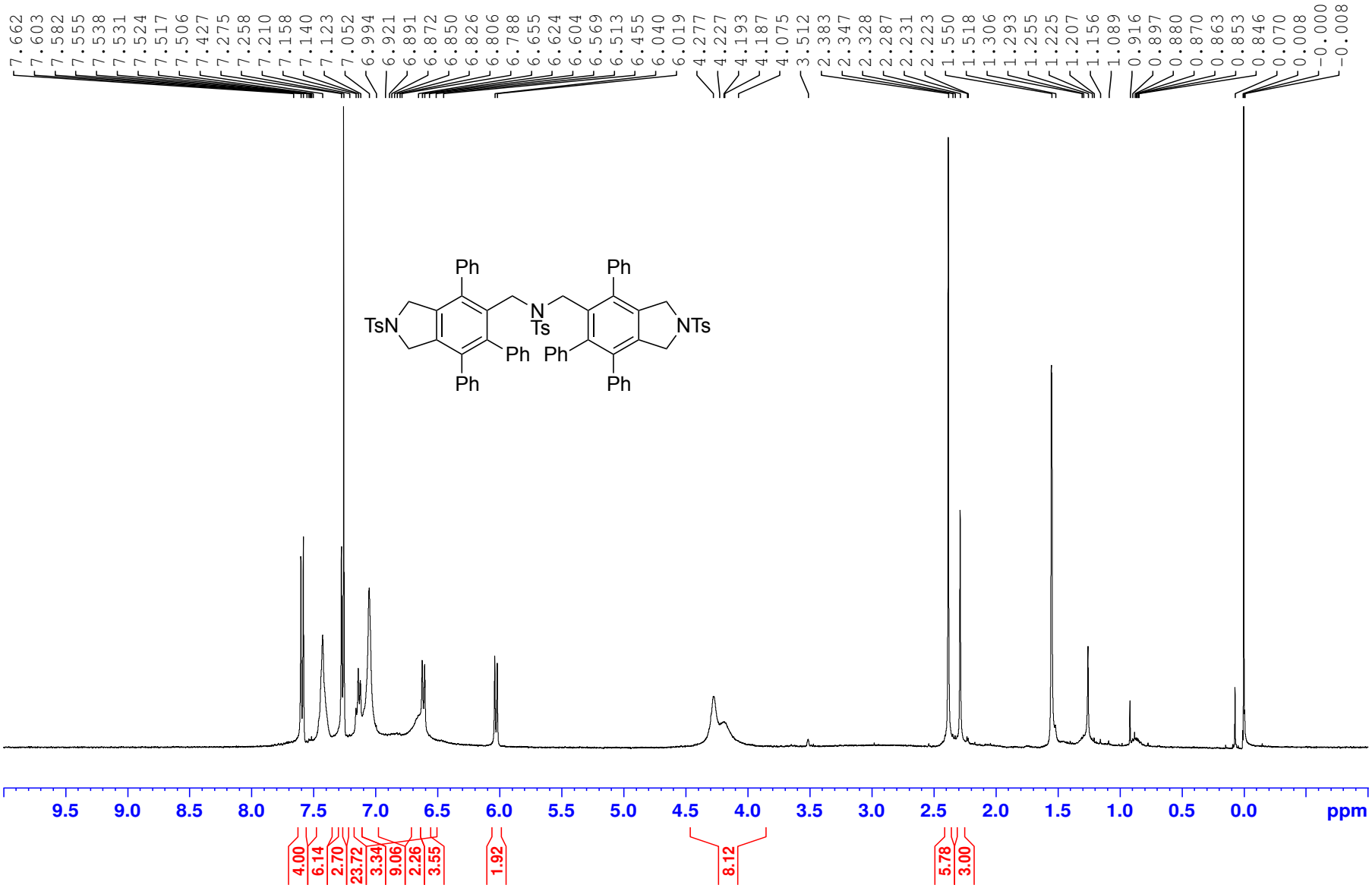
4-Methyl-*N*-{[2-(4-methylbenzenesulfonyl)-4,6,7-triphenyl-2,3-dihydro-1*H*-isoindol-5-yl]methyl}-*N*-(3-phenylprop-2-yn-1-yl)benzene-1-sulfonamide (6a)



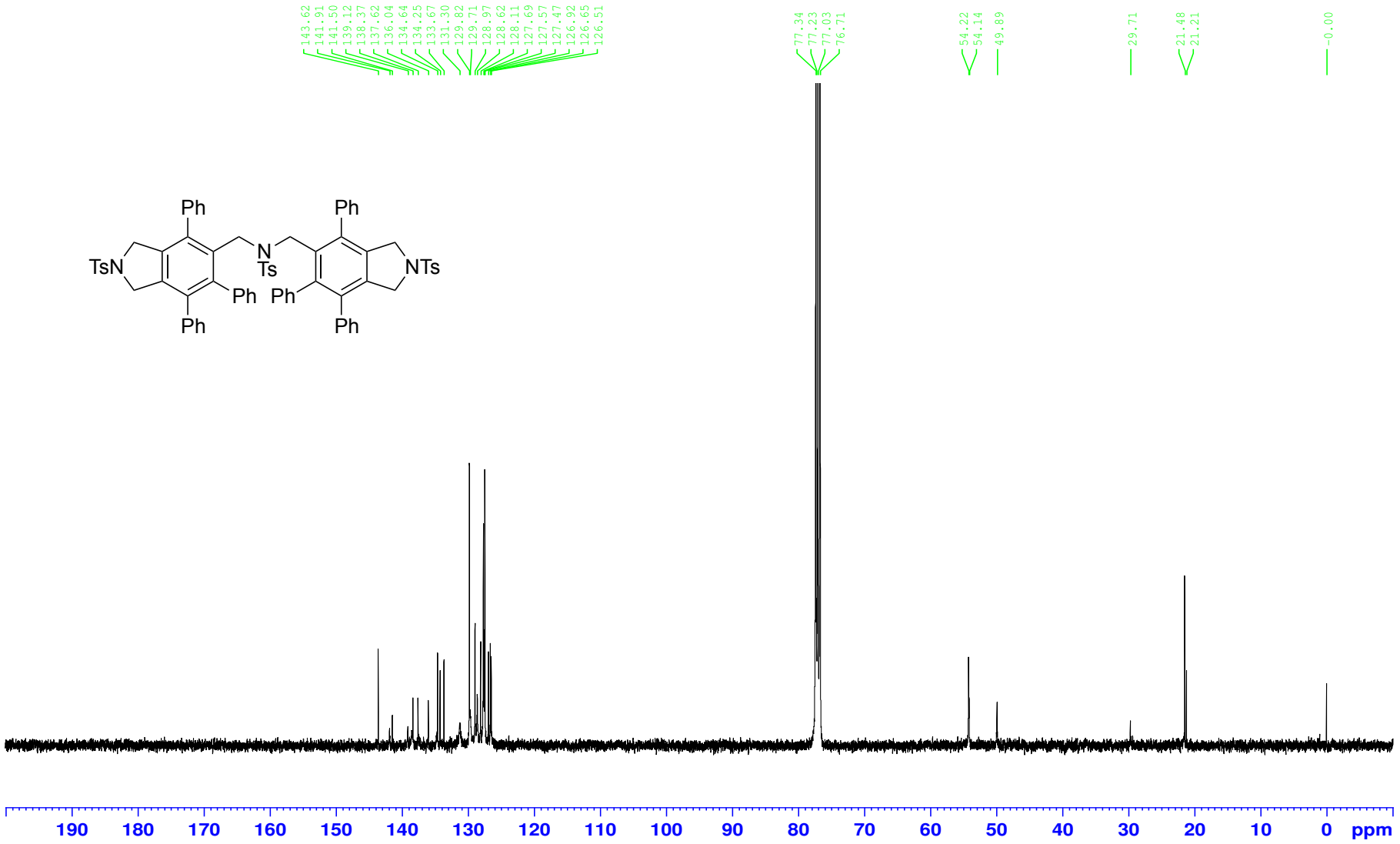
4-Methyl-*N*-{[2-(4-methylbenzenesulfonyl)-4,6,7-triphenyl-2,3-dihydro-1*H*-isoindol-5-yl]methyl}-*N*-(3-phenylprop-2-yn-1-yl)benzene-1-sulfonamide (6a)



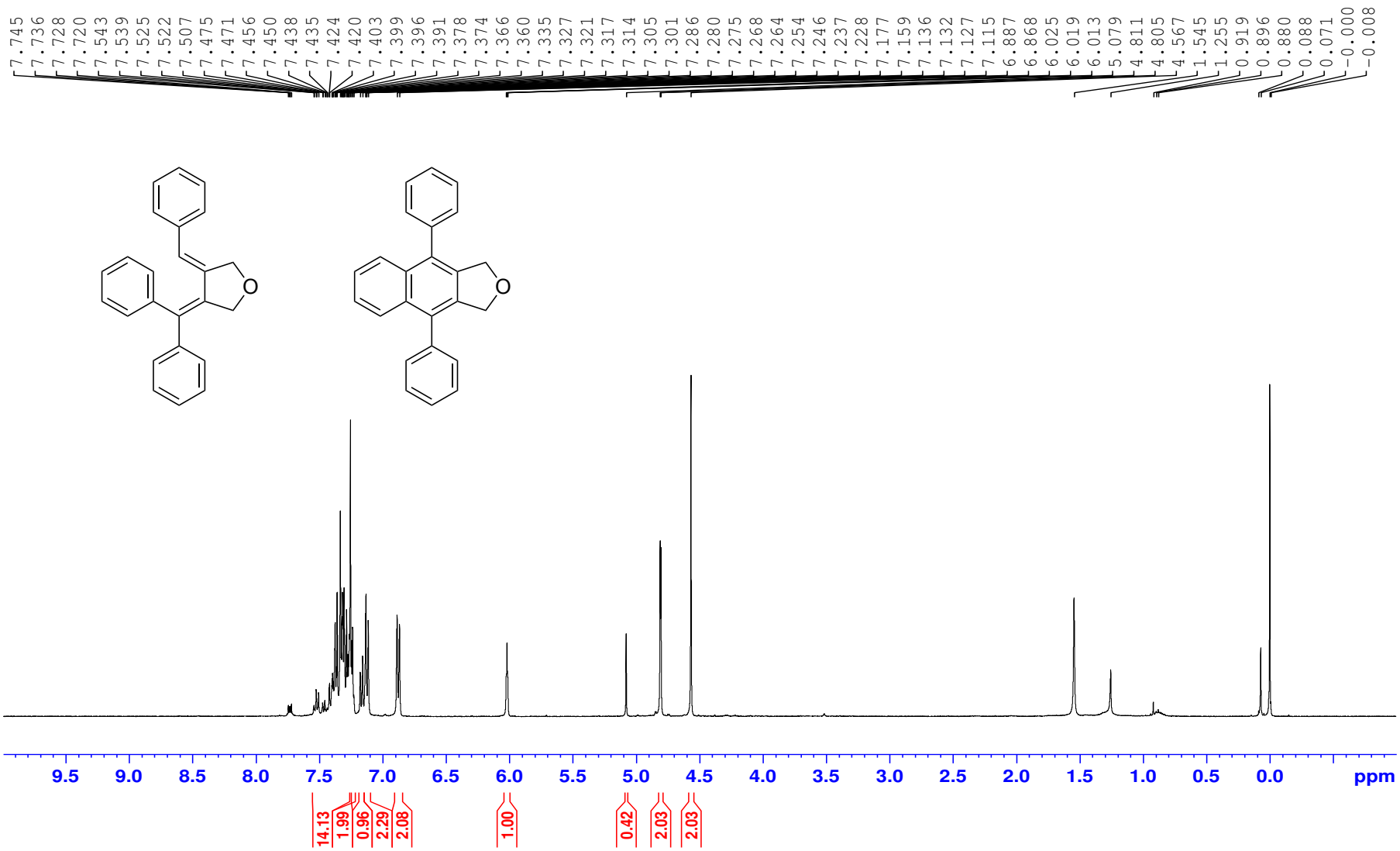
4-Methyl-*N*,*N*-bis({[2-(4-methylbenzenesulfonyl)-4,6,7-triphenyl-2,3-dihydro-1*H*-isoindol-5-yl]methyl})benzene-1-sulfonamide (7a)



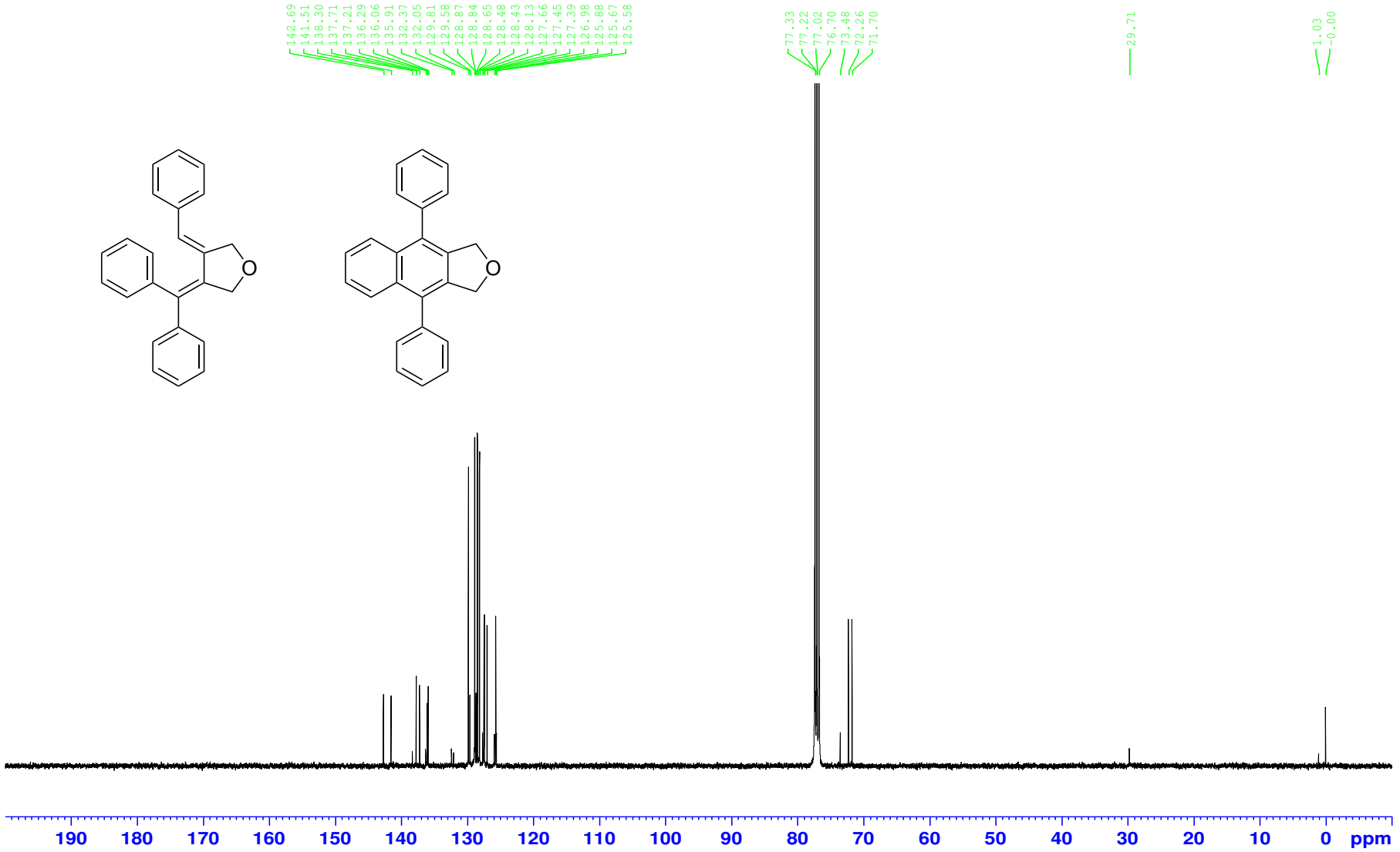
4-Methyl-*N*,*N*-bis({[2-(4-methylbenzenesulfonyl)-4,6,7-triphenyl-2,3-dihydro-1*H*-isoindol-5-yl]methyl})benzene-1-sulfonamide (7a)



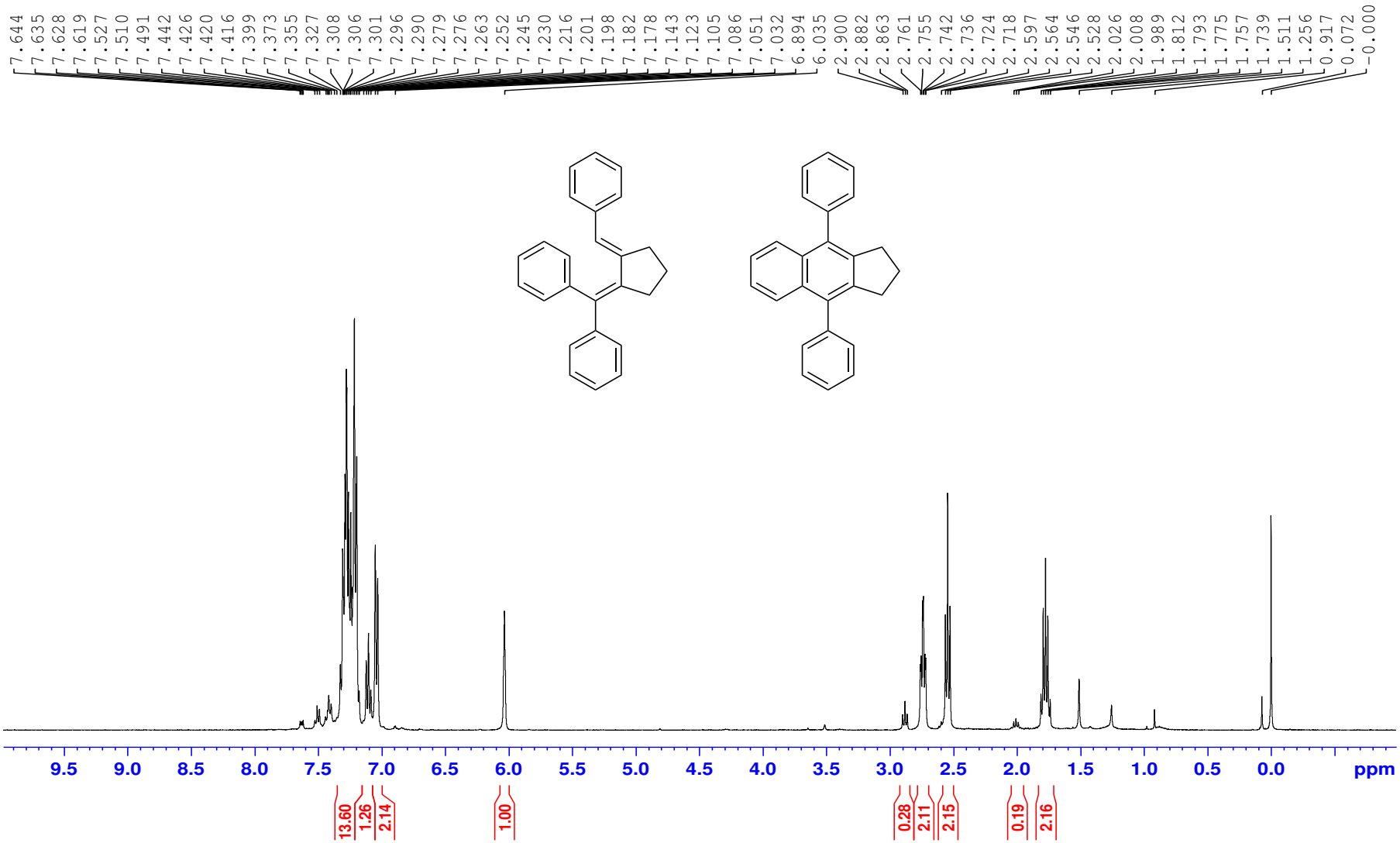
(4*Z*)-3-(Diphenylmethylidene)-4-(phenylmethylidene)oxolane (4ab)
4,9-Diphenyl-1*H*,3*H*-naphtho[2,3-*c*]furan (5ab)
4ab/5ab = 91:9



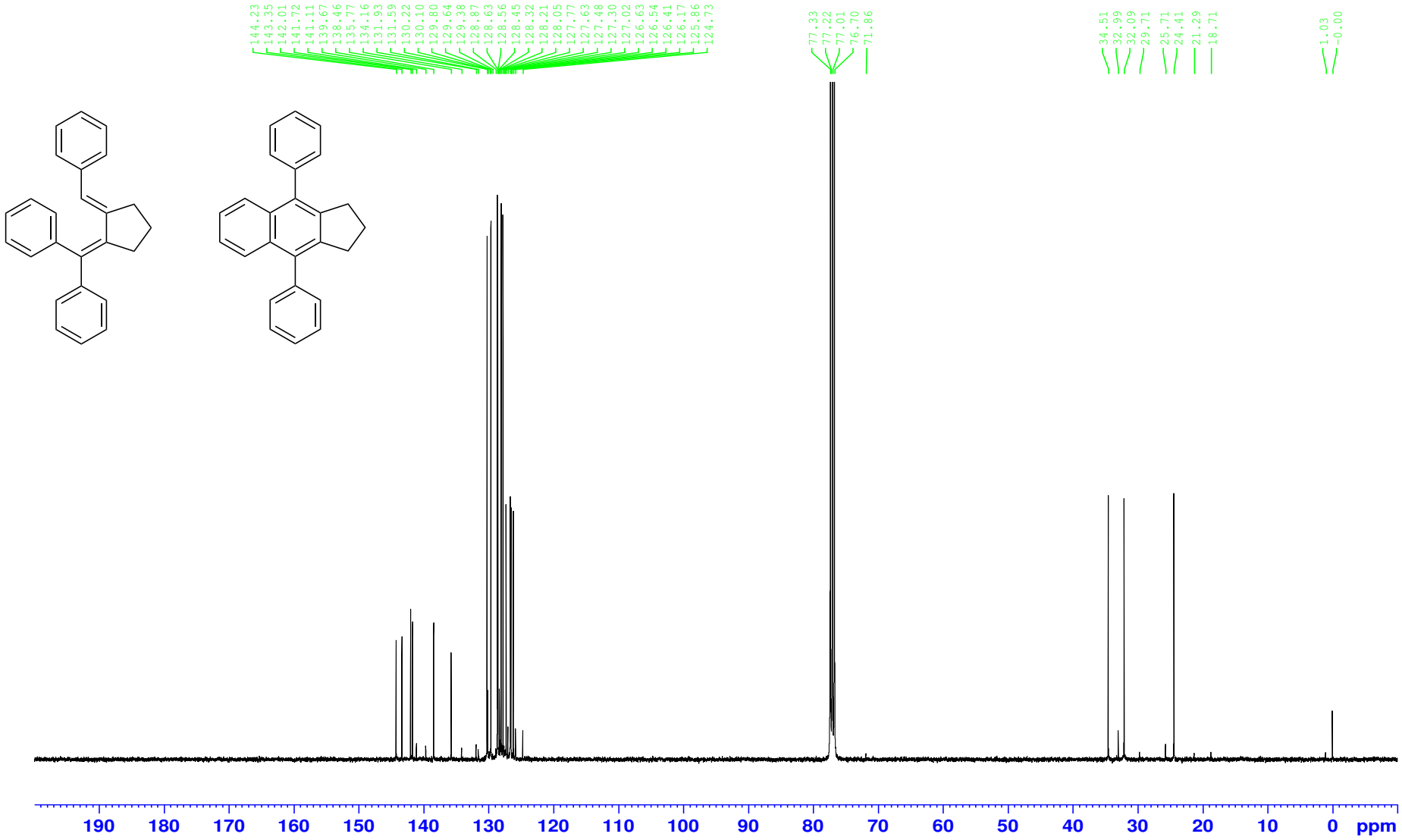
(4*Z*)-3-(Diphenylmethylidene)-4-(phenylmethylidene)oxolane (4ab)
4,9-Diphenyl-1*H*,3*H*-naphtho[2,3-*c*]furan (5ab)
4ab/5ab = 91:9



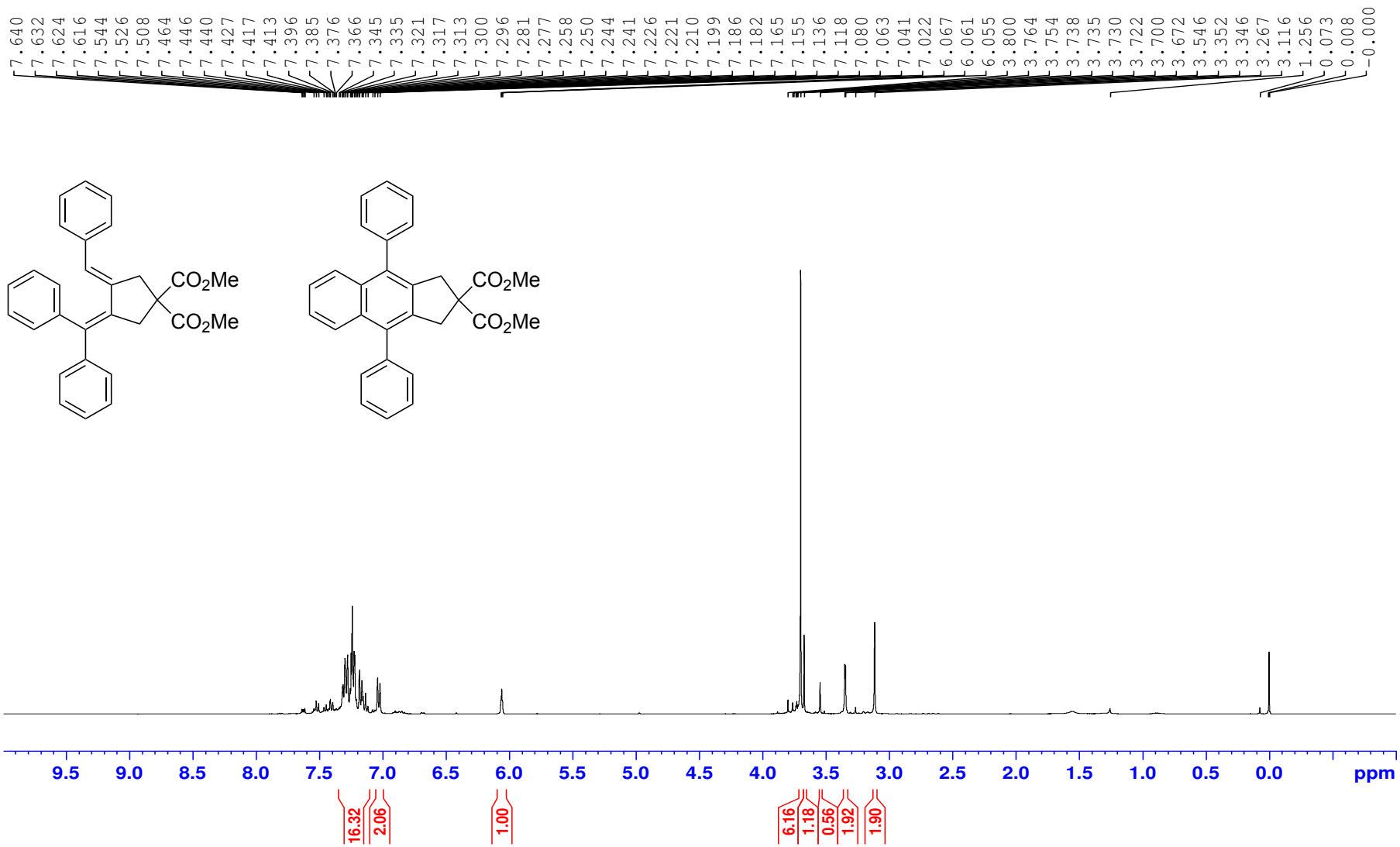
{[(1*E*)-2-(Diphenylmethylidene)cyclopentylidene]methyl}benzene (4ac)
{9-Phenyl-1*H*,2*H*,3*H*-cyclopenta[*b*]naphthalen-4-yl}benzene (5ac)
4ac/5ac = 94:6



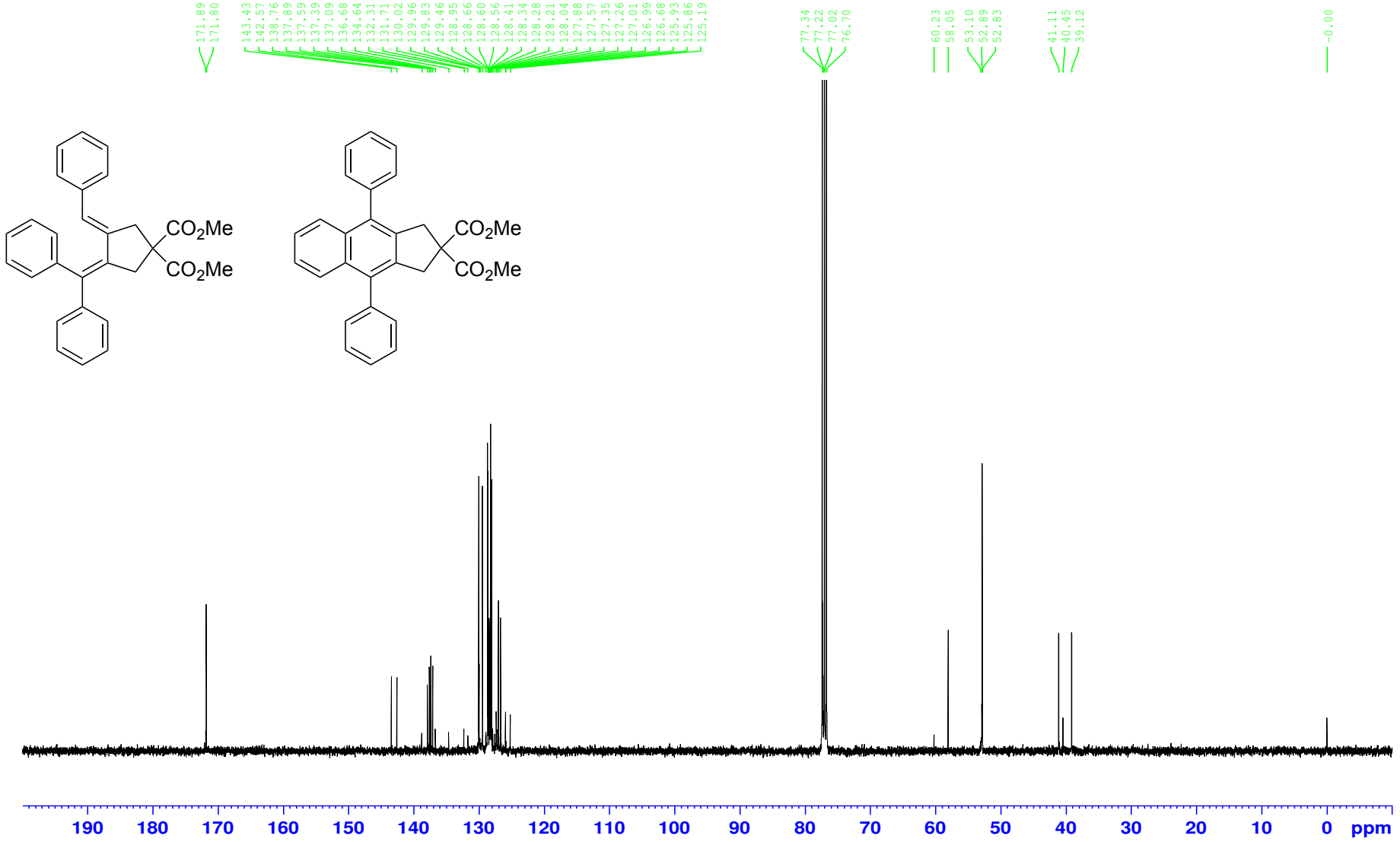
{[(1*E*)-2-(Diphenylmethylidene)cyclopentylidene]methyl}benzene (4ac)
{9-Phenyl-1*H*,2*H*,3*H*-cyclopenta[*b*]naphthalen-4-yl}benzene (5ac)
4ac/5ac = 94:6



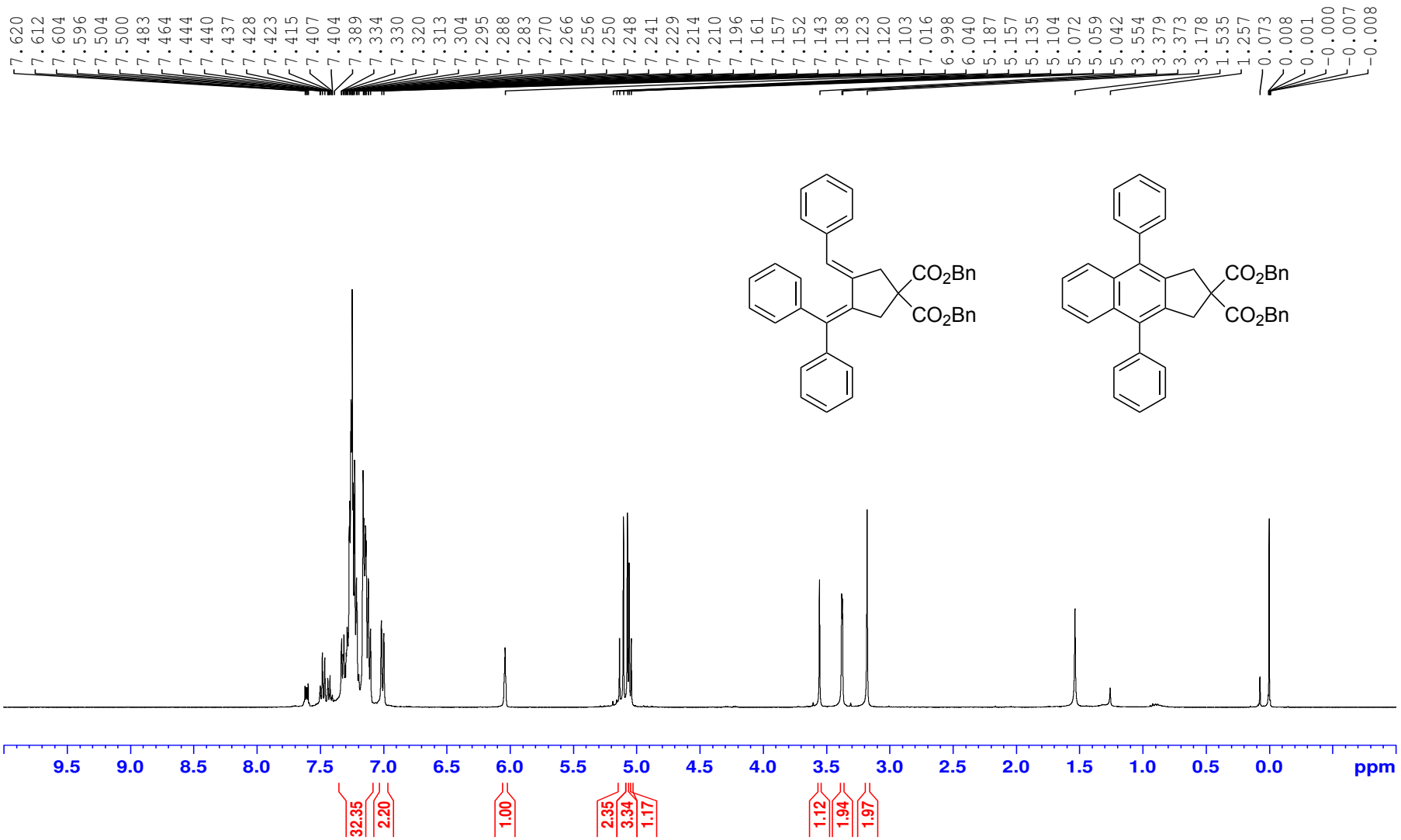
1,1-Dimethyl (4*E*)-3-(diphenylmethylidene)-4-(phenylmethylidene)cyclopentane-1,1- dicarboxylate (4ad)
2,2-Dimethyl 4,9-diphenyl-1*H*,2*H*,3*H*-cyclopenta[*b*]naphthalene-2,2- dicarboxylate (5ad)
4ad/5ad = 90:10



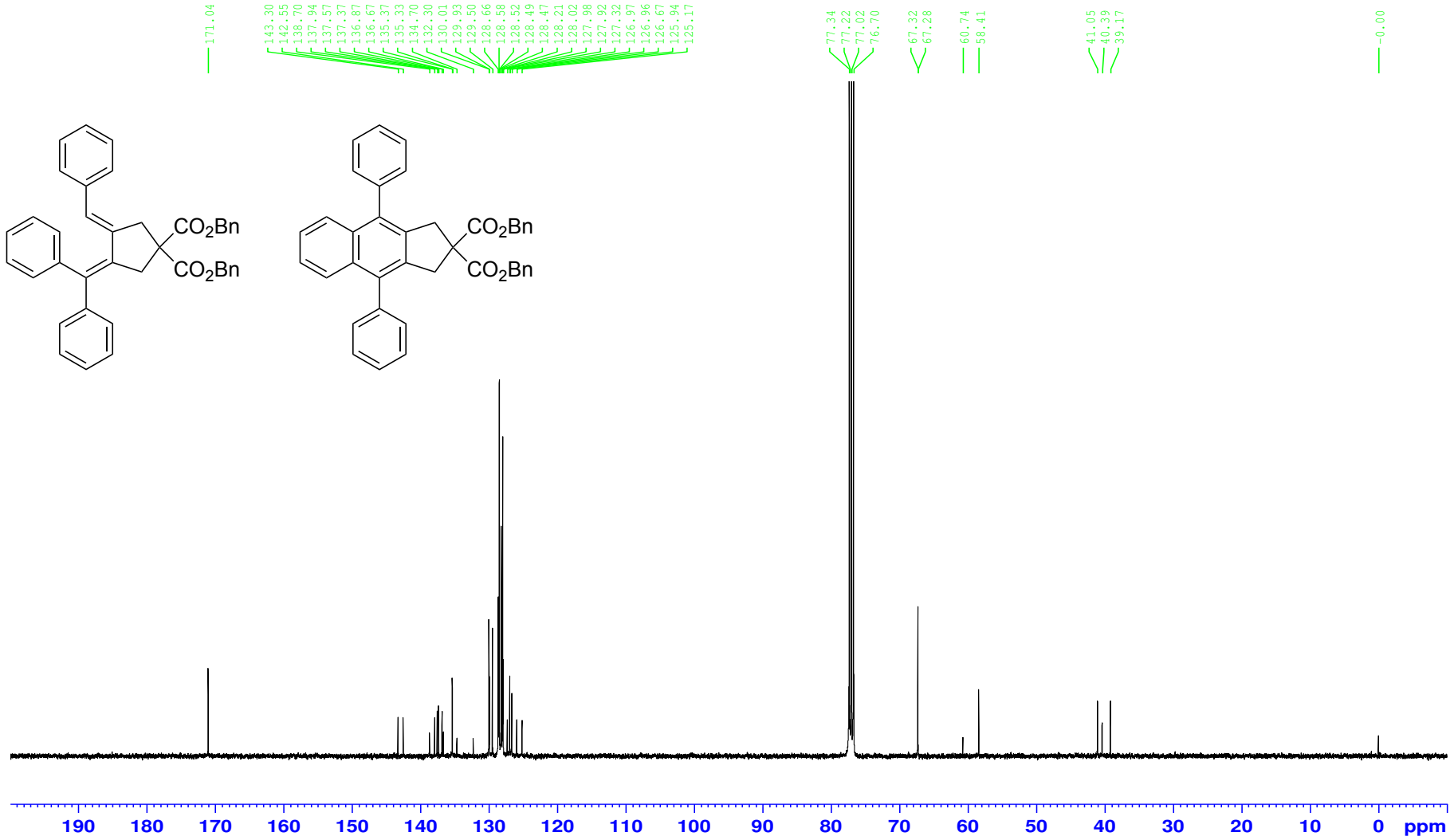
1,1-Dimethyl (4*E*)-3-(diphenylmethylidene)-4-(phenylmethylidene)cyclopentane-1,1- dicarboxylate (4ad)
2,2-Dimethyl 4,9-diphenyl-1*H*,2*H*,3*H*-cyclopenta[*b*]naphthalene-2,2- dicarboxylate (5ad)
4ad/5ad = 90:10



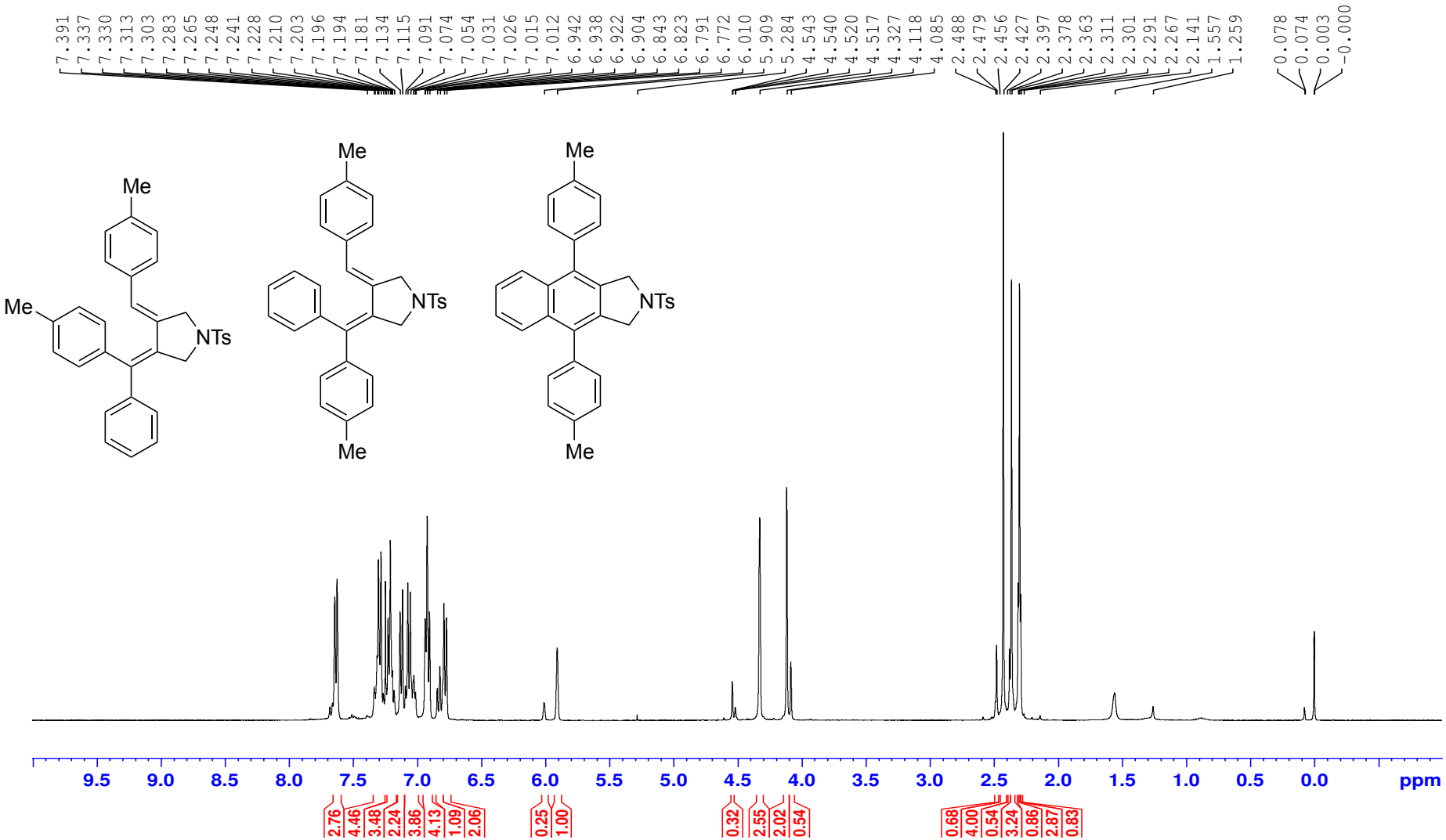
1,1-Dibenzyl (4*E*)-3-(diphenylmethylidene)-4-(phenylmethylidene)cyclopentane-1,1- dicarboxylate (4ae)
2,2-Dibenzyl 4,9-diphenyl-1*H*,2*H*,3*H*-cyclopenta[*b*]naphthalene-2,2- dicarboxylate (5ae)
4ae/5ae = 80:20



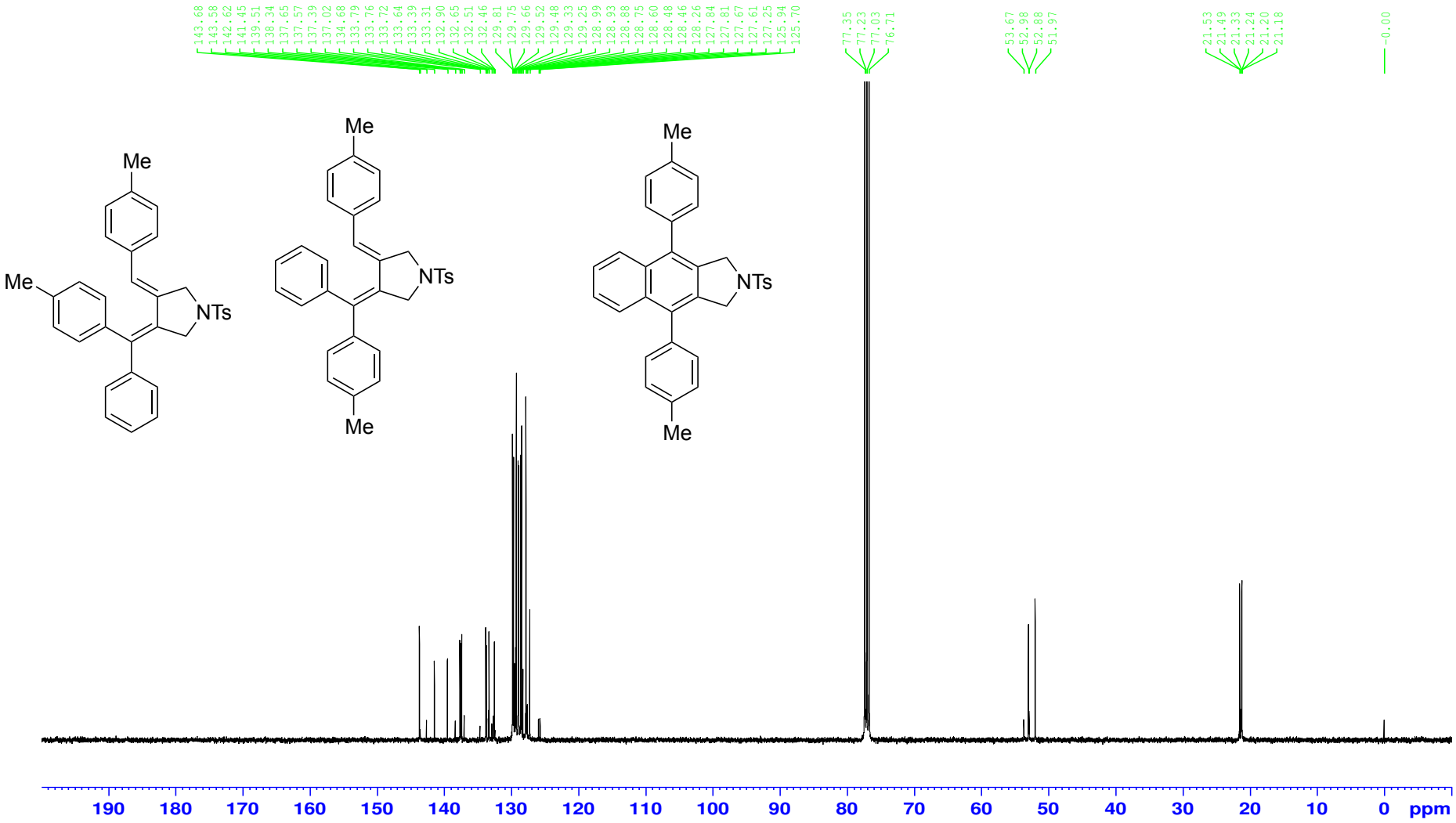
1,1-Dibenzyl (4*E*)-3-(diphenylmethylidene)-4-(phenylmethylidene)cyclopentane-1,1- dicarboxylate (4ae)
2,2-Dibenzyl 4,9-diphenyl-1*H*,2*H*,3*H*-cyclopenta[*b*]naphthalene-2,2- dicarboxylate (5ae)
4ae/5ae = 80:20



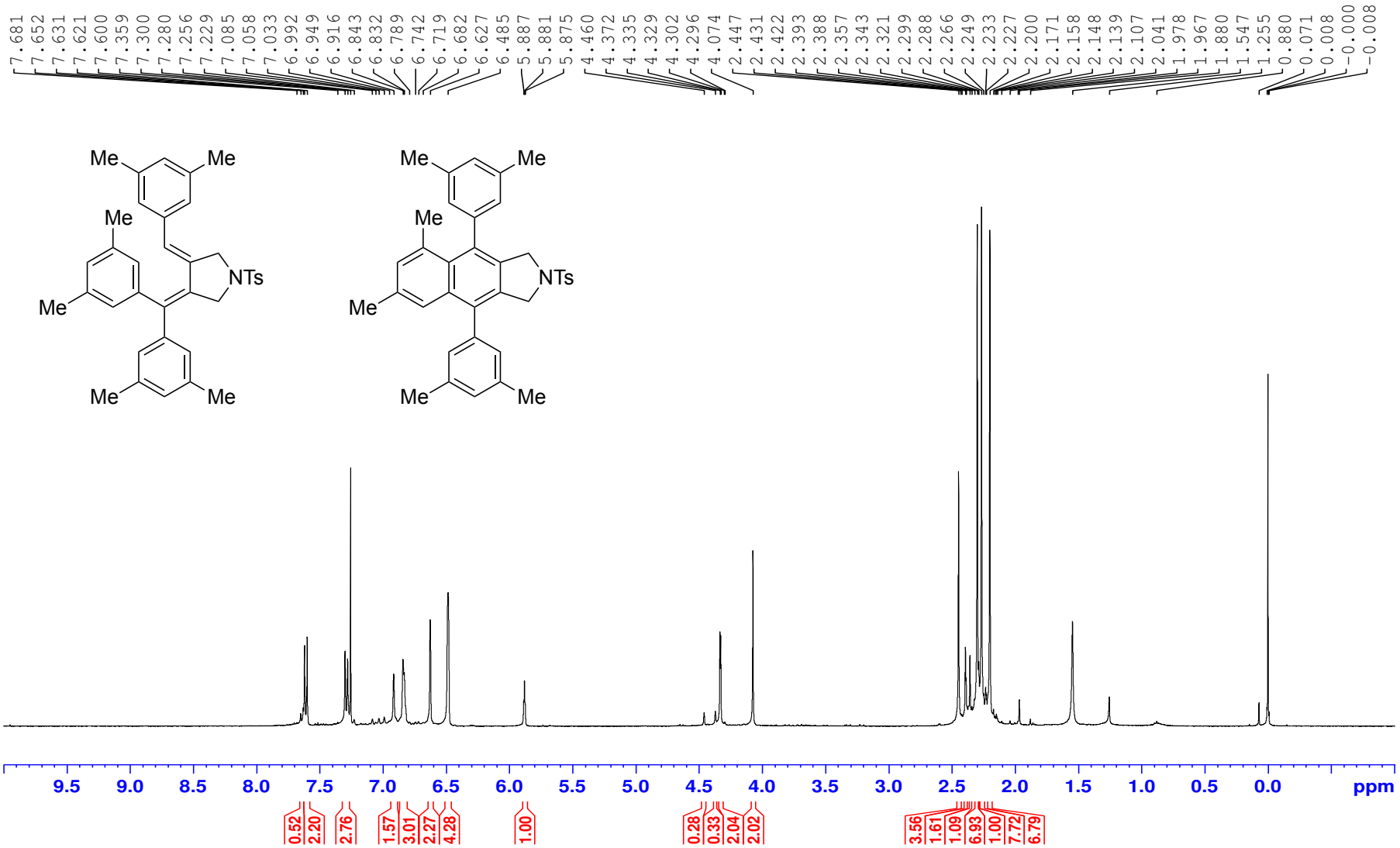
(4*Z*)-1-(4-Methylbenzenesulfonyl)-3-[(4-methylphenyl)(phenyl)methylidene]-4-[(4-methylphenyl)methylidene]pyrrolidine (4af)
6-Methyl-2-(4-methylbenzenesulfonyl)-4-(4-methylphenyl)-9-phenyl-1*H*,2*H*,3*H*-benzo[*f*]isoindole (5af)
4af/5af = 92:8, 4af: *E*/*Z* = 20:80



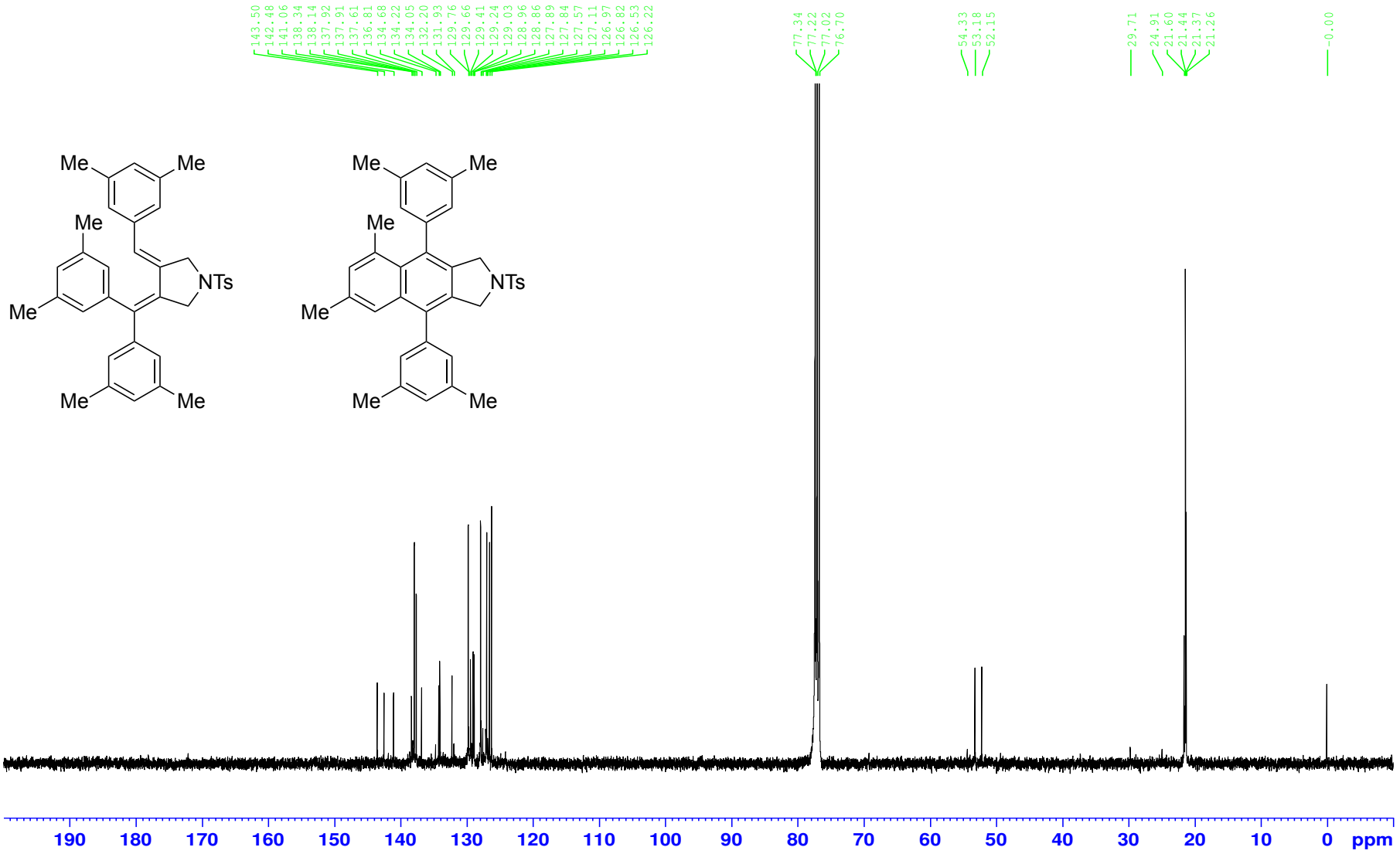
(4*Z*)-1-(4-Methylbenzenesulfonyl)-3-[(4-methylphenyl)(phenyl)methylidene]-4-[(4-methylphenyl)methylidene]pyrrolidine (4af)
6-Methyl-2-(4-methylbenzenesulfonyl)-4-(4-methylphenyl)-9-phenyl-1*H*,2*H*,3*H*-benzo[*f*]isoindole (5af)
4af/5af = 92:8, 4af: *E*/*Z* = 20:80



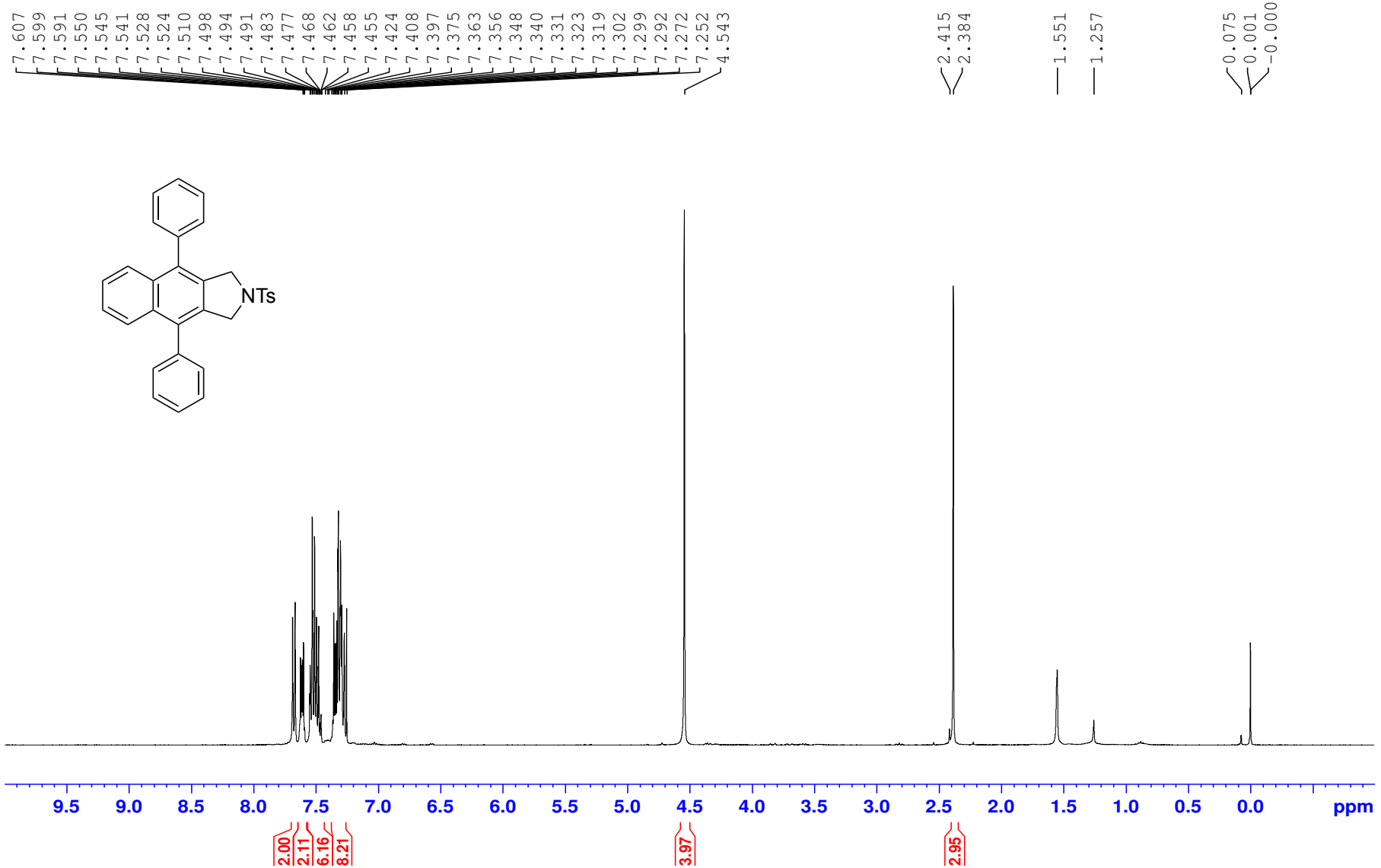
(4*Z*)-3-[Bis(3,5-dimethylphenyl)methylidene]-4-[(3,5-dimethylphenyl)methylidene]-1-(4-methylbenzenesulfonyl)pyrrolidine (4bg)
4,9-Bis(3,5-dimethylphenyl)-5,7-dimethyl-2-(4-methylbenzenesulfonyl)-1*H*,2*H*,3*H*-benzo[*f*]isoindole (5bg)
4bg/5bg = 87:13



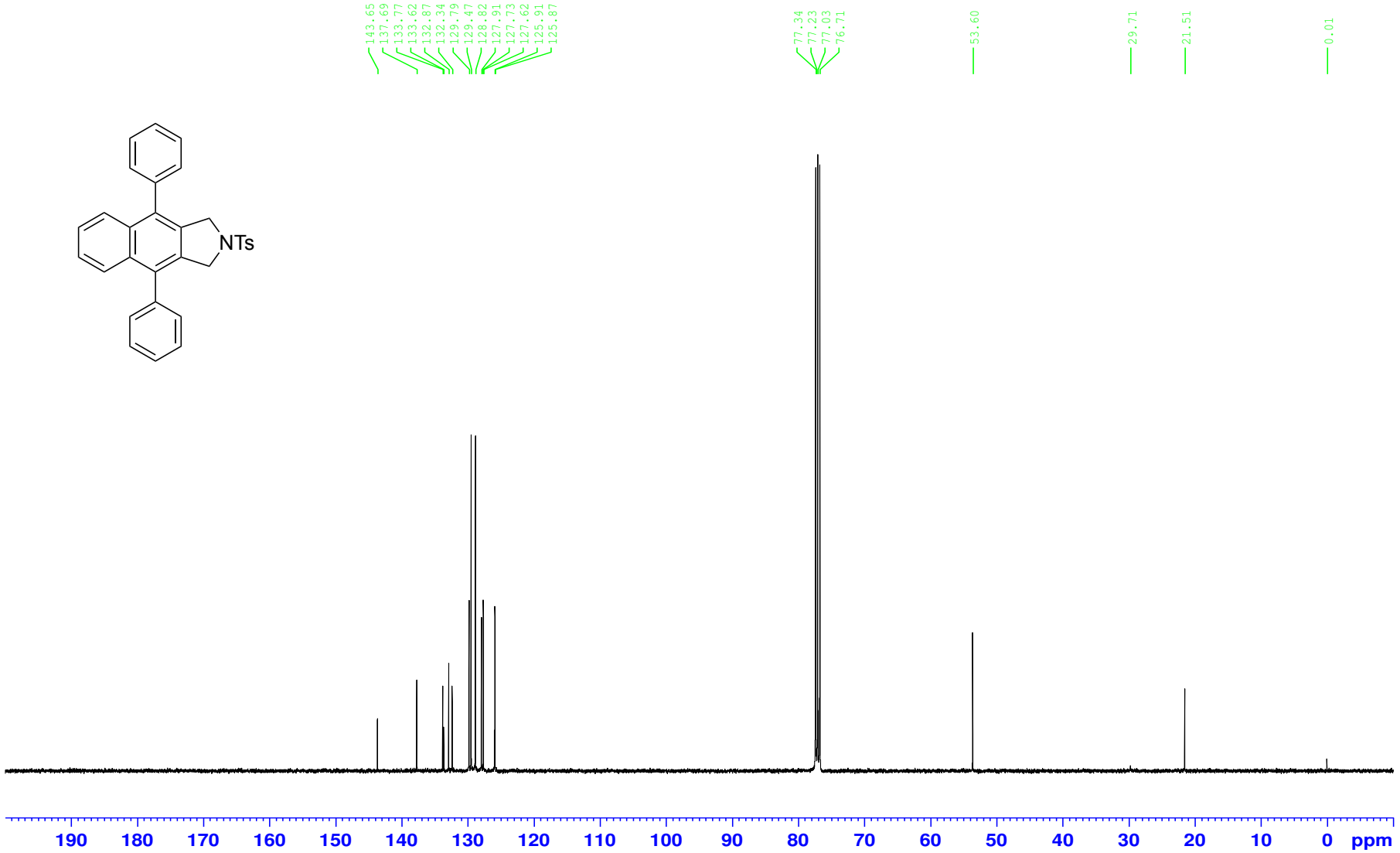
(4*Z*)-3-[Bis(3,5-dimethylphenyl)methylidene]-4-[(3,5-dimethylphenyl)methylidene]-1-(4-methylbenzenesulfonyl)pyrrolidine (4bg)
4,9-Bis(3,5-dimethylphenyl)-5,7-dimethyl-2-(4-methylbenzenesulfonyl)-1*H*,2*H*,3*H*-benzo[*f*]isoindole (5bg)
4bg/5bg = 87:13



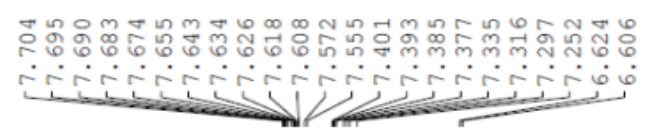
2-(4-Methylbenzenesulfonyl)-4,9-diphenyl-1*H*,2*H*,3*H*-benzo[*f*]isoindole (5aa)

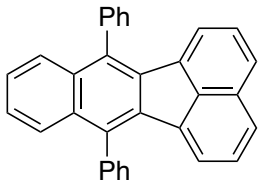


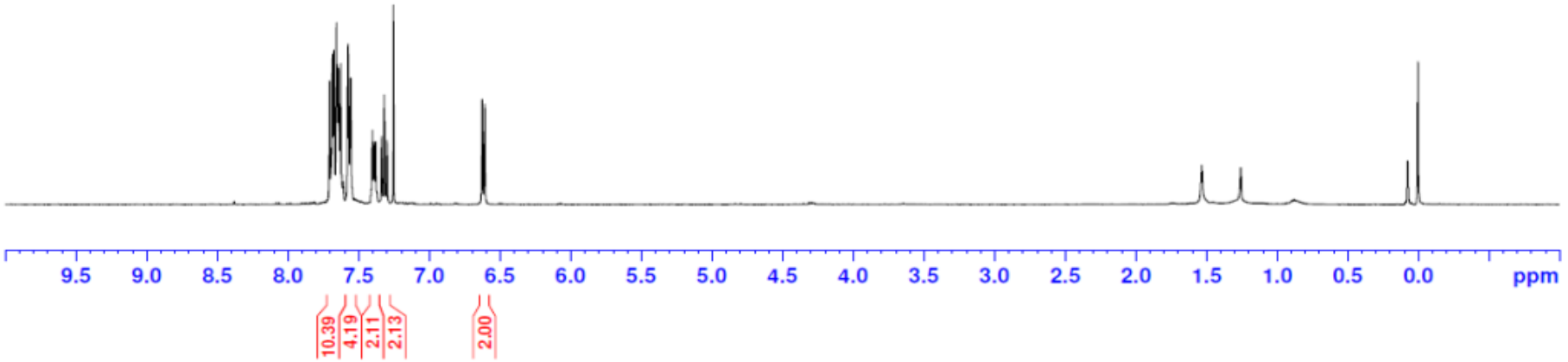
2-(4-Methylbenzenesulfonyl)-4,9-diphenyl-1*H*,2*H*,3*H*-benzo[*f*]isoindole (5aa)



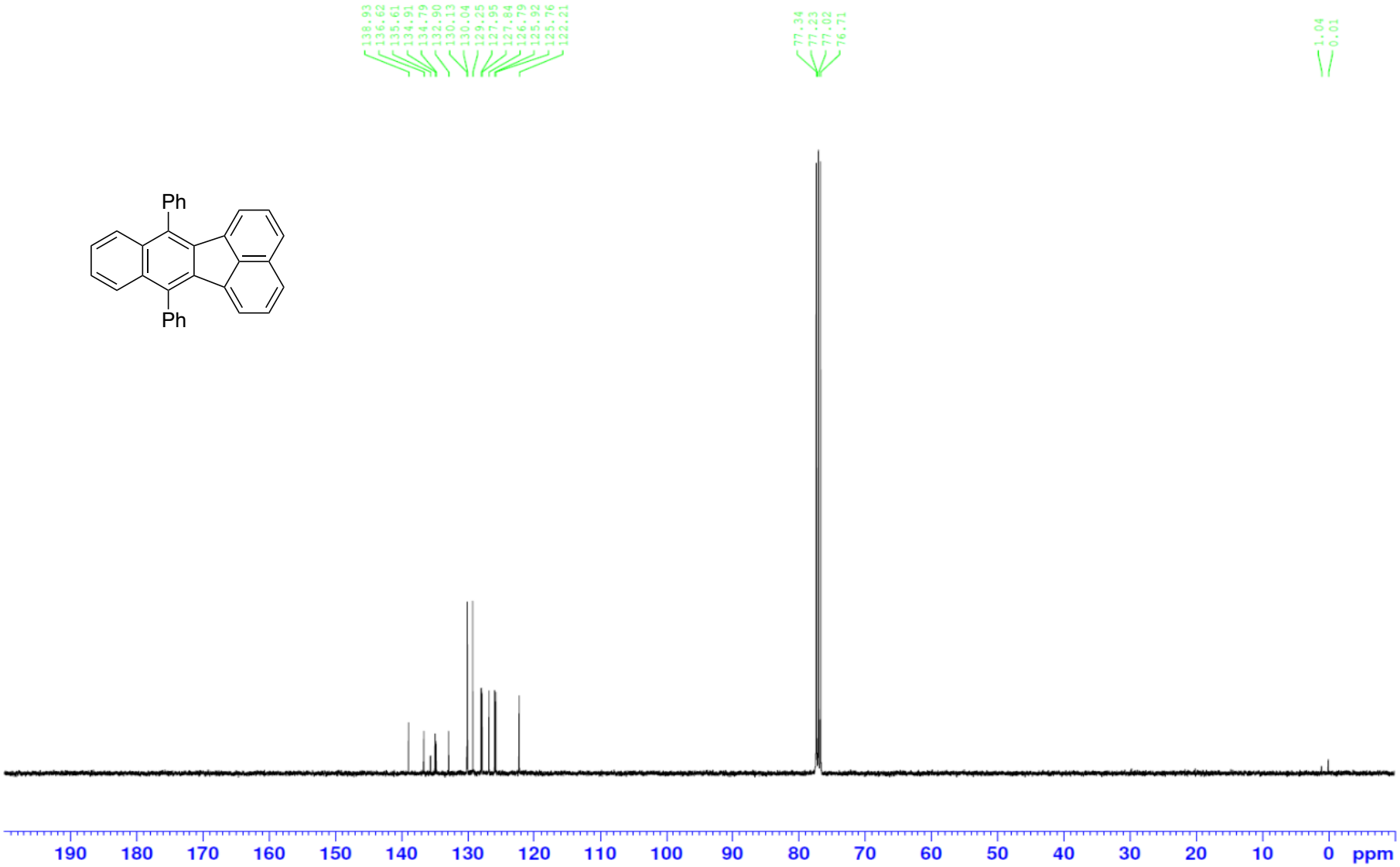
7,12-diphenylbenzo[*k*]fluoranthene (5ah)



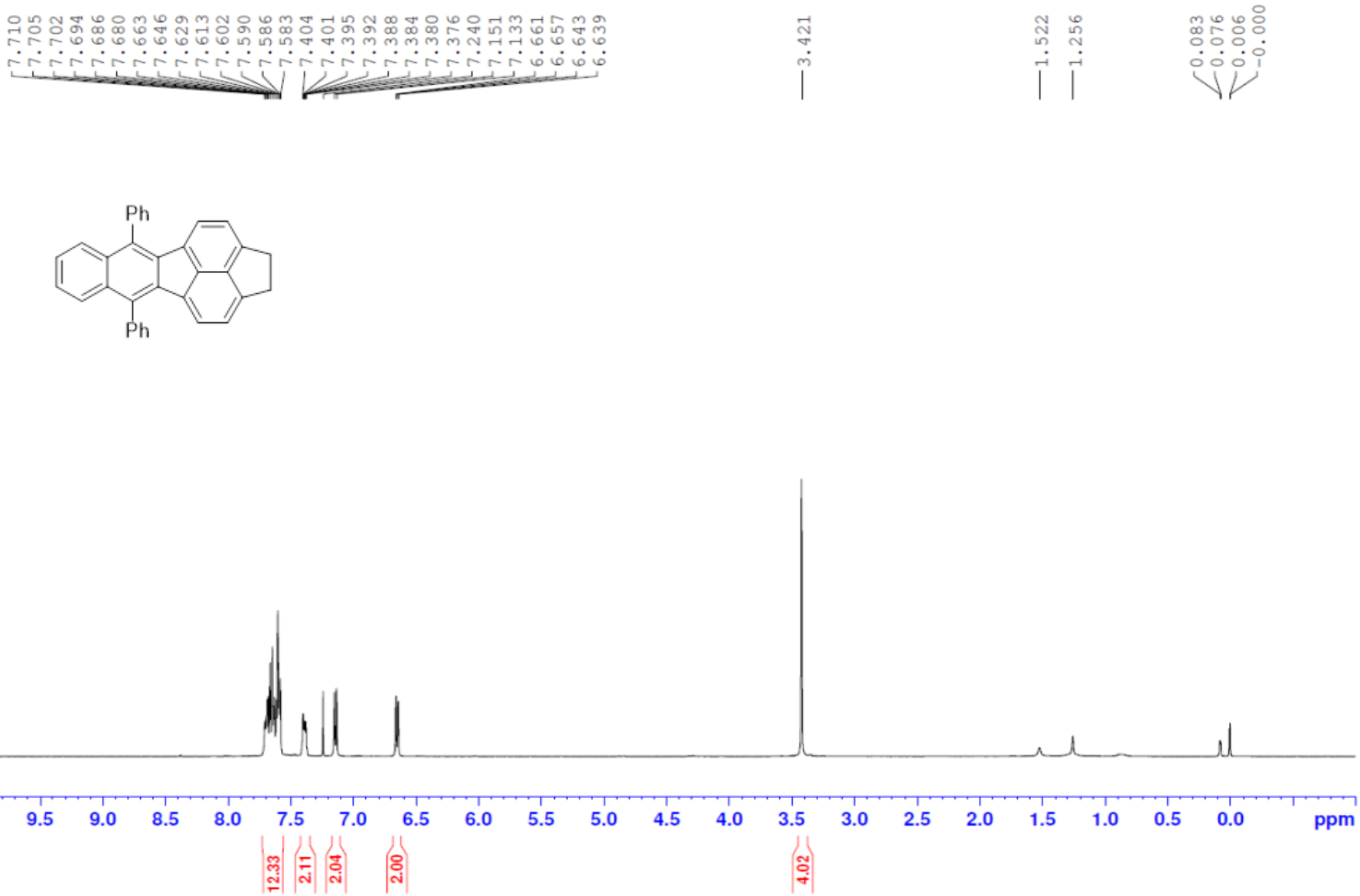




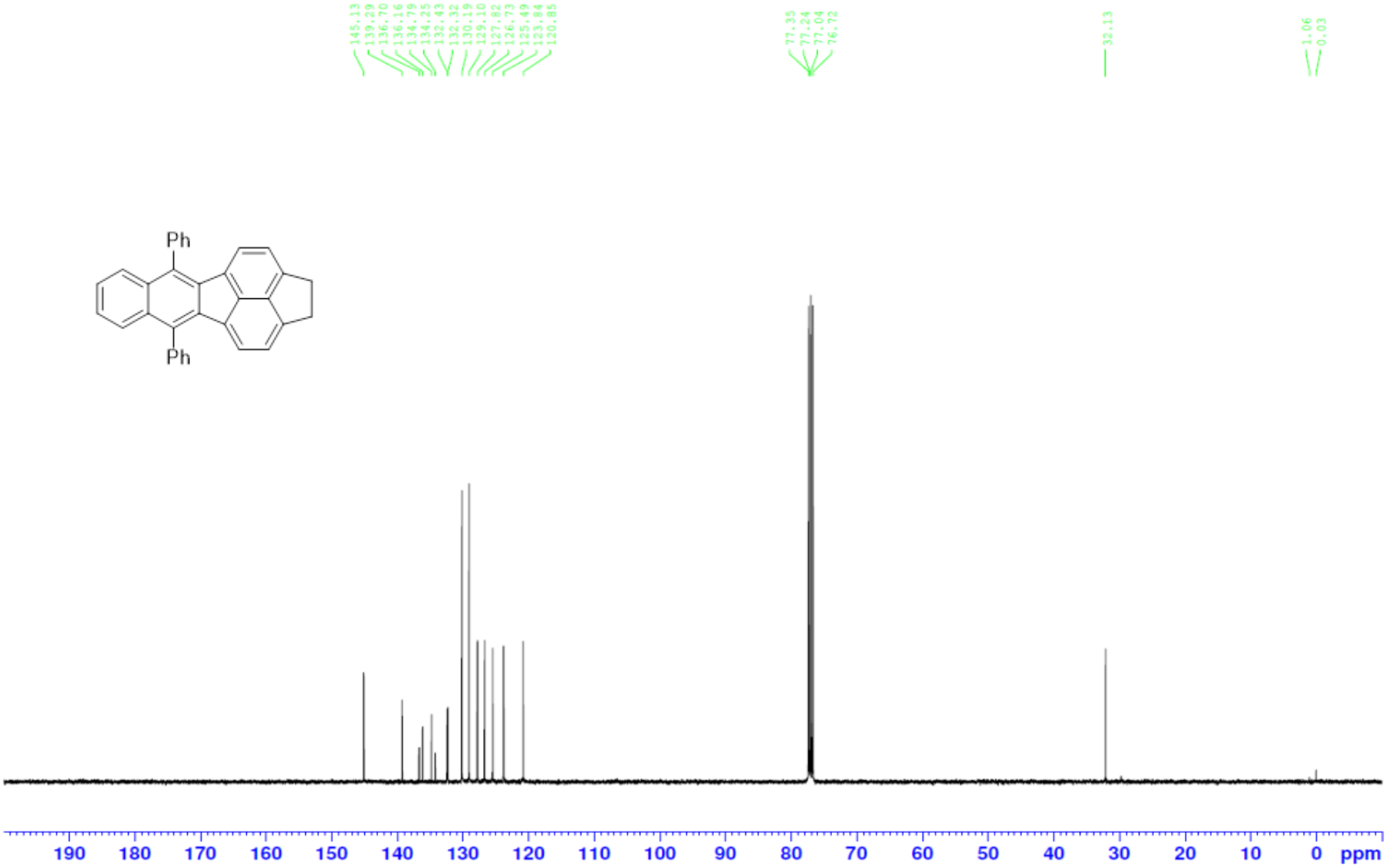
7,12-diphenylbenzo[*k*]fluoranthene (5ah)



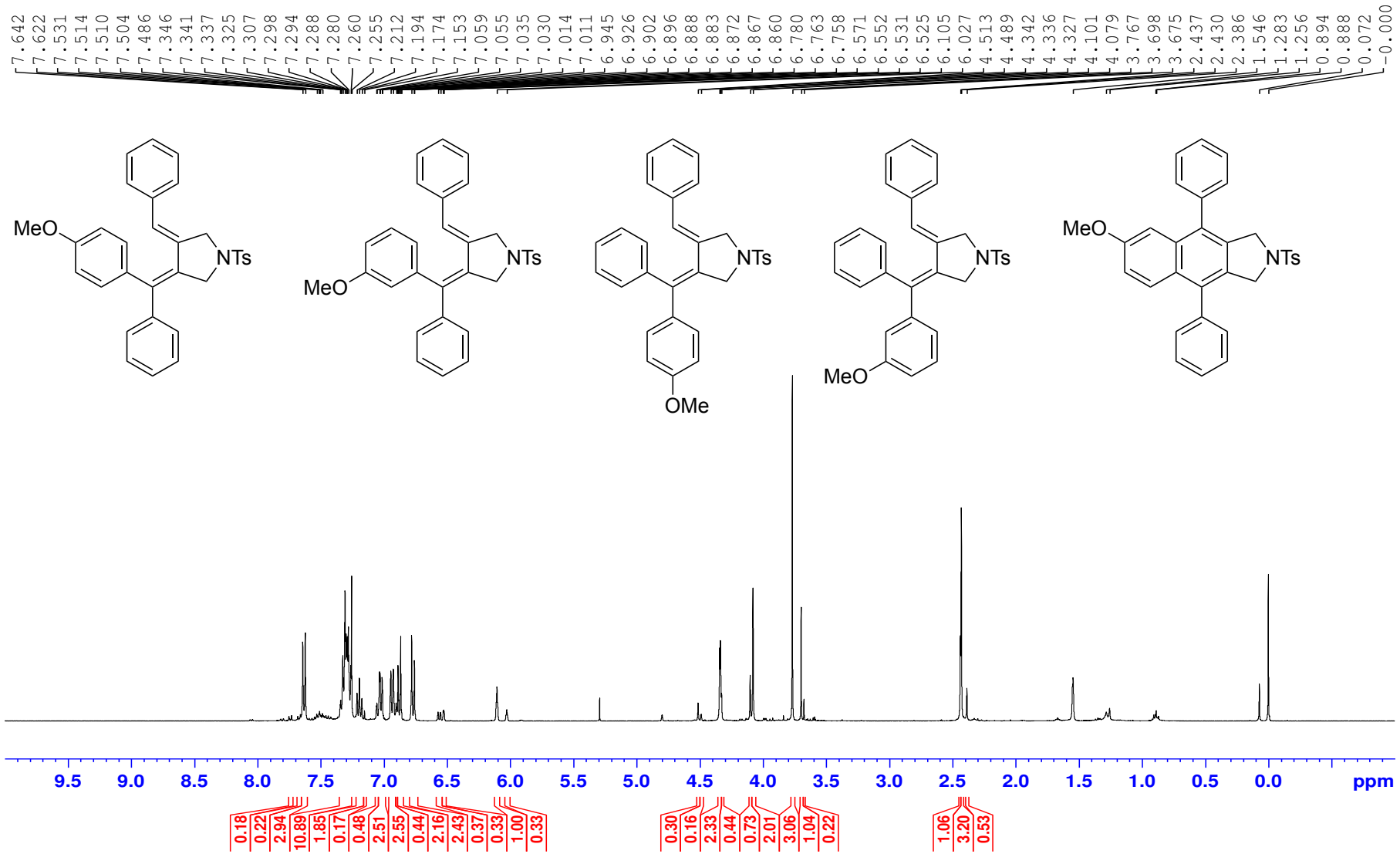
5,10-diphenyl-1,2-dihydrobenzo[*k*]cyclopenta[*cd*]fluoranthene (5ai)



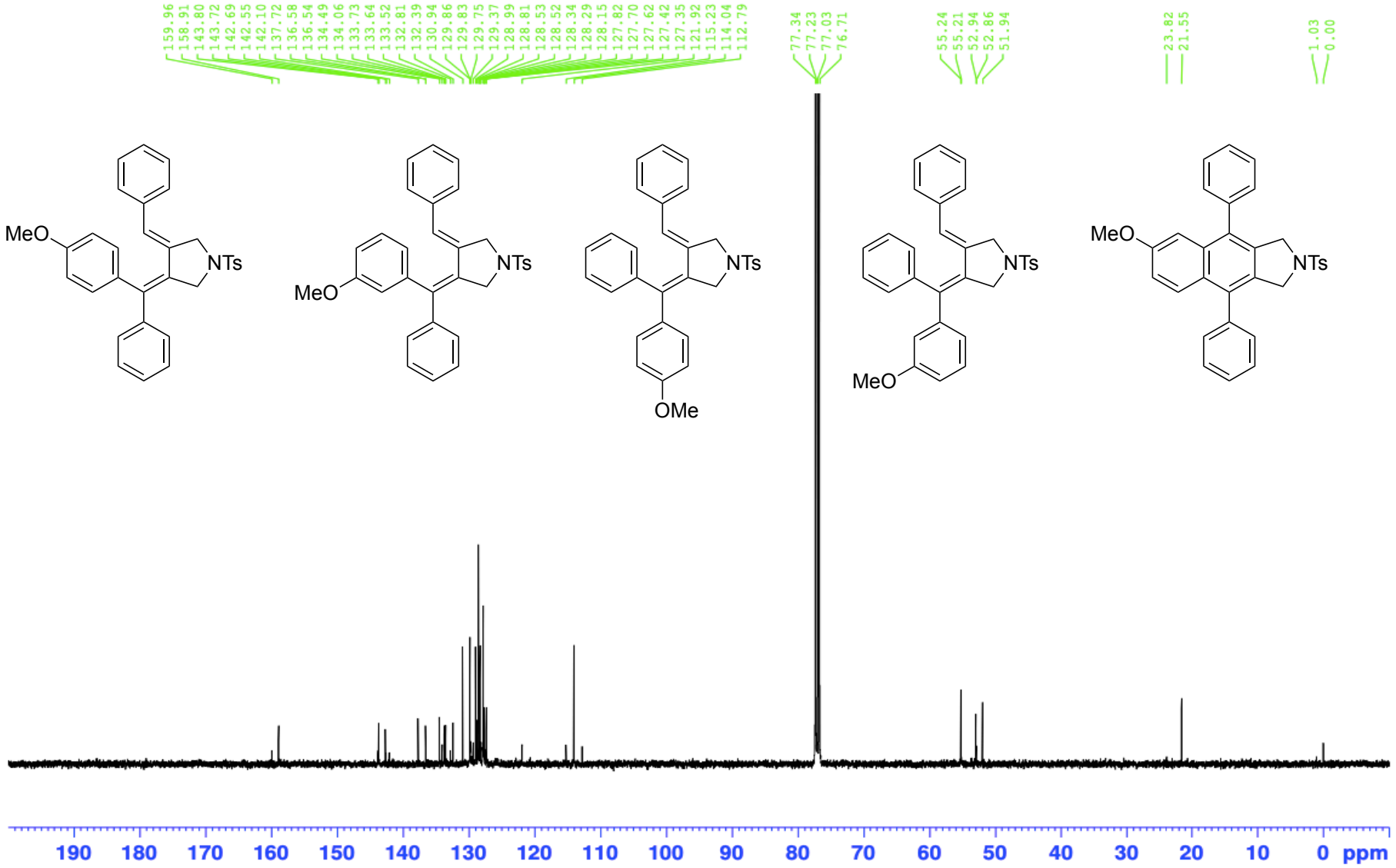
5,10-diphenyl-1,2-dihydrobenzo[*k*]cyclopenta[*cd*]fluoranthene (5ai)



(4*Z*)-3-[(methoxyphenyl)(phenyl)methylidene]-1-(4-methylbenzenesulfonyl)-4-(phenylmethylidene)pyrrolidine (4ca)
6-methoxy-2-(4-methylbenzenesulfonyl)-4,9-diphenyl-1*H*,2*H*,3*H*-benzo[*f*]isoindole (5ca)
4ca/5ca = 92:8, 4ca: 75:25



(4*Z*)-3-[(methoxyphenyl)(phenyl)methylidene]-1-(4-methylbenzenesulfonyl)-4-(phenylmethylidene)pyrrolidine (4ca)
6-methoxy-2-(4-methylbenzenesulfonyl)-4,9-diphenyl-1*H*,2*H*,3*H*-benzo[*f*]isoindole (5ca)
4ca/5ca = 92:8, 4ca: 75:25



(3*Z*)-1-(4-Methylbenzenesulfonyl)-3-[phenyl(²H)methylidene]-4-{phenyl[(2,3,4,5,6-²H₅)phenyl]methylidene}pyrrolidine (4aa-d_6, *E*/*Z* = 81:29)
2-(4-Methylbenzenesulfonyl)-4,9-diphenyl(5,6,7,8-²H₄)-1*H*,2*H*,3*H*-benzo[*f*]isoindole (5aa-d_6)
4aa-d_6/5aa-d_6 = 92:8, 4aa-d_6: *E*/*Z* = 81:29