Supporting Information for:

Atropisomerisation in sterically hindered α,β-disubstituted cyclopentenones derived from an intermolecular cobalt(0)-mediated Pauson-Khand reaction†

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1.0 X-ray diffraction data and information

1.1 General details: Diffraction data were collected at 110 K (unless otherwise specified in the data below) on a Bruker Smart Apex diffractometer with Mo-K_α radiation (λ = 0.71073 Å) using a SMART CCD camera. Diffractometer control, data collection and initial unit cell determination was performed using "SMART".[1] Frame integration and unit-cell refinement was carried out with "SAINT+".[2] Absorption corrections were applied by SADABS.[c] Structures were solved using SHELXS-97 (Sheldrick, 1997),[1] as indicated in the cif files, and refined by full-matrix least squares using SHELXL-97 (Sheldrick, 1997).[2] All non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed using a "riding model" and included in the refinement at calculated positions.

The CCDC reference numbers for compounds **6** and **7β** are 780325 and 780326, respectively.

1.1.1 References

1 "SMART" - control software Bruker SMART Apex X-ray Diffractometer. v5.625, Bruker-AXS GMBH, Karlsruhe, Germany.

2 "SAINT+" - integration software for Bruker SMART detectors. v6.45, Bruker-AXS GMBH, Karlsruhe, Germany.

3 "SADABS" - program for absorption correction. v2.10. G. M. Sheldrick, Bruker AXS Inc., Madison, Wisconsin, USA, 2007.

4 "SHELXS-97" - program for structure solution. G. M. Sheldrick, University of Göttingen, Göttingen, Germany, 1997.

5 "SHELXL-97" - program for the Refinement of Crystal Structures. G. M. Sheldrick, University of Göttingen, Göttingen, Germany, 1997.

1.2 X-ray structures of 6 and 7β

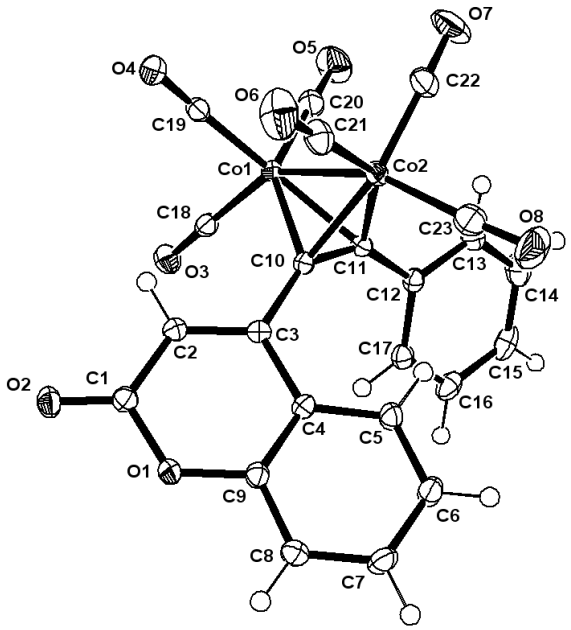


Figure S1. X-ray crystal structure of **6** (determined at 110 K). Thermal ellipsoids are shown at 50% probability.

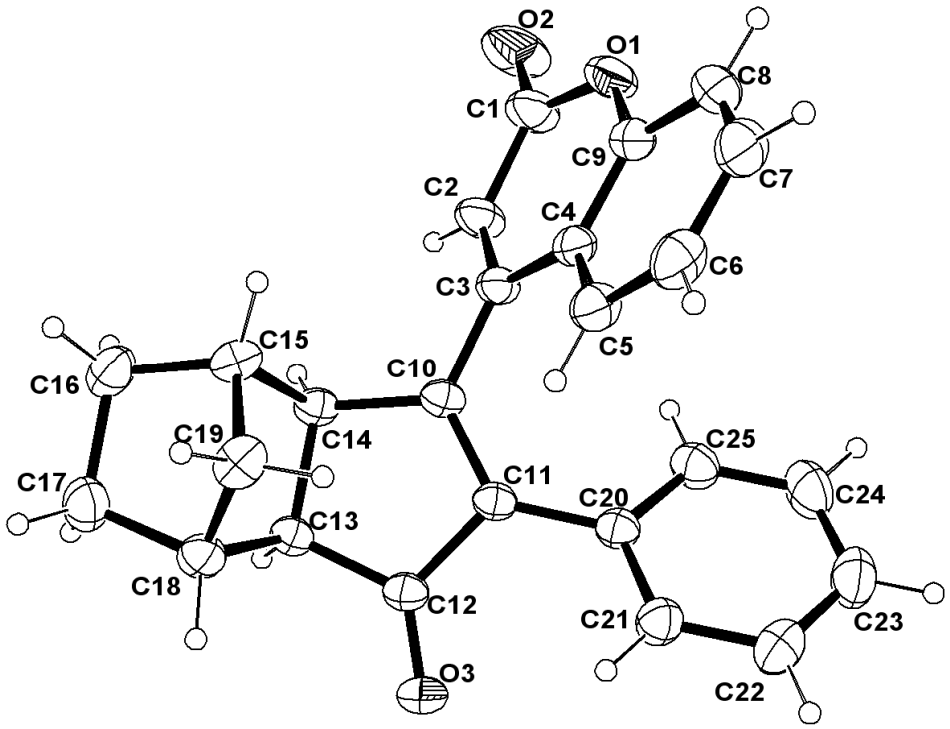


Figure S2. X-ray crystal structure of the major regioisomeric product **7β** (determined at 298 K). Thermal ellipsoids are shown at 30% probability.

Table S1 Key X-ray -data for **6** and **7β.**

Compound reference	ijf0629m	ijf0810a
Chemical formula	$C_{23}H_{10}Co_2O_8$	$C_{25}H_{20}O_3$
Formula Mass	532.17	368.41
Crystal system	Triclinic	Monoclinic
a/Å	8.6456(6)	13.6217(8)
b/Å	8.9910(6)	12.1491(7)
c/Å	14.7003(10)	12.2859(7)
α/°	80.2050(10)	90.00
β/°	74.6770(10)	111.6790(10)
γ/°	73.2410(10)	90.00
Unit cell volume/Å^3	1049.79(12)	1889.40(19)
Temperature/K	110(2)	298(2)
Space group	$P\bar{1}$	*P2(1)/c*
No. of formula units per unit cell, *Z*	2	4
No. of reflections measured	10916	19047
No. of independent reflections	5160	4702
R_{int}	0.0226	0.0258
Final R_1 values ($I > 2\sigma(I)$)	0.0290	0.0464
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.0709	0.1106
Final R_1 values (all data)	0.0346	0.0692
Final $wR(F^2)$ values (all data)	0.0737	0.1213

2.0 Cartesian coordinates of the optimized geometries

2.1 Raw data

$7\beta_A$

E = −1190.0622892 a.u.

C	−1.86677500	3.07658800	−1.85857800
C	−1.87679700	4.30371700	−1.18535200
C	−1.00044800	4.51067400	−0.11419200
C	−0.12373200	3.50010500	0.28834100
C	−0.11623500	2.25170300	−0.37058000
C	−0.99498300	2.06197500	−1.45736700
C	0.80480800	1.18529700	0.07143500
C	2.17690800	1.47583900	0.59519400
C	2.85450900	0.16529400	0.97327100
C	1.81633100	−0.94355200	0.61230200
C	0.60794900	−0.16581000	0.09123200
C	−0.63646500	−0.90348200	−0.24987600
C	−0.73073000	−1.62623500	−1.40531400
C	−1.89792100	−2.41120300	−1.76393800
O	−2.96147700	−2.39938200	−0.82082900
C	−1.75233300	−0.91363500	0.69337900
C	−2.89250000	−1.67866000	0.36429500
C	−1.76091800	−0.21213900	1.91925000
C	−2.86086600	−0.27754300	2.76818800
C	−3.98294500	−1.04788400	2.41256800
C	−4.00238600	−1.75047000	1.20974200
O	−2.04657100	−3.07433600	−2.78924600
O	2.69833800	2.59761300	0.71144700
C	4.09309000	−0.17871000	0.08851200
C	2.59226200	−1.81358200	−0.43654700
C	4.74694900	−1.45679300	0.68253000
C	3.70347200	−2.57998800	0.34009200
C	3.42194300	−0.74313200	−1.19405500
H	3.12218500	0.19367300	2.03532900
H	1.51444400	−1.56433300	1.46559300
H	−2.53158900	2.91079500	−2.70030900
H	−2.55384200	5.09230700	−1.49802100
H	−0.99439000	5.46262900	0.40711800
H	0.56812400	3.67867900	1.10098500
H	−0.98320900	1.12531800	−2.00161000
H	0.06925000	−1.63772000	−2.13366900
H	−0.90052900	0.38877700	2.18829300
H	−2.85369300	0.26934900	3.70439700
H	−4.83983700	−1.09627300	3.07581700
H	−4.85022000	−2.35192700	0.90617600
H	4.93110000	−1.36367000	1.75831300
H	5.71078300	−1.65296500	0.19965500
H	3.30988300	−3.07756800	1.23345300
H	4.14689900	−3.35372700	−0.29595400
H	4.14233200	−1.18036800	−1.89315400
H	2.81277400	−0.00974400	−1.73145200
H	4.77102400	0.66730400	−0.04088800
H	1.95305100	−2.46192500	−1.03825200

$7\beta_B$

E = −1190.0607954 a.u.

C	−1.54526000	3.59247400	−1.21087300
C	−1.01653600	4.82514900	−0.81092800
C	0.19648900	4.86154600	−0.11454800
C	0.87501700	3.67829200	0.18763200
C	0.34410400	2.42723500	−0.19435100
C	−0.87205200	2.40708800	−0.90781800
C	1.05735700	1.18308900	0.15891600
C	2.55160000	1.11097900	0.24030500
C	2.95948500	−0.27544700	0.72353600
C	1.62032500	−1.06880900	0.83789500
C	0.54531100	−0.04048700	0.48435300
C	−0.88657600	−0.39852600	0.68349100
C	−1.46055300	−0.14628700	1.89611800
C	−2.82106400	−0.52552300	2.23171700
O	−3.54088100	−1.20271800	1.20631200
C	−1.66686300	−1.06947600	−0.35196400
C	−2.99008600	−1.45340800	−0.04201800
C	−1.19251500	−1.33651500	−1.65603900
C	−2.00127600	−1.97328100	−2.59259400
C	−3.31013400	−2.35769400	−2.24875400
C	−3.80868000	−2.09685700	−0.97430000
O	−3.39483500	−0.33170100	3.30122100
O	3.35010000	2.02161300	−0.03640400
C	3.79525200	−1.08928300	−0.30952700
C	1.84126000	−2.25828200	−0.16044200
C	4.23099100	−2.41142600	0.38019400
C	2.88371000	−3.21136000	0.49581800
C	2.69103500	−1.59503300	−1.27760300
H	3.49240300	−0.17443000	1.67594100
H	1.42193800	−1.46023100	1.84387100
H	−2.47889700	3.55307000	−1.76304200
H	−1.54062800	5.74618900	−1.04543500
H	0.61860400	5.81285000	0.19323700
H	1.82230000	3.71952100	0.70855300
H	−1.28489800	1.46402800	−1.24508800
H	−0.91369200	0.35692900	2.68321400
H	−0.18804800	−1.03004700	−1.92372700
H	−1.62247900	−2.16952500	−3.58943000
H	−3.93908900	−2.85443200	−2.97954000
H	−4.81433700	−2.37163400	−0.68119600
H	4.70093800	−2.23202700	1.35318100
H	4.95671800	−2.94747100	−0.24158900
H	2.62230400	−3.45093200	1.53239700
H	2.93494100	−4.15681800	−0.05528700
H	3.06464400	−2.31671700	−2.01170800
H	2.17943800	−0.78720600	−1.81118000
H	4.60857500	−0.50943000	−0.75025200
H	0.92214800	−2.75817700	−0.47125700

TS-1 ($7\beta_A \rightarrow 7\beta_B$)

E = −1190.04409 a.u.

C	3.93759500	−1.87585000	1.39381800
C	4.67246900	−2.37344800	0.31090700
C	4.35463500	−1.96607600	−0.98907000
C	3.30566400	−1.06768900	−1.20877700

C	2.54737800	-0.57924000	-0.12976600
C	2.88464600	-0.98340200	1.17692800
C	1.48779300	0.43667600	-0.35586600
C	1.95227900	1.81870200	-0.67246400
C	0.75169800	2.73228100	-0.78635500
C	-0.46561800	1.80418400	-0.48858000
C	0.11101400	0.39160800	-0.31492600
C	-0.73877800	-0.83366100	-0.15410900
C	-0.10451800	-2.04186000	0.00570300
C	-0.75158100	-3.32318500	0.18064000
O	-2.15964300	-3.29942200	0.19139100
C	-2.22611300	-0.86414400	-0.18891900
C	-2.86457700	-2.12056700	-0.00591600
C	-3.10743000	0.22598500	-0.40293800
C	-4.49134500	0.07561500	-0.41913100
C	-5.07519400	-1.18326200	-0.21959600
C	-4.25319600	-2.28354100	-0.01389200
O	-0.18646700	-4.40793900	0.32855000
O	3.13684100	2.16520400	-0.81535900
C	0.69602200	3.81507600	0.33239600
C	-1.06249900	2.44843000	0.82044200
C	-0.53737500	4.71861700	0.05545000
C	-1.75071900	3.78046900	0.39957000
C	0.20530200	2.97698500	1.54134500
H	0.72382300	3.18430100	-1.78401400
H	-1.18416600	1.83311300	-1.31117700
H	4.18378400	-2.18138800	2.40556300
H	5.48721100	-3.06981500	0.48009500
H	4.92560500	-2.34141500	-1.83205600
H	3.07241000	-0.74219600	-2.21700900
H	2.31701500	-0.59870400	2.01871200
H	0.96853700	-2.11340300	0.01893500
H	-2.72305700	1.21504000	-0.56231800
H	-5.11613100	0.94583000	-0.58830100
H	-6.15313300	-1.30096000	-0.22952100
H	-4.64652500	-3.28103700	0.13776500
H	-0.56072400	5.07539300	-0.97991600
H	-0.52321200	5.59991700	0.70637000
H	-2.43065000	3.64784500	-0.45031200
H	-2.34087700	4.18357800	1.22977000
H	-0.03575000	3.58746400	2.41802000
H	0.90286300	2.19114100	1.84610800
H	1.63998700	4.35051100	0.45215100
H	-1.69816400	1.77981500	1.40312100

TS-2 ($7\beta_A \rightarrow 7\beta_B$)

E = -1190.0397672 a.u.

C	1.45863100	3.88499800	1.33715300
C	2.03071700	4.53244000	0.23563500
C	1.74945400	4.07950900	-1.05872500
C	0.90739000	2.98029100	-1.25206700
C	0.35317000	2.30478100	-0.14987000
C	0.61913100	2.78342600	1.14678200
C	-0.62420100	1.20371900	-0.35390400
C	-2.01960900	1.69001400	-0.62133200
C	-2.94816800	0.50951300	-0.77013700
C	-2.03571800	-0.72082300	-0.51362300
C	-0.59524500	-0.17248800	-0.34110700
C	0.49331200	-1.20920700	-0.23475700
C	0.07381800	-2.51397400	-0.37193700
C	0.90880300	-3.69500900	-0.31275500
O	2.27245100	-3.46809000	-0.08268500
C	1.94959200	-1.02113700	-0.02347300
C	2.77310600	-2.17732900	0.04722100
C	2.62885700	0.20867600	0.11231200
C	4.00486000	0.28343800	0.31045700
C	4.77786600	-0.88373200	0.38268300
C	4.15417400	-2.11877000	0.24848000
O	0.51670500	-4.85753900	-0.43927500
O	-2.35204800	2.88344000	-0.69975700
C	-4.03019800	0.43475100	0.34946200
C	-2.68167500	-1.35128300	0.77817200
C	-4.94791900	-0.77958500	0.03595300
C	-4.02084900	-2.01239600	0.33763100
C	-3.19540500	-0.10211800	1.54096300
H	-3.40233700	0.52035300	-1.76720100
H	-2.07789800	-1.42528400	-1.34899800
H	1.66059100	4.23948800	2.34284900
H	2.68118300	5.38832500	0.38414800
H	2.17797000	4.58586100	-1.91764000
H	0.68230000	2.63838800	-2.25692500
H	0.17379700	2.28544600	2.00217100
H	-0.95769900	-2.76869800	-0.53812800
H	2.07640100	1.12495200	0.06012500
H	4.47170300	1.25722900	0.40808100
H	5.84981800	-0.82913300	0.53830500
H	4.70129100	-3.05238000	0.29057200
H	-5.30794600	-0.76566300	-0.99847400
H	-5.82733000	-0.77641200	0.68957900
H	-3.89271400	-2.66679000	-0.53195200
H	-4.42737800	-2.62508400	1.14952000
H	-3.80743400	-0.36357300	2.41058600
H	-2.40094800	0.57670200	1.86639100
H	-4.55320900	1.38163600	0.49744500
H	-2.02038600	-2.01408700	1.33798600

$7\alpha_A$

E = -1190.0653552 a.u.

C	-1.14907800	-0.96263100	0.10853300
C	-1.47610400	-1.88873200	1.05849400
C	-2.84132700	-2.19671200	1.43942400
O	-3.85212700	-1.47625600	0.74320900
C	-2.21757600	-0.28003900	-0.62181600
C	-3.55252400	-0.57191500	-0.26694800
C	-2.00709200	0.63010500	-1.68029600
C	-3.08010600	1.22690800	-2.33454400
C	-4.39861100	0.92730000	-1.94762700
C	-4.63797000	0.02491800	-0.91409800
O	-3.20130600	-2.99295300	2.30517500
H	-0.71362700	-2.44762900	1.58339100
H	-0.99305500	0.85787300	-1.98383200
H	-2.89806500	1.92257000	-3.14631500
H	-5.23430400	1.39372100	-2.45827000
H	-5.63976100	-0.23779500	-0.59742000
C	0.27542200	-0.73371600	-0.21933900
C	1.12708300	-1.86786800	-0.67610700
C	2.50470600	-1.32676200	-1.03588800
C	2.44064400	0.19153700	-0.67858900

C	1.01781800	0.41666200	-0.16862100
O	0.79098800	-3.06254100	-0.72845500
C	3.64909100	-1.87163800	-0.12589200
C	3.56728600	0.34670100	0.39851700
C	4.99137600	-1.32747400	-0.68983000
C	4.93149500	0.20306300	-0.33662400
C	3.47831600	-1.00709600	1.15241800
H	2.70721700	-1.53042100	-2.09318800
H	2.64383100	0.84060100	-1.53926000
H	5.08936500	-1.50932300	-1.76553400
H	5.83997300	-1.81371500	-0.19581900
H	4.98976100	0.84287100	-1.22464000
H	5.75503800	0.48895400	0.32687600
H	4.29206500	-1.14584100	1.87193700
H	2.52618200	-1.16266200	1.66886200
H	3.60936200	-2.95518600	0.00176600
H	3.47623600	1.25079700	1.00422800
C	-0.71888400	3.12021700	1.85601500
C	-0.14418000	4.27937500	1.32065800
C	0.81263700	4.17169900	0.30451300
C	1.19174400	2.91536300	-0.17272100
C	0.60685100	1.73706800	0.34199000
C	-0.35049000	1.86384100	1.37246800
H	-1.45103100	3.19403100	2.65335700
H	-0.43445800	5.25544000	1.69547500
H	1.26534200	5.06491300	-0.11367600
H	1.93484700	2.84975800	-0.95984100
H	-0.78850700	0.97398800	1.80791200

$7\alpha_B$

E = -1190.062993 a.u.

C	-1.25016800	-0.78176100	-0.50159200
C	-1.94194000	-1.38947800	-1.51100800
C	-3.38217700	-1.56259800	-1.50468000
O	-4.05621100	-1.07189300	-0.35128300
C	-1.97474300	-0.32401200	0.68560900
C	-3.37590500	-0.49499100	0.71283000
C	-1.36568900	0.25825500	1.81830300
C	-2.12520200	0.65461000	2.91481100
C	-3.52033200	0.47829500	2.90859000
C	-4.14889900	-0.09860400	1.80770500
O	-4.06543700	-2.07037600	-2.39239400
H	-1.43506000	-1.77897000	-2.38319800
H	-0.29129800	0.39364400	1.82725400
H	-1.63859000	1.09880800	3.77618600
H	-4.11122000	0.78715400	3.76422900
H	-5.21966600	-0.25687400	1.77162000
C	0.22423600	-0.69362600	-0.58301800
C	1.01735000	-1.94759400	-0.71193900
C	2.49819800	-1.59145400	-0.73243200
C	2.52870000	-0.04179500	-0.53751600
C	1.06301500	0.39421500	-0.57225900
O	0.55954200	-3.09945600	-0.79566200
C	3.27290200	-2.15394800	0.49478000
C	3.26818100	0.09758800	0.84977900
C	4.76930800	-1.76876400	0.32873700
C	4.76967200	-0.21872600	0.58651200
C	2.81830600	-1.17687700	1.61087200
H	2.93987000	-1.92408100	-1.67823600
H	3.09453600	0.48088000	-1.31644700
H	5.15243800	-2.03060900	-0.66344100
H	5.38605000	-2.29245400	1.06751300
H	5.16870200	0.34992800	-0.26082600
H	5.37226200	0.03607100	1.46545700
H	3.36148700	-1.31616600	2.55163600
H	1.74498900	-1.21747100	1.81949500
H	3.08743200	-3.21621300	0.66452500
H	3.09581400	1.04498500	1.36405300
C	-0.87589900	3.60208000	-1.22320500
C	0.09192000	4.57457800	-0.94384800
C	1.37312800	4.17573200	-0.54785900
C	1.68052900	2.81961200	-0.42315800
C	0.71010600	1.82189200	-0.67450100
C	-0.57276500	2.24682900	-1.09226000
H	-1.86662300	3.89851000	-1.55157900
H	-0.14667600	5.62832600	-1.04442600
H	2.13580500	4.91963800	-0.34152000
H	2.68326900	2.53754300	-0.12911000
H	-1.32766500	1.51440100	-1.34398700

TS-1 ($7\alpha_A \rightarrow 7\alpha_B$)

E = -1190.0409132 a.u.

C	-1.42633500	0.02824400	-0.05759300
C	-1.54582000	1.39744900	-0.06562400
C	-2.77443800	2.15418800	0.00400900
O	-3.95473200	1.39984900	0.06024300
C	-2.70509200	-0.73283700	-0.01994900
C	-3.91779200	0.01052600	0.02828400
C	-2.86740900	-2.13949100	-0.05329200
C	-4.12228600	-2.74255300	-0.04276600
C	-5.29054700	-1.96984800	0.00509700
C	-5.18141900	-0.58534600	0.04317300
O	-2.86342000	3.38557800	0.01764900
H	-0.68935100	2.04075200	-0.12934000
H	-1.99393800	-2.76796300	-0.04941900
H	-4.18517900	-3.82527900	-0.06529000
H	-6.26795500	-2.44042300	0.01496200
H	-6.04672200	0.06484600	0.08100900
C	-0.02570700	-0.53519800	-0.17747100
C	0.41362700	-1.98137900	-0.19005100
C	1.85427200	-2.08382700	-0.66740200
C	2.35858800	-0.62512300	-0.67414400
C	1.13558700	0.20669700	-0.31384000
O	-0.19174700	-2.99068000	0.21223100
C	2.78590200	-2.80310900	0.35224300
C	3.52089300	-0.64434300	0.37752400
C	4.19629000	-2.90431000	-0.29169800
C	4.70493100	-1.41701700	-0.27270700
C	3.00546000	-1.68460800	1.40822400
H	1.86838500	-2.57574300	-1.64710200
H	2.74120600	-0.27680700	-1.64286000
H	4.15808000	-3.32398200	-1.30299700
H	4.84583300	-3.55223700	0.30718700
H	4.94310600	-1.03897000	-1.27317400
H	5.60787700	-1.31449000	0.33913500
H	3.75855500	-1.94700900	2.15840900
H	2.08874800	-1.38210400	1.92473700
H	2.37019600	-3.74551700	0.71217300

H	3.78467900	0.34275700	0.76142400
C	2.14826400	3.78134400	-1.09118400
C	2.16347400	4.35299000	0.18548500
C	1.81739100	3.57632000	1.29807700
C	1.44743500	2.23883200	1.13641000
C	1.42232900	1.65595400	-0.14737900
C	1.79364700	2.43861500	-1.25741000
H	2.41156100	4.37806000	-1.95833000
H	2.43913000	5.39437900	0.31312200
H	1.82881600	4.01291600	2.29127100
H	1.16613100	1.64381300	1.99920500
H	1.78255900	2.00199300	-2.25121600

TS-2 ($7\alpha_A \rightarrow 7\alpha_B$)

E = -1190.0366235 a.u.

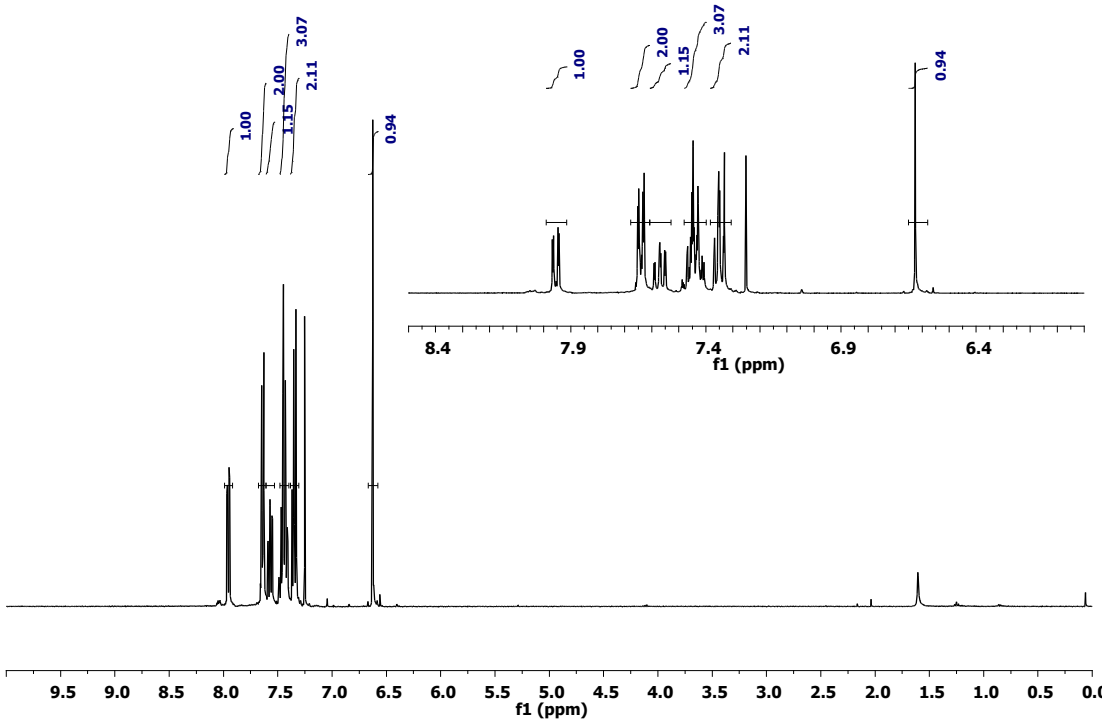
C	-1.35563900	-1.00183700	-0.03975600
C	-1.81197500	-2.29971300	-0.05179400
C	-3.19759400	-2.71760100	-0.02797200
O	-4.15508000	-1.68769400	-0.01346200
C	-2.40436200	0.05055900	0.05155900
C	-3.76621100	-0.35729600	0.04758700
C	-2.20521700	1.44319200	0.16007200
C	-3.25709400	2.35311900	0.23226300
C	-4.58474700	1.90697400	0.20080100
C	-4.83381700	0.54277900	0.11177400
O	-3.60062100	-3.88233800	-0.03779800
H	-1.12405100	-3.12805100	-0.08171200
H	-1.20941900	1.83032400	0.19913200
H	-3.03496200	3.41143800	0.31562300
H	-5.40868200	2.61044000	0.25301800
H	-5.83766000	0.13652200	0.09668900
C	0.14001000	-0.83279100	-0.18271400
C	1.03404400	-2.07131200	-0.29287200
C	2.44264600	-1.67282400	-0.68436000
C	2.43600300	-0.13431300	-0.62569600
C	0.98902100	0.24952800	-0.30047900
O	0.75167600	-3.26066600	-0.06691600
C	3.51465400	-2.09543300	0.36522700
C	3.50484500	0.18126200	0.47890100
C	4.90587400	-1.71125600	-0.20883300
C	4.89820100	-0.14165700	-0.13592700
C	3.31757500	-1.00880000	1.45785300
H	2.66266300	-2.08934000	-1.67393400
H	2.71679800	0.35915200	-1.56504900
H	5.04884100	-2.08604200	-1.22820400
H	5.70569000	-2.13237200	0.41030700
H	5.03390500	0.32800200	-1.11657000
H	5.69638000	0.22890100	0.51671800
H	4.08640900	-1.04258600	2.23668400
H	2.33333300	-1.04091100	1.93642000
H	3.41245000	-3.13588500	0.67801800
H	3.42676100	1.18504200	0.89942100
C	0.73170200	3.90912300	-1.27034400
C	0.80130900	4.53906400	-0.02208000
C	0.90551900	3.76539300	1.13999300
C	0.93007000	2.36926600	1.05781700
C	0.83952300	1.72690500	-0.19340000
C	0.76270100	2.51392200	-1.35825100
H	0.65376400	4.50218900	-2.17580200
H	0.77905100	5.62180000	0.04419300
H	0.96653600	4.24635900	2.11087400
H	0.99822200	1.77269100	1.96164900
H	0.70393700	2.03040000	-2.32827600

2.2 Complete Reference for Ref. 15 – "Gaussian 03" details.

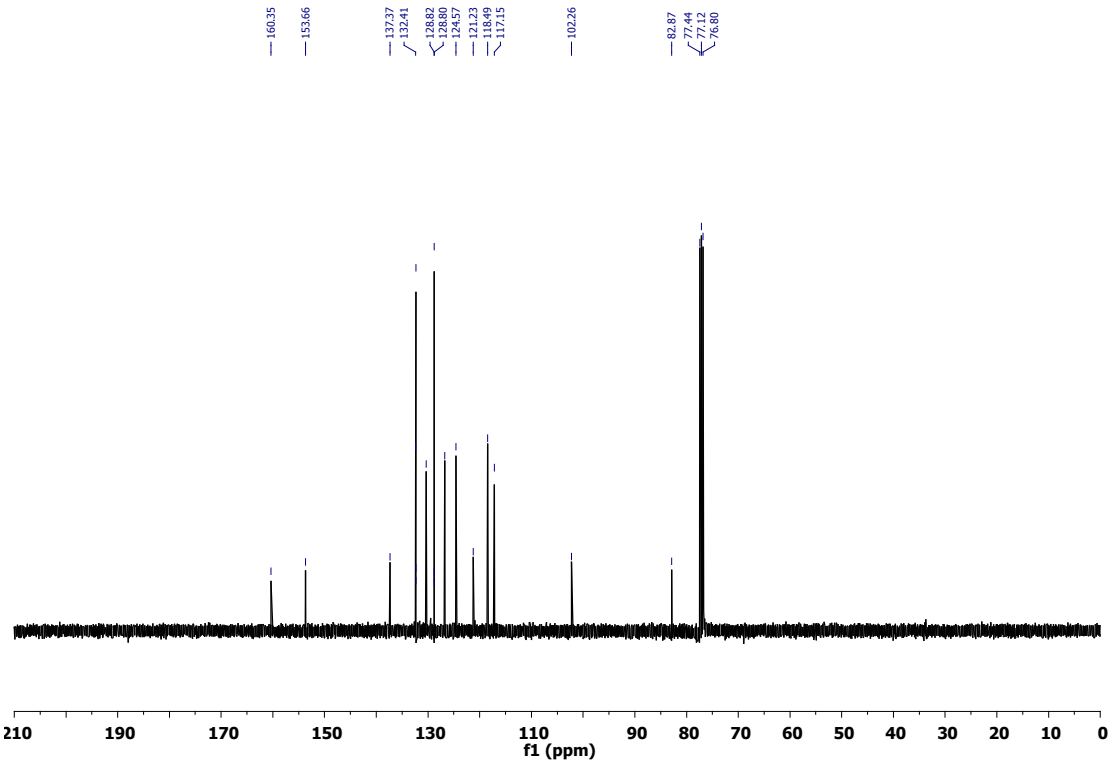
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez and J. A. Pople, *Gaussian 03* (revision B.05), Gaussian, Inc., Pittsburgh, PA, 2003.

3.0 Representative NMR spectra (all run at 298 K in $CDCl_3$).

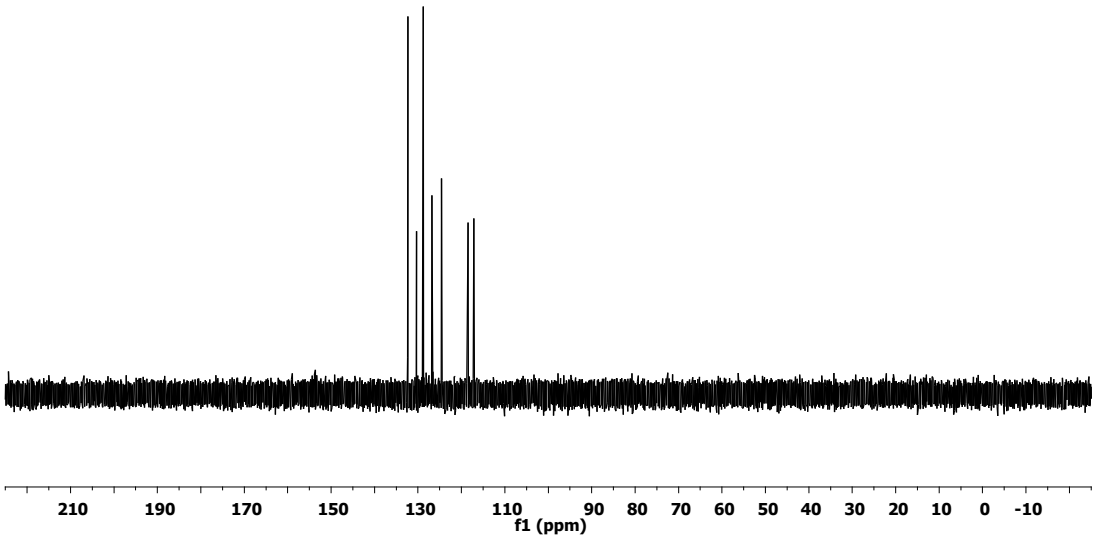
^{1}H NMR (400 Mhz) spectrum of compound **5**.



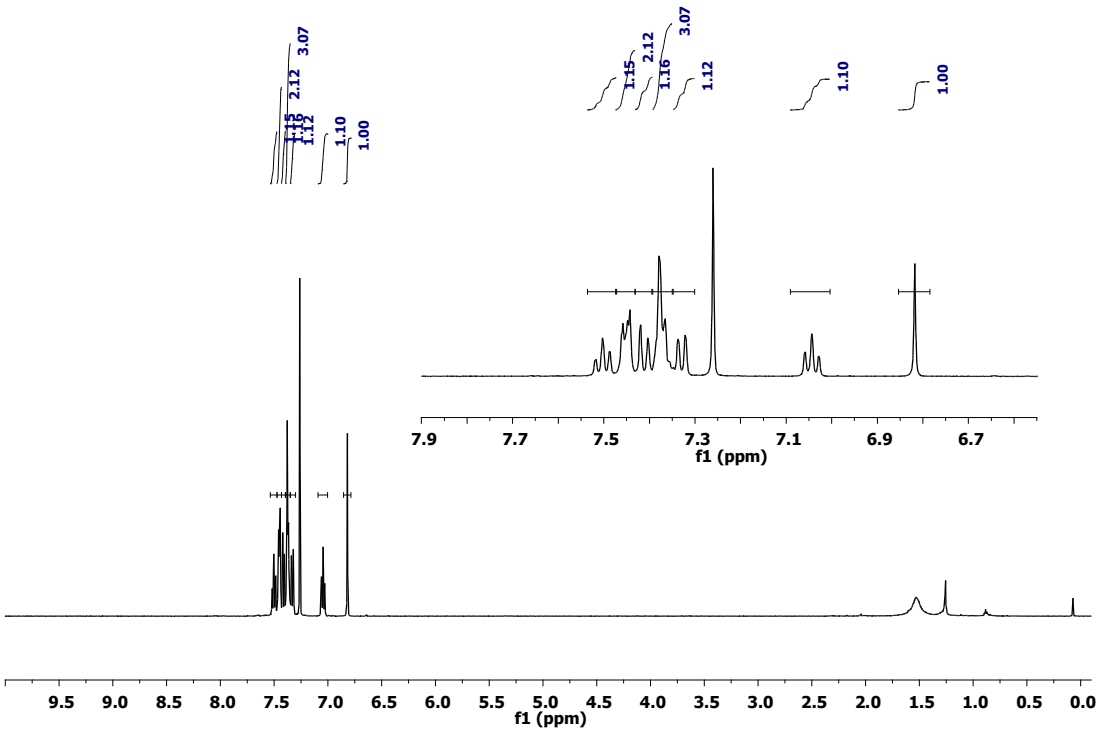
^{13}C{^{1}H} (100 MHz) NMR spectrum of compound **5**.



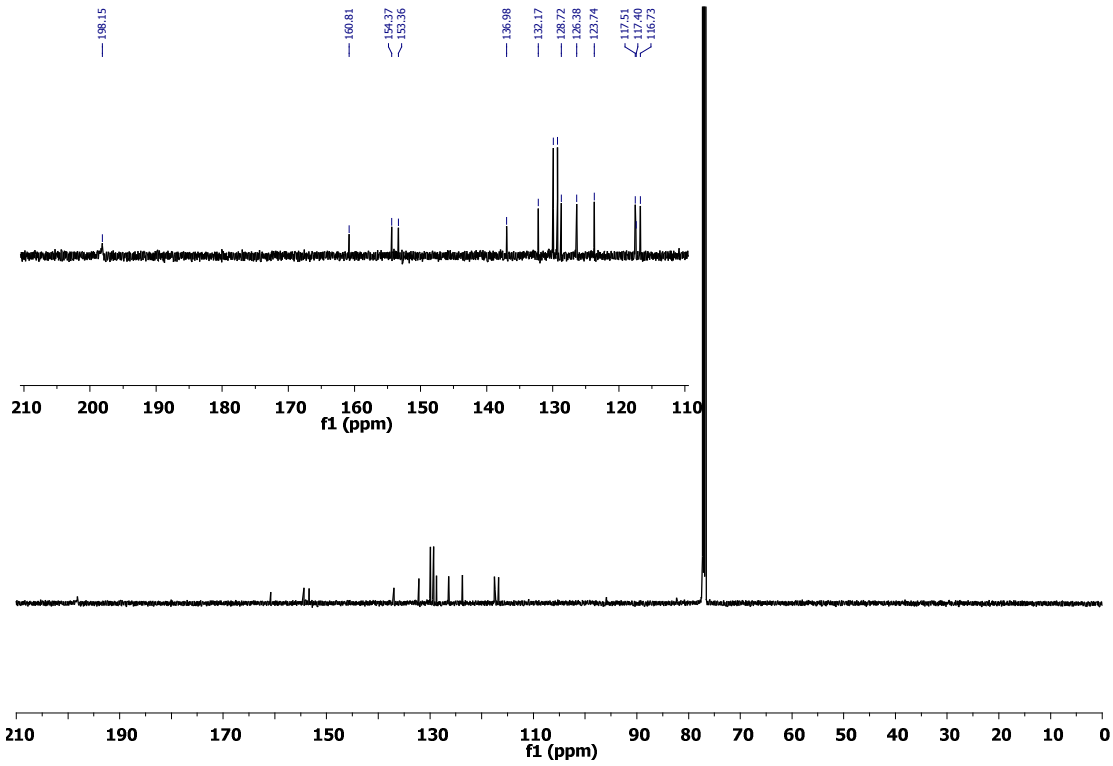
$^{13}C\{^{1}H\}$ DEPT135 (100 Mhz) NMR spectrum of compound **5**.



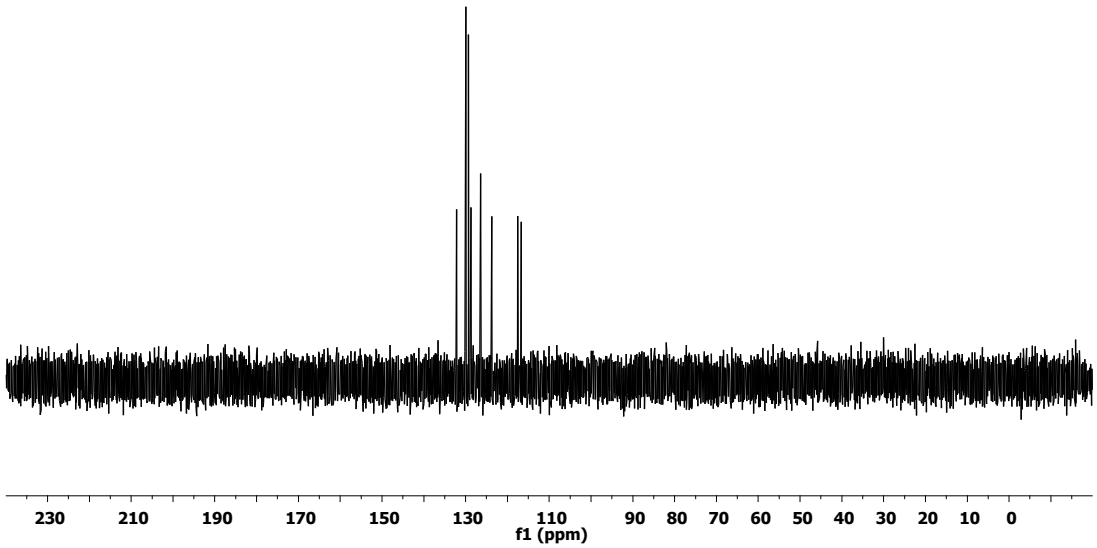
^{1}H NMR (500 Mhz) spectrum of complex **6**.



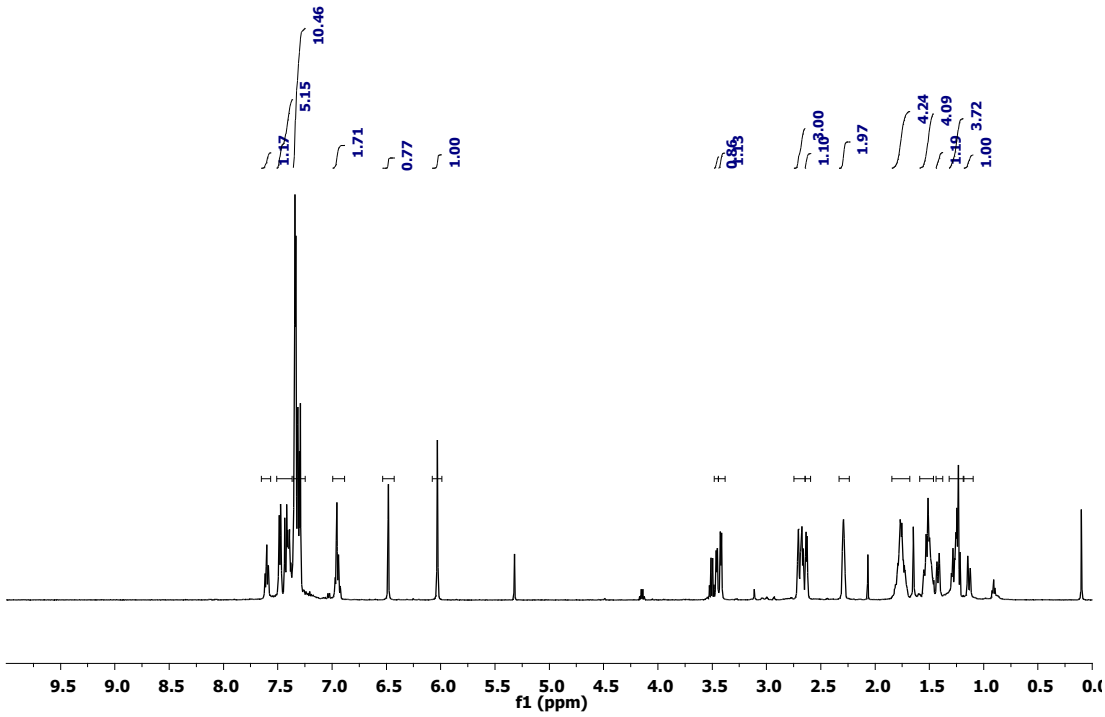
$^{13}C\{^{1}H\}$ (125 MHz) NMR spectrum of complex **6**.



$^{13}C\{^{1}H\}$ DEPT135 (125 MHz) NMR spectrum of complex **6**.

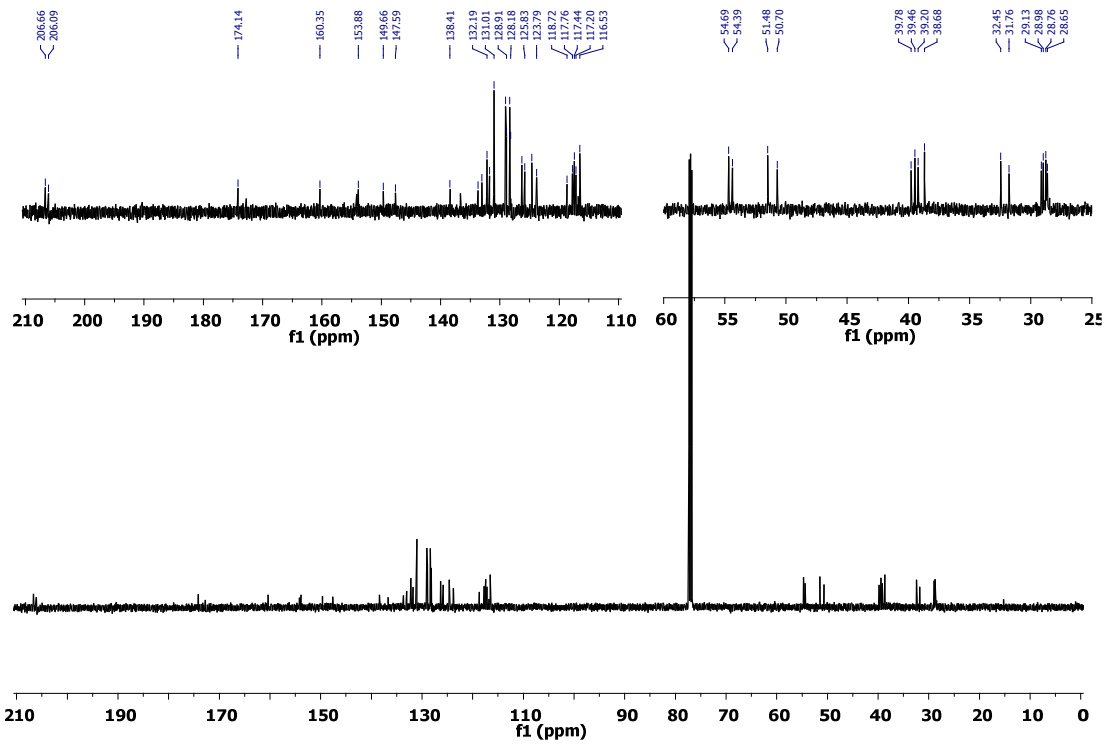


^{1}H NMR (500 Mhz) spectrum of regioisomer **7α**.*

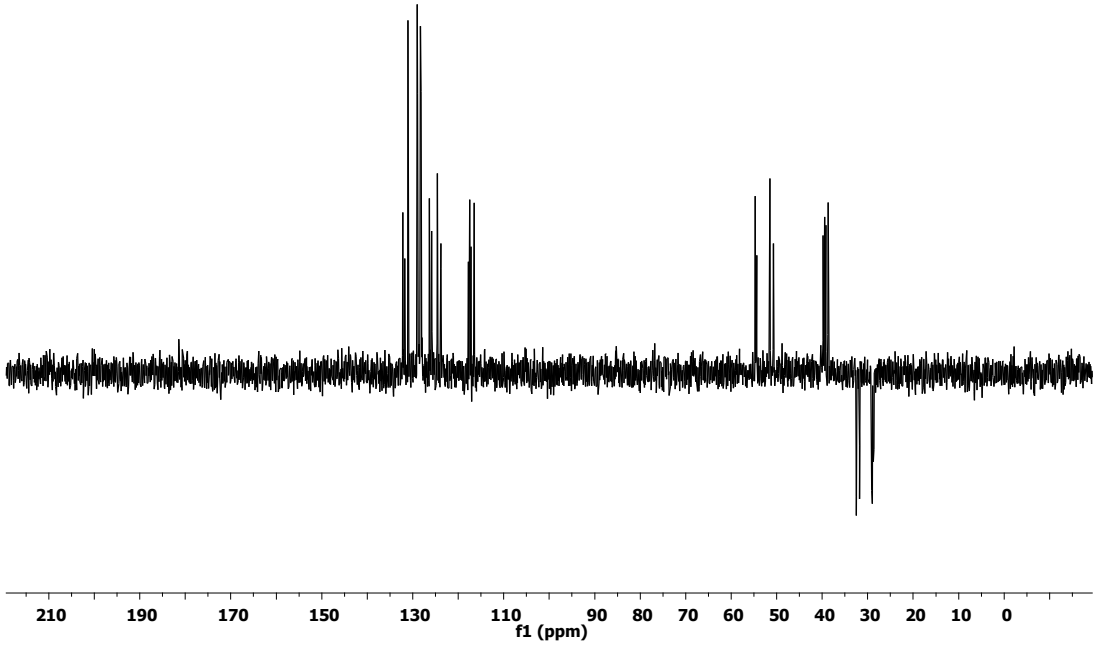


* Note: trace diethyl ether impurity in this ^{1}H NMR spectrum.

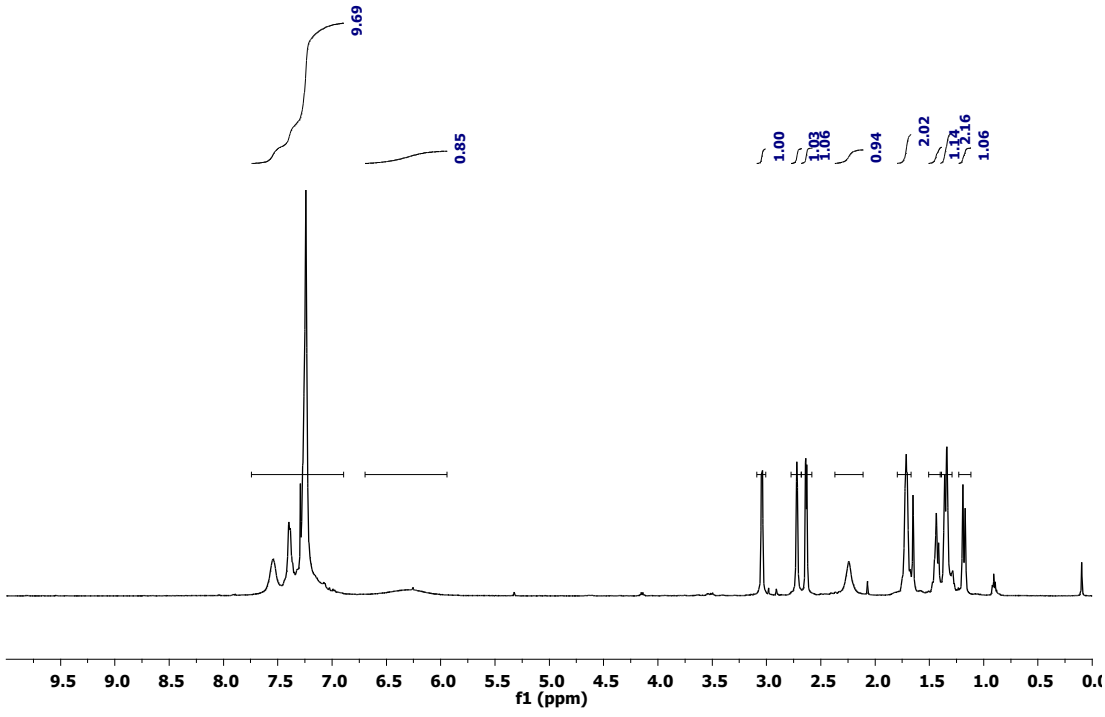
^{13}C{^{1}H} (125 MHz) NMR spectrum of regioisomer **7α**.



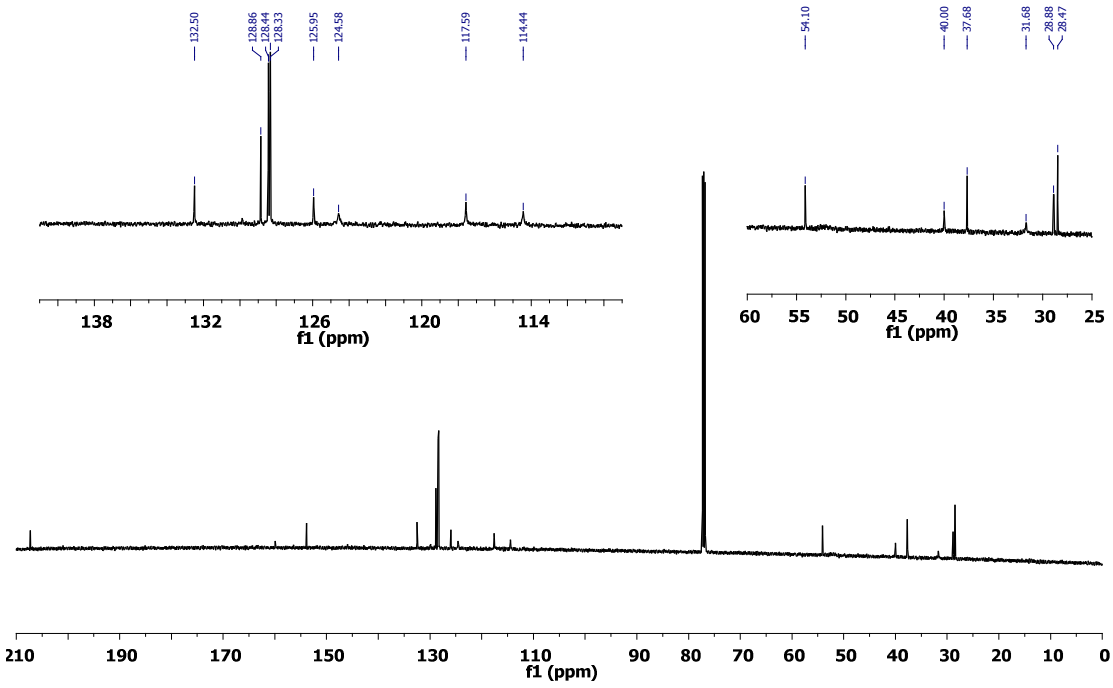
$^{13}C\{^{1}H\}$ DEPT135 (125 MHz) NMR spectrum of regioisomer **7α**.



^{1}H NMR (500 Mhz) spectrum of regioisomer **7β** (mixture of atropisomers at room temperature).



$^{13}C\{^{1}H\}$(125 MHz) NMR spectrum of regioisomer **7β**.



$^{13}C\{^{1}H\}$ DEPT135 (125 MHz) NMR spectrum of regioisomer **7β**.