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Supporting Information

Syntheses and Structures of Facial and Meridional Stereoisomers of κ^2 -*N,S*-Chelated Ruthenium Borate Complexes

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I. Synthetic procedure and experimental details

Syntheses of *cis-mer-2a* and *cis-fac-3a*: In a flame-dried Schlenk tube, solution of *trans-mer*-[PCy₃(κ²-N,S-(NC₇H₄S₂)Ru{κ³-H,S,S'-H₂B(NC₇H₄S₂)₂}], **1a** (30 mg, 34 μmol) dissolved in 5 mL dry toluene. The solution was heated at 90 °C for 24 h, after which all volatiles components were evaporated under vacuum. The residue was dissolved in a minimum amount of dichloromethane and hexane was added to precipitate out the orange isomeric mixture *cis-mer-2a* and *cis-fac-3a* in the ratio of (40:60) (We report the combined spectroscopic data for *cis-mer-2a* and *cis-fac-3a*), (0.015 g, 50% yield).

Syntheses of *cis-mer-2b* and *cis-fac-3b*: Under similar reactions conditions, reaction of *trans-mer*-[Ph₃P(κ²-N,S-(C₇H₄NS₂)Ru{κ³-H,S,S'-H₂B-(C₇H₄NS₂)₂}], **1b** (30 mg, 34 μmol) yielded mixture of orange solid *cis-mer-2b* and *cis-fac-3b* in the ratio of (20:80). (We report the combined spectroscopic data for *cis-mer-2b* and *cis-fac-3b*), (0.016 g, 53% yield).

Spectroscopic data for *cis-mer-2a* and *cis-fac-3a*: MS (ESI⁺): *m/z* calculated for [C₃₉H₄₇PBN₃RuS₆]⁺: 893.0939, found 893.0959; ¹¹B{¹H} NMR (160 MHz, chloroform-d, 22 °C): δ = -4.7 (br, B); ¹³C{¹H} NMR (125 MHz, chloroform-d, 22 °C) 26.9-35.93 (Cy) 113.73-133.80 (Ar_(mbz)), 143(C-N) 145.6-150.7 (C=N) for *cis-mer-2a* and *cis-fac-3a*.

***cis-mer-2a*:** ¹H{¹¹B} NMR (500 MHz, chloroform-d, 22 °C): δ = 8.04 (d, *J* = 8.4 Hz, 1H, Ar_(mbz)), 7.58 (t, *J* = 8.4 Hz, 2H, Ar_(mbz)), 7.51 (t, *J* = 7.9 Hz, 1H, Ar_(mbz)), 7.42 (d, *J* = 7.9 Hz, 1H, Ar_(mbz)), 7.36 – 7.28 (m, 2H, Ar_(mbz)), 7.25 – 7.23 (m, 1H, Ar_(mbz)), 7.20 – 7.13 (m, 2H_(mbz)), 7.07 (m, 1H_(mbz)), 6.99 (q, *J* = 7.5, 6.6 Hz, 1H Ar_(mbz)), .4.91 (d, ²J_{H-H} = 16.0 Hz, 1H, B-H_{terminal}), 1.89-1.09 (m, 33H, PCy₃), -18.60 (t, ²J_{H-P} = 9.1, ²J_{HH} = 16.0 Hz, 1H, Ru-H-B); ³¹P{¹H} NMR (202 MHz, chloroform-d, 22 °C): δ = 52.1 ppm, IR (CH₂Cl₂): $\tilde{\nu}$ = 2515 (B-H_{terminal}), 2129 cm⁻¹ (B-H_b).

***cis-fac-3a*:** ¹H{¹¹B} NMR (500 MHz, chloroform-d, 22 °C): δ = 8.12 (d, *J* = 8.4 Hz, 1H, Ar_(mbz)), 7.65 (t, *J* = 7.8, 7.0, 1.6 Hz, 1H, Ar_(mbz)), 7.45 (d, *J* = 8.0 Hz, 1H Ar_(mbz)), 7.39 – 7.34 (m, 2H Ar_(mbz)), 7.28-7.24 (m, 2H Ar_(mbz)), 7.15– 7.13 (m, 2H, Ar_(mbz)), 6.83 (t, *J* = 7.6 Hz, 1H, Ar_(mbz)), 6.58 (d, *J* = 8.1 Hz, 1H, Ar_(mbz)), 6.45 (t, *J* = 7.7 Hz, 1H, Ar_(mbz)), 4.91 (d, ²J_{H-H} = 12.3 Hz, 1H, B-H_{terminal}), 2.42-0.93 (m, 33H, PCy₃), -16.56 (t, ²J_{H-P} = 16.4, ²J_{HH} = 16.4 Hz, 1H, Ru-H-B); ³¹P{¹H} NMR (202 MHz, chloroform-d, 22 °C): δ = 50.8 ppm, IR (CH₂Cl₂): $\tilde{\nu}$ = 2450 (B-H_{terminal}), 2055 cm⁻¹ (B-H_b).

Combined spectroscopic data for *cis-mer-2b* and *cis-fac-3b*: MS (ESI⁺): *m/z* calculated for [C₃₉H₂₉PBN₃RuS₆]⁺: 874.9554, found 874.9563; ¹¹B{¹H} NMR (160 MHz, Benzene-d₆, 22 °C): δ = -4.3 (br, B) for *cis-mer-2b* and *cis-fac-3b*; ¹³C{¹H} NMR (126 MHz, CDCl₃, 22 °C): δ = 115.0-129.4(Ar_(mbz)), 129.0-135.2 (Ph), 145.1-148.5(C-N), 199.0 (C=S), 200.5 (C=S) for *cis-mer-2b* and *cis-fac-3b*.

***cis-mer-2b*:** ¹H{¹¹B} NMR (500 MHz, chloroform-d, 22 °C): δ = 8.13 (d, *J* = 8.5 Hz, 1H, Ar_(mbz)), 7.81 (d, *J* = 7.8 Hz, 1H, Ar_(mbz)), 7.73 (t, *J* = 7.8, 3.0 Hz, 2H, Ar_(mbz)), 7.48 (d, *J* = 8.1 Hz, 2H, Ar_(mbz)), 7.19 (t, *J* = 8.6 Hz, 10H Ph), 7.13 (t, *J* = 7.7 Hz, 7H, Ph, Ar_(mbz)), 7.00 (m, 4H, Ar_(mbz)), 4.78 (d, ²J_{H-H} = 16.4 Hz, 1H, B-H_{terminal}), -17.21 (t, ²J_{H-P} = 9.2, ²J_{HH} = 16.4 Hz, 1H, Ru-H-B); ³¹P{¹H} NMR (202 MHz, chloroform-d, 22 °C): δ = 59.0 ppm, IR (CH₂Cl₂): $\tilde{\nu}$ = 2515 (B-H_{terminal}), 2129 cm⁻¹ (B-H_b).

***cis-fac-3b*:** ¹H{¹¹B} NMR (500 MHz, chloroform-d, 22 °C): δ = 8.18 (d, *J* = 8.4 Hz, 1H, Ar_(mbz)), 7.56 (m, 1H, Ar_(mbz)), 7.37 (d, *J* = 7.9 Hz, 1H, Ar_(mbz)), 7.30 (dd, *J* = 10.1, 7.6 Hz, 5H Ph), 7.26 – 7.21 (m, 3H, Ph), 7.21 – 7.16 (m, 2H), 7.13 (t, *J* = 7.6 Hz, 1H, Ph), 7.06 (td, *J* = 7.8, 2.2 Hz, 4H, Ph), 6.80 (t, *J* = 7.6 Hz, 1H Ar_(mbz)), 6.49 (t, *J* = 7.7 Hz, 1H Ar_(mbz)), 6.41 (d, *J* = 8.0 Hz, 1H Ar_(mbz)), 4.60 (d, ²J_{H-H} = 16.4 Hz, 1H, B-H_{terminal}), -15.60 (t, ²J_{H-P} = 9.3, ²J_{HH} = 16.4 Hz, 1H, Ru-H-B); ³¹P{¹H} NMR (202 MHz, chloroform-d, 22 °C): δ = 55.6 ppm, IR (CH₂Cl₂): $\tilde{\nu}$ = 2504(B-H_{terminal}), 2131 cm⁻¹ (B-H_b).

Synthesis of *cis-4* and *trans-4*: In a flame-dried Schlenk tube, a solution [Ru(PPh₃)₃Cl₂], (100 mg, 11 mmol) in dry THF (15 mL) was added to a solution of K[C₇H₄NS₂] (42 mg, 22 mmol) in THF (15mL) under Argon, and reaction mixture was stirred for 4 hours at room temperature. Solvent was dried under vacuum and the residue was extracted into hexane/CH₂Cl₂ (60:40 v/v) mixture and passed through Celite. After removal of the solvent, the residue was subjected to chromatographic work-up by using TLC plates. Elution with a hexane/CH₂Cl₂ (30:70 v/v) mixture yielded red solid *cis-4* (70 mg, 70%) along with *trans-mer-1b* (7 mg, 12%),

Combined spectroscopic data *cis-4* and *trans-4*: MS (ESI+): m/z calculated for [C₃₉H₂₉PBN₃RuS₆]⁺: 958. 0446, found 958.0470; ¹H NMR (500 MHz, Benzene-d₆, 22 °C): δ = 6.88-7.94 (all the phenyl and mercaptobenzothiazolyl proton) for *cis-4* and 6.81-7.82 (all the phenyl and mercaptobenzothiazolyl proton of *cis-4* and *trans-4*); ¹³C{¹H} NMR (126 MHz, CDCl₃, 22 °C): δ = 118.2-181.9 (Ar(mbz)), 126.4-135.0 (Ph), 136.0-150.3 (C-N), 181.9 (C=S), for *cis-4* and *trans-4*; ³¹P{¹H} NMR (202 MHz, CDCl₃, 22 °C): δ = 52.3 ppm for *cis-4* and 41.6 ppm for *trans-4*.

II. Spectroscopic details

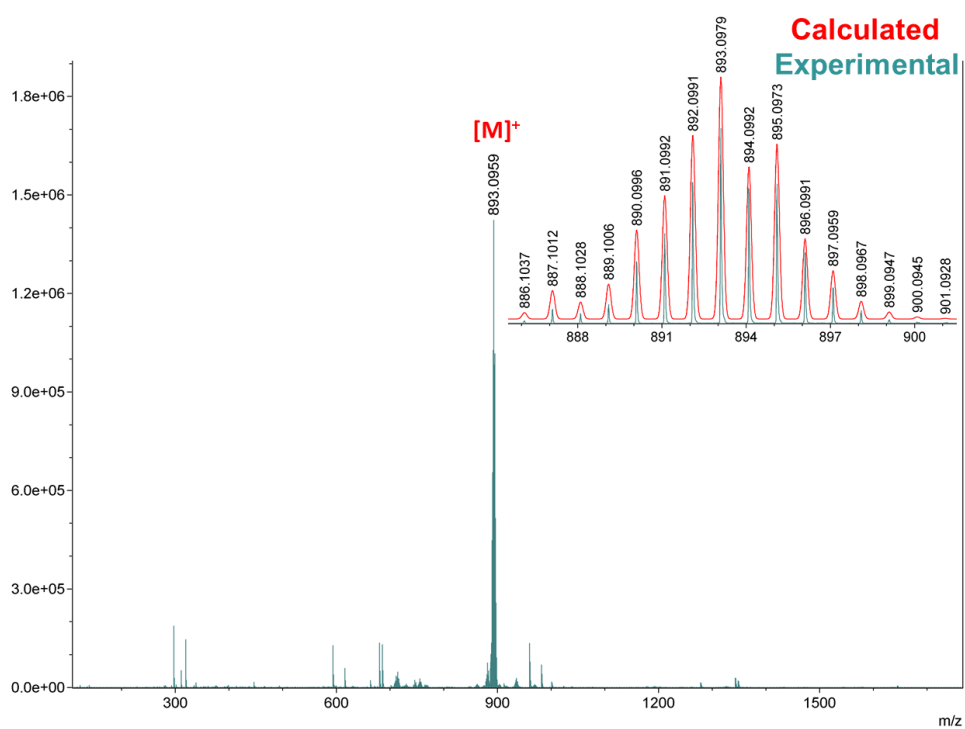


Figure S1. Mass spectral isotopic distribution for the fragment of *cis-mer-2a*, *cis-fac-3a*.

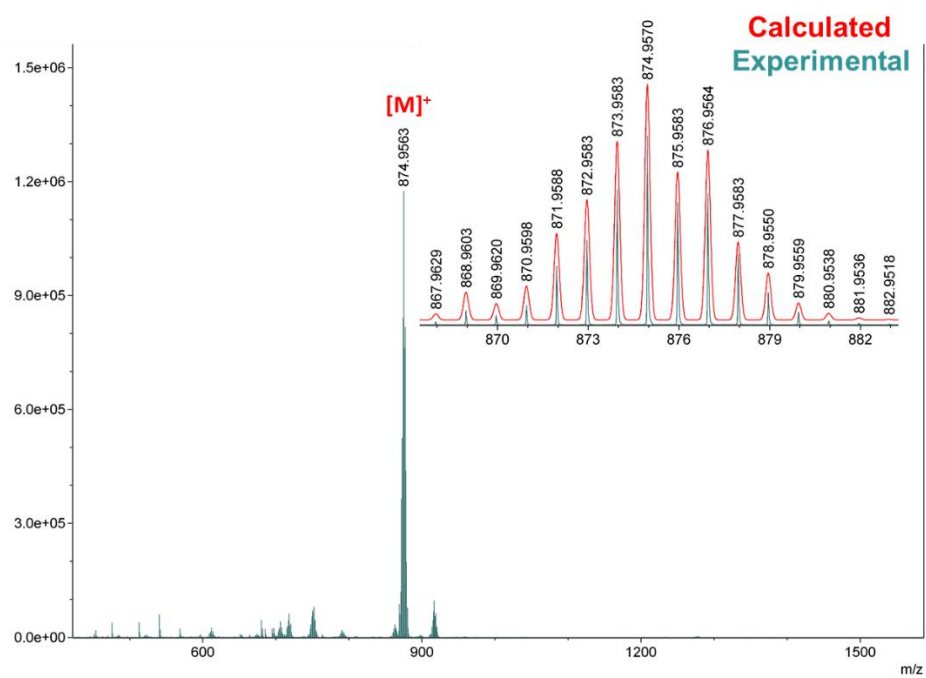


Figure S2. Mass spectral isotopic distribution for the fragment of *cis-mer-2b*, *cis-fac-3b*.

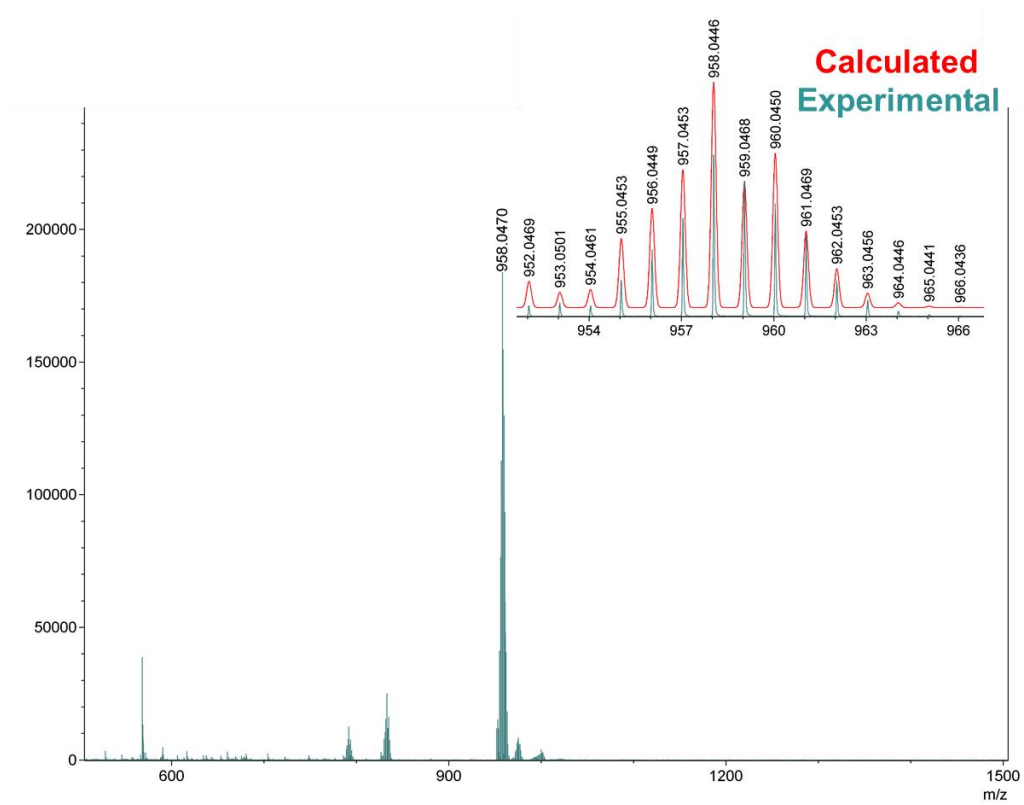


Figure S3. Mass spectral isotopic distribution for the fragment of *cis*-4 and *trans*-4.

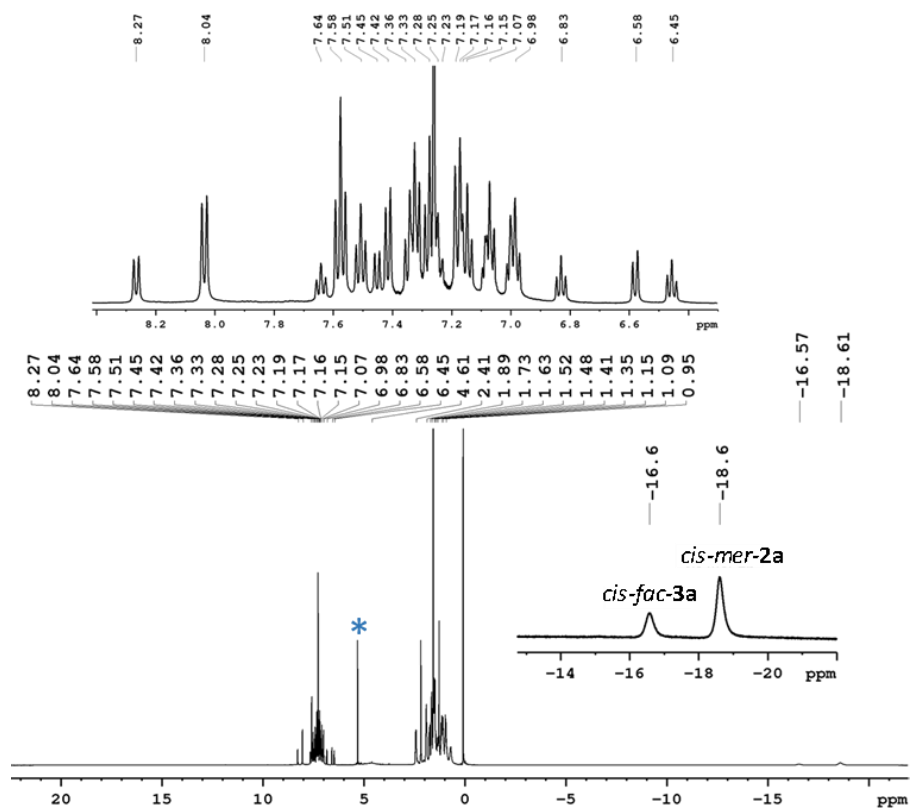


Figure S4. Combined ^1H NMR spectrum of *cis-mer-2a*, *cis-fac-3a* in CDCl_3 (500 MHz) (*= solvent and grease impurities).

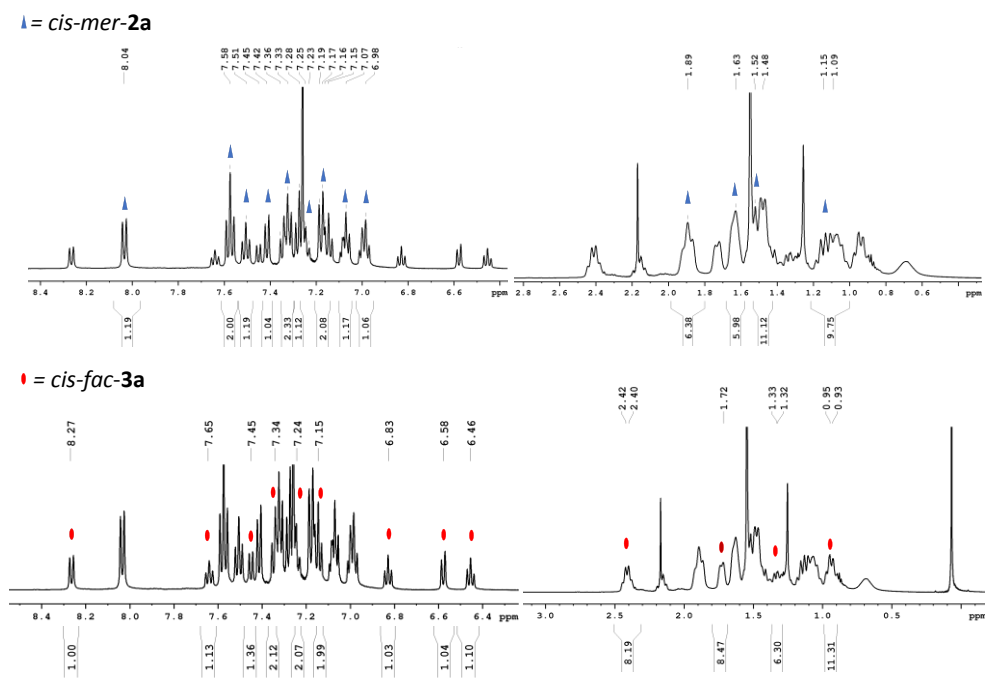


Figure S5. Peak assignment for *cis-mer-2a* and *cis-fac-3a*.

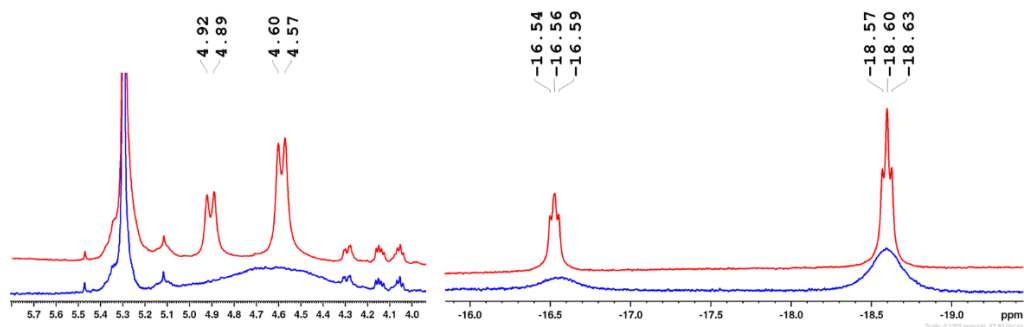


Figure S6. Combined ^1H NMR and $^1\text{H}\{^{11}\text{B}\}$ NMR spectra of *cis-mer-2a*, *cis-fac-3a* in CDCl_3 (500 MHz).

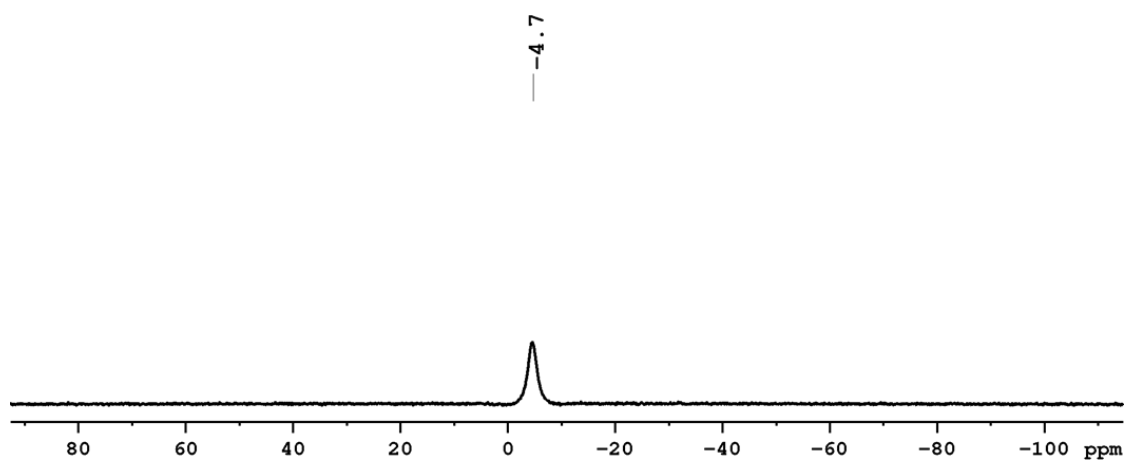


Figure S7. Combined $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of *cis-mer-2a*, *cis-fac-3a* in CDCl_3 (160 MHz).

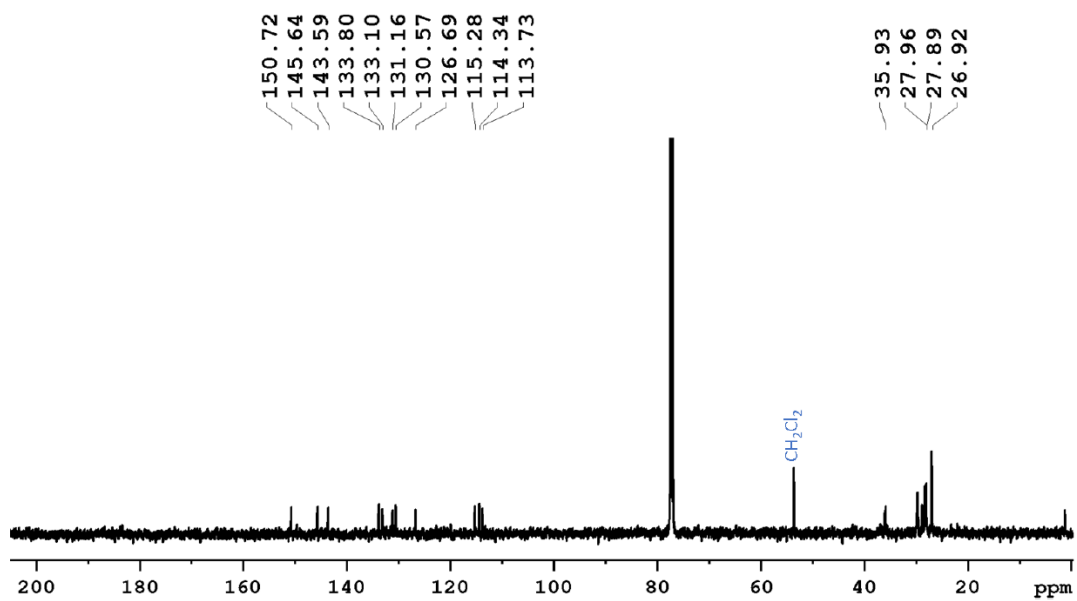


Figure S8. Combined ¹³C{¹H} NMR spectrum of *cis-mer-2a*, *cis-fac-3a* in CDCl₃ (126 MHz).

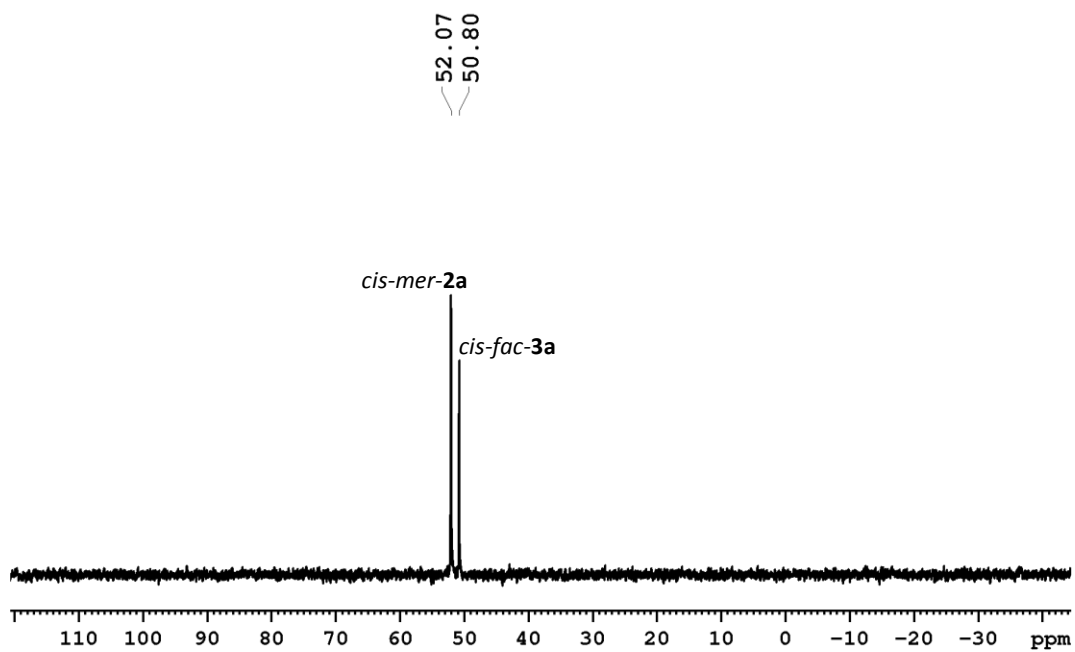


Figure S9. Combined ³¹P{¹H} NMR spectrum of *cis-mer-2a*, *cis-fac-3a* in CDCl₃ (202 MHz).

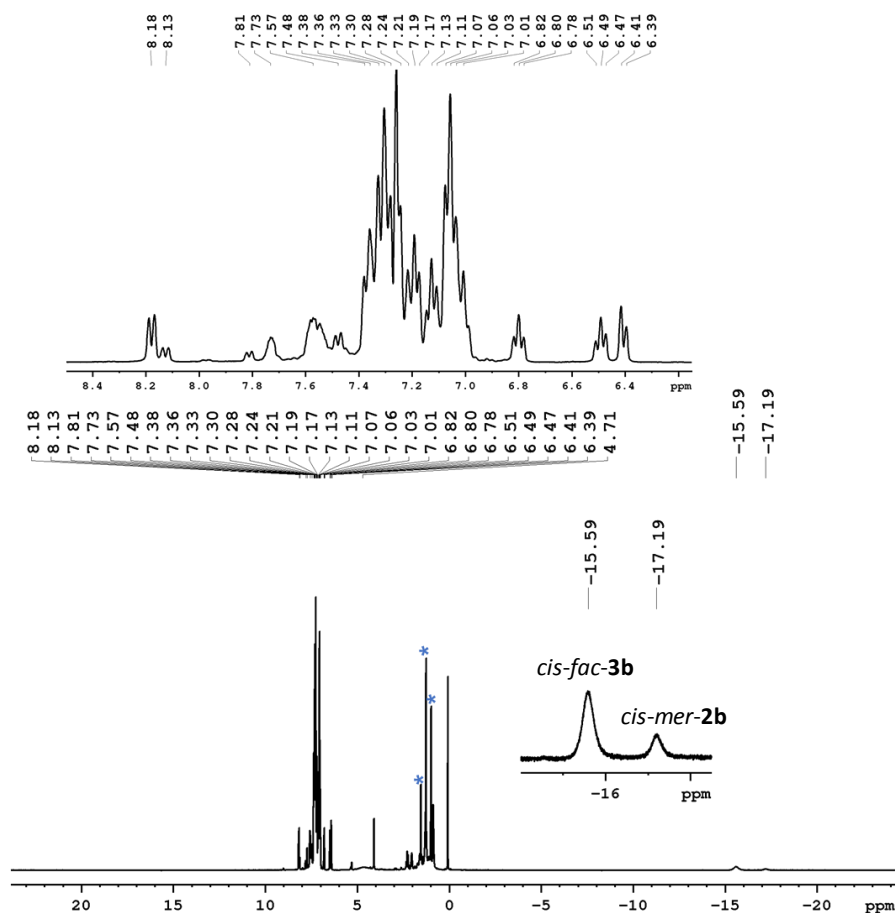


Figure S10. Combined ^1H NMR spectrum of *cis-mer-2b*, *cis-fac-3b* in CDCl_3 (400 MHz) (*= solvent and grease impurities).

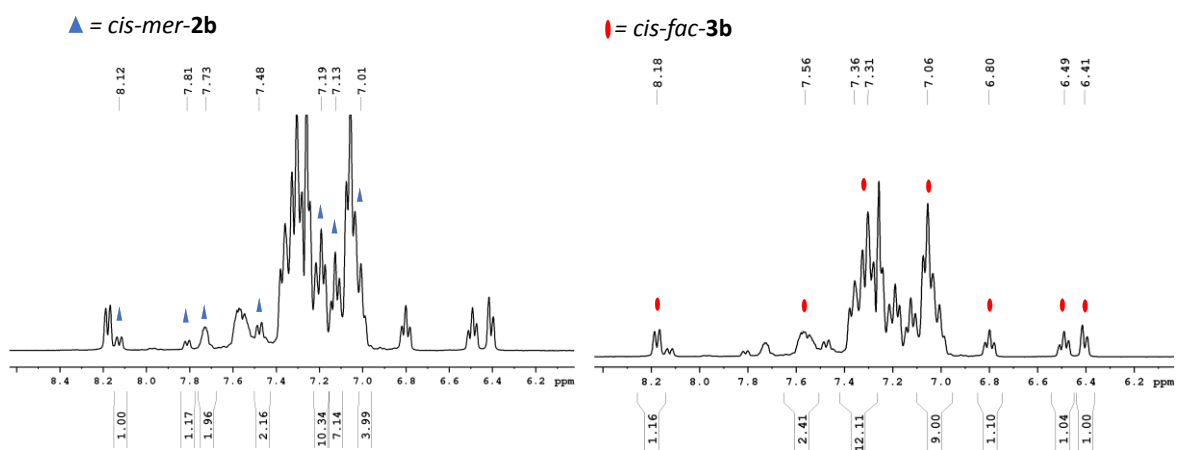


Figure S11. Peak assignment for *cis-mer-2b* and *cis-fac-3b*.

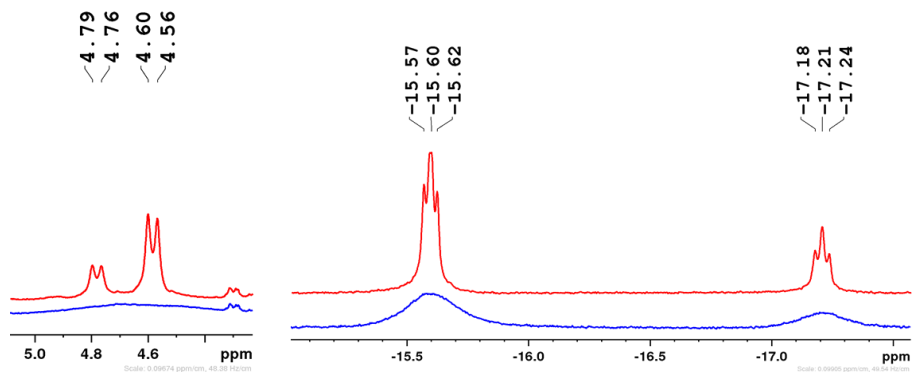


Figure S12. Combined ^1H NMR and $^1\text{H}\{^{11}\text{B}\}$ NMR spectra of *cis-mer-2b*, *cis-fac-3b* in CDCl_3 (500 MHz).

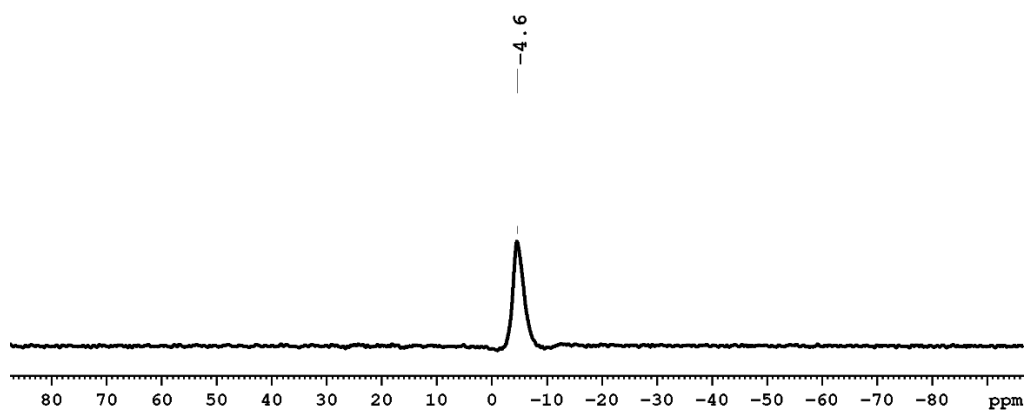


Figure S13. Combined $^{11}\text{B}\{^1\text{H}\}$ NMR spectrum of *cis-mer-2b*, *cis-fac-3b* in benzene- d_6 (160 MHz).

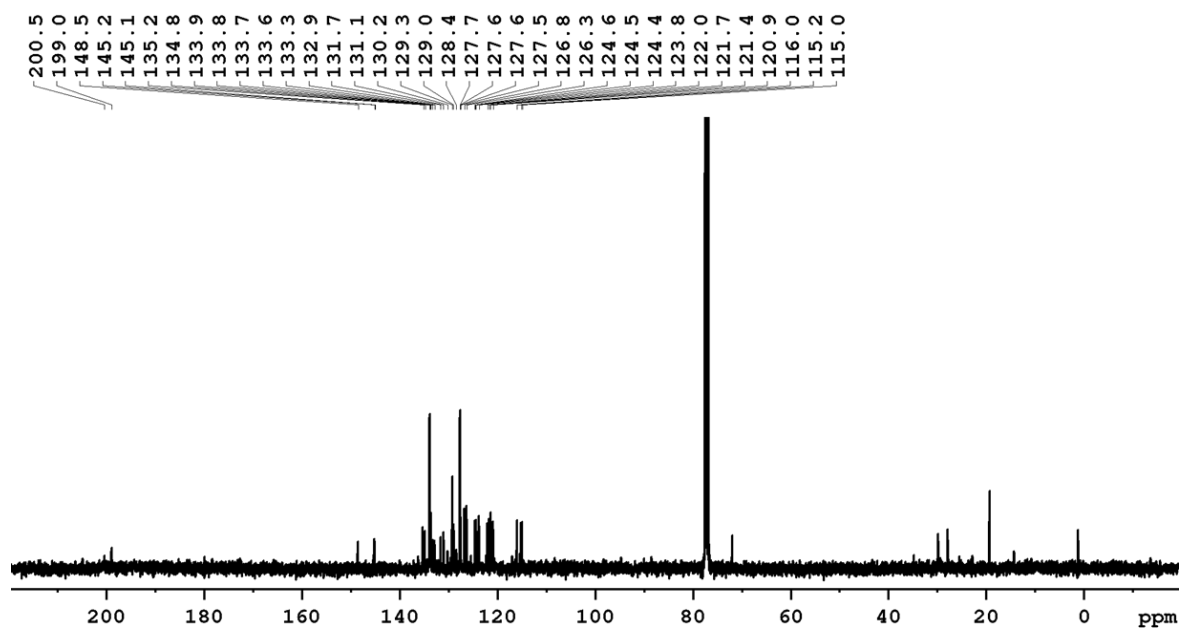


Figure S14. Combined $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of *cis-mer-2b*, *cis-fac-3b* in CDCl_3 (202 MHz).

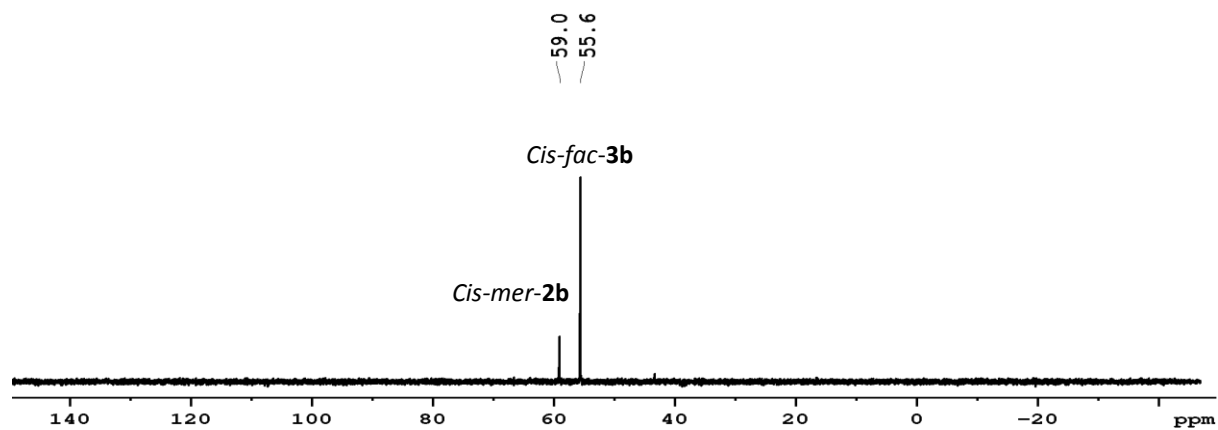


Figure S15. Combined $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of *cis-mer-2b*, *cis-fac-3b* in $\text{benzene-}d_6$ (160 MHz).

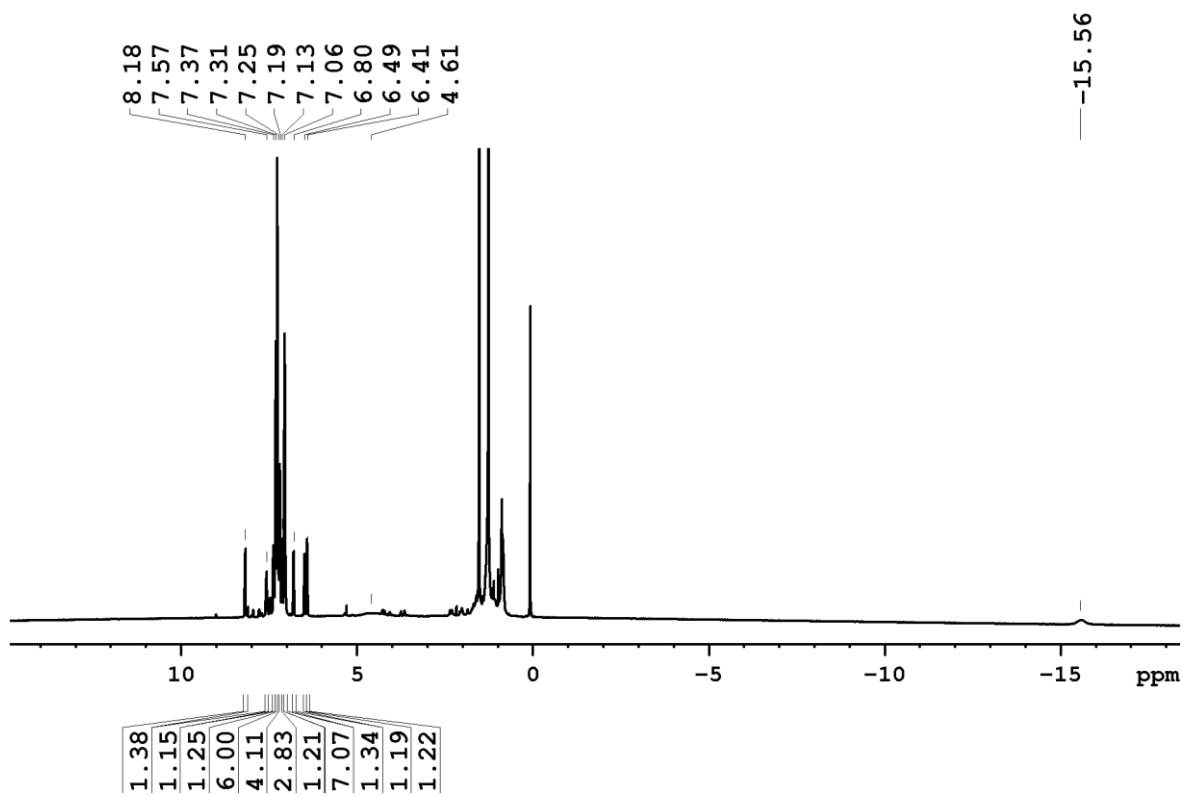


Figure S16. ^1H NMR spectra of *cis-fac-3b* in CDCl_3 (500 MHz).

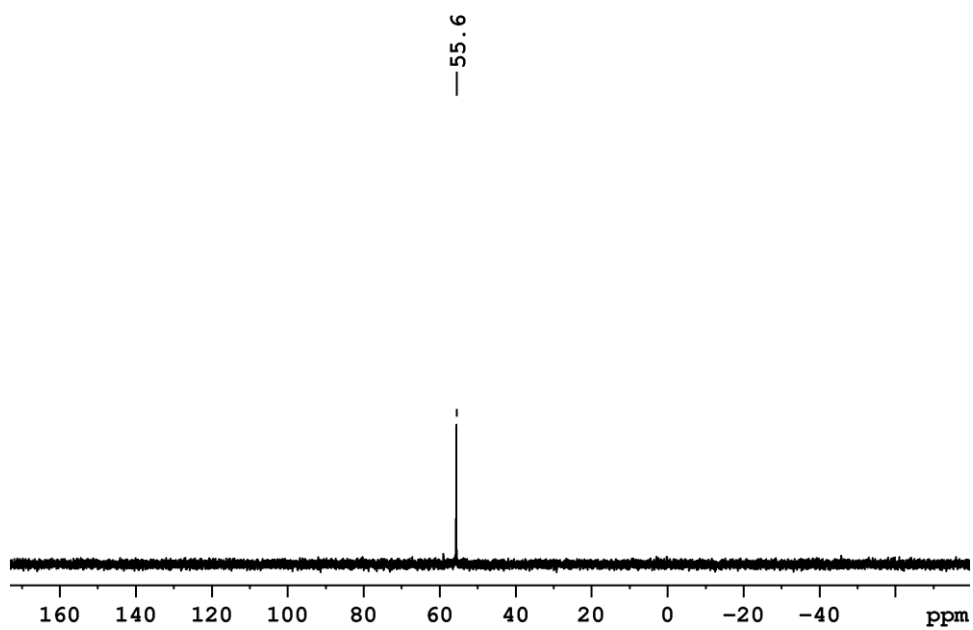


Figure S17. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of *cis-fac-3b*.

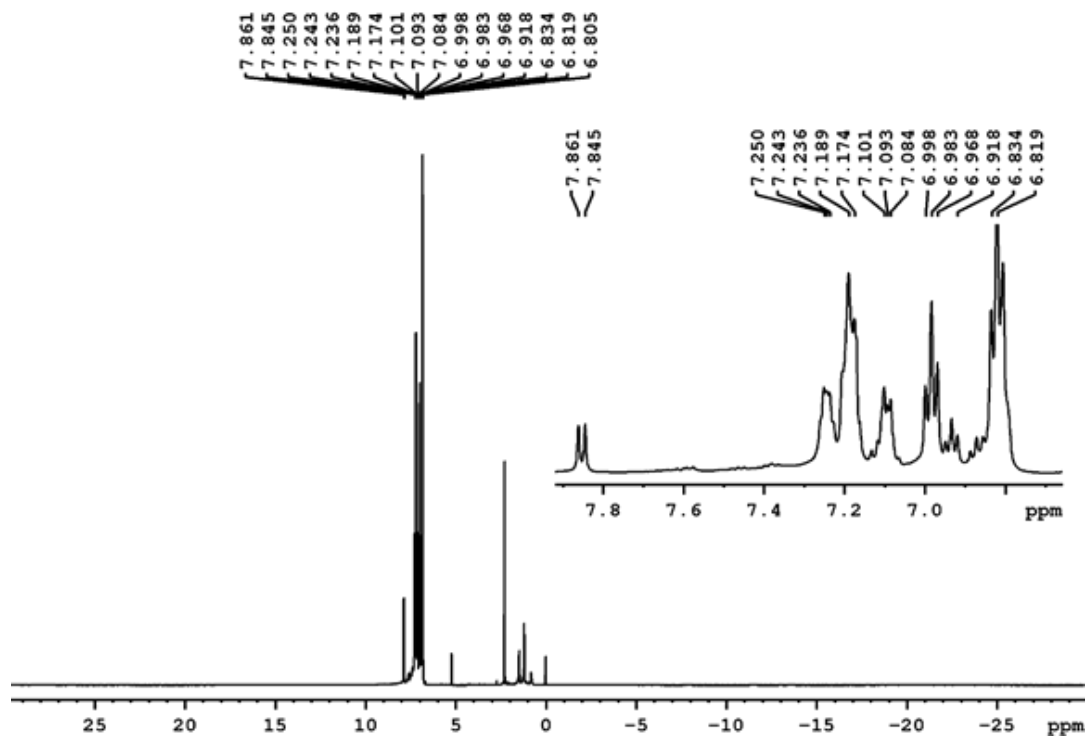


Figure S18. Combined ^1H NMR spectrum of *cis*-4 and *trans*-4 in CDCl_3 (500 MHz).

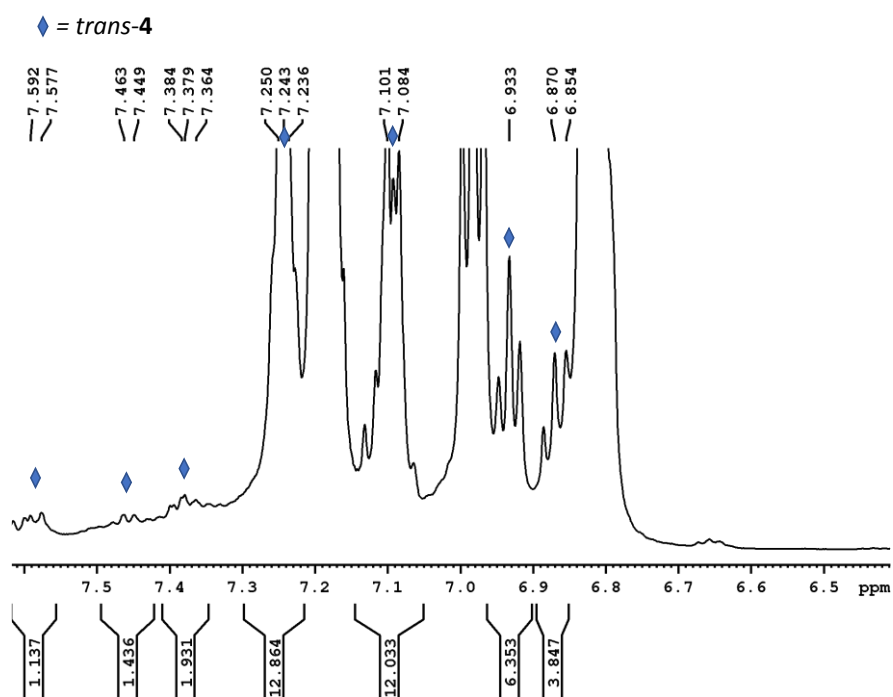


Figure S19. Peak assignment of *trans*-4 in ^1H NMR spectrum of *cis*-4 and *trans*-4 in CDCl_3 (500 MHz).

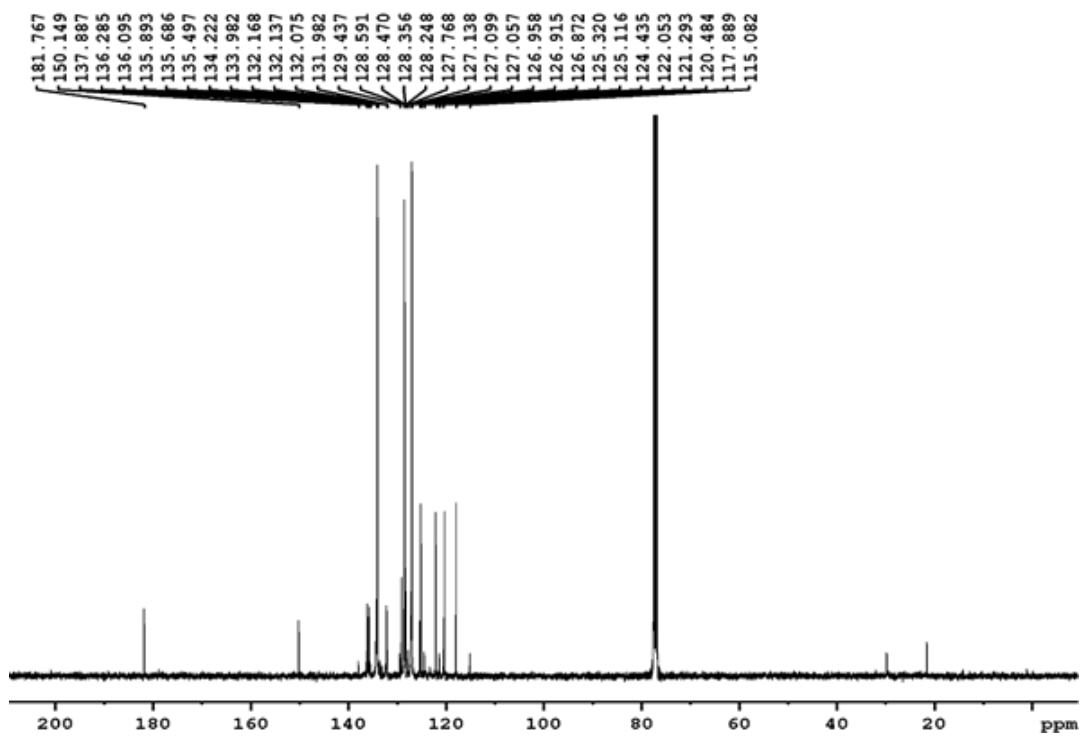


Figure S20. Combined $^{13}\text{C}\{^1\text{H}\}$ spectrum of *cis-4* and *trans-4* in CDCl_3 (202 MHz).

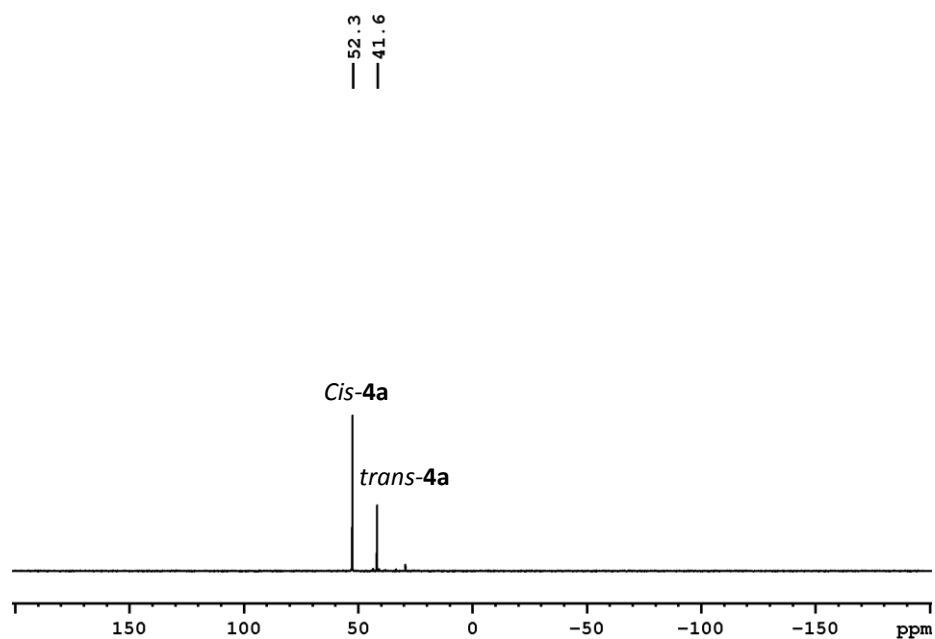


Figure S21. Combined $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of *cis-4* and *trans-4* in CDCl_3 (202 MHz).

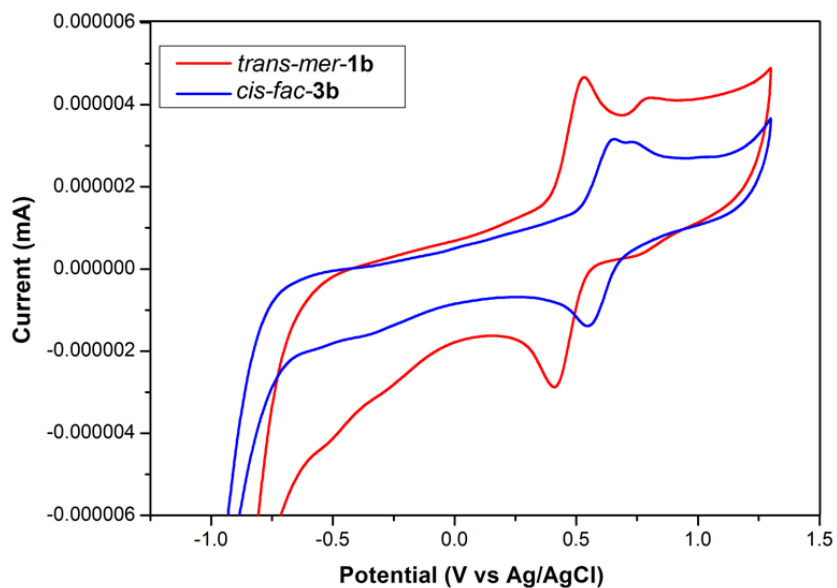


Figure S22. Cyclic voltammetry of *trans-mer-1b* and *cis-fac-3b* collected at 100 mV/s. All CV data were collected in DCM with 0.1 M $(^n\text{Bu}_4\text{N})\text{PF}_6$ using a glassy carbon working electrode, Pt wire counter electrode, and Ag/AgCl-reference electrode.

III. Computational data

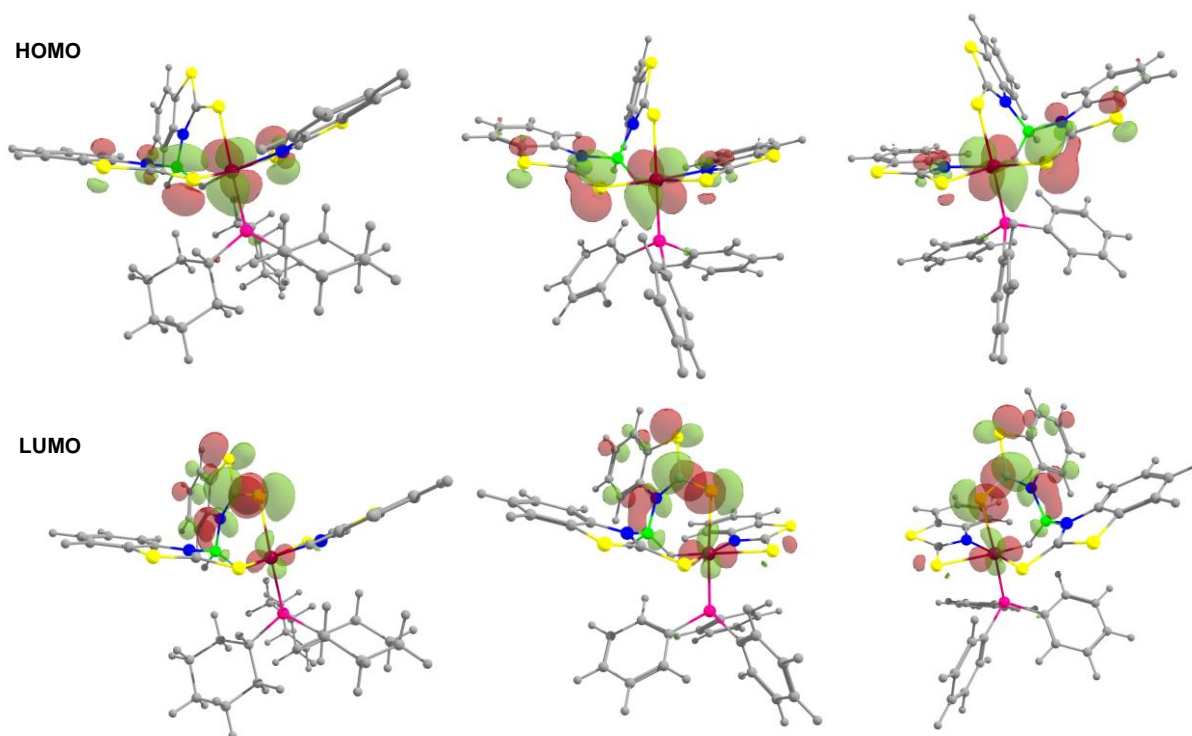


Figure S23. Molecular orbitals (HOMO and LUMO) of *cis-mer-2a* and *cis-fac-3b*. Isosurfaces are plotted at an isovalue of $0.043 a_0^{-3/2}$.

Table S1. Calculated chemical shifts for complexes *trans-mer-1a-b*, *cis-mer-2a* and *cis-fac-3b*.

Comp.	¹ H NMR (ppm)	¹¹ B NMR (ppm)	³¹ P NMR (ppm)
<i>trans-mer-1a</i>	-4.18	-5.40	127.9
<i>trans-mer-1b</i>	-3.11	-5.55	133.3
<i>cis-mer-2a</i>	-15.76	-4.83	155.9
<i>cis-fac-3b</i>	-12.66	-4.98	156.04

Table S2. Calculated natural charges (q), natural valence population (Pop), total energy and HOMO–LUMO gaps of complexes *trans-mer-1a-b*, *cis-mer-2a* and *cis-fac-3b*.

Comp.	q _M	q _P	Pop(M _{val})	Pop(P _{val})	Total Energy (a. u.)	ΔE _{H-L} (eV)
<i>trans-mer-1a</i>	-0.337	1.282	9.116	3.563	-4530.33	1.738
<i>trans-mer-1b</i>	-0.350	1.261	9.157	3.572	-4519.48	1.731
<i>cis-mer-2a</i>	-0.375	1.250	8.354	3.700	-4529.83	1.852
<i>cis-mer-2b</i>	-0.368	1.192	8.348	3.752	-4519.48	1.874
<i>cis-fac-3b</i>	-0.381	1.353	9.208	3.604	-4519.02	1.866

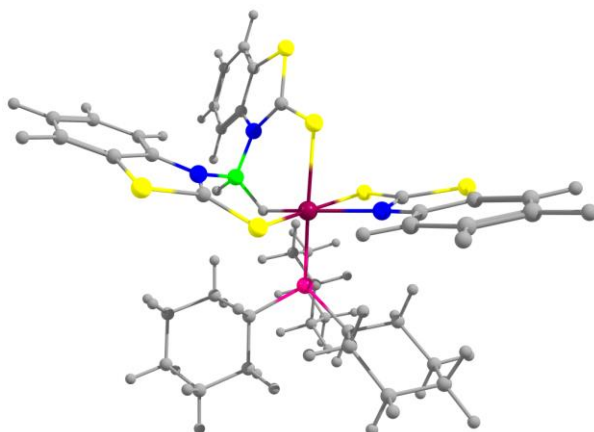


Figure S24. Optimized geometry of *cis-mer-2a*.

Cartesian coordinates for the calculated structure of *cis-mer-2a* (in Å).

Ru	0.331982000	-0.529989000	-0.047168000	C	0.942826000	2.944560000	-0.553616000
B	-2.107458000	0.173188000	0.156623000	H	0.750150000	2.484148000	-1.541553000
H	-2.592288000	1.120863000	0.741779000	C	1.922168000	4.118205000	-0.782815000
H	-0.888468000	0.523188000	0.482197000	H	2.133316000	4.628888000	0.171556000
P	1.543775000	1.432003000	0.434492000	H	2.887567000	3.764165000	-1.171085000
S	0.957385000	-1.542719000	2.150932000	C	1.335148000	5.135138000	-1.779696000
S	3.216741000	-3.594525000	1.335548000	H	2.044827000	5.967739000	-1.916716000
S	0.040759000	0.019347000	-2.273460000	H	1.229004000	4.648585000	-2.766189000
S	-2.381309000	0.573896000	-3.953671000	C	-0.031586000	5.664445000	-1.328265000
S	-0.897293000	-2.622412000	-0.467632000	H	-0.448663000	6.346509000	-2.087117000
S	-3.371367000	-3.622530000	0.958250000	H	0.095629000	6.261951000	-0.406823000
N	1.972828000	-1.881075000	-0.185657000	C	-1.002080000	4.509609000	-1.051093000
N	-2.504826000	0.325683000	-1.362795000	H	-1.233611000	3.989028000	-1.997385000
N	-2.710337000	-1.117396000	0.816023000	H	-1.959222000	4.895541000	-0.663609000
C	3.387928000	1.444009000	0.031954000	C	-0.407716000	3.500852000	-0.054666000
H	3.709354000	2.487123000	0.206506000	H	-1.127494000	2.690354000	0.123900000
C	3.651239000	1.121069000	-1.452546000	H	-0.256821000	4.009839000	0.913542000
H	3.333746000	0.086740000	-1.656187000	C	1.558056000	1.896481000	2.264269000
H	3.045537000	1.765282000	-2.109238000	H	2.155915000	1.065761000	2.683075000
C	5.141611000	1.270580000	-1.801115000	C	0.182384000	1.817152000	2.957749000
H	5.303081000	1.008131000	-2.859375000	H	-0.308272000	0.864754000	2.711483000
H	5.438604000	2.330159000	-1.691557000	H	-0.475199000	2.619344000	2.584455000
C	6.021567000	0.400342000	-0.894244000	C	0.328904000	1.951843000	4.482380000
H	7.087342000	0.558374000	-1.127316000	H	-0.665017000	1.910478000	4.957392000
H	5.808940000	-0.664190000	-1.098091000	H	0.894797000	1.083471000	4.864886000
C	5.749789000	0.696699000	0.586731000	C	1.053502000	3.246538000	4.873440000
H	6.346324000	0.028057000	1.228601000	H	0.425828000	4.113517000	4.596112000
H	6.077727000	1.727173000	0.817714000	H	1.190005000	3.297134000	5.966038000
C	4.258638000	0.550510000	0.936995000	C	2.408095000	3.358494000	4.161570000
H	4.110650000	0.803435000	1.997519000	H	3.082802000	2.566275000	4.533504000
H	3.958762000	-0.502254000	0.821125000	H	2.892129000	4.319755000	4.401265000

C	2.261909000	3.217036000	2.635639000	C	-6.271508000	1.297473000	-2.960919000
H	1.673206000	4.069292000	2.254409000	H	-7.234971000	1.546057000	-3.408560000
H	3.254516000	3.283978000	2.164689000	C	-6.160133000	1.142407000	-1.572855000
C	2.043649000	-2.303702000	1.080579000	H	-7.040845000	1.272263000	-0.941653000
C	3.580356000	-3.577301000	-0.381922000	C	-4.940140000	0.818552000	-0.973718000
C	4.476763000	-4.383045000	-1.087313000	H	-4.877173000	0.698137000	0.105927000
H	5.080166000	-5.132058000	-0.571985000	C	-3.807755000	0.649356000	-1.781329000
C	4.573195000	-4.216914000	-2.471793000	C	-2.303738000	-2.348004000	0.404677000
H	5.264398000	-4.841731000	-3.039809000	C	-3.803159000	-1.163393000	1.694142000
C	3.779896000	-3.267347000	-3.136729000	C	-4.374153000	-0.098429000	2.406132000
H	3.856642000	-3.166240000	-4.220813000	H	-3.957200000	0.904344000	2.317157000
C	2.887937000	-2.454901000	-2.436436000	C	-5.467345000	-0.348938000	3.238692000
H	2.252795000	-1.732171000	-2.950619000	H	-5.909705000	0.478423000	3.796286000
C	2.791227000	-2.596657000	-1.043324000	C	-5.996920000	-1.639995000	3.376199000
C	-1.620059000	0.278006000	-2.399141000	H	-6.851961000	-1.812841000	4.031424000
C	-3.931262000	0.815883000	-3.179737000	C	-5.423861000	-2.714358000	2.691233000
C	-5.150396000	1.135653000	-3.779173000	H	-5.816137000	-3.725714000	2.807332000
H	-5.222828000	1.258553000	-4.860835000	C	-4.326096000	-2.466817000	1.864910000

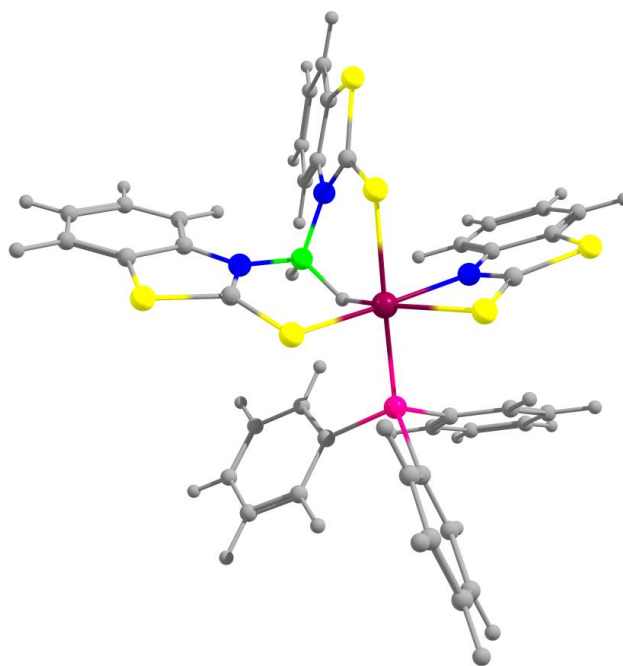


Figure S25. Optimized geometry of *cis-fac-3b*.

Cartesian coordinates for the calculated structure of *cis-fac-3b* (in Å)

Ru	0.491593000	0.034264000	-0.900464000	H	-0.713546000	2.937791000	3.956591000
P	2.165579000	0.922838000	0.426431000	C	0.709614000	4.388421000	3.211415000
C	1.626505000	2.307597000	1.537594000	H	0.353436000	5.194330000	3.856266000
C	0.561342000	2.098735000	2.433242000	C	1.758596000	4.612317000	2.317493000
H	0.067994000	1.126983000	2.475174000	H	2.227774000	5.596684000	2.257608000
C	0.112699000	3.125049000	3.267569000	C	2.216524000	3.581363000	1.490226000

H	3.038118000	3.777404000	0.801343000	C	1.315302000	-5.555688000	0.244779000
C	3.636954000	1.675450000	-0.423253000	H	1.811542000	-6.434572000	-0.169902000
C	3.524080000	2.177357000	-1.728716000	C	1.434071000	-4.308155000	-0.371685000
H	2.579557000	2.085994000	-2.265422000	S	-1.168787000	-0.858344000	-2.456137000
C	4.612092000	2.791218000	-2.355935000	S	-3.669397000	-2.450397000	-1.897962000
H	4.503278000	3.170319000	-3.374043000	C	-2.419460000	-1.312993000	-1.428087000
C	5.833373000	2.909248000	-1.687620000	N	-2.548094000	-0.910721000	-0.134696000
H	6.685971000	3.381802000	-2.179768000	C	-3.551695000	-1.605141000	0.559429000
C	5.958643000	2.413639000	-0.386145000	C	-3.838529000	-1.551370000	1.931414000
H	6.908997000	2.499158000	0.145125000	H	-3.240168000	-0.924345000	2.591851000
C	4.869492000	1.803200000	0.241746000	C	-4.886158000	-2.324800000	2.436964000
H	4.982756000	1.419712000	1.257248000	H	-5.107228000	-2.284778000	3.504991000
C	3.010271000	-0.255429000	1.580617000	C	-5.648423000	-3.153099000	1.601295000
C	2.897768000	-0.199104000	2.978120000	H	-6.463448000	-3.747442000	2.016904000
H	2.324350000	0.599848000	3.449605000	C	-5.357102000	-3.238014000	0.237741000
C	3.533573000	-1.151972000	3.782459000	H	-5.928998000	-3.896877000	-0.417212000
H	3.436899000	-1.089872000	4.868630000	C	-4.303864000	-2.472801000	-0.266388000
C	4.293311000	-2.169758000	3.202585000	S	-0.008648000	2.157505000	-1.680732000
H	4.788926000	-2.912579000	3.830869000	S	-2.403333000	3.932238000	-1.551023000
C	4.420366000	-2.228149000	1.810167000	C	-1.555779000	2.464465000	-1.092931000
H	5.017210000	-3.015814000	1.345883000	N	-2.271883000	1.690439000	-0.227574000
C	3.783657000	-1.282049000	1.006183000	C	-3.498073000	2.280636000	0.131292000
H	3.899156000	-1.329481000	-0.078931000	C	-4.452483000	1.777579000	1.024645000
S	2.088439000	-0.811483000	-2.567548000	H	-4.294099000	0.827408000	1.529797000
S	2.328637000	-3.887642000	-1.823043000	C	-5.619566000	2.509390000	1.258593000
C	1.797109000	-2.218013000	-1.635796000	H	-6.361541000	2.113702000	1.954196000
N	1.019299000	-2.010247000	-0.574633000	C	-5.852794000	3.731768000	0.615036000
C	0.789125000	-3.157926000	0.160874000	H	-6.772738000	4.285762000	0.808072000
C	0.020565000	-3.272763000	1.328074000	C	-4.909651000	4.247706000	-0.277397000
H	-0.468403000	-2.389240000	1.740257000	H	-5.077034000	5.200535000	-0.781774000
C	-0.096204000	-4.520617000	1.939123000	C	-3.742668000	3.517499000	-0.507558000
H	-0.694659000	-4.618748000	2.846567000	B	-1.765685000	0.340913000	0.399971000
C	0.541667000	-5.652688000	1.404664000	H	-1.959075000	0.399583000	1.596314000
H	0.434407000	-6.620190000	1.897922000	H	-0.476105000	0.203191000	0.510403000