

Electronic Supporting Information

Stereospecific control of the metal-centred chirality of rhodium(III) and iridium(III) complexes bearing tetradentate CNN'P ligands

María Carmona,^a Ricardo Rodríguez,^{*,a} Isabel Méndez,^a Vincenzo Passarelli,^{*,a,b} Fernando J. Lahoz,^a Pilar García-Orduña^a and Daniel Carmona^{*,a}

^a Instituto de Síntesis Química y Catálisis Homogénea (ISQCH), CSIC - Universidad de Zaragoza, Departamento de Química Inorgánica, Pedro Cerbuna 12, 50009 Zaragoza, Spain, E-mail: dcarmona@unizar.es (D. C.), riromar@unizar.es (R. R.), passarel@unizar.es (V. P.)

^b Centro Universitario de la Defensa, Ctra. Huesca s/n, 50090 Zaragoza, Spain

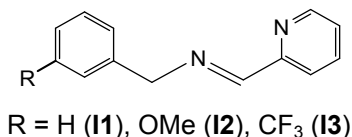
E-mails: dcarmona@unizar.es (D. C.); riromar@unizar.es (R. R.); passarel@unizar.es (V. P.)

Table of Contents

1- Preparation and characterization of the imines I1-I3 and amines A1-A3	S2
2- Selected NMR spectra of compound 1b-3b and 5	S5
3- Atomic coordinates of calculated structures	S14
4- Energies from relaxed PSE calculations	S49
5- References	S50

1- Preparation and characterization of the imines **I1-I3** and amines **A1-A3**.

Amines **A1-A3** were obtained by condensation of 2-pyridinecarboxaldehyde with the corresponding benzylamine followed by reduction of the resulting imine (**I1-I3**) with NaBH₄ in methanol, according to described procedures for similar ligands.^{S1-S3}

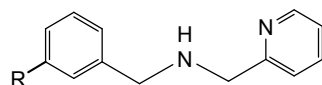


Imine **I1**. ¹H NMR (400.16 MHz, CDCl₃, RT, ppm): δ = 8.52 (m, 1H, 6-CH(Py)), 8.43 (brs, 1H, NCH), 7.96 (brd, *J* = 7.9 Hz, 1H, H(Ar)), 7.49 (ptd, *J* = 7.7, 1.9 Hz, 1H, H(Ar)), 7.33-7.20 (m, 4H, H(Ar)), 7.17 (m, 1H, H(Ar)), 7.07 (m, 1H, H(Ar)), and 4.74 (s, 2H, NCH₂).
¹³C{¹H} NMR (100.62 MHz, CDCl₃, RT, ppm): δ = 162.73 (s, NCH), 154.58 (s, 2-C(Py)), 149.33 (s, 6-CH(Py)), 138.85 (s, C(Ar)), 136.34 (s, CH(Ar)), 128.52 (s, 2C, CH(Ar)), 128.14 (s, 2C, CH(Ar)), 127.09 (s, CH(Ar)), 124.70 (s, CH(Ar)), 121.19 (s, CH(Ar)), and 64.81 (s, NCH₂).

Imine **I2**. ¹H NMR (300.13 MHz, CDCl₃, RT, ppm): δ = 8.61 (brd, *J* = 4.7 Hz, 1H, 6-CH(Py)), 8.46 (brs, 1H, NCH), 8.04 (brd, *J* = 8.0 Hz, 1H, H(Ar)), 7.66 (ptd, *J* = 7.8, 1.7 Hz, 1H, H(Ar)), 7.32-7.13 (m, 2H, H(Ar)), 6.99-6.69 (m, 3H, H(Ar)), 4.82 (s, 2H, NCH₂), and 3.75 (s, 3H, OMe). ¹³C{¹H} NMR (75.48 MHz, CDCl₃, RT, ppm): δ = 162.83 (s, NCH), 159.82 (s, C(OMe)), 154.52 (s, 2-C(Py)), 149.35 (s, 6-CH(Py)), 140.31 (s, C(Ar)), 136.46 (s, CH(Ar)), 129.53 (s, CH(Ar)), 124.78 (s, CH(Ar)), 121.29 (s, CH(Ar)), 120.44 (s, CH(Ar)), 113.78 (s, CH(Ar)), 112.57 (s, CH(Ar)), 64.75 (s, NCH₂), and 55.11 (s, OMe).

Imine **I3**. ¹H NMR (400.16 MHz, CDCl₃, RT, ppm): δ = 8.57 (ddd, *J* = 4.9, 1.7, 1.0 Hz, 1H, 6-CH(Py)), 8.43 (brs, 1H, NCH), 7.98 (ptd, *J* = 8.9, 1.1 Hz, 1H, H(Ar)), 7.66 (ptdd, *J* = 7.8,

1.7, 0.6 Hz, 1H, H(Ar)), 7.55 (brs, 1H, H(Ar)), 7.49-7.31 (m, 3H, H(Ar)), 7.24 (ddd, $J = 7.6, 4.9, 1.2$ Hz, 1H, H(Ar)), and 4.82 (s, 2H, NCH₂). $^{13}\text{C}\{^1\text{H}\}$ NMR (100.62 MHz, CDCl₃, RT, ppm): $\delta = 163.50$ (s, NCH), 154.26 (s, 2-C(Py)), 149.51 (s, 6-CH(Py)), 139.85 (s, C(Ar)), 136.63 (s, CH(Ar)), 131.41 (s, CH(Ar)), 130.71 (q, $J = 32.2$ Hz, C(CF₃)), 128.97 (s, CH(Ar)), 125.03 (s, CH(Ar)), 124.79 (q, $J = 3.8$ Hz, CH(Ar)), 124.62 (q, $J = 272.3$ Hz, CF₃), 123.98 (q, $J = 3.8$ Hz, CH(Ar)), 121.45 (s, CH(Ar)), and 64.26 (s, NCH₂). $^{19}\text{F}\{^1\text{H}\}$ NMR (376.48 MHz, CDCl₃, RT, ppm): $\delta = -62.52$ (s).



R = H (**A1**), OMe (**A2**), CF₃ (**A3**)

Amine **A1**. ^1H NMR (300.13 MHz, CDCl₃, RT): $\delta = 8.52$ (d, $J = 4.6$ Hz, 1H, 6-CH(Py)), 7.54 (ptd, $J = 7.7, 1.8$ Hz, 1H, H(Ar)), 7.38-7.15 (m, 6H, H(Ar)), 7.07 (ddd, $J = 7.3, 4.8, 0.5$ Hz, 1H, H(Ar)), 3.89 (s, 2H, CH₂), 3.80 (s, 2H, CH₂), and 2.32 (brs, 1H, NH).

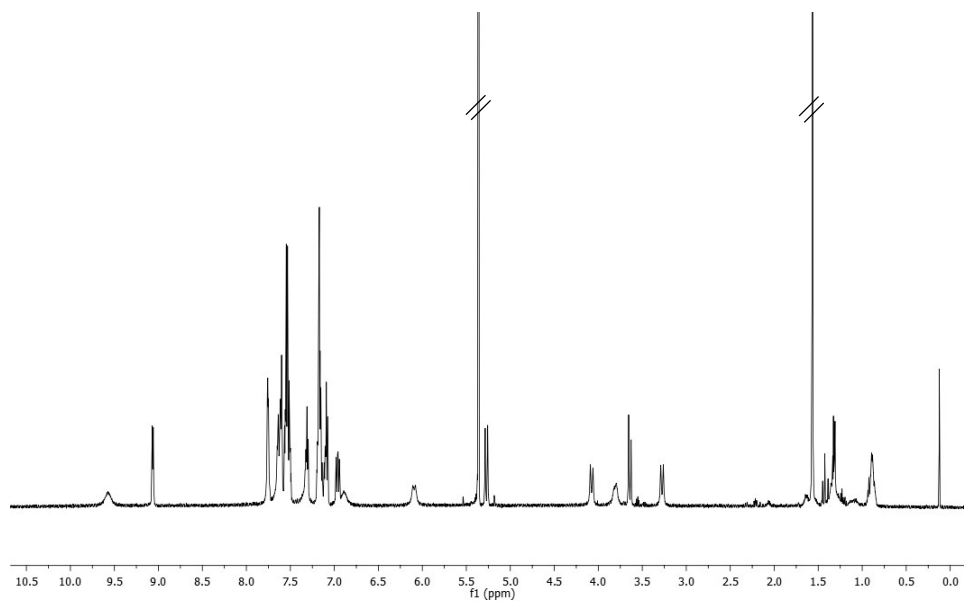
$^{13}\text{C}\{^1\text{H}\}$ NMR (100.62 MHz, CDCl₃, RT, ppm): $\delta = 159.82$ (s, 2-C(Py)), 148.86 (s, 6-CH(Py)), 140.24 (s, C(Ar)), 135.84 (s, CH(Ar)), 128.03 (s, 2C, CH(Ar)), 127.90 (s, 2C, CH(Ar)), 126.57 (s, CH(Ar)), 121.76 (s, CH(Ar)), 121.43 (s, CH(Ar)), 54.20 (s, 2H, CH₂), and 53.09 (s, CH₂).

Amine **A2**. ^1H NMR (300.13 MHz, CDCl₃, RT): $\delta = 8.58$ (brd, $J = 4.8$ Hz, 1H, 6-CH(Py)), 7.67 (ptd, $J = 7.7, 1.8$ Hz, 1H, H(Ar)), 7.39-7.11 (m, 3H, H(Ar)), 7.01-6.79 (m, 3H, H(Ar)), 3.98 (s, 2H, CH₂), 3.88 (s, 2H, CH₂), 3.83 (s, 3H, OMe), and 3.27 (brs, 1H, NH). $^{13}\text{C}\{^1\text{H}\}$ NMR (100.62 MHz, CDCl₃, RT, ppm): $\delta = 157.81$ (s, 2-C(Py)), 157.75 (s, C(OMe)), 147.37 (s, 6-CH(Py)), 139.85 (s, C(Ar)), 134.52 (s, CH(Ar)), 127.46 (s, CH(Ar)), 120.45 (s, CH(Ar)), 120.04 (s, CH(Ar)), 118.63 (s, CH(Ar)), 111.69 (s, CH(Ar)), 110.64 (s, CH(Ar)), 53.27 (s, OMe), 52.52 (s, CH₂), and 51.52 (s, CH₂).

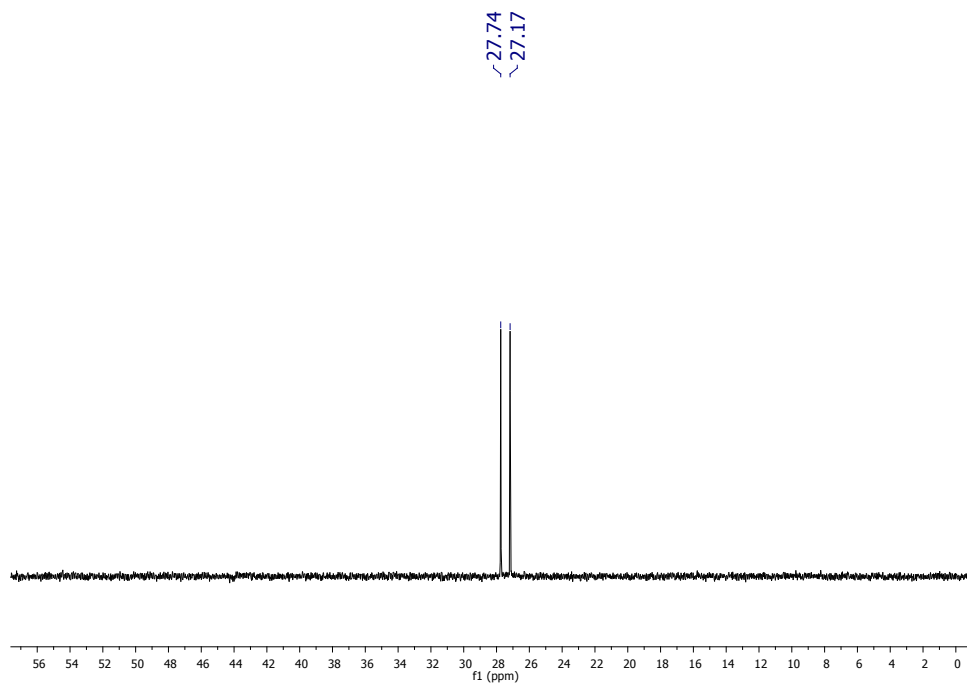
Amine **A3**. ^1H NMR (400.16 MHz, CDCl_3 , RT): δ = 8.58 (brd, J = 4.9 Hz, 1H, 6-CH(Py)), 7.66 (m, 2H, H(Ar)), 7.58 (brd, J = 7.5 Hz, 1H, H(Ar)), 7.52 (brd, J = 7.8 Hz, 1H, H(Ar)), 7.45 (brd, J = 7.5 Hz, 1H, H(Ar)), 7.31 (brd, J = 7.8 Hz, 1H, H(Ar)), 7.18 (brdd, J = 7.5, 4.8 Hz, 1H, H(Ar)), 3.95 (s, 2H, CH_2), 3.91 (s, 2H, CH_2), and 2.38 (brs, 1H, NH). $^{13}\text{C}\{^1\text{H}\}$ NMR (100.62 MHz, CDCl_3 , RT, ppm): δ = 159.31 (s, 2-C(Py)), 149.37 (s, 6-CH(Py)), 141.11 (s, C(Ar)), 136.52 (s, CH(Ar)), 131.59 (s, CH(Ar)), 130.84 (q, J = 31.9 Hz, C(CF_3)), 128.80 (s, CH(Ar)), 124.95 (q, J = 3.8 Hz, CH(Ar)), 124.22 (q, J = 272.2 Hz, CF_3), 123.85 (q, J = 3.8 Hz, CH(Ar)), 122.39 (s, CH(Ar)), 122.09 (s, CH(Ar)), 54.45 (s, CH_2), and 52.97 (s, CH_2). $^{19}\text{F}\{^1\text{H}\}$ NMR (376.48 MHz, CDCl_3 , RT, ppm): δ = -62.49 (s).

2- Selected NMR spectra of compound 1b-3b and 5.

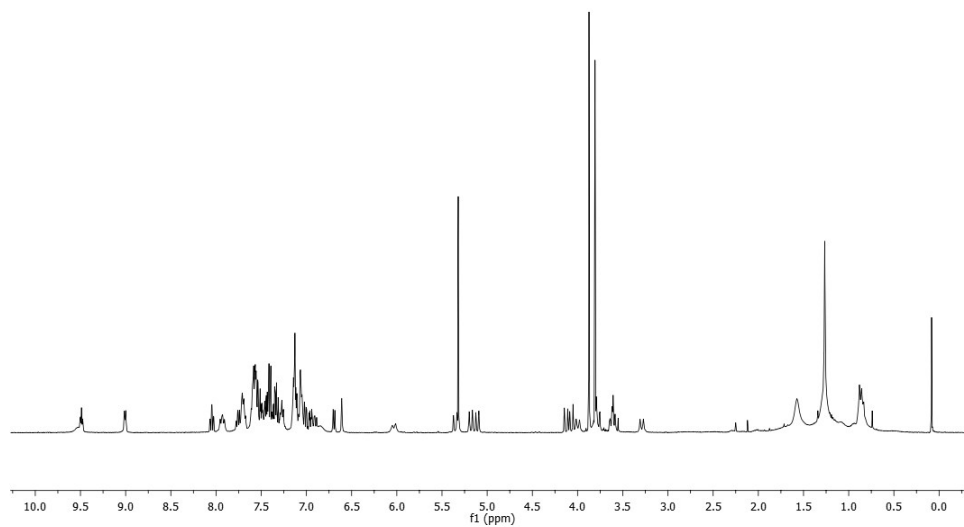
^1H NMR (500.13 MHz, CD_2Cl_2 , RT) of 1b



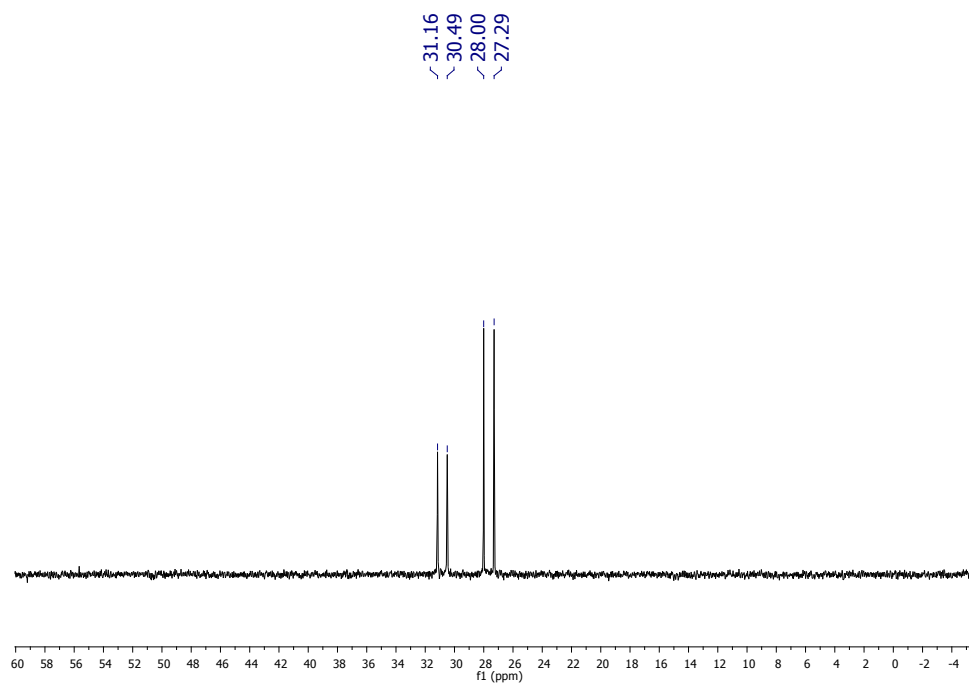
$^{31}\text{P}\{^1\text{H}\}$ NMR (202.46 MHz, CD_2Cl_2 , RT) of 1b



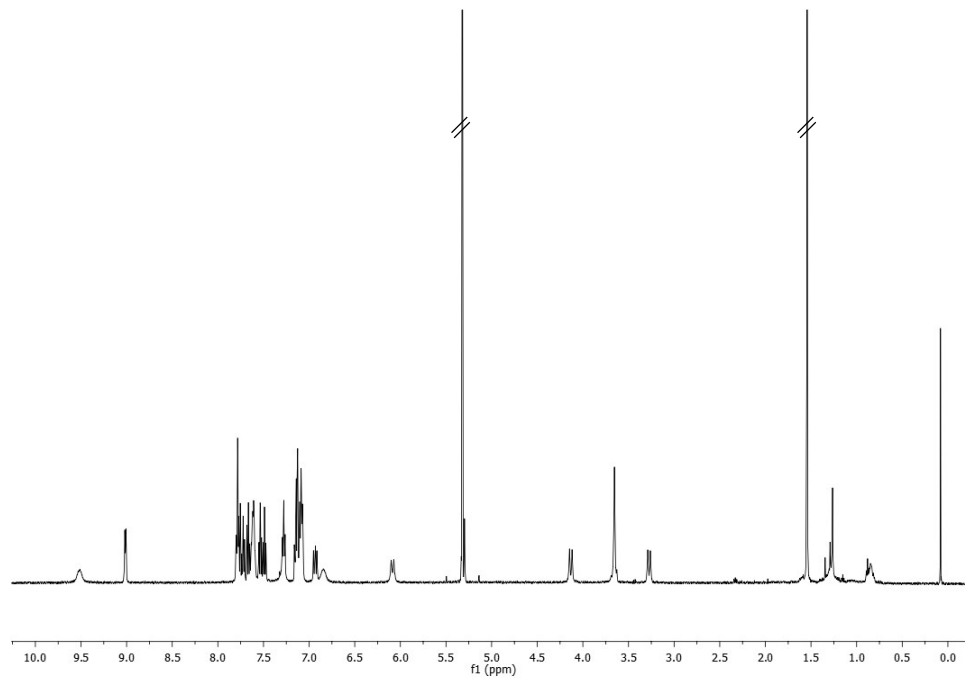
^1H NMR (400.16 MHz, CD_2Cl_2 , RT) of 2a/2b mixture (molar ratio 40/60)



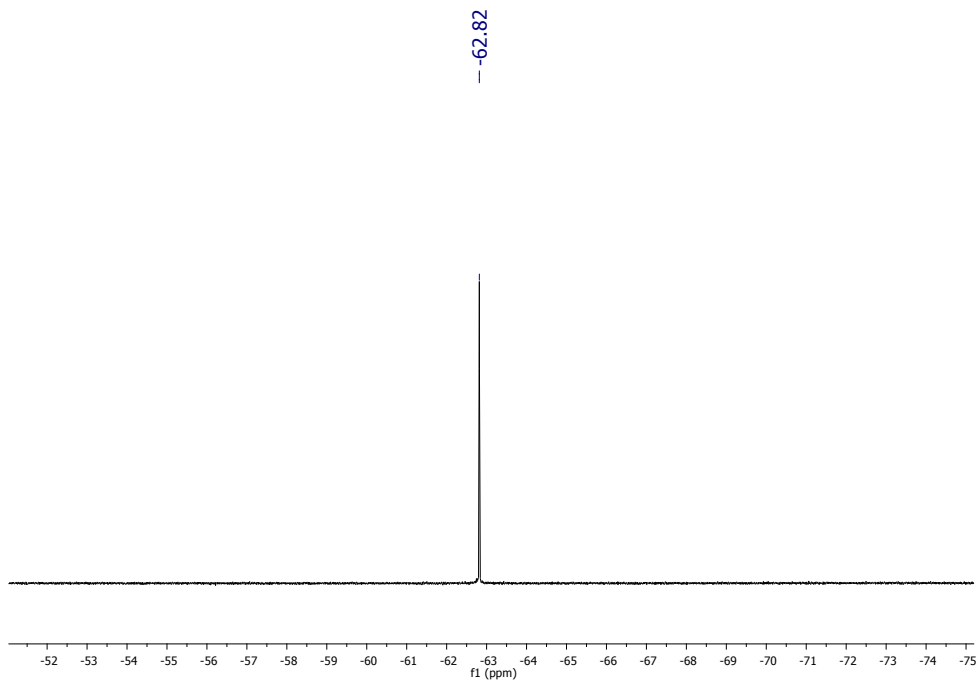
$^{31}\text{P}\{^1\text{H}\}$ NMR (161.98 MHz, CD_2Cl_2 , RT) of 2a/2b mixture (molar ratio 40/60)



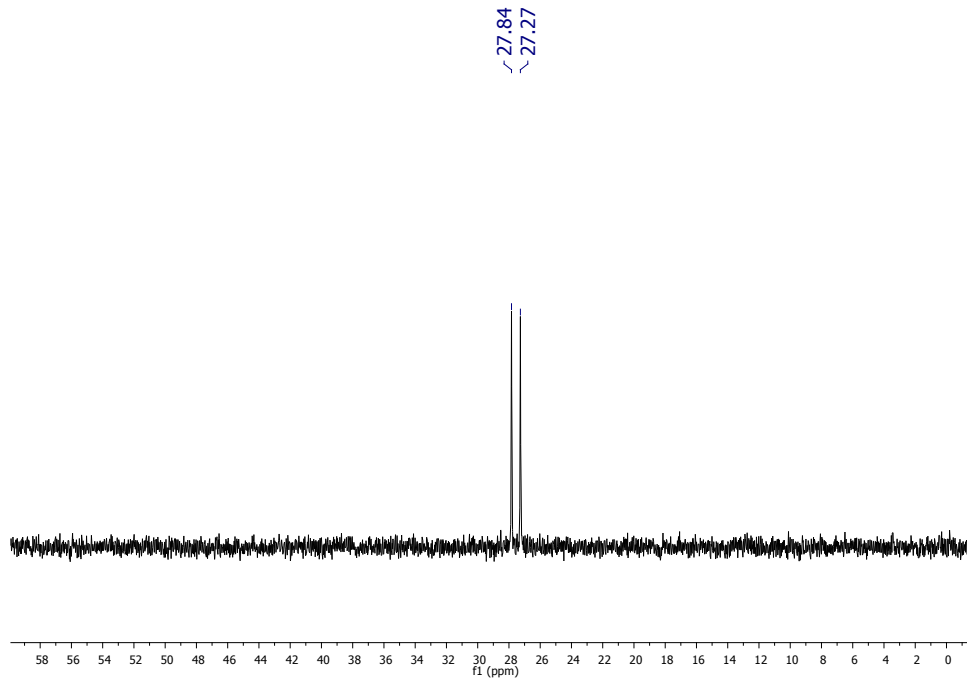
^1H NMR (500.13 MHz, CD_2Cl_2 , RT) of 3b



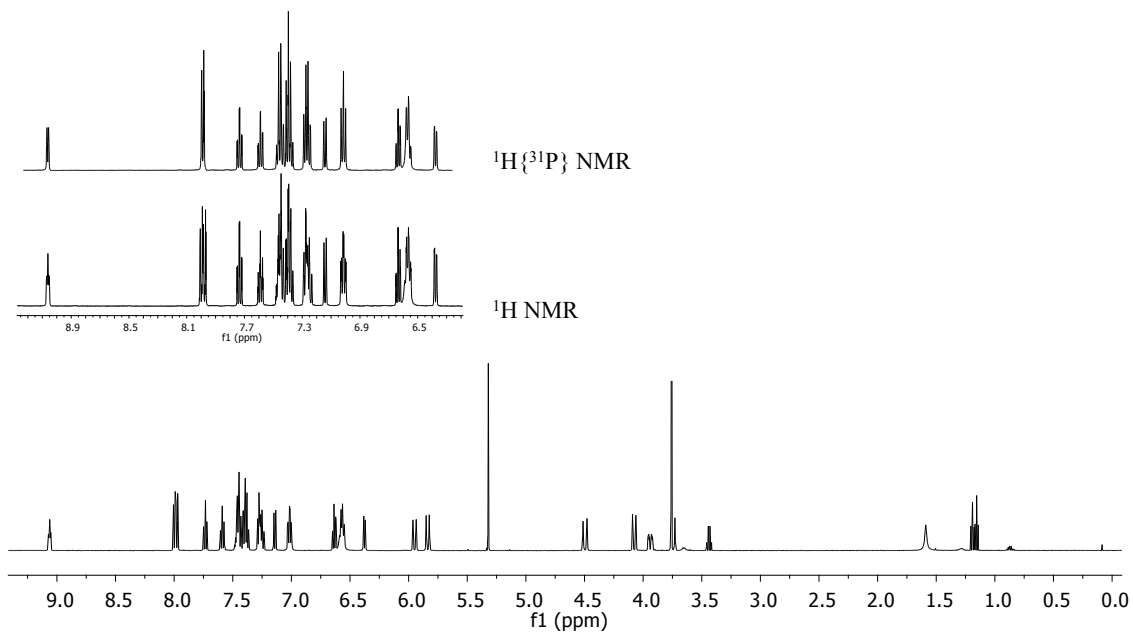
$^{19}\text{F}\{^1\text{H}\}$ NMR (282.33 MHz, CD_2Cl_2 , RT) of 3b



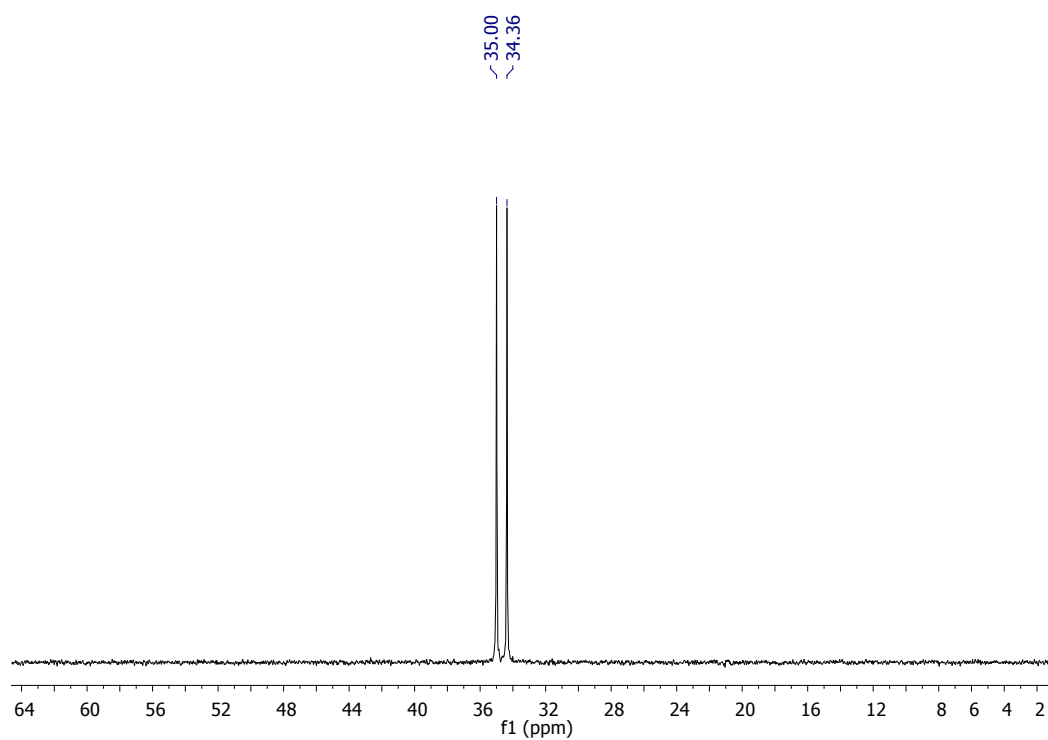
$^{31}\text{P}\{^1\text{H}\}$ NMR (202.46 MHz, CD_2Cl_2 , RT) of 3b



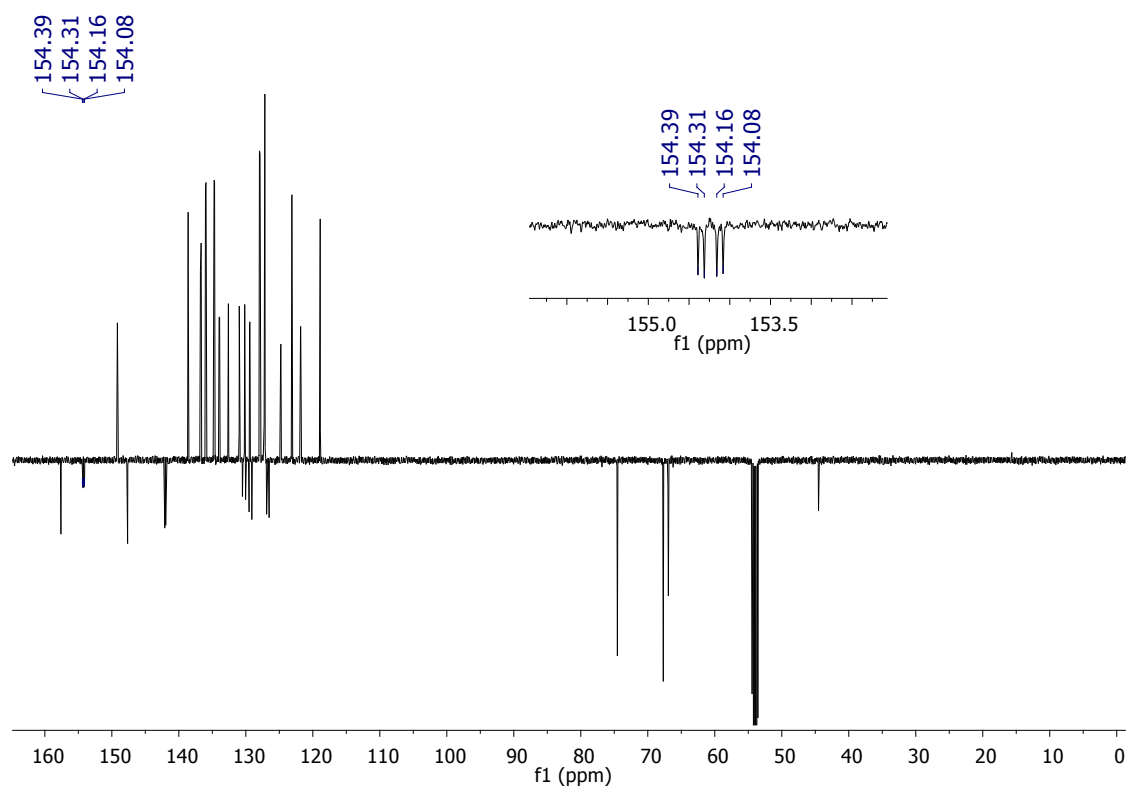
^1H NMR (500.13 MHz, CD_2Cl_2 , RT) of 5



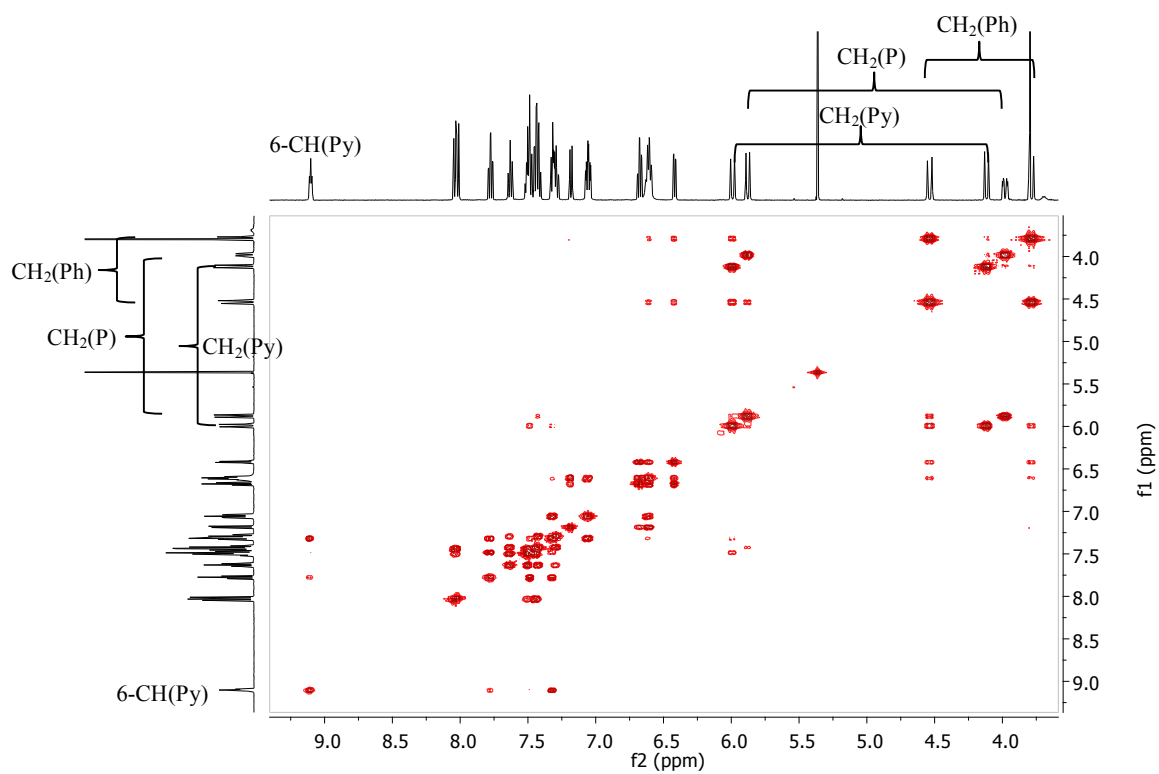
$^{31}\text{P}\{^1\text{H}\}$ NMR (202.46 MHz, CD_2Cl_2 , RT) of 5



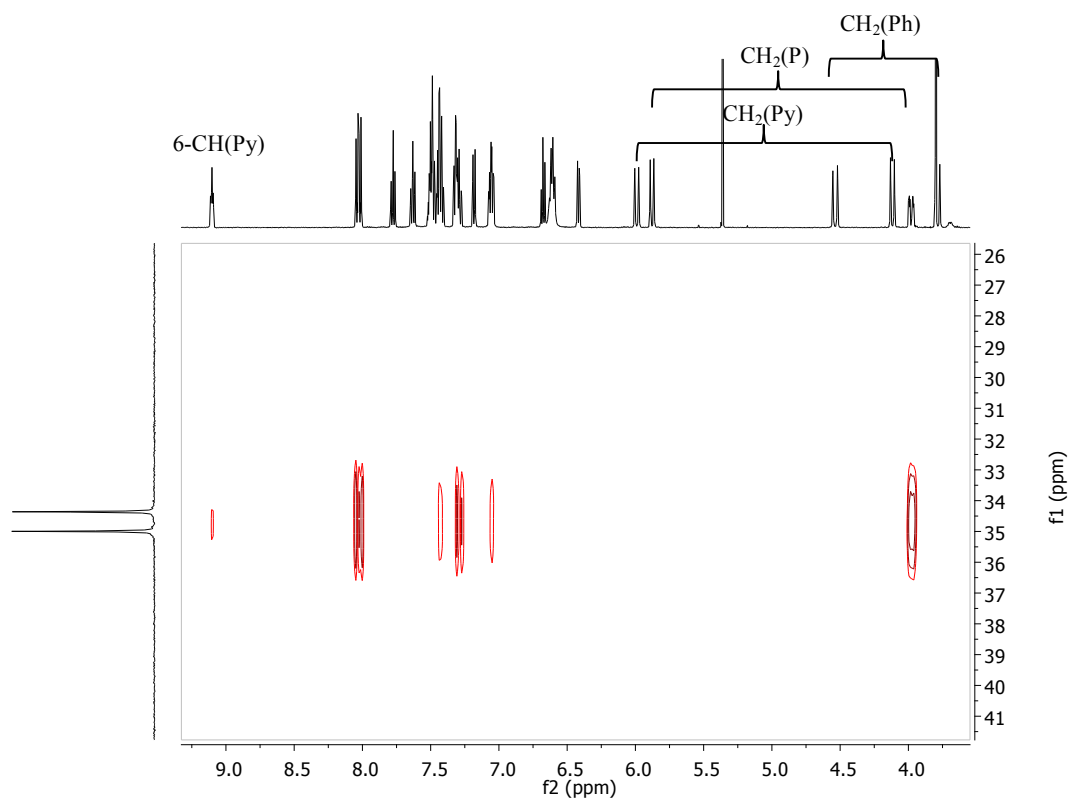
$^{13}\text{C}\{^1\text{H}\}$ NMR (125.77 MHz, CD_2Cl_2 , RT) of **5**



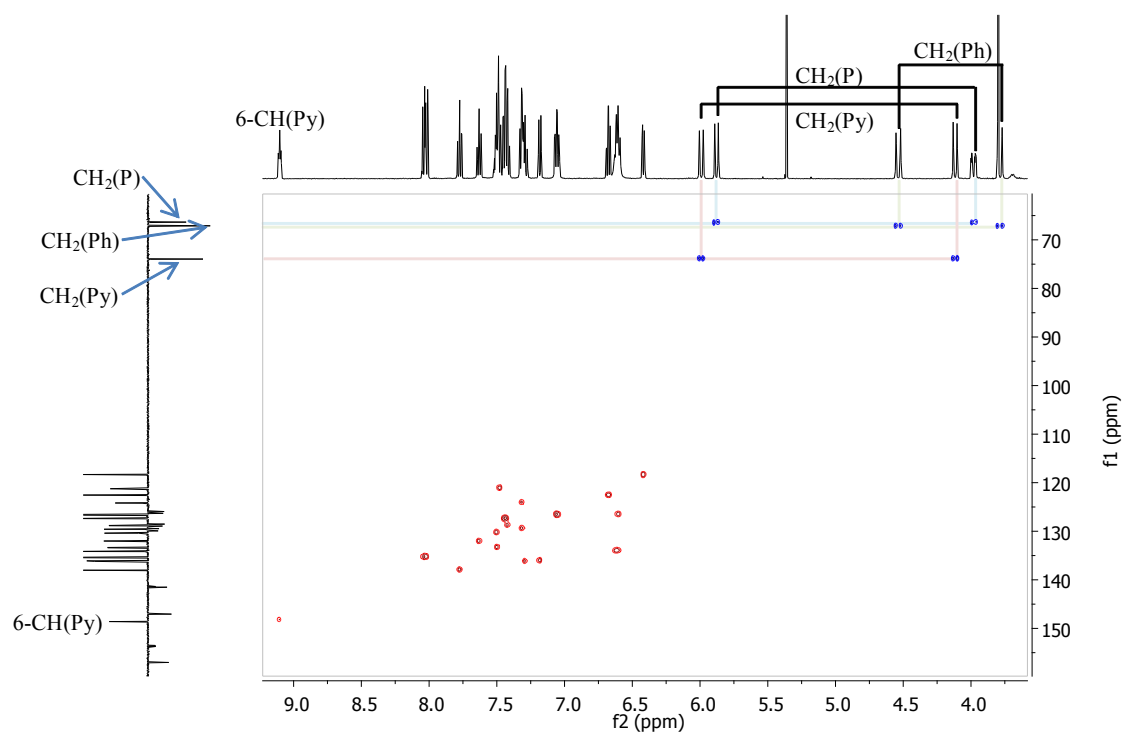
^1H - ^1H COSY (CD_2Cl_2 , RT) of **5**



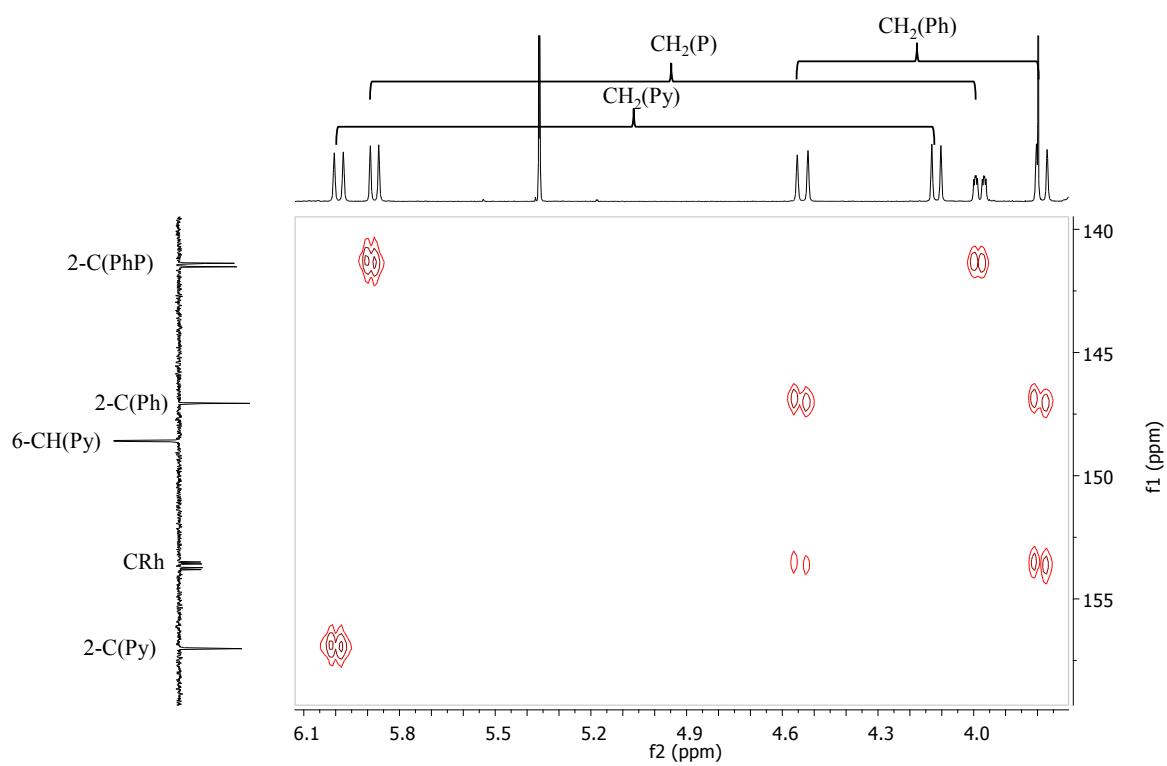
^1H - ^{31}P HMBC (CD_2Cl_2 , RT) of 5



^1H - ^{13}C HSQC (CD_2Cl_2 , RT) of 5

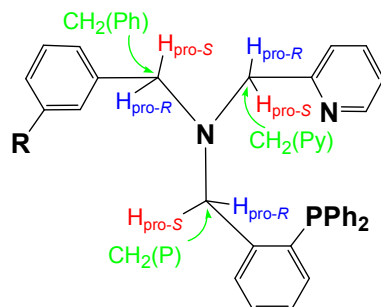


^1H - ^{13}C HMBC (CD_2Cl_2 , RT) of **5**

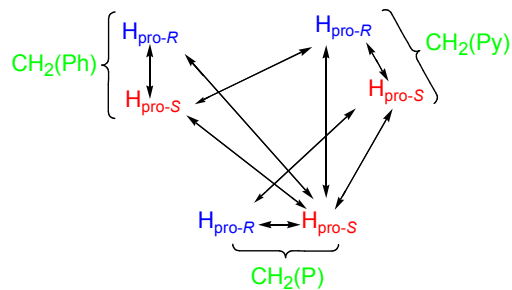


Assignment of the Methylene Descriptors (A) and NOE Relationship Pattern (B) on (*R*_{Nam})-OC-6-54-C Isomers

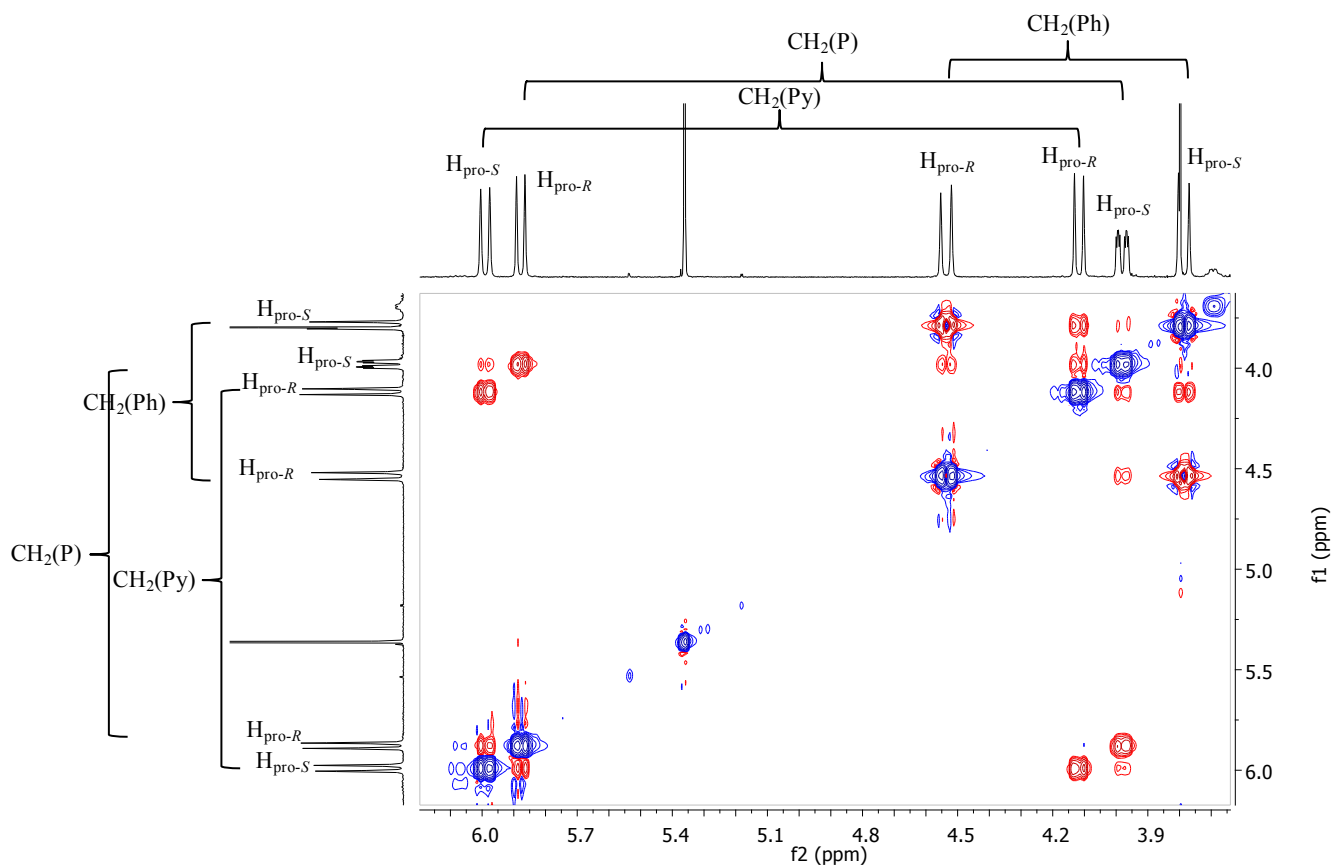
A: Methylene descriptors



B: NOE pattern



¹H-¹H NOESY (CD₂Cl₂, RT) of 5



RhCl ₃ (κ ³ N,N',P-LH1) (1a)							
Rh	-0.04322500	-1.20185200	0.03905900	C	3.21870100	-1.53722600	-1.85109400
Cl	1.48797100	-2.98142200	0.58420900	C	4.41214000	-2.09184700	-2.31618300
Cl	0.29052200	-1.70818400	-2.31190100	C	5.47324800	-2.32610700	-1.43993300
P	1.70539500	0.38157000	0.02607100	C	5.33667300	-2.00580500	-0.08812700
N	-1.60972600	0.23166800	-0.52778300	C	4.14791600	-1.44811700	0.38411600
N	-1.74181300	-2.47974900	-0.00277500	C	0.60231000	-2.01112600	0.85862200
C	2.92870400	0.22293000	-1.34853100	C	1.22052900	-3.26816000	0.90552000
C	3.29734600	1.32529100	-2.13469800	C	0.56070900	-4.36876700	1.45434700
H	2.84753800	2.29684100	-1.96937700	C	-0.72164600	-4.21640700	1.97581700
C	4.25329100	1.18436600	-3.14406300	C	-1.34723300	-2.97012300	1.91915200
C	4.52534700	2.04666100	-3.74540000	C	-0.71655500	-1.86118700	1.34119800
C	4.85468200	-0.05262000	-3.37629300	C	-1.43506800	-0.53049200	1.35770100
H	5.59973300	-0.15887400	-4.15923500	C	-2.36672100	1.42823900	0.31539200
C	4.48886200	-1.15584200	-2.60062100	H	-2.86822500	1.76136200	-0.59523500
C	4.94575200	-2.12464600	-2.77972800	H	-3.10916100	1.35113100	1.11416700
C	3.52554000	-1.02503400	-1.60071600	C	-1.32345800	2.45563800	0.64250000
H	3.22450100	-1.89154600	-1.02276200	C	-1.58342000	3.54039800	1.47624700
C	2.73324300	0.47252000	1.55540800	C	-0.62801500	4.54698500	1.60302400
C	2.20267200	1.05843700	2.71852200	C	0.56399400	4.43670600	0.89030900
H	1.20148900	1.47185400	2.71287600	C	0.77519400	3.31453500	0.09743900
C	2.96065500	1.12024600	3.88697200	C	-2.74222500	-0.76167200	-0.77446400
H	2.53925600	1.58329000	4.77417800	C	-4.14538800	-0.91110000	-0.21248300
C	4.25263000	0.58885500	3.91745800	C	-4.51356100	-2.06088300	0.50227300
H	4.84043200	0.63671000	4.82930600	C	-5.81612800	-2.22835400	0.97719000
C	4.78535200	0.00244900	2.76919500	C	-6.78008400	-1.24825700	0.73504700
H	5.79077600	-0.40741200	2.77972900	C	-6.43779000	-0.11168800	-0.00182000
C	4.03335800	-0.05350500	1.59329800	C	-5.13591000	0.04981500	-0.47715000
C	1.02997600	2.08489900	-0.17422000	H	3.31985700	1.68623600	0.46632000
C	1.80464000	3.16674300	0.28231500	H	4.15121400	2.99630400	2.38308200
C	2.72585400	2.97592600	0.82033200	H	3.40004100	2.45122200	4.69174500
H	1.42806900	4.48655100	0.04115000	H	1.81735300	0.56911100	5.06233200
H	2.04884600	5.30000400	0.40289000	H	0.99435500	-0.75483600	3.15919300
C	0.26385700	4.74498200	-0.67860500	H	2.40048200	-1.36118600	-2.53548800
H	-0.03916200	5.76530100	-0.89158600	H	4.51018700	-2.33759600	-3.36937500
C	-0.52046800	3.68139000	-1.12139200	H	6.40064100	-2.75553700	-1.80721600
H	-1.42848800	3.88998000	-1.67861700	H	6.15373300	-2.18591700	0.60378400
C	-0.17300000	2.34454600	-0.87086200	H	4.06360300	-1.20720700	1.43749300
C	-1.08630200	1.28746100	-1.46460300	H	2.22675200	-3.39043600	0.52337000
H	-1.94790300	1.79512400	-1.90991400	H	1.05715600	-5.33352300	

C	1.11258100	-2.37733400	0.64421000	H	-5.61039400	-0.17451500	2.72377300
C	1.26618500	-3.47526900	1.48932300	H	-3.16764400	-0.14973100	2.51078900
C	0.27991500	-4.45779900	1.51797300	H	-2.49337600	3.13598700	0.24465900
C	-0.83276400	-4.32200300	0.68810600	H	-2.13614500	5.21116500	-1.01024000
C	-0.93969300	-3.19207700	-0.11343500	H	-0.33051500	5.31367600	-2.73987000
C	2.86045000	0.55411700	-0.97189500	H	1.11256400	3.35502300	-3.11086800
C	4.22421800	0.74403100	-0.33504500	H	4.37412700	-2.66262500	-0.19218900
C	4.56828800	1.96144700	0.27568400	H	4.05258800	-4.36595700	1.61146500
C	5.83658000	2.15612800	0.82532400	H	1.75860300	-4.65850100	2.59918500
C	6.78924800	1.13673900	0.76451500	H	-0.11552400	-3.27354800	1.69375700
C	6.47064000	-0.07055700	0.13852200	H	1.19836600	1.54825500	0.51173500
C	5.20185500	-0.26110700	-0.41115000	H	1.87336200	0.05028900	1.11353600
H	-4.09728400	1.81480300	-0.47968900	H	4.27060700	-0.24736600	1.23019600
H	-6.39614700	0.96717800	-0.44626000	H	6.51482600	0.77469500	1.15959900
H	-6.88289100	-1.32623600	0.38964700	H	6.83877300	3.00785900	0.10939900
H	-5.01403200	-2.75730400	1.20466600	H	4.88265800	4.21431100	-0.84341600
H	-2.71277500	-1.92161700	1.17386500	H	2.63819900	3.20168900	-0.75970400
H	-1.03678400	2.79654600	2.22079400	H	3.42099200	-0.61893800	-1.34161600
H	-1.29363900	5.23750900	2.08232300	H	2.14759700	-1.48402600	-2.23497100
H	-2.04243700	6.30296500	-0.03780200	H	0.74489700	0.43310600	-2.89828700
H	-2.51595000	4.88768800	-2.02857000	H	2.07541700	1.46714300	-2.36241500
H	-2.21240900	2.44730400	-1.91597500				
H	-2.69541900	-0.08518300	2.91719600	TS_25B-B25			
H	-1.72205500	-0.53266800	5.13036700	Rh	-0.08760800	0.47985700	-1.17748400
H	0.74673600	-0.40565700	5.45532200	P	1.47581500	-0.54678500	0.22148500
H	2.20196900	0.22646600	3.55753700	Cl	1.75828700	1.19442400	-2.53957300
H	2.15904700	-3.55839600	2.09884300	Cl	-0.29446300	-1.55213100	-2.46087200
H	0.38476100	-5.32046800	2.16740900	Cl	-1.57696800	1.63767300	-2.85972400
H	-1.61550900	-5.07104600	0.65988200	N	-1.86582200	0.08547900	0.11360300
H	-1.77873400	-3.02623100	-0.77726400	N	-0.12899600	2.25887200	-0.10388000
H	3.84288800	2.77005200	0.30732000	C	2.85422500	0.56009300	0.76899900
H	6.08172900	3.10556600	1.29201800	C	4.11412500	0.57448900	0.15190000
H	7.77743200	1.28708200	1.18908500	C	5.11619600	1.43179100	0.61079600
H	7.21216100	-0.86084200	0.06816500	C	4.87580700	2.28761200	1.68668400
H	4.97931800	-1.19428700	-0.92096500	C	3.62588800	2.27949200	2.30905500
H	1.15179200	1.79980700	0.59931700	C	2.62285400	1.42329500	1.85518300
H	2.48718800	1.10145500	1.50855900	C	2.26610800	-2.05353000	-0.49694900
H	2.93052100	-0.09219800	-1.84533600	C	2.09244400	-3.31247200	0.09937600
H	2.45235700	1.50966200	-1.29773000	C	2.69580100	-4.44631200	-0.45022900
				C	3.47827900	-4.34116900	-1.59964900
				C	3.63736800	-3.09594600	-2.21249000
				C	3.02668000	-1.96310000	-1.67671200
				C	0.81112100	-1.08942600	1.83550200
				C	1.77196600	-1.58782100	2.75010700
				C	1.41761000	-2.04448700	4.00845800
				C	0.07238000	-2.00197600	4.38930800
				C	-0.87236900	-1.50174600	3.50819100
				C	-0.53350600	-1.03211600	2.21860700
				C	-1.77786800	-0.51628800	1.50004800
				C	-2.39034200	1.48774300	0.25435800
				H	-2.80953400	1.76807400	-0.71448500
				H	-3.18254800	1.53794900	1.00443900
				C	-1.29823300	2.47317400	0.54498700
				C	-1.49531700	3.61497700	1.31611500
				C	-0.48437900	4.57346100	1.38441100
				C	0.69756500	4.35930900	0.67940300
				C	0.84672700	3.18239100	-0.04712300
				C	-2.85464700	-0.74569500	-0.70992900
				C	-4.26597900	-0.87780900	-0.16766300
				C	-4.65855100	-2.03713100	0.52128900
				C	-5.96532200	-2.18921000	0.98911900
				C	-6.90854300	-1.18452600	0.76589900
				C	-6.54121900	-0.03714500	0.05837800
				C	-5.23474300	0.11054700	-0.40936300
				H	4.33277300	-0.08980000	-0.67341100
				H	6.08760400	1.42280900	0.12590400
				H	5.65837400	2.95113900	2.04203600
				H	3.42850600	2.93559200	3.15122600
				H	1.66467100	1.41980700	2.36356500
				H	1.48731800	-3.42405200	0.99022200
				H	2.54953200	-5.41076400	0.02669100
				H	3.95136600	-5.22273100	-2.02179900
				H	4.22799300	-3.00466100	-3.11912800
				H	3.11204000	-1.01611400	-2.19570100
				H	2.81594200	-1.61440900	2.45752000
				H	2.17649500	-2.42453400	4.68456300
				H	-0.23525600	-2.35094100	5.37013400
				H	-1.91321600	-1.46188100	3.81887500
				H	-2.43596400	3.75206800	1.83739500
				H	-0.62241600	5.47344700	1.97431400
				H	1.50629800	5.08050800	0.69381900
				H	1.74491300	2.95705200	-0.60664000
				H	-2.86776500	-0.28449100	-1.69635300
				H	-2.39085800	-1.72590600	-0.80890300
				H	-3.94160000	-2.83972600	0.67638900
				H	-6.24617000	-3.09467900	1.51876600
				H	-7.92617200	-1.30069100	1.12683700
				H	-7.27428400	0.73931100	-0.13941600
RhCl3(κ^3N,N',P-LH1) (1c)							
Rh	-0.39424000	-1.30492100	-0.78768000				
P	-1.32713800	0.53128800	0.30840800				
Cl	-2.15117400	-2.76589000	-0.05723700				
Cl	-1.75452100	-0.51574400	-2.61758400				
Cl	0.29998900	-3.13362700	-2.42320200				
N	1.40943100	0.02805600	-0.95984800				
N	1.08089500	-2.24351900	0.36647700				
C	-0.76694500	0.83182600	2.04029900				
C	-0.62629700	-0.27444800	2.89402200				
C	-0.24707700	-0.09659900	4.22558000				
C	0.00463700	1.18630000	4.71590600				
C	-0.13116500	2.29086300	3.87222800				
C	-0.51746300	2.11896100	2.54196100				
C	-3.16614700	0.55056900	0.45982800				
C	-3.98387500	0.94301400	-0.61416300				
C	-5.37217100	0.93599400	-0.48167300				
C	-5.96565200	0.53044500	0.71583600				
C	-5.16104200	0.13758900	1.78598400				
C	-3.77093800	0.14893200	1.66225500				
C	-0.89475000	2.03359900	-0.69799000				
C	-1.69264700	3.17356400	-0.48530700				
C	-1.50034600	4.35299600	-1.20221500				
C	-0.49457000	4.40925300	-2.16258600				
C	0.31815300	3.29646400	-2.37175400				
C	0.14988400	2.09882100	-1.66134100				
C	1.13804000	0.99533800	-2.04820800				
C	2.41002400	-1.03039700	-1.27744400				
C	2.31387400	-2.07000200	-0.17943500				
C	3.39971500	-2.82119300	0.25601200				
C	3.21579800	-3.76970700	1.26339800				
C	1.94742900	-3.93520000	1.81456300				
C	0.89927200	-3.15557400	1.33498200				
C	1.90838600	0.76099500	0.29047900				
C	3.29406200	1.37737500	0.19718100				
C	4.40228800	0.72016400	0.75451100				
C	5.67147000	1.30006900	0.72156400				
C	5.85239500	2.55444100	0.13533000				
C	4.75500100	3.22977100	-0.40343000				
C	3.48604500	2.64946200	-0.36613500				
H	-0.82686900	-1.27342800	2.52423900				
H	-0.14592600	-0.96081300	4.87467100				
H	0.30644600	1.32453800	5.74956000				
H	0.06418100	3.29099600	4.24664400				
H	-0.61220800	2.98893400	1.90184900				
H	-3.53939300	1.25406400	-1.55002900				
H	-5.98896100	1.24979200	-1.31840400				
H	-7.04698800	0.52560600	0.81501300				

H	-4.97464900	0.99543500	-0.98261300	C	-5.72199100	1.44821400	0.12363200
H	-2.20659800	0.21879900	2.18395700	C	-6.22962000	0.31079700	0.75075100
H	-2.47725000	-1.35106400	1.51474100	C	-5.34905400	-0.65959500	1.23475700
RhCl₃(κ³N,N',P-LH2) (2a)							
Rh	0.39581900	-1.22589900	0.04176500	C	-0.84978700	3.46275900	0.89872000
Cl	2.04538600	-2.88692100	0.61477000	C	-0.70108600	4.83086900	0.66095700
Cl	0.78206100	-1.73002200	-2.30169600	C	-1.08175000	5.37580800	-0.56558800
P	2.03198800	0.47216000	0.03472100	C	-1.60964700	4.54711100	-1.55888200
N	-1.26218300	0.09063400	-0.54766900	C	-1.74700600	3.17763500	-1.33360700
N	-1.20886500	-2.61951200	-0.01301100	C	-0.90643600	0.55903100	1.89983200
C	3.26111100	0.40072000	-1.34215700	C	-1.68933800	0.53040800	3.06197600
C	3.55540300	1.52956800	-2.12219800	C	-1.10483800	0.30683500	4.31034900
H	3.04293000	2.46842900	-1.95026900	C	0.27153600	0.11545000	4.40925700
C	4.51652200	1.45747200	-3.13388000	C	1.06052200	0.16700200	3.25908200
H	4.73055400	2.33923200	-3.73043800	C	0.49134800	0.38609600	1.99922100
C	5.19671600	0.26365000	-3.37461900	C	1.40887100	0.54564100	0.80968900
H	5.94534800	0.21081300	-4.15958600	C	1.60526700	-1.88494500	0.40668500
C	4.90513200	-0.86575600	-2.60517500	H	2.03824100	-2.52541700	-0.36525600
H	5.42375000	-1.80160500	-2.79124000	H	2.32485200	-1.81401900	1.22621400
C	3.93741100	-0.80408900	-1.60283000	C	0.34042300	-2.56615700	0.84817000
H	3.69467700	-1.69175600	-1.02963500	C	0.34717100	-3.56076000	1.82492600
C	3.05355800	0.63000900	1.56184700	C	-0.80844400	-4.30419200	2.05027700
C	2.48446500	1.16846500	2.72962900	C	-1.94153300	-4.04064700	1.28097300
H	1.45540000	1.50656100	2.72886800	C	-1.89250100	-3.01926400	0.34029200
C	3.23912800	1.27866600	3.89671500	C	2.47919700	-0.25260700	-1.23847300
H	2.78737900	1.70413900	4.78777700	C	3.90538800	-0.28494500	-0.72071200
C	4.56657800	0.84304700	3.92100600	C	4.52314500	0.88772200	-0.27574100
H	5.15178600	0.92821700	4.83179900	C	5.85488300	0.88168800	0.16782600
C	5.13763500	0.30375400	2.76808700	C	6.58658500	-0.31231200	0.15662300
H	6.17023400	-0.03196800	2.77395300	C	5.97511900	-1.47995500	-0.30948000
C	4.38858500	0.19965500	1.59370100	C	4.65344800	-1.47556800	-0.74861500
C	1.24018500	2.12306600	-0.16560000	H	-3.97729000	2.51607300	-0.50524700
C	1.93018300	3.25549700	0.30341900	H	-6.39510700	2.21449900	-0.24840200
H	2.85620600	3.12810800	0.85165100	H	-7.30135800	0.18292000	0.86817200
H	1.46296200	4.54596700	0.06172500	H	-5.72994900	-1.54482600	1.73467200
C	2.01936000	5.40043600	0.43355500	H	-3.31245500	-1.25669800	1.47931000
C	0.29232200	4.72293100	-0.67196000	H	-0.56336500	3.06069000	1.86369000
H	-0.08032900	5.71968400	-0.88607800	H	-0.29279400	5.46696100	1.44027300
C	-0.40871900	3.60757000	-1.12726500	H	-0.96934800	6.44033400	-0.74770000
H	-1.32256400	3.75270800	-1.69483700	H	-1.90942400	4.96395200	-2.51546600
C	0.02958900	2.29815300	-0.87514900	H	-2.13809000	2.54524400	-2.12027800
C	-0.80089900	1.17995300	-1.47979700	H	-2.75857900	0.69076400	3.00180800
H	-1.68967100	1.62736600	-1.93645700	H	-1.72807500	0.29003600	5.19880400
H	-0.24247400	0.67220300	-2.26984600	H	0.73416700	-0.05967100	5.37537000
C	-2.14364500	-0.83101600	-1.34535000	H	2.13720100	0.04862000	3.34060300
H	-1.65720600	-0.98783800	-2.31015500	H	1.25646300	-3.75359500	2.38310300
H	-3.11441200	-0.36378300	-1.52373600	H	-0.81973100	-5.08448600	2.80393300
C	-2.29487400	-2.16885600	-0.67484200	H	-2.85688300	-4.60754400	1.40457500
C	-3.45077600	-2.94169800	-0.77314700	H	-2.73665000	-2.76601600	-0.28848100
H	-4.31177800	-2.55809700	-1.30928100	H	3.99209400	1.83493800	-0.27775600
C	-3.47418900	-4.20324200	-0.17897800	H	6.54862200	-2.40184900	-0.33533700
H	-4.36309100	-4.82184700	-0.24556200	H	4.21068800	-2.38983600	-1.13138000
C	-2.34571500	-4.65329500	0.50536700	H	1.19679000	1.47502700	0.27427300
H	-2.32438000	-5.62494500	0.98526300	H	2.43330400	0.61446100	1.18379100
C	-1.22837000	-3.82695300	0.57266300	H	2.34409900	-0.98690900	-2.03084700
H	-0.32014700	-4.11627700	1.08800500	H	2.24041300	0.72722100	-1.64918400
C	-2.03013900	0.63989100	0.64852000	H	7.61695700	-0.34149300	0.48930400
H	-2.18712800	-0.20823400	1.31135300	O	6.34131900	2.08620000	0.58018600
H	-1.34921400	1.31849200	1.16040400	C	7.69058700	2.14987800	1.03780100
C	-3.36006600	1.32611000	0.38268300	H	7.86407000	3.19026300	1.31430000
C	-3.44847300	2.72111300	0.24259200	H	7.84713100	1.51088600	1.91461000
C	-4.69026800	3.32890600	0.06924500	H	8.39560000	1.86183300	0.24944200
H	-4.75103600	4.40826000	-0.03534300	RhCl₃(κ³N,N',P-LH2) (2b-B₂s)			
C	-5.86748600	2.57660900	0.03915800	Rh	-0.58439900	-0.86214300	-1.14597900
C	-5.79057500	1.18786100	0.20395100	P	-1.63833500	0.78636200	0.17143900
C	-4.54061600	0.57591100	0.38241500	Cl	-2.71467500	-1.41448500	-2.11743500
H	-4.52123100	-0.49798100	0.54144200	Cl	-0.18182600	0.85993000	-2.79218500
H	4.85606300	-0.20860500	0.70574000	Cl	0.46638600	-2.53528400	-2.67849800
H	-2.55328500	3.32899300	0.29494000	N	1.36573500	-0.61075000	-0.13274100
Cl	-0.00579600	-0.99816400	2.40812400	N	-0.71123600	-2.41026900	0.23777100
H	-6.82048500	3.07375000	-0.09467200	C	-2.27429600	0.16927600	1.78615100
O	-6.86316700	0.34733300	0.21844400	C	-3.41878800	-0.64863500	1.77623200
C	-8.16522600	0.91065500	0.07100600	C	-3.94695100	-1.13627300	2.97023200
H	-8.27535900	1.41941800	-0.89362200	C	-3.33928800	-0.81842700	4.18830300
H	-8.86100900	0.07247500	0.11807200	C	-2.20935800	-0.00037900	4.20730600
H	-8.39069100	1.61522800	0.87984500	C	-1.67939100	0.49673000	3.01359700
RhCl₃(κ³N,N',P-LH2) (2b-²⁻⁵B)							
Rh	-0.56531500	-0.74922500	-1.23470500	C	-3.08730200	1.71726900	-0.49255100
P	-1.62686200	0.82507900	0.22959800	C	-3.28275000	1.91555900	-1.86763300
Cl	-2.67739200	-1.15251400	-2.31601800	C	-4.35678100	2.68358300	-2.32031100
Cl	-0.06939900	0.90458000	-2.90958800	C	-5.24499900	3.26375600	-1.41304300
Cl	0.43701300	-2.51635700	-2.68113400	C	-5.05459500	3.07578400	-0.04288400
N	1.37498900	-0.54691300	-0.22423900	C	-3.98536100	2.30650200	0.41737800
N	-0.78030900	-2.28457200	0.14674400	C	-0.38329200	2.05987700	0.58290700
C	-3.45088500	0.64343300	0.44595800	C	-0.69806600	3.42387600	0.50888000
C	-4.34370000	1.61748700	-0.02612800	C	0.23863800	4.39392000	0.86826400
				C	1.49750100	4.00514400	1.31978400

C	1.82142800	2.64906800	1.38130300	C	3.27828800	2.40115700	-0.70615000
C	0.90781000	1.66113000	0.99257900	H	-1.06969300	-1.21195800	2.55877400
C	1.31149500	0.21063400	1.13137700	H	-0.19720700	-0.92475300	4.84886700
C	1.67881100	-2.01456400	0.28964500	H	0.47682000	1.33131700	5.65374000
H	1.99718500	-2.55505100	-0.60398000	H	0.25995200	3.29561500	4.14413800
H	2.49555400	-2.02613500	1.01606300	H	-0.60947700	3.01881200	1.85969300
C	0.46863800	-2.72306300	0.82272200	H	-3.89178400	1.44396800	-1.34814600
C	0.55732300	-3.73241700	1.77792400	H	-6.31469400	1.59018500	-0.94590100
C	-0.58370900	-4.46169200	2.10701500	H	-5.73775200	0.18061200	3.07792600
C	-1.78414700	-4.15694100	1.46916200	H	-3.31908300	0.05637200	2.69459000
C	-1.81310100	-3.11823800	0.54571700	H	-2.60717100	3.27224800	0.33487300
C	2.42568900	-0.10388400	-1.09668400	H	-2.21332500	5.30652500	-0.97317000
C	3.87140400	-0.16819900	-0.63256800	H	-0.53103100	5.27814900	-2.82576900
C	4.50678500	0.98684800	-0.17233300	H	0.75830900	3.22876700	-2.26750800
C	5.85510900	0.96976900	0.21883300	H	3.84073800	-2.94199800	-0.48066800
C	6.58752700	-0.22002300	0.13736200	H	3.54081400	-4.59925900	1.36917500
C	5.95953500	-1.37002700	-0.35145300	H	1.30504700	-4.73945500	2.51193900
C	4.62260200	-1.35350800	-0.74001900	H	-0.53934600	-3.25487900	1.71080500
H	-3.90831800	-0.88719100	0.83697900	H	0.99513100	1.46489500	0.36430800
H	-4.83364100	-1.76231300	2.94868900	H	1.61509900	-0.06839900	0.93955800
H	-3.75116700	-1.19995400	5.11760100	H	3.99100300	-0.51320000	0.91139300
H	-1.74080900	0.26329100	5.15044900	H	4.75427800	3.84418100	-1.30245300
H	-0.81921300	1.15609800	3.05133200	H	2.44751700	3.00351800	-1.05748800
H	-2.59689700	1.47220300	-2.57606800	H	2.93624500	-0.86343100	-1.60159700
H	-4.49815500	2.82444900	-3.38774300	H	1.55095900	-1.65815800	-2.38968300
H	-6.08021200	3.85874900	-1.77046000	H	0.22437100	0.33672900	-2.98620200
H	-5.73699500	3.52423800	0.67266100	H	1.65138300	1.29265000	-2.56390000
H	-3.85488900	2.17298300	1.48497700	C	-6.19110200	0.88822700	1.09080100
H	-1.68256300	3.73436200	0.18079200	H	-7.26114400	0.94916100	1.26524200
H	-0.02509500	5.44499100	0.80676900	H	6.67258500	2.55185800	-0.45799800
H	2.22799400	4.74866700	1.62251000	O	6.41782200	0.12918700	0.80641200
H	2.79918500	2.35036000	1.74452700	C	7.77077900	0.57467200	0.72769100
H	0.62669800	-0.31389700	1.80325400	H	8.36875000	-0.19922600	1.20966200
H	2.30197000	0.16576400	1.59486600	H	8.09577400	0.68807200	-0.31291400
H	1.51415000	-3.94626700	2.24061900	H	7.91107600	1.52411200	1.25704400
H	-0.53288000	-5.25647900	2.84370800	RhCl₃(κ³N,N',P-LH3) (3a)			
H	-2.69544700	-4.70353100	1.68192000	Rh	0.67389000	-1.21937600	0.02413000
H	-2.71519800	-2.84102400	0.01775400	Cl	2.28167800	-2.92105600	0.58307900
H	2.29221000	-0.70061500	-1.99879400	Cl	1.05781800	-1.70626400	-2.32293800
H	2.14524100	0.92081400	-1.33382800	P	2.34373500	0.44707800	0.04094000
H	3.97675300	1.93168500	-0.12945200	N	-0.95415000	0.14200600	-0.55567700
H	6.53316500	-2.28823600	-0.43718200	N	-0.96422800	-2.57680400	-0.04457300
H	4.17281400	-2.25347500	-1.14587700	C	3.57563100	0.36620700	-1.33227000
H	7.62946100	-0.25963100	0.43065200	C	3.89703000	1.49789300	-2.09735100
O	6.35336500	2.16142800	0.65453600	H	3.40378000	2.44533300	-1.91637500
H	7.71981700	2.21445900	1.05949800	C	4.86105400	1.41737100	-3.10559100
H	7.90174500	3.24508000	1.36554100	H	5.09641600	2.30134700	-3.69070000
H	7.91322000	1.54540300	1.90598800	C	5.51712800	0.21235500	-3.35736900
H	8.39303000	1.95712100	0.23357400	H	6.26813600	0.15303500	-4.13958400
RhCl₃(κ³N,N',P-LH2) (2c)				C	5.19858000	-0.91966900	-2.60259800
Rh	-0.86783600	-1.30106500	-0.77549100	H	5.69844600	-1.86389000	-2.79738000
P	-1.60106200	0.60069200	0.35865800	C	4.22769600	-0.84945700	-1.60390600
Cl	-2.65438500	-2.64178100	0.09364900	H	3.96387400	-1.73834000	-1.04198400
Cl	-2.30853400	-0.44703000	-2.51302800	C	3.36231700	0.56780000	1.57351100
Cl	-0.40371600	-3.18966900	-2.42510200	C	2.80028300	1.10467000	2.74550600
N	1.00152800	-0.08490100	-1.09335800	H	1.77852700	1.46421700	2.74537200
N	0.62376200	-2.31600500	0.28945400	C	3.55306900	1.18612100	3.91613900
C	-0.89980000	0.87934400	2.04110600	H	3.10707900	1.61072300	4.81050200
C	-0.77374300	-0.22591100	2.89843500	C	4.87121800	0.72309300	3.93974600
C	-0.28577400	-0.06204000	4.19594200	H	5.45485200	0.78591500	4.85334900
C	0.09037000	1.20468500	4.64712700	C	5.43514900	0.18537900	2.78259900
C	-0.03104700	2.30804800	3.79966900	H	6.46064200	-0.17141600	2.78794000
C	-0.52604300	2.15075400	2.50410100	C	4.68823700	0.11002200	1.60467200
C	-3.42018300	0.73697600	0.63966500	C	1.58450700	2.11598200	-0.14286500
C	-4.28690200	1.16901100	-0.37942800	C	2.29239500	3.22925400	0.34452200
C	-5.66029600	1.24705200	-0.15027600	H	3.21401800	3.07818100	0.89414500
C	-5.33783600	0.45694800	2.10709400	C	1.84849600	4.53118700	0.12002500
C	-3.96174600	0.38328700	1.88646300	H	2.41860700	5.37009400	0.50616900
C	-1.14977800	2.06134300	-0.69938500	C	0.68368400	4.73982800	-0.61445800
C	-1.85893200	3.25131100	-0.44925500	H	0.32929900	5.74602500	-0.81477400
C	-1.64627300	4.40855800	-1.19605300	C	-0.03453500	3.64360800	-1.08946400
C	-0.70914100	4.39195500	-2.22486200	H	-0.94170100	3.81327500	-1.66127100
C	0.01626200	3.22826600	-2.47373900	C	0.38081800	2.32346900	-0.85567100
C	-0.17449100	2.05111100	-1.73544500	C	-0.46563500	1.22776200	-1.47785700
C	0.71227600	0.88371900	-2.17585500	H	-1.34111200	1.69550200	-1.94009700
C	1.90859800	-1.20901400	-1.46133200	H	0.08880000	0.71420500	-2.26689700
C	1.82501700	-2.22565500	-0.34095000	C	-1.85054300	-0.75693700	-1.36252000
C	2.89104600	-3.03570100	0.03391000	H	-1.35388300	-0.92957800	-2.31942600
C	2.71939800	-3.95814300	1.06731400	H	-2.80523600	-0.26569600	-1.56117800
C	1.48343600	-4.03913700	1.70435100	C	-2.04404600	-2.08808300	-0.69009800
C	0.45384000	-3.20336000	1.28270800	C	-3.22962900	-2.81664800	-0.76805200
C	1.63402600	0.62932400	0.10529000	H	-4.09008200	-2.39587200	-1.27683300
C	3.04610900	1.15505000	-0.09658700	C	-3.28724800	-4.07903000	-0.17704100
C	4.13418700	0.43495900	0.40295200	H	-4.19960800	-4.66408200	-0.22707600
C	5.44459800	0.92264000	0.27864900	C	-2.16275200	-4.57251400	0.48300000
C	5.67137300	2.15292000	-0.35040100	H	-2.16721900	-5.54660300	0.95834000
C	4.57975300	2.88122900	-0.83169900	C	-1.01650800	-3.78502500	0.53676400

H	-0.11212000	-4.10649500	1.03978500	C	6.89155500	-0.28830300	0.07668900
C	-1.71053700	0.69896200	0.64220900	F	6.96160100	-0.98296100	1.23937300
H	-1.88235300	-0.14650200	1.30499200	F	6.76421700	-1.19978100	-0.91321100
H	-1.02156800	1.36684700	1.15711300	F	8.09066300	0.31671800	-0.08275500
C	-3.02923400	1.40337600	0.37181300	H	5.02734500	3.84338100	1.14644500
C	-4.22132400	0.66738800	0.33494900	RhCl₃(κ³N,N',P-LH3) (3b-B_{2,5})			
C	-5.44726500	1.30037000	0.12087900	Rh	-0.98954200	-0.92441400	-1.13002400
C	-5.51007300	2.68763100	-0.03007600	P	-1.77768100	0.89013400	0.14995800
C	-4.33471300	3.43371000	0.04604900	Cl	-3.20013700	-1.21374200	-2.03016300
C	-3.10864800	2.79825300	0.24851200	Cl	-0.40100800	0.67597800	-2.84105000
H	-2.20668000	3.39472600	0.32583200	Cl	-0.21058300	-2.77967700	-2.62390300
H	5.15042400	-0.29764500	0.71367700	N	1.00229400	-0.90484900	-0.17346500
H	-4.19870600	-0.40761700	0.48012300	N	-1.28480700	-2.39366200	0.31379100
Cl	0.26785700	-1.00602700	2.38970100	C	-2.44099700	0.41352200	1.80176200
H	-6.46373000	3.17518100	-0.19807600	C	-3.68919000	-0.23328700	1.85186000
C	-6.70436000	0.47502800	0.11202700	C	-4.24201800	-0.60478900	3.07613500
F	-7.15016300	0.21946700	1.36609600	C	-3.55618200	-0.34116700	4.26526800
F	-7.71264400	1.08835500	-0.54463900	C	-2.32147200	0.30710100	4.22468300
F	-6.51209700	-0.72946800	-0.47882300	C	-1.76601000	0.68819700	3.00034900
H	-4.37366900	4.51401900	-0.04935100	C	-3.11102100	1.98163400	-0.51072100
RhCl₃(κ³N,N',P-LH3) (3b-2⁵B)				C	-3.31265300	2.16643000	-1.88687900
Rh	-0.65474000	-0.46543700	-1.29093200	C	-4.29026400	3.05373600	-2.34006400
P	-2.18282800	0.50426700	0.28499000	C	-5.07485600	3.76735800	-1.43243200
Cl	-2.51979800	-1.30068800	-2.55417600	C	-4.87675000	3.59358300	-0.06159400
Cl	-0.61638600	1.48571800	-2.70155500	C	-3.90385400	2.70594900	0.39944800
Cl	0.86101700	-1.63858500	-2.88266300	C	-0.35467600	2.00048600	0.48462000
N	1.10673500	0.13970200	-0.12637200	C	-0.49199000	3.39064000	0.36872700
N	-0.44842400	-2.17837400	-0.13589100	C	0.57399300	4.24113000	0.66493500
C	-3.87384200	-0.23332900	0.34160600	C	1.78613200	3.70630300	1.09393500
C	-5.00029100	0.49087000	-0.07719800	C	1.93401700	2.32237400	1.19789400
C	-6.26819100	-0.09431200	-0.05353700	C	0.88696000	1.45012100	0.87217400
C	-6.43230600	-1.40535700	0.39278800	C	1.10044700	-0.03584200	1.05655400
C	-5.31899000	-2.13107300	0.82300500	C	1.13706800	-2.32153500	0.29789000
C	-4.05122500	-1.55267300	0.79481500	H	1.35685800	-2.93021900	-0.58164700
C	-2.46930300	2.32344800	0.21102800	H	1.96223700	-2.41646200	1.00886800
C	-2.27240700	3.12686900	1.34637800	C	-0.14204600	-2.84310300	0.88328000
C	-2.53903800	4.49677200	1.29609700	C	-0.16233400	-3.82352500	1.87177600
C	-3.01509600	5.07723400	0.12010700	C	-1.38119500	-4.38134200	2.25307400
C	-3.22095200	4.28370900	-1.01114700	C	-2.54704100	-3.93903100	1.63198000
C	-2.94275500	2.91757200	-0.97254100	C	-2.46242600	-2.93720500	0.67177900
C	-1.46698200	0.22019300	1.95349200	C	2.08771800	-0.58890300	-1.18722100
C	-2.24025700	-0.19859300	3.04502300	C	3.52397800	-0.78772400	-0.73658800
C	-1.65246400	-0.42135600	4.29208400	C	4.29623700	0.31819900	-0.36993300
C	-0.28445500	-0.22095800	4.46180400	C	5.62551400	0.16456600	0.03493800
C	0.48738200	0.22081900	3.38620800	C	6.21718900	-1.09781800	0.05307500
C	-0.08403700	0.44546500	2.12835500	C	5.46924400	-2.20428200	-0.35445700
C	0.78049100	1.03524800	1.03870800	C	4.14095300	-2.05122100	-0.74890400
C	1.70409800	-1.15028200	0.34335000	H	-4.23842100	-0.42645100	0.93577200
H	2.33149900	-1.52187700	-0.47051800	H	-5.20899600	-1.09767000	3.10078700
H	2.34107200	-0.99216900	1.21758000	H	-3.98766800	-0.63209300	5.21812700
C	0.68478600	-2.22525500	0.59947600	H	-1.78953800	0.52899500	5.14465700
C	0.95728600	-3.30721300	1.43489800	H	-0.82056400	1.21928500	2.99265900
C	0.06524200	-4.37535800	1.48117900	H	-2.70629800	1.61991100	-2.59581500
C	-1.07359100	-4.33888700	0.67711400	H	-4.43815300	3.18283900	-3.40807500
C	-1.30062500	-3.22148900	-0.11694200	H	-5.83558700	4.45484300	-1.79016100
C	2.10169100	0.88026800	-1.01475000	H	-5.47846600	4.14514600	0.65428300
C	3.43789400	1.23799800	-0.39059800	H	-3.76648300	2.58645500	1.46776500
C	3.64544000	2.50301400	0.18182300	H	-1.43766700	3.81624000	0.05599400
C	4.88617000	2.85871300	0.71275300	H	0.44717500	5.31501400	0.57171700
C	5.94759400	1.95659700	0.67534000	H	2.61668400	4.35756400	1.34704100
C	5.75904700	0.70140100	0.08956300	H	2.87909000	1.91615600	1.54350400
C	4.51858700	0.34669300	-0.44411000	H	0.37587300	-0.44031000	1.76861600
H	-4.90340300	1.51407900	-0.41664200	H	2.09032500	-0.19573100	1.49530700
H	-7.12674900	0.48375600	-0.38123800	H	0.76990400	-4.14890100	2.31956900
H	-7.41935800	-1.85713700	0.41240600	H	-1.41706800	-5.15093800	3.01686100
H	-5.43397300	-3.14868900	1.18338900	H	-3.51695700	-4.35091500	1.88509500
H	-3.20771400	-2.13076700	1.15016000	H	-3.33377200	-2.56001600	0.15423800
H	-1.91884600	2.69250000	2.27438000	H	1.86387800	-1.22115000	-2.04661000
H	-2.37880700	5.10461300	2.18125300	H	1.92775500	0.44460900	-1.48850500
H	-3.22576100	6.14181800	0.08410900	H	3.86285200	1.31133400	-0.41050100
H	-3.59204300	4.72755100	-1.92982500	H	3.58760900	-2.92262300	-1.08428500
H	-3.08620900	2.31928500	-1.86302000	H	7.24789900	-1.21336100	0.36760000
H	-3.30688500	-0.34696400	2.93150700	C	6.38219500	1.39065600	0.46194800
H	-2.26890400	-0.74396000	5.12513400	F	5.79537100	1.98413200	1.53474600
H	0.18073600	-0.39237700	5.42730200	F	7.65810900	1.12198400	0.80580200
H	1.54786600	0.40806900	3.52841000	F	6.41588100	2.32743800	-0.51522300
H	1.86706100	-3.31059500	2.02454000	H	5.92679200	-3.18813700	-0.37013000
H	0.26288800	-5.22658200	2.12399200	RhCl₃(κ³N,N',P-LH3) (3c)			
H	-1.78555500	-5.15585900	0.66271800	Rh	-1.13865100	-1.30201200	-0.78826500
H	-2.16479600	-3.13324400	-0.76319900	P	-1.88765700	0.57218700	0.38328800
H	2.83281800	3.22385500	0.19836900	Cl	-2.84977800	-2.70050600	0.12914700
H	4.40623300	-0.61969700	-0.92354600	Cl	-2.66423500	-0.47544800	-2.46334000
H	0.31762100	1.92923500	0.61240700	Cl	-0.68111500	-3.15991100	-2.46908300
H	1.72445800	1.34444400	1.49412800	N	0.68738000	-0.02674700	-1.15959200
H	2.24202700	0.24274700	-1.88653300	N	0.41840800	-2.27972700	0.21762300
H	1.58494400	1.78004400	-1.34431600	C	-1.13983000	0.86241800	2.04345800
H	6.91671800	2.22990700	1.07843200				

C	-0.95458300	-0.24384300	2.88870400	H	4.78585000	0.75414000	4.85545700
C	-0.43066400	-0.07400200	4.17129700	C	4.75303200	0.11835300	2.79527400
C	-0.07665500	1.20027700	4.61909100	H	5.76004700	-0.28744100	2.81583600
C	-0.25584400	2.30464100	3.78330500	C	4.01215500	0.05898700	1.61196500
C	-0.78713200	2.14119700	2.50292700	C	1.03315100	2.18762500	-0.18529000
C	-3.69980400	0.65246000	0.72391800	C	1.80908700	3.26954500	0.26692400
C	-4.61127700	1.07678200	-0.25869500	H	2.72843000	3.07838400	0.80832500
C	-5.97805100	1.11116900	0.01630700	C	1.43610900	4.58925300	0.01880900
C	-5.55951500	0.29051600	2.24688100	H	2.05789800	5.40332100	0.37760900
C	-4.18997400	0.26056800	1.98048400	C	0.27331900	4.84731500	-0.70375000
C	-1.51135400	2.05291000	-0.67651000	H	-0.02672900	5.86745100	-0.92192300
C	-2.24444300	3.22046300	-0.39244800	C	-0.51343700	3.78363100	-1.14208300
C	-2.08705100	4.39020200	-1.13354500	H	-1.42044300	3.99152200	-1.70139800
C	-1.18198300	4.40989800	-2.19052300	C	-0.16783200	2.44762000	-0.88415400
C	-0.43313400	3.26908500	-2.47396500	C	-1.07994800	1.38849400	-1.47437200
C	-0.56925400	2.08005500	-1.74275100	H	-1.94884300	1.89040200	-1.91054800
C	0.33317800	0.94077800	-2.22369900	H	-0.56940100	0.84872900	-2.27500300
C	1.60917300	-1.12515600	-1.56731000	C	-2.55884000	-0.52053200	-1.33002700
C	1.59667600	-2.14636200	-0.44787600	H	-2.10060300	-0.69789000	-2.30479700
C	2.70274400	-2.91583900	-0.10468600	H	-3.49581100	0.01734500	-1.48419900
C	2.59399800	-3.84615500	0.93054800	C	-2.78710300	-1.84945900	-0.66761700
C	1.37987600	-3.97519400	1.60021500	C	-3.98896900	-2.54752400	-0.74979500
C	0.30921100	-3.17540100	1.21186400	H	-4.82958300	-2.11065200	-1.27729400
C	1.33713700	0.69432300	0.02281900	C	-4.08618300	-3.80368400	-0.15160400
C	2.72525900	1.26141400	-0.22494000	H	-5.01297800	-4.36503100	-0.20631800
C	2.90454800	2.52798400	-0.80373700	C	-2.98078400	-4.32014900	0.52285900
C	4.18312000	3.05214800	-0.99646600	H	-3.01551600	-5.28862800	1.00820900
C	5.30794600	2.32663600	-0.60469300	C	-1.81222600	-3.56838300	0.57578200
C	5.13901200	1.07680800	-0.00516100	H	-0.92009400	-3.91271800	1.08397500
C	3.85920700	0.55329400	0.19109000	C	-2.31121100	0.92961900	0.67212100
H	-1.23300000	-1.23585300	2.55163400	H	-2.53199100	0.09176600	1.32998900
H	-0.29697400	-0.93776100	4.81506100	H	-1.57068400	1.54409500	1.18214700
H	0.33757600	1.33204600	5.61391700	C	-3.58089500	1.72162400	0.41882700
H	0.01789500	3.29803900	4.12513100	C	-4.82931800	1.07599700	0.41679600
H	-0.91578900	3.01061500	1.86791900	C	-6.01215700	1.79683300	0.24820700
H	-4.25670700	1.37979600	-1.23466100	C	-5.97001900	3.18471800	0.09613100
H	-6.66766500	1.44917200	-0.75126000	C	-4.74006900	3.84450800	0.13033600
H	-5.91926000	-0.01489800	3.22468500	C	-3.55859700	3.11879300	0.29611100
H	-3.51241100	-0.06291000	2.76094200	H	-2.61289100	3.64654400	0.35023300
H	-2.96826800	3.21323700	0.41454200	H	4.46093600	-0.38576200	0.73167800
H	-2.67150100	5.26979100	-0.88403400	H	-4.87947900	0.00124300	0.56869600
H	-1.04687500	5.30651300	-2.78708800	Cl	-0.42284200	-0.89506800	2.40523600
H	0.28332400	3.29748500	-3.29045700	H	-6.88945000	3.74833900	-0.03146400
H	3.63657900	-2.78101000	-0.63900600	H	-4.69819300	4.92583300	0.03845200
H	3.44715400	-4.45572700	1.20865900	H	-6.96493700	1.27582000	0.24856200
H	1.224996100	-4.68377900	2.40979000				
H	-0.66808500	-3.26239600	1.66985400	IrCl₃(κ³N,N',P-LH1) (4b-^{2,5}B)			
H	0.68437200	1.50785600	0.31494600	Ir	-0.03268800	-0.52350500	-1.12381400
H	1.37045700	-0.01108500	0.85035700	P	-1.44275800	0.65653700	0.33512800
H	2.04083500	3.11795700	-1.09328000	Cl	-1.93989400	-1.25702400	-2.41158600
H	3.74804900	-0.41199100	0.67315700	Cl	0.22594600	1.31264100	-2.67570200
H	2.62091400	-0.75453100	-1.75232200	Cl	1.37798500	-1.92331300	-2.62603900
H	1.22621900	-1.58116100	-2.48213000	N	1.76086800	-0.03604600	0.00825700
H	-0.16825800	0.38452700	-3.01948400	N	0.00268300	-2.17447500	0.10713200
H	1.24564200	1.37687900	-2.64524600	C	-3.20031000	0.08361800	0.41884800
C	-6.45746400	0.71539000	1.26700800	C	-4.25433700	0.87609900	-0.05947600
H	-7.52249100	0.74253500	1.47702200	C	-5.57074600	0.41048700	-0.01449600
H	6.30356400	2.72714300	-0.75904900	C	-5.85675600	-0.84717900	0.51557000
C	6.32959600	0.29962000	0.48582100	C	-4.81673100	-1.63871100	1.00859500
F	6.15510100	-1.03490600	0.33614900	C	-3.50158200	-1.17917600	0.95873700
F	7.46280000	0.63411200	-0.16834500	C	-1.57835500	2.48764800	0.14218300
F	6.56067300	0.51153200	1.80432700	C	-1.32966700	3.34499000	1.22622000
H	4.30238100	4.03110000	-1.44911900	C	-1.47545500	4.72687500	1.08374800
IrCl₃(κ³N,N',P-LH1) (4a)				C	-1.88123500	5.26794900	-0.13637800
Ir	-0.03757600	-1.09054300	0.02869500	C	-2.13894800	4.42203500	-1.21803900
Cl	1.47858900	-2.89655500	0.57239500	C	-1.98227200	3.04229300	-1.08548500
Cl	0.28847300	-1.60696900	-2.32259800	C	-0.79270200	0.43574000	2.04205500
P	1.68775500	0.47618600	0.02414600	C	-1.61726000	0.17479600	3.14435100
N	-1.59267600	0.32338900	-0.53497400	C	-1.07105900	-0.01220700	4.41626200
N	-1.71842700	-2.36484800	-0.01796600	C	0.30758400	0.06645200	4.59979600
C	2.93236200	0.32131200	-1.33663000	C	1.13373000	0.35163000	3.51150200
C	3.32279000	1.42318200	-2.11254800	C	0.60268100	0.53933000	2.23017700
H	2.87968100	2.39809500	-1.94891800	C	1.53143100	0.96211800	1.11700000
C	4.28966500	1.27897300	-3.11125700	C	2.23648800	-1.34286900	0.57408100
H	4.57661000	2.14176400	-3.70506300	H	2.84391300	-1.81822700	-0.19940900
C	4.88253600	0.03782700	-3.34297400	H	2.86886200	-1.18425900	1.45027200
H	5.63600500	-0.07150500	-4.11746600	C	1.11707600	-2.29997600	0.86777600
C	4.49685600	-1.06540300	-2.57712900	C	1.26931000	-3.36032800	1.75761200
H	4.94714600	-2.03759400	-2.75510800	C	0.27886200	-4.33592900	1.83550800
C	3.52254700	-0.92991800	-1.58819800	C	-0.83699600	-4.22863400	1.00579500
H	3.20827000	-1.79674100	-1.01771800	C	-0.94516700	-3.13467900	0.15772100
C	2.71039500	0.57858800	1.56051900	C	2.85019400	0.55236500	-0.90062900
C	2.16736400	1.16340700	2.71813500	C	4.21556200	0.76951300	-0.27865300
H	1.16469700	1.57349000	2.70193100	C	4.56405700	2.01401500	0.27232900
C	2.91311600	1.22903000	3.89437200	C	5.83563600	2.23325800	0.80459300
H	2.48123000	1.69083300	4.77727400	C	6.78740800	1.21134800	0.78603800
C	4.20708200	0.70317700	3.93795300	C	6.46445700	-0.02366600	0.21921600
				C	5.19254700	-0.23865200	-0.31382800

H	-4.06332400	1.86163800	-0.46464600	H	-1.31253800	-5.07543200	1.27102200
H	-6.37082800	1.04019900	-0.39158000	H	-1.65177100	-3.12741600	-0.25095100
H	-6.88086800	-1.20597800	0.55201500	H	2.76305200	0.31875800	-1.66813600
H	-5.02608200	-2.61484600	1.43539200	H	2.26594400	1.78922300	-0.83917700
H	-2.71663900	-1.80434300	1.36542100	H	3.79732900	2.89971000	0.73524200
H	-1.02759200	2.94307800	2.18647600	H	4.87440500	-0.86765800	-1.03223600
H	-1.27538100	5.37544000	1.93119000	H	7.80674000	1.41165100	1.12135500
H	-1.99741300	6.34212400	-0.24498600	H	7.17656800	-0.60132600	-0.19972300
H	-2.45641600	4.83488800	-2.17072500	H	6.10228400	3.16869300	1.57175700
H	-2.16632700	2.40161100	-1.93836900	IrCl₃(κ³N,N',P-LH1) (4c)			
H	-2.69157500	0.12073700	3.01937700	Ir	-0.39702200	-1.21683200	-0.63232400
H	-1.72717800	-0.21313900	5.25729500	P	-1.24398600	0.69109200	0.35122200
H	0.74041700	-0.07933500	5.58441700	Cl	-2.21462200	-2.60839400	0.11188900
H	2.20578500	0.44388800	3.66047900	Cl	-1.75488500	-0.51673100	-2.51700100
H	2.16626900	-3.42162700	2.36359400	Cl	0.22109400	-3.14974300	-2.14466500
H	0.38324900	-5.17067200	2.52030200	N	1.42972700	-0.00775900	-0.93008300
H	-1.62342700	-4.97430400	1.01236700	N	1.02796100	-2.13431400	0.55677500
H	-1.78578000	-2.99469600	-0.50909600	C	-0.66301400	1.13607100	2.04854600
H	3.83913600	2.82357600	0.27095000	C	-0.49374900	0.10106600	2.98201100
H	4.96713300	-1.19431900	-0.77865600	C	-0.09723100	0.38308600	4.29045000
H	1.16929100	1.87084900	0.62945400	C	0.14447000	1.70232600	4.67845700
H	2.50355900	1.19252700	1.55765900	C	-0.01842300	2.73737400	3.75525700
H	2.91623500	-0.13079600	-1.74555300	C	-0.42317900	2.45992900	2.44832000
H	2.43813800	1.49219400	-1.26458600	C	-3.08271900	0.77566800	0.53080000
H	7.77806900	1.38049800	1.19753500	C	-3.91175100	1.11362100	-0.55253000
H	6.08388500	3.20323200	1.22508300	C	-5.29780600	1.14336100	-0.39818100
H	7.20510500	-0.81696500	0.18157500	C	-5.06314700	0.49061800	1.91277500
IrCl₃(κ³N,N',P-LH1) (4b-B₂S)				C	-3.67508700	0.46699000	1.76607200
Ir	0.00540900	-0.61476200	-1.04419700	C	-0.79305800	2.10524900	-0.77593600
P	-1.48812700	0.59353100	0.25850700	C	-1.55471000	3.28121300	-0.64811100
Cl	-1.81280200	-1.58480700	-2.30003000	C	-1.34246500	4.39326300	-1.46107200
Cl	0.11375400	1.26664700	-2.57062100	C	-0.34863000	4.34405800	-2.43405000
Cl	1.54852600	-1.84799000	-2.56765700	C	0.42989100	3.19516400	-2.56227200
N	1.74526700	-0.00149000	0.13128600	C	0.23858500	2.06283900	-1.75664400
N	0.16040700	-2.25092400	0.19946700	C	1.19357500	0.90716200	-2.07633700
C	-2.06424100	-0.26584600	1.78702600	C	2.41990600	-1.10318500	-1.16075200
C	-2.95652100	-1.34389900	1.64619300	C	2.27650600	-2.05413200	0.01185500
C	-3.42973000	-2.02061000	2.76932200	C	3.32688900	-2.81031000	0.51628800
C	-3.01668200	-1.63419500	4.04759300	C	3.09963700	-3.66979100	1.59226600
C	-2.13879800	-0.56047800	4.19709500	C	1.82105300	-3.74223300	2.14022000
C	-1.66769700	0.12539300	3.07406800	C	0.80710200	-2.96332900	1.59415400
C	-3.08024900	1.18811900	-0.46793600	C	1.95635700	0.80280100	0.27154100
C	-3.21979500	1.44958300	-1.83951900	C	3.35283700	1.38275600	0.13296600
C	-4.41699200	1.96505600	-2.33949400	C	3.56454700	2.61831400	-0.50026700
C	-5.48694400	2.22913700	-1.48281100	C	4.84290900	3.17384600	-0.57371900
C	-5.35489200	1.97864000	-0.11582500	C	5.93074000	2.51069200	-0.00166800
C	-4.16201900	1.46065300	0.39023400	C	5.73071500	1.29415700	0.65405500
C	-0.64210200	2.11226900	0.85136200	C	4.45207000	0.73895900	0.72332400
C	-1.28264100	3.35793700	0.82896100	H	-0.68082200	-0.92558400	2.68985700
C	-0.64164200	4.50050500	1.31122500	H	0.02620600	-0.42843700	5.00091300
C	0.64488600	4.40198700	1.83532900	H	0.45997900	1.92257800	5.69369900
C	1.29270300	3.16574700	1.84914000	H	0.17026900	3.76539700	4.04918900
C	0.67961600	2.01459300	1.33864500	H	-0.53762700	3.27773400	1.74584500
C	1.41799400	0.69856500	1.43315000	H	-3.47824000	1.35229900	-1.51454400
C	2.36982500	-1.31379400	0.51901500	H	-5.92278400	1.41380800	-1.24403500
H	2.90051400	-1.68907000	-0.35721400	H	-5.50216100	0.24892900	2.87600400
H	3.08970400	-1.17516900	1.32870700	H	-3.06300400	0.21250500	2.62292000
C	1.33183000	-2.33454900	0.87945200	H	-2.34642800	3.32487300	0.09138300
C	1.58562900	-3.37831500	1.76361500	H	-1.95300400	5.28119000	-1.33264100
C	0.63473700	-4.38431700	1.92420700	H	-0.16774700	5.19403200	-3.08445900
C	-0.54762500	-4.31188600	1.19111700	H	1.21494400	3.17200800	-3.31327600
C	-0.75645700	-3.22937900	0.34604600	H	4.30914400	-2.72545200	0.06524800
C	2.73420700	0.81614700	-0.70012000	H	3.90956600	-4.26897100	1.99420900
C	4.14116200	0.96552400	-0.15166100	H	1.59775700	-4.39465700	2.97620000
C	4.52223500	2.11163300	0.56232800	H	-0.21342500	-3.01450200	1.95119700
C	5.83085600	2.27194900	1.02265900	H	1.26536400	1.61902200	0.43723300
C	6.78803800	1.28896800	0.76566900	H	1.90887600	0.15202900	1.14133800
C	6.43300100	0.15654000	0.02845200	H	2.72464700	3.16200200	-0.92160400
C	5.12503100	0.00205200	-0.43181300	H	4.30624800	-0.19750000	1.25385800
H	-3.30106600	-1.64005100	0.66008100	H	3.43842200	-0.71438200	-1.23094900
H	-4.12235400	-2.84748100	2.64568400	H	2.16590200	-1.61595500	-2.08961700
H	-3.38527200	-2.16265200	4.92151300	H	0.78634300	0.30928700	-2.89444800
H	-1.82438800	-0.24468000	5.18713100	H	2.14760700	1.32940700	-2.40814600
H	-1.01015400	0.97671100	3.21279200	C	-5.87861300	0.82884100	0.83235000
H	-2.39477400	1.25218400	-2.50987900	H	-6.95805500	0.85183100	0.94867400
H	-4.51063000	2.15747900	-3.40418400	H	6.92457700	2.94492800	-0.05551100
H	-6.41709100	2.62815400	-1.87659700	H	4.98528100	4.13008300	-1.06818300
H	-6.17863600	2.18287200	0.56141100	H	6.56659800	0.77977300	1.11862400
H	-4.08145200	1.27433000	1.45494200	I (M = Rh)			
H	-2.29123700	3.43965700	0.44218600	Rh	-0.05168400	-1.20433300	-0.08689500
H	-1.15498100	5.45658000	1.28648600	Cl	-1.61229600	-2.98348700	-0.29975800
H	1.14671400	5.27859000	2.23262200	P	-1.76057100	0.38182400	0.03489700
H	2.28652400	3.09095200	2.27805800	N	1.54351200	0.18698900	0.39991600
H	0.84479600	-0.02033200	2.02498200	N	1.62490800	-2.53087800	0.02925400
H	2.36193600	0.86100300	1.96156000	C	-2.37389000	0.40311200	1.76771300
H	2.52622500	-3.40269200	2.30206900	C	-2.62683500	1.62185900	2.42225700
H	0.81783600	-5.20983700	2.60362400	H	-2.45933500	2.56493100	1.91432600

C	-3.10517000	1.62579300	3.73236100	C	-2.42296700	1.94477200	0.59808100
H	-3.30105000	2.57191100	4.22717100	C	-3.42541600	2.77874800	1.08691200
C	-3.33137400	0.42144600	4.40345200	C	-3.55878300	4.05904100	0.54781800
H	-3.70099600	0.42988000	5.42421600	C	-2.69174800	4.47063700	-0.46493800
C	-3.08169200	-0.79225600	3.76000500	C	-1.71030500	3.58862000	-0.90213900
H	-3.25747700	-1.73107400	4.27583900	C	-2.64551300	-0.59291300	-1.01505100
C	-2.60325800	-0.80647600	2.44896300	C	-3.94371000	-1.23913600	-0.57377800
H	-2.41389100	-1.75348500	1.95513600	C	-4.09240500	-2.63538800	-0.60378200
C	-3.21387000	0.19678300	-1.05684700	C	-5.30076500	-3.23327200	-0.24274500
C	-3.07789400	0.36471400	-2.44698300	C	-6.38514800	-2.44252900	0.14396600
H	-2.11910500	0.62999200	-2.87639700	C	-6.25841100	-1.05175700	0.15673700
C	-4.18170800	0.19560100	-3.28167200	C	-5.04883700	-0.45616200	-0.20448200
H	-4.06888200	0.33355500	-4.35242800	H	4.72902600	-0.18608700	-0.25811700
C	-5.42462000	-0.14978700	-2.74402400	H	6.39312700	1.42331600	0.58452200
H	-6.28112800	-0.28320200	-3.39767300	H	5.68744700	3.31403700	2.03491900
C	-5.56418200	-0.31816900	-1.36552600	H	3.29050500	3.57850100	2.64762300
H	-6.52817900	-0.58046000	-0.94106000	H	1.61441900	1.97878200	1.81214200
C	-4.46608500	-0.14435300	-0.52122500	H	2.13942800	-3.27410900	0.61517600
C	-1.05718000	2.04937600	-0.22362200	H	3.28710000	-5.03064300	-0.67884200
C	-1.79215300	3.03566100	-0.89708500	H	4.40027700	-4.47470400	-2.83057000
H	-2.75057200	2.78850100	-1.33802100	H	4.34255200	-2.14296600	-3.69155500
C	-1.31597600	4.34443600	-0.98884600	H	3.16610000	-0.38100000	-2.42474400
H	-1.89988300	5.09423500	-1.51264300	H	2.97966200	-0.79276900	-2.74067200
C	-0.10651600	4.68063200	-0.38673100	H	2.19942300	-1.74817700	4.86732800
C	0.26547100	5.69916600	-0.43061800	H	-0.13899600	-2.59525500	5.06580800
C	0.63344300	3.70151800	0.27900700	H	-1.64721900	-2.50401500	3.11074700
H	1.57001300	3.97516800	0.75357100	H	-4.08757600	2.43059100	1.87170800
C	0.19384800	2.37477400	0.35475000	H	-4.33482500	4.72405100	0.91202800
C	1.03253000	1.39205800	1.15132900	H	-2.76941500	5.45561400	-0.91019600
H	1.89613700	1.92137900	1.56577000	H	-0.99529900	3.85235000	-1.67329400
H	0.45972900	0.99989200	1.99759300	H	-3.26393400	-3.25942600	-0.92775800
C	2.32730300	-0.65501800	1.37494400	H	-5.39694600	-4.31434700	-0.27360200
H	1.71795800	-0.76005500	2.27922300	H	-7.32677500	-2.90670100	0.42138000
H	3.24825800	-0.14275800	1.66388000	H	-7.10229200	-0.42910700	0.43802500
C	2.60864900	-2.02253400	0.80183300	H	-4.97078600	0.62730900	-0.21559500
C	3.76655300	-2.74905700	1.06379000	H	-2.84375900	0.36933800	-1.48664000
H	4.54281700	-2.32828700	1.69289200	H	-2.14319400	-1.21838500	-1.74979300
C	3.90375800	-4.02042200	0.50298900	C	-1.16673700	-1.65706100	0.63539200
H	4.79766900	-4.60482000	0.69345100	H	-0.73298600	-2.20174100	-0.20807600
C	2.88839800	-4.52421000	-0.30891900	H	-2.05690200	-2.20463200	0.95325400
H	2.96430500	-5.50281500	-0.76815900	II (M = Rh)			
C	1.75532500	-3.74592200	-0.52585600	Rh	-0.03159700	0.28950700	-1.25955300
H	0.92673600	-4.08393200	-1.13714700	P	1.47871800	-0.39873200	0.29007600
C	2.39888000	0.57457800	-0.80317100	Cl	1.61983200	1.06876800	-2.80063100
C	2.62130300	-0.35777500	-1.32081300	Cl	-0.07550600	-1.81031000	-2.38281200
H	1.74746000	1.15578200	-1.45428600	N	-1.75940500	-0.19334600	-0.09050000
C	3.68551500	1.33323100	-0.53233100	N	-0.39821000	2.18046300	-0.46582300
C	3.75018700	2.71979900	-0.73501200	C	2.59610000	0.96474600	0.78421100
C	4.94511900	3.41804400	-0.55072300	C	3.91866200	1.02804100	0.31632100
H	4.97173700	4.49094300	-0.71573200	C	4.74471200	2.08734600	0.69458100
C	6.10249000	2.73707600	-0.16922300	C	4.26393700	3.08780900	1.54057800
H	7.03277600	3.27835700	-0.02560500	C	2.95110300	3.02674000	2.01594300
C	6.06259900	1.35160400	0.00304900	C	2.11835200	1.97544200	1.63884100
H	6.96362200	0.80808500	0.27076300	C	2.51856400	-1.80974500	-0.25078400
C	4.86779100	0.65660900	-0.18766600	C	2.61318800	-2.95558100	0.55661400
H	4.86631800	-0.42498600	-0.09432000	C	3.43834700	-4.01450800	0.17282100
H	-4.59025100	-0.27248600	0.54784400	C	4.17169100	-3.94250700	-1.01135800
H	2.86573400	3.25473900	-1.06310100	C	4.07221300	-2.80838800	-1.82248600
Cl	0.13395400	-1.01172300	-2.37653100	C	3.24391000	-1.75027900	-1.45418900
TS I-II (M = Rh)				C	0.64472000	-0.94234900	1.82530500
Rh	0.01387200	0.85657700	-0.73469400	C	1.41349600	-0.93258300	3.00407600
P	1.76412500	-0.38075500	0.13894100	C	0.89418100	-1.41554600	4.20324700
C	1.42917800	2.47529800	-1.74548800	C	-0.41021800	-1.90404800	4.23931300
Cl	0.09089100	-0.40687000	-2.67664700	C	-1.18583500	-1.89666800	3.08070900
N	-1.60334100	-0.33124000	0.08053400	C	-0.68270300	-1.42719000	1.85931000
N	-1.58329800	2.35566600	-0.37988800	C	-1.61716800	-1.48608300	0.66780100
C	3.05285500	0.78572300	0.70839200	C	-2.03194300	0.94663100	0.84624900
C	4.40454000	0.63647500	0.36803200	H	-3.10121800	1.01399900	1.05676200
C	5.34763700	1.54839400	0.84810500	H	-1.54254100	0.72750900	1.79790000
C	4.95050900	2.60855400	1.66366900	C	-1.48654300	2.24957800	0.33936500
C	3.60333300	2.75855300	2.00888000	C	-2.00337300	3.47645300	0.74862000
C	2.65714000	1.85408900	1.53529800	C	-1.37751900	4.65096700	0.33698600
C	2.57976200	-1.70332400	-0.81067200	C	-0.24908300	4.56734400	-0.47784600
C	2.61113300	-3.02061800	-0.32755700	C	0.21043000	3.31634000	-0.86621300
C	3.26503400	-4.01416100	-1.05869600	C	-2.88270900	-0.31915000	-1.13232100
C	3.89011200	-3.70022000	-2.26615800	C	-4.27688000	-0.59049300	-0.60487300
C	3.85925000	-2.38894900	-2.75139400	C	-4.73009800	-1.90817900	-0.42918500
C	3.20013800	-1.39266600	-2.03482800	C	-6.02533400	-2.16124500	0.02429400
C	1.11536300	-1.11201000	1.69351100	C	-6.89189700	-1.10029900	0.29782200
C	1.96523500	-1.16649000	2.81197100	C	-6.46242400	0.21386800	0.10231100
C	1.52379400	-1.70603000	4.01929000	C	-5.16636900	0.46597100	-0.35124800
C	0.21881800	-2.18229700	4.12814200	H	4.31471900	0.25347700	-0.32831600
C	-0.63237000	-2.12762500	3.02440600	H	5.76649900	2.12249700	0.33055500
C	-0.20529800	-1.60178200	1.79862500	H	4.91033300	3.90879500	1.83470800
C	-2.17355900	0.55790700	1.14398200	H	2.57384200	3.79519400	2.68294500
H	-3.09001500	0.12396800	1.55443200	H	1.10776700	1.94067400	2.03054000
H	-1.44502400	0.61459000	1.95800500	H	2.05427200	-3.03348800	1.48054900

H	3.50313000	-4.89421000	0.80525800	H	-4.27647700	-1.17831300	1.46799300
H	4.81295300	-4.76757000	-1.30573500	N	-3.83404100	2.32153400	-0.77266400
H	4.63214900	-2.74947600	-2.75054000	N	-1.60845100	0.08486900	-0.28183800
H	3.14344800	-0.89339600	-2.10953500				
H	2.42937100	-0.55442200	2.98507700	IV (M = Rh)			
H	1.50712000	-1.40434700	5.09831100	N	-1.66963500	-0.00806500	-0.11366100
H	-0.83142500	-2.27789800	5.16694400	C	-2.39331500	1.32450400	-0.21767300
H	-2.20883500	-2.25788700	3.12265600	C	-1.63829000	2.59185600	0.14475900
H	-2.87960800	3.50128100	1.38627300	N	-1.49377300	2.86727300	1.45585800
H	-1.76626300	5.61496800	0.64724600	C	-1.24557800	3.49308200	-0.85359800
H	0.27038800	5.45420200	-0.82102200	C	-0.68908000	4.71819300	-0.48122000
H	1.06800700	3.19144200	-1.51397600	C	-0.53734500	5.00160600	0.87290500
H	-4.07372100	-2.74168500	-0.66319700	C	-0.94708100	4.03855300	1.79873000
H	-6.35928200	-3.18613500	0.15415700	C	-1.37995800	-0.24085300	1.35011800
H	-7.90066700	-1.29740300	0.64783400	C	-0.60495800	-1.48354600	1.73833200
H	-7.13689200	1.04309700	0.29254100	C	0.74786600	-1.69408300	1.38541700
H	-4.85490700	1.49203900	-0.52883300	P	1.58434200	-0.47675100	0.31329100
H	-1.29656700	-2.23299700	-0.06230800	C	1.43304600	-2.81764900	1.86930400
H	-2.60469700	-1.77454500	1.03326000	C	0.79941000	-3.73041800	2.71359600
H	-2.88329100	0.61831200	-1.69511400	C	-0.52406100	-3.51579200	3.08958900
H	-2.56426100	-1.11708400	-1.80275400	C	-1.20999800	-2.39910100	2.60823100
III (M = Rh)				C	-2.59054300	-1.09265600	-0.66889900
Cl	-0.02511000	-2.46981900	1.22132000	C	-4.00590400	-1.18018800	-0.12331200
Rh	0.10069800	-1.20496100	-0.80608100	C	-5.04188700	-0.40245900	-0.66842200
C	-1.54088900	1.44793100	-0.95891500	C	-6.35316900	-0.53061200	-0.20965600
C	-2.53038500	2.50860400	-0.49549500	C	-6.65860900	-1.45272700	0.79482000
P	1.55378100	0.19443400	0.18428100	C	-5.64695900	-2.25622700	1.32316300
Cl	-0.07050000	-0.44287800	-3.06606800	C	-4.33536300	-2.12287300	0.86195500
Cl	1.78132500	-2.72561000	-1.55897600	C	3.22420100	-1.18028100	-0.12135700
C	-2.06640100	3.67584500	0.12431200	C	1.94751400	0.98651300	1.35382400
C	-2.97874100	4.67401700	0.46668100	C	2.31754300	2.18917800	0.72677800
C	-4.32931000	4.47274900	0.19129300	C	2.67681900	3.29499000	1.49740000
C	-4.70367900	3.27768600	-0.42484300	C	2.65995700	3.21395000	2.89211600
C	-1.71350000	0.25673600	1.19399100	C	2.28140400	2.02452900	3.51876700
C	-0.61944900	1.04590700	1.89423600	C	1.92739900	0.91074400	2.75576900
C	0.76338300	1.05058100	1.60324000	C	4.40251900	-0.57154700	0.33974900
C	-1.05521600	1.77081800	3.01731500	C	5.64744200	-1.12067900	0.02565400
C	-0.17642000	2.47091500	3.83719800	C	5.73045500	-2.27999000	-0.74561400
C	1.18734800	2.47389000	3.54549000	C	4.56115600	-2.89273600	-1.20437900
C	1.64591400	1.76675300	2.43976000	C	3.31478300	-2.34854600	-0.89904600
C	3.05971000	-0.58123000	0.90160000	Rh	0.13526200	0.12742300	-1.41779000
C	2.16548600	1.48178600	-0.97531900	Cl	-1.30975200	0.81197000	-3.32303500
C	2.12227800	2.84812000	-0.65387300	Cl	0.07652600	-2.07445800	-2.12294500
C	2.63388900	3.79391200	-1.54518600	Cl	2.02310200	0.65715000	-2.76422000
C	3.19697700	3.38745300	-2.75502700	H	-3.26560100	1.26501700	0.44013500
C	3.24306100	2.02878400	-3.07987000	H	-2.73403100	1.39997800	-1.24785700
C	2.72194000	1.07921500	-2.20297000	H	-1.38423600	3.23260100	-1.89707000
C	4.30082100	-0.50079400	0.25066400	H	-0.38881000	5.43672900	-1.23779100
C	5.43394300	-1.07890800	0.82488600	H	-0.11725500	5.94253100	1.21211800
C	5.34257800	-1.73852200	2.05100200	H	-0.84019400	4.22391700	2.86546600
C	4.11169300	-1.81429800	2.70823800	H	-2.34401000	-0.26051100	1.86890100
C	2.97518600	-1.24224800	2.14002900	H	-0.86442100	0.65188100	1.70676800
C	-2.86664900	-0.60642500	-0.82586600	H	2.46914500	-2.97891900	1.59646000
C	-3.25182300	-1.95785300	-0.26784200	H	1.34560900	-4.59311500	3.08137300
C	-2.97317300	-3.12440500	-0.99558300	H	-1.02486800	-4.20841600	3.75866000
C	-3.39207400	-4.37477700	-0.53728700	H	-2.23226500	-2.22588500	2.92782100
C	-4.10853200	-4.47584200	0.65692700	H	-2.62078900	-0.91338000	-1.74326200
C	-4.41715900	-3.31945700	1.37868300	H	-2.06964700	-2.03407500	-0.50198200
C	-4.00251200	-2.07107600	0.91324400	H	-4.82557700	0.29902200	-1.46878400
H	-0.53365800	1.83579600	-0.82512700	H	-7.13752600	0.08186800	-0.64449300
H	-1.66910300	1.26559200	-2.02432400	H	-7.67967700	-1.55474300	1.15038000
H	-1.00954300	3.80484600	0.32944100	H	-5.87721800	-2.99401200	2.08613600
H	-2.63801500	5.58890500	0.94143400	H	-3.56391000	-2.77778400	1.25311800
H	-5.07640000	5.21858700	0.44084700	H	2.33981600	2.25103500	-0.35660300
H	-5.74831500	3.08337900	-0.65903500	H	2.96742900	4.21890000	1.00759700
H	-2.66549400	0.75204500	1.40849200	H	2.93964600	4.07655600	3.48924700
H	-1.75345700	-0.74217700	1.62879700	H	2.26654400	1.95865200	4.60225700
H	-2.11560000	1.77737400	3.25182600	H	1.64856900	-0.01309300	3.25127200
H	-0.55703800	3.01427900	4.69630700	H	4.35872900	0.32651000	0.94363500
H	1.88948300	3.01631400	4.17004400	H	6.54989900	-0.63870400	0.38882100
H	2.70873300	1.76557600	2.22373300	H	6.69958300	-2.70569500	-0.98768100
H	1.70173600	3.18411900	0.28632500	H	4.61716800	-3.79616400	-1.80396800
H	2.59118600	4.84735000	-1.28697000	H	2.41547400	-2.82558500	-1.26827400
H	3.59569900	4.12502300	-3.44478800	V (M = Rh)			
H	3.67541500	1.70666400	-4.02200900	Cl	-1.87017900	-0.57106600	2.43524900
H	2.73441100	0.02996100	-2.47567900	Rh	-2.47478900	-1.25918700	0.22959200
H	4.39841200	0.01930400	-0.69371600	C	-2.05000700	0.76486700	-1.77717900
H	6.38769700	-1.00577000	0.31167200	C	-3.32507500	1.11197500	-1.06633300
H	6.22612900	-2.18574300	2.49630100	N	-3.70316100	0.25163200	-0.08825400
H	4.03391600	-2.31843800	3.66653600	P	3.01741500	0.16074500	-0.53438800
H	2.02652100	-1.31159000	2.65693400	Cl	-3.10645900	-2.24745200	-1.87357800
H	-2.68965900	-0.69051200	-1.89951000	Cl	-4.02632500	-2.75616400	1.26222600
H	-3.68434700	0.10462500	-0.68178900	C	-4.12171700	2.20933800	-1.37652300
H	-2.42295400	-3.04929300	-1.93030000	C	-5.31082000	2.41233800	-0.67863500
H	-3.16549200	-5.26553200	-1.11580300	C	-5.67034700	1.51983100	0.33047900
H	-4.43820900	-5.44652200	0.10554100	C	-4.84016100	0.44252000	0.61092600
H	-4.99318900	-3.38792800	2.29682800	C	-0.00216000	-0.59778300	-1.58039400

C	0.79198100	-1.63971400	-0.80165700	C	7.13658600	-2.56071200	0.98751200
C	2.09199600	-1.43486100	-0.27113600	C	7.05514600	-1.38220200	0.24339400
C	0.22624800	-2.92614300	-0.70498200	C	5.83998300	-0.70062500	0.13325200
C	0.87051200	-3.97027300	-0.04348800	C	3.94120400	2.28007200	0.81736200
C	2.13066700	-3.75678300	0.51181900	C	4.24393600	3.55380400	0.33636900
C	2.73312000	-2.50783500	0.37565800	C	4.01373500	3.86805700	-1.00598600
C	4.75339800	-0.43140900	-0.78399700	C	3.48561200	2.89951000	-1.86099300
C	3.07806900	0.92462900	1.15177000	C	3.19635000	1.61789800	-1.38309600
C	2.69189600	0.28706400	2.34172300	H	-2.18968400	0.99264900	1.99702800
C	2.74640900	0.96575900	3.56273700	H	-0.95847000	-0.01346300	2.77797100
C	3.19418100	2.28673800	3.61524600	H	-2.51755200	-1.33729200	4.21903000
C	3.58016600	2.93354100	2.43781500	H	-4.30664600	-3.08507200	4.30312900
C	3.51177400	2.26205900	1.21274500	H	-5.43774900	-3.75756600	2.16083800
C	5.11380100	-0.81263000	-2.08877200	H	-4.73681500	-2.63339800	0.03348800
C	6.40988100	-1.24252200	-2.37447500	H	0.56204100	-1.13345600	1.59080700
C	7.37392200	-1.27978800	-1.36313200	H	-0.72892200	-2.14497400	0.93987900
C	7.03218600	-0.88934200	-0.06687500	H	3.93278600	-1.50341600	-1.80290100
C	5.73104700	-0.46962700	0.22280600	H	2.90517000	-2.94141700	-3.51365700
C	-0.51505300	1.18026000	0.13203900	H	0.53649500	-3.69064900	-3.23487900
C	-0.29908400	2.57770500	-0.42794300	H	-0.75898300	-2.93267500	-1.28901600
C	0.69564600	2.90599600	-1.36423400	H	0.76842000	1.00262600	1.02713700
C	0.84935500	4.22009900	-1.81068800	H	0.20847600	1.06860100	-0.65097600
C	0.02280500	5.23459500	-1.32237300	H	-0.14205600	2.48988500	2.76595300
C	-0.95883400	4.92695500	-0.37905300	H	-0.90737200	4.79218300	3.21322100
C	-1.11717800	3.61094000	0.05878100	H	-1.80919100	6.18995800	1.36139100
H	-1.60652900	1.64521000	-2.24468200	H	-1.93671600	5.25215000	-0.93884000
H	-2.27689100	0.03196300	-2.55348200	H	-1.21394100	2.91973300	-1.37163400
H	-3.80062400	2.89268400	-2.15377600	H	3.91122400	-2.75091900	2.04903900
H	-5.94244800	3.26222800	-0.91327900	H	6.05386500	-3.96617700	2.21696900
H	-6.58061100	1.64636500	0.90430200	H	8.08193900	-3.08863200	1.07200200
H	-5.06087200	-0.28943100	1.37505700	H	7.93725700	-0.99106800	-0.25566600
H	0.66084400	0.15948300	-2.00438200	H	5.79156100	0.21398700	-0.44892500
H	-0.50566500	-1.10330100	-2.40485900	H	4.10641700	2.05425000	1.86805100
H	-0.72604900	3.11710100	-1.19007700	H	4.64835700	4.30279000	1.01103200
H	0.39969600	-4.94712000	0.01077500	H	4.23901700	4.86236900	-1.38020900
H	2.65446000	-4.55958700	1.02187500	H	3.29941900	3.13677000	-2.90455900
H	3.73571200	-2.36624800	0.76570500	H	2.79150700	0.87727200	-2.06441300
H	2.34547200	-0.74070600	2.32265000	I (M = Ir)			
H	2.44093200	0.45695800	4.47253900	Ir	-0.04107700	-1.10121600	-0.05322900
H	3.23671800	2.81120700	4.56528500	Cl	-1.59837400	-2.90239500	-0.25829500
H	3.92316400	3.96364900	2.46809200	P	-1.73898000	0.47992200	0.03246000
H	3.79473700	2.78223500	0.30561900	N	1.54433100	0.28697100	0.42604600
H	4.37681600	-0.76869600	-2.88694800	N	1.61597700	-2.41496900	0.09452400
H	6.66964900	-1.53714900	-3.38717500	C	-2.41599200	0.52983400	1.74470900
H	8.38598500	-1.60465400	-1.58613800	C	-2.76321400	1.75047600	2.34887400
H	7.77748600	-0.91195900	0.72316200	H	-2.63719800	2.68450200	1.81253900
H	5.48024500	-0.16949700	1.23520200	C	-3.27619000	1.77010800	3.64602700
H	-1.19474000	1.25864700	0.97543100	H	-3.54190100	2.71859200	4.10245300
H	0.40666900	0.75364600	0.52652800	C	-3.44572600	0.57771100	4.35410400
H	1.37404400	2.14394800	-1.73101700	H	-3.84191400	0.59777100	5.36477200
H	1.62485500	4.45132900	-2.53507800	C	-3.10558600	-0.63909600	3.75999500
H	0.14833800	6.25627000	-1.66846700	H	-3.23887500	-1.56917700	4.30385600
H	-1.60133500	5.70752300	0.01747300	C	-2.59177200	-0.66736700	2.46206000
H	-1.88096300	3.38426600	0.79769000	H	-2.34027400	-1.61834500	2.00453200
N	-1.09915000	0.12246100	-0.80790100	C	-3.17257400	0.29853100	-1.09290200
VI (M = Rh)				C	-3.00146300	0.45148900	-2.48043700
Cl	-4.39875800	-1.28088200	-2.13550100	H	-2.03169500	0.71328900	-2.88769400
Rh	-2.64460400	-0.46751500	-0.73939600	C	-4.08280700	0.27284600	-3.34259800
N	-0.99262400	-0.06714300	0.63192400	H	-3.94200000	0.39909000	-4.41158500
C	-1.68389800	0.02591600	1.95845300	C	-5.33957200	-0.06732400	-2.83434900
C	-2.70708100	-1.06599700	2.09945800	H	-6.17854600	-0.20870900	-3.50883000
N	-3.32865900	-1.44050000	0.95656300	C	-5.51478700	-0.22053600	-1.45840100
Cl	-1.66005900	0.57731100	-2.64703600	H	-6.48935300	-0.47950300	-1.05632600
C	-3.03770300	-1.64766600	3.32000000	C	-4.43841500	-0.03607500	-0.58788900
C	-4.03335500	-2.62248600	3.36067100	C	-1.04772900	2.15711600	-0.21450500
C	-4.66357300	-2.99936300	2.17543100	C	-1.78062900	3.14437300	-0.88732700
C	-4.28430700	-2.38821400	0.98626400	H	-2.73396400	2.89396700	-1.33806400
Cl	-3.92075100	1.34281600	-0.11827900	C	-1.30934200	4.45586800	-0.96950100
C	-0.07405200	-1.30142000	0.71634600	H	-1.89186100	5.20608800	-1.49441600
C	0.79165000	-1.67409800	-0.47650000	C	-0.10551000	4.79364700	-0.35704700
C	2.15558900	-1.29989700	-0.60090200	H	0.26293300	5.81382800	-0.39292700
P	3.03879700	-0.34648500	0.73936200	C	0.63384200	3.81336700	0.30764500
C	2.88580800	-1.77178700	-1.70694600	H	1.56666700	4.08806800	0.78916200
C	2.31264000	-2.59852100	-2.67078400	C	0.19822300	2.48429300	0.37317400
C	0.98871900	-3.00956200	-2.52064100	C	1.03612900	1.50284000	1.17247000
C	0.25344400	-2.56164500	-1.42680400	H	1.90319000	2.02982600	1.58091500
C	-0.10842400	1.14598000	0.38780700	H	0.46283800	1.11350400	2.01940200
C	-0.65862000	2.52798100	0.66719500	C	2.35508200	-0.53116700	1.40911400
C	-0.56308900	3.07944600	1.95564700	H	1.76109500	-0.61718100	2.32522100
C	-0.98556800	4.38524100	2.20938800	H	3.28116900	-0.01298200	1.66575400
C	-1.48818600	5.17024800	1.16913500	C	2.61878100	-1.90677300	0.85024900
C	-1.56090300	4.64234100	-0.12221600	C	3.77436000	-2.63881700	1.09851600
C	-1.14975700	3.33216700	-0.37085900	H	4.56230900	-2.21707100	1.71206800
C	3.42491200	1.28885300	-0.03801800	C	3.89628200	-3.91562900	0.54636900
C	4.68852200	-1.18857700	0.77071400	H	4.78930900	-4.50385800	0.72841000
C	4.78678700	-2.36801300	1.53026000	C	2.86620900	-4.41823900	-0.24700900
C	5.99739800	-3.05394100	1.63001100	H	2.92958100	-5.40008900	-0.70099000

C	1.73474300	-3.63693800	-0.45530500	II (M = Ir)		
H	0.89693600	-3.97365100	-1.05345700	Ir	-0.02823700	0.30495200
C	2.40033500	0.67741100	-0.78318300	P	1.45286900	-0.44084500
C	2.63345600	-0.25754100	-1.29090100	Cl	1.63545000	1.09821800
H	1.73995900	1.24344600	-1.43836800	Cl	-0.12063900	-1.73707700
C	3.67851500	1.45184300	-0.52422000	N	-1.76179000	-0.19169100
C	3.72698200	2.83796400	-0.73512300	N	-0.36483900	2.16191000
C	4.91702300	3.54885300	-0.56933000	C	2.64318800	0.86336000
H	4.93100900	4.62099400	-0.74069600	C	3.94006300	0.90446300
C	6.08584800	2.88138300	-0.19891800	C	4.81899600	1.92622100
H	7.01247100	3.43262800	-0.07034100	C	4.41755900	2.91275100
C	6.06207600	1.49651500	-0.01894200	C	3.13215100	2.87300700
H	6.97189800	0.96342800	0.23972300	C	2.24774200	1.85829000
C	4.87203100	0.78881000	-0.19131300	C	2.45943600	-1.87965100
H	4.88254800	-0.29250300	-0.09391600	C	2.60896600	-2.99872900
H	-4.59003800	-0.15254400	0.47921600	C	3.41683600	-4.06711900
H	2.83326400	3.36218100	-1.05499300	C	4.08204000	-4.03057700
Cl	0.20846600	-0.98767300	-2.35210700	C	3.93045100	-2.92287900
TS_I-II (M = Ir)				C	3.11783800	-1.85680700
Ir	-0.00022300	0.83466200	-0.63603800	C	0.63084600	-0.98715400
P	1.73530300	-0.45035000	0.16619900	C	1.39016600	-1.00013500
Cl	1.43520100	2.51199900	-1.56548800	C	0.85392600	-1.48199300
Cl	0.09195500	-0.34766700	-2.64635600	C	-0.45868500	-1.94862600
N	-1.59579700	-0.37956200	0.14692300	C	-1.22503000	-1.92223500
N	-1.54075500	2.31085600	-0.19361900	C	-0.70328900	-1.45258000
C	3.11771400	0.63070800	0.70683400	C	-1.62320700	-1.49739000
C	4.45207100	0.37418400	0.36478200	C	-2.05217500	0.93282600
C	5.46691700	1.21891700	0.82365100	H	-3.12702100	1.01683000
C	5.15893200	2.31674600	1.62704800	H	-1.60828000	0.67852400
C	3.82948100	2.57121900	1.98055100	C	-1.46101300	2.23609100
C	2.81373200	1.73557300	1.52386300	C	-1.94256900	3.46078100
C	2.47511600	-1.82453400	-0.78877900	C	-1.27574700	4.63092700
C	2.43416800	-3.14144800	-0.30602400	C	-0.13978000	4.54330900
C	3.01771900	-4.17569800	-1.04124900	C	0.28533800	3.29707200
C	3.64882600	-3.90332400	-2.25532800	C	-2.89911600	-0.32026400
C	3.69444300	-2.59262600	-2.74076800	C	-4.29174500	-0.58768600
C	3.10484400	-1.55686000	-2.01816000	C	-4.74947200	-1.90386200
C	1.12026700	-1.17758400	1.74075400	C	-6.04725700	-2.15255300
C	1.97211000	-1.23253700	2.85545300	C	-6.91256300	-1.08878600
C	1.53106700	-1.76426700	4.06747200	C	-6.47924900	0.22383100
C	0.22601700	-2.23882700	4.18234300	C	-5.18060500	0.47143000
C	-0.62730700	-2.18920100	3.07966800	H	4.27612600	0.14030200
C	-0.19980900	-1.66661900	1.85276900	H	5.82000800	1.94274600
C	-2.19613700	0.46415200	1.23634000	H	5.10444700	3.70437100
H	3.12582100	0.01793600	1.59815300	H	2.81593600	3.62848100
H	-1.48927500	0.48105900	2.07046300	H	1.26379100	1.83568300
C	-2.41947900	1.87040700	0.74123000	H	2.10411900	-3.05032900
C	3.43064200	2.69567200	1.22190400	H	3.52147100	-4.92633000
C	-3.53727000	3.99427900	0.72237900	H	4.71080600	-4.86192200
C	-2.63300500	4.43473200	-0.24525400	H	4.43818200	-2.89002100
C	-1.64117900	3.56588200	-0.67890300	H	2.98147300	-1.01863400
C	-2.63867800	-0.63549400	-0.95926000	H	2.41227500	-0.63885700
C	-3.92949300	-1.30635800	-0.53907200	H	1.46037400	-1.48747000
C	-4.05726100	-2.70444000	-0.58567900	H	-0.89253400	-2.32153500
C	-5.26056000	-3.32336900	-0.24440700	H	-2.25331000	-2.26960600
C	-6.36091300	-2.55243600	0.13742200	H	-2.82505100	3.48672600
C	-6.25546700	-1.16014200	0.16461600	H	-1.63775300	5.59334800
C	-5.05075000	-0.54332800	-0.17628900	H	0.41279600	5.42592400
H	4.70936200	-0.47940900	-0.25077500	H	1.14526300	3.17220400
H	6.49738500	1.01133800	0.55270000	H	-4.09495400	-2.73976200
H	5.94997400	2.96959500	1.98316800	H	-6.38436100	-3.17629400
H	3.58446000	3.41985900	2.61162500	H	-7.92349500	-1.28258900
H	1.78543500	1.94276000	1.80468300	H	-7.15294500	1.05509000
H	1.96029300	-3.36512900	0.64317400	H	-4.86593200	1.49601600
H	2.98198700	-5.19070600	-0.65818700	H	-1.29333500	-2.23218100
H	4.10599300	-4.70812500	-2.82280300	H	-2.61478600	-1.78976500
H	4.18623900	-2.37654700	-3.68400200	H	-2.89810600	0.61638900
H	3.13723600	-0.54550600	-2.40877000	H	-2.58363400	-1.11886500
H	2.98772000	-0.86318400	2.77909800	III (M = Ir)		
H	2.20802200	-1.80306800	4.91476700	Cl	-0.13058800	-2.38327700
H	-0.12983800	-2.64684300	5.12294700	Ir	0.09011000	-1.12618700
H	-1.64219200	-2.56534200	3.16843800	C	-1.50015400	1.53985300
H	-4.12201000	2.32532300	1.97014400	C	-2.45638700	2.63991200
H	-4.32223400	4.65155600	1.08106300	P	1.53819000	0.26851900
H	-2.69095200	5.43395200	-0.66026400	Cl	-0.01397400	-0.39184900
H	-0.90078400	3.84914400	-1.41724200	Cl	1.72429500	-2.72630900
H	-3.21640600	-3.31317900	-0.90664100	C	-1.95340700	3.81000000
H	-5.34038400	-4.40534100	-0.28696300	C	-2.83153200	4.84741600
H	-7.29861000	-3.03324000	0.39926900	C	-4.18875000	4.68199500
H	-7.11193900	-0.55286000	0.44116200	C	-4.60356200	3.48143000
H	-4.98928500	0.54140800	-0.17706900	C	-1.71936000	0.40930100
H	-2.84551700	0.33481800	-1.41109400	C	-0.62161600	1.20197900
H	-2.12325000	-1.23853800	-1.70365100	C	0.76337100	1.18383900
C	-1.15763500	-1.71723200	0.68743100	C	-1.06055400	1.95858900
H	-0.72082900	-2.24899200	-0.16212600	C	-0.18115200	2.66824700
H	-2.04996800	-2.26605000	0.99484800	C	1.18556200	2.64808900
				C	1.64518400	1.90943400
						2.46196100

C	3.02206000	-0.51468800	1.01172400	Cl	-1.34085900	0.69845500	-3.19404600
C	2.22055500	1.52326200	-0.92207000	Cl	0.04184100	-2.16373600	-1.95263800
C	2.21318900	2.89724400	-0.63546900	Cl	1.97757300	0.54510600	-2.74646100
C	2.76988800	3.80688000	-1.53822200	H	-3.30142400	1.18750400	0.54289900
C	3.34544600	3.35594200	-2.72612500	H	-2.77796000	1.33034200	-1.14655500
C	3.35793400	1.98897900	-3.01712300	H	-1.42076500	3.16958900	-1.80961500
C	2.79111900	1.07732400	-2.12800900	H	-0.47011800	5.39905900	-1.16995000
C	4.28139200	-0.46990700	0.39464600	H	-0.27433400	5.95985800	1.27501000
C	5.38702600	-1.06600100	1.00496300	H	-1.03150500	4.27174600	2.94417500
C	5.25005100	-1.70689800	2.23645600	H	-2.32647800	-0.24252900	1.99193900
C	4.00101400	-1.74624100	2.86191700	H	-0.85725300	0.68221600	1.79716700
C	2.89307900	-1.15623300	2.25617400	H	2.53051200	-2.88309000	1.77336200
C	-2.88828600	-0.46772000	-0.78836900	H	1.43919100	-4.48743400	3.29652400
C	-3.34391400	-1.77291600	-0.17815600	H	-0.93568200	-4.13182100	3.97208600
C	-3.09624600	-2.98409900	-0.84102500	H	-2.18203800	-2.19018800	3.10165200
C	-3.58107600	-4.19153700	-0.33518500	H	-2.61592400	-1.02086600	-1.59042500
C	-4.33066500	-4.20414300	0.84307800	H	-2.05359300	-2.08269900	-0.30376900
C	-4.60578100	-3.00238700	1.50104500	H	-4.82763400	0.16492400	-1.39018000
C	-4.12636900	-1.79679300	0.98728100	H	-7.14351500	-0.04435300	-0.57576000
H	-0.48136100	1.89998100	-0.84446600	H	-7.67834900	-1.59602800	1.29537200
H	-1.63957700	1.33448300	-2.02275300	H	-5.86401500	-2.95960900	2.31730500
H	-0.89231800	3.91066500	0.25627500	H	-3.54703000	-2.75310600	1.49279600
H	-2.45949800	5.76486900	0.81710500	H	2.36493500	2.25105800	-0.34133800
H	-4.91038900	5.45922000	0.33321500	H	2.97498600	4.27589400	0.94553300
H	-5.65463400	3.31432500	-0.69909400	H	2.90467800	4.24343700	3.43033100
H	-2.66546700	0.92569800	1.40572400	H	2.20901500	2.17708400	4.62363000
H	-1.78142000	-0.57613100	1.68256900	H	1.60756000	0.14914400	3.34910100
H	-2.12296900	1.98335000	3.23848700	H	4.30943500	0.19837900	1.36274500
H	-0.56314800	3.23683200	4.66711000	H	6.51462500	-0.79199700	0.91001300
H	1.88790000	3.19677300	4.16548000	H	6.73360600	-2.69518000	-0.67725100
H	2.71007300	1.88777100	2.25632300	H	4.70892400	-3.59223400	-1.81198000
H	1.78315900	3.26806800	0.28733900	H	2.49587000	-2.59396800	-1.37556900
H	2.75257900	4.86723600	-1.30618800	V (M = Ir)			
H	3.77963700	4.06481700	-3.42461500	Cl	-1.68701700	-0.40037800	2.41423100
H	3.80007300	1.63110500	-3.94182200	Ir	-2.30284900	-1.07678000	0.19855600
H	2.77996600	0.02155200	-2.37462100	C	-1.81822600	0.95393200	-1.79831700
H	4.41480000	0.03657000	-0.55301900	C	-3.08529000	1.33314800	-1.09170400
H	6.35504400	-1.02116500	0.51541800	N	-3.47744500	0.46910000	-0.11646100
H	6.11163800	-2.16757500	2.71038200	P	3.25132700	0.17101200	-0.54308300
H	3.88727600	-2.23540500	3.82455200	Cl	-2.97275800	-2.02049500	-1.92014400
H	1.93005700	-1.19754600	2.74960700	Cl	-3.88943200	-2.55037800	1.22589300
H	-2.69679800	-0.60691600	-1.85386700	C	-3.84907700	2.45474600	-1.39143100
H	-3.67064400	0.28787500	-0.68692800	C	-5.02892600	2.69059700	-0.68824600
H	-2.52066600	-2.97818900	-1.76333500	C	-5.40766900	1.80098700	0.31638300
H	-3.37922100	-5.11848700	-0.86386600	C	-4.61003500	0.69816700	0.58726900
H	-4.71069500	-5.14154900	1.23855600	C	0.19197500	-0.45770900	-1.60409000
H	-5.20543400	-3.00156600	2.40656400	C	0.95121800	-1.53111700	-0.83858600
H	-4.37404500	-0.86748800	1.49233700	C	2.24862400	-1.37795800	-0.28639800
N	-3.76655200	2.48744200	-0.79339800	C	0.34052600	-2.79684400	-0.76557200
N	-1.59902600	0.18868600	-0.25221800	C	0.93191200	-3.86826700	-0.09818800
IV (M = Ir)				C	2.18487600	-3.70229600	0.48887000
N	-1.66249400	-0.03693000	-0.00252000	C	2.83519700	-2.47592900	0.37054100
C	-2.43427700	1.27554800	-0.11624400	C	4.95335900	-0.51780100	-0.78383700
C	-1.72414300	2.56851800	0.23854500	C	3.34471200	0.92947500	1.14303200
N	-1.62428800	2.87485700	1.54666000	C	2.86654400	0.33448700	2.32136100
C	-1.31454900	3.45344300	-0.76842600	C	2.94970800	1.00879000	3.54338900
C	-0.78423600	4.69311100	-0.40717600	C	3.51873800	2.28147100	3.60845500
C	-0.67472600	5.00725000	0.94465500	C	3.99781500	2.88546900	2.44234100
C	-1.10224500	4.06080700	1.87908800	C	3.90030600	2.22050800	1.22038400
C	-1.36426400	-0.22660100	1.47126100	C	5.28754500	-0.94839300	-2.08021700
C	-0.56969300	-1.44532600	1.89172000	C	6.55550200	-1.45958600	-2.35794600
C	0.78642400	-1.63542200	1.54256700	C	7.51845200	-1.53080300	-1.34730100
P	1.57799500	-0.43269600	0.41491600	C	7.20346800	-1.09169100	-0.05993000
C	1.49260400	-2.73490300	2.04791300	C	5.92982700	-0.59014000	0.22204100
C	0.87732600	-3.64181500	2.91271800	C	-0.28104900	1.31277200	0.12257600
C	-0.44928700	-3.44417800	3.28732600	C	-0.00776000	2.69871500	-0.43989300
C	-1.15749900	-2.35159200	2.78298300	C	1.02668600	2.99283500	-1.34409700
C	-2.58351200	-1.15474900	-0.51009800	C	1.23550100	4.29933500	-1.79053200
C	-3.99856900	-1.23208400	0.03498500	C	0.42483200	5.34096700	-1.33449900
C	-5.04135700	-0.49878600	-0.55750100	C	-0.59622900	5.06787200	-0.42273400
C	-6.35453000	-0.62250100	-0.10385000	C	-0.80847600	3.75978900	0.01578300
C	-6.65568000	-1.49709000	0.94359200	H	-1.33957300	1.82253200	-2.25173500
C	-5.63737600	-2.25775600	1.52016000	H	-2.05732500	0.23336900	-2.58199400
C	-4.32359800	-2.12887300	1.06365000	H	-3.50939800	3.13266400	-2.16567100
C	3.23886600	-1.12733200	0.02651000	H	-5.63605400	3.56032000	-0.91422700
C	1.93826600	1.06344900	1.41557900	H	-6.31084100	1.95055100	0.89600200
C	2.32388400	2.23657100	0.74373300	H	-4.85086700	-0.02995100	1.34867200
C	2.67282000	3.37498000	1.47032500	H	0.87072600	0.29640700	-2.00619200
C	2.63274300	3.35583500	2.86711400	H	-0.31665000	-0.93415400	-2.44260400
C	2.24189800	2.19555000	3.53859000	H	-0.60826100	-2.94775100	-1.27040700
C	1.89727600	1.04996700	2.81816400	H	0.42573000	-4.82813500	-0.06203700
C	4.38496000	-0.62714600	0.66506800	H	2.66714700	-4.52502300	1.00806900
C	5.63735900	-1.19073700	0.40974700	H	3.83347200	-2.37185000	0.78264100
C	5.75930600	-2.25796200	-0.48023700	H	2.42659500	-0.65665800	2.29180600
C	4.62226900	-2.76229000	-1.11712300	H	2.57168900	0.53372700	4.44413900
C	3.36974500	-2.20204200	-0.86985700	H	3.58408600	2.80223300	4.55923200
Ir	0.13089800	0.06620400	-1.30638100	H	4.43633200	3.87833400	2.48247900

H	4.25854000	2.70887400	0.31761000	Cl	0.56503700	-3.10129000	-0.14814600
H	4.55186900	-0.88103400	-2.87801500	P	-1.41505300	-0.05874100	-0.02458600
H	6.79448800	-1.79235900	-3.36393200	N	1.35866400	-0.40505200	1.70249200
H	8.50882200	-1.92037000	-1.56395400	N	2.95747900	-0.85651400	-0.49395000
H	7.94794400	-1.14077100	0.72970300	C	-2.56592700	-1.46374900	-0.35774500
H	5.69996000	-0.25342600	1.22783900	C	-3.54056300	-1.85759000	0.57166700
H	-0.96529800	1.41927800	0.95864800	H	-3.62952500	-1.35118900	1.52562600
H	0.62026900	0.85201900	0.52598000	C	-4.41110400	-2.91084500	0.27903200
H	1.69450400	2.20984300	-1.68550700	H	-5.15747300	-3.20598300	1.01060100
H	2.04193700	4.50281500	-2.48904100	C	-4.32413700	-3.57625900	-0.94401800
H	0.59321200	6.35665300	-1.68008300	H	-5.00393600	-4.39228400	-1.17095900
H	-1.22679800	5.86976100	-0.05032800	C	-3.35390300	-3.19139500	-1.87321100
H	-1.60153400	3.56097200	0.73135900	H	-3.27440100	-3.70895300	-2.82476800
N	-0.90059400	0.26748900	-0.81984000	C	-2.47228100	-2.15108700	-1.58050000
				H	-1.70326700	-1.87501800	-2.29341700
VI (M = Ir)				C	-2.12620800	1.35543300	-0.97679100
Cl	-4.20944700	-1.13674800	-2.04697500	C	-1.74768100	2.66942900	-0.64889300
Ir	-2.41513500	-0.39524800	-0.63555500	H	-1.05841200	2.85259700	0.16744600
N	-0.77377200	-0.02476400	0.72442000	C	-2.26105100	3.75208500	-1.36219900
C	-1.44970900	0.07442300	2.06391300	H	-1.96305900	4.76062800	-1.09167700
C	-2.49134800	-1.00009700	2.19705600	C	-3.14926100	3.54131600	-2.42000900
N	-3.10536800	-1.35867500	1.04018800	H	-3.54591200	4.38578000	-2.97579200
Cl	-1.43578300	0.66294600	-2.55994600	C	-3.52729300	2.24080700	-2.75481400
C	-2.84045900	-1.58314000	3.41050100	H	-4.22140700	2.06558600	-3.57135100
C	-3.84905800	-2.54473700	3.43974100	C	-3.02332200	1.15384600	-2.03618100
C	-4.47210200	-2.90657000	2.24588500	C	-1.75057900	0.39196900	1.73303300
C	-4.07496100	-2.29772400	1.06275400	C	-2.87768600	1.17471400	2.03571800
Cl	-3.66410200	1.43369000	0.02951100	H	-3.51477800	1.52975100	1.23359300
C	0.14758200	-1.26046800	0.81872500	C	-3.20152200	1.50437100	3.35132800
C	0.98209300	-1.66312400	-0.38716800	H	-4.08065800	2.10736800	3.55567800
C	2.34776400	-1.30889000	-0.54698400	C	-2.39008900	1.05672900	4.39177600
P	3.27119300	-0.33429200	0.75053300	H	-2.62408600	1.30917700	5.42128100
C	3.04860700	-1.81085500	-1.65897000	C	-1.26561300	0.28433100	4.10403200
C	2.44577200	-2.64687400	-2.59614300	H	-0.63159900	-0.05849800	4.91672600
C	1.11902400	-3.03506600	-2.41391400	C	-0.92808700	-0.06471700	2.78779700
C	0.41309300	-2.55859500	-1.31320600	C	0.28077200	-0.95714800	2.59987100
C	0.12779200	1.18358300	0.48279500	H	0.72439800	-1.14333800	3.58450000
C	-0.40406800	2.57188000	0.76398900	H	0.00251100	-1.92133000	2.16643800
C	-0.29964000	3.12081300	2.05281500	C	2.54744600	-1.31609500	1.83497000
C	-0.70213700	4.43269400	2.30780200	H	2.16608500	-2.33964300	1.77755600
C	-1.19280700	5.22622800	1.26829300	H	3.02648500	-1.16958600	2.80821400
C	-1.27417900	4.70042900	-0.02338900	C	3.51800700	-1.12304300	0.70435700
C	-0.88359500	3.38421300	-0.27305500	C	4.89567600	-1.27623300	0.84270300
C	3.66185100	1.27285900	-0.08189200	H	5.32143800	-1.48145300	1.81861000
C	4.91182800	-1.19398500	0.77345000	C	5.70392800	-1.16280700	-0.28829200
C	5.03039100	-2.31402700	1.61514300	H	6.77953600	-1.27924700	-0.20515300
C	6.23579200	-3.01004200	1.71166200	C	5.11252000	-0.89079100	-1.52157900
C	7.34952000	-2.58535500	0.98194200	H	5.70534200	-0.79131700	-2.42366300
C	7.24861400	-1.46502500	0.15444800	C	3.73110500	-0.73403800	-1.58369300
C	6.03866700	-0.77402100	0.04893100	H	3.20924400	-0.51176900	-2.50750200
C	4.24380000	2.26933900	0.72397600	C	1.73641300	1.01096600	2.09627600
C	4.55444300	3.52344000	0.19893300	H	0.99394200	1.37129000	2.81198700
C	4.26681700	3.81398300	-1.13786100	H	2.69212100	0.98274100	2.62896300
C	3.67247800	2.84114900	-1.94281700	C	1.79860000	1.92602700	0.90245300
C	3.37514900	1.57838400	-1.42133100	C	1.35995200	1.45301500	-0.34745300
H	-1.93518400	1.05077800	2.11053300	C	1.43177000	2.31453000	-1.45113300
H	-0.71774100	0.01377400	2.87542100	H	1.11026800	1.96509500	-2.42568400
H	-2.32367300	-1.28261000	4.31483600	C	1.91156700	3.62024900	-1.30880600
H	-4.13702900	-3.00797200	4.37736200	H	1.95689100	4.27261400	-2.17744700
H	-5.25634000	-3.65411100	2.22012800	C	2.32998500	4.08769800	-0.06010400
H	-4.52199000	-2.53456300	0.10576000	H	2.70161100	5.10219600	0.05234800
H	0.80381900	-1.07512600	1.67329600	C	2.27481500	3.23698700	1.04364800
H	-0.50601400	-2.09550800	1.07481800	H	2.60684600	3.58839900	2.01840300
H	4.09645800	-1.55782400	-1.78246700	H	-3.34135600	0.15264300	-2.30155600
H	3.01702800	-3.01287500	-3.44396500				
H	0.64221800	-3.72012100	-3.10806000	(R_{Nam}) -OC-6-43-C RhCl₂(κ¹C,N,N',P-L1)			
H	-0.60483300	-2.90669600	-1.15156800	Rh	-0.94634600	-0.58752700	-0.46367400
H	1.00189700	1.02714100	1.12163300	P	1.51947300	-0.11356900	-0.07208800
H	0.44161000	1.10246900	-0.55646500	N	-1.29813100	-0.75898400	1.62565900
H	0.11308300	2.52438200	2.86238900	N	-1.42019600	1.39060500	-0.11191000
H	-0.61738100	4.83758900	3.31194000	C	1.85560700	1.66571300	-0.43702900
H	-1.49797800	6.25063500	1.46145600	C	1.92655500	2.65174400	0.55932600
H	-1.64113200	5.31649100	-0.83937500	H	1.87079300	2.37859700	1.60710000
H	-0.95529600	2.97240900	-1.27355900	C	2.08074000	3.99827700	0.21776500
H	4.17536900	-2.64099400	2.20188600	H	2.13772300	4.74553200	1.00390200
H	6.30839400	-3.87572300	2.36372900	C	2.16843300	4.38031900	-1.12127100
H	8.29112200	-3.12042700	1.06336000	H	2.29462300	5.42634100	-1.38438600
H	8.11160400	-1.12692400	-0.41218700	C	2.09043500	3.40782400	-2.12186900
H	5.97453800	0.09569700	-0.59722000	H	2.15365100	3.69407900	-3.16768500
H	4.45561100	2.06271800	1.77027000	C	1.92665200	2.06429600	-1.78489300
H	5.01044200	4.27630700	0.83534800	H	1.84876500	1.32227200	-2.57224900
H	4.49894800	4.79333500	-1.54580200	C	2.89428600	-1.00542300	-0.93216300
H	3.44102400	3.05976300	-2.98139200	C	2.75842200	-2.38692600	-1.14837200
H	2.91942100	0.83347600	-2.06483900	H	1.83822800	-2.88792200	-0.86661700
				C	3.79339400	-3.11493000	-1.73890000
				H	3.67275100	-4.18215300	-1.90140900
(R_{Nam}) -OC-6-54-C RhCl₂(κ¹C,N,N',P-L1) (5)				C	4.97356100	-2.47612900	-2.12480900
Rh	0.85859500	-0.50721300	-0.36664600	H	5.77614100	-3.04329200	-2.58718400
Cl	0.54270800	-0.62058200	-2.77540500				

C	5.11571400	-1.10257000	-1.91633700	C	-4.59900300	-0.50812200	-1.05175400
H	6.02936800	-0.59647800	-2.21433000	H	-5.31398400	-0.05579600	-1.72957600
C	4.08540800	-0.37053600	-1.32301500	C	-3.23692900	-0.43108500	-1.32554600
C	1.97846800	-0.30178600	1.71388100	H	-2.86217200	0.06397000	-2.21505200
C	3.24865200	0.13079000	2.13287100	C	0.79983100	-2.95924700	1.26385400
H	3.93693300	0.54557300	1.40367100	C	2.03649300	-2.50358800	0.53032300
C	3.65121000	0.04461700	3.46352900	C	1.85883300	-1.63127300	-0.56790800
H	4.63944200	0.38678100	3.75478100	C	2.95843800	-1.37249600	-1.39265900
C	2.77176700	-0.47858400	4.41039500	H	2.83605300	-0.74571500	-2.27054600
H	3.06102600	-0.54612200	5.45458900	C	4.21452300	-1.92419800	-1.10841600
C	1.51368700	-0.92155700	4.00916600	H	5.05598700	-1.70858100	-1.76251200
H	0.83891200	-1.33970800	4.75053600	C	4.39188300	-2.73902100	0.01144300
C	1.09469700	-0.85942300	2.66821600	H	5.36973400	-3.15225900	0.24186000
C	-0.23403900	-1.53266200	2.36782200	C	3.29676500	-3.03321100	0.82821600
C	-1.46232500	0.61957100	2.20163200	H	3.41783800	-3.69164100	1.68595100
H	-0.52697200	0.88724200	2.70154500	H	2.93991400	1.23147000	-1.08204100
H	-2.23961000	0.61474300	2.97117700	Cl	-0.53294100	-3.31493000	-1.72936400
C	-1.74496900	1.67586600	1.16846900	Cl	0.11025600	-0.19456800	-3.00369900
C	-2.24401600	2.92781900	1.52492700	H	-1.92334800	-2.57474800	2.36767400
H	-2.50159700	3.12604100	2.55964000	H	-1.61946400	-3.44135600	0.85757500
C	-2.39867100	3.90442500	0.54465200	H	1.04934700	-0.63243000	2.25294600
H	-2.78565800	4.88428300	0.80403600	H	-0.05399400	-1.54283400	3.27869200
C	-2.05259500	3.60014800	-0.77180400	H	0.38724000	-3.82781700	0.74724600
H	-2.15695200	4.32768200	-1.56840400	H	0.99304100	-3.23820900	2.30599500
C	-1.57488800	2.32952600	-1.06553600	(R _{Ham}) -OC-6-54-C RhCl ₂ (κ ⁴ C,N,N',P-L2) (C-4 metallated) (6)			
H	-1.30813300	2.02297800	-2.06892200	Rh	0.38558900	-0.98931800	-0.38313600
C	-2.58045000	-1.55295000	1.76170300	Cl	0.10661500	-0.84368900	-2.79402500
H	-2.29072100	-2.60365100	1.67231500	Cl	-0.87359600	-3.27906800	-0.31894400
H	-2.99348100	-1.40110600	2.76560000	P	-1.55692600	0.27233600	-0.02553600
C	-3.53934300	-1.20448000	0.66011700	N	0.84349800	-1.18287600	1.68878100
C	-2.97137000	-0.83171300	-0.57068700	N	2.19704000	-2.10066700	-0.52412500
C	-3.81836400	-0.57466600	-1.65262600	C	-3.15449400	-0.56186200	-0.43204800
H	-3.39878000	-0.27592700	-2.60830200	C	-4.25232600	-0.52196800	0.44102300
C	-5.20690900	-0.70122100	-1.51027000	H	-4.17694200	-0.02128600	1.39912400
H	-5.85457100	-0.50314700	-2.36111300	C	-5.45968500	-1.12928000	0.08636000
C	-5.76304500	-1.06803900	-0.28222500	H	-6.29897500	-1.09223600	0.77456100
H	-6.84033300	-1.15415600	-0.17185600	C	-5.58673500	-1.77612600	-1.14335300
C	-4.92617900	-1.31731400	0.80846600	H	-6.52718300	-2.24419700	-1.41909100
H	-5.35046000	-1.60178500	1.76897400	C	-4.49613300	-1.82403600	-2.01559800
H	4.21266600	0.69621800	-1.17502800	H	-4.58425700	-2.33266000	-2.97121200
H	-0.67092600	-1.83648200	3.32517400	C	-3.28372300	-1.23240900	-1.66053600
H	-0.07528300	-2.43662200	1.77515800	H	-2.43167300	-1.29594700	-2.32785600
Cl	-0.70520000	-3.00883400	-0.69860300	C	-1.65764300	1.89305100	-0.90572900
Cl	-0.64532600	-0.31640400	-2.86534300	C	-0.82303200	2.95279600	-0.50880500
(R _{Ham}) -OC-6-42-A RhCl ₂ (κ ⁴ C,N,N',P-L1)				H	-0.13477500	2.82630600	0.31898000
Rh	-0.06970900	-1.05034700	-0.74886800	C	-0.87698700	4.18032000	-1.16838100
P	0.25939900	1.13083800	0.10670200	H	-0.23036300	4.99037300	-0.84459000
N	-0.26237300	-1.88252500	1.20715500	C	-1.75350200	4.36595300	-2.24052500
N	-2.30547500	-0.97207500	-0.52349000	H	-1.79269200	5.32224100	-2.75372000
C	-0.17654200	2.54582400	-0.99655500	C	-2.58073800	3.31789900	-2.64522500
C	-1.48518400	2.64308400	-1.49973300	H	-3.26885000	3.45280700	-3.47440300
H	-2.22767100	1.90292300	-1.23156500	C	-2.53698100	2.08953600	-1.98097500
C	-1.85442500	3.70172600	-2.32688300	C	-1.72957100	0.73478500	1.75366200
H	-2.87281500	3.76082300	-2.69881900	C	-2.47480700	1.87595600	2.09581800
C	-0.91848800	4.67903100	-2.67603300	H	-2.90882100	2.48621900	1.31202600
H	-1.20410200	5.50174200	-3.32454100	C	-2.67540400	2.24213300	3.42631700
C	0.38178100	4.59408100	-2.18012000	H	-3.25900200	3.12692000	3.66044800
H	1.11594400	5.35161500	-2.43718600	C	-2.12151400	1.46731800	4.44313700
C	0.75201800	3.53838700	-1.34224000	H	-2.26248800	1.74073500	5.48416500
H	1.76492300	3.50406100	-0.96135500	C	-1.37361200	0.33688300	4.11675000
C	1.91285300	1.58748700	0.78702200	H	-0.93607500	-0.26072800	4.91133600
C	2.07083500	2.01465500	2.11526300	C	-1.16726200	-0.05201700	2.78461800
H	1.21655000	2.06910500	2.78044800	C	-0.38190600	-1.32642600	2.55462100
C	3.32991100	2.38322300	2.59468900	H	-0.06162700	-1.70984800	3.53003200
H	3.43481900	2.70806400	3.62536900	H	-0.99385000	-2.09493400	2.07511900
C	4.44253900	2.34155000	1.75370500	C	1.59371600	-2.48302200	1.77600000
H	5.41998500	2.63153700	2.12722500	H	0.85380300	-3.28086700	1.66441800
C	4.29298400	1.92903600	0.42741700	H	2.07050000	-2.57644700	2.75678000
H	5.15189800	1.89830600	-0.23591800	C	2.58850500	-2.61987100	0.65833500
C	3.03956400	1.54902800	-0.05195100	C	3.80002000	-3.29505600	0.78922000
C	-0.87179800	1.29825400	1.54892000	H	4.09436400	-3.69506400	1.75321300
C	-1.68418800	2.42142000	1.75033200	C	4.61287000	-3.44578200	-0.33399700
H	-1.65131600	3.24847500	1.05140200	H	5.55981200	-3.96999700	-0.25708400
C	-2.53893200	2.49363000	2.85305100	C	4.19569500	-2.90848500	-1.55139400
H	-3.15958100	3.37304100	2.99391700	H	4.79936300	-3.00079700	-2.44703300
C	-2.58493100	1.44423900	3.76829800	C	2.98122600	-2.23117200	-1.60560700
H	-3.24546100	1.49378400	4.62824600	H	2.60456100	-1.78124500	-2.51712300
C	-1.76936800	0.32664900	3.58063200	C	1.72215200	-0.03775700	2.15962500
H	-1.79219400	-0.48350900	4.30399900	H	1.15953300	0.53905500	2.89704900
C	-0.91295800	0.23610500	2.47813000	H	2.58679000	-0.45360800	2.68594400
C	0.00919300	-0.95173900	2.35860800	C	2.14602600	0.84775500	1.01870400
C	-1.64467000	-2.45016800	1.31657500	C	1.58388500	0.63686600	-0.25444400
C	-2.69756000	-1.65710000	0.57111400	C	2.00125900	1.46820200	-1.29775800
C	-4.04461000	-1.75669600	0.92457900	H	1.59650100	1.32369000	-2.29304700
H	-4.32923500	-2.29889700	1.81999100	C	2.93318300	2.49407300	-1.09340200
C	-5.00749800	-1.16956100	0.10630100	H	3.22643300	3.11709600	-1.93068000
H	-6.05958500	-1.23782200	0.36348500	C	3.46971300	2.70043100	-1.18301900

C	-2.91364600	4.27130900	-0.71312800	H	-1.85397100	-0.28330000	3.28023700
H	-3.24270500	5.29347600	-0.87512400	C	-1.40332100	1.22450900	1.82429700
C	-3.32597900	3.25590000	-1.57632700	C	-1.83160900	2.35442100	2.51989100
H	-3.97888800	3.48155800	-2.41421000	H	-1.97299100	2.30012000	3.59386100
C	-2.91009900	1.93906300	-1.36422900	C	-2.07157600	3.53472100	1.82136600
C	-1.83924000	-0.41310700	1.77205600	H	-2.40763500	4.42234600	2.34714900
C	-2.91385300	0.25857700	2.37908500	C	-1.87838600	3.55528100	0.43992600
H	-3.48273700	0.98376700	1.80865300	H	-2.05693800	4.45087000	-0.14385300
C	-3.27408600	0.00812300	3.70283200	C	-1.45570900	2.39619400	-0.19749400
H	-4.11110200	0.54014800	4.14400800	H	-1.30253800	2.33369300	-1.26696600
C	-2.55475700	-0.92522000	4.44613800	C	-2.08614600	-2.15671900	1.68226200
H	-2.81916400	-1.13023300	5.47883100	H	-1.75992800	-3.10269400	1.24281500
C	-1.48178900	-1.59315100	3.85765800	H	-2.35390300	-2.34055800	2.72953600
H	-0.91741500	-2.31406100	4.44216800	C	-3.21371800	-1.57877700	0.88044700
C	-1.10729700	-1.35848600	2.52616200	C	-2.85849200	-0.81529700	-0.24135300
C	0.04447600	-2.17628000	1.98046300	C	-3.91268800	-0.24599000	-0.98982100
H	0.42899500	-2.80668200	2.79036800	C	-5.25196900	-0.51453100	-0.65787800
H	-0.27348100	-2.83105000	1.16520500	H	-6.05718400	-0.09152200	-1.24687300
C	2.32076800	-2.33963100	1.17128800	C	-5.56438500	-1.31053300	0.44670700
H	1.88357400	-3.20035100	0.65809300	C	-4.54663500	-1.83474200	1.23496500
H	2.75668600	-2.67350300	2.11813100	H	-4.77520800	-2.43275300	2.11333800
C	3.35663400	-1.73689600	0.26504200	H	4.30773000	0.97641400	-1.23677100
C	4.71390900	-2.04145800	0.34236400	H	-0.01070100	-2.64000800	2.93723000
H	5.07645700	-2.69684500	1.12651300	H	0.43247000	-2.80207200	1.23756900
C	5.58314100	-1.49323200	-0.60052500	Cl	-0.59103700	-2.84454300	-1.22135200
H	6.64409200	-1.71738800	-0.56105900	Cl	-0.57412000	0.26363000	-2.66490500
C	5.07192800	-0.64935800	-1.58625100	H	-6.60553400	-1.49848400	0.69345500
H	5.71429500	-0.19968400	-2.33475800	O	-3.57635100	0.58097500	-2.02514400
C	3.70746400	-0.37607400	-1.59489400	C	-4.61241400	1.18399800	-2.78642600
H	3.24604700	0.27536300	-2.32783700	H	-5.25363000	1.82573500	-2.16880300
C	1.64760700	-0.32585600	2.42624300	H	-4.11277500	1.79602000	-3.53910200
H	0.91905700	-0.28690400	3.23941400	H	-5.23773100	0.43648200	-3.29063400
H	2.59145200	-0.65002100	2.87546600				
C	1.79142000	1.03187500	1.79676600	(R_{Ham}) -OC-6-42-A RhCl₂(κ⁴C,N,N',P-L2) (C-2 metallated)			
C	1.39509600	1.22914000	0.46426100	Rh	-0.02825700	-1.06420100	-0.62387100
C	1.55896300	2.53996000	-0.05808500	P	-0.04474300	1.15627800	0.20008200
C	2.07881700	3.57343900	0.73684300	N	-0.46287600	-1.86624900	1.30435300
H	2.19346500	4.56947600	0.32704100	N	-2.25042800	-1.18379100	-0.76288500
C	2.45133900	3.33611900	2.06119400	C	-0.40374500	2.51192400	-1.00011400
C	2.31116200	2.06455800	2.59618100	C	-1.61973000	2.50493200	-1.70507700
H	2.60020100	1.86023800	3.62412200	H	-2.33970100	1.71379100	-1.54015700
H	-3.25339100	1.16233600	-2.03750000	C	-1.92684400	3.52300600	-2.60537300
H	2.85110500	4.14820300	2.66181800	H	-2.87538500	3.50303100	-3.13338100
O	1.18666600	2.75915000	-1.35005300	C	-1.01756600	4.56062800	-2.82876600
C	1.32775200	4.05949700	-1.90163000	H	-1.25454400	5.35166300	-3.53385200
H	0.98010100	3.98271300	-2.93317900	C	0.19244600	4.57625900	-2.13632300
H	0.71435300	4.79736500	-1.36978300	H	0.90409700	5.38057800	-2.29630700
H	2.37270300	4.39469500	-1.89967300	C	0.49757300	3.56303700	-1.22320800
				H	1.43759600	3.60607100	-0.68762700
				C	1.40721900	1.78462000	1.15621100
				C	1.26424900	2.29292100	2.45770600
				H	0.29526500	2.30108300	2.94301900
				C	2.36968500	2.80138000	3.14347200
				H	2.24233900	3.18630500	4.15073700
				C	3.62610200	2.82030500	2.53686900
				H	4.48397100	3.21838100	3.07050400
				C	3.77425200	2.32691000	1.23850700
				H	4.74732300	2.34090200	0.75686200
				C	2.67571600	1.80634500	0.55323700
				C	-1.41500600	1.23886100	1.42804200
				C	-2.35117900	2.28021400	1.45770900
				H	-2.28957400	3.08843100	0.73903200
				C	-3.36751200	2.29785300	2.41631000
				H	-4.08200500	3.11507600	2.42530900
				C	-3.45321500	1.27584200	3.35924300
				H	-4.23808800	1.28416400	4.10903500
				C	-2.51753100	0.23970800	3.34241600
				H	-2.57338800	-0.54857700	4.08792200
				C	-1.49820700	0.20401800	2.38473700
				C	-0.46616300	-0.89567300	2.45442800
				C	-1.79209400	-2.55364500	1.20683400
				C	-2.76852000	-1.86673000	0.27915300
				C	-4.14481300	-2.05619900	0.41418600
				H	-4.53447100	-2.59713600	1.26983400
				C	-4.99832600	-1.55724500	-0.56801000
				H	-6.07138300	-1.69409100	-0.48138800
				C	-4.45135600	-0.89382300	-1.66616500
				H	-5.07557100	-0.50737800	-2.46387500
				C	-3.07097800	-0.72681500	-1.72228700
				H	-2.58231400	-0.23008700	-2.55378100
				C	0.65354800	-2.84530900	1.56563300
				C	1.95881800	-2.30128600	1.04344400
				C	1.91665400	-1.45397500	-0.08408200
				C	3.15592700	-1.12156200	-0.67371400
				C	4.36504000	-1.58829700	-0.13288600
				H	5.30954500	-1.32010900	-0.59118500
				C	4.36698700	-2.39406500	1.00692400
				C	3.16291400	-2.75344800	1.60180300
(R_{Ham}) -OC-6-43-C RhCl₂(κ⁴C,N,N',P-L2) (C-2 metallated)							
Rh	-0.79967900	-0.55463500	-0.37504300				
P	1.69157300	-0.08032400	-0.16641500				
N	-0.88739200	-1.24048200	1.62955000				
N	-1.21835100	1.26006500	0.48659400				
C	1.96375900	1.74794400	-0.18645800				
C	2.03449800	2.50749000	0.99270000				
H	2.01289700	2.02083800	1.96142700				
C	2.14570600	3.89909100	0.93859200				
H	2.20455800	4.46670800	1.86270200				
C	2.18793800	4.55484800	-0.29247700				
H	2.28122300	5.63606300	-0.33347700				
C	2.10909900	3.81044400	-1.47202400				
H	2.13913200	4.31025300	-2.43588500				
C	1.98998800	2.42113500	-1.42159400				
H	1.91545200	1.85897900	-2.34539400				
C	2.97185100	-0.72702200	-1.33574400				
C	2.78854900	-2.00474900	-1.88865400				
H	1.87748500	-2.55484600	-1.67728500				
C	3.76111000	-2.55995600	-2.72335100				
H	3.60352800	-3.54808400	-3.14615200				
C	4.92513700	-1.84843000	-3.01974700				
H	5.67874000	-2.28007800	-3.67197300				
C	5.11402000	-0.57544400	-2.47675300				
H	6.01487700	-0.01268200	-2.70364400				
C	4.14627600	-0.01734300	-1.63984000				
C	2.35907500	-0.59155300	1.48548800				
C	3.64022000	-0.16130400	1.87148600				
C	4.22592400	0.44829000	1.19170600				
H	4.18158400	-0.49329400	3.11131700				
H	5.17497900	-0.14708200	3.37940300				
C	3.43442100	-1.26597400	3.99951000				
H	3.83413100	-1.52793700	4.97428500				
C	2.16685300	-1.70746400	3.62748300				
H	1.59494500	-2.32034800	4.31832200				
C	1.61090800	-1.39690400	2.37404200				
C	0.29687500	-2.08102300	2.04692700				
C	-1.07713300	-0.05938200	2.54376400				
H	-0.14888900	0.09181600	3.10211500				

H	3.14864300	-3.39639200	2.47820600	(R_{Nam}) -OC-6-43-C RhCl₂(κ⁴C,N,N',P-L3) (C-4 metallated)		
H	2.80310800	1.42307500	-0.45214200	Rh	-0.31588200	-0.44596200
Cl	-0.10577000	-3.40087400	-1.56498600	P	2.18352200	-0.23789800
Cl	0.17717100	-0.26300200	-2.90313300	N	-0.67221300	-0.53218000
H	-2.22446600	-2.68824000	2.20319400	N	-0.56464400	1.58012100
H	-1.60706400	-3.54447700	0.78511800	C	2.71038600	1.48396100
H	0.54632600	-0.48731900	2.51030200	C	2.88016100	2.48326500
H	-0.63086500	-1.47543400	3.36920000	H	2.78899500	2.24641800
H	0.40674000	-3.75373600	1.01361200	C	3.18270400	3.79514700
H	0.69193700	-3.09094200	2.63320700	H	3.31526600	4.55296700
H	5.31119400	-2.73664700	1.42048200	C	3.32105000	4.12841500
O	3.12860700	-0.31427500	-1.78334100	H	3.56246800	5.14685700
C	4.34270500	-0.06447600	-2.48155700	C	3.14513000	3.14309600
H	4.06733000	0.52854100	-3.35495100	H	3.24709700	3.39180200
H	5.05740400	0.50381900	-1.87317000	C	2.83375400	1.83492700
H	4.81686500	-0.99639500	-2.81209400	H	2.68291900	1.08499600
(R_{Nam}) -OC-6-54-C RhCl₂(κ⁴C,N,N',P-L3) (C-4 metallated) (7)				C	3.44016900	-1.29514800
Rh	0.21335100	1.18633900	-0.35717500	C	3.13980200	-2.65029400
Cl	0.55779300	1.09016000	-2.75951400	H	2.16430500	-3.03494600
Cl	2.10715800	2.95627100	-0.10284200	C	4.08282400	-3.49903300
P	1.65887000	-0.63416100	-0.01900800	H	3.83535000	-4.54424700
N	-0.26291000	1.40505900	1.70649300	C	5.33351000	-3.00800800
N	-1.15432000	2.81449200	-0.48406600	H	6.06441300	-3.66889300
C	3.45005100	-0.31293600	-0.32509300	C	5.63912800	-1.66102600
C	4.43707900	-0.69953400	0.59431300	H	6.60858900	-1.26927200
H	4.16462200	-1.17720700	1.52816500	C	4.70110600	-0.80891100
C	5.78752500	-0.47331700	0.31586100	C	2.63488500	-0.42890200
H	6.53985700	-0.77487300	1.03859500	C	3.94711300	-0.12161200
C	6.16677600	0.13276600	-0.88227300	H	4.66855300	0.19988200
H	7.21725300	0.30412700	-1.09821200	C	4.35050100	-0.21592100
C	5.18850000	0.52374400	-1.80031700	H	5.37187300	0.02750300
H	5.47508200	1.00311100	-2.73177100	C	3.42987000	-0.61951600
C	3.83802200	0.31418700	-1.52154700	H	3.72022700	-0.69087300
H	3.07994500	0.64397700	-2.22302300	C	2.12819800	-0.93637000
C	1.28795300	-2.15487700	-0.99943600	H	1.41982300	-1.26154500
C	0.15870400	-2.92908400	-0.67970300	C	1.70576000	-0.86391100
H	-0.47791500	-2.65173100	0.15287800	C	0.30994900	-1.39832500
C	-0.14965700	-4.06983500	-1.42010300	C	-0.69025100	0.86750800
H	-1.02164100	-4.66008800	-1.15495100	H	0.26316600	1.04162400
C	0.65560300	-4.44877500	-2.49714200	C	-1.47076900	0.96243900
H	0.41314300	-5.33662700	-3.07351000	C	-0.84835700	1.92758600
C	1.77510300	-3.68331700	-2.82492100	C	-1.19775600	3.23610200
H	2.41067800	-3.97174900	-3.65678100	H	-1.42466300	3.48491100
C	2.09276500	-2.54495400	-2.08003300	C	-1.24458500	4.20260400
C	1.59317000	-1.21518400	1.73129700	H	-1.51525300	5.22569100
C	1.93890200	-2.54556100	2.02394600	C	-0.94256400	3.83276900
H	2.20431800	-3.22023900	1.21791000	H	-0.96696800	4.55032200
C	1.95249700	-3.02144700	3.33462800	C	-0.61443400	2.51009100
H	2.22752900	-4.05288800	3.53115900	H	-0.38848300	2.15339100
C	1.61043100	-2.16642900	4.38014000	C	-2.02883500	-1.18503300
H	1.61052100	-2.52192200	5.40576400	H	-1.85361500	-2.26169900
C	1.25829100	-0.84639200	4.10240400	H	-2.42061100	-0.97282200
H	0.98557300	-0.18401800	4.91886100	C	-2.95106100	-0.76116100
C	1.24639800	-0.34680500	2.79156900	C	-2.35230000	-0.47374000
C	0.90439500	1.11761700	2.61646500	C	-3.17483900	-0.15034000
H	0.67262300	1.53570400	3.60231500	C	-4.56523700	-0.12799300
H	1.74563400	1.67836700	2.20095300	H	-5.19628600	0.12365400
C	-0.58045600	2.86810100	1.85550100	C	-5.14573800	-0.40958700
H	0.37452100	3.40029700	1.82467900	C	-4.33668500	-0.72524000
H	-1.05699900	3.05188000	2.82349800	H	-4.78789900	-0.93708700
C	-1.42350700	3.36847600	0.71675300	H	4.95431700	0.23555600
C	-2.36910400	4.38235000	0.85192400	H	-0.14737800	-1.63010400
H	-2.57273200	4.80453800	1.82964300	H	0.36415100	-2.32760500
C	-3.03724700	4.83742600	-0.28456800	Cl	-0.35556700	-2.88299000
C	-3.77670800	5.62739500	-0.20396400	Cl	-0.00462400	-0.26238800
H	-2.74850000	4.25871900	-1.52005600	C	-6.63700700	-0.43430100
H	-3.24878000	4.58039800	-2.42630000	F	-7.15094500	-1.67676900
C	-1.80408900	3.23849900	-1.57951400	F	-7.03570100	-0.05685300
H	-1.54163500	2.73941500	-2.50536200	F	-7.25786900	0.38145500
C	-1.47128300	0.56436400	2.07240400	H	-2.73393900	0.08660700
H	-1.14838800	-0.20153700	2.78096300	(R_{Nam}) -OC-6-42-A RhCl₂(κ⁴C,N,N',P-L3) (C-4 metallated)		
H	-2.19166200	1.19476500	2.60246700	Rh	-0.24189200	-0.92426500
C	-2.09104300	-0.07963200	0.86098200	P	-0.90917800	1.16552600
C	-1.43110500	0.01641500	-0.37857900	N	0.02496200	-1.77033600
C	-2.02572300	-0.58337000	-1.49864100	N	-2.25548900	-1.85776100
C	-3.23146600	-1.27505700	-1.38721400	C	-1.98258900	2.22466700
H	-3.67885400	-1.73008800	-2.26548200	C	-3.22700800	1.73102600
C	-3.86793300	-1.37635500	-0.14560300	H	-3.56078400	0.74915800
C	-3.29770400	-0.77615600	0.97831700	C	-4.06036700	2.50348300
H	-3.79850000	-0.84302500	1.93981700	H	-5.02057400	2.10553500
H	2.97423300	-1.97158100	-2.34187500	C	-3.66106100	3.78081000
C	-5.12858300	-2.17639600	-0.01255200	H	-4.30791000	4.38094700
F	-5.88822800	-1.77250700	1.03327400	C	-2.43047600	4.28157600
F	-5.90267800	-2.10098900	-1.12151800	H	-2.11251100	5.27596700
F	-4.87736300	-3.49761200	0.18550700	C	-1.59711800	3.51287400
H	-1.54328100	-0.50895000	-2.46599700	H	-0.65263600	3.93120800
				C	0.38808500	2.31724600

C	0.38807900	2.75901100	2.08426500	H	-3.58155700	-2.13411100	4.93676900
H	-0.37457100	2.41952200	2.77572500	C	-2.11457700	-2.35038900	3.37812700
C	1.36557300	3.64908800	2.53462100	H	-1.66950600	-3.23279200	3.82894300
C	1.35250400	3.97787700	3.56926400	C	-1.58359400	-1.86425700	2.17304500
H	2.34688000	4.11723700	1.66017600	C	-0.45615500	-2.66078500	1.55538100
H	3.10462200	4.81114700	2.01124500	H	-0.17573200	-3.45437000	2.25688500
C	2.34856600	3.69203400	0.32953200	H	-0.76733900	-3.13060000	0.61960800
C	3.10515700	4.05449100	-0.35954500	C	1.84033000	-2.89952100	0.85929100
C	1.38091900	2.79465900	-0.12181000	H	1.34916300	-3.62639100	0.20697300
C	-1.93448400	0.79947000	1.60368100	H	2.18988900	-3.41554500	1.75905100
C	-3.15016000	1.44573500	1.86167600	C	2.98083700	-2.29764700	0.09048800
H	-3.51441900	2.20854200	1.18433000	C	4.28220000	-2.79157600	0.15122400
C	-3.90236500	1.12266600	2.99365600	H	4.52115100	-3.60274500	0.82998300
H	-4.84064200	1.63624900	3.17855600	C	5.25639000	-2.22770600	-0.67177000
C	-3.44294600	0.15156900	3.88076900	H	6.27641000	-2.59667500	-0.64299900
H	-4.02170800	-0.10469900	4.76256200	C	4.90389300	-1.17897100	-1.52069800
C	-2.22552900	-0.48715200	3.63756000	H	5.63302600	-0.70678900	-2.16916600
H	-1.85721100	-1.22937200	4.34006500	C	3.58875000	-0.72463000	-1.51879300
C	-1.46268800	-0.17802300	2.50630900	H	3.25466000	0.10113200	-2.13438900
C	-0.11283300	-0.82914300	2.33269300	C	1.23480100	-1.07451700	2.41356900
C	-0.95032900	-2.90182300	1.29141200	H	0.35345600	-0.89280500	3.03295200
C	-2.26826900	-2.65729000	0.58644600	H	1.92603000	-1.66610300	3.02274500
C	-3.41776300	-3.35312000	0.96451700	C	1.82652600	0.24776500	2.01674900
H	-3.40494200	-3.97495400	1.85312300	C	1.53044100	0.80904900	0.74936200
C	-4.56374800	-3.25082800	0.17842800	C	2.03605900	2.12008100	0.53605800
H	-5.46649500	-3.78566000	0.45519000	C	2.80100100	2.77600500	1.51748300
C	-4.52675400	-2.46462400	-0.97306100	H	3.17188600	3.77241300	1.31423100
H	-5.38718400	-2.37341000	-1.62614900	C	3.09101500	2.17803200	2.73669500
C	-3.35191200	-1.78194200	-1.27275400	C	2.59282100	0.90658400	2.98436000
H	-3.26313500	-1.15927700	-2.15645000	H	2.79122700	0.41548400	3.93406500
C	1.45915100	-2.25187700	1.17363500	H	-3.14165000	2.04185000	-1.56640200
C	2.33233500	-1.28620900	0.41061300	C	1.84673900	2.92844400	-0.72909600
C	1.74183500	-0.58022700	-0.66469900	F	2.64851100	2.49904800	-1.73819500
C	2.58046200	0.14541800	-1.51776400	F	0.57980800	2.94541600	-1.17695900
C	3.95691000	0.21574500	-1.28660100	F	2.17918700	4.23883200	-0.54902100
H	4.59147000	0.78935100	-1.95474900	H	3.69024400	2.69845200	3.47694600
C	4.51554600	-0.43595900	-0.18410900	(R_{Ham}) -OC-6-43-C RhCl₂($\kappa^4\text{C}, \text{N}, \text{N}', \text{P-L3}$) (C-2 metallated)			
C	3.70115100	-1.19646300	0.66252400	Rh	-0.67916400	0.36707300	-0.42342800
H	4.13862200	-1.72619900	1.50416000	P	1.81396600	0.24868400	0.00367200
H	1.39704800	2.47587500	-1.15631700	N	-0.53595700	-1.25091700	-1.79687400
Cl	0.34500600	-3.13919900	-1.79330300	N	-0.96945300	-1.15404300	0.93479100
Cl	-0.54189200	-0.05655500	-3.00989000	C	2.12380900	-0.42509300	1.69777700
H	-1.11165000	-3.15181000	2.34462600	C	2.37679400	-1.78891000	1.91878700
H	-0.49559300	-3.76948900	0.80715100	H	2.47680200	-2.47198800	1.08301600
H	0.67230700	-0.07804400	2.21119300	C	2.52049000	-2.28642700	3.21619500
H	0.12390500	-1.39729500	3.23885400	H	2.72045500	-3.34368600	3.36348300
H	1.46885400	-3.21142100	0.65390000	C	2.41602500	-1.43136100	4.31395900
H	1.79376000	-2.41480800	2.20411800	H	2.53511700	-1.81813700	5.32170400
C	5.99453300	-0.39370000	0.05125100	C	2.15676100	-0.07452800	4.10703400
F	6.56789800	0.71761100	-0.46786700	H	2.07170400	0.60038300	4.95369900
F	6.30509400	-0.42465900	1.37048100	C	2.00365000	0.42454300	2.81298100
F	6.63559700	-1.45254500	-0.51198600	H	1.78639500	1.47631000	2.66968300
H	2.16021500	0.65477900	-2.37864600	C	2.92431800	1.72340300	-0.11246200
(R_{Ham}) -OC-6-54-C RhCl₂($\kappa^4\text{C}, \text{N}, \text{N}', \text{P-L3}$) (C-2 metallated)				C	2.70779100	2.64610100	-1.14924200
Rh	0.64423200	-0.62847700	-0.48658000	H	1.85638400	2.52316300	-1.80994200
Cl	0.65088100	0.43448900	-2.66358400	C	3.56910200	3.73161000	-1.31969400
Cl	-0.12963600	-2.73642600	-1.78141300	H	3.38637600	4.43882200	-2.12364800
P	-1.58085300	-0.00481600	-0.01469200	C	4.65475500	3.91257700	-0.46021500
N	0.79403400	-1.88205100	1.23097100	H	5.32136300	4.75975900	-0.59239200
N	2.65151500	-1.28512600	-0.73710000	C	4.87779600	2.99914400	0.57184900
C	-2.86173600	-0.58768500	-1.21453200	H	5.71953400	3.13020900	1.24556500
C	-3.95648400	-1.36143100	-0.79867900	C	4.02126000	1.91013900	0.74522500
H	-4.06574300	-1.64863900	0.23996100	C	2.67405000	-0.96987800	-1.09412400
C	-4.92260000	-1.77486500	-1.71954000	C	4.01166600	-1.30605900	-0.82274500
H	-5.76077000	-2.37596100	-1.37964400	H	4.52248500	-0.83445900	0.01011000
C	-4.81323100	-1.41736400	-3.06339100	C	4.70198700	-2.23640600	-1.59581400
H	-5.56714400	-1.73629200	-3.77707300	H	5.73506300	-2.47493900	-1.36270100
C	-3.72382600	-0.65166200	-3.48643400	C	4.05275500	-2.85728300	-2.66271100
H	-3.62466900	-0.37469000	-4.53196000	H	4.57062700	-3.59237100	-3.27093200
C	-2.74968200	-0.24682600	-2.57386800	C	2.73124100	-2.52508600	-2.95053600
C	-1.88824000	0.31364900	-2.91830700	H	2.23465100	-3.00083300	-3.79134900
H	-1.91781700	1.79937600	0.19992900	C	2.02482400	-1.57536200	-2.19194200
C	-1.37114100	2.46134800	1.31329200	C	0.65851800	-1.18815300	-2.72067000
H	-0.77018300	1.91619200	2.03242100	C	-0.57468400	-2.54765800	-1.03611100
C	-1.60213900	3.82101100	1.51200600	H	0.42987200	-2.98028600	-1.05065800
H	-1.17810200	4.31562200	2.38081800	H	-1.22822300	-3.25922800	-1.54876100
C	-2.37440700	4.54398200	0.59833200	C	-0.99392200	-2.39573900	0.40228300
H	-2.55283700	5.60391300	0.75346700	C	-1.32367400	-3.50572800	1.17847000
C	-2.91893200	3.89554700	-0.50971600	H	-1.33973100	-4.49025500	0.72394100
H	-3.52583500	4.44628200	-1.22222400	C	-1.62115300	-3.33038700	2.52715300
C	-2.69660000	2.52987700	-0.70757400	H	-1.88128200	-4.18318800	3.14537800
C	-2.15477300	-0.70725800	1.59804100	C	-1.57907700	-2.04491500	3.06681800
C	-3.23459900	-0.08521500	2.24923500	H	-1.80009700	-1.86137100	4.11185800
H	-3.67938500	0.80424300	1.81742200	C	-1.25423200	-0.97769300	2.23983500
C	-3.75655900	-0.58991600	3.43885200	H	-1.21919400	0.04473800	2.58952600
H	-4.59460700	-0.09090100	3.91515000	C	-1.74086300	-1.12116600	-2.68177700
C	-3.19279200	-1.73098200	4.00685300	H	-1.50635800	-0.33098900	-3.39987100

H	-1.88525100	-2.05427200	-3.23855800	F	4.79650000	-0.32029800	-1.64075200
C	-2.94639600	-0.72390900	-1.88742600	H	4.99181200	-2.20298400	2.55779200
C	-2.75854200	0.16133500	-0.80112500	(R_{Ham}) -OC-6-54-C IrCl₂(κ⁴C,N,N',P-L1) (8)			
C	-3.94789600	0.60522300	-0.17210200	Ir	0.77885400	-0.45654700	-0.29372400
C	-5.21286000	0.16198400	-0.59975300	Cl	0.48329600	-0.70008500	-2.68066400
H	-6.09755300	0.52586500	-0.09258200	Cl	0.54684100	-2.97786400	0.04690000
C	-5.34878900	-0.73405400	-1.65268000	P	-1.47171400	-0.04894800	0.00176800
C	-4.20247800	-1.17607800	-2.30292700	N	1.29177700	-0.24528100	1.75970300
H	-4.27653200	-1.86827500	-3.13812400	N	2.85683500	-0.81267000	-0.40596100
H	4.21086300	1.21464200	1.55491900	C	-2.61782500	-1.48137800	-0.22272800
H	0.43511500	-1.84643500	-3.56702300	C	-3.69123200	-1.71958900	0.64890500
H	0.67299900	-0.16251000	-3.09676600	H	-3.85541800	-1.08074000	1.50904600
Cl	-0.59010500	2.00162500	-2.23608800	C	-4.56231100	-2.78764900	0.42279200
Cl	-0.56266100	2.17612700	1.20926100	H	-5.38542700	-2.96228100	1.10978800
C	-3.97269500	1.60252000	0.96096200	C	-4.37548700	-3.62451100	-0.67758900
F	-3.45060600	2.79728600	0.60507700	H	-5.05374400	-4.45478900	-0.85289100
F	-5.23758700	1.87218800	1.38633900	C	-3.30804300	-3.39460700	-1.54819900
F	-3.31333400	1.17052300	2.06277600	H	-3.14879500	-4.04741600	-2.40138500
H	-6.33205100	-1.07648000	-1.95920400	C	-2.42659200	-2.33762700	-1.32058000
(R_{Ham}) -OC-6-42-A RhCl₂(κ⁴C,N,N',P-L3) (C-2 metallated)							
Rh	-0.07546000	-1.10703100	-0.43951300	H	-1.58524800	-2.18043500	-1.98577900
P	-0.20725500	1.20100900	0.15742100	C	-2.21278500	1.27339200	-1.05676200
N	-0.72129300	-1.69483500	1.51118800	C	-1.87333500	2.61914900	-0.83500700
N	-2.26886900	-1.29404300	-0.78478500	H	-1.19956800	2.88753100	-0.02938600
C	-0.32788900	2.43515200	-1.20559100	C	-2.40022800	3.62420300	-1.64538400
C	-1.38403500	2.35238900	-2.12927500	H	-2.12982000	4.65922000	-1.45793100
H	-2.12743800	1.57098300	-2.03887500	C	-3.26230400	3.30188100	-2.69611800
C	-1.49831800	3.28117700	-3.16172200	H	-3.66845000	4.08592800	-3.32872500
H	-2.32665700	3.20693300	-3.85969400	C	-3.59852900	1.96829800	-2.92824000
C	-0.54800700	4.29635900	-3.30154900	H	-4.26764100	1.70619000	-3.74255400
H	-0.63383900	5.01580500	-4.11029600	C	-3.08075500	0.95971300	-2.11246500
C	0.50869400	4.38150300	-2.39556200	C	-1.82300900	0.53037500	1.72354100
H	1.25076300	5.16813600	-2.49249900	C	-2.94484600	1.33769500	1.97271400
C	0.61766900	3.46087800	-1.35006700	H	-3.57513500	1.64376800	1.14529800
H	1.43889800	3.55389200	-0.65021100	C	-3.27177200	1.75631300	3.26244500
C	1.00499400	1.96344200	1.34041500	H	-4.14824300	2.37672900	3.42286900
C	0.55348300	2.65530900	2.47858500	C	-2.46766500	1.37405000	4.33357600
H	-0.50516000	2.72697500	2.69598600	H	-2.70489700	1.69342900	5.34383900
C	1.46089500	3.26673200	3.34553700	C	-1.34468900	0.58186500	4.09949300
H	1.09018000	3.79285800	4.22000300	H	-0.71445500	0.29077500	4.93559500
C	2.83104000	3.20661000	3.08875300	C	-1.00328700	0.14670400	2.81010200
H	3.53542700	3.68238400	3.76438700	C	0.21107400	-0.75070100	2.68572200
C	3.28887800	2.53662200	1.95307800	H	0.65085700	-0.87252600	3.68294400
H	4.35165000	2.49093300	1.73555900	H	-0.05753900	-1.74023300	2.30573800
C	2.38561100	1.91877100	1.08688000	C	2.48448000	-1.14555800	1.94716100
C	-1.78360100	1.34241400	1.09968000	H	2.10242200	-2.17114700	1.94978000
C	-2.75547800	2.31482600	0.83711500	H	2.97169100	-0.93663400	2.90542900
H	-2.60369100	3.03613800	0.04302900	C	3.44041400	-1.02173800	0.79505300
C	-3.92354500	2.37752100	1.60221000	C	4.81758400	-1.18275200	0.91416500
H	-4.66581400	3.13950100	1.38588000	H	5.25964100	-1.34177200	1.89184100
C	-4.12443500	1.47317800	2.64268700	C	5.60473100	-1.14248200	-0.23649500
H	-5.02684100	1.51936800	3.24409000	H	6.68057800	-1.26835100	-0.16821800
C	-3.15438400	0.50657200	2.91621200	C	4.99046700	-0.93336400	-1.47005100
H	-3.30441500	-0.18952000	3.73665800	H	5.56516200	-0.89363100	-2.38844500
C	-1.98572600	0.42321200	2.15300100	C	3.61054000	-0.76262500	-1.51719000
C	-0.93589200	-0.59773300	2.51983400	H	3.06781300	-0.59123300	-2.43979900
C	-1.99206500	-2.47024200	1.33145300	C	1.66782300	1.19442100	2.08657300
C	-2.88065800	-1.91323800	0.24645000	H	0.92630600	1.57838400	2.79141000
H	-4.25631300	-2.14616400	0.24702700	H	2.62731000	1.18973300	2.61434300
H	-4.72002400	-2.63489300	1.09707500	C	1.71973900	2.05905900	0.85222500
C	-5.01113700	-1.75585700	-0.85716700	C	1.26966100	1.51616000	-0.37025700
H	-6.08231800	-1.92850600	-0.87693900	C	1.32765300	2.34596300	-1.50428400
C	-4.36644700	-1.15165400	-1.93603200	C	1.79984000	3.65828400	-1.42122900
H	-4.90989400	-0.84674400	-2.82315700	H	1.83069400	4.27526300	-2.31625700
C	-2.99378600	-0.93786300	-1.85766000	C	2.23020700	4.18130300	-0.19876000
H	-2.43163800	-0.49003800	-2.66944400	C	2.19063400	3.37508600	0.93869300
C	0.38836400	-2.56435300	2.02747100	H	2.52985400	3.76950400	1.89518200
C	1.72814700	-2.02779200	1.59455800	H	-3.35857000	-0.07041700	-2.30213500
C	1.83178000	-1.38696600	0.32979000	H	0.99386500	1.95652100	-2.46015800
C	3.15093500	-1.13768900	-0.11988800	H	2.59717100	5.20175700	-0.13232500
C	4.26849300	-1.44004200	0.67978300	(R_{Ham}) -OC-6-43-C IrCl₂(κ⁴C,N,N',P-L1)			
H	5.26086900	-1.22748800	0.30205800	Ir	-0.81457200	-0.56019500	-0.32131800
C	4.12113300	-1.99658000	1.94358400	P	1.55203500	-0.09583300	-0.02590400
C	2.84047400	-2.30193400	2.39451500	N	-1.20140600	-0.44727000	1.76054000
H	2.69989800	-2.77277100	3.36449700	N	-1.33254500	1.42264800	-0.25705900
H	2.75816600	1.42255300	0.20463000	C	1.89897900	1.68130600	-0.41291300
Cl	-0.00292900	-3.52189900	-1.09770600	C	2.11152500	2.66147000	0.56720800
Cl	0.22948800	-0.57018600	-2.78145100	H	2.16165600	2.38607000	1.61514700
H	-2.52818200	-2.54430600	2.28269100	C	2.27999300	4.00252000	0.20872800
H	-1.70993100	-3.47950100	1.02298600	H	2.44865300	4.74640100	0.98234200
H	0.03872000	-0.12933400	2.67690600	C	2.24218500	4.38169800	-1.13265900
H	-1.21851600	-1.07502400	3.46453200	H	2.38121700	5.42240500	-1.41085400
H	0.25063300	-3.54968800	1.57799200	C	2.02383900	3.41362100	-2.11698500
H	0.30817400	-2.67097700	3.11500600	H	1.98896800	3.69899600	-3.16452800
C	3.47258500	-0.59386500	-1.49204500	C	1.84481500	2.07699400	-1.76261700
F	3.16831400	-1.46668300	-2.47770700	H	1.65160700	1.33710500	-2.53328300
F	2.83680500	0.57364600	-1.77102900	C	2.87284500	-0.98326400	-0.96773300

C	-4.68701500	3.64416300	0.45548600	C	-0.14072200	-4.51369500	0.17411100
H	-4.67216100	4.72757100	0.38450900	H	-0.80641000	-4.80417400	-0.64131100
C	-5.90306500	2.96294400	0.53838500	H	0.88751800	-4.71372000	-0.14705500
H	-6.83886000	3.51357200	0.52467000	H	-0.34800600	-5.11163700	1.06286000
C	-5.91011700	1.57120200	0.65702700	TS_VIII-IXa			
H	-6.85017000	1.03478600	0.74321700	Rh	-0.78373500	-0.23054700	-0.51775400
C	-4.70628200	0.86596100	0.67927500	Cl	-0.26274200	-0.06502700	-2.87677500
H	-4.72308600	-0.21395300	0.79919400	P	1.56099400	0.10667600	-0.01480500
H	4.36992800	-0.23419500	1.00281400	N	-1.16439200	1.84187100	-0.39691100
O	-2.54491000	3.47809600	0.43667600	N	-2.78491700	-0.32509700	-1.13491200
H	1.18753300	-2.53017800	0.80616900	C	2.68826500	-0.52104700	-1.33069600
C	0.71714600	-2.17586300	1.94452200	C	3.73179600	0.26700500	-1.83844000
O	-0.16846700	-1.24908000	1.92535800	H	3.87718700	1.28212500	-1.48984800
C	1.19223200	-2.78125500	3.22352200	C	4.59778400	-0.24887700	-2.80566100
H	1.61335600	-3.77090800	3.04230400	H	5.39874900	0.37459500	-3.19104800
H	1.97225900	-2.13723300	3.64410900	C	4.43518300	-1.55316000	-3.27241600
H	0.37198100	-2.83714000	3.94143900	H	5.11139800	-1.95250800	-4.02222000
VIIIa				C	3.39308500	-2.34115600	-2.77681700
Rh	-0.69780400	-0.25350800	-0.48587600	H	3.25234300	-3.35391000	-3.14191000
Cl	-0.22108300	-0.27726300	-2.78554100	C	2.51850800	-1.82809300	-1.81994200
P	1.61007900	0.14624700	0.00811700	H	1.69313100	-2.43758300	-1.47367000
N	-1.19336500	1.83086500	-0.58246200	C	2.20889200	-0.61559400	1.55353200
N	-2.72496400	-0.44918400	-1.06084800	C	1.70999300	-0.13624000	2.77736400
C	2.76795100	-0.44620600	-1.28869900	H	0.95539000	0.64381100	2.80047100
C	3.81422200	0.36024800	-1.75942100	C	2.17856400	-0.65486600	3.98188700
H	3.93828500	1.37264800	-1.39368000	H	1.78671000	-0.27270100	4.91947100
C	4.70945500	-0.13826100	-2.70883900	C	3.14951000	-1.66138500	3.98234000
H	5.51435100	0.49539900	-3.06837300	H	3.51383000	-2.06547400	4.92191200
C	4.57084100	-1.44029600	-3.19055000	C	3.65031900	-2.14052800	2.77239500
H	5.27012400	-1.82563600	-3.92642600	H	4.40864000	-2.91750100	2.76367700
C	3.52537600	-2.24528700	-2.72946600	C	3.18527600	-1.62100300	1.56088400
H	3.40638400	-3.25588000	-3.10799300	C	1.98284000	1.89128000	0.18047400
C	2.62072700	-1.75114100	-1.79083500	C	3.18491100	2.20851300	0.83897400
H	1.79002700	-2.36624600	-1.46393100	H	3.81364800	1.41291700	1.22272100
C	2.23075900	-0.58472500	1.58173600	C	3.59128300	3.53029400	1.00930800
C	1.77151200	-0.07864700	2.81033400	H	4.52775000	3.74542800	1.51368800
H	1.07358500	0.75106300	2.84519100	C	2.78313700	4.56357400	0.53883600
C	2.22207600	-0.62369500	4.01052800	H	3.07886700	5.59917700	0.67309000
H	1.86205900	-0.21886100	4.95131300	C	1.57853500	4.26255400	-0.09335000
C	3.13582000	-1.68157100	4.00253600	H	0.94371600	5.07125200	-0.44303600
H	3.48672200	-2.10486000	4.93874600	C	1.16126500	2.93796600	-0.29131300
C	3.59990600	-2.18541000	2.78767300	C	-0.13501900	2.74461100	-1.04355100
H	4.31600700	-3.00129200	2.77156100	H	-0.60211700	3.72666200	-1.16627100
C	3.15211500	-1.64168200	1.58135300	H	0.04327200	2.32929800	-2.03749900
C	1.93794500	1.94742800	0.21429600	C	-2.45500000	2.08134800	-1.14728000
C	3.08164900	2.32186000	0.94223300	H	-2.17593800	2.34225100	-2.17218100
H	3.72150300	1.55715000	1.36770200	H	-2.97222200	2.94418400	-0.71830600
C	3.41543600	3.66191600	1.13018700	C	-3.36452700	0.88529100	-1.23973000
H	4.30819300	3.92146200	1.68980700	C	-4.71923500	1.00697600	-1.54385600
C	2.59196100	4.65460400	0.60406300	H	-5.17113100	1.99009500	-1.61367900
H	2.83028500	5.70325300	0.75045800	C	-5.46724500	-0.14774500	-1.76563500
C	1.44825800	4.29629300	-0.10771900	H	-6.52264000	-0.07511400	-2.00592900
H	0.80591500	5.07432900	-0.50911300	C	-4.84454300	-1.39347200	-1.67795400
C	1.10347500	2.95414800	-0.32448200	H	-5.39029200	-2.31362100	-1.85052400
H	-0.11435300	2.69954700	-1.18710300	C	-3.49586400	-1.44457400	-1.34795700
C	-0.56849400	3.66581100	-1.42943000	H	-2.95686500	-2.37902900	-1.24610000
H	0.16625900	2.21897200	-2.12632700	C	-1.30427800	2.17836500	1.06628900
C	-2.38201100	1.90904300	-1.50808100	H	-0.29529300	2.25225800	1.47514700
H	-1.98779400	1.93921300	-2.52756300	H	-1.76388400	3.16733600	1.16552000
H	-2.92397000	2.84256300	-1.33143700	C	-2.09486100	1.11778700	1.77180700
C	-3.29766800	0.71738300	-1.41646100	C	-3.14810800	1.49146000	2.61044200
C	-4.64135000	0.77516300	-1.77978600	C	-3.98629100	0.53018300	3.17644400
H	-5.08673000	1.72468700	-2.05476900	H	-4.79478800	0.83277800	3.83455200
C	-5.38813700	-0.40211000	-1.79010800	C	-3.79807100	-0.81318700	2.85604100
H	-6.43538900	-0.38005000	-2.07252700	H	-4.45803800	-1.57367000	3.26211000
C	-4.77548600	-1.60411400	-1.43448700	C	-2.75528900	-1.18844700	2.00888700
H	-5.32139600	-2.54024400	-1.43347400	H	-2.62131500	-2.24252600	1.79814600
C	-3.43494200	-1.58828600	-1.06705600	C	-1.83905000	-0.24754800	1.48724200
H	-2.89721400	-2.48286100	-0.77790900	H	-0.77463500	-1.08938900	1.41236500
C	-1.56168500	2.34398900	0.78914400	H	3.59158800	-2.00021800	0.63039600
H	-0.62899600	2.57186000	1.30848900	H	-3.32792100	2.54552400	2.80134000
H	-2.10700600	3.28637300	0.67615300	O	-0.56111900	-2.29807900	-0.64225600
C	-2.35891900	1.33763100	1.57158500	C	-0.29844100	-2.91652700	0.45024700
C	-3.61833500	1.64537900	2.08743900	O	-0.24058000	-2.33138400	1.56941700
C	-4.34860600	0.68118100	2.79049000	C	-0.02091700	-4.39462000	0.37311300
H	-5.32485200	0.93626200	3.19102700	H	-0.52045500	-4.90930000	1.19629500
C	-3.83506200	-0.60553400	2.96705800	H	-0.34158200	-4.80243800	-0.58514400
H	-4.40708100	-1.35114200	3.51003300	H	1.05699800	-4.55130300	0.48667300
C	-2.58205600	-0.93228300	2.44635400	IXa			
H	-2.15505500	-1.91899600	2.57338600	Rh	-0.86579600	-0.35529200	-0.17062800
C	-1.84255900	0.04383200	1.77014700	P	1.46938700	0.05682600	-0.08831700
H	-0.77709200	-0.20440800	1.56887000	N	-1.23635700	1.14406100	-1.59513100
C	3.52995200	-2.04230500	0.64820000	N	-2.97287900	-0.53566400	-0.33021600
H	-4.03436000	2.63684200	1.93579200	C	2.54994800	-1.21164500	-0.88115600
O	-0.46339400	-2.29144800	-0.56390800	C	3.58892600	-0.84293900	-1.75008200
C	-0.27865500	-3.03433300	0.50251700	H	3.75860100	0.19876600	-1.99473800
O	-0.19338400	-2.61279300	1.65611300				

C	4.42061200	-1.81581700	-2.30920600	C	-0.10532900	-2.02849900	4.48372500
H	5.21815100	-1.51368100	-2.98107600	C	0.79638700	-1.92958700	3.42789300
C	4.23043800	-3.16414100	-2.00532600	C	0.43048700	-1.38109100	2.18726700
H	4.87992400	-3.91831300	-2.43918900	C	1.69727600	0.98068300	0.82046300
C	3.19721000	-3.54059500	-1.143392600	C	1.38617200	2.08145100	-0.15379600
H	3.03657600	-4.58756900	-0.90603000	C	1.93426300	3.35698000	-0.06574800
C	2.35719600	-2.57321300	-0.59370000	C	1.55648900	4.32482600	-0.99615100
H	1.54842900	-2.88788900	0.05279100	C	0.64830900	3.98497900	-1.99696700
C	2.16149000	0.27301600	1.60622700	C	0.13739300	2.69294500	-2.03566700
C	1.90882300	1.45971200	2.31720000	C	2.90336200	-0.57125100	-0.70362900
H	1.33420900	2.25886200	1.86345100	C	4.22537500	-0.52759000	0.03430400
C	2.40782100	1.62705000	3.60841000	C	4.79058400	-1.69748000	0.56721200
H	2.21285300	2.55288500	4.14086700	C	6.02727900	-1.66173500	1.21322500
C	3.14889200	0.60959500	4.21446800	C	6.72419500	-0.45652700	1.32551600
H	3.53365600	0.74171400	5.22120600	C	6.18609300	0.70942600	0.77640500
C	3.39642200	-0.57451600	3.51902800	C	4.94940000	0.67165300	0.13050400
H	3.97635300	-1.36866200	3.97917800	H	-2.91456400	1.96192900	-0.97955600
C	2.91017400	-0.74272700	2.22074100	H	-3.54838900	4.29184600	-0.46851100
C	1.87772200	1.61586800	-0.97483400	H	-2.97903200	5.28909500	1.73803100
C	3.01176200	2.35473000	-0.60016300	H	-1.78151100	3.92598500	3.43827200
H	3.61618800	2.02522500	0.23714100	H	-1.17666600	1.59259300	2.95805800
C	3.38202300	3.50811600	-1.29187000	H	-2.03545800	-2.80803400	-0.45241700
H	4.26423500	4.06047300	-0.98459100	H	-4.08602900	-4.13985800	-0.77813500
C	2.61593600	3.93985600	-2.37250800	H	-6.31751700	-3.12758200	-0.35195300
H	2.88997600	4.83704900	-2.91830600	H	-6.47778500	-0.77128600	0.42587700
C	1.48610800	3.21502200	-2.75080000	H	-4.43824900	0.56373900	0.77178000
H	0.88930300	3.55654000	-3.59140700	H	-2.81186900	-0.65288700	2.98967600
C	1.10043300	2.05142500	-2.07121800	H	-2.12893600	-1.64025400	5.13621400
C	-0.11283600	1.31200800	-2.59124600	H	0.21411900	-2.46211400	5.42596700
H	-0.51062800	1.86397700	-3.44891200	H	1.80983600	-2.29604000	3.56110800
H	0.14145900	0.30575100	-2.93316500	H	2.64439700	3.58222500	0.72173900
C	-2.43228600	0.63881600	-2.36208600	H	1.97257400	5.32511700	-0.94312300
H	-2.07985600	-0.16121100	-3.01829100	H	0.33419800	4.70280900	-2.74547000
H	-2.84197900	1.44237600	-2.98075800	H	-0.57006800	2.36877900	-2.78830200
C	-3.46614400	0.07292700	-1.42971700	H	2.88354600	0.18813100	-1.48545700
H	-4.83494200	0.11204400	-1.68258700	H	2.77615600	-1.53871600	-1.18455100
C	-5.20698900	0.61318500	-2.56917100	H	4.27067800	-2.64582500	0.46191800
C	-5.70467800	-0.50102000	-0.78109800	H	6.44927100	-2.57616500	1.61882500
H	-6.77466800	-0.48665900	-0.95923600	H	7.68755800	-0.42873100	1.82565300
C	-5.18390500	-1.11872200	0.35583100	H	6.73163600	1.64589600	0.84100900
H	-5.82666800	-1.59582300	1.08630700	H	4.55387200	1.57864000	-0.31912300
C	-3.80764800	-1.10577400	0.55377700	O	1.11301400	-1.09222500	-2.95618400
H	-3.35311600	-1.54683700	1.43266500	O	-0.11169900	-2.28397300	-1.58745700
C	-1.57974900	2.46823600	-0.91895500	C	0.82363500	-3.44310000	-3.48804200
H	-0.85372800	3.21550900	-1.24577000	H	-0.05786600	-3.59428000	-4.12034200
C	-2.55460800	2.79771800	-1.28912000	H	0.93364200	-4.32107200	-2.84793200
C	-1.58575500	2.34063000	0.57946700	H	1.69935500	-3.32379600	-4.12693500
C	-1.23975700	1.11023000	1.15650500	C	0.61458200	-2.21677100	-2.65364700
C	-1.29527800	0.95948900	2.54575600	H	0.95507400	0.98825500	1.62223400
H	-1.04391100	0.00791300	3.00049100	H	2.67165300	1.12498400	1.29253800
C	-1.66945900	2.03831900	3.35324300	C	1.49358200	-1.47965500	1.10754400
H	-1.70682400	1.91286700	4.43205800	H	2.45370400	-1.60811800	1.61140800
C	-1.98903100	3.27209600	2.77982600	H	1.31695300	-2.37230900	0.49966000
H	-2.27472200	4.11087100	3.40761400	VIIb			
C	-1.95052300	3.42156700	1.39338400	Rh	-0.58718400	0.55344300	-0.31736600
H	-2.21227700	4.37506400	0.94043700	P	1.50339700	-0.32519700	0.01104200
H	3.13047000	-1.66188000	1.69070000	Cl	-0.21044900	0.75689100	-2.66956600
Cl	-0.71705200	-2.20774400	-2.03399000	N	-1.19472100	0.39156000	1.70572100
O	-0.71808900	-1.77194300	1.41967800	N	-1.59132500	-1.26144400	-0.47536400
C	-0.81083200	-3.01508700	1.48515500	C	2.84960400	0.89602700	-0.24387900
C	-0.80817200	-3.71555400	2.81021200	C	2.92251200	1.65222100	-1.42712700
H	0.05379100	-4.38725200	2.85984400	C	3.98586400	2.53048300	-1.62899800
H	-0.76521500	-2.99220700	3.62233700	C	4.97531900	2.67866200	-0.65239700
H	-1.70867000	-4.32979000	2.89725000	C	4.89732100	1.94324000	0.52998100
O	-0.90714500	-3.80480200	0.44802700	C	3.84047000	1.05463900	0.73860300
H	-0.87949600	-3.29043900	-0.42048700	C	1.85129400	-1.76772300	-1.05902100
VIIb				C	1.22584400	-2.99983500	-0.79430500
Rh	-0.02380900	-0.23399300	-1.22147500	C	1.47855700	-4.10281900	-1.60756600
P	-1.53808600	-0.10966100	0.51338000	C	2.35044300	-3.98965600	-2.69365700
Cl	-1.79882500	0.08496200	-2.80682000	C	2.97593900	-2.77067500	-2.95967200
N	1.63584200	-0.35057100	0.13356600	C	2.73038800	-1.66205300	-2.14887000
N	0.49517700	1.76607300	-1.12593000	C	1.68878500	-0.91953700	1.73341400
C	-2.00751700	1.60508300	0.95508500	C	2.64205100	-1.92376800	1.97901900
C	-2.67437100	2.38461200	-0.00918900	C	2.90218600	-2.36344200	3.27588600
C	-3.02668500	3.70187800	0.27853000	C	2.19937500	-1.81021000	4.34410900
C	-2.70606700	4.26146500	1.51883300	C	1.23802500	-0.82786700	4.10745700
C	-2.03418200	3.49776000	2.47345400	C	0.96713800	-0.36163100	2.81398600
C	-1.68598900	2.17352200	2.19759800	C	-0.08277400	0.71856300	2.67119300
C	-3.09160600	-1.02819100	0.18399400	C	-1.75521300	-0.98297900	1.94802000
C	-3.00219700	-2.36265800	-0.24906100	C	-2.14620700	-1.69553100	0.68096900
C	-4.16221800	-3.11087500	-0.44030900	C	-2.98140600	-2.81103000	0.70477400
C	-5.41629900	-2.54111500	-0.20116600	C	-3.24158100	-3.49379100	-0.48034900
C	-5.50755700	-1.21886900	0.23404400	C	-2.66074000	-3.04058800	-1.66489000
C	-4.35074300	-0.46014400	0.42827900	C	-1.84339200	-1.91988900	-1.62622200
C	-0.88751700	-0.89960100	2.03704900	C	-2.27830500	1.44195500	1.89064700
C	-1.79401500	-1.00937300	3.10937500	C	-3.40466900	1.27068000	0.90149400
C	-1.41244000	-1.56842300	4.32459000	C	-3.20499100	1.62629700	-0.44375800

C	-4.20091800	1.37942700	-1.39492000	H	-3.28406900	0.30648000	-2.40715800
C	-5.41427000	0.81015500	-1.00494200	H	-3.46316000	2.11902100	1.05649600
C	-5.63050300	0.48849600	0.33810900	H	-3.98139900	2.96008000	3.30987100
C	-4.62846200	0.71094900	1.28602600	H	-2.63211600	2.18618700	5.26250700
H	2.14558600	1.56388200	-2.17759200	H	-0.78358200	0.58849400	4.91833400
H	4.03598700	3.10479900	-2.54885400	H	-0.28032900	-1.56267200	2.34985200
H	5.79893200	3.36775800	-0.81208500	H	0.48313500	-0.72838700	3.70585600
H	5.65713800	2.05610600	1.29691200	H	2.92654400	3.60639600	1.65012600
H	3.80012900	0.49197900	1.66282400	H	3.27262500	4.82807700	-0.50264700
H	0.55811700	-3.11272200	0.05222700	H	2.41978900	3.78713200	-2.62931800
H	0.99536000	-5.04987400	-1.38972000	H	1.29025800	1.55793100	-2.49706400
H	2.54508300	-4.85051400	-3.32574200	H	2.76723600	-0.89823400	3.06247500
H	3.66144100	-2.67836800	-3.79605000	H	1.97251300	-2.14090700	2.08398200
H	3.23374300	-0.72711600	-2.36231900	H	2.24307200	-2.20404900	-0.59520000
H	3.19482700	-2.35835200	1.15412700	H	3.43351500	-0.90677200	-2.43405000
H	3.64745300	-3.13400400	3.44321100	H	5.81421700	-0.34761300	-1.99507100
H	2.38693400	-2.14717200	5.35849900	H	6.63889400	-0.18564400	0.34008700
H	0.67997700	-0.41509400	4.94230500	H	5.08895500	-0.53777600	2.24483500
H	0.34632200	1.65886000	2.31657600	O	0.02072600	-2.42029600	0.12781500
H	-0.53060300	0.89834500	3.65321100	O	1.83166000	-3.43112000	-0.71494100
H	-3.41518800	-3.13483000	1.64415100	C	-0.03073300	-4.79104200	-0.04891100
H	-3.88929100	-4.36398200	-0.47847400	H	-0.22179000	-4.94934100	1.01657300
H	-2.83609300	-3.53985200	-2.61050000	H	-0.99794100	-4.76713300	-0.55755100
H	-1.37275300	-1.51524500	-2.51300200	H	0.58120900	-5.60423200	-0.43745000
H	-2.64002500	1.36645800	2.92151700	C	0.66104500	-3.46525400	-0.23426000
H	-1.78680000	2.40906500	1.76898900	H	2.49054200	1.26640400	2.65736300
H	-2.32495900	2.20785900	-0.74477800	H	0.81597900	1.75841500	2.49414600
H	-4.03408000	1.65559100	-2.43163300				
H	-6.19374100	0.63126700	-1.73913600	xTb			
H	-6.57842500	0.05990400	0.64868200	Rh	-0.95432500	0.16570500	-0.27796700
H	-4.80378700	0.45031700	2.32607800	P	1.56383100	0.10371900	0.03167500
O	0.28093400	2.35513300	0.14450500	Cl	-0.69017000	0.72142800	-2.65036700
O	-0.98387500	3.72425200	-1.14117400	N	-1.33148100	-0.31805100	1.73474600
C	0.88267600	4.63501200	0.08296100	N	-1.07322000	-1.84608700	-0.54825100
H	0.93334000	4.65982700	1.17519400	C	2.34805900	1.76425300	0.16947400
H	1.89468700	4.44653600	-0.28793600	C	2.05559400	2.72858500	-0.81217400
H	0.52750300	5.59524900	-0.29267400	C	2.62369000	4.00118400	-0.74330700
C	-0.04209700	3.51772700	-0.37582000	C	3.47515700	4.33304600	0.31444400
H	-2.60149100	-0.92448600	2.63713900	C	3.76206700	3.38480700	1.29740700
H	-0.98914000	-1.58124700	2.44662600	C	3.20569400	2.10525000	1.22607700
				C	2.55630600	-0.80189000	-1.23184200
TS_VIII-1xb				C	2.41174000	-2.19648600	-1.34819300
Rh	0.74234600	-0.50488400	-0.26478500	C	3.09745800	-2.90048600	-2.33771600
P	-1.53723900	0.20026500	-0.00401700	C	3.93089400	-2.22416800	-3.23229400
Cl	0.42466900	-0.84982000	-2.63286100	C	4.07959500	-0.84095300	-3.12519500
N	1.20295400	-0.20169600	1.78438600	C	3.39881100	-0.13251700	-2.13202600
N	1.48193700	1.40965200	-0.44816500	C	1.95515500	-0.74542500	1.61963900
C	-2.77722400	-1.14576500	-0.21222900	C	3.15153100	-1.46177300	1.77741800
C	-2.68720200	-2.01214800	-1.31606800	C	3.44629700	-2.12337700	2.97015300
C	-3.63892000	-3.01547000	-1.49961600	C	2.53937600	-2.07799100	4.02652700
C	-4.67800800	-3.17904000	-0.57931100	C	1.34974800	-1.36287900	3.88418800
C	-4.76416700	-2.33117000	0.52516400	C	1.03685200	-0.68956800	2.69472900
C	-3.82072300	-1.31796800	0.71047900	C	-0.23669500	0.13269200	2.67753000
C	-2.05418700	1.55309000	-1.13639800	C	-1.60262300	-1.79894500	1.84290200
C	-1.56724600	2.85693300	-0.93277700	C	-1.33697600	-2.55875200	0.57126400
C	-1.91370400	3.88397000	-1.81006400	C	-1.42115700	-3.94971800	0.53340100
C	-2.74200400	3.62364600	-2.90470200	C	-1.26056700	-4.61249200	-0.67993100
C	-3.22819200	2.33241000	-3.11370700	C	-1.01568700	-3.86376100	-1.83111000
C	-2.88880700	1.30091700	-2.23595800	C	-0.92217200	-2.48303400	-1.72910700
C	-1.83300300	0.85372600	1.68955200	C	-2.59010800	0.44476100	2.09903100
C	-2.87272500	1.77512500	1.89830400	C	-3.56214400	0.34046000	0.95653400
C	-3.16895900	2.25344600	3.17438000	C	-3.00225300	0.22700000	-0.32908000
C	-2.41712300	1.81929900	4.26396900	C	-3.85085400	0.13430400	-1.43494100
C	-1.37437700	0.91420700	4.06731000	C	-5.24058300	0.17723600	-1.25936500
C	-1.06575200	0.41398400	2.79414700	C	-5.78987000	0.29727300	0.01947000
C	0.06665000	-0.58883100	2.70337500	C	-4.94952700	0.37117100	1.13311000
C	1.62681900	1.22950300	1.98842400	H	1.38824800	2.48239700	-1.63276400
C	1.92583500	1.95870400	0.70541100	H	2.39687600	4.73309200	-1.51269900
C	2.57698800	3.19115100	0.71132100	H	3.91073100	5.32603400	0.37136700
C	2.76592300	3.86899200	-0.49000000	H	4.42231200	3.63611200	2.12203500
C	2.29613200	3.29572300	-1.67144900	H	3.44413900	1.37747100	1.99392200
C	1.66237200	2.06209800	-1.61478000	H	1.78436400	-2.74393200	-0.65293200
C	2.37150900	-1.12244700	2.06657500	H	2.97982600	-3.97765000	-2.40744000
C	3.39502300	-0.96115400	0.97612400	H	4.46281700	-2.77296000	-4.00351600
C	2.90674500	-1.08204700	-0.34906300	H	4.73071500	-0.30673100	-3.81061300
C	3.79390900	-0.83015000	-1.41185500	H	3.53485600	0.94047000	-2.06031800
C	5.13364900	-0.52028900	-1.16650300	H	3.86217000	-1.50501800	0.95965900
C	5.59855500	-0.43107500	0.14842700	H	4.38040300	-2.66749000	3.06832100
C	4.72688300	-0.63791700	1.22528100	H	2.75352300	-2.59064400	4.95894400
H	-1.87157100	-1.90396800	-2.02220000	H	0.65266800	-1.31746900	4.71613400
H	-3.56347800	-3.67327600	-2.36027200	H	-0.03791500	1.17507900	2.41801900
H	-5.41355700	-3.96498400	-0.72185300	H	-0.66100600	0.12421000	3.68673200
H	-5.56555200	-2.45293500	1.24750100	H	-1.62241900	-4.49675500	1.44791500
H	-3.90674200	-0.66861100	1.57347100	H	-1.32885600	-5.69402900	-0.72610400
H	-0.93703000	3.08474800	-0.07974000	H	-0.88883100	-4.33426000	-2.79889000
H	-1.53697500	4.88699600	-1.63532200	H	-0.72251200	-1.85331200	-2.58556700
H	-3.01019200	4.42448900	-3.58698900	H	-2.98373300	0.05569600	3.04467100
H	-3.87856000	2.12313400	-3.95746000	H	-2.28630200	1.48134400	2.26328900

H	-1.47250700	2.46695800	-1.97704100	XIb			
H	-3.43903200	0.03626200	-2.43486200	Rh	2.53868600	-0.62583500	-0.02848400
H	-5.89342000	0.11123300	-2.12597900	Cl	4.37347500	-2.01983500	-0.74658700
H	-6.86761600	0.32182900	0.15120800	P	-2.78366900	0.26105300	-0.45067400
H	-5.37119900	0.44966200	2.13234000	N	1.07163000	0.76240500	0.68827200
O	-0.94805500	2.21169000	0.31449100	N	3.72136000	1.03568700	0.27105100
O	-1.65452900	3.33217500	-1.51366700	C	-3.03854900	-1.51356400	0.01532500
C	-1.38887000	4.55431300	0.49698900	C	-3.42445200	-1.95061200	1.29353700
H	-1.38771100	4.37314000	1.57070100	H	-3.60361600	-1.22701100	2.08278100
H	-0.50980200	5.15178800	0.23210200	C	-3.57686500	-3.31287900	1.56211700
H	-2.27714500	5.11462500	0.19870400	H	-3.87519400	-3.63568300	2.55550000
C	-1.32247600	3.25818200	-0.24960400	C	-3.34803600	-4.25763900	0.55815000
H	-2.65506900	-1.93700200	2.10400600	H	-3.46668600	-5.31637800	0.76917700
H	-1.01371100	-2.22067200	2.65982500	C	-2.96265100	-3.83558400	-0.71703000
				H	-2.77862700	-4.56447400	-1.50091700
Xb				C	-2.80244900	-2.47438200	-0.98318000
Rh	-0.93302000	-0.37817100	-0.26804900	H	-2.48659500	-2.15515500	-1.97321200
P	1.57606700	-0.05448500	-0.03547700	C	-4.48618400	0.83276100	-0.89421800
N	-1.23850700	-0.07262300	1.80523400	C	-4.58163900	1.96993300	-1.71528400
N	-1.23168800	1.66176200	-0.35703200	H	-3.67621200	2.47397400	-2.04387700
C	2.09247800	1.50928500	-0.86717500	C	-5.82580500	2.45797000	-2.11833000
C	2.22040700	2.72480600	-0.17597200	H	-5.88129500	3.34030500	-2.74929600
H	2.11136500	2.75520800	0.90237200	C	-6.99448300	1.80355200	-1.72148200
C	2.49898300	3.90877600	-0.86366000	H	-7.96320900	2.17566900	-2.04201900
H	2.59986800	4.83749300	-0.30961400	C	-6.91246100	0.66432000	-0.91692900
C	2.65328300	3.89856000	-2.25059500	H	-7.81788200	0.14913000	-0.60891400
H	2.87609000	4.81855900	-2.78284500	C	-5.66832500	0.18295700	-0.50354900
C	2.51600300	2.69691800	-2.95027000	C	-2.48321300	1.06397000	1.20733300
H	2.62916800	2.67791000	-4.03031200	C	-3.46658800	1.86219100	1.81396100
C	2.22873400	1.51457300	-2.26777000	H	-4.42405000	1.99367700	1.32286900
H	2.10667000	0.59361300	-2.82738100	C	-3.24815900	2.48297100	3.04450600
C	2.79332600	-1.31853700	-0.61776100	H	-4.02982900	3.09361100	3.48680300
C	2.46234300	-2.67586700	-0.46278500	C	-2.03967000	2.29137600	3.71082000
H	1.49549000	-2.95452000	-0.05663000	H	-1.86619600	2.74179800	4.68328000
C	3.37203900	-3.66763600	-0.83648400	C	-1.05371700	1.49900700	3.12396800
C	3.10270400	-4.71281700	-0.71335900	H	-0.13109900	1.32188000	3.66838100
H	4.61535700	-3.32193500	-1.37001100	C	-1.23409800	0.90683800	1.86424200
H	5.31886600	-4.09580300	-1.66317300	C	-0.11337200	0.04497900	1.29983000
C	4.94988800	-1.97505800	-1.52731500	H	0.30366400	-0.57696400	2.09366800
H	5.91453300	-1.69635700	-1.94155500	H	-0.47642900	-0.62800600	0.52525300
C	4.04708900	-0.97817200	-1.15253600	C	1.84669100	1.53508800	1.71076500
C	2.06635300	0.19114000	1.73394800	H	2.00039300	0.87618700	2.57199600
C	3.36211600	0.64927800	2.02738700	H	1.29526000	2.41744800	2.04764100
H	4.05773400	0.83736500	1.21587900	C	3.18527200	1.92714800	1.13850300
C	3.77974800	0.87351900	3.33747200	C	3.85387000	3.10016200	1.47468100
H	4.78740900	1.22718400	3.53280100	H	3.39785100	3.80037800	2.16549400
C	2.89156300	0.64291700	4.38722700	C	5.10358000	3.35348700	0.90868900
H	3.19419400	0.82001700	5.41467900	H	5.64311900	4.26084800	1.15879200
C	1.60833100	0.17508500	4.11261000	C	5.64095700	2.43265600	0.01045400
H	0.92702500	-0.01733700	4.93648100	H	6.60437700	2.59564800	-0.45857400
C	1.17297800	-0.07216200	2.79890300	C	4.91802100	1.28373400	-0.29176800
C	-0.18705900	-0.73429100	2.66482800	H	5.28253000	0.52763800	-0.97584000
C	-1.33374500	1.40298400	2.07398600	C	0.66482900	1.67512900	-0.45315600
H	-0.40462400	1.71882300	2.55684000	H	-0.40487700	1.88120300	-0.38463900
H	-2.14078300	1.60226400	2.78480200	H	1.17624600	2.63234500	-0.31283400
C	-1.51141500	2.23920600	0.83226500	C	1.03879200	1.08344700	-1.78492300
C	-1.88094100	3.58143700	0.91312500	C	1.99531800	0.05307900	-1.81449900
H	-2.10413400	4.01734400	1.88081900	C	2.39605400	-0.47595300	-3.04743100
C	-1.95448900	4.34054300	-0.25178700	H	3.13075000	-1.27266400	-3.08068600
H	-2.24172000	5.38584900	-0.20688400	C	1.84846400	0.02060700	-4.23633700
C	-1.65642600	3.73460900	-1.47262300	H	2.16738900	-0.39749300	-5.18777700
H	-1.70060700	4.28549900	-2.40501600	C	0.89567100	1.04170400	-4.20480700
C	-1.30559700	2.39112000	-1.48747300	H	0.46714900	1.42138700	-5.12779600
H	-1.07806000	1.85665400	-2.40101400	C	0.48949900	1.56914700	-2.97775600
C	-2.54691900	-0.76581100	2.12033500	H	-0.25545400	2.36104600	-2.94476800
H	-2.30320600	-1.82759900	2.21637700	H	-5.61887100	-0.70222400	0.12241900
H	-2.91738500	-0.41616600	3.09108600	O	2.32942500	-2.09237700	1.91194700
C	-3.52284400	-0.56647400	0.99714500	C	1.58610500	-2.75424800	1.14205800
C	-2.97014800	-0.46842900	-0.29206100	C	0.99175700	-4.08078900	1.54867800
C	-3.83525300	-0.32707000	-1.38206800	H	1.54560100	-4.88762400	1.05669800
H	-3.43012600	-0.23972200	-2.38570800	H	1.06030400	-4.21453400	2.62906300
C	-5.22262100	-0.31070100	-1.18919300	H	-0.04984800	-4.14873900	1.22498100
H	-5.88367100	-0.20834100	-2.04666800	O	1.31814100	-2.31202900	-0.04152800
C	-5.76172500	-0.41718200	0.09606200				
H	-6.83789100	-0.39554900	0.24283300	XIIB			
C	-4.90805700	-0.53964700	1.19503700	Rh	-0.84906600	0.22436800	-0.27781400
H	-5.31750400	-0.61408300	2.20016500	Cl	-0.57111500	0.63717800	-2.65951300
H	4.32146200	0.06228500	-1.28841300	P	1.46956200	0.02857800	-0.01328700
H	-0.60848700	-0.82702500	3.67140300	N	-1.28931600	-0.14438500	-1.76199700
H	-0.08445300	-1.73921600	2.24814000	N	-2.96962600	0.35272500	-0.34607000
Cl	-0.66926700	-0.68898700	-2.67282500	C	2.39350900	1.62345600	-0.11385600
O	-0.66379000	-2.39007800	0.17203800	C	3.40982400	1.94530500	0.79874900
C	-1.09857700	-3.54270100	-0.26916300	H	3.66069500	1.26685300	1.60611800
C	-2.26205700	-3.57699200	-1.24612200	C	4.11137900	3.14756900	0.67812200
H	-2.40827500	-4.59875800	-1.60089400	H	4.89320300	3.38484700	1.39353500
C	-3.17386400	-3.23166500	-0.75093900	C	3.81040800	4.03655300	-0.35445800
H	-2.07837200	-2.90261600	-2.08447800	H	4.35770000	4.97004700	-0.44723600
O	-0.58052500	-4.59633200	0.12173000	C	2.79894500	3.72240300	-1.26608500

H	2.55639000	4.41134000	-2.06993700	H	-3.41547100	-1.75103200	1.09714700
C	2.08784400	2.52846800	-1.14471800	C	-2.80259300	-2.13515600	3.11758900
H	1.29193000	2.29586900	-1.84321900	H	-3.60374200	-2.84539500	3.29657600
C	2.35268300	-1.09469700	-1.17845200	C	-1.88707600	-1.83546900	4.12325600
C	2.17346500	-2.48525300	-1.07528700	H	-1.96167700	-2.31142100	5.09578400
H	1.53906000	-2.89806300	-0.29951800	C	-0.87142900	-0.90925700	3.87848400
C	2.81660500	-3.34810500	-1.96240400	H	-0.17106000	-0.66236500	4.67161800
H	2.67298200	-4.42006700	-1.86527500	C	-0.74335100	-0.28000600	2.63399700
C	3.63718300	-2.83701800	-2.97115600	C	0.33597900	0.77197000	2.47787500
H	4.13538100	-3.51056600	-3.66216400	C	2.09958600	-0.90384800	1.89880200
C	3.81706300	-1.45779800	-3.08325600	H	1.78604000	-1.22476800	2.89422700
H	4.45676500	-1.05109400	-3.86080300	H	3.18528400	-0.77650300	1.92490900
C	3.18225300	-0.59034300	-2.19117900	C	1.78675000	-1.95761000	0.87499500
C	1.88814100	-0.63327300	1.65608000	C	1.98672300	-3.31507600	1.11250500
C	3.08298800	-1.34617600	1.84834000	H	2.30457600	-3.63956400	2.09685000
H	3.73752000	-1.53434100	1.00498400	C	1.78705900	-4.22943800	0.08188200
C	3.45201900	-1.81578600	3.10909200	H	1.94209900	-5.28896000	0.25354800
H	4.38280600	-2.36094200	3.23043200	C	1.39027700	-3.76305000	-1.17171000
C	2.62102900	-1.57925000	4.20197200	H	1.23014000	-4.43669200	-2.00501400
H	2.89196200	-1.94121900	5.18889600	C	1.18657900	-2.40282300	-1.35401900
C	1.42991300	-0.87633900	4.02228200	H	0.86698000	-1.97892600	-2.29600700
H	0.78215000	-0.69669100	4.87554100	C	2.52831700	1.51779300	1.67769200
C	1.04443200	-0.39170700	2.76418300	H	1.99005700	2.46985900	1.62769700
C	-0.23773900	0.40985200	2.68933100	H	3.00595100	1.45701100	2.66260700
H	-0.66920700	0.46267100	3.69530700	C	3.50250700	1.36922300	0.53683000
H	-0.05763600	1.42963600	2.33812000	C	2.99889800	0.80179800	-0.64868100
C	-2.54299100	0.64946200	2.00342200	C	3.85570300	0.60128700	-1.73348700
H	-2.24467600	1.70038200	2.03053600	H	3.48359500	0.14688100	-2.64667400
H	-2.97950200	0.37991700	2.97014500	C	5.19478400	1.00320300	-1.64896600
C	-3.52396500	0.46510000	0.87924300	H	5.85555000	0.85573100	-2.49909000
C	-4.90589000	0.46607000	1.05322300	C	5.68507200	1.58707200	-0.47779500
H	-5.32538500	0.54951500	2.04960000	H	6.72589300	1.89030900	-0.41444800
C	-5.72636200	0.35870500	-0.06994900	C	4.84150000	1.76387400	0.62226300
H	-6.80583200	0.35836400	0.04003300	H	5.22610700	2.19810300	1.54190100
C	-5.14158700	0.24242900	-1.33089300	H	-3.55425000	1.36977300	1.78024100
H	-5.74411500	0.15152000	-2.22741900	H	0.76657500	0.98122200	3.46310700
C	-3.75347900	0.23411900	-1.42896300	H	-0.07899200	1.71047000	2.10096400
H	-3.23506100	0.14031000	-2.37634600	Cl	0.60829900	0.62710400	-2.86623300
C	-1.54279500	-1.62071700	2.00530700				
H	-0.80971700	-1.97660200	2.73325900	XIVa			
H	-2.52426500	-1.72982400	2.47752100	Ir	-0.07199100	-0.67154800	-0.60234000
C	-1.46281000	-2.42188300	0.73046500	Cl	0.14528000	-0.28665700	-2.93182700
C	-1.10422400	-1.77350700	-0.46717200	P	1.47807500	0.99015900	-0.09756900
C	-1.07030700	-2.53277500	-1.64631000	N	-1.76494000	0.58465500	-0.56945100
H	-0.80841500	-2.05161600	-2.58216900	N	-1.56335600	-2.09249300	-1.06944900
C	-1.36507100	-3.89972600	-1.63142600	C	2.73732200	1.27265600	-1.39902100
H	-1.33005200	-4.46765300	-2.55805000	C	3.07281400	2.55701200	-1.84873100
C	-1.69948700	-4.53669500	-0.43321300	H	2.57006100	3.43050500	-1.44993500
H	-1.92521300	-5.59923300	-0.41774700	C	4.05916300	2.72123800	-2.82387500
C	-1.75061700	-3.79379100	0.74634900	H	4.30925700	3.71969300	-3.16900700
H	-2.02125000	-4.27849000	1.68237900	C	4.71728300	1.61055600	-3.35189400
H	3.34227600	0.47749000	-2.28613400	H	5.48425700	1.74186900	-4.10903500
O	-0.69793800	2.34939400	0.35568400	C	4.38332400	0.32743100	-2.91019000
C	-1.12455300	3.52136200	0.00359600	H	4.88620700	-0.54113000	-3.32379400
C	-2.06626600	3.61361300	-1.19736800	C	3.39273200	0.15469000	-1.94546100
H	-2.19889100	4.65731400	-1.48949800	H	3.12819100	-0.84733200	-1.62356900
H	-1.68824800	3.02681600	-2.03733100	C	2.42734600	0.65305800	1.44621900
H	-3.04473100	3.19944800	-0.93007700	C	1.75150800	0.64862800	2.68040900
O	-0.82103400	4.55818600	0.61631500	H	0.68956600	0.86637800	2.72815200
				C	2.43791400	0.36742600	3.85971100
				H	1.90422300	0.36957200	4.80502700
XIIIb				C	3.80622400	0.08411400	3.82483500
Rh	1.00293600	0.41345000	-0.50123300	H	4.33934200	-0.13586200	4.74463700
P	-1.47701500	0.21186700	-0.03293300	C	4.48409300	0.08719600	2.60622800
N	1.48371300	0.42806400	1.55666000	H	5.54770200	-0.12706500	2.57154000
N	1.37420200	-1.52703600	-0.34224900	C	3.80147200	0.37105700	1.42073100
C	-2.59059600	-0.68747700	-1.18394800	C	0.65793900	2.59961900	0.22142000
C	-2.38657300	-2.06052700	-1.41254700	C	1.38103700	3.57129700	0.93625500
H	-1.62517400	-2.60215900	-0.86073500	H	2.36762900	3.32946700	1.31699800
C	-3.17485100	-2.74769900	-2.33497200	C	0.86043000	4.84346200	1.16148500
H	-3.01228600	-3.80932800	-2.49410400	H	1.44218700	5.57775100	1.70918500
C	-4.16673800	-2.07241000	-3.05169400	C	-0.40678700	5.15894400	0.67540400
H	-4.77738500	-2.60767000	-3.77241500	H	-0.82762900	6.14665000	0.83467400
C	-4.37001500	-0.70867300	-2.83649600	C	-1.14346200	4.19437000	-0.00959900
H	-5.14026800	-0.17778000	-3.38771600	H	-2.13263700	4.44864900	-0.37852800
C	-3.58903700	-0.01745300	-1.90704400	C	-0.64142500	2.90437700	-0.24478900
H	-3.76129400	1.04110200	-1.74732100	C	-1.52090400	1.99006900	-1.07835400
C	-2.21151300	1.88900800	0.16439500	H	-2.50062900	2.46481500	-1.18380200
C	-1.76144800	2.92823600	-0.66999400	H	-1.09904700	1.86778700	-2.07878900
H	-1.00165300	2.73694000	-1.42257000	C	-2.75890300	-0.04275600	-1.51888700
C	-2.29712300	4.21171100	-0.54544000	H	-2.44212600	0.22492800	-2.52954400
H	-1.94564200	5.00606300	-1.19686900	H	-3.75390200	0.37017600	-1.34293900
C	-3.27671100	4.47244600	0.41528800	C	-2.75009100	-1.54196200	-1.41234400
H	-3.68798600	5.47245400	0.51468400	C	-3.85178300	-2.33522800	-1.71914400
C	-3.72585900	3.44574600	1.24979800	H	-4.79416100	-1.86894500	-1.98437500
H	-4.48724400	3.64466300	1.99791000	C	-3.71721000	-3.72306200	-1.68901900
C	-3.19848500	2.15951800	1.12643800	H	-4.56218000	-4.35945100	-1.93004100
C	-1.67561000	-0.58731200	1.61262500	C	-2.48533500	-4.27940400	-1.34674400
C	-2.69541300	-1.51280700	1.87170400				

[illegible]

XVIa

Ir	0.63734000	-0.31269100	-0.35731500
P	-1.64671100	0.14214400	-0.03684900
N	0.34137700	-2.31662300	-0.87016400
N	2.63993700	-0.90350900	-0.66993200
C	-2.48816700	1.10811100	-1.36464500
C	-3.68685800	0.66458200	-1.94388400
H	-4.13395900	-0.27289900	-1.63552700
C	-4.32310900	1.42838900	-2.92510900
H	-5.24796300	1.06851200	-3.36536300
C	-3.77797300	2.64472900	-3.33435300
H	-4.27553500	3.23759300	-4.09561400
C	-2.58583900	3.09609300	-2.76305600
H	-2.15049800	4.03930700	-3.07805800
C	-1.94243200	2.32989600	-1.79311000
H	-1.01169200	2.69198400	-1.37420600
C	-2.07360800	1.01832000	1.52840600
C	-1.93881000	0.34644300	2.75687000
H	-1.61309300	-0.68651000	2.78428300
C	-2.23746700	0.99798900	3.95251600
H	-2.13470700	0.46399400	4.89214400
C	-2.66292800	2.32841600	3.94237400
H	-2.89263100	2.83398400	4.87539700
C	-2.79910000	3.00197200	2.72861800
H	-3.13865700	4.03300200	2.71011900
C	-2.51164200	2.35159400	1.52652400
C	-2.59879800	-1.43145200	0.02902600
C	-3.77942400	-1.50473600	0.78378000
H	-4.09834400	-0.64773000	1.36583500
C	-4.55810800	-2.66240400	0.79487200
H	-5.46862800	-2.69346100	1.38471600
C	-4.16221200	-3.76829700	0.04610700
H	-4.75855100	-4.67512700	0.04574400
C	-2.98758600	-3.70830800	-0.70383600
H	-2.67991100	-4.57331100	-1.28482200
C	-2.19422100	-2.55319900	-0.72834700
C	-0.96128400	-2.56885400	-1.60432800
H	-0.88518200	-3.55142200	-2.08177300
H	-1.01158000	-1.81426700	-2.39334300
C	1.45554700	-2.63949500	-1.83999500
H	1.19968300	-2.17060900	-2.79418400
H	1.51828600	-3.72165300	-1.98721100
C	2.75569900	-2.06644800	-1.35083400
C	3.99838500	-2.64079600	-1.59791800
H	4.06239800	-3.57659500	-2.14202200
C	5.14558900	-1.99474000	-1.13782500
H	6.12541500	-2.42193800	-1.32337700
C	5.01452600	-0.80321400	-0.42546000
H	5.87918300	-0.27687100	-0.03833800
C	3.74222000	-0.29202500	-0.19918200
H	3.58723200	0.61638600	0.36996300
C	0.45590800	-3.22671100	0.36091400
H	-0.49123800	-3.75900700	0.46860100
H	1.22119000	-3.97955400	0.15147300
C	0.78428500	-2.44706500	1.60685000
C	0.87146500	-1.04700200	1.51417900
C	1.22482800	-0.32112200	2.66180100
H	1.30735200	0.76007900	2.61676900
C	1.46044900	-0.97679500	3.87340800
H	1.72973400	-0.39851400	4.75305800
C	1.34650800	-2.36675000	3.95953400
H	1.52494500	-2.87510600	4.90216300
C	1.01186100	-3.10254600	2.82272000
H	0.93544900	-4.18616900	2.88072200
H	-2.64596800	2.88543300	0.59339100
Cl	0.66565500	0.44874900	-2.82781000
O	1.21193200	1.61452500	0.30124000
C	1.61905300	2.62608500	-0.28848500
C	2.23108700	3.73905300	0.58782300
O	1.65488800	2.85684700	-1.55489000
H	1.31623100	2.05085000	-2.09858000
F	1.60270300	3.80003800	1.76382200
F	2.16863600	4.92516700	-0.01345400
F	3.52305800	3.42231000	0.80417900

XIVb

P	1.70167700	-0.27905400	0.57720000
Cl	1.57759700	1.58887200	-2.17289000
N	-1.49886700	-0.48847200	0.41949900
N	-0.17312200	-1.17771000	-1.83942700
C	2.52200800	-1.76453400	-0.12236900
C	3.21877700	-1.62546300	-1.33760100
C	3.83009800	-2.73238900	-1.92411500
C	3.74153400	-3.98907500	-1.31841600
C	3.04000500	-4.13587400	-0.12177300
C	2.43296700	-3.02973400	0.47796200
C	3.02422600	0.94900500	0.90542100
C	2.65861200	2.24098800	1.32053400

C	3.64266100	3.16988000	1.65261500
C	4.99406500	2.82283900	1.57667300
C	5.36053400	1.54023200	1.16931000
C	4.38184400	0.60209300	0.83422700
C	1.12549200	-0.74701900	2.25884300
C	2.11795600	-1.15498100	3.16940200
C	1.79600400	-1.54943900	4.46428300
C	0.46137300	-1.54358200	4.86859500
C	-0.52812400	-1.13528400	3.97825300
C	-0.22409000	-0.71788100	2.67184400
C	-1.29330500	-1.95305800	0.15708600
C	-0.91247800	-2.17220200	-1.27936200
C	-1.24521400	-3.31419200	-1.99793700
C	-0.80716100	-3.44413900	-3.31607200
C	-0.05454300	-2.41690100	-3.88089300
C	0.24382300	-1.29402000	-3.11912200
C	-2.89036100	-0.05591800	-0.08409800
C	-4.08687400	-0.76715100	0.50824700
C	-4.73798200	-0.24948400	1.63970700
C	-5.86743500	-0.87908500	2.16370600
C	-6.37167600	-2.03056900	1.55574800
C	-5.75116700	-2.54081300	0.41353200
C	-4.62151200	-1.90968700	-0.10899300
H	3.28215700	-0.65467400	-1.81951100
H	4.37589400	-2.61225500	-2.85484900
H	4.21938400	-4.84887200	-1.77793500
H	2.96894500	-5.10888900	0.35444200
H	1.90824800	-3.15929500	1.41805000
H	1.61536800	2.52935100	1.37075400
H	3.35221300	4.16753400	1.96680000
H	5.75746300	3.55074400	1.83367900
H	6.40860200	1.26399400	1.10826700
H	4.68369100	-0.38987500	0.51891900
H	3.15828700	-1.15771900	2.86074000
H	2.58056200	-1.85748300	5.14768000
H	0.18930000	-1.85372000	5.87246600
H	-1.56369900	-1.12589000	4.30578300
H	-1.83923000	-4.08877800	-1.52562100
H	-1.05785900	-4.32869900	-3.89188300
H	0.29916700	-2.46974300	-4.90394100
H	0.81489600	-0.45911500	-3.50526300
H	-2.86760400	-0.18280900	-1.16700300
H	-2.95844600	0.10150600	0.11880700
H	-4.37365900	0.66431700	2.10178100
H	-6.36006000	-0.46292700	3.03698600
H	-4.16750000	-2.29418400	-1.01894800
O	-1.47445600	1.95382100	-1.66278000
O	-0.32864200	2.41907800	0.14952600
C	-1.85106700	4.13059100	-0.65484900
C	-1.15998800	2.76484800	-0.75539100
H	-0.47782200	-2.29646900	0.79790000
H	-2.18293900	-2.52370900	0.43159700
C	-1.39999800	-0.16699100	1.88518700
H	-2.31124000	-0.52766800	2.36633200
H	-1.40467800	0.92602300	1.94313500
H	-7.25365400	-2.51795100	1.95963000
H	-6.15379200	-3.42076400	-0.07864800
Ir	0.00669100	0.52507400	-0.72724500
F	-1.10365700	5.00220600	0.02686800
F	-2.11167000	4.62193800	-1.86740300
F	-3.01876300	3.95877800	0.00200800

XVb

P	-1.19414500	1.09175100	0.01260600
Cl	0.25371800	-0.34004200	-2.69282200
N	1.05378300	-0.52861600	1.72192000
N	2.03333300	1.03686200	-0.32978500
C	-2.84108900	0.38721000	-0.38909700
C	-3.05689100	-0.25305200	-1.62235100
C	-4.32315900	-0.73660400	-1.94501500
C	-5.38102300	-0.60343800	-1.04280400
C	-5.16846100	0.01700500	0.18799600
C	-3.90569600	0.51152400	0.51859500
C	-1.01595300	2.64855600	-0.93891200
C	-0.08593200	3.61954500	-0.52568500
C	0.07700100	4.79336400	-1.25886400
C	-0.67756700	5.00870200	-2.41516400
C	-1.60108500	4.04920800	-2.83091900
C	-1.77391400	2.87394300	-2.09820100
C	-1.29874000	1.60016800	1.77353600
C	-1.92598500	2.82134600	2.07537900
C	-2.11782400	3.22746600	3.39529500
C	-1.67106100	2.41660700	4.43629700
C	-1.03005100	1.21208200	4.14779200
C	-0.83776700	0.77796900	2.82856100
C	-0.15224200	-0.55839300	2.63703200
C	1.98688800	0.60054000	2.07667700
C	2.63106900	1.23806100	0.87227100

C	3.74520800	2.06329000	0.99495700	H	5.49377100	3.56570200	-0.61908700
C	4.25393000	2.69994900	-0.13489200	H	5.66676500	1.96956800	1.27986200
C	3.63045600	2.49062800	-1.36405400	H	3.98466600	0.20185500	1.57199200
C	2.52613000	1.65272000	-1.42814500	H	0.99888600	-3.45665200	-0.09874000
C	1.77108000	-1.86417600	1.87403400	H	1.56764300	-5.22221200	-1.71291400
C	2.89233000	-1.98287900	0.87420400	H	2.96317800	-4.69869600	-3.70472200
C	2.58120300	-2.13121200	-0.49044400	H	3.78479700	-2.37879400	-4.05903300
C	3.59683400	-2.10969000	-1.45480300	H	3.22535300	-0.60248400	-2.44904800
C	4.92865200	-1.98143000	-1.06011100	H	3.48771700	-2.52140700	1.00655600
C	5.24350600	-1.86947500	0.29746600	H	4.01824400	-3.42802300	3.23230900
C	4.22972700	-1.85694200	1.26016700	H	2.68668700	-2.70390200	5.21556200
H	-2.23666200	-0.38649800	-2.31815800	H	0.84505200	-1.08737000	4.92894200
H	-4.47806500	-1.22904300	-2.89992600	H	0.33517800	1.13842600	2.43732800
H	-6.36412100	-0.98847300	-1.29571800	H	-0.43020100	0.25850600	3.76416200
H	-5.98309300	0.11728000	0.89843900	H	-2.86119900	-4.01408000	1.57195900
H	-3.76365200	0.98909200	1.48002600	H	-3.18013600	-5.17395200	-0.62022500
H	0.49832800	3.47646400	0.37729700	H	-2.31577600	-4.05920400	-2.70535100
H	0.79022900	5.54063000	-0.92503000	H	-1.20381500	-1.82802300	-2.49690000
H	-0.54899800	5.92352500	-2.98537400	H	-2.71967600	0.46879300	3.13299200
H	-2.19532900	4.21309100	-3.72422400	H	-1.91455100	1.73959600	2.20059500
H	-2.50356300	2.14443300	-2.42824500	H	-2.23407300	1.88815100	-0.50582900
H	-2.27949600	3.45748400	1.27166700	H	-5.76327400	0.15455000	-1.94992200
H	-2.61305500	4.17054900	3.60245400	H	-5.07330300	0.27234200	2.29801500
H	-1.81019400	2.72036300	5.46888800	O	0.02355300	2.08492500	0.15611500
H	-0.67163300	0.59119000	4.96384100	O	-1.83359200	3.11462600	-0.58699400
H	-0.82330300	-1.30697600	2.20830000	C	0.08877600	4.45221600	-0.02763900
H	0.17828300	-0.92054100	3.61589900	C	-0.65213700	3.10506200	-0.16801400
H	4.20292300	2.20161400	1.96850500	H	-2.47722100	-1.67211400	2.63710900
H	5.12262400	3.34505300	-0.05547000	H	-0.79707900	-2.16906600	2.50709200
H	3.99063500	2.96255300	-2.27077300	H	-6.61781300	0.01631500	0.37420000
H	2.00766900	1.44082200	-2.35452900	Ir	-0.68692100	0.15176600	-0.21844200
H	2.13748300	-1.93748700	2.90338500	F	0.96578000	4.57893700	-1.03731800
H	1.01349100	-2.63633400	1.72389400	F	0.76300400	4.48976200	1.13216900
H	1.58014800	-2.44438800	-0.81827900	F	-0.76301100	5.47836100	-0.06449500
H	3.33866000	-2.22412200	-2.50254600	H	-3.35187700	0.59499500	-2.36253400
H	5.72031100	-1.98575100	-1.80266400				
H	6.28037800	-1.78629900	0.60864200	xvib			
H	4.48475100	-1.75495800	2.31164200	Ir	-0.53926300	-0.54364200	-0.27227900
O	-0.86234200	-1.85363600	-0.01952600	P	1.53938100	0.73745600	0.02149900
O	-0.09400500	-3.53683300	-1.34854100	Cl	-0.54811500	-0.07666900	-2.67224700
C	-2.02774300	-3.87746200	0.04970000	N	-0.69698000	-1.03322000	1.76526000
C	-0.86940000	-3.04087400	-0.55010400	N	0.40766700	-2.32083900	-0.40537100
H	2.74716900	0.25101600	2.78031700	C	1.30983400	2.56456300	0.00051900
H	1.40327000	1.36630200	2.59351400	C	0.62983900	3.15054200	-1.08320500
Ir	0.52761100	-0.36243500	-0.32472900	C	0.41779800	4.52856500	-1.12173700
F	-1.84462600	-3.99463900	1.38870000	C	0.87137700	5.33801700	-0.07704700
F	-3.22077300	-3.28920700	-0.14921700	C	1.54349600	4.76435400	1.00243200
F	-2.06858900	-5.10483700	-0.47343400	C	1.76517200	3.38574900	1.04292700
				C	2.90885000	0.38826800	-1.16163200
TS_xv-xvib				C	3.52244000	-0.87774800	-1.13931500
P	1.56406000	-0.56181600	0.00819100	C	4.52395500	-1.19567400	-2.05552300
C	-0.40430000	0.57963300	-2.56724200	C	4.92221500	-0.25982300	-3.01345500
N	-1.15797500	-0.19355900	1.82151400	C	4.31914100	0.99738000	-3.04280000
N	-1.42112700	-1.73668800	-0.44626900	C	3.31979100	1.32306900	-2.12259100
C	2.82325300	0.77120300	-0.16662600	C	2.26997500	0.37498500	1.67516100
C	2.72363700	1.68352000	-1.23166500	C	3.65708800	0.44809400	1.87483300
C	3.68693700	2.67889900	-1.39356500	C	4.22526300	0.17437900	3.11971600
C	4.74919100	2.78551800	-0.49325600	C	3.40675800	-0.18107100	4.18908000
C	4.84699600	1.89033000	0.57238700	C	2.02564700	-0.25305600	4.00493600
C	3.89085900	0.88681200	0.73782700	C	1.43645500	0.02137500	2.76240000
C	2.06113800	-1.89207200	-1.16121200	C	-0.07644800	-0.00462900	2.69220900
C	1.59656000	-3.20549500	-0.96924600	C	-0.10868300	-2.40926100	1.99102400
C	1.92362200	-4.21000700	-1.87936300	C	0.48928800	-3.02360400	0.75157500
C	2.70871700	-3.91582800	-2.99684600	C	1.07944600	-4.28416100	0.78702800
C	3.16975300	-2.61434100	-3.19609200	C	1.57454100	-4.84545800	-0.38709400
C	2.85075500	-1.60598700	-2.28453600	C	1.46631900	-4.12226400	-1.57431000
C	1.86816600	-1.26795700	1.68305500	C	0.88156600	-2.86468000	-1.54993400
C	2.90451900	-2.19892000	1.86200400	C	-2.18963200	-1.07194900	2.07351800
C	3.20723100	-2.71526500	3.12203500	C	-2.90031400	-1.76021400	0.94152800
C	2.46524900	-2.30961600	4.22890900	C	-2.31786600	-1.60003500	-0.33318900
C	1.42543700	-1.39499100	4.06355500	C	-2.95450500	-2.19852000	-1.42797500
C	1.11154000	-0.85750200	2.80660500	C	-4.14261800	-2.91883000	-1.25574800
C	-0.01600700	0.15379200	2.75589400	C	-4.70623800	-3.06531900	0.01375900
C	-1.59541800	-1.62917000	1.99246100	C	-4.07943900	-2.48922900	1.12076200
C	-1.87087900	-2.32981000	0.68690100	H	0.27447300	2.53213900	-1.90193400
C	-2.50769300	-3.56713700	0.64891300	H	-0.10354300	4.96816500	-1.96652600
C	-2.68198400	-4.21130400	-0.57393400	H	0.70094900	6.40981700	-0.10564900
C	-2.20644800	-3.59689200	-1.73124000	H	1.90016700	5.38784700	1.81664500
C	-1.58359400	-2.36030400	-1.63448500	H	2.29420600	2.95750200	1.88691100
C	-2.32377500	0.72586700	2.14485700	H	3.24102800	-1.61139100	-0.39069400
C	-3.34680100	0.61329200	1.04862800	H	4.99478400	-2.17351400	-2.01867900
C	-2.83046400	0.71315100	-0.27256200	H	5.70106500	-0.50864900	-3.72767700
C	-3.72556500	0.52027700	-1.34509500	H	4.62722300	1.73370400	-3.77872600
C	-5.08198900	0.28033700	-1.11385700	H	2.87154400	2.30933400	-2.15610900
C	-5.56340000	0.20403400	0.19482500	H	4.30352800	0.72238200	1.04875900
C	-4.69316500	0.35636200	1.28331300	H	5.30092800	0.24232700	3.24815800
H	1.89234900	1.62054700	-1.92488000	H	3.83498200	-0.39813300	5.16251700
H	3.59880000	3.37749200	-2.21967300	H	1.38945900	-0.51709300	4.84546200

H	-0.47922400	0.95871300	2.37044300
H	-0.46436300	-0.20287200	3.69683400
H	1.13494500	-4.81885500	1.72924800
H	2.02987600	-5.82997400	-0.37525600
H	1.82907900	-4.51796800	-2.51574600
H	0.77449600	-2.25965600	-2.43960600
H	-2.33935100	-1.55274100	3.04692700
H	-2.50475500	-0.02885300	2.16337400
H	-2.03951100	1.11812700	-2.25541700
H	-2.52996400	-2.10178100	-2.42310700
H	-4.62672600	-3.37107500	-2.11722300
H	-5.62400100	-3.63102400	0.14300300
H	-4.50856400	-2.60622800	2.11330200
O	-1.69213600	1.18565500	0.13722800
O	-2.67608200	1.77735600	-1.82547600
C	-3.33708700	2.91391800	0.15874500
C	-2.48220400	1.84332800	-0.55145900
H	-0.89784300	-3.06972400	2.35867800
H	0.65457100	-2.34924000	2.77023400
F	-2.73071200	4.10452300	0.04383600
F	-4.55051600	2.98669000	-0.38994000
F	-3.45714500	2.61308300	1.45710400

XVII (LH2)

Rh	-0.46926700	-0.37293700	-1.22329400
P	-1.85592000	0.04921900	0.57299900
Cl	-2.29476000	0.01847700	-2.73392800
N	1.24742700	-0.56841900	0.04870100
N	0.26850500	1.55675600	-1.32482200
C	-2.11122100	1.83412600	0.89781500
C	-2.72461500	2.61395500	-0.10099600
C	-2.91945500	3.97938000	0.09903500
C	-2.49248900	4.58477200	1.28459400
C	-1.87148500	3.81940800	2.27183500
C	-1.68108000	2.44852700	2.08432900
C	-3.51399200	-0.71648800	0.40141200
C	-3.58940100	-2.09543200	0.13594000
C	-4.83119500	-2.72362500	0.06497700
C	-6.00495200	-1.98927400	0.25906300
C	-5.93297800	-0.62215300	0.52686900
C	-4.69299800	0.01716200	0.59891900
C	-1.20215100	-0.69251900	2.11956600
C	-2.04967000	-0.62618900	3.24265000
C	-1.65418300	-1.12885300	4.47799100
C	-0.39258600	-1.70961600	4.60663700
C	0.44928700	-1.78684500	3.50076400
C	0.06653700	-1.29898000	2.24025500
C	1.49277500	0.79651300	0.61651800
C	1.24709400	1.84453400	-0.43141200
C	1.93592900	3.05211900	-0.48257700
C	1.60875300	3.98006500	-1.47111000
C	0.60800300	3.66819200	-2.38915100
C	-0.04165300	2.44341300	-2.29032100
C	2.42759800	-0.99379700	-0.83406600
C	3.78871600	-1.05604800	-0.17066000
C	4.24988700	-2.25067300	0.41023000
C	5.52076500	-2.30015900	0.97832200
C	6.35816000	-1.18145300	0.97513000
C	5.91258700	0.00544800	0.37895400
C	4.63263500	0.05772200	-0.19548100
H	-3.04598900	2.15313200	-1.02964900
H	-3.40134300	4.57033400	-0.67351400
H	-2.64260700	5.64929600	1.43566100
H	-1.53590700	4.28347500	3.19388100
H	-1.20870300	1.86894800	2.86901700
H	-2.68704800	-2.67256300	-0.02940500
H	-4.88157500	-3.78806100	-0.14267500
H	-6.97048400	-2.48274600	0.20358300
H	-6.83986300	-0.04625900	0.68297400
H	-4.65515300	1.07861500	0.81313500
H	-3.03238000	-0.17599000	3.14743700
H	-2.32487700	-1.06426400	5.32843700
H	-0.06249900	-2.10153700	5.56337200
H	1.42657600	-2.24734000	3.60992000
H	2.71533200	3.25704500	0.24244900
H	2.13448400	4.92723400	-1.52621300
H	0.32777500	4.35567800	-3.17849500
H	-0.82499300	2.14314500	-2.97463600
H	2.44663600	-0.29572600	-1.67131200
H	2.16318400	-1.97170400	-1.23033100
H	3.62727400	-3.13993000	0.39879600
H	5.87562000	-3.22424700	1.42452900
H	4.32815100	0.98207900	-0.67725800
O	0.45923000	-1.47497600	-2.94092100
O	-0.79462700	-2.42037900	-1.41546300
C	-0.11056200	-3.81214200	-3.26687700
H	-1.03884900	-3.90704400	-3.84051500
H	-0.06001800	-4.64845800	-2.56642700

H	0.73390200	-3.83933300	-3.95641600
C	-0.13474000	-2.51283300	-2.52210100
H	0.80221100	0.95130500	1.44855300
H	2.50279500	0.86528100	1.02673300
C	1.04307000	-1.59791600	1.11690900
H	2.01336400	-1.80164800	1.57466500
H	0.72743600	-2.50513500	0.59271200
H	7.34337500	-1.24783700	1.41991800
O	6.64031300	1.15223900	0.29594000
C	7.95542900	1.16202000	0.85058400
H	8.34600700	2.16449800	0.67452300
H	7.93619400	0.96378700	1.92826600
H	8.60294600	0.42813000	0.35743000

XVIII (LH2, C-4)

Rh	-0.28428100	0.58938500	-0.29617300
P	1.79497600	-0.36526400	-0.00679400
Cl	0.07205900	0.78940900	-2.65889500
N	-0.84626300	0.42324700	1.74324800
N	-1.34596700	-1.19171200	-0.44850300
C	3.18235500	0.80620900	-0.28428000
C	3.26715400	1.54884300	-1.47527800
C	4.35274700	2.39552700	-1.69451600
C	5.35421700	2.52567400	-0.72774100
C	5.26565500	1.80345300	0.46207500
C	4.18625300	0.94645500	0.68739300
C	2.08047700	-1.82210900	-1.07962900
C	1.40471500	-3.02648800	-0.81112500
C	1.60382900	-4.13966800	-1.62555900
C	2.47256400	-4.06504700	-2.71746500
C	3.14832600	-2.87426900	-2.98743000
C	2.95643700	-1.75598800	-2.17481200
C	2.00226800	-0.96964000	1.71219800
C	2.93079000	-2.00108500	1.93759000
C	3.20000600	-2.45561400	3.22750700
C	2.53067700	-1.88928600	4.31040500
C	1.59349300	-0.87933800	4.09460300
C	1.31455700	-0.39856100	2.80797400
C	0.29386900	0.71203100	2.68850000
C	-1.43490700	-0.94066500	1.98195000
C	-1.87601500	-1.62953000	0.71740400
C	-2.72975500	-2.73092400	0.75223300
C	-3.03632000	-3.39415500	-0.43280900
C	-2.48304000	-2.93504300	-1.62824000
C	-1.64472500	-1.82949700	-1.59955300
C	-1.89726500	1.49717000	1.95364800
C	-2.98657600	1.38173700	0.91699400
C	-2.69518000	1.74403600	-0.41522300
C	-3.64680400	1.49993100	-1.41348100
C	-4.88591500	0.94078900	-1.10973400
C	-5.18423700	0.61904000	0.22527200
C	-4.22126700	0.82861800	1.23167900
H	2.48261700	1.47392000	-2.21930100
H	4.41122900	2.95909900	-2.62057900
H	6.19538900	3.18991300	-0.90089000
H	6.03489500	1.90206300	1.22163300
H	4.13799100	0.39362700	1.61719900
H	0.73852300	-3.11130500	0.03999800
H	1.08132900	-5.06480300	-1.40390900
H	2.62558500	-4.93362600	-3.35047800
H	3.83191800	-2.81149100	-3.82819400
H	3.49886800	-0.84400200	-2.39219800
H	3.45697700	-2.44638700	1.10097100
H	3.92616000	-3.24758600	3.37844800
H	2.72548400	-2.23704900	5.31980600
H	1.06096400	-0.45551500	4.94057200
H	0.74443100	1.63968700	2.32763900
H	-0.12990600	0.90168900	3.67950700
H	-3.14161700	-3.05890400	1.70005500
H	-3.69840200	-4.25342200	-0.42246800
H	-2.69506200	-3.41849600	-2.57459900
H	-1.19263900	-1.42033100	-2.49390000
H	-2.28917100	1.39678000	2.97100500
H	-1.37794500	2.45416100	1.87418500
H	-1.83436800	2.37755900	-0.65967100
H	-3.42602700	1.77507400	-2.44022900
H	-5.61046300	0.77764500	-1.89774300
H	-4.47148700	0.54429800	2.24898100
O	0.66595300	2.35155300	0.17610600
O	-0.48907200	3.82185200	-1.10261400
C	1.41459100	4.58909700	0.15901300
H	1.47562400	4.57579500	1.25077400
H	2.41165400	4.35888800	-0.22869300
H	1.11018100	5.57894400	-0.18297300
C	0.42630300	3.53963600	-0.32846700
H	-2.26052800	-0.87129800	2.69491600
H	-0.66917100	-1.56249400	2.45137000
O	-6.35656700	0.09330900	0.64492900

C	-7.38466800	-0.15724800	-0.31826000	N	-0.85502600	0.18505600	1.79809500
H	-7.05575500	-0.88382900	-1.06862800	N	-1.15821900	-1.43053900	-0.42760300
H	-8.22210500	-0.56903200	0.24434300	C	3.10552200	1.16840500	-0.24426500
H	-7.69672100	0.76813900	-0.81362000	C	2.98658800	2.03298900	-1.34687100
XVIII (LH2, C-2)							
Rh	-0.45243800	0.44642300	-0.02663300	C	3.92220500	3.04852900	-1.54666900
P	1.74644600	-0.18423400	-0.16480400	C	4.97394700	3.22625600	-0.64348800
Cl	-0.46276800	1.09714900	-2.32935100	C	5.08909300	2.38018400	0.45982600
N	-0.70619700	-0.14996400	1.99176100	C	4.16204200	1.35479300	0.66063300
N	-1.28625900	-1.42642800	-0.39289400	C	2.41475600	-1.54194400	-1.14661900
C	2.90137100	1.22732900	-0.37148300	C	1.92037900	-2.84415000	-0.95034700
C	2.69994600	2.18231800	-1.38374300	C	2.27491700	-3.87279000	-1.82248500
C	3.62037300	3.21351300	-1.56384400	C	3.11919200	-3.61586600	-2.90581900
C	4.73873700	3.31617200	-0.73134700	C	3.61283300	-2.32644600	-3.10792600
C	4.93381600	2.38061500	0.28429500	C	3.26538200	-1.29355200	-2.23451000
C	4.02172900	1.33932800	0.46816100	C	2.20288400	-0.83283000	1.67376300
C	2.05983500	-1.36702000	-1.52442200	C	3.25352000	-1.74233500	1.87884300
C	1.63227100	-2.70119300	-1.39663800	C	3.56260000	-2.21542200	3.15394000
C	1.85166600	-3.60910600	-2.43073900	C	2.81243900	-1.78785800	4.24731000
C	2.49197100	-3.19710300	-3.60256400	C	1.75843000	-0.89504500	4.05481400
C	2.91983700	-1.87505700	-3.73414100	C	1.43654000	-0.40091700	2.78233000
C	2.70675600	-0.96043700	-2.70229000	C	0.29208600	0.58908300	2.69784700
C	2.27296800	-1.03717700	1.36781400	C	-1.25559300	-1.25128400	2.01049100
C	3.36309000	-1.92140700	1.28164500	C	-1.57765000	-1.98225500	0.73390800
C	3.87775800	-2.53834900	2.42053600	C	-2.22007300	-3.21915400	0.75232400
C	3.29624300	-2.28738000	3.66156800	C	-2.42441600	-3.89993600	-0.44486500
C	2.20265900	-1.42679300	3.75346200	C	-1.97911200	-3.32444600	-1.63465500
C	1.67614500	-0.78477400	2.62446600	C	-1.35442800	-2.08553400	-1.59021300
C	0.50498900	0.14871400	2.84021300	C	-2.02874000	1.09157400	2.10105500
C	-1.06520200	-1.60932000	2.03484400	C	-3.05589900	0.93588800	1.01358100
C	-1.58922400	-2.13073800	0.72314900	C	-2.55842800	1.05887600	-0.31576000
C	-2.28578600	-3.33551800	0.64858700	C	-3.46201900	0.79848700	-1.36535200
C	-2.67124700	-3.82385200	-0.59670700	C	-4.80412100	0.50697200	-1.12958400
C	-2.35315100	-3.09057300	-1.74015400	C	-5.26995000	0.42985100	0.19386900
C	-1.66280000	-1.89496200	-1.60135400	C	-4.37891500	0.62822200	1.27150300
C	-1.85126900	0.69526100	2.52330800	H	2.16086600	1.91330300	-2.03960500
C	-3.10094500	0.53860000	1.69193700	H	3.82446700	3.70473700	-2.40636900
C	-3.18591700	1.18898400	0.45269900	H	5.69684300	4.02159600	-0.79837100
C	-4.30645500	0.98181200	-0.37714800	H	5.90070500	2.51283600	1.16878600
C	-5.34304900	0.13725700	0.04575200	H	4.27082200	0.70672300	1.52222500
C	-5.25315500	-0.48255200	1.29338200	H	1.27704600	-3.06878700	-0.10620800
C	-4.14251400	-0.29391500	2.11739800	H	1.89188700	-4.87440500	-1.65300400
H	1.82171200	2.12534500	-2.01580200	H	3.39350300	-4.41772400	-3.58451300
H	3.45770100	3.94184100	-2.35227800	H	4.27534400	-2.11957400	-3.94285800
H	5.44991600	4.12434500	-0.87202300	H	3.66613800	-0.30025900	-2.40035700
H	5.79560300	2.45503100	0.94001000	H	3.84211700	-2.08174700	1.03382400
H	4.19509000	0.62454400	1.26273500	H	4.38359600	-2.91286600	3.28592100
H	1.14844600	-3.04334500	-0.48846700	H	3.03733100	-2.15044800	5.24527000
H	1.52442900	-4.63776700	-2.31838700	H	1.16893800	-0.57443900	4.90873700
H	2.66133500	-3.90625200	-4.40687200	H	0.62383500	1.56337200	2.33144400
H	3.42582300	-1.55118300	-4.63806900	H	-0.11169400	0.73271100	3.70497800
H	3.05534500	0.05873100	-2.81632300	H	-2.55015800	-3.63595300	1.69747800
H	3.82241800	-2.12144200	0.32048400	H	-2.92400800	-4.86283300	-0.44788600
H	4.72502900	-3.21023200	2.33181900	H	-2.11535200	-3.81796800	-2.58976300
H	3.68243600	-2.76545600	4.55597900	H	-1.00265000	-1.57868600	-2.47936400
H	1.74283500	-1.24891400	4.72079500	H	-2.41557900	0.85508300	3.09742200
H	0.76710900	1.18587900	2.61810200	H	-1.64003100	2.11397900	2.12288400
H	0.20474500	0.08973200	3.89103000	H	-1.97698600	2.23282600	-0.55261700
H	-2.51638600	-3.87661600	1.55933100	H	-3.11100100	0.86053600	-2.39188800
H	-3.21372000	-4.76021400	-0.67245100	H	-5.47454600	0.34345500	-1.96445900
H	-2.63541000	-3.43131700	-2.72934800	H	-4.75885600	0.52468500	2.28337300
H	-1.39707800	-1.27647100	-2.44895300	O	0.27535100	2.41605900	0.11662500
H	-2.02982100	0.39682000	3.56154500	O	-1.55675000	3.44477300	-0.66244200
H	-1.49580500	1.72713000	2.51815200	C	0.33038200	4.78767500	-0.03794900
H	-2.47223500	1.96552300	0.15819500	H	0.51871400	4.95062700	1.02754500
H	-6.21749800	-0.02701100	-0.57148600	H	1.29882400	4.75572200	-0.54334200
H	-4.09211800	-0.78680500	3.08338700	H	-0.27620800	5.60300500	-0.43061300
O	0.29293600	2.23441100	0.65986900	C	-0.37051600	3.46512900	-0.21656200
O	-1.30554200	3.63601400	-0.11867000	H	-2.09994200	-1.30164700	2.70292000
C	0.63770300	4.54605300	0.97899300	H	-0.42323400	-1.76959400	2.49153200
H	0.13144900	5.50362600	0.85217500	O	-6.54486500	0.15661300	0.54281100
H	0.85878200	4.38172900	2.03751000	C	-7.50953000	-0.08121600	-0.48796400
H	1.59155200	4.55977200	0.44312500	H	-7.23641600	-0.95350300	-1.09076800
C	-0.23114400	3.41883100	0.44187400	H	-8.45007800	-0.27383200	0.02733800
H	-1.77982200	-1.79569300	2.84040200	H	-7.61929900	0.79484100	-1.13543700
H	-0.16329800	-2.17363200	2.28246400	TS_XVIII-XIX (LH2, C-2)			
H	-6.06519900	-1.12333900	1.62346500	Rh	-0.60675900	0.42403300	-0.01879000
O	-4.30418800	1.66321400	-1.54947800	P	1.73926100	-0.12397100	-0.12917100
C	-5.42782300	1.52884500	-2.42253900	Cl	-0.49609000	0.96810500	-2.37134900
H	-5.21168900	2.16114300	-3.28333900	N	-0.73498900	-0.07510900	2.03883100
H	-5.55240500	0.49228200	-2.75410600	N	-1.26058300	-1.50540600	-0.27178000
H	-6.34875800	1.87238200	-1.93891200	C	2.86312200	1.32476300	-0.31177000
TS_XVIII-XIX (LH2, C-4)							
Rh	-0.43236900	0.48779200	-0.25901600	C	2.60068300	2.29492900	-1.29552600
P	1.88007100	-0.18895100	-0.20326000	C	3.46056400	3.38145700	-1.45753500
Cl	-0.15086100	0.83688600	-2.63457800	C	4.57978900	3.52502800	-0.63301000
				C	4.83825700	2.57317200	0.35355400
				C	3.98750900	1.47727900	0.51544500
				C	2.18428700	-1.30158500	-1.46736200

C	1.76738000	-2.64126100	-1.37205200	C	1.83589500	-1.16511100	3.93015500
C	2.05624200	-3.54403500	-2.39474500	C	1.47631700	-0.56023100	2.71678000
C	2.75808000	-3.12173800	-3.52679500	C	0.19143500	0.24417100	2.70262200
C	3.17583100	-1.79403000	-3.62757000	C	-1.14351400	-1.73308500	1.92866400
C	2.89265600	-0.88650300	-2.60474500	C	-1.02756100	-2.49069000	0.63172800
C	2.30093400	-0.94421300	1.41726300	C	-1.20829300	-3.87261100	0.59209500
C	3.39279400	-1.82677200	1.38083200	C	-1.13591600	-4.53787900	-0.62819400
C	3.87700400	-2.42226500	2.54544700	C	-0.88039600	-3.80146200	-1.78497900
C	3.26636800	-2.14519300	3.76696600	C	-0.69593400	-2.43001300	-1.68323200
C	2.17548600	-1.27726300	3.81341800	C	-2.17539200	0.49864300	2.16681600
C	1.67833500	-0.66393400	2.65484500	C	-3.17638600	0.35656200	1.05323300
C	0.51212400	0.28722900	2.81510300	C	-2.64243800	0.26927800	-0.25185200
C	-1.07719600	-1.53740400	2.17050900	C	-3.53356600	0.12554400	-1.31815400
C	-1.51107200	-2.17524800	0.87618000	C	-4.92252200	0.10647500	-1.10884800
C	-2.09701300	-3.43963200	0.85519100	C	-5.43128500	0.20650100	0.19070100
C	-2.42657800	-4.01912200	-0.36723900	C	-4.54772600	0.32101000	1.27871100
C	-2.16259200	-3.31687300	-1.54310000	H	1.72836400	2.39967200	-1.76281600
C	-1.58122800	-2.05917400	-1.45909500	H	2.88553100	4.58318700	-1.85640400
C	-1.86700400	0.76754200	2.57392800	H	4.58813200	5.16983900	-0.13963600
C	-3.05376800	0.62122900	1.66452700	H	5.14188400	3.54168800	1.65636800
C	-2.81081800	0.85743300	0.28558200	H	4.02037800	1.34959400	1.73579800
C	-3.89771700	0.62579600	-0.60197600	H	2.02670700	-2.80850100	-0.45529500
C	-5.15362800	0.21546700	-0.11675500	H	3.07153200	-4.21989000	-2.17325500
C	-5.33984500	0.01533500	1.24729800	H	4.47181400	-3.19660900	-3.95935400
C	-4.29008100	0.20985200	2.15173300	H	4.81172900	-0.73231500	-3.99514600
H	1.72289700	2.19925000	-1.92421800	H	3.76832900	0.69184500	-2.28085800
H	3.25097600	4.11917800	-2.22635300	H	4.23703600	-1.47230000	0.92775500
H	5.24358700	4.37525800	-0.75786800	H	4.83966800	-2.50800900	3.07856800
H	5.70323000	2.67736200	1.00149100	H	3.28431000	-2.32350000	5.02208900
H	4.21014500	0.74907800	1.28615300	H	1.16711100	-1.07809100	4.78171800
H	1.23721700	-2.99141600	-0.49278600	H	0.37221300	1.28199600	2.41249000
H	1.73440000	-4.57690700	-2.30431000	H	-0.21226800	0.25609400	3.7023500
H	2.98191000	-3.82574200	-4.32247000	H	-1.41137000	-4.41036700	1.51176000
H	3.72830600	-1.45963500	-4.50033800	H	-1.27978300	-5.61199600	-0.67508800
H	3.23185200	0.13883900	-2.69539100	H	-0.81884300	-4.27486400	-2.75774500
H	3.87535400	-2.04636100	0.43516100	H	-0.49234900	-1.80516700	-2.54279700
H	4.72587600	-3.09645000	2.49310300	H	-2.54187200	0.12798800	3.13039100
H	3.63020600	-2.60437200	4.68060400	H	-1.88779500	1.54503900	2.30317900
H	1.69679800	-1.07066600	4.76609600	H	-2.36531000	2.19737900	-1.05886000
H	0.76779600	1.30254700	2.50187800	H	-3.15803600	0.03513100	-2.33355000
H	0.24334900	0.32567000	3.87547500	H	-5.58474300	0.00508300	-1.96058500
H	-2.28814000	-3.95565400	1.78969200	H	-4.96034600	0.37704600	2.28211200
H	-2.88479000	-5.00185500	-0.40006200	O	-0.42055200	2.28594200	0.23688800
H	-2.40428600	-3.72819400	-2.51610300	O	-2.14528700	3.15201800	-0.93118400
H	-1.36302600	-1.45533200	-2.33028900	C	-0.68784700	4.65800400	0.18864400
H	-2.08483900	0.46176900	3.60282000	H	-0.90786700	4.81370900	1.24965300
H	-1.50638500	1.79964200	2.59880600	H	0.38812400	4.77897600	0.04817500
H	-2.28901500	2.08112100	0.01619100	H	-1.23906000	5.38651700	-0.40452300
H	-5.98258600	0.05292500	-0.79433700	C	-1.07747600	3.26019600	-0.17814000
H	-4.43756800	0.03115700	3.21241000	H	-2.14154100	-1.89908800	2.34243600
O	0.01574700	2.36521700	0.44104800	H	-0.43143400	-2.14158500	2.64897900
O	-1.95899700	3.29123300	-0.07792100	O	-6.75623900	0.18988300	0.51088200
C	-0.12156000	4.74039400	0.43934500	C	-7.70452800	0.05163400	-0.54517900
H	-0.79646600	5.52038800	0.08833900	H	-7.56836100	-0.89286000	-1.08460200
H	0.08004600	4.88870500	1.50496800	H	-8.68569100	0.05768900	-0.06952200
H	0.83259800	4.79157600	-0.08975900	H	-7.63995300	0.88541300	-1.25389900
C	-0.73357800	3.37763300	0.24421700	XIX (LH2, C-2)			
H	-1.85050100	-1.66617600	2.93225300	Rh	-0.78057400	0.20009700	-0.05516200
H	-0.19181500	-2.06746600	2.52820100	P	1.75605200	0.07606400	-0.08547900
H	-6.31300300	-0.30437300	1.60817700	Cl	-0.66694900	0.65937200	-2.46644000
O	-3.67007400	0.86690100	-1.91237500	N	-0.86700400	-0.16068200	2.01365000
C	-4.74072100	0.72789200	-2.84794500	N	-0.99386900	-1.81460300	-0.18744600
H	-4.31897600	0.99016000	-3.81817700	C	2.59806900	1.71307800	-0.03725100
H	-5.11227200	-0.30201400	-2.88040300	C	2.22141300	2.69150600	-0.97517800
H	-5.56678500	1.40796200	-2.61324800	C	2.83178900	3.94599900	-0.96915500
XIX (LH2, C-4)				C	3.81091600	4.24557900	-0.01761800
Rh	-0.58315200	0.21675900	-0.24432700	C	4.18346900	3.28285100	0.92159900
P	1.92225000	0.09299400	-0.00582300	C	3.58445500	2.02067800	0.91216600
Cl	-0.38985900	0.76695800	-2.59834800	C	2.54971800	-0.84311600	-1.47176700
N	-0.91255100	-0.24778100	1.79067100	C	2.32155500	-2.22588800	-1.59409000
N	-0.76356700	-1.79127600	-0.49544000	C	2.85741000	-2.94128000	-2.66444700
C	2.80045500	1.71250700	-0.01471600	C	3.62186600	-2.28732200	-3.63420400
C	2.48236200	2.64278500	-1.02059700	C	3.85259500	-0.91588200	-3.52153300
C	3.13178900	3.87731100	-1.06871200	C	3.32223400	-0.19642400	-2.44782300
C	4.08926200	4.20595600	-0.10483200	C	2.32616700	-0.79572500	1.43247600
C	4.40047300	3.29221600	0.90323000	C	3.47586200	-1.59958100	1.42785800
C	3.76338300	2.04981200	0.94869900	C	3.89119600	-2.27053100	2.57911900
C	2.80624200	-0.94618900	-1.24659500	C	3.15666200	-2.14471000	3.75622000
C	2.62027100	-2.34056500	-1.23393000	C	2.01572900	-1.34157000	3.77479700
C	3.21990000	-3.14467300	-2.20294800	C	1.58338900	-0.66138400	2.62824600
C	4.00671400	-2.57002000	-3.20435900	C	0.38226100	0.25051200	2.76120000
C	4.19587700	-1.18762600	-3.22534400	C	-1.21443000	-1.61145600	2.24132600
C	3.60179600	-0.37903700	-2.25335500	C	-1.12074900	-2.45495700	0.99778100
C	2.35430700	-0.67491400	1.61330300	C	-1.24046800	-3.84234900	1.05196100
C	3.55778800	-1.38123800	1.76806700	C	-1.26477900	-4.57311400	-0.13291000
C	3.90077800	-1.97143600	2.98482000	C	-1.16835900	-3.89537600	-1.34843500
C	3.03389000	-1.86606300	4.07018200	C	-1.02772400	-2.51451500	-1.34029200

C	-1.99851100	0.71088500	2.51264400	H	-4.67289100	1.86855800	0.23628700
C	-3.15595000	0.58362800	1.56109000	H	-7.02088900	1.20087800	-0.04266800
C	-2.83620100	0.30765600	0.22304900	H	-7.64604100	-1.20648200	-0.09484000
C	-3.90050100	0.09257400	-0.67706200	H	-5.87925200	-2.94386800	0.14192900
C	-5.22990900	0.24524400	-0.24740700	H	-3.53257800	-2.29282000	0.42111500
C	-5.51200300	0.56339200	1.08322900	H	-1.97579300	1.79705000	3.08351700
C	-4.47986900	0.71464200	2.00366900	H	-2.07159100	4.19433400	3.64667200
H	1.45715000	2.46744400	-1.71293100	H	-2.34721900	5.89247100	1.85160000
H	2.53901900	4.68949000	-1.70442800	H	-2.52396000	5.16985400	-0.52040100
H	4.28001900	5.22483200	-0.00932200	H	-2.40031800	2.77625900	-1.10219300
H	4.94400000	3.50897100	1.66292400	H	-3.41155900	-1.26459200	2.71414900
H	3.89047400	1.28075200	1.64374300	H	-2.45584900	-2.49716600	4.61749300
H	1.74482700	-2.75601700	-0.84392200	H	0.00760700	-2.48873500	4.99604300
H	2.67720300	-4.00946100	-2.73851800	H	1.47741900	-1.18982600	3.49215400
H	4.03723700	-2.84457700	-4.46836300	H	1.75175900	-4.02792300	0.59114900
H	4.45089200	-0.39961700	-4.26627400	H	0.03343100	-5.77755900	0.09687700
C	3.51913900	0.86691900	-2.37469200	H	-2.08538000	-5.08679600	-1.07137500
H	4.05505300	-1.70413300	0.51752800	H	-2.40907900	-2.67232900	-1.62985900
H	4.78633800	-2.88393000	2.55155400	H	2.79126700	2.77690700	1.36554600
C	3.46815700	-2.66245700	4.65786100	H	4.35673800	-0.42213700	-1.05227100
H	1.45407700	-1.23240300	4.69837200	H	0.45135600	1.39687900	1.40658200
H	0.60732600	1.26475600	2.42231900	H	1.78669500	0.37318900	1.91997300
H	0.11370000	0.31336800	3.82085300	H	2.20868200	0.72166200	-1.63179100
H	-1.32717500	-4.43327600	2.01521100	H	1.53784800	1.97211300	-0.58036000
H	-1.36306200	-5.65307900	-0.10742000	H	6.88131400	1.54726400	1.80539800
H	-1.19175100	-4.42154600	-2.29544400	C	6.85259800	-0.45243300	-0.01938600
H	-0.93552600	-1.93281800	-2.24731100	F	6.98368800	-1.47109100	0.86525700
H	-2.25477200	0.41451500	3.53624100	F	6.68493300	-1.01209500	-1.23785200
H	-1.61200300	1.73168400	2.54522000	F	8.03678000	0.20027300	-0.03326600
H	-1.53409700	2.35692400	-1.79935600	H	4.99370100	3.02704000	2.45372500
H	-6.04985800	0.10251500	-0.94116000	O	-0.47012700	1.82056900	-2.13731900
H	-4.69269200	0.92355300	3.04847300	C	0.20300300	1.35011600	-3.12674800
O	-0.66249900	2.27850400	0.39266400	O	0.50066200	0.11213800	-3.09701800
O	-1.69797700	3.24292900	-1.36589400	C	0.59542000	2.23577800	-4.26779600
C	-1.14831700	4.61803900	0.48257500	H	-0.23264500	2.27022100	-4.98426600
H	-0.32512400	5.20175300	0.05648100	H	-0.78249400	3.25142600	-3.91418500
H	-2.07923300	5.14798000	0.27233100	H	1.47604200	1.83655100	-4.77289000
H	-0.99390100	4.51664000	1.55580900				
C	-1.16123600	3.27167500	-0.17269600	XVIII (LH3, C-4)			
H	-2.24551600	-1.66103300	2.60101700	Rh	-0.49623400	-0.73864100	-0.70396800
H	-0.57966700	-2.02495800	3.02741500	P	-2.27393000	0.33196100	0.31542900
H	-6.54633500	0.66792200	1.39769400	Cl	-1.79410900	-0.90045700	-2.71764500
O	-3.57821800	-0.27668300	-1.95105600	N	0.82999600	-0.50932600	0.98846600
C	-4.62571300	-0.48112300	-2.89207200	N	0.54282300	0.94709300	-1.33247800
H	-4.13650000	-0.75097600	-3.82888600	C	-3.61111500	-0.87996500	0.67052400
H	-5.29371200	-1.29555000	-2.58626100	C	-4.19122400	-1.63712700	-0.36360900
H	-5.21705900	0.42984700	-3.04429300	C	-5.22611300	-2.52825200	-0.08461400
				C	-5.68489500	-2.69039300	1.22507600
				C	-5.10570500	-1.95234800	2.25740400
				C	-4.07525600	-1.05045600	1.98638700
				C	-3.00761100	1.72591500	-0.61635700
				C	-2.3160500	2.87295600	-0.86243000
				C	-2.77178500	3.94753400	-1.56615900
				C	-4.08666500	3.88960200	-2.03639600
				C	-4.86229500	2.75583800	-1.79256200
				C	-4.32960100	1.67676200	-1.08459500
				C	-1.82632900	0.99334900	1.95916600
				C	-2.54695500	2.08027600	2.47868200
				C	-2.3039100	2.54487800	3.77095000
				C	-1.32829600	1.92805200	4.55221900
				C	-0.59186400	0.86258600	4.03291000
				C	-0.82359400	0.37518000	2.74003300
				C	0.04108600	-0.77533400	2.26491500
				C	1.35555500	0.89781700	0.95518500
				C	1.44777800	1.42894900	-0.44537800
				C	2.34781600	2.42960400	-0.80291300
				C	2.31337400	2.94744900	-2.09528200
				C	1.38041100	2.44360800	-3.00087600
				C	0.51400800	1.43969400	-2.58875100
				C	1.99692000	-1.51717400	0.97491500
				C	3.22854800	-1.14269700	0.17304700
				C	3.34565700	-1.39122300	-1.20316000
				C	4.51552200	-1.05853200	-1.88816000
				C	5.59213700	-0.48506000	-1.21398700
				C	5.49484400	-0.25843000	0.16146100
				C	4.32629900	-0.59054800	0.84953400
				H	-3.82899200	-1.53470400	-1.37907600
				H	-5.66930300	-3.10088200	-0.89352000
				H	-6.48767100	-3.38950900	1.43870600
				H	-5.45385800	-2.07189300	3.27858700
				H	-3.64720300	-0.48338100	2.80340800
				H	-1.21277400	2.94319700	-0.49932500
				H	-2.16477200	4.82920800	-1.74583300
				H	-4.50426700	4.72725900	-2.58638300
				H	-5.88657700	2.70673800	-2.14838800
				H	-4.94799000	0.80746700	-0.89652200
				H	-3.31065200	2.55918600	1.87638500
				H	-2.87426400	3.38196400	4.15914900

H	-1.12799800	2.28024600	5.55899100	H	3.08281800	1.45544900	-0.00727900
H	0.18301900	0.40380600	4.63936300	H	6.62367200	-0.88614100	-0.69526200
H	-0.53586100	-1.68463400	2.07689400	H	3.47055200	-0.85332600	-3.61042500
H	0.75274400	-0.99881500	3.06321000	O	-0.66090400	2.39842000	-0.37666200
H	3.06323100	2.78948600	-0.07233500	O	1.42905700	2.90207100	0.19384200
H	3.00713900	3.72720000	-2.39083000	C	-0.07111200	4.70612100	-0.40371300
H	1.32020000	2.81236600	-4.01803000	H	-0.53847500	4.82393300	-1.38520500
H	-0.22181700	1.00156600	-3.25021300	H	-0.80248400	5.01974300	0.34781500
H	2.30341300	-1.63094500	2.01762000	H	0.81472700	5.33801900	-0.33449700
H	1.58897200	-2.46893100	0.64402900	C	0.29598300	3.25889900	-0.17119500
H	2.52411900	-1.85721500	-1.73178100	H	1.50639700	-1.74054700	-2.61283400
H	6.49931200	-0.22158800	-1.74679100	H	-0.11887200	-2.03146400	-2.04288900
H	4.27562000	-0.42120500	1.92049500	C	5.41100800	0.75470000	1.12685700
O	-1.14998400	-2.62962400	-0.15275200	F	6.73626000	0.54184900	1.26841000
O	0.54882200	-2.61814000	-1.53195400	F	4.79546400	0.09276500	2.14041400
C	-0.43990700	-4.77107600	-1.00681700	F	5.18703700	2.07194700	1.34146200
H	0.50417400	-5.20280000	-1.34122100	H	5.70172600	-1.61793600	-2.88696700
H	-0.73818300	-5.19916000	-0.04757700	TS_XVIII-XIX (LH3, C-4)			
H	-1.21645400	-5.01103800	-1.74118500	Rh	-0.07957000	0.50556300	-0.30739500
C	-0.32308700	-3.28057800	-0.89966600	P	2.17316300	-0.19711000	0.04326500
H	2.31587500	0.96657400	1.46823600	Cl	0.32719700	0.84491500	-2.65895700
H	0.66434300	1.53395700	1.50849400	N	-0.63323000	0.20014700	1.72069100
C	6.67775600	0.28465300	0.91478700	N	-0.81120300	-1.41158200	-0.52313200
F	7.41051600	1.13318900	0.15930900	C	3.41894400	1.14799400	-0.13258600
F	6.30834600	0.95342500	2.03046000	C	3.36696100	2.01122100	-1.24121000
F	7.51621900	-0.70308000	1.31341400	C	4.32893300	3.00897800	-1.39865600
H	4.58867500	-1.25342600	-2.95330900	C	5.34054000	3.16986100	-0.44792500
XVIII (LH3, C-2)				C	5.38841300	2.32534000	0.66142100
Rh	0.00381900	0.54305600	0.20054800	C	4.43421000	1.31805500	0.82170900
P	-2.16707800	-0.16337300	0.09441300	C	2.71423800	-1.55477500	-1.06987500
Cl	-0.25522300	1.13175000	2.50699000	C	2.25262000	-2.86530900	-0.85179900
N	0.50448100	-0.02348200	-1.80505700	C	2.61454900	-3.89332600	-1.72169700
N	0.88492700	-1.30495100	0.61093900	C	3.43258900	-3.62696600	-2.82248800
C	-3.35002000	1.23728500	0.18437700	C	3.89375600	-2.32874700	-3.04536500
C	-3.30033100	2.15885500	1.24524200	C	3.53897000	-1.29608800	-2.17554900
C	-4.23865300	3.18608600	1.32261300	C	2.40538900	-0.84155200	1.74837000
C	-5.22270500	3.31943200	0.33912100	C	3.44446100	-1.75416400	1.99634000
C	-5.26620200	2.41816400	-0.72454400	C	3.69730200	-2.22782100	3.28327300
C	-4.33543700	1.38079100	-0.80689400	C	2.90181000	-1.79834100	4.34326200
C	-2.61577600	-1.36777100	1.39639500	C	1.85951300	-0.90215200	4.10690100
C	-2.08167000	-2.66886000	1.35746600	C	1.59430500	-0.40579200	2.82260000
C	-2.41653600	-3.59361000	2.34436900	C	0.46023300	0.59015800	2.68912800
C	-3.28126400	-3.23299400	3.38125300	C	-1.06177400	-1.23266500	1.90509800
C	-3.81795900	-1.94561600	3.42282500	C	-1.30727000	-1.95968700	0.60960200
C	-3.49027200	-1.01421100	2.43668300	C	-1.96235300	-3.18961000	0.58647100
C	-2.51528800	-0.97844200	-1.50524100	C	-2.10135600	-3.86602200	-0.62249600
C	-3.56793500	-1.90768300	-1.56234700	C	-1.57786600	-3.29415600	-1.78184000
C	-3.94999900	-2.47978200	-2.77502300	C	-0.94220000	-2.06322900	-1.69683200
C	-3.27282100	-2.13452900	-3.94284200	C	-1.81465700	1.11749400	1.95084400
C	-2.21075500	-1.23168200	-3.88919400	C	-2.79397600	0.95027100	0.82083900
C	-1.81402200	-0.63776500	-2.68384900	C	-2.26424800	1.08200100	-0.48548100
C	-0.64348300	0.32082800	-2.73514100	C	-3.10993800	0.82768600	-1.57730600
C	0.80368800	-1.49573600	-1.81457500	C	-4.45316900	0.50002000	-1.38347200
C	1.30700100	-1.98278500	-0.48462900	C	-4.95708200	0.39849700	-0.08473400
C	2.09437200	-3.12574200	-0.36650100	C	-4.12683900	0.60858800	1.02481200
C	2.44515400	-3.58304700	0.90152800	H	2.57295200	1.90551600	-1.97160700
C	2.00220100	-2.88082500	2.02215900	H	4.28269600	3.66447100	-2.26308400
C	1.22830100	-1.74274300	1.84010100	H	6.08435000	3.95133700	-0.57055100
C	1.72390400	0.77280100	-2.30637500	H	6.16789100	2.44536600	1.40755700
C	3.08512700	0.30757300	-1.82868400	H	4.48988200	0.67219200	1.68965200
C	3.63435700	0.75182600	-0.62034700	H	1.63103900	-3.09685400	0.00644800
C	4.89599400	0.31023900	-0.21420800	H	2.25778600	-4.90167100	-1.53632100
C	5.64263400	-0.55473800	-1.01598800	H	3.71247300	-4.42856400	-3.49914000
C	5.12052900	-0.96682500	-2.24236000	H	4.53607700	-2.11493200	-3.89407200
C	3.85620700	-0.53749900	-2.64481800	H	3.91465500	-0.29611200	-2.35763700
H	-2.52395600	2.07865500	1.99617400	H	4.06813900	-2.09444600	1.17742500
H	-4.19424700	3.88806500	2.14949300	H	4.50994400	-2.92746100	3.44986500
H	-5.94813400	4.12490300	0.40041100	H	3.08266000	-2.16220500	5.34958800
H	-6.02356700	2.51639600	-1.49586900	H	1.23525300	-0.58025600	4.93511500
H	-4.38905100	0.69055300	-1.63925800	H	0.81560700	1.56762000	2.35429800
H	-1.41997000	-2.97704900	0.55646100	H	0.00117800	0.72214300	3.67378800
H	-2.00288400	-4.59601600	2.30013300	H	-2.35421900	-3.60369700	1.50890000
H	-3.53957000	-3.95565300	4.14902800	H	-2.61102800	-4.82292800	-0.65791100
H	-4.49806300	-1.66161900	4.21954200	H	-1.66142200	-3.78443800	-2.74457900
H	-3.92521700	-0.02321000	2.47791700	H	-0.52957700	-1.56053100	-2.56175000
H	-4.10263700	-2.17637700	-0.65840200	H	-2.25089700	0.89631500	2.93016500
H	-4.77027000	-3.18947100	-2.80072300	H	-1.42194000	2.13786400	1.97943000
H	-3.55751400	-2.57462800	-4.89308400	H	-1.55656100	2.18007800	-0.71253900
H	-1.67165100	-0.98668500	-4.79922700	H	-5.10352800	0.31954400	-2.23222600
H	-0.93406600	1.34386700	-2.48257700	H	-4.52327500	0.49047300	2.02833600
H	-0.26346400	0.32561200	-3.76000700	O	0.62117800	2.41930100	0.11900800
H	2.42328700	-3.64359500	-1.26011600	O	-1.15041800	3.41201600	-0.82152800
H	3.05792600	-4.47140100	1.01163800	C	0.66738900	4.78935400	-0.07105400
H	2.25351000	-3.19893300	3.02711000	H	0.04689000	5.60141600	-0.44794800
H	0.86782800	-1.14766000	2.66912400	H	0.85881800	4.93154900	0.99629800
H	1.70048000	0.70060400	-3.39759600	H	1.63424300	4.78445500	-0.58155500
H	1.54900100	1.81098400	-2.02858500	C	-0.00698100	3.45893200	-0.28109600

H	-1.95144500	-1.27196500	2.53899500	P	2.21376800	0.15591100	0.05192500
H	-0.27127800	-1.76092400	2.44260900	Cl	-0.00991300	0.66878900	-2.66823900
C	-6.41474700	0.09640700	0.14233600	N	-0.68610000	-0.37759700	1.70681200
F	-6.98186500	-0.51550300	-0.91844900	N	-0.32888900	-1.90233100	-0.56627600
F	-6.60023100	-0.70201900	1.21820200	C	2.92880000	1.84629700	0.19715200
F	-7.12310900	1.22801500	0.37174000	C	2.61266400	2.79786500	-0.78948200
H	-2.71872900	0.91174900	-2.58692900	C	3.13244700	4.09064400	-0.71552600
TS XVIII-XIX (LH3, C-2)							
Rh	0.44194400	0.33064100	-0.14286800	C	3.76089100	2.21921000	1.26341900
P	-1.88415100	-0.04089900	0.19633700	C	3.25586500	-0.71190100	-1.19652100
Cl	0.51402700	1.12362100	2.12635500	C	3.17104300	-2.11164700	-1.30830100
N	0.38885100	-0.40324300	-2.13159000	C	3.89627600	-2.78972700	-2.28767300
N	0.99279600	-1.60398300	0.28930700	C	4.71011100	-2.08190900	-3.17588000
C	-2.88574800	1.50317200	0.28253700	C	4.79960500	-0.69327900	-3.07286900
C	-2.51436400	2.54767900	1.14836900	C	4.07902800	-0.01035700	-2.09004700
C	-3.29447000	3.70080400	1.23176300	C	2.61111300	-0.67287700	1.64810200
C	-4.44161000	3.83667700	0.44523000	C	3.83009300	-1.34479800	1.82640100
C	-4.80791500	2.81024700	-0.42504700	C	4.13112900	-1.98948200	3.02685600
C	-4.03730600	1.64832100	-0.50858200	C	3.20845600	-1.97129700	4.07027900
C	-2.27977300	-1.02482900	1.69350200	C	1.99578900	-1.30064800	3.90730900
C	-1.97372100	-2.39723700	1.71897000	C	1.67583400	-0.64586900	2.70954600
C	-2.23962300	-3.15618600	2.85797600	C	0.37154800	0.12485300	2.66696600
C	-2.80723300	-2.55613000	3.98484600	C	-0.89366000	-1.86930700	1.81825000
C	-3.11533000	-1.19505600	3.96502000	C	-0.58927100	-2.62100200	0.55010300
C	-2.85475000	-0.43026200	2.82660700	C	-0.62988800	-4.01388100	0.51296300
C	-2.61472900	-0.98703800	-1.19733900	C	-0.42713400	-4.67266100	-0.69620600
C	-3.75153700	-1.78056600	-0.97018100	C	-0.18440800	-3.91831600	-1.84418300
C	-4.37578400	-2.45820600	-2.01710300	C	-0.13635000	-2.53530700	-1.74325700
C	-3.86266700	-2.35596000	-3.30858000	C	-1.98133700	0.33287500	2.04393200
C	-2.72765300	-1.57974200	-3.54255900	C	-2.92581900	0.18892100	0.88263600
C	-2.09113400	-0.88437100	-2.50558000	C	-2.33777100	0.09313100	-0.39218500
C	-0.88515800	-0.04551600	-2.86380500	C	-3.16319500	-0.03809600	-1.51215500
C	0.63127700	-1.89119200	-2.11777600	C	-4.55334800	-0.04839100	-1.36636600
C	1.11218700	-2.41284100	-0.78894600	C	-5.12591300	0.05601100	-0.09488700
C	1.60453300	-3.71014100	-0.66122600	C	-4.31258000	0.16759500	1.03682200
C	1.97500600	-4.17921400	0.59638500	H	1.96582900	2.52586400	-1.61820800
C	1.84316500	-3.33627600	1.69936500	H	2.88832400	4.81286800	-1.48871000
C	1.35123400	-2.05225900	1.50997800	H	4.35650000	5.46284700	0.41247800
C	1.52410600	0.29779500	-2.83251500	H	4.90977000	3.79463300	2.17114300
C	2.78230800	0.14802000	-2.02388500	H	4.01720700	1.50136000	2.03483900
C	2.74775600	0.58709200	-0.67782800	H	2.55984400	-2.68174700	-0.61685100
C	3.93201100	0.38705000	0.07259300	H	3.82492100	-3.87110000	-2.35437500
C	5.06270000	-0.21875900	-0.48709300	H	5.27295000	-2.61050300	-3.93920500
C	5.05250400	-0.64366600	-1.81367500	H	5.43502500	-0.13473800	-3.75356700
C	3.90769400	-0.45795700	-2.58622700	H	4.16896100	1.06764600	-2.02134400
H	-1.61497700	2.46045300	1.74624700	H	4.55359500	-1.36671600	1.01917700
H	-3.00018800	4.49602500	1.91001600	H	5.08261900	-2.49920600	3.14104400
H	-5.04311000	4.73836600	0.50939100	H	3.42784900	-2.47098400	5.00846500
H	-5.69501400	2.90671700	-1.04339500	H	1.28558700	-1.27628500	4.72900800
H	-4.34398400	0.86417400	-1.18998700	H	0.53131300	1.17299900	2.40367500
H	-1.54889600	-2.88467300	0.84798200	H	-0.06999500	0.10432200	3.66857900
H	-2.00446200	-4.21590300	2.86194500	H	-0.83004600	-4.56590700	1.42468800
H	-3.01308200	-3.14860200	4.87103100	H	-0.46146900	-5.75581800	-0.74170600
H	-3.56414100	-0.72337000	4.83369300	H	-0.02552200	-4.38591400	-2.80861600
H	-3.10808200	0.62324000	2.82468900	H	0.05804600	-1.90028100	-2.59689300
H	-4.15997500	-1.86367200	0.03045000	H	-2.37917800	-0.06898700	2.98205800
H	-5.25670100	-3.06019000	-1.81903900	H	-1.72607700	1.38210000	2.20916400
H	-4.33625000	-2.88135200	-4.13168200	H	-0.84600700	2.39989900	-2.02572300
H	-2.32410300	-1.51169700	-4.54840800	H	-5.18993400	-0.14889600	-2.23978500
H	-1.05288400	1.01597800	-2.66480800	H	-4.75972300	0.22838500	2.02418800
H	-0.69427500	-0.15513100	-3.93594200	O	-0.38504800	2.15872700	0.28254100
H	1.69065700	-4.33812000	-1.54097800	O	-1.06962000	3.25779200	-1.56697600
H	2.36114300	-5.18637500	0.71146300	C	-0.91344500	4.48380000	0.45279000
H	2.11910300	-3.65855400	2.69647400	H	-1.80230400	5.02055200	0.11597400
H	1.23922000	-1.34633900	2.32140500	H	-0.95465900	4.29906200	1.52513000
H	1.62747100	-0.11709600	-3.84055100	H	-0.03967200	5.10541200	0.22922500
H	1.23475000	1.34742300	-2.93035300	C	-0.77728400	3.19297700	-0.29316600
H	2.21142400	1.84490000	-0.47852100	H	-1.93869200	-2.05415500	2.08017800
H	5.95801400	-0.34103200	0.11101400	H	-0.28696500	-2.26145700	2.63681400
H	3.88953400	-0.78670200	-3.62145900	C	-6.61921800	0.10047000	0.05107600
O	-0.10860800	2.23123100	-0.78784100	F	-7.24731500	-0.64888400	-0.88467800
O	1.95814900	3.06240200	-0.54842700	F	-7.02960100	-0.34336900	1.26205500
C	0.18429600	4.56957000	-1.11609300	F	-7.10343500	1.36229400	-0.08053200
H	-0.05571100	4.60564100	-2.18362400	H	-2.73144900	-0.12718600	-2.50387000
H	-0.73889200	4.74645000	-0.56026100	XIX (LH3, C-2)			
H	0.92338700	5.33697200	-0.88829700	Rh	0.64282100	0.14658600	-0.08284100
C	0.71889600	3.20176900	-0.78557800	P	-1.88150500	0.15568100	0.13589700
H	1.33985100	-2.15516100	-2.90725100	Cl	0.64962700	0.63553600	2.31781200
H	-0.30737800	-2.39461300	-2.35750300	N	0.54398500	-0.23268600	-2.14844700
C	4.05637700	0.85531100	1.50434400	N	0.68030100	-1.88411500	0.04235100
F	5.35219200	0.98146700	1.88396700	C	-2.62108100	1.83905900	0.04540400
F	3.49553800	-0.01753600	2.37767300	C	-2.13369500	2.84112500	0.90411400
F	3.47997100	2.05691400	1.70306100	C	-2.67503000	4.12626100	0.86680300
H	5.93345700	-1.11139000	-2.24115300	C	-3.69444300	4.43245700	-0.03912700
XIX (LH3, C-4)				C	-4.17607700	3.44610300	-0.90091700
Rh	-0.29184800	0.11400400	-0.30151400	C	-3.64676100	2.15382800	-0.85896300

C	-2.62228800	-0.62509400	1.63211700
C	-2.53993500	-2.01913700	1.79972900
C	-3.03599500	-2.62584900	2.95353300
C	-3.61722000	-1.85138000	3.96026400
C	-3.70739400	-0.46806600	3.80075000
C	-3.21509800	0.14306900	2.64553700
C	-2.60586000	-0.76291700	-1.28473000
C	-3.77696300	-1.52392600	-1.15462900
C	-4.29789500	-2.23281200	-2.23850700
C	-3.65118000	-2.18786000	-3.47164800
C	-2.49318900	-1.42280800	-3.61600300
C	-1.95594700	-0.70628600	-2.53881600
C	-0.75648400	0.17615400	-2.80136500
C	0.86318300	-1.68705000	-2.38125100
C	0.69382200	-2.53015600	-1.14810400
C	0.64993800	-3.92062900	-1.21047200
C	0.62236900	-4.65665900	-0.02835800
C	0.63428800	-3.97951000	1.19041700
C	0.65440200	-2.59116900	1.19030100
C	1.62834500	0.61961700	-2.75048100
C	2.87039200	0.48576100	-1.91456100
C	2.71294200	0.19775100	-0.53910600
C	3.90623000	0.01872400	0.19542400
C	5.16430700	0.18867700	-0.40866700
C	5.27901300	0.50646900	-1.75678200
C	4.12221400	0.63589400	-2.51843900
H	-1.33892000	2.61215200	1.60702200
H	-2.29757700	4.88757000	1.54281600
H	-4.11025500	5.43492900	-0.07190700
H	-4.96862000	3.67685200	-1.60630900
H	-4.03890700	1.39659800	-1.52910200
H	-2.11391000	-2.64231100	1.02190500
H	-2.96956700	-3.70415400	3.06166800
H	-4.00198600	-2.32415800	4.85874700
H	-4.16570900	0.14224200	4.57306100
H	-3.30254200	1.21776100	2.53879600
H	-4.29095900	-1.56488400	-0.20145300
H	-5.20738500	-2.81222000	-2.11481900
H	-4.04627000	-2.73640000	-4.32074300
H	-2.00416200	-1.37023800	-4.58464000
H	-0.93908500	1.20495900	-2.48050200
H	-0.57533400	0.20038400	-3.88102200
H	0.65019700	-4.41156800	-2.17716600
H	0.59432600	-5.74054900	-0.05945900
H	0.61684100	-4.50981800	2.13520900
H	0.64944000	-2.01156700	2.10272400
H	1.78826800	0.31720900	-3.79174100
H	1.25581400	1.64593500	-2.75269900
H	1.64993900	2.26021200	1.60563000
H	6.05863900	0.05537600	0.18810300
H	4.18659800	0.84720100	-3.58271700
O	0.61886800	2.22647800	-0.52392100
O	1.82832800	3.13263600	1.15457500
C	1.22094400	4.53563600	-0.65380900
H	2.18226800	5.02636500	-0.49175200
H	1.00768900	4.44015900	-1.71749000
H	0.44411800	5.15245500	-0.18890600
C	1.20964900	3.19063700	0.00316000
H	1.91155100	-1.75312600	-2.68443600
H	0.26249000	-2.07596000	-3.20603800
C	3.94363100	-0.32259100	1.66467800
F	5.15624000	-0.79656500	2.04788800
F	3.05098000	-1.27663800	2.01133500
F	3.70842000	0.75999600	2.44919400
H	6.25785000	0.62652600	-2.20952100

CH₃COOH

C	-1.39577900	-0.11140400	0.00000700
H	-1.68180100	-0.69242700	-0.88158800
H	-1.91822500	0.84420700	0.00005100
H	-1.68174500	-0.69247400	0.88158900
C	0.09210500	0.12129100	-0.00004100
O	0.64301500	1.20441600	0.00001100
O	0.77928400	-1.04227200	0.00000600
H	1.72542600	-0.81577900	0.00002300

CH₃COO⁻

C	1.35286200	-0.00003000	-0.00426000
H	1.75739400	0.89433500	-0.48889300
H	1.75737800	-0.89457800	-0.48856600
H	1.71214300	0.00016800	1.03353100
C	-0.20015900	0.00000000	-0.01235600
O	-0.75897700	-1.13120200	0.00273900
O	-0.75891500	1.13123300	0.00271400

4- Energies (kcal·mol⁻¹) from relaxed PSE calculations on 1a, 1b-^{2,5}B, 4a, 4b-^{2,5}B (ethanol, 298 K)

1a	
d_{MCl}	ΔE
2.4	0.0
2.9	8.9
3.4	16.7
3.9	17.0
4.4	16.7
4.9	16.5
5.4	16.5
5.9	16.9
6.4	17.8
6.9	17.1
7.9	17.7
8.9	18.0
11.9	18.4
14.9	18.5
19.9	18.8
BDE	20.0

1b-^{2,5}B	
d_{MCl}	ΔE
2.5	0.0
3.0	5.4
3.5	9.3
4.0	9.2
4.5	9.3
5.0	9.4
5.5	9.8
6.0	10.2
6.5	11.0
7.0	10.8
8.0	11.1
9.0	11.3
12.0	11.6
15.0	11.8
20.0	12.1
BDE	11.0

4a	
d_{MCl}	ΔE
2.4	0.0
2.9	10.9
3.4	19.8
3.9	19.7
4.4	19.5
4.9	19.7
5.4	19.6
5.9	20.3
6.4	20.4
6.9	20.4
7.9	21.1
8.9	21.4
11.9	21.8
14.9	21.8
19.9	22.2
BDE	23.3

4b-^{2,5}B	
d_{MCl}	ΔE
2.5	0.0
3.0	7.0
3.5	11.4
4.0	10.4
4.5	10.6
5.0	10.9
5.5	11.4
6.0	11.6
6.5	12.1
7.0	11.4
8.0	12.2
9.0	12.4
12.0	13.0
15.0	13.2
20.0	13.5
BDE	12.4

5- References.

- S1 (a) E. C. Volpe, P. T. Wolczanski and E. B. Lobkovsky, *Organometallics* 2010, **29**, 364-377. (b) R. M. Ceder, G. Muller, M. Ordinas and J. I. Ordinas, *Dalton Trans.* 2007, 83-90. (c) T. V. Laine, U. Piironen, K. Lappalainen, K. Klinga, E Aitola and M. Leskelä, *J. Organomet. Chem.* 2000, **606**, 112-124.
- S2 R. O. Hutchins, A. B. Hutchins In *Comprehensive Organic Chemistry*, B. M. Trost and I. Fleming, Eds.; Pergamon: Oxford, 1991; Vol. 8, Chapter 1.2.
- S3 A. F. Abdel-Magid and S. J. Mehrman, *Org. Process Res. Dev.* 2006, **10**, 971-1031.