Electronic supplementary information

for

Syntheses and structures of cationic osmium bis(σ-B–H) borane complexes

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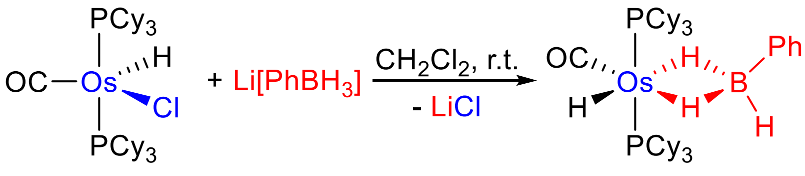
Contents

General information

X-ray diffraction: Single-crystal X-ray diffraction data were collected on a Bruker D8 Venture diffractometer equipped with a Photon 100 CMOS detector using Mo Kα radiation (λ = 0.71073 Å). All of the data were corrected for absorption effects using the multi-scan technique. Final unit cell parameters were based on all observed reflections from integration of all frame data. The structures were solved with the ShelXT structure solution program using Intrinsic Phasing and refined with the ShelXL refinement package using Least Squares minimization that implanted in Olex2. For all compounds, all non-H atoms were refined anisotropically unless otherwise stated, and hydrogen atoms were introduced at their geometric positions and refined as riding atoms unless otherwise stated. For **2a** and **2e** the Cy groups and NTf^- counter anions were found disordered over two positions, and several restraints were used in order to improve refinement stability. For **2a**, the distance between Os and terminal H is kept during refinement at the value of 1.576 Å using DFIX restraint. For **2e**, the distance between Os and terminal H is kept during refinement at the value of 1.585 Å using DFIX restraint. CCDC 2434259 (**2e**) and 2434260 (**2a**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/structures/.

NMR spectra of 1a



Scheme S1

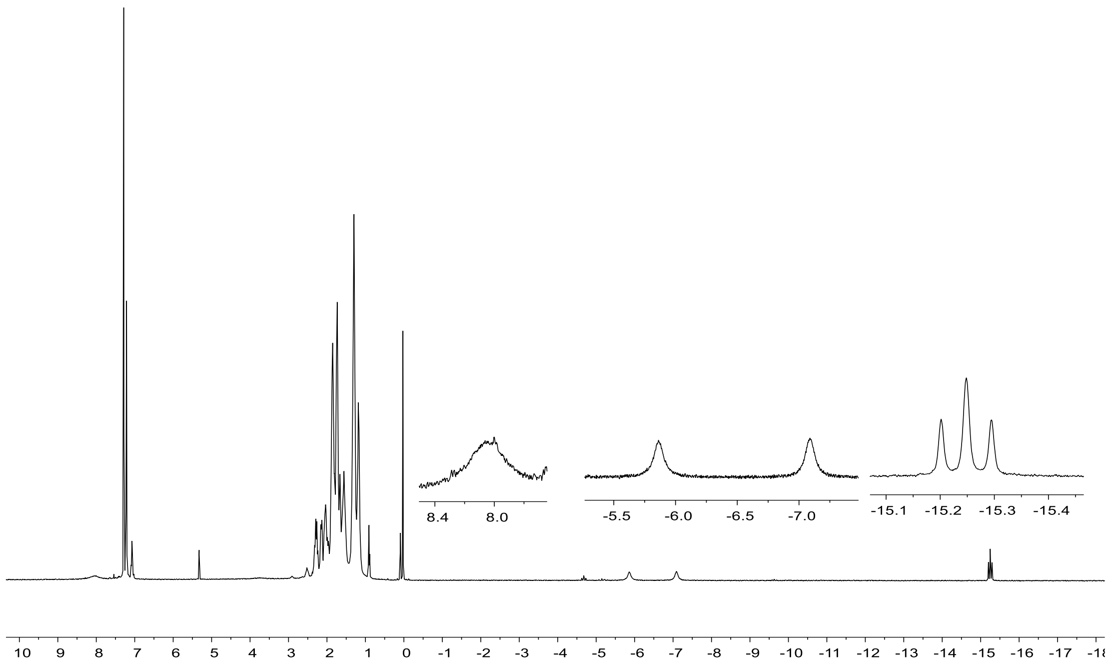


Fig. S1 ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) spectrum of **1a**.

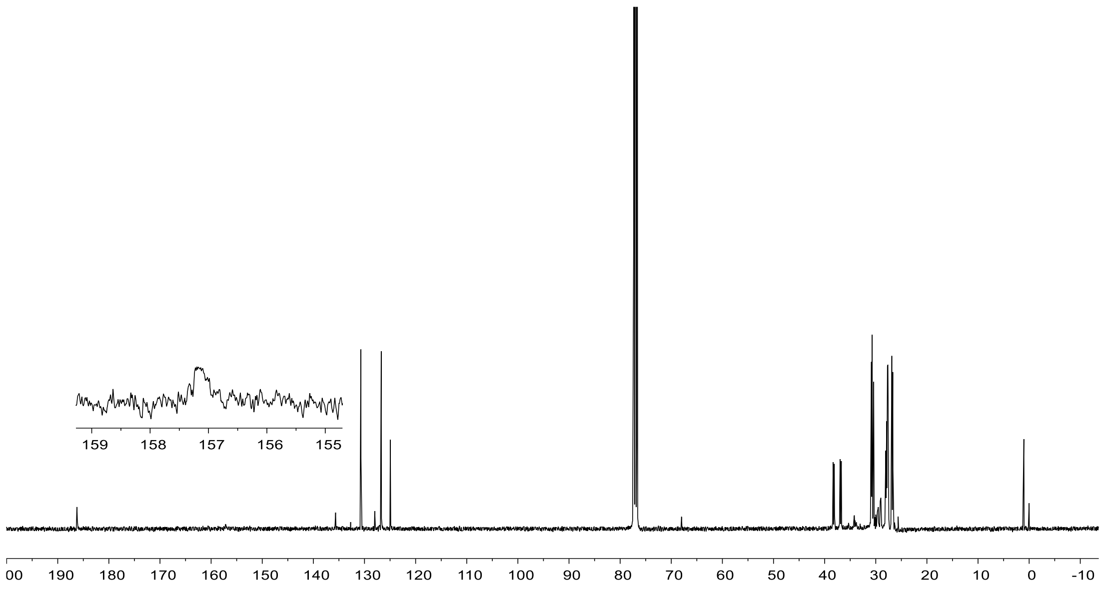


Fig. S2. $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$) spectrum of **1a**.

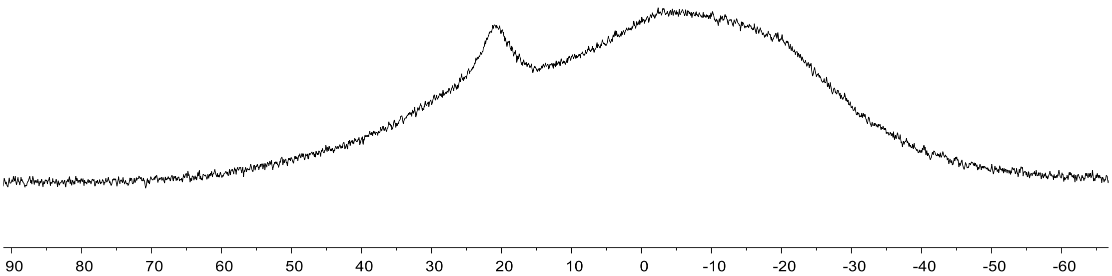


Fig. S3 $^{11}B\{^1H\}$ NMR (128 MHz, 298 K, $CDCl_3$) spectrum of **1a**.

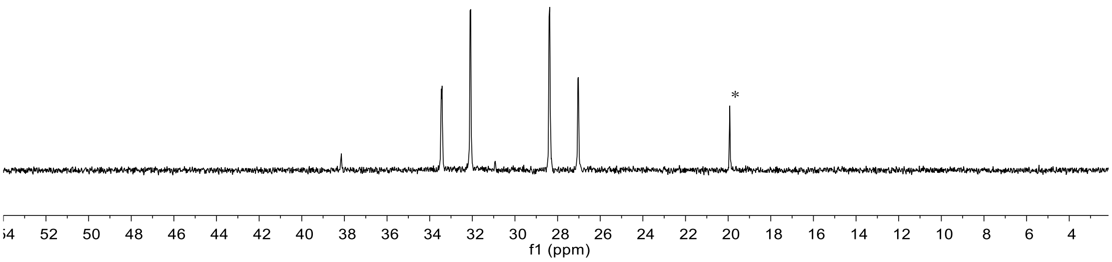
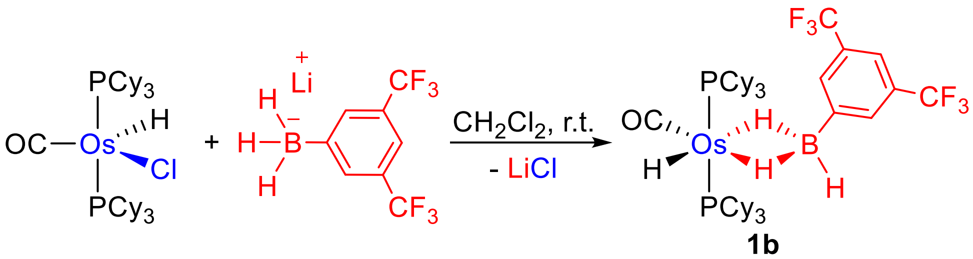


Fig. S4 $^{31}P\{^1H\}$ NMR (162 MHz, 298 K, $CDCl_3$) spectrum of **1a** (* unidentified species). [Comment: The unidentified species was formed during the synthesis of $OsHCl(CO)(PCy_3)_2$, which might be one of the oxidation products of PCy_3.]

NMR spectra of 1b



Scheme S2

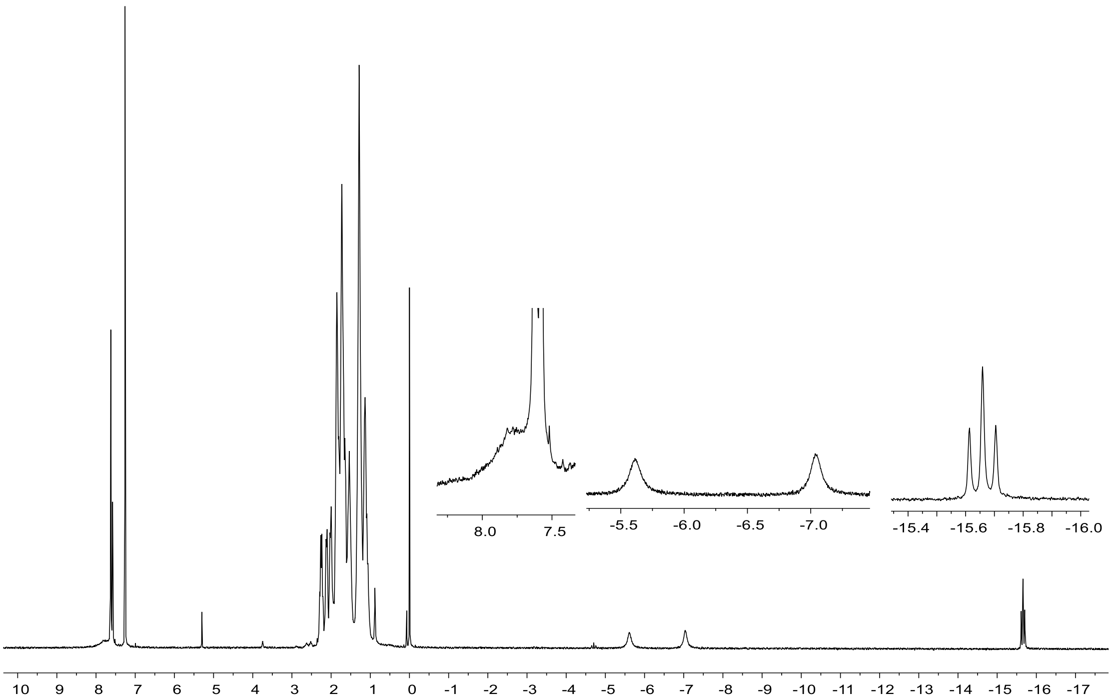


Fig. S5 ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) spectrum of **1b**.

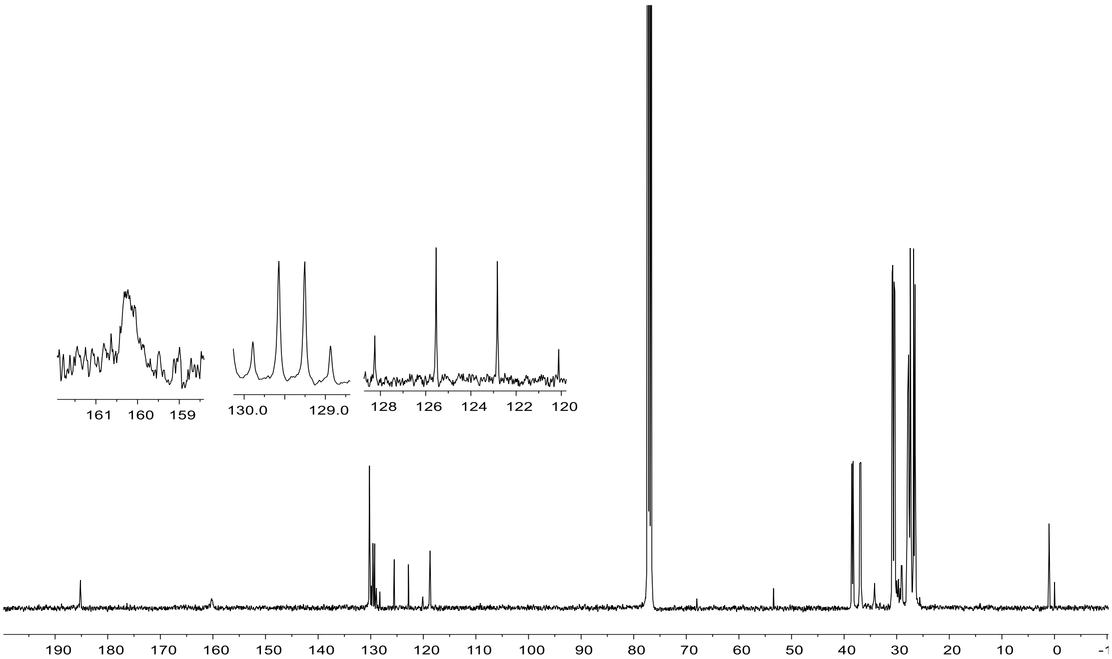


Fig. S6 $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$) spectrum of **1b**.

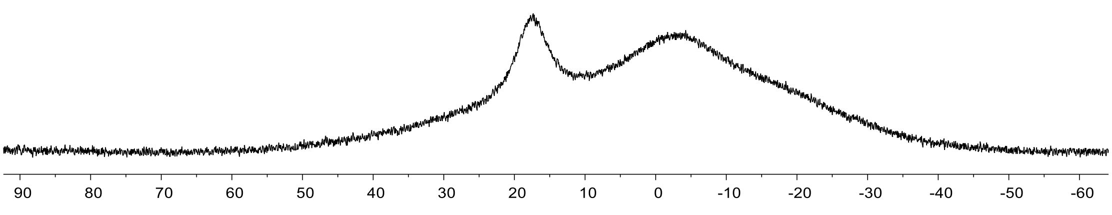


Fig. S7 $^{11}B\{^{1}H\}$ NMR (128 MHz, 298 K, $CDCl_3$) spectrum of **1b**.

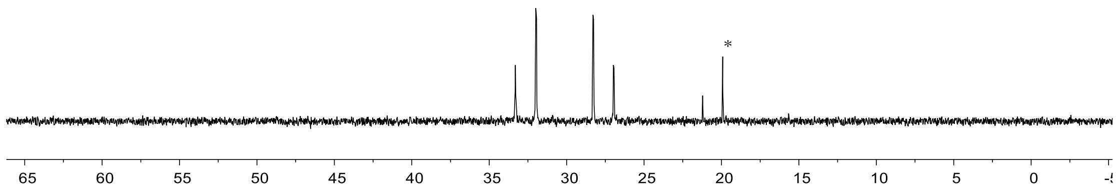


Fig. S8 $^{31}P\{^1H\}$ NMR (162 MHz, 298 K, $CDCl_3$) spectrum of **1b** (* unidentified species). [Comment: The unidentified species was formed during the synthesis of $OsHCl(CO)(PCy_3)_2$, which might be one of the oxidation products of PCy_3.]

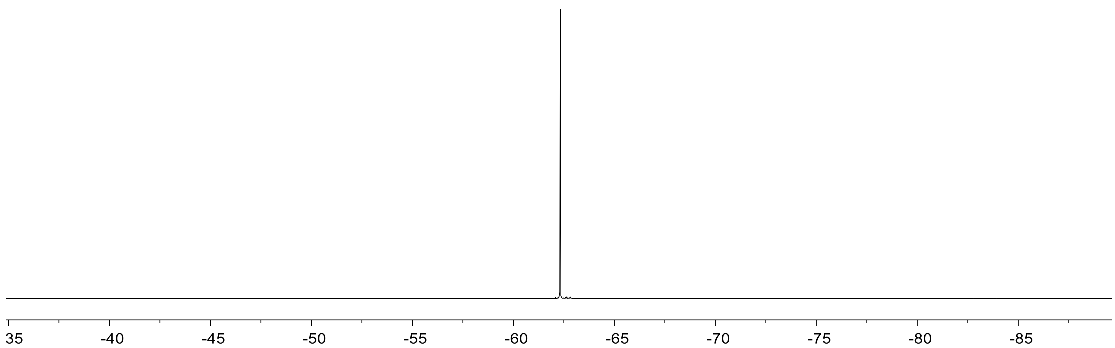
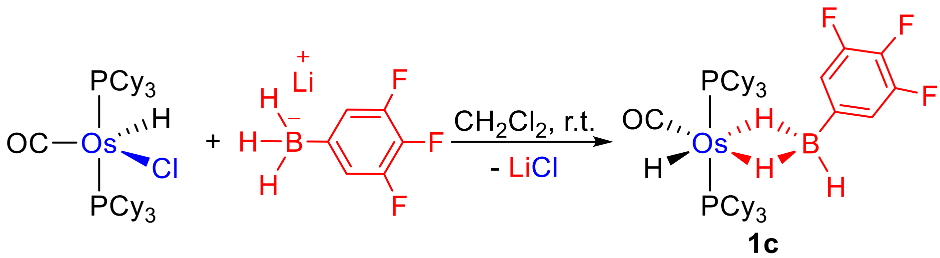


Fig. S9 $^{19}F\{^1H\}$ NMR (377 MHz, 298 K, $CDCl_3$) spectrum of **1b**.

NMR spectra of 1c



Scheme S3

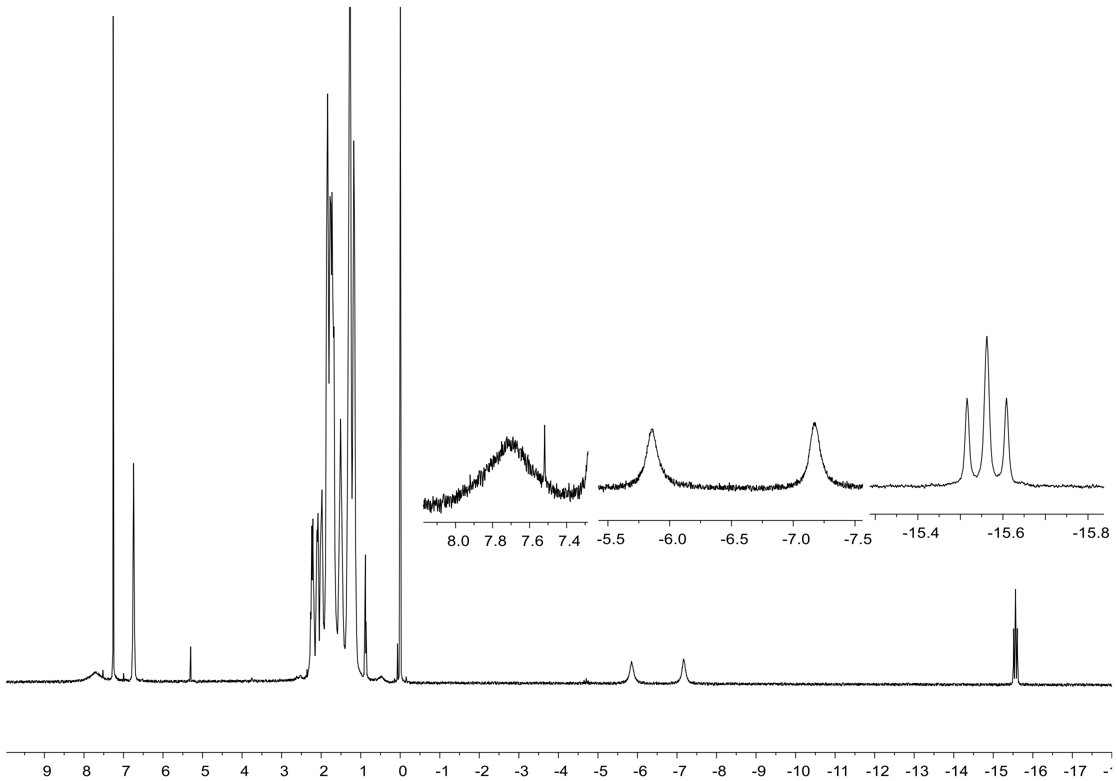


Fig. S10 ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) spectrum of **1c**.

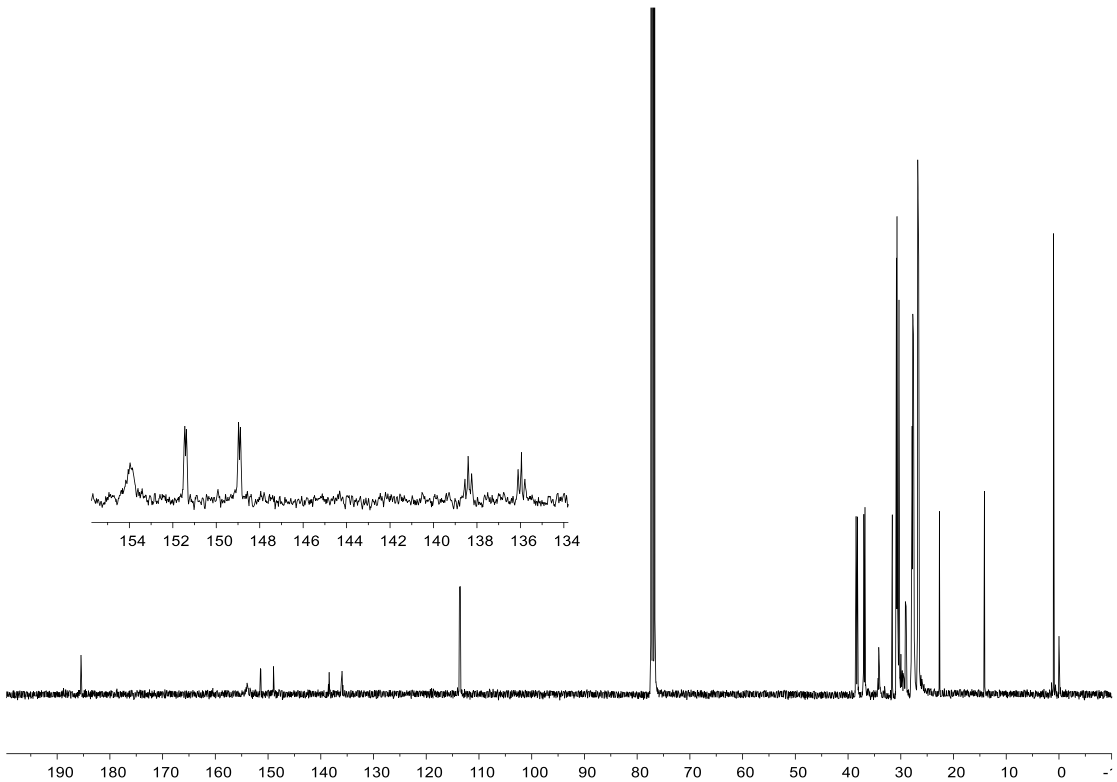


Fig. S11 $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$) spectrum of **1c** .

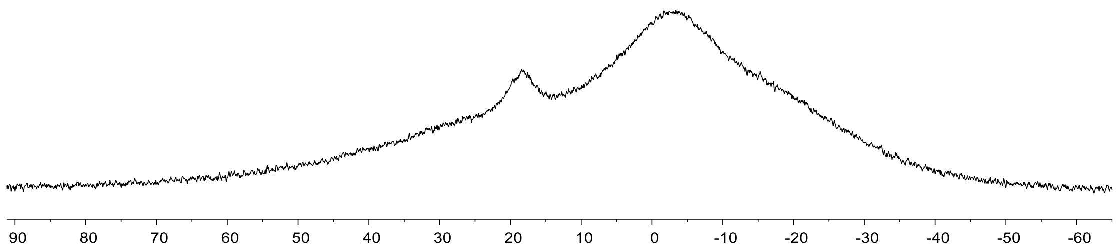


Fig. S12 $^{11}B\{^1H\}$ NMR (128 MHz, 298 K, $CDCl_3$) spectrum of **1c**.

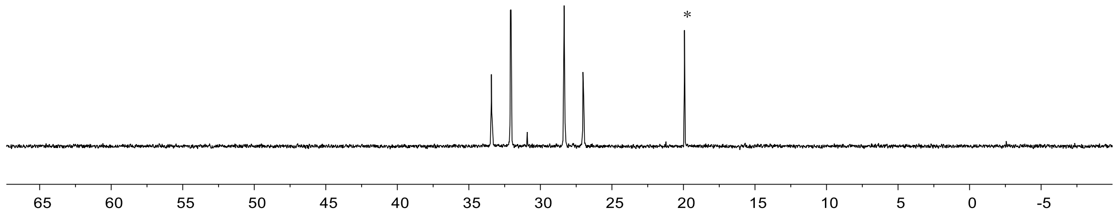


Fig. S13 $^{31}P\{^1H\}$ NMR (162 MHz, 298 K, $CDCl_3$) spectrum of 1c (* unidentified species). [Comment: The unidentified species was formed during the synthesis of $OsHCl(CO)(PCy_3)_2$, which might be one of the oxidation products of PCy_3.]

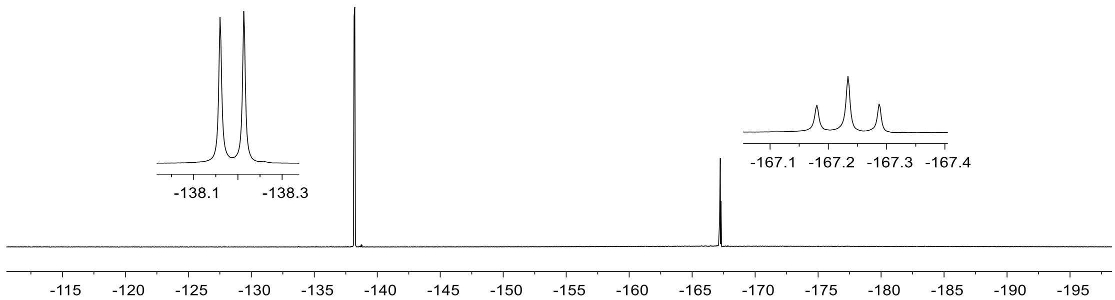
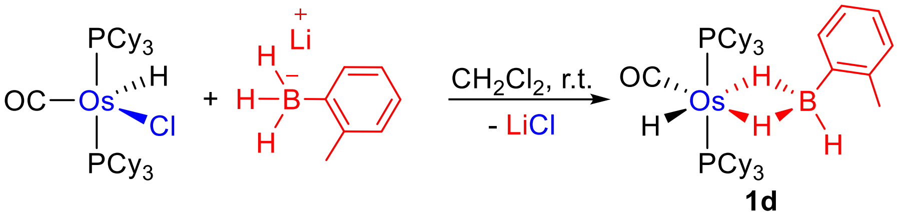


Fig. S14 $^{19}F\{^1H\}$ NMR (377 MHz, 298 K, $CDCl_3$) spectrum of **1c**.

NMR spectra of 1d



Scheme S4

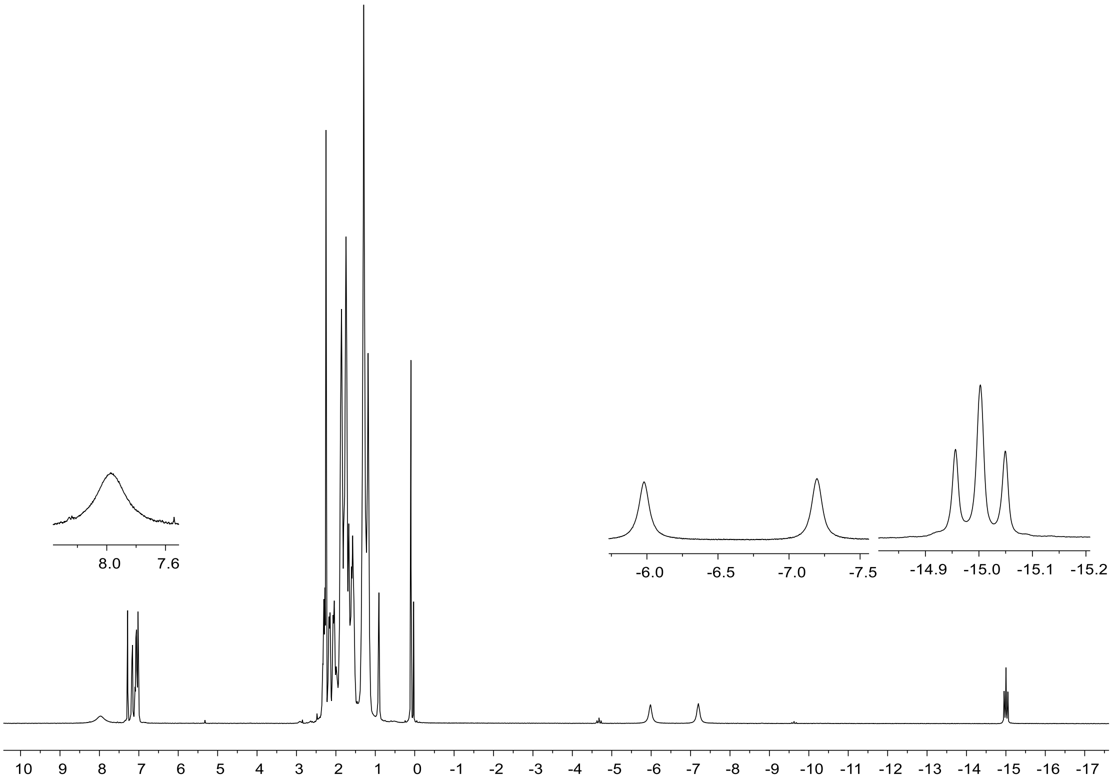


Fig. S15 ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) spectrum of **1d**.

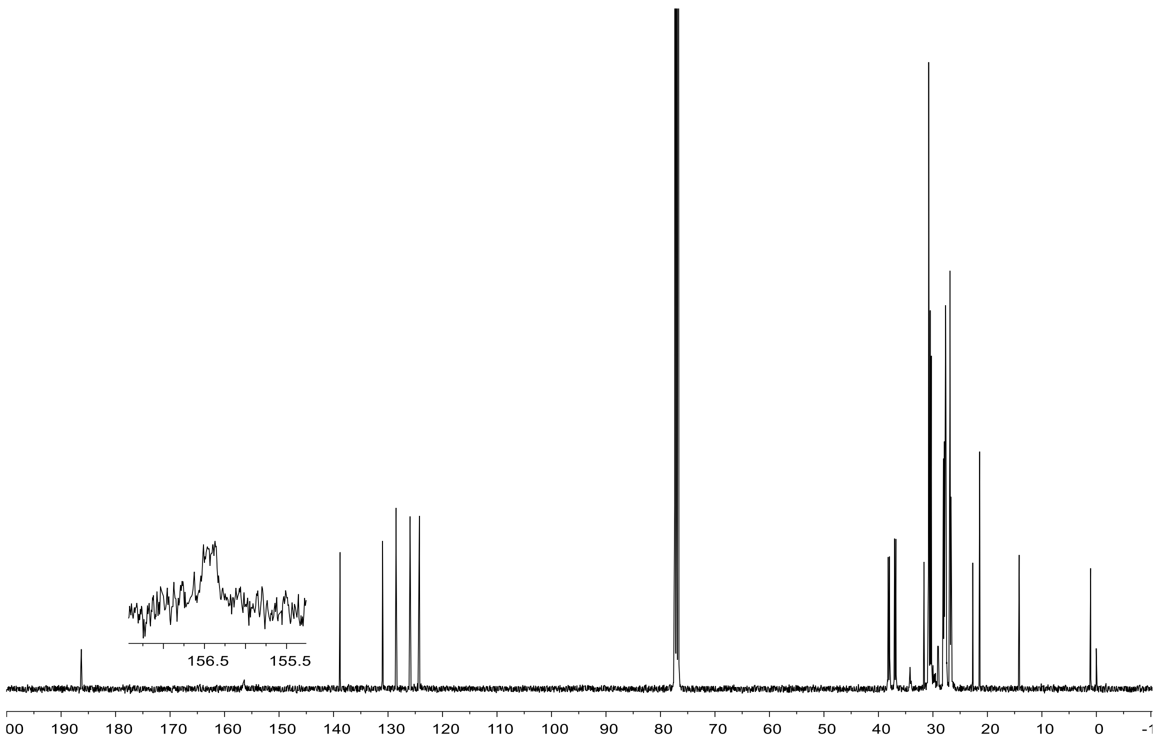


Fig. S16 $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$) spectrum of **1d**.

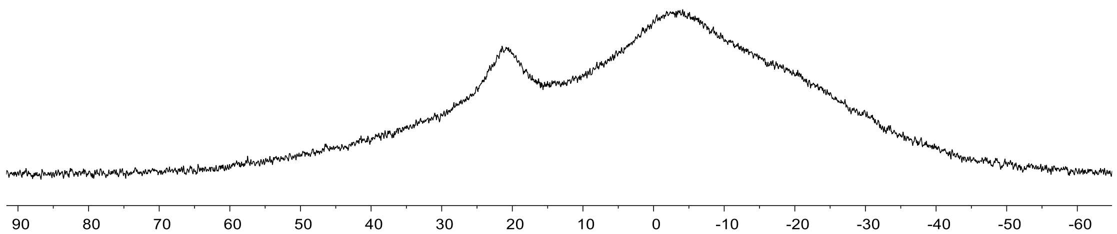


Fig. S17 $^{11}B\{^{1}H\}$ NMR (128 MHz, 298 K, $CDCl_3$) spectrum of **1d**.

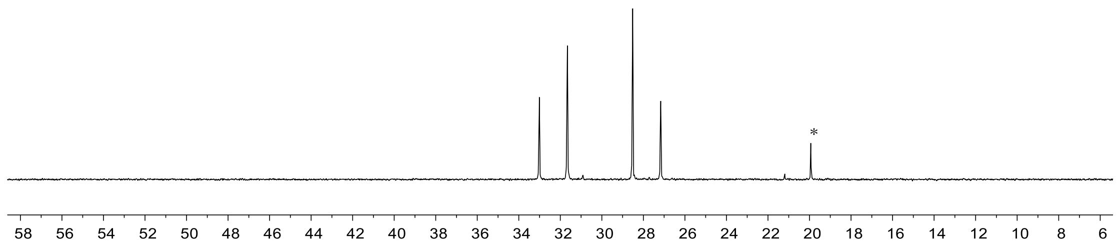
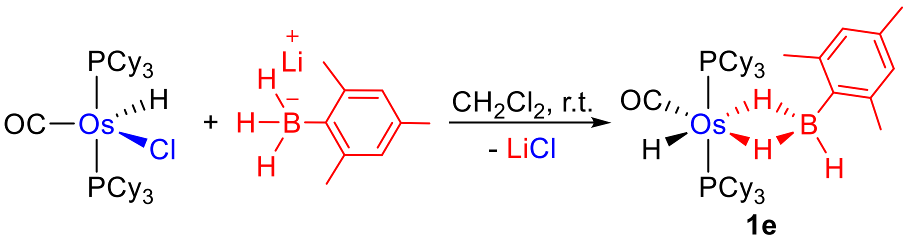


Fig. S18 $^{31}P\{^{1}H\}$ NMR (162 MHz, 298 K, $CDCl_3$) spectrum of **1d** (* unidentified species). [Comment: The unidentified species was formed during the synthesis of $OsHCl(CO)(PCy_3)_2$, which might be one of the oxidation products of PCy_3.]

NMR spectra of 1e



Scheme S5

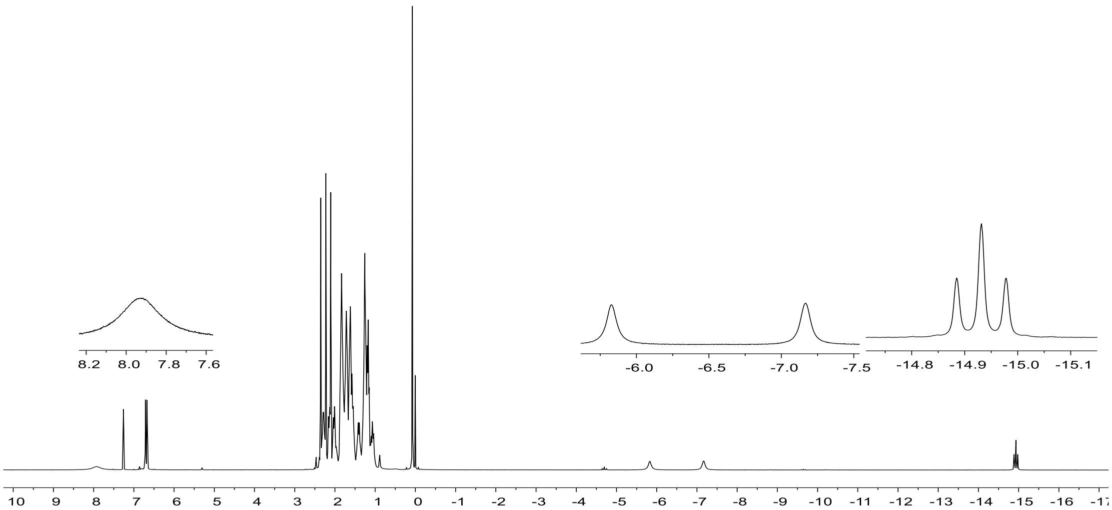


Fig. S19 ^1H NMR (400 MHz, 298 K, $CDCl_3$) spectrum of **1e**.

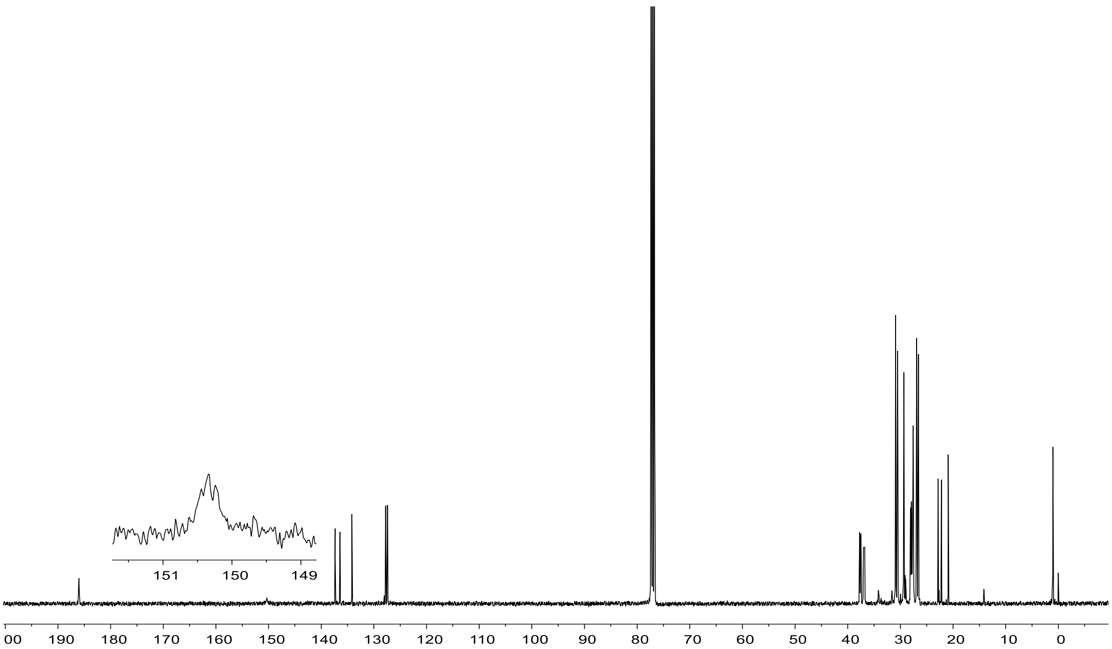


Fig. S20 $^{13}C\{^1H\}$ NMR (101 MHz, 298 K, $CDCl_3$) spectrum of **1e**.

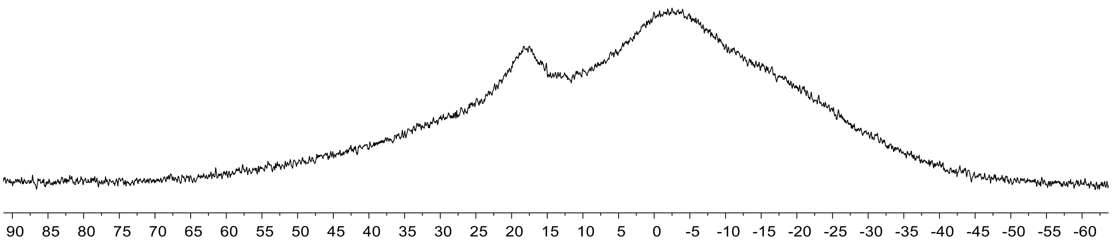


Fig. S21 $^{11}B\{^1H\}$ NMR (128 MHz, 298 K, $CDCl_3$) spectrum of **1e**.

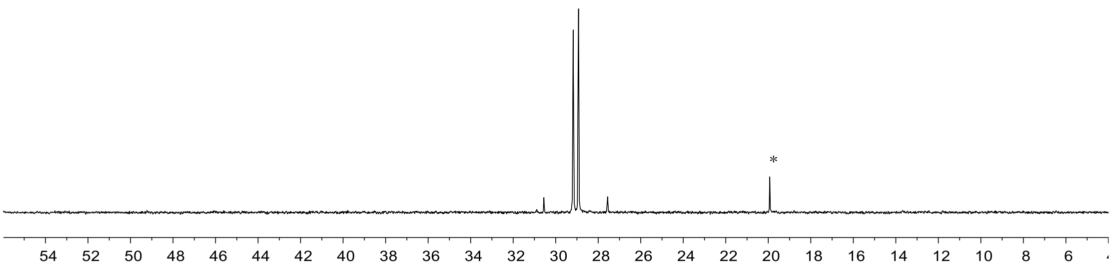
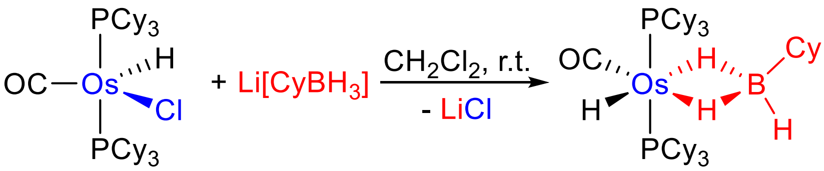


Fig. S22 $^{31}P\{^1H\}$ NMR (162 MHz, 298 K, $CDCl_3$) spectrum of **1e** (* unidentified species). [Comment: The unidentified species was formed during the synthesis of $OsHCl(CO)(PCy_3)_2$, which might be one of the oxidation products of PCy_3.]

NMR spectra of 1f



1f

Scheme S6

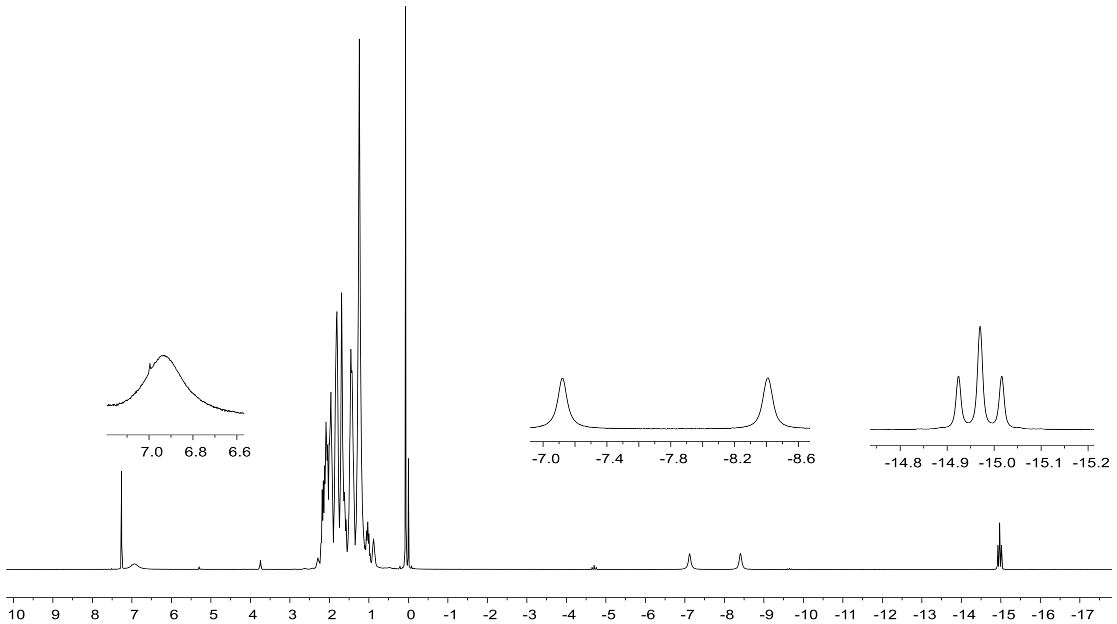


Fig. S23 ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) spectrum of **1f**.

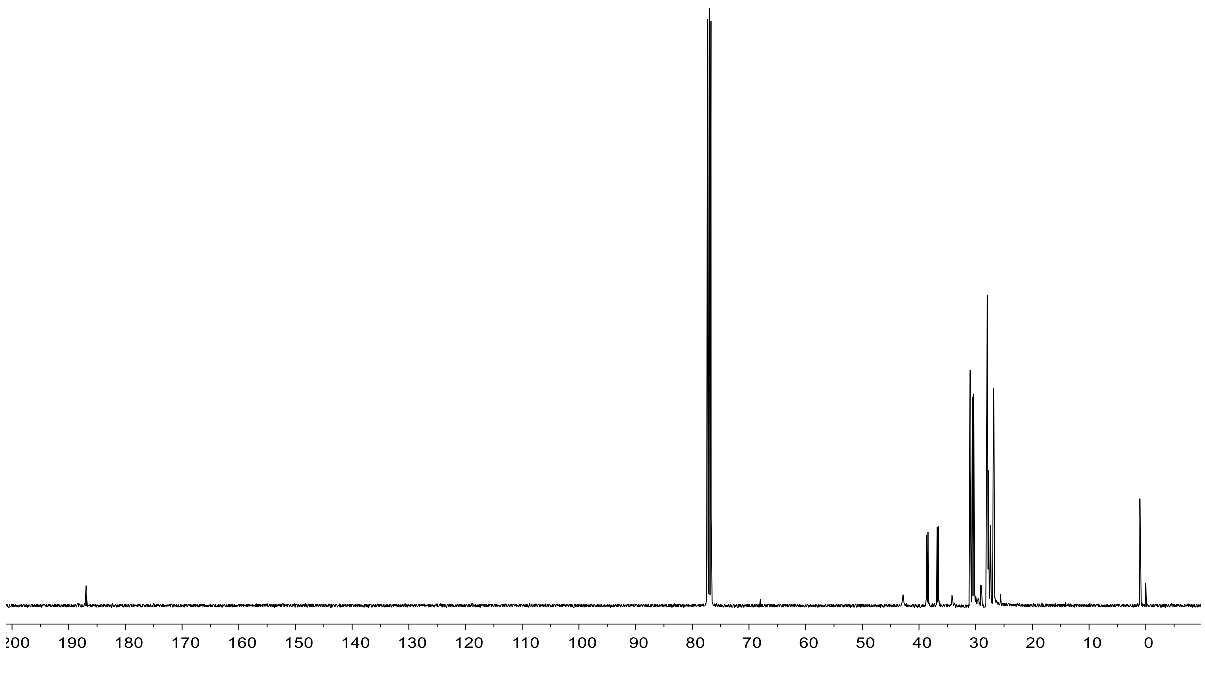


Fig. S24 $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$) spectrum of **1f**.

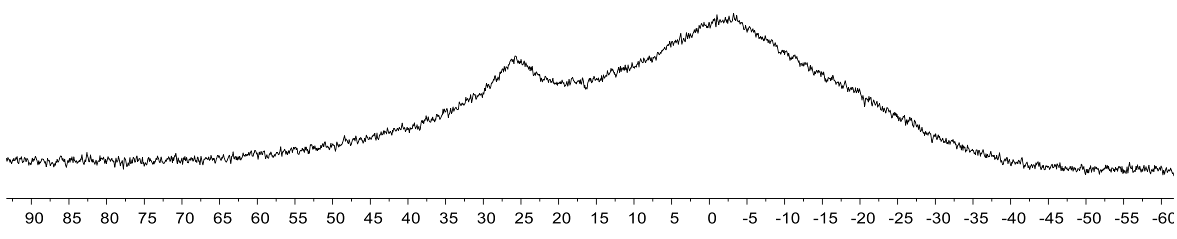


Fig. S25 $^{11}B\{^{1}H\}$ NMR (128 MHz, 298 K, $CDCl_3$) spectrum of **1f**.

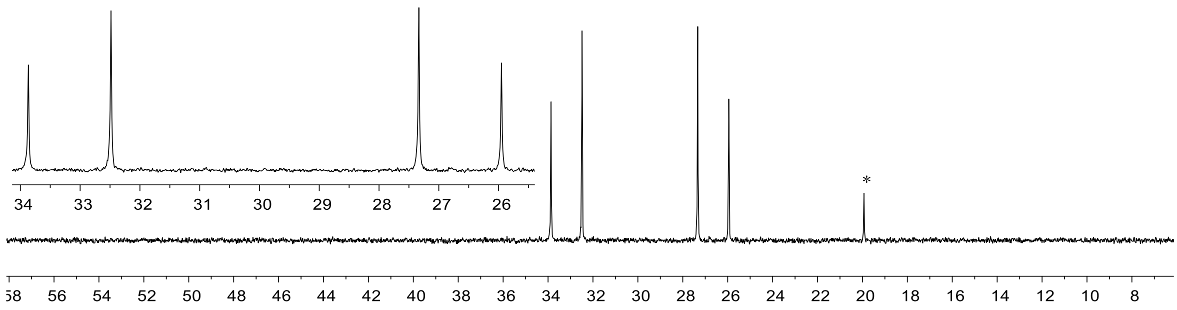
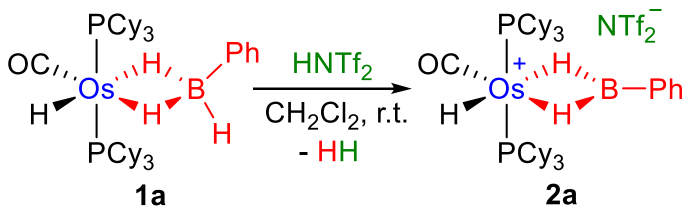


Fig. S26 $^{31}P\{^1H\}$ NMR (162 MHz, 298 K, $CDCl_3$) spectrum of **1f** (* unidentified species). [Comment: The unidentified species was formed during the synthesis of $OsHCl(CO)(PCy_3)_2$, which might be one of the oxidation products of PCy_3.]

NMR spectra and crystallographic data of 2a



Scheme S7

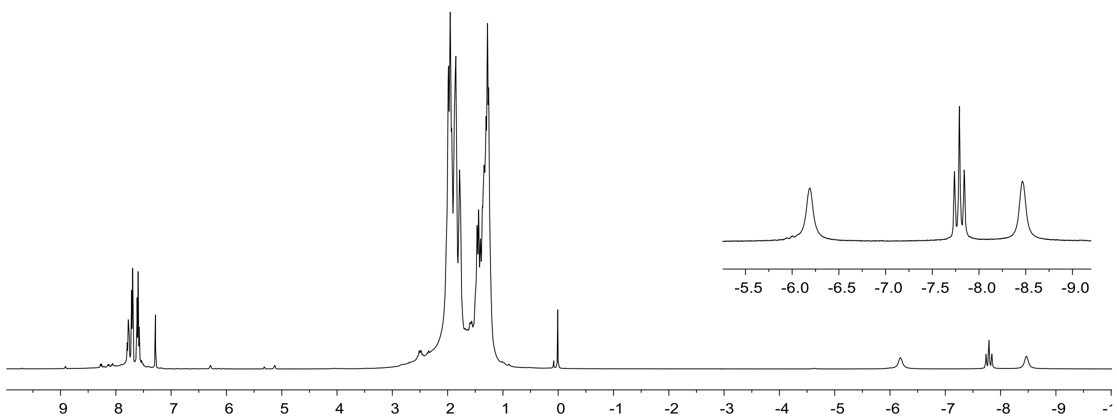


Fig. S27 ^1H NMR (400 MHz, 298 K, $CDCl_3$) spectrum of **2a**.

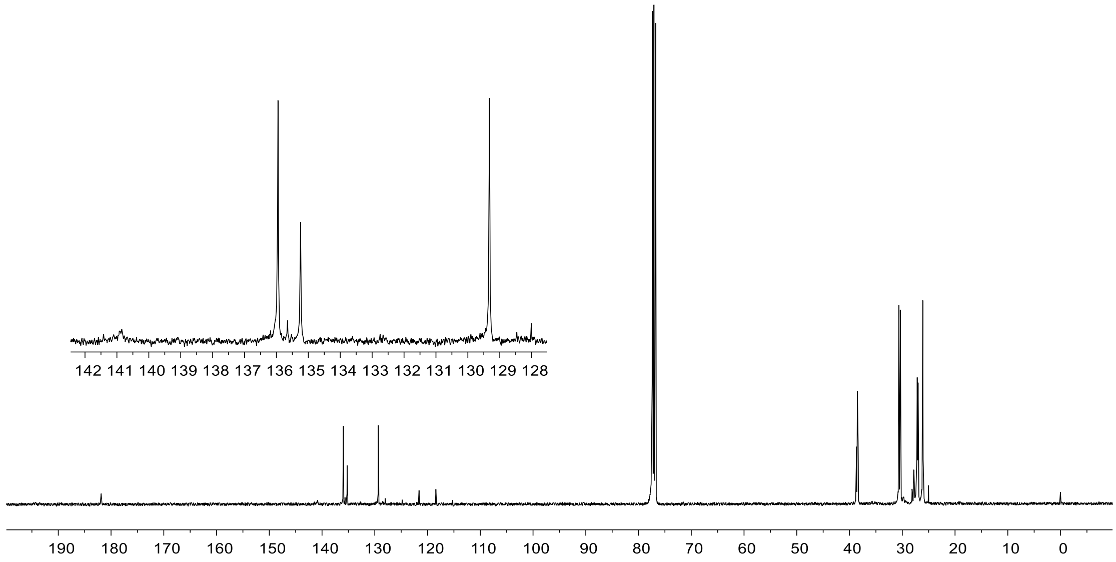


Fig. S28 $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$) spectrum of **2a**.

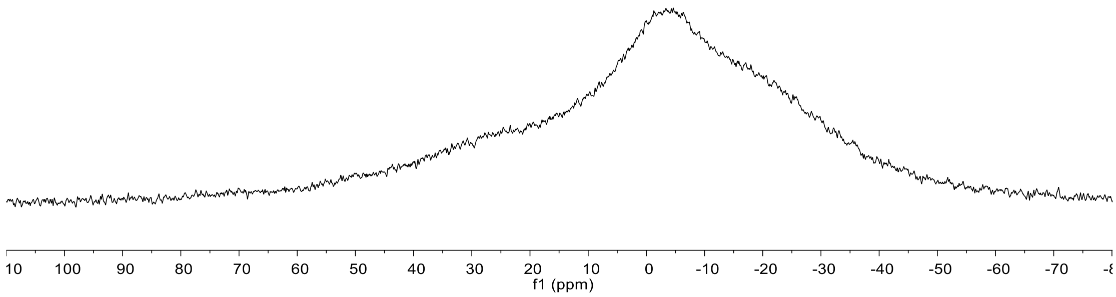


Fig. S29 $^{11}B\{^{1}H\}$ NMR (128 MHz, 298 K, $CDCl_3$) spectrum of **2a**.

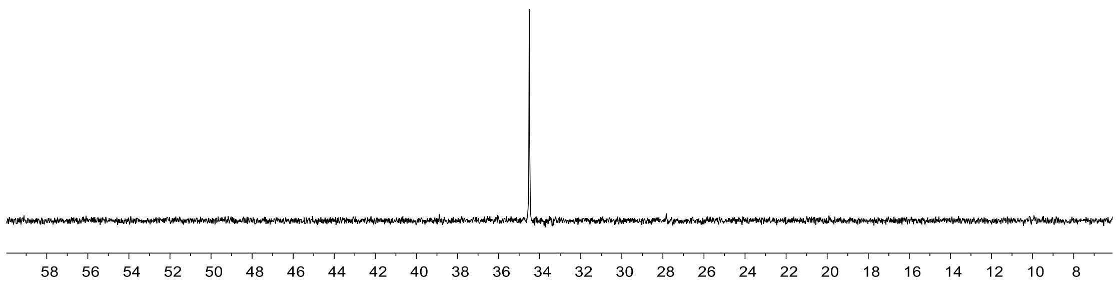


Fig. S30 $^{31}P\{^{1}H\}$ NMR (162 MHz, 298 K, $CDCl_3$) spectrum of **2a**.

X-ray crystal structure analysis of complex 2a: formula $C_{46}H_{76}BCl_2F_6NO_5OsP_2S_2$, M = 1235.04 g/mol, dull light orange crystal, 0.18 × 0.13 × 0.1 mm, a = 16.850(4), b = 18.960(5), c = 16.990(4) Å, α =

90, β = 94.936(7), γ = 90°, V = 5408(2) Å^3, ρ_{calc} = 1.517 g·cm^{-3}, μ = 2.657 mm^{-1}, empirical absorption correction (0.5202 ≤ T ≤ 0.7463), Z = 4, monoclinic, space group $P2_1/n$, λ = 0.71073 Å, T = 120 K, ω and φ scans, 98977 reflections collected (±h, ±k, ±l), 9513 independent (R_{int} = 0.0900) and 8174 observed reflections [I>2σ(I)], 692 refined parameters, R = 0.0364, wR^2 = 0.0963, max. (min.) residual electron density 1.58 (-1.23) e.Å^{-3}.

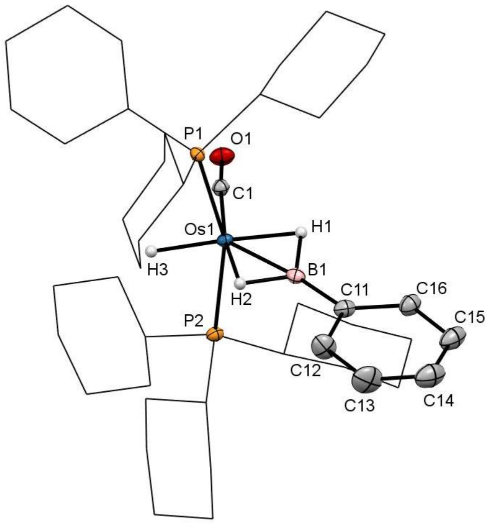
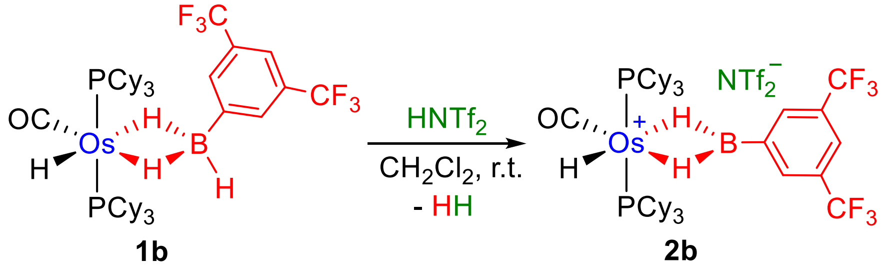


Fig. S31 Molecular structure of **2a** (thermal ellipsoids are shown at the 30% probability level).

NMR spectra of 2b



Scheme S8

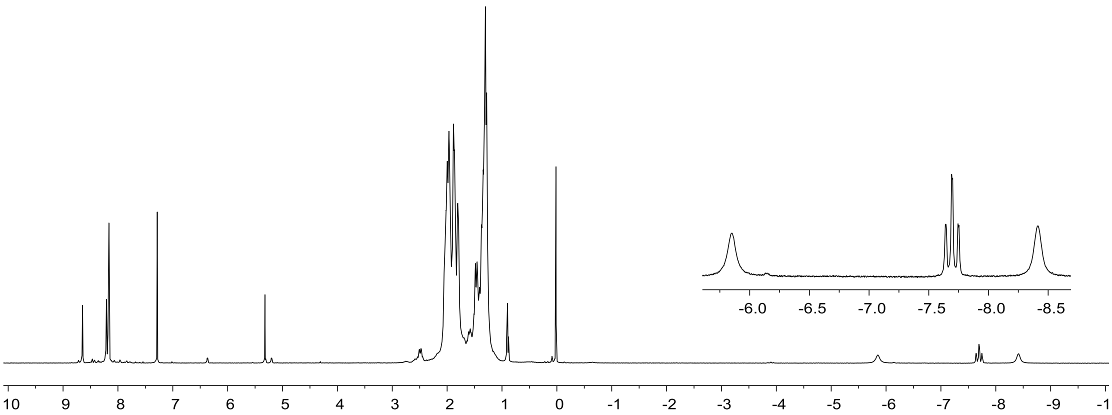


Fig. S32 ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) spectrum of **2b**.

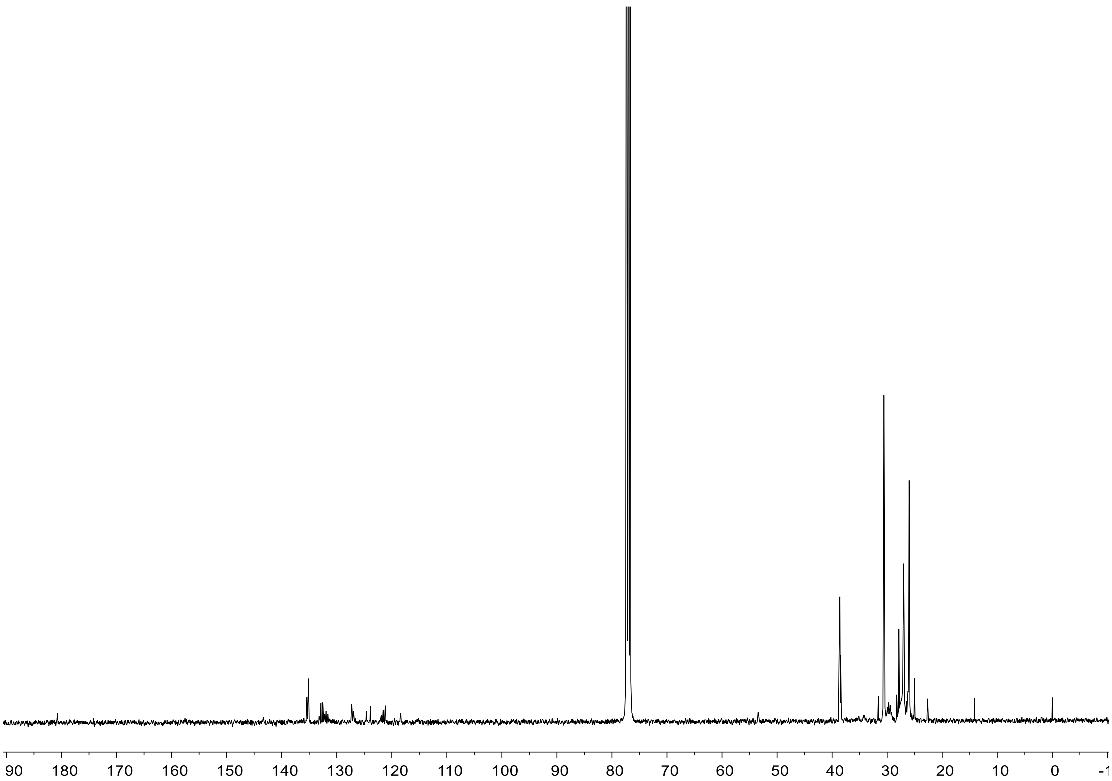


Fig. S33 $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$) spectrum of **2b**.

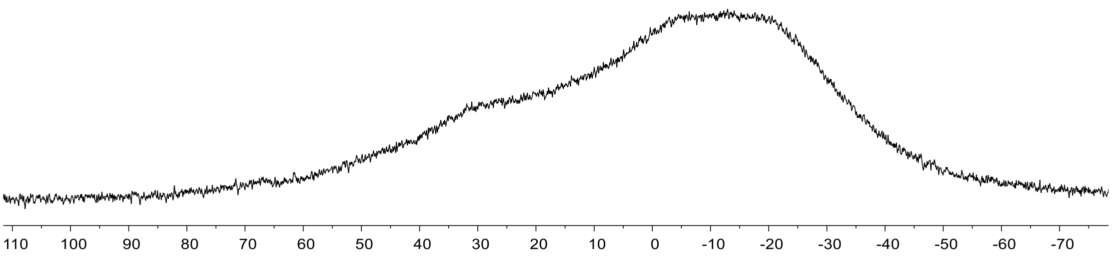


Fig. S34 $^{11}B\{^{1}H\}$ NMR (128 MHz, 298 K, $CDCl_3$) spectrum of **2b**.

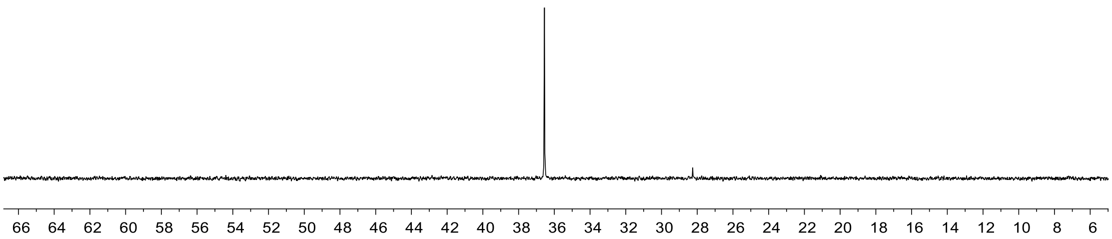


Fig. S35 $^{31}P\{^{1}H\}$ NMR (162 MHz, 298 K, $CDCl_3$) spectrum of **2b**.

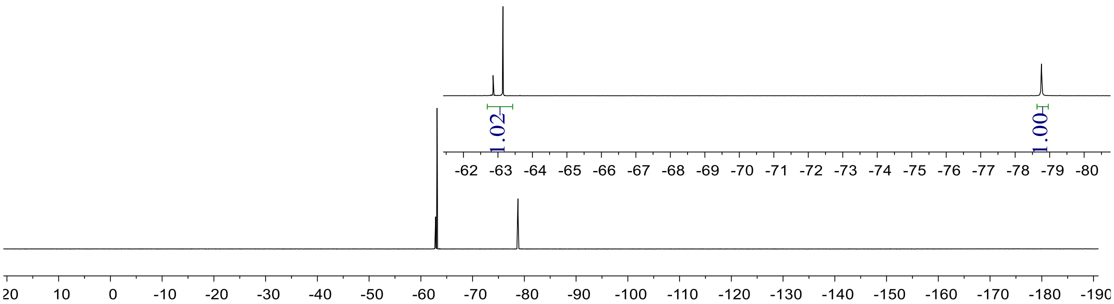
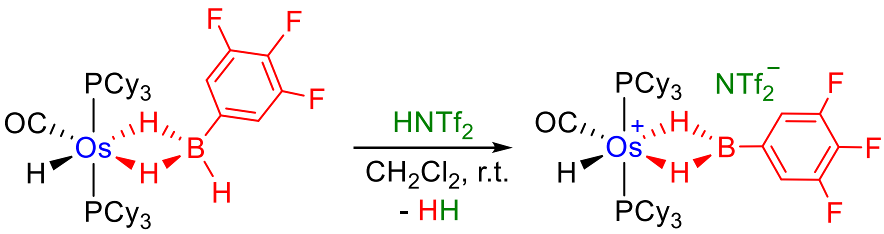


Fig. S36 $^{19}F\{^{1}H\}$ NMR (377 MHz, 298 K, $CDCl_3$) spectrum of **2b**.

NMR spectra of 2c



1c **2c**

Scheme S9

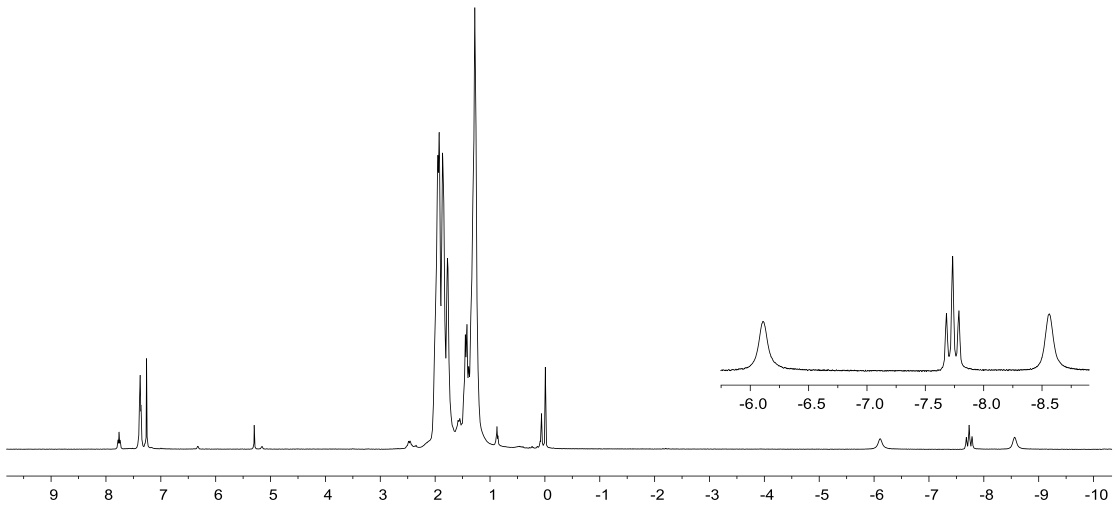


Fig. S37 ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) spectrum of **2c**.

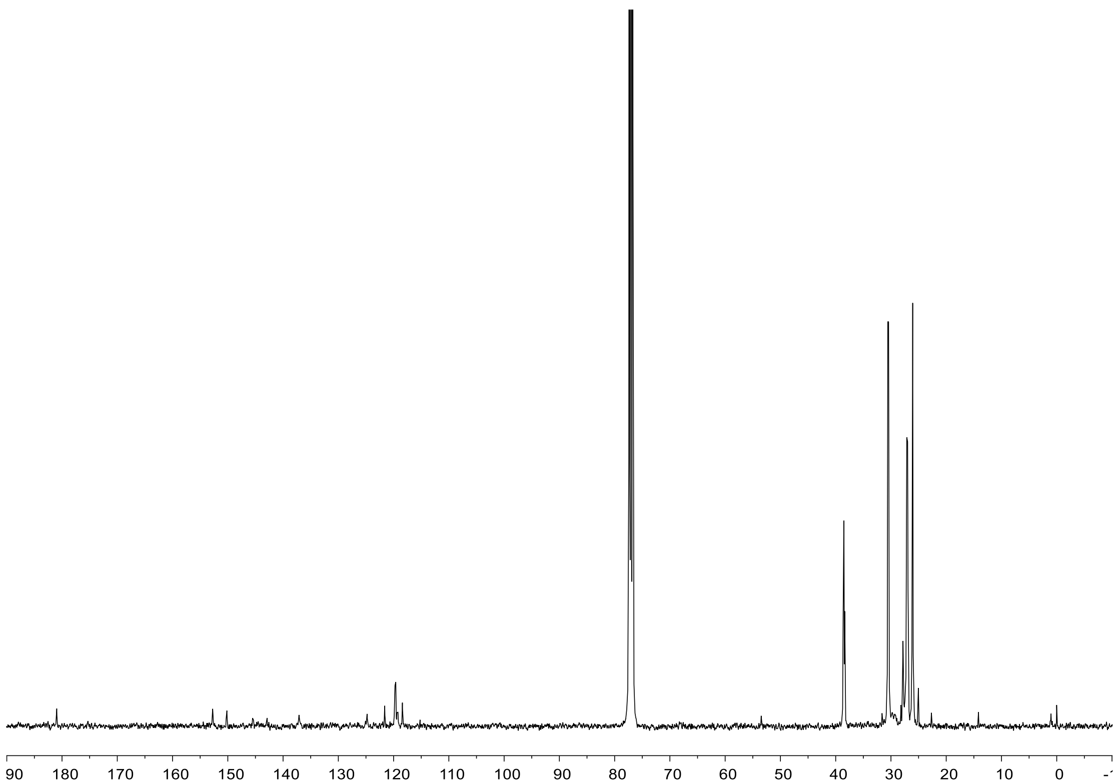


Fig. S38 $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$) spectrum of **2c**.

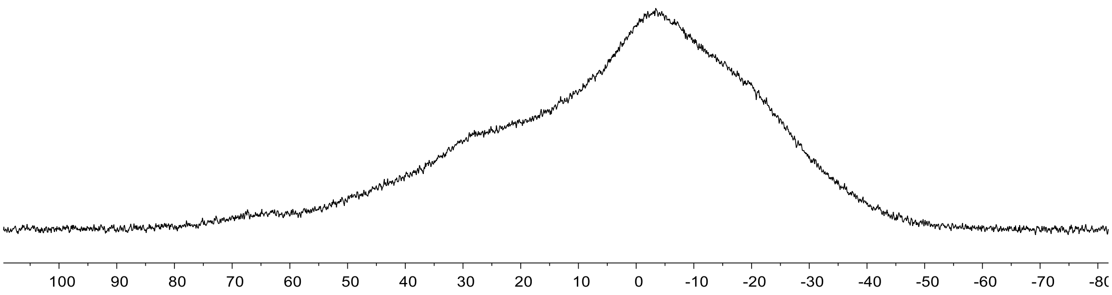


Fig. S39 $^{11}B\{^1H\}$ NMR (128 MHz, 298 K, $CDCl_3$) spectrum of **2c**.

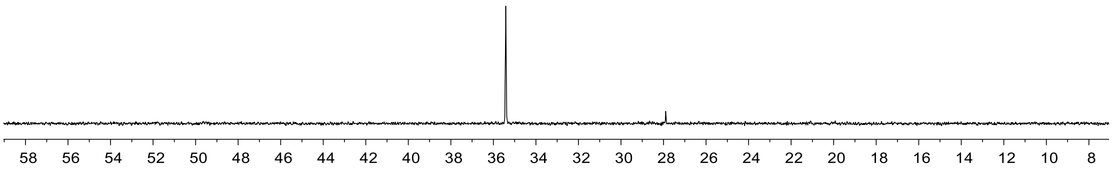


Fig. S40 $^{31}P\{^1H\}$ NMR (162 MHz, 298 K, $CDCl_3$) spectrum of **2c.**

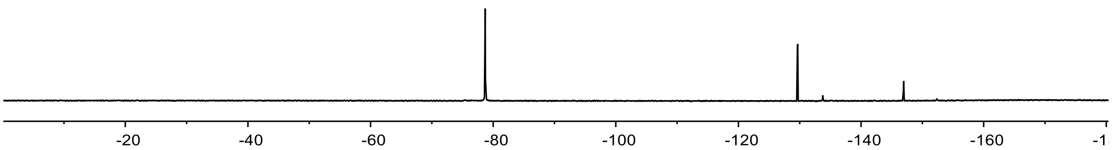
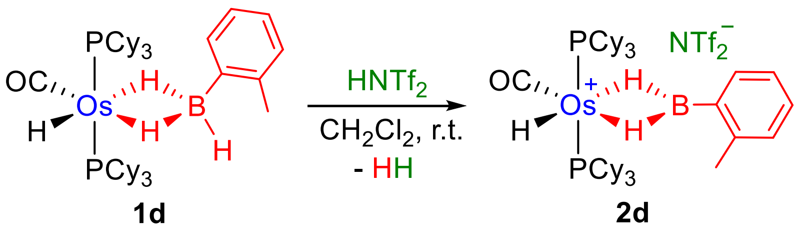


Fig. S41 $^{19}F\{^1H\}$ NMR (377 MHz, 298 K, $CDCl_3$) spectrum of **2c**.

NMR spectra of 2d



Scheme S10

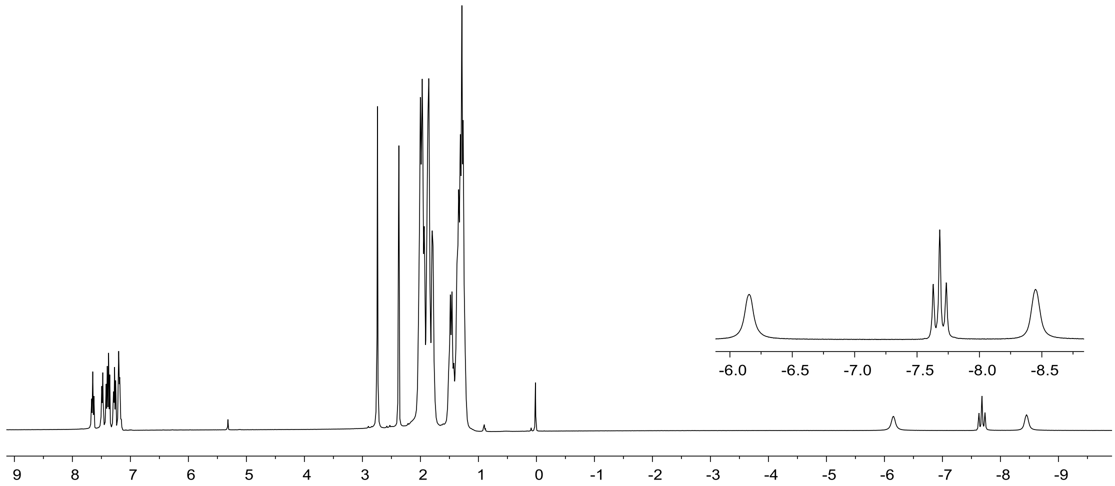


Fig. S42 ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) spectrum of **2d**.

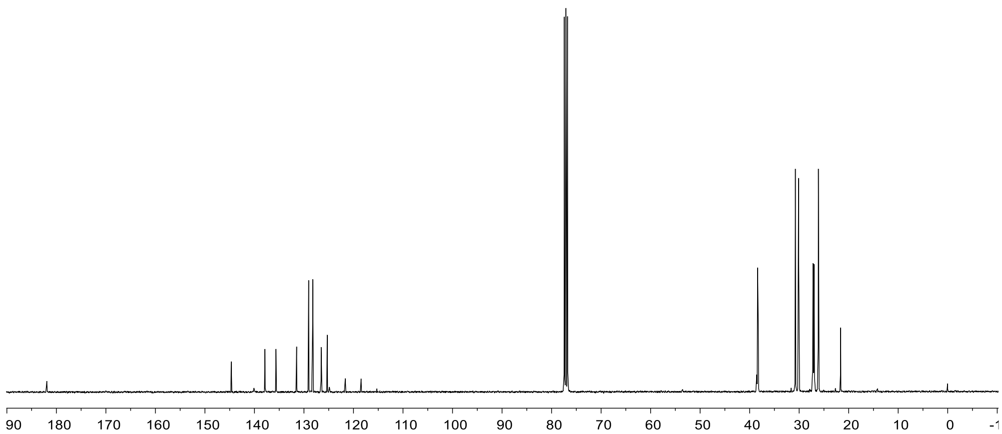


Fig. S43 $^{13}C\{^{1}H\}$ NMR (101 MHz, 298 K, $CDCl_3$) spectrum of **2d**.

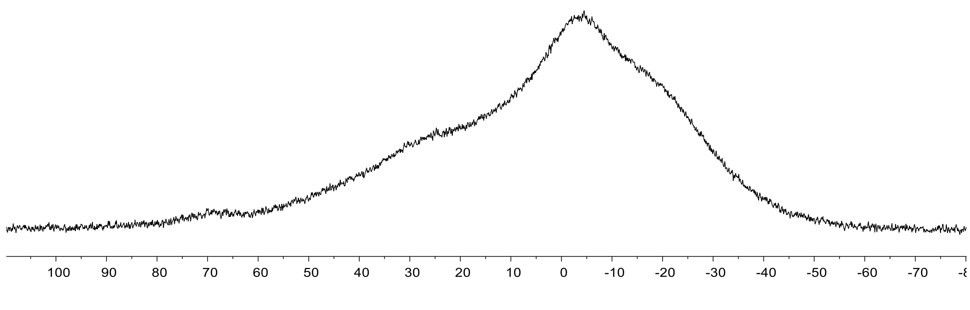


Fig. S44 $^{11}B\{^{1}H\}$ NMR (128 MHz, 298 K, $CDCl_3$) spectrum of **2d**.

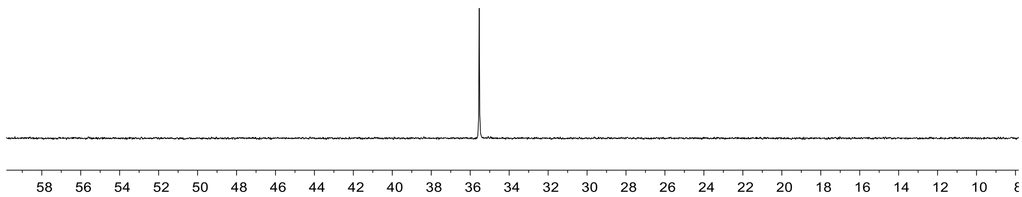
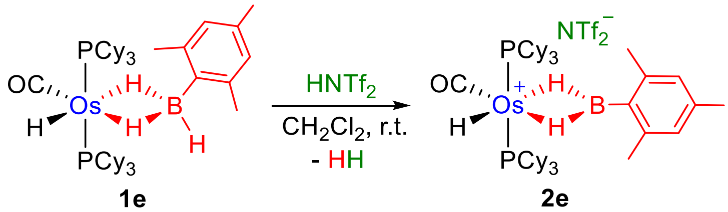


Fig. S45 $^{31}P\{^{1}H\}$ NMR (162 MHz, 298 K, $CDCl_3$) spectrum of **2d**.

NMR spectra and crystallographic data of 2e



Scheme S11

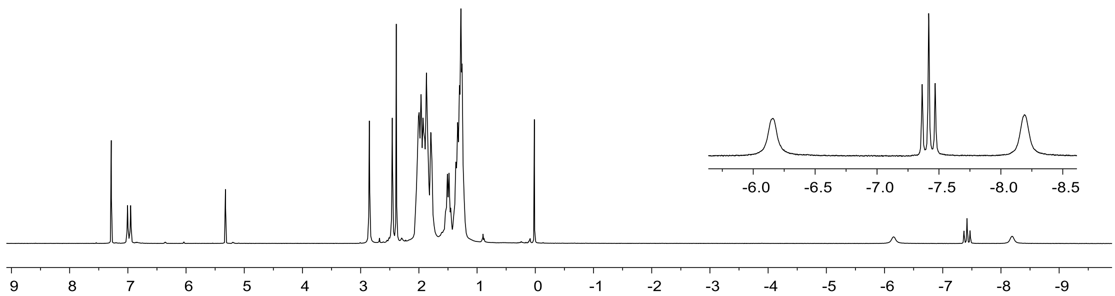


Fig. S46 ^{1}H NMR (400 MHz, 298 K, $CDCl_3$) spectrum of **2e**.

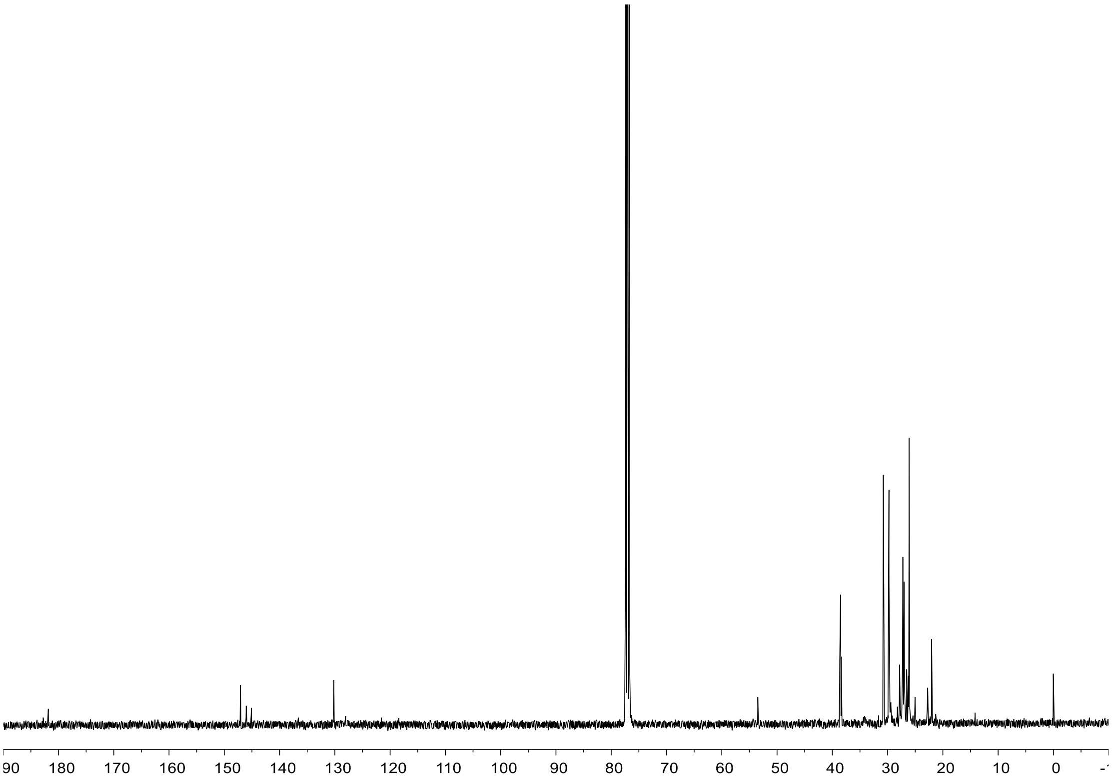


Fig. S47 $^{13}C\{^1H\}$ NMR (101 MHz, 298 K, $CDCl_3$) spectrum of **2e**.

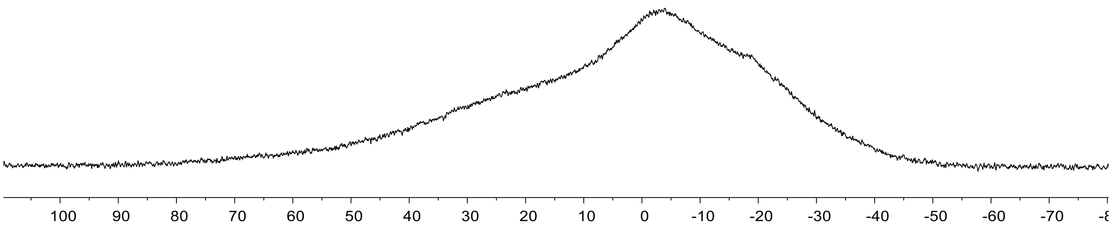


Fig. S48 $^{11}B\{^1H\}$ NMR (128 MHz, 298 K, $CDCl_3$) spectrum of **2e**.

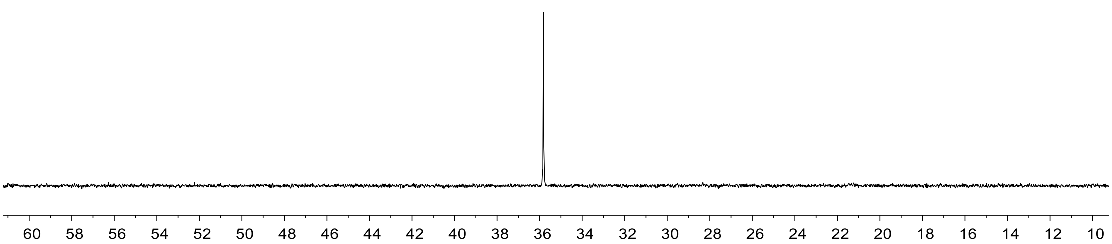


Fig. S49 $^{31}P\{^1H\}$ NMR (162 MHz, 298 K, $CDCl_3$) spectrum of **2e**.

X-ray crystal structure analysis of complex 2e: formula $C_{48}H_{80}BF_6NO_5OsP_2S_2$, M = 1192.20 g/mol, clear light orange crystal, 0.26 × 0.15 × 0.1 mm, a = 16.553(2), b = 16.8037(18), c = 19.306(2) Å, α = 90,

β = 90, γ = 90°, V = 5370.0(11) Å^3, ρ_{calc} = 1.475 g·cm^{-3}, μ = 2.576 mm^{-1}, empirical absorption correction (0.4492 ≤ T ≤ 0.7460), Z = 4, orthorhombic, space group $P2_12_12_1$, λ = 0.71073 Å, T = 120 K, ω and φ scans, 55997 reflections collected (±h, ±k, ±l), 15354 independent (R_{int} = 0.0979) and 12197 observed reflections [I>2σ(I)], 794 refined parameters, R = 0.0443, wR^2 = 0.0875, max. (min.) residual electron density 1.60 (-1.18) e.Å^{-3}.

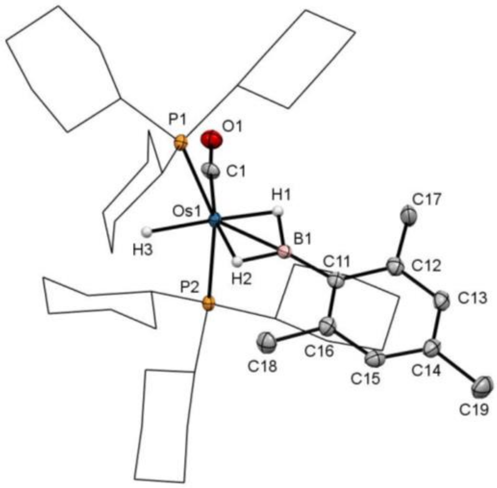


Fig. S50 Molecular structure of **2e** (thermal ellipsoids are shown at the 30% probability level).

IR spectra of 1a-1f and 2a-2e

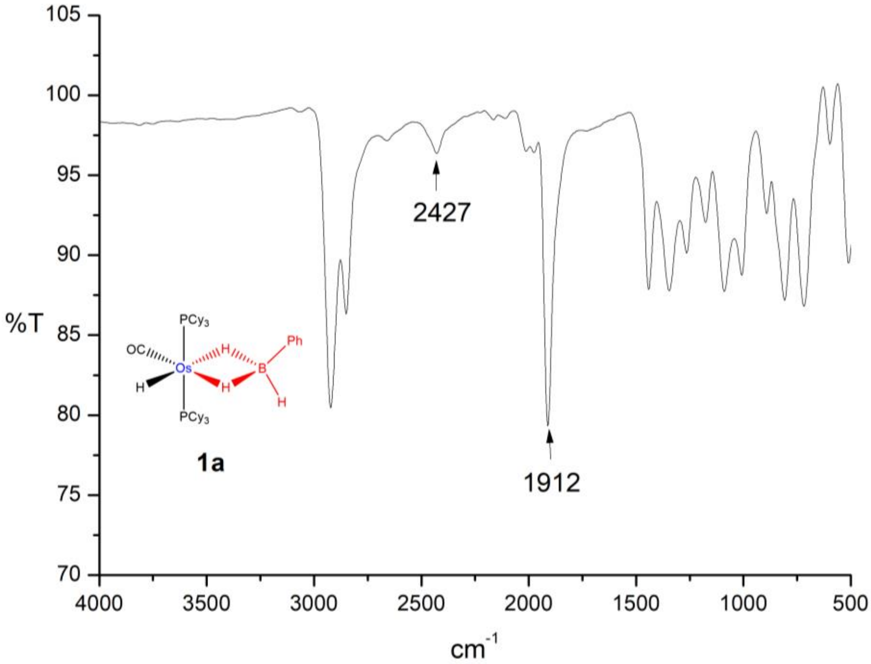


Fig. S51 IR spectrum of **1a**.

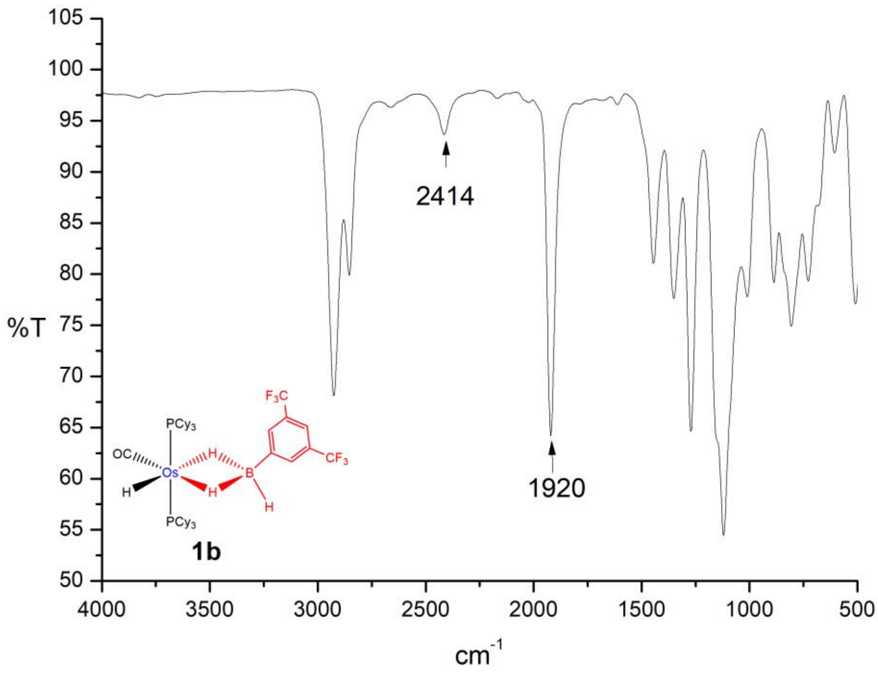


Fig. S52 IR spectrum of **1b**.

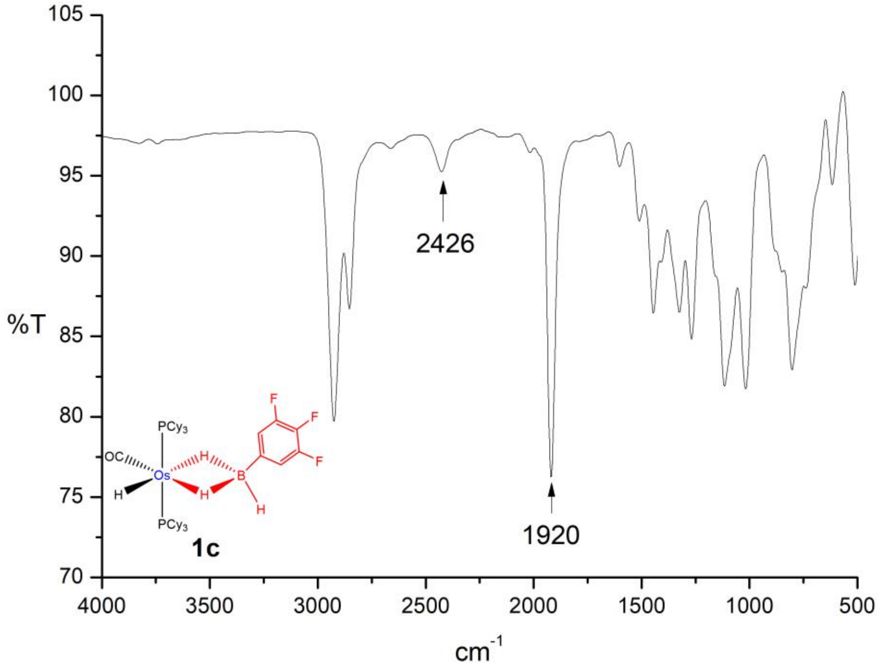


Fig. S53 IR spectrum of **1c**.

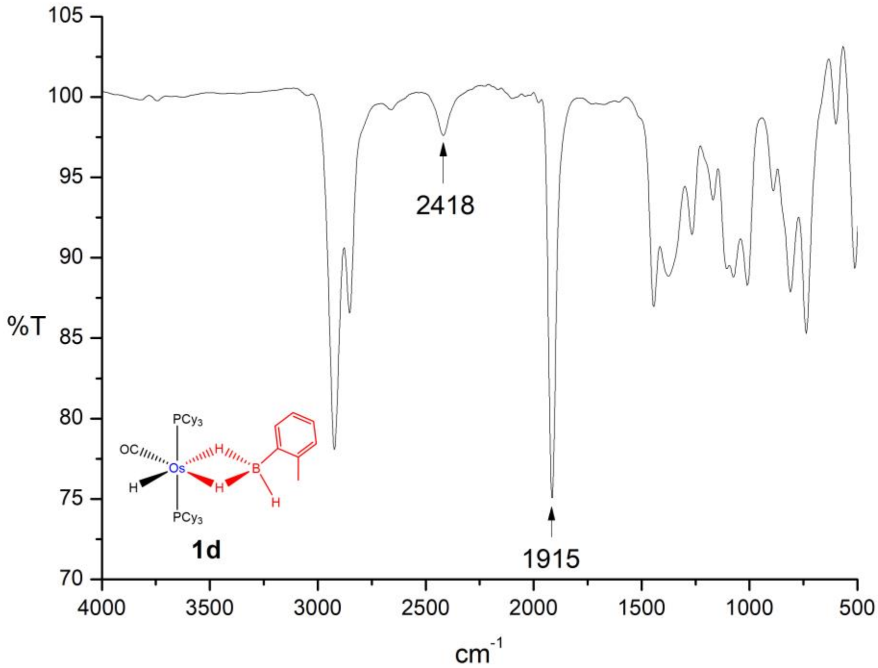


Fig. S54 IR spectrum of **1d**.

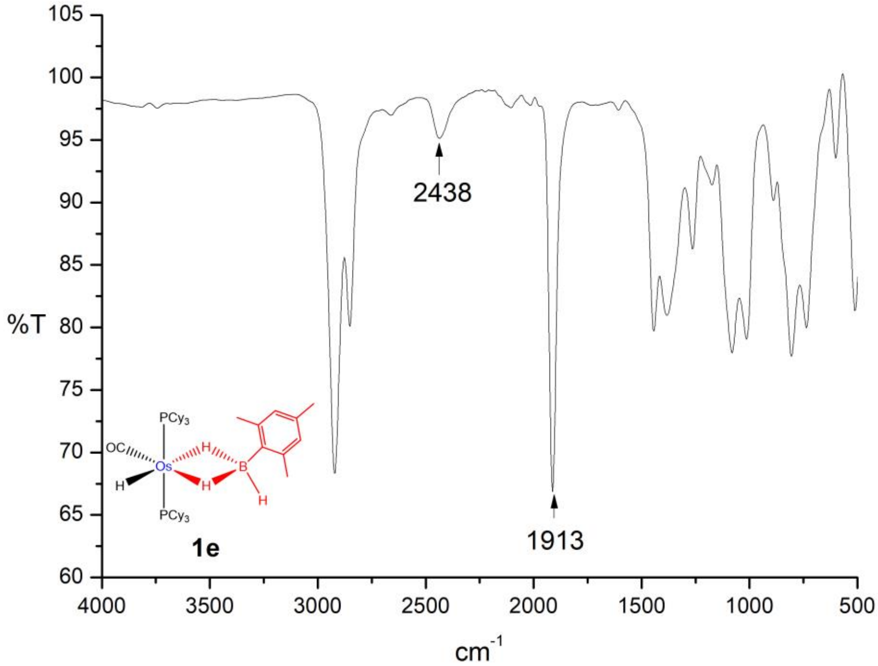


Fig. S55 IR spectrum of **1e**.

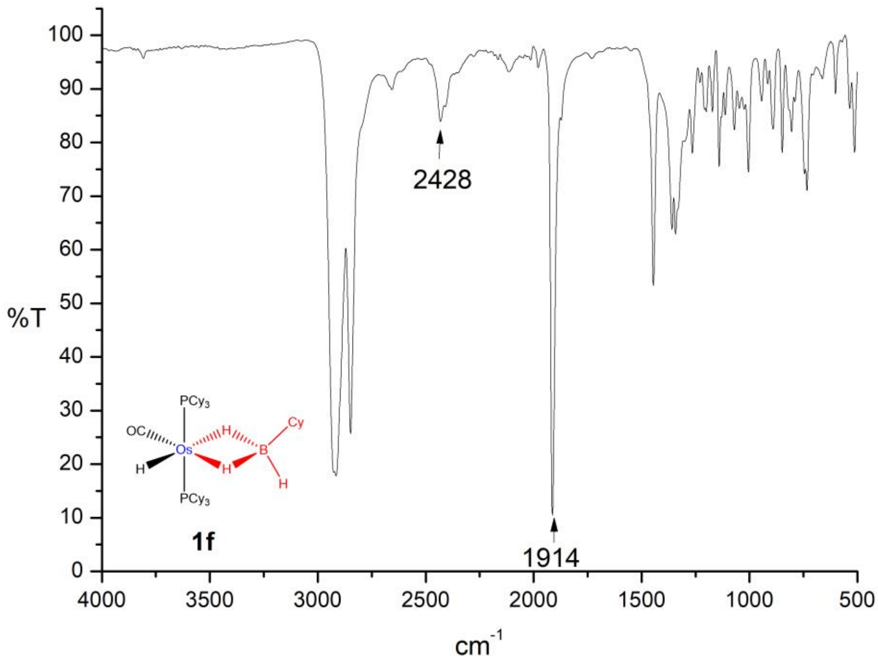


Fig. S56 IR spectrum of **1f**.

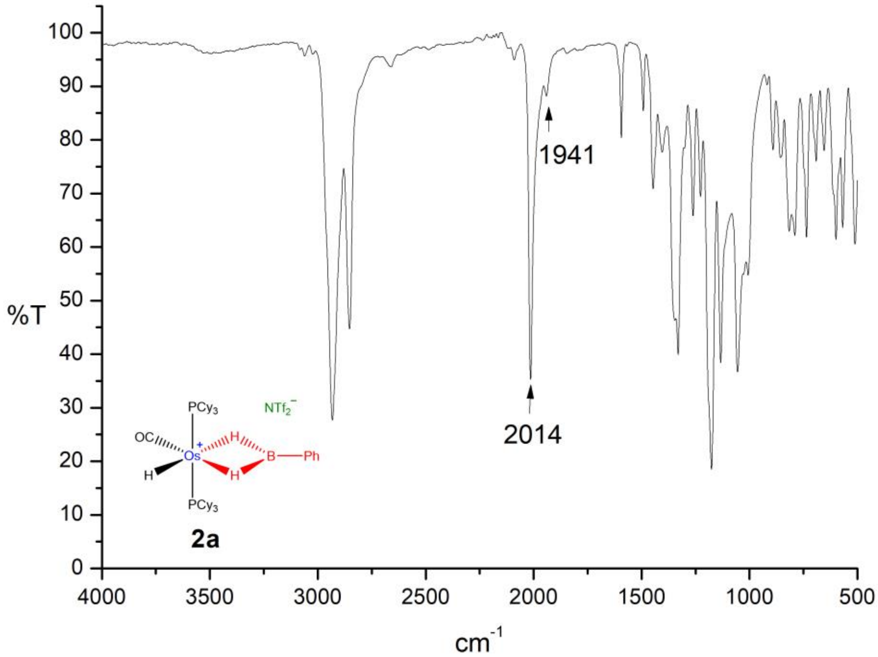


Fig. S57 IR spectrum of **2a**.

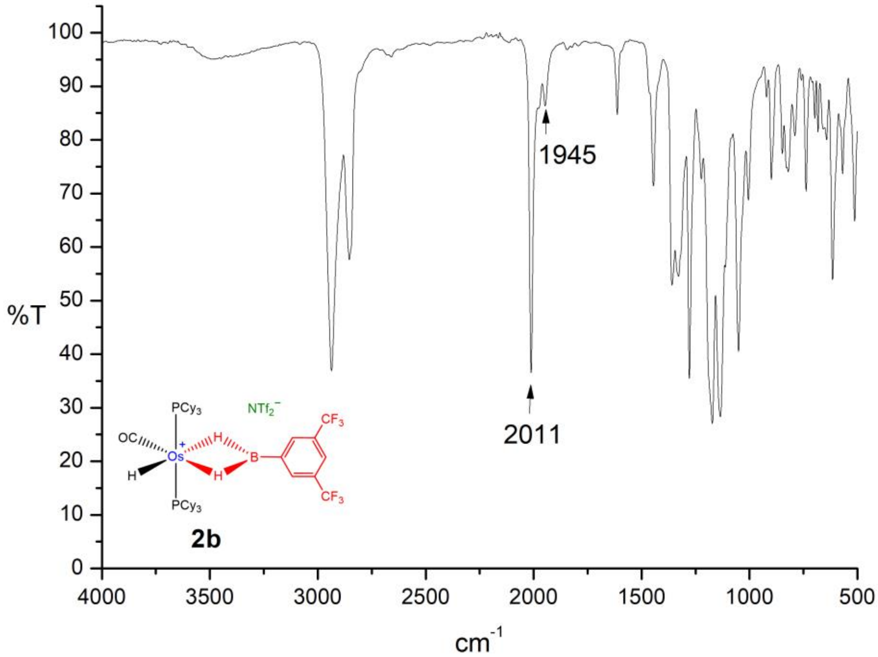


Fig. S58 IR spectrum of **2b**.

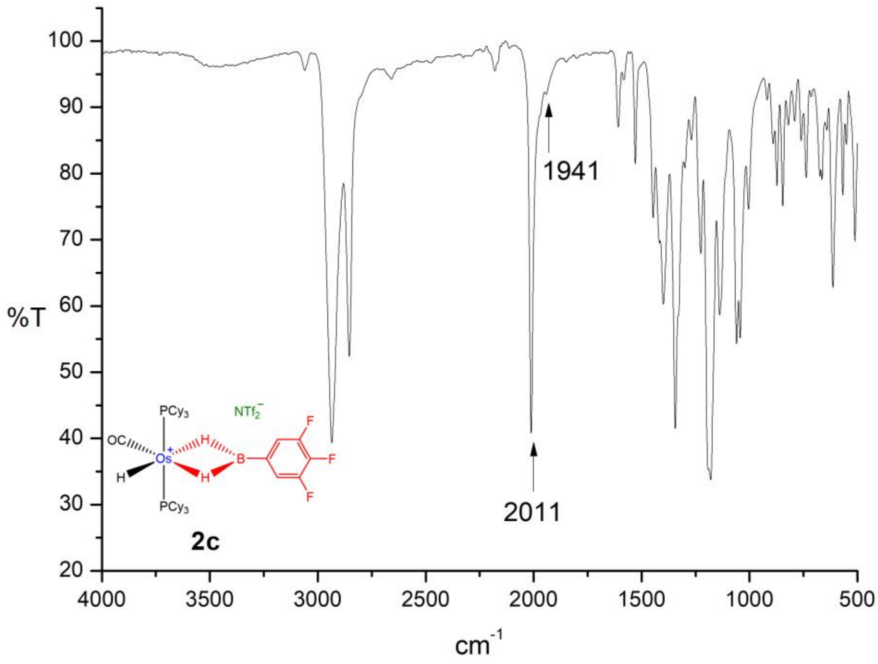


Fig. S59 IR spectrum of **2c**.

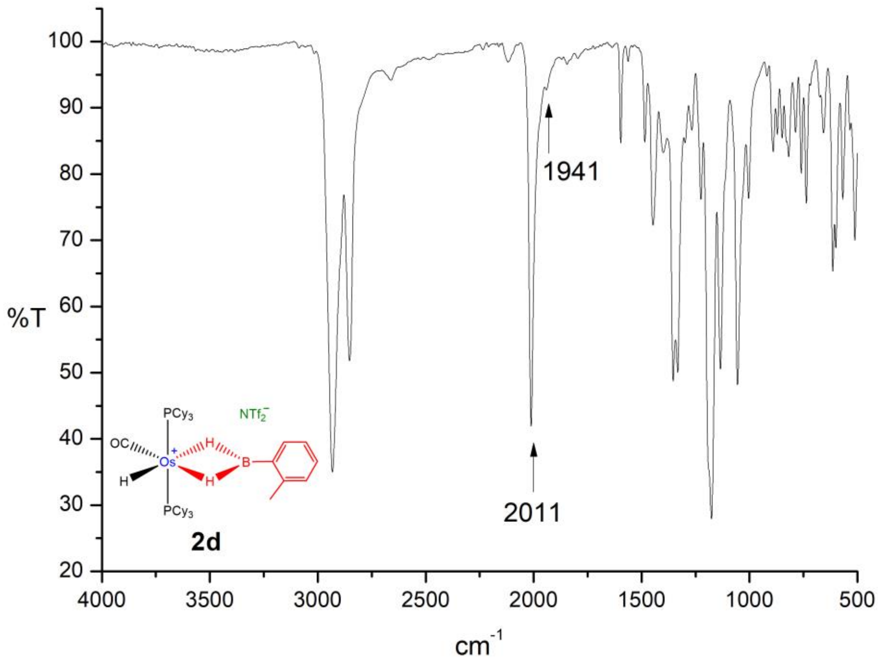


Fig. S60 IR spectrum of **2d**.

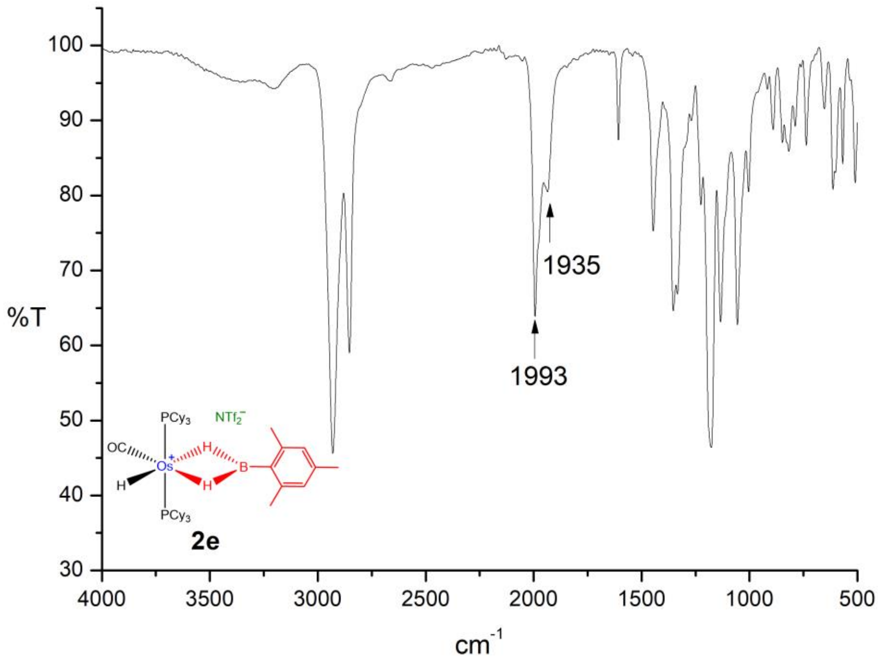


Fig. S61 IR spectrum of **2e**.

Computational Details

Geometry optimizations of **1a** and **2a** were performed at the PBE0[1] /def2-SVP[2,3] level, in combination with RIJOCSX[4] and the def2/J[5] auxiliary basis set planted in the ORCA5.0.1[6-8] suite of programs. During the calculations, the D3 dispersion correction suggested by Grimme et al[9,10] was used. All species were characterized as local minima by analytic frequency calculations. For AIM analysis, single-point calculations on the computationally optimized geometries were performed with in M06-L[11] /def2-SVP level, in combination with Split-RI-J[12] and the def2/J auxiliary basis set. The topology of the electron density was conducted through the Multiwfn program package.[13]

1a

Os	4.420492000	4.740779000	16.310368000
P	4.519154000	5.365920000	14.004702000
P	4.186911000	4.619323000	18.686492000
O	1.529229000	3.939601000	16.094739000
C	2.636904000	4.285053000	16.161388000
C	3.946587000	2.934803000	19.444400000
H	3.676440000	3.113593000	20.500511000
C	2.629569000	5.513100000	19.218462000
H	1.902937000	5.166624000	18.461598000
C	6.132702000	6.664134000	19.079811000
H	5.410347000	7.453445000	19.341400000
H	6.188187000	6.645951000	17.981957000
C	5.644304000	5.310632000	19.605992000
H	6.421118000	4.576573000	19.323484000
C	7.489384000	7.011588000	19.683466000
H	7.828138000	7.992272000	19.311447000
H	8.235827000	6.272624000	19.340693000
C	4.318670000	4.017658000	12.746040000
H	4.288815000	4.508694000	11.758097000
C	2.737274000	7.031849000	19.057116000
H	3.172268000	7.277748000	18.076896000
H	3.423955000	7.430556000	19.823324000
C	2.779329000	2.212271000	18.764805000
H	3.037189000	2.057965000	17.703162000
H	1.869255000	2.831907000	18.768552000
C	0.686657000	5.852622000	20.784186000
H	0.291553000	5.617851000	21.786013000
H	-0.030545000	5.425331000	20.060430000
B	6.504618000	3.740890000	16.508061000
C	3.002320000	3.264711000	12.951686000
H	2.144381000	3.955105000	12.945028000
H	3.014246000	2.802369000	13.953256000
C	5.550149000	5.331698000	21.131903000
H	5.204309000	4.362453000	21.524490000
H	4.803498000	6.082531000	21.443398000
C	6.427737000	6.464545000	12.114615000
H	5.739527000	7.252949000	11.764571000
H	6.247341000	5.580111000	11.484330000
C	5.487152000	3.036802000	12.762564000
H	5.542974000	2.578465000	13.761492000
H	6.448965000	3.550452000	12.614800000
C	2.041275000	5.172605000	20.591750000
H	2.732284000	5.496097000	21.387650000

H	1.915003000	4.086663000	20.710613000
C	6.417476000	7.394188000	14.448038000
H	6.239656000	7.162697000	15.509640000
H	5.697733000	8.189191000	14.181738000
C	7.861870000	6.954349000	11.928127000
H	8.051617000	7.166328000	10.863262000
H	8.558018000	6.147315000	12.218214000
C	5.191180000	2.045968000	19.433848000
H	6.033054000	2.540975000	19.941691000
H	5.512316000	1.884324000	18.393266000
C	7.436425000	7.010724000	21.207554000
H	8.432252000	7.222012000	21.629841000
H	6.776311000	7.830399000	21.545842000
C	6.152941000	6.154378000	13.586503000
H	6.869398000	5.376715000	13.903238000
C	1.378646000	7.701429000	19.228147000
H	1.480702000	8.792941000	19.114254000
H	0.704744000	7.365914000	18.419333000
C	5.313048000	1.945963000	11.711993000
H	6.160456000	1.243191000	11.765479000
H	5.349146000	2.400096000	10.704701000
C	4.909632000	0.701380000	20.098021000
H	5.815448000	0.074659000	20.065071000
H	4.680733000	0.862465000	21.167613000
C	3.990687000	1.208293000	11.885508000
H	4.009418000	0.658055000	12.843595000
H	3.860776000	0.452035000	11.094244000
C	6.902585000	5.688150000	21.746582000
H	7.622405000	4.882733000	21.514530000
H	6.819850000	5.724753000	22.845147000
C	7.682886000	3.390576000	15.495259000
C	2.496850000	0.864004000	19.418999000
H	2.149940000	1.027136000	20.455953000
H	1.670954000	0.359536000	18.891908000
C	7.806174000	2.114753000	14.922262000
H	7.048470000	1.355404000	15.141376000
C	0.763710000	7.360601000	20.580159000
H	-0.236652000	7.812606000	20.678270000
H	1.384491000	7.803641000	21.380375000
C	2.815533000	2.179319000	11.896378000
H	2.721013000	2.651103000	10.901212000
H	1.870555000	1.641301000	12.075693000
C	8.699086000	4.313313000	15.204053000
H	8.660933000	5.307272000	15.660354000

C	2.945964000	6.689050000	11.980245000
H	3.859883000	6.673379000	11.371148000
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C	7.832343000	7.930038000	14.245015000
H	8.555961000	7.194314000	14.633976000
H	7.971243000	8.848197000	14.838714000
C	1.116964000	7.910500000	13.917222000
H	1.652270000	8.831489000	14.213288000
H	0.181211000	7.896713000	14.499428000
C	3.270185000	6.670916000	13.479394000
H	3.807891000	7.607685000	13.715985000
C	8.135539000	8.191746000	12.774835000
H	7.502899000	9.023461000	12.413977000
H	9.179896000	8.521693000	12.651410000
C	3.739947000	-0.016722000	19.436613000
H	4.016167000	-0.272457000	18.397743000
H	3.531375000	-0.970530000	19.947962000
C	8.860674000	1.788472000	14.071252000
H	8.919639000	0.786823000	13.636459000
C	1.970098000	6.701248000	14.286335000
H	1.394483000	5.777978000	14.103580000
H	2.199368000	6.714937000	15.359823000
C	9.757921000	4.002758000	14.350376000
H	10.525930000	4.752244000	14.139017000
C	2.101771000	7.905364000	11.609381000
H	1.876165000	7.887150000	10.530604000
H	2.690957000	8.823297000	11.787944000
C	0.816689000	7.962697000	12.424866000
H	0.239594000	8.867996000	12.175469000
H	0.178840000	7.101900000	12.153712000
C	9.838220000	2.737362000	13.770688000
H	10.662353000	2.488112000	13.097636000
H	3.942564000	6.279483000	16.485341000
H	5.385261000	3.124128000	16.170418000
H	6.246958000	5.041433000	16.462423000
H	6.828033000	3.464495000	17.648295000

2a

Os	4.338530000	4.678248000	16.182333000
P	4.455960000	5.430994000	13.895607000
P	4.171017000	4.715145000	18.585105000
O	1.397252000	3.974105000	15.989827000
C	2.495724000	4.305548000	16.047995000
C	4.336981000	3.037164000	19.361035000

H	4.156075000	3.188381000	20.439964000
C	2.512238000	5.320893000	19.158011000
H	1.829453000	4.695853000	18.553286000
C	5.745274000	7.094208000	18.702952000
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H	5.723119000	7.039835000	17.604852000
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H	6.434142000	5.099695000	18.979581000
C	7.051606000	7.720411000	19.181067000
H	7.158333000	8.730582000	18.754910000
H	7.899207000	7.127766000	18.790533000
C	4.165940000	4.137203000	12.605716000
H	4.167014000	4.680948000	11.645188000
C	2.229047000	6.778275000	18.781984000
H	2.497943000	6.964151000	17.731098000
H	2.864229000	7.441713000	19.393124000
C	3.263408000	2.086916000	18.820089000
H	3.379662000	2.005326000	17.724945000
H	2.255795000	2.496364000	18.993599000
C	0.691031000	5.415662000	20.882077000
H	0.451556000	5.249899000	21.944125000
H	0.051887000	4.719939000	20.309131000
B	5.999645000	3.556149000	15.895637000
C	2.798208000	3.472126000	12.778567000
H	1.994652000	4.224106000	12.813239000
H	2.778692000	2.949941000	13.750839000
C	5.598532000	5.768309000	20.837381000
H	5.470993000	4.771124000	21.286807000
H	4.754589000	6.383671000	21.191357000
C	6.465020000	6.493091000	12.115487000
H	5.867017000	7.381650000	11.852655000
H	6.184596000	5.697885000	11.407670000
C	5.267595000	3.080189000	12.554714000
H	5.300556000	2.551632000	13.521665000
H	6.258396000	3.539650000	12.417177000
C	2.156051000	5.066264000	20.626324000
H	2.797297000	5.678837000	21.280163000
H	2.334000000	4.016729000	20.904402000
C	6.555302000	7.209600000	14.520110000
H	6.347034000	6.919755000	15.560990000
H	5.930276000	8.097814000	14.320268000
C	7.944401000	6.837313000	11.957124000
H	8.148059000	7.132377000	10.915956000
H	8.548782000	5.932003000	12.147102000

C	5.738143000	2.445036000	19.202961000
H	6.492395000	3.096329000	19.670453000
H	5.995006000	2.390041000	18.130088000
C	7.127545000	7.770963000	20.702506000
H	8.095539000	8.184142000	21.026063000
H	6.354121000	8.463367000	21.080235000
C	6.163750000	6.083378000	13.558501000
H	6.799261000	5.210071000	13.796342000
C	0.763711000	7.120929000	19.031982000
H	0.578189000	8.174761000	18.770944000
H	0.133883000	6.516641000	18.354495000
C	5.005790000	2.067476000	11.442783000
H	5.799920000	1.304297000	11.445165000
H	5.070592000	2.578516000	10.465778000
C	5.831765000	1.046056000	19.806731000
H	6.840278000	0.639171000	19.633570000
H	5.710617000	1.116517000	20.902213000
C	3.634965000	1.417742000	11.585108000
H	3.617438000	0.803262000	12.503650000
H	3.449341000	0.726417000	10.748457000
C	6.907166000	6.393585000	21.315527000
H	7.745415000	5.728292000	21.040317000
H	6.909795000	6.454846000	22.414999000
C	7.283013000	2.799839000	15.569526000
C	3.375208000	0.697247000	19.438556000
H	3.151832000	0.758709000	20.518503000
H	2.609722000	0.036377000	19.002900000
C	7.250898000	1.418675000	15.291928000
H	6.297716000	0.883131000	15.323694000
C	0.367742000	6.848749000	20.478236000
H	-0.703085000	7.056038000	20.629078000
H	0.913092000	7.545080000	21.140257000
C	2.531292000	2.465278000	11.664062000
H	2.461890000	3.001060000	10.700561000
H	1.552410000	1.986365000	11.822204000
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H	8.572724000	4.534302000	15.749534000
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H	3.927042000	6.936587000	11.372676000
H	2.386569000	6.124349000	11.652138000
C	8.025723000	7.584676000	14.358650000
H	8.651589000	6.731256000	14.676988000
H	8.272899000	8.418298000	15.034824000
C	1.242111000	8.190742000	13.977113000

H	1.833575000	9.050550000	14.340778000
H	0.300905000	8.199268000	14.549247000
C	3.311531000	6.844914000	13.473249000
H	3.911749000	7.723214000	13.775854000
C	8.363618000	7.943843000	12.917071000
H	7.839408000	8.877149000	12.644319000
H	9.439703000	8.154403000	12.816291000
C	4.768249000	0.113980000	19.242244000
H	4.951361000	-0.038718000	18.162652000
H	4.840134000	-0.879127000	19.712015000
C	8.415631000	0.728932000	14.978031000
H	8.379228000	-0.341905000	14.766455000
C	2.007644000	6.904729000	14.273363000
H	1.375222000	6.036165000	14.020914000
H	2.221755000	6.839746000	15.348710000
C	9.690082000	2.776407000	15.209205000
H	10.646698000	3.302484000	15.177963000
C	2.255113000	8.271784000	11.682004000
H	2.043727000	8.339181000	10.603323000
H	2.904313000	9.131910000	11.925790000
C	0.966854000	8.360866000	12.488969000
H	0.457774000	9.318405000	12.298339000
H	0.273223000	7.568915000	12.154157000
C	9.634624000	1.409361000	14.932897000
H	10.550083000	0.867917000	14.682872000
H	4.019723000	6.261625000	16.384753000
H	4.863729000	2.922593000	16.041197000
H	6.143592000	4.791472000	16.370328000

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