

Oxidation-induced C-H bond activation in iridium pincer complexes

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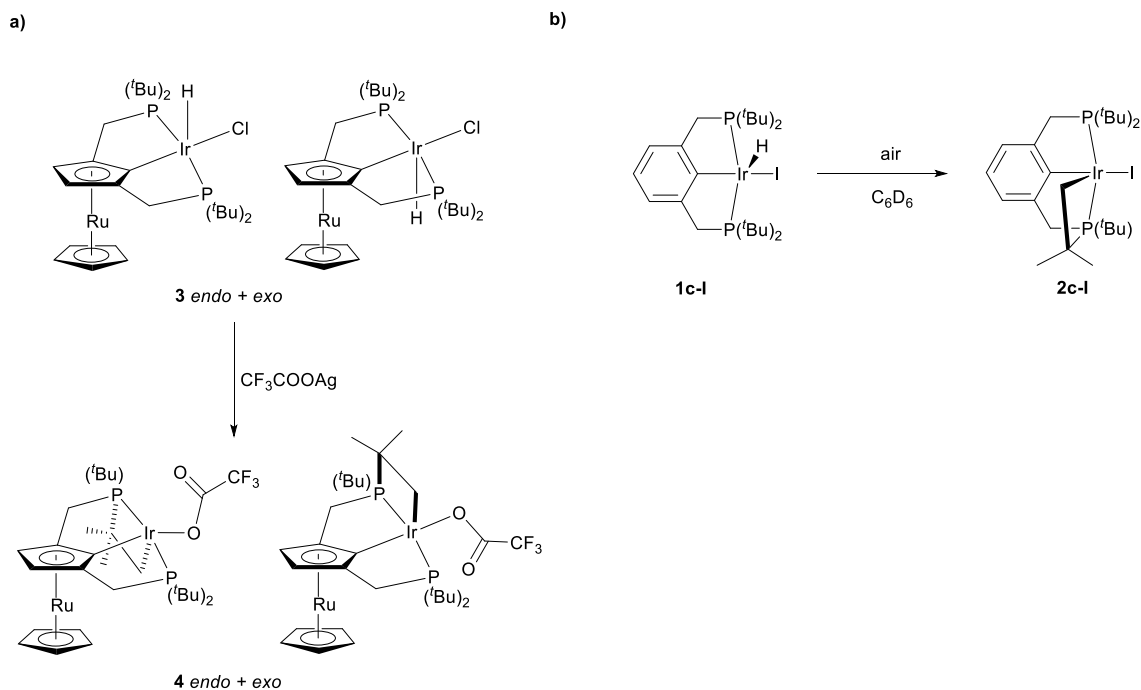
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Supporting Information

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1. Observation of other plausible oxidation-induced C-H bond activations



Scheme S1. Observation of other plausible oxidation-induced C-H bond activations.

a) Addition of the CF_3COOAg to the CDCl_3 solution of ruthenocene-based complex **3** resulted in the disappearance of signals of **3** and formation of the two AX-systems in the $^{31}\text{P}\{^1\text{H}\}$ NMR

spectrum (85.2 and 25.3 ppm, d, $^2J_{PP} = 346.6$ Hz; 76.4 and 36.0 ppm, d, $^2J_{PP} = 332.2$ Hz) lacking any detectable hydride resonances in the ^1H NMR spectrum. We ascribe these signals to the type **4** structures with *exo* and *endo* cyclometallated *tert*-butyl groups (Scheme S1); unfortunately, **4** appeared to be unstable and decomposed during purification attempt.

b) A solution of (PCP)IrHI (**1c-I**) in C_6D_6 in the NMR tube was left for ca. 4 weeks, with the standard plastic cap allowing the inert atmosphere to be substituted with air. The starting material was fully consumed and compound **2c-I** was formed in more than 80% NMR yield. ^1H NMR (400 MHz, C_6D_6) δ 7.22-7.08 (m, overlapping, 3 H, Ar-H), 3.56 (ddd, $J_1 = 6.3$ Hz, $J_2 = 5.1$ Hz, $J_3 = 1.5$ Hz, 1H, Ir-CH₂-), 3.38 – 2.83 (m, 4H, -CH₂-P), 1.93 (ddd, $J_1 = 7.7$, $J_2 = 5.1$ Hz, $J_3 = 2.8$ Hz, 1H, Ir-CH₂-), 1.44 (d, $^3J_{PH} = 13.8$ Hz, 9H, -C(CH₃)₃), 1.39 (d, $^3J_{PH} = 13.8$ Hz, 3H, -CH₃), 1.28 (d, $^3J_{PH} = 13.0$ Hz, 9H, -C(CH₃)₃), 1.09 (d, $^3J_{PH} = 12.5$ Hz, 9H, -C(CH₃)₃), 0.62 (d, $^3J_{PH} = 12.7$ Hz, 3H, -CH₃). ^{31}P NMR (162 MHz, C_6D_6) δ 48.69 (d, $^2J_{PP} = 339.4$ Hz), 8.57 (d, $^2J_{PP} = 339.4$ Hz).

2. Additional Electrochemical Data

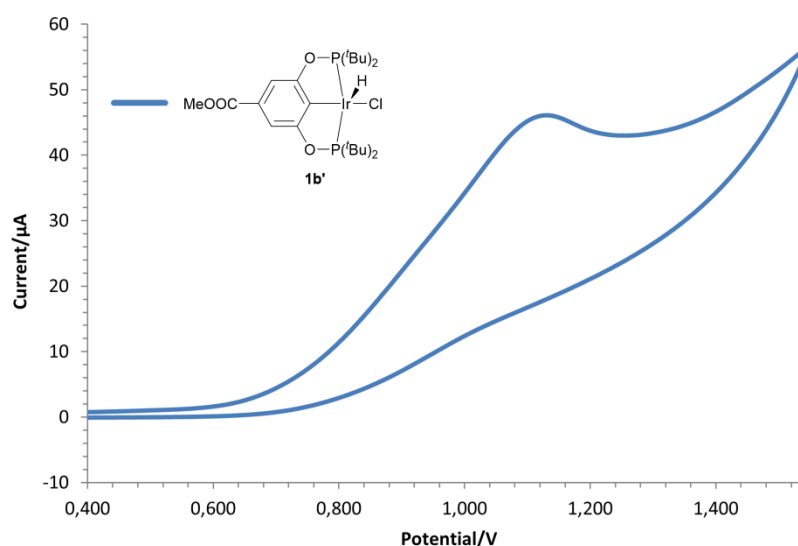


Figure S1. Cyclic voltammogram of **1b'** in THF, scan rate 0.05 V/s.

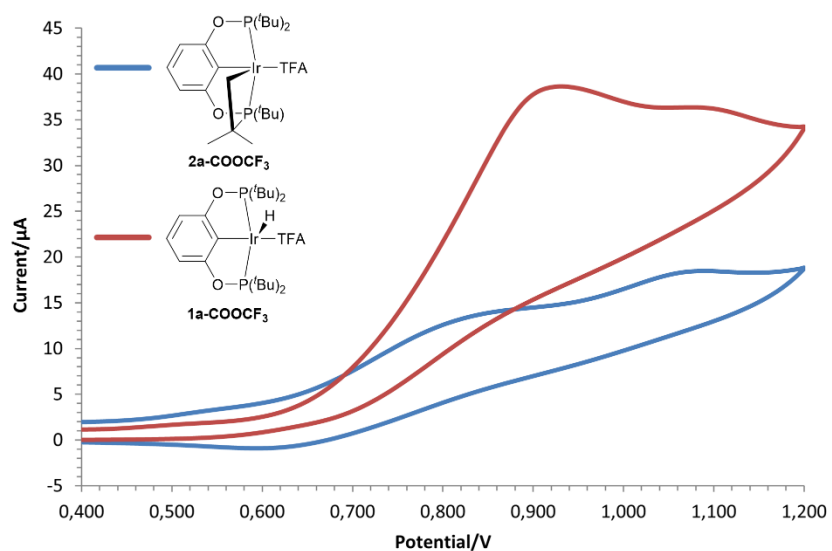


Figure S2. Cyclic voltammograms of complexes **1a-COOCF₃** and **2a-COOCF₃** in THF, scan rate 0.05 V/s.

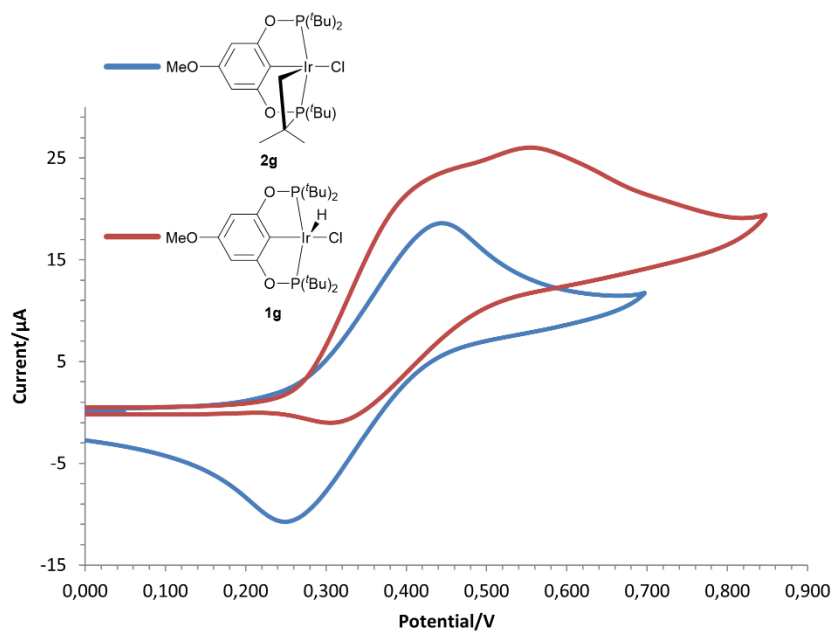


Figure S3. Cyclic voltammograms of complexes **1g** and **2g** in THF, scan rate 0.05 V/s.

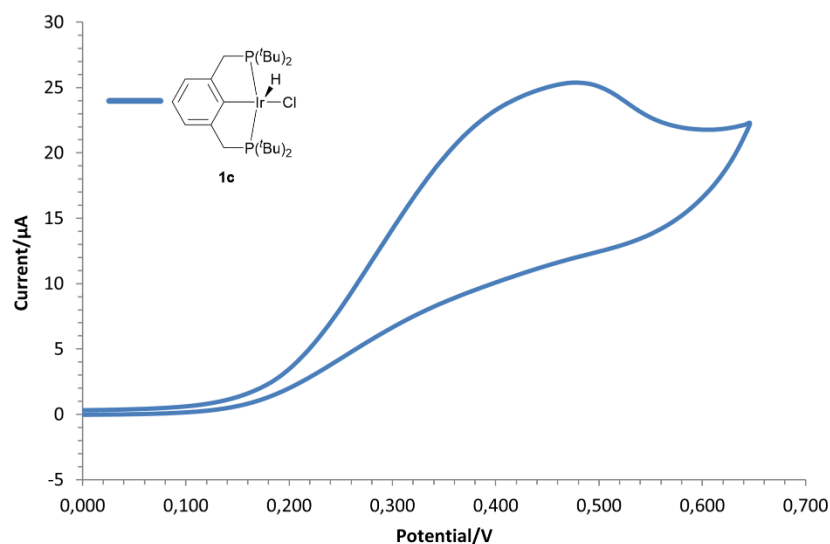


Figure S4. Cyclic voltammogram of complexes **1c** in THF, scan rate 0.05 V/s.

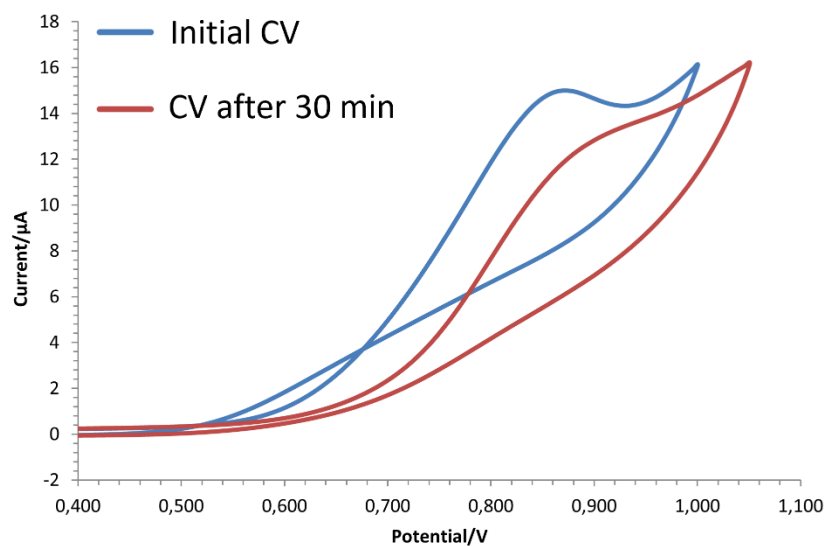
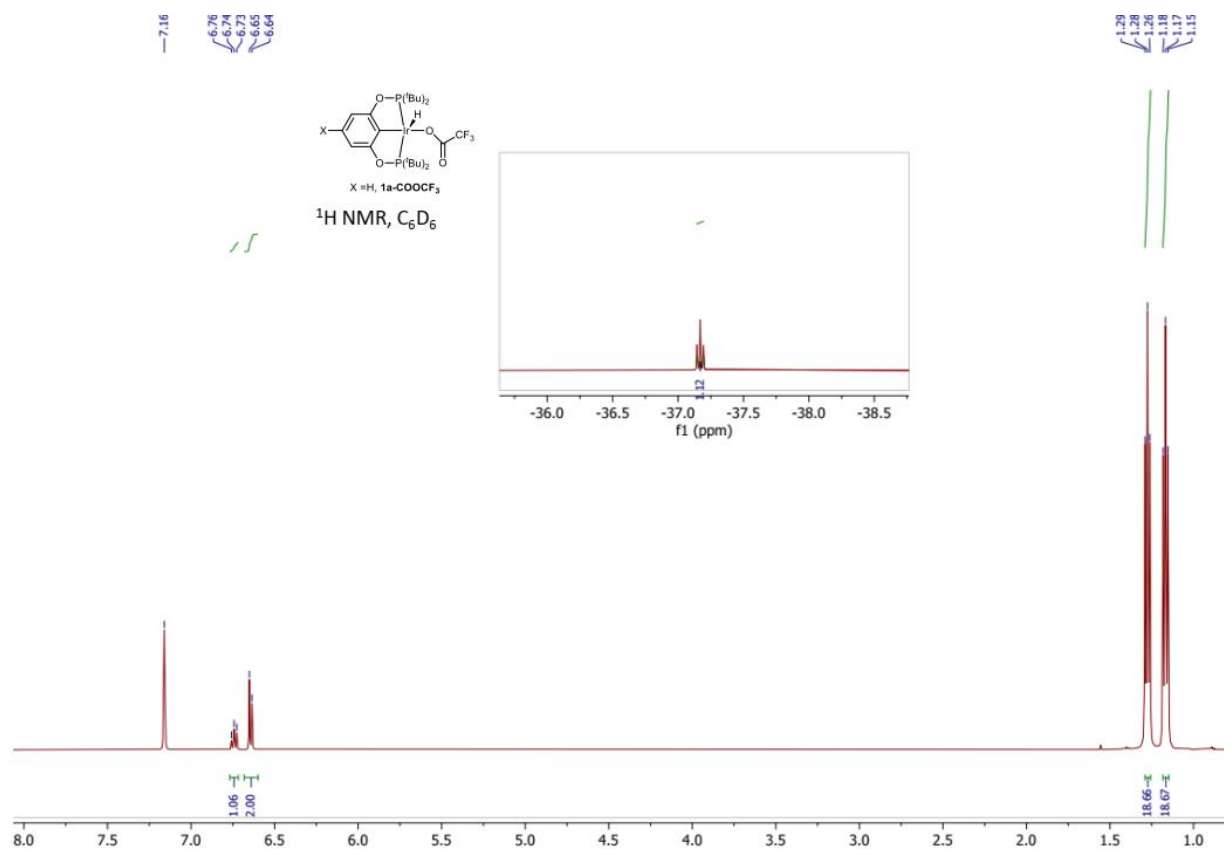
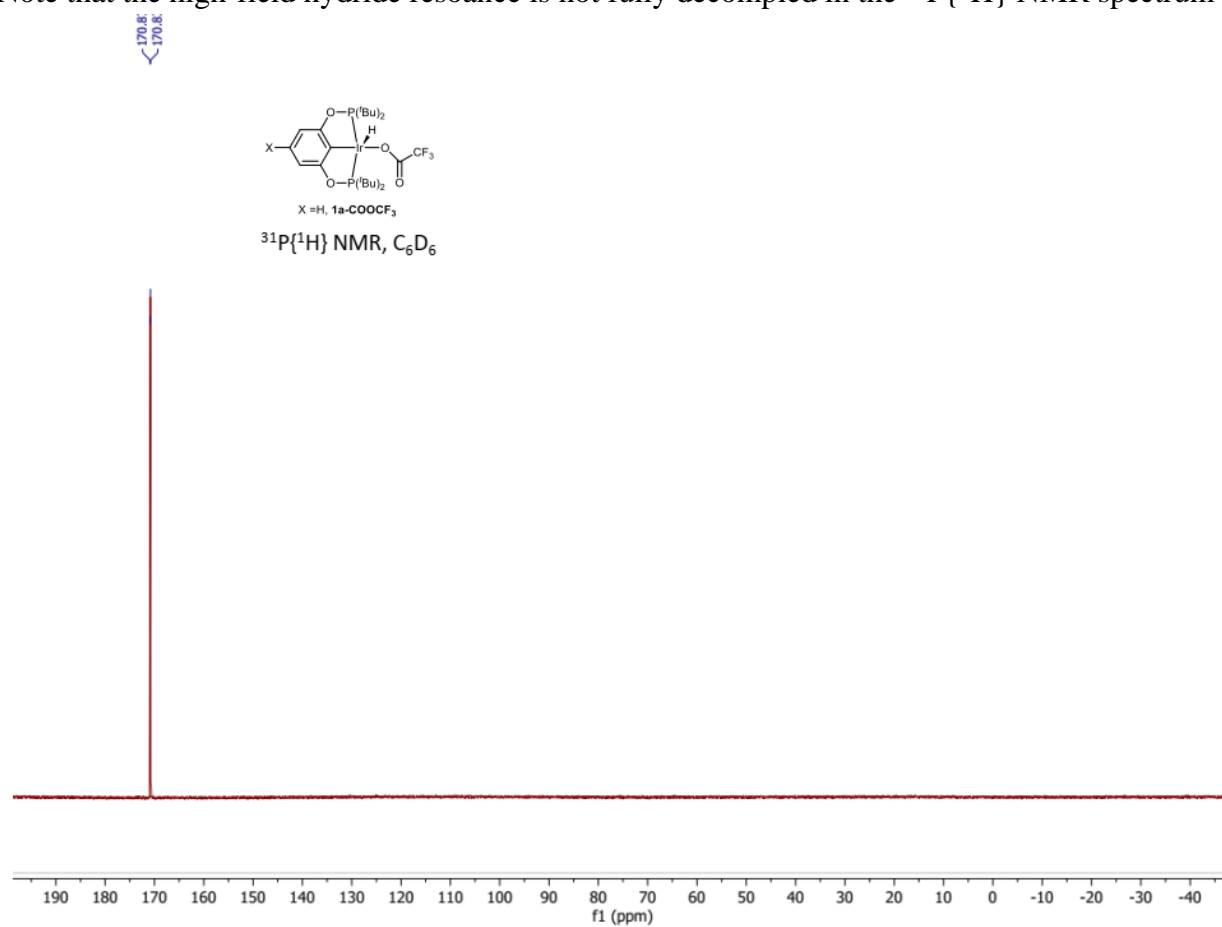
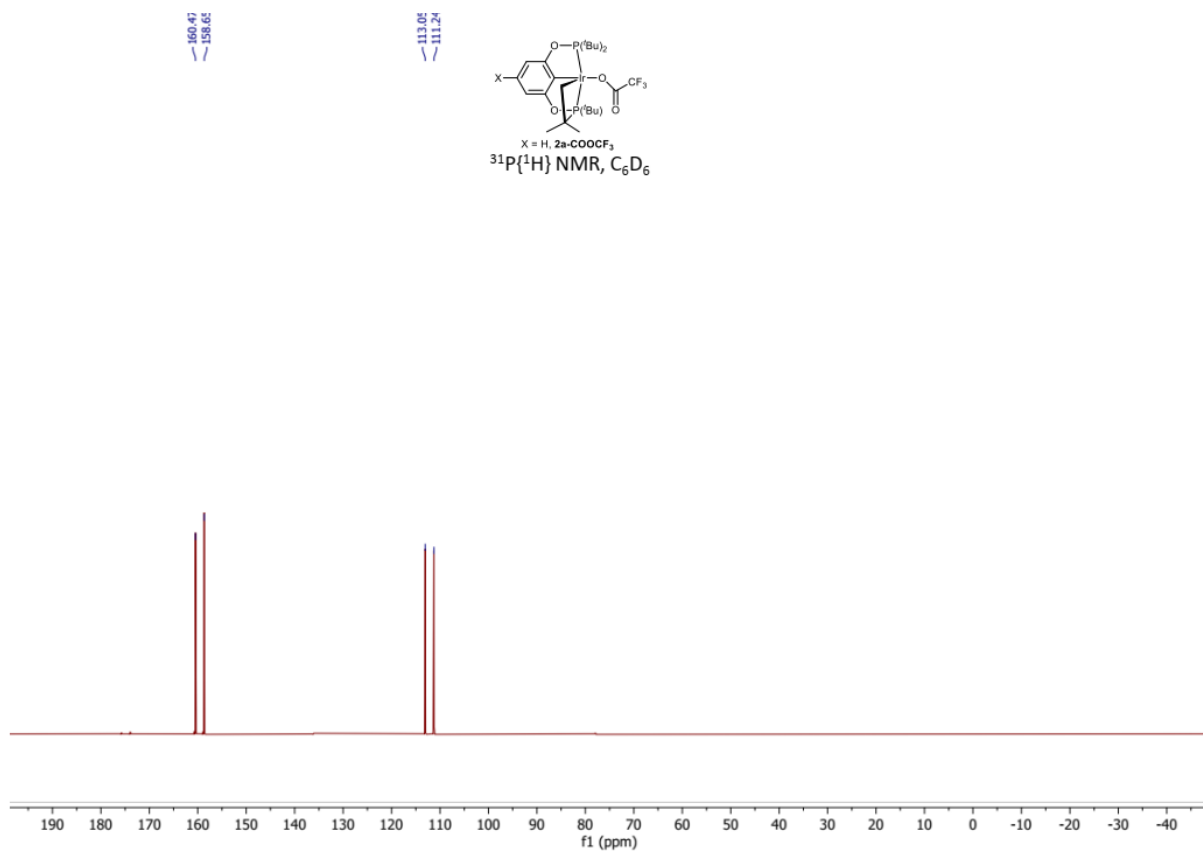
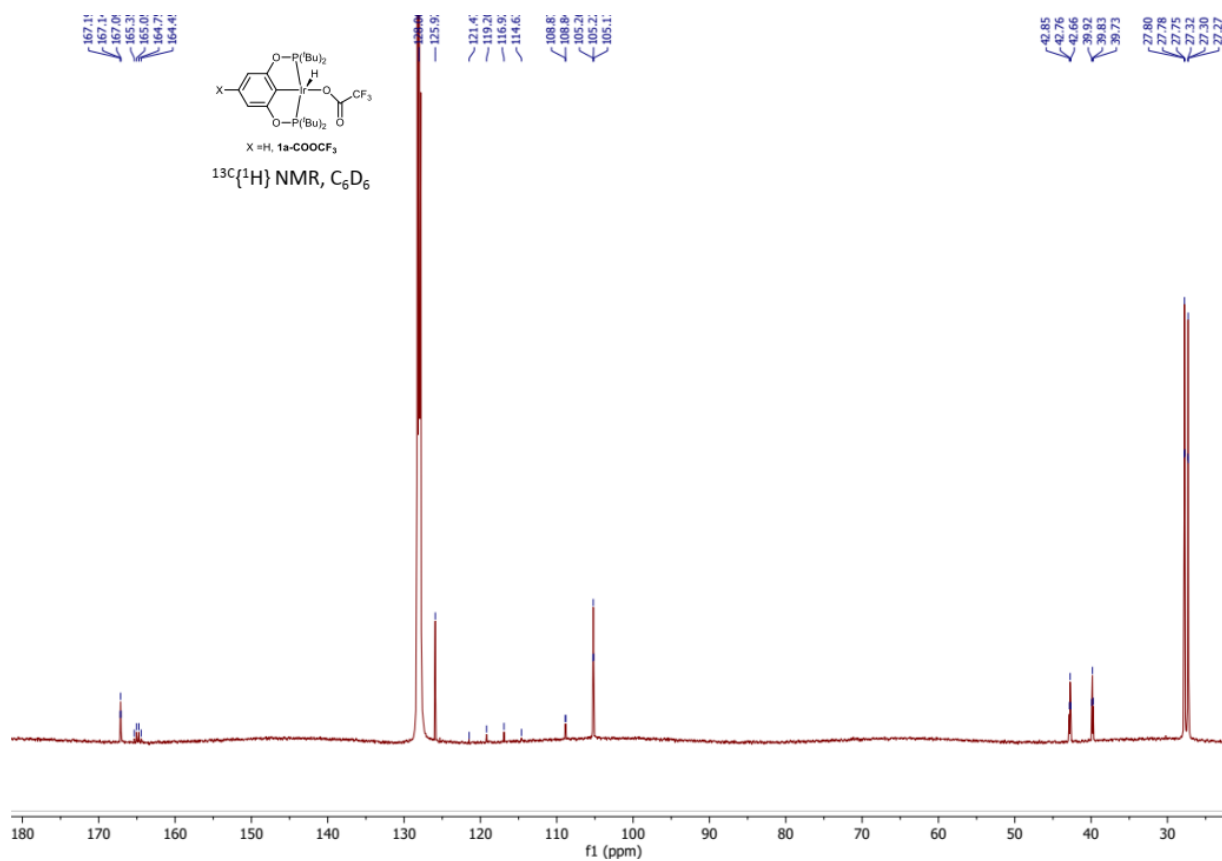


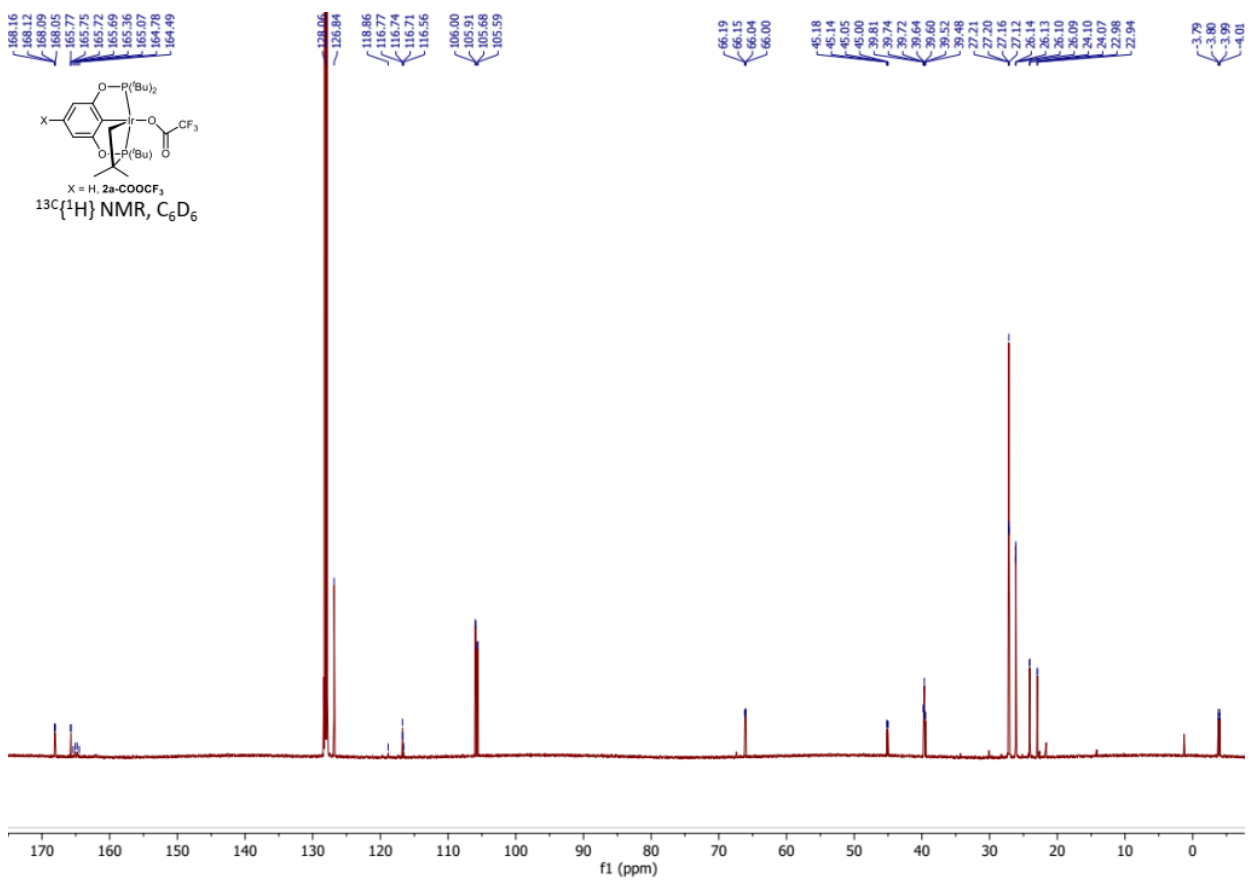
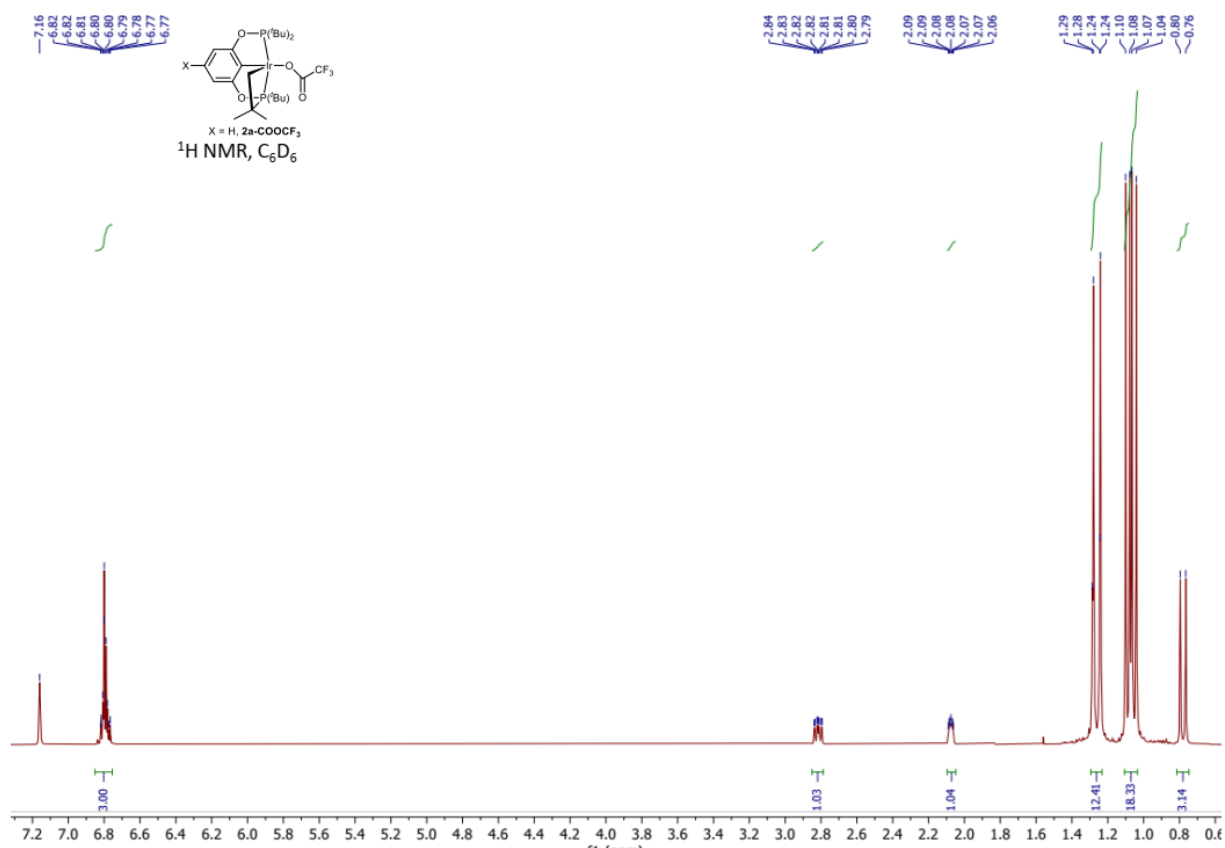
Figure S5. Two cyclic voltammograms of complex **1a** recorded with ca. 30 min time gap. The second CV demonstrates weaker oxidation wave, that is presumably associated with adsorption of **1a** or its oxidation products on the electrode. If CVs are extended to negative potential (-2.5...-3 V), a much better stability of CVs with time is observed.

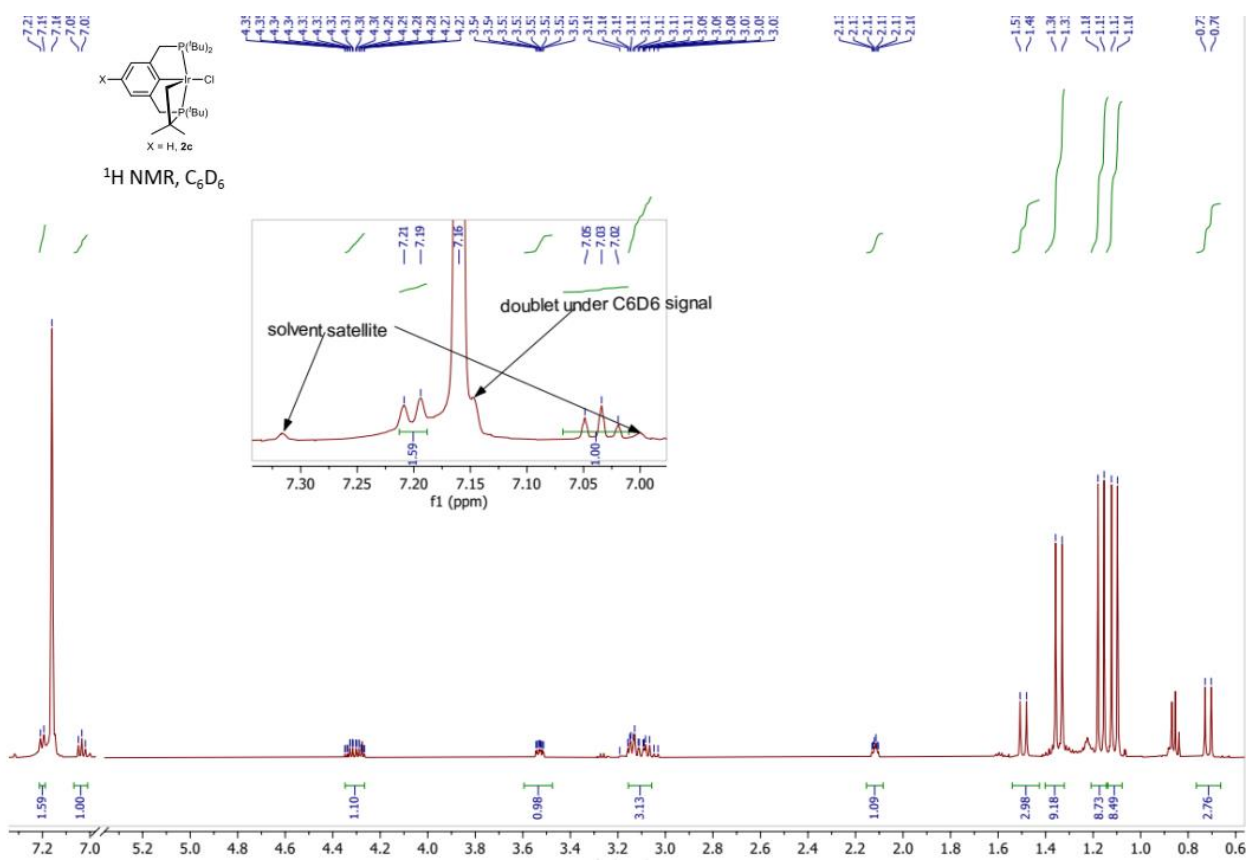
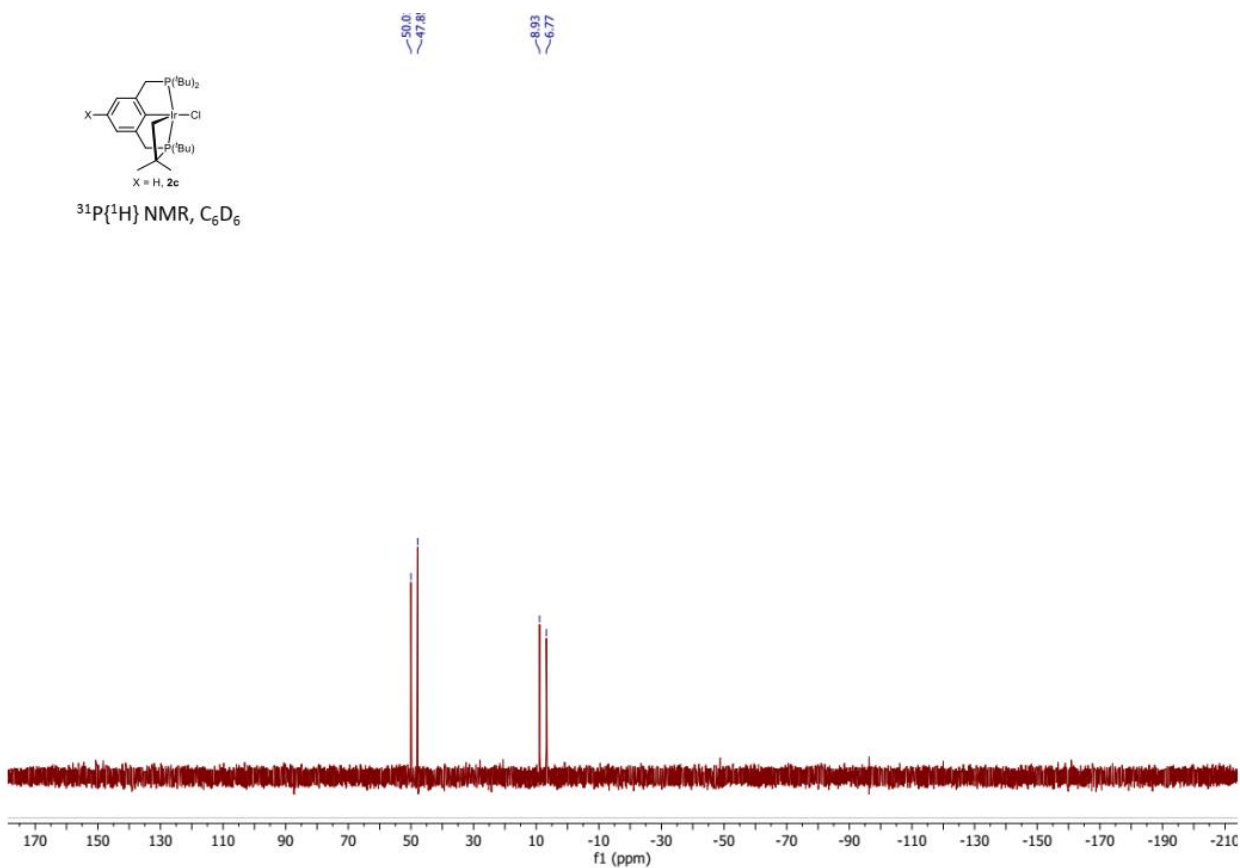
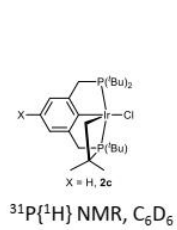
3. NMR spectra of the new compounds

Note that the high-field hydride resonance is not fully decoupled in the $^3\text{P}\{^1\text{H}\}$ NMR spectrum









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H	2.491221000	1.265870000	-2.441702000
H	3.443737000	2.718711000	-1.981191000
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C	4.200720000	1.781239000	0.587465000
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Cl	0.122695000	-0.239396000	-2.886846000

(POCOP)IrHCl⁺ (**1a⁺**), E = -2258.90616256362

68

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(POCOP)IrCl double cyclometallated (**2a**), E = -2257.88507993071

66

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H	-3.365073000	1.644024000	1.348155000
H	-2.484025000	2.321691000	-0.066285000
H	-4.272911000	2.444144000	0.018433000
Cl	0.231284000	0.100121000	-2.862686000

(POCOP)IrCl⁺ double cyclometallated (**2a⁺**), E = -2257.69159710438

66

C	-1.044978000	-0.837904000	3.671210000
C	-1.028060000	-0.691636000	2.282417000
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C	1.431306000	-0.655152000	2.300858000
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O	-2.204791000	-0.660506000	1.593303000
P	2.538638000	-0.429204000	-0.070070000
P	-2.070261000	-0.567351000	-0.112363000
Ir	0.205531000	-0.386965000	-0.411501000
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H	2.440200000	-2.005408000	-2.483047000
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H	5.274914000	1.089246000	0.398724000
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H	4.125008000	1.406174000	1.743118000
C	1.965155000	2.207239000	0.168270000
H	1.080444000	2.031518000	-0.489375000
H	1.669034000	2.050773000	1.224267000
H	2.229935000	3.278337000	0.048527000
C	-2.474409000	-2.523379000	-2.116562000
H	-2.022083000	-1.783261000	-2.806323000
H	-2.197198000	-3.535451000	-2.476630000
H	-3.577122000	-2.438890000	-2.164056000
C	-3.592026000	0.719583000	-2.028227000
H	-4.387144000	1.463786000	-2.239084000
H	-2.627761000	1.134536000	-2.383966000
H	-3.819658000	-0.189941000	-2.613509000
C	-0.402165000	-2.382558000	-0.653000000
H	0.005892000	-2.980768000	0.181558000
H	0.056778000	-2.685628000	-1.614554000
C	-2.590410000	-3.370327000	0.281091000
H	-3.693468000	-3.270111000	0.290225000
H	-2.342278000	-4.397657000	-0.056724000
H	-2.217991000	-3.251182000	1.316707000
C	-4.841000000	-0.290712000	-0.044874000
H	-5.721323000	0.359004000	-0.231275000
H	-4.995425000	-1.234700000	-0.603391000
H	-4.806804000	-0.516769000	1.038574000
C	-3.390044000	1.776862000	0.256234000
H	-3.360978000	1.619637000	1.351323000
H	-2.463336000	2.300126000	-0.055272000
H	-4.249414000	2.438932000	0.024153000
Cl	0.179303000	0.250708000	-2.731287000

(POCOP)IrCl⁺ (ii), E = -2258.28756808506

67

C	-1.113736000	-1.086102000	3.630252000
C	-1.129877000	-0.864440000	2.253229000
C	0.109479000	-0.629846000	1.512486000
C	1.346096000	-0.548085000	2.289624000
C	1.346446000	-0.771696000	3.666413000
C	0.119297000	-1.028141000	4.310178000
H	-2.049970000	-1.301831000	4.161967000
H	2.291181000	-0.746898000	4.225568000
H	0.124944000	-1.197054000	5.397910000

O	2.499476000	-0.286271000	1.655163000
O	-2.293270000	-0.898263000	1.584902000
P	2.416609000	-0.213068000	-0.080145000
P	-2.180827000	-0.804108000	-0.147578000
Ir	0.117846000	-0.475272000	-0.398054000
C	3.438215000	-1.716842000	-0.571727000
C	3.231795000	1.464034000	-0.341869000
C	-2.773110000	-2.517221000	-0.659526000
C	-3.386469000	0.611477000	-0.443569000
C	3.200759000	-1.903474000	-2.084294000
H	3.697483000	-2.843391000	-2.402344000
H	2.120579000	-1.995281000	-2.320725000
H	3.622084000	-1.077440000	-2.687773000
C	3.583472000	1.603714000	-1.833857000
H	2.708135000	1.411700000	-2.485913000
H	3.918052000	2.645814000	-2.016962000
H	4.412137000	0.932089000	-2.131238000
C	2.830234000	-2.909074000	0.194396000
H	2.982623000	-2.822616000	1.287640000
H	1.744949000	-3.018631000	-0.007422000
H	3.334343000	-3.835962000	-0.147901000
C	4.932043000	-1.588159000	-0.249213000
H	5.426150000	-2.552269000	-0.490549000
H	5.425657000	-0.803415000	-0.853299000
H	5.106081000	-1.380228000	0.824465000
C	4.473367000	1.653251000	0.546356000
H	5.304898000	0.982002000	0.268665000
H	4.827561000	2.696848000	0.415421000
H	4.238668000	1.506412000	1.617726000
C	2.155585000	2.496425000	0.056153000
H	1.265738000	2.438724000	-0.598463000
H	1.830660000	2.369912000	1.108546000
H	2.593556000	3.511299000	-0.039958000
C	-2.442970000	-2.637655000	-2.161365000
H	-1.365408000	-2.461115000	-2.358350000
H	-2.682042000	-3.670263000	-2.489899000
H	-3.031898000	-1.939522000	-2.785787000
C	-3.718236000	0.658290000	-1.945976000
H	-4.300274000	1.581701000	-2.145805000
H	-2.804028000	0.694557000	-2.571408000
H	-4.340609000	-0.201009000	-2.262868000
C	-1.912495000	-3.518447000	0.137207000
H	-0.827995000	-3.350905000	-0.025121000
H	-2.121274000	-3.474473000	1.223643000
H	-2.154079000	-4.541986000	-0.215505000
C	-4.261718000	-2.768504000	-0.389256000
H	-4.915412000	-2.132569000	-1.015990000
H	-4.489178000	-3.825638000	-0.639520000
H	-4.519686000	-2.611450000	0.676116000
C	-4.660442000	0.479845000	0.408387000
H	-5.264238000	1.398919000	0.258741000
H	-5.285861000	-0.381300000	0.114519000
H	-4.426696000	0.399204000	1.486975000
C	-2.619019000	1.883081000	-0.022986000

H	-2.301615000	1.842438000	1.038493000
H	-1.726182000	2.053512000	-0.653351000
H	-3.297583000	2.753422000	-0.137278000
Cl	-0.003494000	0.699170000	-2.424437000

1a-TS1, E = -2258.25968803897

67

C	-1.134233000	-0.838701000	3.669580000
C	-1.095405000	-0.784064000	2.275881000
C	0.142174000	-0.599115000	1.555184000
C	1.355653000	-0.548097000	2.332816000
C	1.323749000	-0.589452000	3.731140000
C	0.080865000	-0.730187000	4.376573000
H	-2.090543000	-0.974571000	4.192019000
H	2.259247000	-0.521987000	4.302700000
H	0.057109000	-0.764977000	5.476203000
O	2.550078000	-0.451540000	1.695717000
O	-2.249462000	-0.954178000	1.562089000
P	2.495346000	-0.294956000	-0.022282000
P	-2.082911000	-0.753623000	-0.127819000
Ir	0.164172000	-0.398285000	-0.405040000
C	3.538967000	-1.765296000	-0.560165000
C	3.295966000	1.402905000	-0.209494000
C	-2.014711000	-2.484534000	-0.905438000
C	-3.509410000	0.390642000	-0.503132000
C	3.383346000	-1.896201000	-2.087627000
H	3.899378000	-2.821929000	-2.415161000
H	2.321723000	-1.970260000	-2.396876000
H	3.836114000	-1.046554000	-2.632077000
C	3.704116000	1.586888000	-1.681699000
H	2.858556000	1.386242000	-2.370119000
H	4.016768000	2.642151000	-1.825773000
H	4.563399000	0.946035000	-1.959400000
C	2.928831000	-2.993974000	0.143761000
H	3.056421000	-2.943987000	1.241845000
H	1.848805000	-3.117425000	-0.072629000
H	3.447952000	-3.902234000	-0.224291000
C	5.015758000	-1.624936000	-0.163436000
H	5.537814000	-2.570477000	-0.418346000
H	5.521094000	-0.808957000	-0.713820000
H	5.136373000	-1.455535000	0.924201000
C	4.491338000	1.597518000	0.736673000
H	5.346775000	0.945933000	0.484451000
H	4.832603000	2.649458000	0.641569000
H	4.211083000	1.423837000	1.792864000
C	2.176795000	2.401198000	0.160324000
H	1.321650000	2.329763000	-0.542744000
H	1.811148000	2.250492000	1.196199000
H	2.585023000	3.431244000	0.097050000
C	-3.165003000	-2.917925000	-1.819589000
H	-3.355818000	-2.198496000	-2.637097000
H	-2.905991000	-3.892587000	-2.281598000
H	-4.096187000	-3.059654000	-1.238166000
C	-3.495288000	0.654335000	-2.019070000
H	-4.219342000	1.466819000	-2.234243000

H	-2.495579000	0.980300000	-2.373287000
H	-3.809125000	-0.231172000	-2.603189000
C	-0.729989000	-2.244904000	-1.719313000
H	0.300494000	-1.973123000	-1.019537000
H	-0.186090000	-3.192854000	-1.950027000
H	-0.837126000	-1.654289000	-2.645584000
C	-1.783252000	-3.512860000	0.212284000
H	-2.675637000	-3.607091000	0.859074000
H	-1.584852000	-4.499217000	-0.254538000
H	-0.914989000	-3.256872000	0.851809000
C	-4.831163000	-0.225604000	-0.021725000
H	-5.643301000	0.510258000	-0.198194000
H	-5.088092000	-1.148176000	-0.576036000
H	-4.805735000	-0.451895000	1.061807000
C	-3.182569000	1.686262000	0.266038000
H	-3.149641000	1.522183000	1.360527000
H	-2.218154000	2.123777000	-0.062180000
H	-3.981440000	2.426163000	0.054241000
Cl	0.245685000	0.686378000	-2.622719000

iii, E = -2258.28613428535

67

C	-1.043015000	-0.618663000	3.685326000
C	-1.015773000	-0.798852000	2.299912000
C	0.232336000	-0.799461000	1.609170000
C	1.456745000	-0.619157000	2.318630000
C	1.429743000	-0.434720000	3.706269000
C	0.182501000	-0.441445000	4.360886000
H	-2.000369000	-0.605824000	4.223390000
H	2.366159000	-0.284358000	4.260215000
H	0.162309000	-0.291559000	5.450772000
O	2.627153000	-0.652863000	1.622458000
O	-2.159772000	-0.974230000	1.572250000
P	2.566399000	-0.487183000	-0.101953000
P	-2.047098000	-0.745782000	-0.134076000
Ir	0.205516000	-0.572160000	-0.486370000
C	3.763066000	-1.819726000	-0.639250000
C	3.129569000	1.302587000	-0.268654000
C	-2.033150000	-2.470760000	-0.898256000
C	-3.481836000	0.421708000	-0.402383000
C	3.656586000	-1.907411000	-2.174567000
H	4.232576000	-2.791557000	-2.516697000
H	2.606361000	-2.031627000	-2.507910000
H	4.076766000	-1.016469000	-2.677665000
C	3.466820000	1.572110000	-1.745071000
H	2.647654000	1.258771000	-2.423647000
H	3.615730000	2.664154000	-1.875640000
H	4.404791000	1.069632000	-2.050943000
C	3.232788000	-3.120137000	-0.002699000
H	3.275145000	-3.086698000	1.102890000
H	2.192536000	-3.339516000	-0.315255000
H	3.867241000	-3.962093000	-0.347436000
C	5.203852000	-1.549258000	-0.183972000
H	5.826624000	-2.430036000	-0.444797000

H	5.642561000	-0.669730000	-0.692523000
H	5.269071000	-1.400435000	0.911553000
C	4.305862000	1.654095000	0.652742000
H	5.241923000	1.150458000	0.350621000
H	4.478824000	2.748848000	0.590594000
H	4.091595000	1.401754000	1.708711000
C	1.879213000	2.110446000	0.151065000
H	0.998760000	1.884401000	-0.496319000
H	1.604238000	1.945377000	1.211632000
H	2.086678000	3.193506000	0.024938000
C	-2.770977000	-2.521820000	-2.242848000
H	-2.411213000	-1.741828000	-2.941946000
H	-2.574665000	-3.508673000	-2.709666000
H	-3.865863000	-2.419695000	-2.113835000
C	-3.525583000	0.799492000	-1.893187000
H	-4.244691000	1.635629000	-2.013421000
H	-2.537080000	1.138584000	-2.263400000
H	-3.873096000	-0.035462000	-2.528203000
C	-0.491152000	-2.474859000	-1.116077000
H	0.355087000	-1.728546000	0.863923000
H	0.024473000	-3.261358000	-0.532034000
H	-0.202480000	-2.530515000	-2.181937000
C	-2.512876000	-3.559424000	0.065223000
H	-3.599346000	-3.468400000	0.261716000
H	-2.327799000	-4.551985000	-0.394517000
H	-1.978479000	-3.524155000	1.034406000
C	-4.781009000	-0.250809000	0.068561000
H	-5.613525000	0.474545000	-0.044901000
H	-5.029175000	-1.144690000	-0.536710000
H	-4.726361000	-0.544025000	1.134795000
C	-3.150523000	1.663615000	0.449021000
H	-3.096586000	1.426033000	1.528731000
H	-2.195200000	2.130923000	0.135130000
H	-3.958490000	2.409541000	0.302498000
Cl	0.159507000	0.206995000	-2.731858000

1a-TS2, E = -2258.28288977988

67

C	-1.005436000	-0.526760000	3.678938000
C	-0.996211000	-0.778089000	2.307204000
C	0.258441000	-0.897211000	1.598747000
C	1.498006000	-0.676909000	2.309422000
C	1.481712000	-0.423888000	3.683198000
C	0.233418000	-0.360964000	4.335647000
H	-1.955098000	-0.437076000	4.223017000
H	2.420192000	-0.260186000	4.229439000
H	0.222935000	-0.148101000	5.415549000
O	2.650304000	-0.747555000	1.610048000
O	-2.139915000	-0.916172000	1.597060000
P	2.559291000	-0.546707000	-0.124907000
P	-2.022303000	-0.704324000	-0.131003000
Ir	0.224528000	-0.558958000	-0.486656000
C	3.787533000	-1.837263000	-0.684203000
C	3.074737000	1.261583000	-0.244926000

C	-2.014358000	-2.446230000	-0.848481000
C	-3.478732000	0.434130000	-0.398485000
C	3.733815000	-1.852388000	-2.225115000
H	4.291306000	-2.740504000	-2.587060000
H	2.692940000	-1.922023000	-2.601896000
H	4.203471000	-0.955449000	-2.670081000
C	3.392720000	1.575445000	-1.717085000
H	2.586000000	1.237196000	-2.399223000
H	3.491904000	2.675383000	-1.826876000
H	4.351183000	1.121115000	-2.033915000
C	3.240425000	-3.169069000	-0.131349000
H	3.226737000	-3.184647000	0.975809000
H	2.219683000	-3.378975000	-0.507501000
H	3.900068000	-3.990445000	-0.478633000
C	5.208226000	-1.577008000	-0.165039000
H	5.849959000	-2.438194000	-0.444740000
H	5.654457000	-0.669951000	-0.615642000
H	5.232771000	-1.479033000	0.937859000
C	4.239991000	1.641072000	0.677188000
H	5.191437000	1.176659000	0.359447000
H	4.374115000	2.742314000	0.635725000
H	4.043442000	1.360435000	1.729493000
C	1.791604000	2.007873000	0.193745000
H	0.901302000	1.726903000	-0.429211000
H	1.550107000	1.851245000	1.263236000
H	1.926114000	3.098453000	0.036770000
C	-2.668783000	-2.488364000	-2.236500000
H	-2.246995000	-1.719706000	-2.913773000
H	-2.465724000	-3.482121000	-2.685779000
H	-3.767185000	-2.361715000	-2.176616000
C	-3.511452000	0.803950000	-1.892940000
H	-4.234169000	1.634977000	-2.026443000
H	-2.521035000	1.144920000	-2.257051000
H	-3.845967000	-0.037909000	-2.525979000
C	-0.458776000	-2.494092000	-0.971437000
H	0.332758000	-1.916769000	1.111917000
H	-0.010732000	-3.249838000	-0.294373000
H	-0.112341000	-2.671465000	-2.007094000
C	-2.587650000	-3.510051000	0.090516000
H	-3.682919000	-3.391392000	0.208349000
H	-2.395337000	-4.513845000	-0.341359000
H	-2.123220000	-3.473743000	1.095235000
C	-4.772897000	-0.255418000	0.059999000
H	-5.616600000	0.454944000	-0.065406000
H	-4.999015000	-1.155957000	-0.544256000
H	-4.725632000	-0.544011000	1.127989000
C	-3.176846000	1.686428000	0.448255000
H	-3.134806000	1.456723000	1.530251000
H	-2.222507000	2.163273000	0.145348000
H	-3.991363000	2.421838000	0.285258000
Cl	0.190201000	0.085891000	-2.797355000

iv, E = -2258.28381068069

67

C	-1.001324000	-0.672839000	3.667025000
C	-1.011551000	-0.870337000	2.287883000
C	0.244156000	-1.066622000	1.540195000
C	1.499741000	-0.837402000	2.278528000
C	1.492305000	-0.637455000	3.658816000
C	0.247041000	-0.568929000	4.316708000
H	-1.942165000	-0.561014000	4.222253000
H	2.433820000	-0.500067000	4.207090000
O	2.639849000	-0.873843000	1.584905000
O	-2.155621000	-0.920267000	1.597667000
P	2.523622000	-0.587839000	-0.152181000
P	-2.027069000	-0.675618000	-0.144199000
Ir	0.214664000	-0.516467000	-0.475487000
C	3.734543000	-1.862669000	-0.782108000
C	3.075302000	1.215202000	-0.172367000
C	-1.995572000	-2.409726000	-0.877720000
C	-3.514705000	0.428079000	-0.380109000
C	3.658419000	-1.806346000	-2.321651000
H	4.196286000	-2.685530000	-2.731969000
H	2.611590000	-1.839457000	-2.686660000
H	4.136814000	-0.897117000	-2.731060000
C	3.394660000	1.596949000	-1.628536000
H	2.581839000	1.301701000	-2.323828000
H	3.507716000	2.699609000	-1.684839000
H	4.346765000	1.146542000	-1.969373000
C	3.188060000	-3.215473000	-0.282332000
H	3.192001000	-3.281711000	0.823203000
H	2.160626000	-3.403236000	-0.650199000
H	3.838632000	-4.023026000	-0.676171000
C	5.164871000	-1.635439000	-0.274280000
H	5.796667000	-2.485104000	-0.606990000
H	5.609346000	-0.709641000	-0.686826000
H	5.208813000	-1.592634000	0.831569000
C	4.246279000	1.534585000	0.764661000
H	5.190566000	1.071344000	0.424836000
H	4.396851000	2.634509000	0.773648000
H	4.046960000	1.209479000	1.803588000
C	1.801461000	1.954974000	0.303317000
H	0.905549000	1.715337000	-0.331761000
H	1.561267000	1.754145000	1.365788000
H	1.945810000	3.050326000	0.195202000
C	-2.605543000	-2.426872000	-2.286584000
H	-2.164938000	-1.641946000	-2.932989000
H	-2.381894000	-3.410282000	-2.749050000
H	-3.706181000	-2.307542000	-2.261029000
C	-3.546987000	0.829083000	-1.867611000
H	-4.282628000	1.650722000	-1.988279000
H	-2.560235000	1.192622000	-2.220279000
H	-3.863892000	-0.005570000	-2.519137000
C	-0.434825000	-2.448197000	-0.951849000
H	0.273953000	-2.185315000	1.399437000
H	-0.011039000	-3.193979000	-0.248483000
H	-0.062196000	-2.649916000	-1.974689000
C	-2.598522000	-3.491590000	0.021131000

H	-3.698095000	-3.380825000	0.100989000
H	-2.385576000	-4.487130000	-0.420410000
H	-2.171721000	-3.473054000	1.043044000
C	-4.795147000	-0.301665000	0.052834000
H	-5.655340000	0.390545000	-0.061818000
H	-4.995122000	-1.192844000	-0.574080000
H	-4.748588000	-0.614741000	1.113997000
C	-3.249483000	1.670120000	0.493390000
H	-3.208356000	1.419603000	1.570842000
H	-2.304497000	2.174890000	0.206654000
H	-4.079992000	2.389591000	0.339710000
Cl	0.192213000	0.183544000	-2.801145000
H	0.248299000	-0.388752000	5.403087000

i, E = -2258.47246674245

67

C	-1.013293000	-1.125455000	3.561823000
C	-0.948760000	-1.010017000	2.165342000
C	0.284834000	-0.739251000	1.481074000
C	1.456648000	-0.584059000	2.297410000
C	1.408580000	-0.697428000	3.694364000
C	0.170229000	-0.967555000	4.307792000
H	-1.974651000	-1.334340000	4.051552000
H	2.325812000	-0.574065000	4.287051000
H	0.126150000	-1.057347000	5.404104000
O	2.651441000	-0.316478000	1.695523000
O	-2.091614000	-1.152999000	1.437792000
P	2.575846000	-0.154296000	-0.028734000
P	-1.889365000	-1.051146000	-0.282123000
Ir	0.355477000	-0.565500000	-0.478777000
C	3.825376000	-1.481214000	-0.523422000
C	3.185388000	1.626432000	-0.198594000
C	-2.470877000	-2.800765000	-0.838148000
C	-3.121709000	0.349317000	-0.599584000
C	4.008205000	-1.411309000	-2.050771000
H	4.529899000	-2.329507000	-2.393428000
H	3.034247000	-1.347678000	-2.579151000
H	4.625960000	-0.544234000	-2.353992000
C	3.284579000	1.955087000	-1.699632000
H	2.376079000	1.636988000	-2.251669000
H	3.399312000	3.052867000	-1.820001000
H	4.163351000	1.474795000	-2.171147000
C	3.135558000	-2.809761000	-0.146446000
H	2.972181000	-2.890334000	0.946736000
H	2.152237000	-2.909551000	-0.649466000
H	3.786249000	-3.652611000	-0.460524000
C	5.169508000	-1.376252000	0.211114000
H	5.763122000	-2.291414000	0.002666000
H	5.766778000	-0.510279000	-0.128545000
H	5.030301000	-1.303578000	1.307446000
C	4.510648000	1.901428000	0.526133000
H	5.372201000	1.430449000	0.017722000
H	4.691178000	2.997179000	0.537667000
H	4.482062000	1.550441000	1.576197000

C	2.064119000	2.472801000	0.441794000
H	1.084970000	2.280068000	-0.041950000
H	1.959348000	2.262623000	1.524817000
H	2.316202000	3.547375000	0.323185000
C	-3.745667000	-2.810267000	-1.696026000
H	-3.631275000	-2.225546000	-2.628344000
H	-3.952807000	-3.859978000	-1.993049000
H	-4.634194000	-2.443407000	-1.149775000
C	-3.226776000	0.572259000	-2.119300000
H	-3.736427000	1.540882000	-2.305581000
H	-2.224210000	0.614004000	-2.593852000
H	-3.818662000	-0.215719000	-2.620801000
C	-1.306998000	-3.369903000	-1.674767000
H	-0.368941000	-3.413698000	-1.085487000
H	-1.568809000	-4.396845000	-2.006534000
H	-1.103364000	-2.748915000	-2.569613000
C	-2.682481000	-3.668676000	0.414590000
H	-3.516051000	-3.299631000	1.042271000
H	-2.925428000	-4.700970000	0.084862000
H	-1.772602000	-3.719242000	1.044400000
C	-4.491294000	0.108944000	0.052794000
H	-5.107787000	1.025925000	-0.059430000
H	-5.048839000	-0.722177000	-0.416979000
H	-4.388558000	-0.101500000	1.135116000
C	-2.460844000	1.586061000	0.047092000
H	-2.336335000	1.461660000	1.140961000
H	-1.462660000	1.785569000	-0.392378000
H	-3.111456000	2.468607000	-0.127324000
Cl	0.419984000	-0.248836000	-2.884888000

1a-TS3, E = -2258.42980580841

67

C	-1.126791000	-0.980298000	3.647277000
C	-1.075351000	-0.850339000	2.249409000
C	0.141004000	-0.604629000	1.563990000
C	1.326586000	-0.540449000	2.336288000
C	1.303273000	-0.663994000	3.736211000
C	0.070520000	-0.879552000	4.379166000
H	-2.090788000	-1.161031000	4.143833000
H	2.241954000	-0.594930000	4.304580000
H	0.042973000	-0.976660000	5.475075000
O	2.535959000	-0.354274000	1.700101000
O	-2.247850000	-0.973178000	1.521444000
P	2.477144000	-0.246930000	-0.013746000
P	-2.061887000	-0.772113000	-0.166202000
Ir	0.190342000	-0.414188000	-0.448024000
C	3.552881000	-1.727634000	-0.506333000
C	3.323185000	1.428633000	-0.252166000
C	-2.051777000	-2.499899000	-0.966034000
C	-3.505529000	0.375051000	-0.512073000
C	3.341699000	-1.950633000	-2.016081000
H	3.883674000	-2.868717000	-2.325767000
H	2.267643000	-2.081477000	-2.255987000
H	3.727793000	-1.109559000	-2.623521000

C	3.700425000	1.583033000	-1.735639000
H	2.823704000	1.408351000	-2.392382000
H	4.054294000	2.621601000	-1.907946000
H	4.520874000	0.900190000	-2.031868000
C	3.006300000	-2.936407000	0.278118000
H	3.160678000	-2.819880000	1.368009000
H	1.924759000	-3.098404000	0.096627000
H	3.542954000	-3.848659000	-0.055479000
C	5.042827000	-1.552663000	-0.179506000
H	5.571619000	-2.501938000	-0.408869000
H	5.515124000	-0.757130000	-0.786660000
H	5.204868000	-1.328299000	0.892913000
C	4.541364000	1.619668000	0.666733000
H	5.397235000	0.982033000	0.383836000
H	4.872600000	2.676875000	0.590441000
H	4.284191000	1.418242000	1.724428000
C	2.245220000	2.467850000	0.123781000
H	1.372737000	2.406360000	-0.555662000
H	1.895222000	2.334188000	1.167322000
H	2.686478000	3.483477000	0.040095000
C	-3.193678000	-2.859183000	-1.924257000
H	-3.280244000	-2.143159000	-2.762802000
H	-2.989202000	-3.859042000	-2.361439000
H	-4.169087000	-2.915245000	-1.400403000
C	-3.564559000	0.640210000	-2.026589000
H	-4.281210000	1.467257000	-2.213184000
H	-2.573580000	0.943358000	-2.424175000
H	-3.921001000	-0.240501000	-2.592918000
C	-0.707764000	-2.318126000	-1.692543000
H	0.348868000	-1.974743000	-0.279902000
H	-0.092767000	-3.236733000	-1.758897000
H	-0.767168000	-1.793765000	-2.662911000
C	-1.941394000	-3.547407000	0.152415000
H	-2.869760000	-3.602468000	0.753203000
H	-1.763459000	-4.540828000	-0.309791000
H	-1.097997000	-3.337699000	0.840949000
C	-4.816223000	-0.215538000	0.028252000
H	-5.633573000	0.521151000	-0.122315000
H	-5.100864000	-1.145895000	-0.500567000
H	-4.744846000	-0.431714000	1.112065000
C	-3.142200000	1.678354000	0.227150000
H	-3.052784000	1.520451000	1.319757000
H	-2.187701000	2.098132000	-0.150342000
H	-3.943421000	2.425761000	0.049832000
Cl	0.130927000	0.935569000	-2.520784000

v, E = -2258.43569147583

67

C	-1.140833000	-0.864901000	3.678874000
C	-1.089151000	-0.793562000	2.277620000
C	0.115412000	-0.490924000	1.591871000
C	1.305514000	-0.403648000	2.355408000
C	1.278884000	-0.465730000	3.759445000
C	0.049510000	-0.684066000	4.407883000

H	-2.096062000	-1.074939000	4.180541000
H	2.215112000	-0.360711000	4.326396000
H	0.021235000	-0.735332000	5.506822000
O	2.514467000	-0.276362000	1.710948000
O	-2.239643000	-1.057544000	1.548481000
P	2.475678000	-0.274302000	-0.012451000
P	-2.067943000	-0.845503000	-0.139416000
Ir	0.166984000	-0.509958000	-0.438831000
C	3.564392000	-1.782963000	-0.402465000
C	3.332937000	1.390786000	-0.301696000
C	-2.029989000	-2.487402000	-1.076505000
C	-3.480205000	0.350389000	-0.462455000
C	3.358535000	-2.088315000	-1.898399000
H	3.913213000	-3.013725000	-2.160127000
H	2.286408000	-2.245437000	-2.131620000
H	3.736080000	-1.274560000	-2.548214000
C	3.615126000	1.540565000	-1.806067000
H	2.689671000	1.408174000	-2.402054000
H	4.001266000	2.564056000	-1.998568000
H	4.384265000	0.825126000	-2.159325000
C	3.022533000	-2.948759000	0.446326000
H	3.158828000	-2.763447000	1.529287000
H	1.947068000	-3.139644000	0.256523000
H	3.578613000	-3.870684000	0.177113000
C	5.054946000	-1.591776000	-0.088931000
H	5.577084000	-2.558205000	-0.252445000
H	5.529649000	-0.845299000	-0.753272000
H	5.222362000	-1.293091000	0.964014000
C	4.614258000	1.563016000	0.533065000
H	5.459501000	0.961883000	0.156594000
H	4.916820000	2.630222000	0.482674000
H	4.441712000	1.310672000	1.597223000
C	2.308611000	2.450026000	0.159359000
H	1.375847000	2.400286000	-0.433295000
H	2.062479000	2.333597000	1.233738000
H	2.760336000	3.455188000	0.022323000
C	-3.207821000	-2.868813000	-1.977284000
H	-3.417390000	-2.104528000	-2.748093000
H	-2.956257000	-3.812077000	-2.506458000
H	-4.132272000	-3.049009000	-1.392100000
C	-3.586837000	0.638208000	-1.969122000
H	-4.319392000	1.459715000	-2.114771000
H	-2.613167000	0.964641000	-2.386533000
H	-3.953255000	-0.234742000	-2.540385000
C	-0.751180000	-2.060710000	-1.845675000
H	0.441738000	-1.958295000	0.101138000
H	-0.045134000	-2.895005000	-2.023062000
H	-0.975038000	-1.518345000	-2.783713000
C	-1.756751000	-3.614518000	-0.069656000
H	-2.650661000	-3.827860000	0.548662000
H	-1.492988000	-4.534688000	-0.631686000
H	-0.914136000	-3.380733000	0.611396000
C	-4.783522000	-0.240388000	0.099766000
H	-5.599018000	0.501583000	-0.033374000

H	-5.080555000	-1.166007000	-0.431280000
H	-4.695583000	-0.463973000	1.180616000
C	-3.082978000	1.638733000	0.284519000
H	-2.956975000	1.465216000	1.371253000
H	-2.141018000	2.055066000	-0.124858000
H	-3.886944000	2.391908000	0.148589000
Cl	-0.036804000	1.246676000	-2.176878000

1g, E = -2373.54614224156

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C	-0.285323000	1.190784000	-3.625752000
C	-0.148731000	1.177763000	-2.232078000
C	-0.087348000	-0.024343000	-1.483624000
C	-0.152841000	-1.229636000	-2.216161000
C	-0.290049000	-1.267478000	-3.616177000
C	-0.354586000	-0.042480000	-4.315235000
H	-0.337251000	2.134885000	-4.184815000
H	-0.341289000	-2.237897000	-4.124416000
O	-0.078857000	-2.431747000	-1.535970000
O	-0.070562000	2.384465000	-1.561973000
P	0.036255000	-2.298929000	0.170412000
P	0.046642000	2.269364000	0.145303000
Ir	0.088378000	-0.012723000	0.522120000
H	1.615190000	-0.017281000	0.304312000
C	1.581931000	-3.327277000	0.497748000
C	-1.584083000	-3.122413000	0.685109000
C	1.597616000	3.293933000	0.459096000
C	-1.568805000	3.106017000	0.653796000
C	1.921024000	-3.212863000	1.996118000
H	2.940295000	-3.618879000	2.165125000
H	1.898406000	-2.160099000	2.343991000
H	1.220579000	-3.792331000	2.626451000
C	-1.517709000	-3.446752000	2.187232000
H	-1.165900000	-2.574350000	2.777154000
H	-2.535091000	-3.714469000	2.542622000
H	-0.854961000	-4.309201000	2.395354000
C	2.698897000	-2.666695000	-0.335913000
H	2.473055000	-2.690757000	-1.419648000
H	2.866238000	-1.613107000	-0.035996000
H	3.644038000	-3.222585000	-0.164954000
C	1.424695000	-4.794216000	0.070530000
H	2.406830000	-5.303450000	0.166505000
H	0.705790000	-5.339552000	0.711473000
H	1.099114000	-4.881135000	-0.984810000
C	-1.932793000	-4.361216000	-0.152716000
H	-1.248970000	-5.207893000	0.038398000
H	-2.959040000	-4.692178000	0.113214000
H	-1.914984000	-4.132640000	-1.235737000
C	-2.644481000	-2.026619000	0.440339000
H	-2.466676000	-1.141291000	1.086344000
H	-2.666676000	-1.694267000	-0.616971000
H	-3.648315000	-2.426665000	0.694926000
C	1.938231000	3.195253000	1.958248000
H	1.910326000	2.146818000	2.318591000

H	2.960003000	3.597451000	2.121118000
H	1.241963000	3.786012000	2.582669000
C	-1.497411000	3.449401000	2.151449000
H	-2.512897000	3.725255000	2.506010000
H	-1.147196000	2.583334000	2.751560000
H	-0.831197000	4.312162000	2.346913000
C	2.710412000	2.618631000	-0.368286000
H	2.873388000	1.567836000	-0.056340000
H	2.483359000	2.631179000	-1.451962000
H	3.658287000	3.172152000	-0.204957000
C	1.446414000	4.756463000	0.015085000
H	0.730487000	5.312330000	0.650298000
H	2.430828000	5.262514000	0.104309000
H	1.120223000	4.832452000	-1.040906000
C	-1.914358000	4.335294000	-0.199246000
H	-2.937980000	4.675031000	0.065685000
H	-1.225599000	5.180964000	-0.021764000
H	-1.901216000	4.092321000	-1.279191000
C	-2.634145000	2.011395000	0.426109000
H	-2.660104000	1.664610000	-0.626490000
H	-2.458274000	1.134395000	1.083942000
H	-3.635896000	2.418763000	0.677175000
O	-0.487520000	0.047346000	-5.671405000
C	-0.555662000	-1.157092000	-6.421000000
H	0.364965000	-1.769582000	-6.300680000
H	-1.433914000	-1.774470000	-6.129810000
H	-0.657206000	-0.860456000	-7.481167000
Cl	0.037208000	0.000733000	2.992865000

1g⁺, E = -2373.36581469379

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C	-0.278129000	1.199043000	-3.607736000
C	-0.149960000	1.201262000	-2.227864000
C	-0.087987000	-0.025105000	-1.468626000
C	-0.158444000	-1.261560000	-2.211965000
C	-0.287357000	-1.289821000	-3.598018000
C	-0.346276000	-0.051750000	-4.291210000
H	-0.325350000	2.132589000	-4.183054000
H	-0.337683000	-2.253485000	-4.117570000
O	-0.095528000	-2.434769000	-1.534451000
O	-0.078635000	2.386057000	-1.562608000
P	0.025437000	-2.329740000	0.186799000
P	0.037207000	2.300348000	0.154582000
Ir	0.068045000	-0.013399000	0.487546000
H	1.603235000	-0.016569000	0.273991000
C	1.591773000	-3.317838000	0.499352000
C	-1.594036000	-3.149494000	0.685706000
C	1.607398000	3.282755000	0.465403000
C	-1.578859000	3.131270000	0.646519000
C	1.958143000	-3.137111000	1.985357000
H	2.949406000	-3.604045000	2.159463000
H	2.025824000	-2.067571000	2.267123000
H	1.232362000	-3.626724000	2.661196000
C	-1.519042000	-3.491978000	2.184126000

H	-1.196704000	-2.621245000	2.791289000
H	-2.531524000	-3.789451000	2.527427000
H	-0.837113000	-4.341331000	2.382239000
C	2.680299000	-2.679017000	-0.386277000
H	2.449454000	-2.774269000	-1.464702000
H	2.834813000	-1.606889000	-0.149491000
H	3.638253000	-3.202849000	-0.191077000
C	1.430728000	-4.802114000	0.138101000
H	2.418095000	-5.297703000	0.243133000
H	0.726070000	-5.321883000	0.814689000
H	1.093267000	-4.939282000	-0.907818000
C	-1.927392000	-4.383884000	-0.165983000
H	-1.227057000	-5.220490000	0.006516000
H	-2.942804000	-4.732763000	0.115439000
H	-1.935732000	-4.144997000	-1.246585000
C	-2.657144000	-2.054821000	0.449400000
H	-2.493409000	-1.176030000	1.107723000
H	-2.687964000	-1.716408000	-0.606028000
H	-3.657315000	-2.465713000	0.698133000
C	1.963534000	3.127319000	1.956565000
H	2.016704000	2.062854000	2.259993000
H	2.959245000	3.585929000	2.127431000
H	1.239863000	3.638781000	2.618265000
C	-1.505633000	3.493146000	2.140228000
H	-2.517945000	3.797331000	2.478179000
H	-1.185900000	2.629933000	2.759328000
H	-0.822250000	4.343632000	2.328115000
C	2.698395000	2.622429000	-0.401254000
H	2.850077000	1.555748000	-0.139077000
H	2.471810000	2.693269000	-1.482475000
H	3.656636000	3.148830000	-0.214483000
C	1.457079000	4.761149000	0.075705000
H	0.750538000	5.296933000	0.737650000
H	2.446277000	5.253638000	0.178154000
H	1.127093000	4.880447000	-0.974806000
C	-1.907047000	4.355663000	-0.221571000
H	-2.922459000	4.710702000	0.052089000
H	-1.204946000	5.192543000	-0.057339000
H	-1.912115000	4.103091000	-1.299062000
C	-2.645580000	2.037340000	0.422892000
H	-2.676299000	1.685469000	-0.628136000
H	-2.485013000	1.166435000	1.092501000
H	-3.644844000	2.454142000	0.665377000
O	-0.469023000	0.040587000	-5.617383000
C	-0.545595000	-1.149105000	-6.415476000
H	0.374676000	-1.756831000	-6.301567000
H	-1.432655000	-1.752494000	-6.135719000
H	-0.640519000	-0.804718000	-7.459493000
Cl	-0.107296000	0.004875000	2.894728000

1b', E = -2486.8412664915

74

C	-0.286191000	1.168603000	-3.631908000
C	-0.147245000	1.166194000	-2.239680000

C	-0.081470000	-0.037928000	-1.491881000
C	-0.149484000	-1.255532000	-2.216983000
C	-0.288606000	-1.288126000	-3.610079000
C	-0.356146000	-0.065422000	-4.317058000
H	-0.338664000	2.110749000	-4.194078000
H	-0.341465000	-2.248087000	-4.139095000
O	-0.076432000	-2.449513000	-1.526730000
O	-0.072039000	2.372797000	-1.572594000
P	0.037589000	-2.312617000	0.178182000
P	0.045339000	2.268350000	0.134277000
Ir	0.087894000	-0.019036000	0.505373000
H	1.608899000	-0.023896000	0.246853000
C	1.585944000	-3.331952000	0.514123000
C	-1.583061000	-3.131126000	0.696181000
C	1.598739000	3.287632000	0.446683000
C	-1.570697000	3.103422000	0.639951000
C	1.924322000	-3.204571000	2.011619000
H	2.940696000	-3.616003000	2.184270000
H	1.910950000	-2.148232000	2.348513000
H	1.220056000	-3.772606000	2.647982000
C	-1.517964000	-3.450741000	2.199298000
H	-1.170589000	-2.575894000	2.787886000
H	-2.535328000	-3.720414000	2.552900000
H	-0.853294000	-4.310786000	2.410770000
C	2.701462000	-2.675783000	-0.324864000
H	2.476901000	-2.708767000	-1.408599000
H	2.868875000	-1.619961000	-0.032332000
H	3.647174000	-3.229018000	-0.149186000
C	1.429907000	-4.802543000	0.098929000
H	2.412410000	-5.309603000	0.201067000
H	0.710436000	-5.342849000	0.743432000
H	1.106710000	-4.898994000	-0.956292000
C	-1.928862000	-4.373426000	-0.137979000
H	-1.244852000	-5.218804000	0.058046000
H	-2.955155000	-4.703555000	0.128306000
H	-1.910353000	-4.149679000	-1.221952000
C	-2.642971000	-2.036259000	0.445275000
H	-2.467766000	-1.148313000	1.088330000
H	-2.665899000	-1.709512000	-0.613807000
H	-3.646782000	-2.435667000	0.700394000
C	1.940098000	3.188722000	1.945603000
H	1.924938000	2.139194000	2.303013000
H	2.957849000	3.600925000	2.107978000
H	1.238642000	3.770709000	2.572395000
C	-1.500720000	3.453041000	2.136147000
H	-2.516198000	3.733920000	2.486453000
H	-1.155664000	2.588815000	2.741555000
H	-0.832219000	4.314529000	2.328828000
C	2.709611000	2.610459000	-0.381641000
H	2.872742000	1.559632000	-0.069342000
H	2.483115000	2.623837000	-1.465390000
H	3.658187000	3.162561000	-0.218293000
C	1.447585000	4.750220000	0.002458000
H	0.731967000	5.306228000	0.637772000

H	2.432381000	5.255212000	0.091978000
H	1.122018000	4.826692000	-1.053652000
C	-1.913871000	4.329910000	-0.218334000
H	-2.938067000	4.669542000	0.044026000
H	-1.225880000	5.176269000	-0.041428000
H	-1.899253000	4.084162000	-1.297575000
C	-2.635203000	2.007564000	0.414051000
H	-2.661287000	1.658457000	-0.637817000
H	-2.461740000	1.132930000	1.075529000
H	-3.637110000	2.415959000	0.662292000
Cl	-0.001381000	0.004763000	2.963275000
C	-0.501465000	-0.021479000	-5.795610000
O	-0.565625000	1.005819000	-6.463523000
O	-0.557011000	-1.257573000	-6.350589000
C	-0.695094000	-1.294988000	-7.777521000
H	-1.627276000	-0.787011000	-8.096806000
H	0.164271000	-0.796913000	-8.269881000
H	-0.727468000	-2.363516000	-8.053748000

1b⁺⁺, E = -2486.64140888882

74

C	-0.281501000	1.179883000	-3.616551000
C	-0.153037000	1.191091000	-2.229192000
C	-0.090619000	-0.036924000	-1.469945000
C	-0.163912000	-1.278276000	-2.206764000
C	-0.292652000	-1.295625000	-3.595649000
C	-0.349882000	-0.063147000	-4.285944000
H	-0.327129000	2.114408000	-4.190667000
H	-0.345256000	-2.247994000	-4.136823000
O	-0.102694000	-2.449032000	-1.527661000
O	-0.081359000	2.373999000	-1.571833000
P	0.023385000	-2.345202000	0.192556000
P	0.036469000	2.300800000	0.149877000
Ir	0.066139000	-0.019531000	0.482905000
H	1.603375000	-0.024102000	0.269519000
C	1.594548000	-3.323517000	0.504934000
C	-1.596724000	-3.159355000	0.696202000
C	1.609521000	3.279217000	0.451246000
C	-1.583221000	3.128983000	0.632148000
C	1.966452000	-3.124312000	1.987266000
H	2.950516000	-3.604524000	2.165437000
H	2.054615000	-2.051826000	2.251162000
H	1.235256000	-3.590985000	2.673382000
C	-1.518786000	-3.501561000	2.194521000
H	-1.200560000	-2.630795000	2.803311000
H	-2.530459000	-3.802646000	2.536757000
H	-0.834467000	-4.349017000	2.392308000
C	2.675530000	-2.691646000	-0.394385000
H	2.442439000	-2.805553000	-1.470386000
H	2.826301000	-1.615080000	-0.174917000
H	3.636994000	-3.206694000	-0.193748000
C	1.431884000	-4.811778000	0.161468000
H	2.420328000	-5.304548000	0.268363000
H	0.730834000	-5.324053000	0.847377000

H	1.090803000	-4.961475000	-0.881472000
C	-1.930481000	-4.394289000	-0.154636000
H	-1.228476000	-5.229898000	0.015702000
H	-2.944125000	-4.743770000	0.131947000
H	-1.944316000	-4.156151000	-1.235228000
C	-2.657309000	-2.062545000	0.458635000
H	-2.493895000	-1.183567000	1.116950000
H	-2.689474000	-1.726121000	-0.597420000
H	-3.658029000	-2.471443000	0.707957000
C	1.968678000	3.119298000	1.941425000
H	2.040753000	2.054043000	2.237788000
H	2.957996000	3.591396000	2.112043000
H	1.239526000	3.616347000	2.608048000
C	-1.509644000	3.502068000	2.123186000
H	-2.522175000	3.810763000	2.455992000
H	-1.193745000	2.644091000	2.751040000
H	-0.825337000	4.353029000	2.304994000
C	2.695197000	2.617879000	-0.420998000
H	2.845763000	1.549769000	-0.163215000
H	2.467852000	2.694612000	-1.501571000
H	3.655319000	3.140328000	-0.233426000
C	1.456237000	4.758134000	0.065196000
H	0.751566000	5.292047000	0.730570000
H	2.445842000	5.249692000	0.166748000
H	1.124443000	4.880075000	-0.984330000
C	-1.910676000	4.346978000	-0.245040000
H	-2.923520000	4.706326000	0.032035000
H	-1.205585000	5.183091000	-0.090549000
H	-1.923147000	4.086433000	-1.320449000
C	-2.645850000	2.030132000	0.413928000
H	-2.675758000	1.671677000	-0.634920000
H	-2.486359000	1.164722000	1.091028000
H	-3.646352000	2.446395000	0.651670000
Cl	-0.123727000	0.004165000	2.874826000
C	-0.486188000	-0.016317000	-5.780903000
O	-0.540207000	1.021579000	-6.424611000
O	-0.540445000	-1.244414000	-6.323021000
C	-0.669375000	-1.296516000	-7.755726000
H	-1.600265000	-0.789573000	-8.077630000
H	0.195636000	-0.800949000	-8.238776000
H	-0.699619000	-2.367578000	-8.018317000

1a-COOCF₃, E = -2324.98845763412

74

C	-1.164224000	-0.633842000	3.626920000
C	-1.094936000	-0.666896000	2.223453000
C	0.119318000	-0.479973000	1.520923000
C	1.290479000	-0.334550000	2.302090000
C	1.257379000	-0.296955000	3.706726000
C	0.020045000	-0.438753000	4.359256000
H	-2.134282000	-0.770079000	4.126232000
H	2.193668000	-0.168945000	4.268796000
H	-0.020299000	-0.408896000	5.458630000
O	2.515913000	-0.244307000	1.666309000

O	-2.254381000	-0.907623000	1.508720000
P	2.477292000	-0.368379000	-0.035219000
P	-2.084483000	-0.940220000	-0.189244000
Ir	0.196756000	-0.558523000	-0.486103000
H	0.379242000	-2.067601000	-0.177926000
C	3.453666000	-1.963888000	-0.357135000
C	3.437028000	1.209575000	-0.452664000
C	-2.631923000	-2.702742000	-0.626616000
C	-3.365533000	0.388223000	-0.618770000
C	3.125547000	-2.390049000	-1.801569000
H	3.644728000	-3.345864000	-2.023527000
H	2.036995000	-2.543476000	-1.938713000
H	3.461458000	-1.642875000	-2.547535000
C	3.742539000	1.224479000	-1.959716000
H	2.828449000	1.116894000	-2.575457000
H	4.202504000	2.199665000	-2.224204000
H	4.457328000	0.430554000	-2.252796000
C	2.919930000	-3.014409000	0.636404000
H	3.159163000	-2.742705000	1.682478000
H	1.823212000	-3.149734000	0.555675000
H	3.398689000	-3.989644000	0.410106000
C	4.971873000	-1.834994000	-0.166320000
H	5.427901000	-2.838577000	-0.300019000
H	5.435974000	-1.161949000	-0.911886000
H	5.234097000	-1.480579000	0.849172000
C	4.723391000	1.363677000	0.378539000
H	5.525608000	0.673341000	0.067211000
H	5.101672000	2.398298000	0.239861000
H	4.525101000	1.217898000	1.457878000
C	2.481811000	2.365467000	-0.088908000
H	1.556321000	2.339270000	-0.692398000
H	2.211467000	2.342463000	0.985785000
H	3.001772000	3.326242000	-0.286265000
C	-2.126187000	-2.969596000	-2.058110000
H	-1.026026000	-2.858563000	-2.124565000
H	-2.392556000	-4.007650000	-2.347669000
H	-2.582484000	-2.285265000	-2.800571000
C	-3.573578000	0.415844000	-2.141777000
H	-4.258358000	1.252055000	-2.395753000
H	-2.628508000	0.590596000	-2.691068000
H	-4.035355000	-0.516965000	-2.521047000
C	-1.921931000	-3.643187000	0.366530000
H	-0.821672000	-3.512997000	0.352224000
H	-2.276881000	-3.482875000	1.402681000
H	-2.142269000	-4.692154000	0.079032000
C	-4.145776000	-2.943950000	-0.538190000
H	-4.709963000	-2.364689000	-1.293506000
H	-4.341042000	-4.019237000	-0.734749000
H	-4.546274000	-2.709221000	0.466820000
C	-4.700935000	0.187735000	0.120539000
H	-5.302029000	1.113816000	0.003119000
H	-5.297872000	-0.647615000	-0.283292000
H	-4.541489000	0.023007000	1.203556000
C	-2.738941000	1.714425000	-0.139293000

H	-2.546490000	1.698966000	0.952109000
H	-1.794910000	1.937385000	-0.668803000
H	-3.457024000	2.535982000	-0.343792000
O	0.276604000	-0.489798000	-2.762718000
C	0.103299000	0.762691000	-2.819933000
O	-0.040700000	1.496071000	-1.804520000
C	0.072395000	1.446336000	-4.203426000
F	0.201856000	0.566570000	-5.210591000
F	1.079505000	2.347738000	-4.299796000
F	-1.094242000	2.112552000	-4.372789000

1a-COOCF₃⁺, E = -2324.79466267829

74

C	-1.166282000	-0.704350000	3.622270000
C	-1.110227000	-0.775298000	2.229747000
C	0.137348000	-0.616790000	1.514567000
C	1.338228000	-0.485955000	2.310831000
C	1.285258000	-0.414991000	3.703502000
C	0.032226000	-0.518387000	4.340128000
H	-2.131750000	-0.806178000	4.135601000
H	2.212298000	-0.293546000	4.279575000
H	-0.010286000	-0.465664000	5.438272000
O	2.539377000	-0.439854000	1.684172000
O	-2.245590000	-1.005422000	1.525589000
P	2.518196000	-0.416414000	-0.035424000
P	-2.117157000	-0.973098000	-0.189130000
Ir	0.215809000	-0.734260000	-0.429789000
H	0.376866000	-2.232759000	-0.020785000
C	3.673080000	-1.840008000	-0.454122000
C	3.198544000	1.325314000	-0.314720000
C	-2.867546000	-2.630638000	-0.665336000
C	-3.176007000	0.554540000	-0.534867000
C	3.605245000	-2.041397000	-1.980867000
H	4.189962000	-2.948619000	-2.237607000
H	2.567395000	-2.193581000	-2.337163000
H	4.046822000	-1.193256000	-2.538157000
C	3.534279000	1.505620000	-1.804633000
H	2.671549000	1.296864000	-2.465624000
H	3.820277000	2.565057000	-1.969533000
H	4.391187000	0.879433000	-2.119193000
C	3.101879000	-3.078247000	0.265028000
H	3.099842000	-2.956578000	1.365513000
H	2.073074000	-3.318139000	-0.070150000
H	3.743060000	-3.948384000	0.016516000
C	5.116529000	-1.593754000	0.010069000
H	5.695698000	-2.526059000	-0.152779000
H	5.610812000	-0.792891000	-0.570897000
H	5.171407000	-1.345848000	1.087860000
C	4.428931000	1.607899000	0.565205000
H	5.320597000	1.039008000	0.250068000
H	4.670176000	2.686841000	0.469943000
H	4.229102000	1.398194000	1.633103000
C	2.055371000	2.275869000	0.100832000
H	1.164424000	2.164035000	-0.544487000

H	1.759493000	2.135904000	1.159638000
H	2.418000000	3.318777000	-0.005596000
C	-2.632005000	-2.810089000	-2.178150000
H	-1.560995000	-2.723512000	-2.447373000
H	-2.974992000	-3.825390000	-2.465198000
H	-3.205417000	-2.082453000	-2.783853000
C	-3.448273000	0.651947000	-2.045406000
H	-3.972257000	1.610197000	-2.241675000
H	-2.519351000	0.662420000	-2.647162000
H	-4.104368000	-0.163260000	-2.406579000
C	-2.081788000	-3.699897000	0.119228000
H	-1.001567000	-3.690906000	-0.128506000
H	-2.197898000	-3.582580000	1.214007000
H	-2.477858000	-4.696381000	-0.163932000
C	-4.360878000	-2.732042000	-0.320446000
H	-4.980876000	-2.067685000	-0.950830000
H	-4.690091000	-3.773732000	-0.514417000
H	-4.558895000	-2.508156000	0.745709000
C	-4.491954000	0.532169000	0.262673000
H	-4.976324000	1.522891000	0.139473000
H	-5.200853000	-0.231926000	-0.100175000
H	-4.315880000	0.373138000	1.343434000
C	-2.323145000	1.751196000	-0.062084000
H	-2.070243000	1.684663000	1.014877000
H	-1.392488000	1.857003000	-0.649663000
H	-2.918131000	2.676418000	-0.204890000
O	0.356904000	-1.266950000	-2.671300000
C	0.221030000	-0.055088000	-2.998843000
O	0.081659000	0.857438000	-2.128005000
C	0.222702000	0.354473000	-4.486338000
F	0.365889000	-0.709437000	-5.286417000
F	1.236214000	1.214863000	-4.723681000
F	-0.936942000	0.974704000	-4.792819000

2a-COOCF₃, E = -2323.77517756488

72

C	-1.048950000	-0.919147000	3.690904000
C	-1.004366000	-0.711843000	2.301380000
C	0.214481000	-0.538227000	1.601091000
C	1.409253000	-0.639045000	2.355275000
C	1.400587000	-0.836610000	3.746326000
C	0.162940000	-0.969600000	4.402682000
H	-2.017759000	-1.044265000	4.195383000
H	2.350959000	-0.893897000	4.296222000
H	0.143710000	-1.125850000	5.491963000
O	2.626572000	-0.551677000	1.699636000
O	-2.191738000	-0.688912000	1.588297000
P	2.530565000	-0.395905000	0.000305000
P	-2.015213000	-0.492859000	-0.099735000
Ir	0.245038000	-0.284977000	-0.388937000
C	3.654762000	-1.791998000	-0.572274000
C	3.237024000	1.338654000	-0.237495000
C	-1.869330000	-2.255862000	-0.770705000
C	-3.582317000	0.473179000	-0.455197000

C	3.463931000	-1.933537000	-2.094623000
H	4.001647000	-2.840843000	-2.440559000
H	2.394635000	-2.039721000	-2.365476000
H	3.871109000	-1.068520000	-2.651417000
C	3.560220000	1.544542000	-1.727668000
H	2.721600000	1.238256000	-2.385350000
H	3.754966000	2.622281000	-1.908900000
H	4.466043000	0.986181000	-2.034968000
C	3.143730000	-3.060052000	0.139848000
H	3.255534000	-2.983192000	1.238371000
H	2.081840000	-3.266285000	-0.091251000
H	3.740965000	-3.927079000	-0.211245000
C	5.129957000	-1.559799000	-0.215053000
H	5.708772000	-2.468932000	-0.482585000
H	5.567864000	-0.711521000	-0.775052000
H	5.265921000	-1.379788000	0.869524000
C	4.451306000	1.638530000	0.652421000
H	5.351007000	1.074449000	0.346835000
H	4.690640000	2.720245000	0.574619000
H	4.236307000	1.410943000	1.714375000
C	2.060267000	2.252280000	0.177830000
H	1.162069000	2.105939000	-0.470342000
H	1.773987000	2.103178000	1.237719000
H	2.360869000	3.314360000	0.053651000
C	-2.291265000	-2.320289000	-2.245609000
H	-1.801362000	-1.531006000	-2.850129000
H	-1.980157000	-3.301401000	-2.661596000
H	-3.389553000	-2.238519000	-2.364422000
C	-3.615972000	0.843824000	-1.948135000
H	-4.502749000	1.487209000	-2.126753000
H	-2.715362000	1.417267000	-2.241946000
H	-3.706956000	-0.040084000	-2.605936000
C	-0.317844000	-2.272684000	-0.638276000
H	0.008774000	-2.871049000	0.234417000
H	0.183364000	-2.629956000	-1.561246000
C	-2.564467000	-3.325850000	0.073597000
H	-3.667046000	-3.256011000	-0.013673000
H	-2.257609000	-4.332014000	-0.282134000
H	-2.294259000	-3.241601000	1.144174000
C	-4.809169000	-0.358656000	-0.048407000
H	-5.723266000	0.258245000	-0.179107000
H	-4.921250000	-1.262526000	-0.679345000
H	-4.756117000	-0.671439000	1.012663000
C	-3.473223000	1.757050000	0.390486000
H	-3.445441000	1.533851000	1.474102000
H	-2.565800000	2.335312000	0.121956000
H	-4.358834000	2.394605000	0.187088000
O	0.314178000	-0.027456000	-2.558781000
C	-0.069671000	1.125093000	-2.968317000
O	-0.379600000	2.121999000	-2.301407000
C	-0.169912000	1.180579000	-4.516478000
F	-1.155386000	0.348614000	-4.952206000
F	0.985345000	0.785766000	-5.102717000
F	-0.457787000	2.417422000	-4.962871000

2a-COOCF₃⁺, E = -2323.58322784433

72

C	-1.152228000	-0.640827000	3.607707000
C	-1.117908000	-0.540544000	2.216903000
C	0.127641000	-0.458280000	1.492384000
C	1.344008000	-0.580693000	2.259621000
C	1.315992000	-0.676963000	3.653758000
C	0.069952000	-0.695212000	4.309013000
H	-2.116575000	-0.693111000	4.130613000
H	2.257967000	-0.749769000	4.213839000
H	0.048635000	-0.773785000	5.406203000
O	2.537408000	-0.623548000	1.612975000
O	-2.285514000	-0.537331000	1.511859000
P	2.500095000	-0.343020000	-0.082979000
P	-2.120636000	-0.628226000	-0.188817000
Ir	0.141484000	-0.342778000	-0.454152000
C	3.553920000	-1.741387000	-0.779809000
C	3.328236000	1.363505000	-0.108738000
C	-1.908575000	-2.462892000	-0.563154000
C	-3.631271000	0.319862000	-0.728224000
C	3.198259000	-1.805425000	-2.280216000
H	3.768841000	-2.637544000	-2.741238000
H	2.120376000	-1.995511000	-2.446169000
H	3.468423000	-0.876421000	-2.819850000
C	3.598370000	1.752859000	-1.572123000
H	2.683798000	1.731905000	-2.194880000
H	3.982916000	2.793485000	-1.593459000
H	4.364299000	1.107823000	-2.044423000
C	3.110760000	-3.031855000	-0.065480000
H	3.355229000	-3.005466000	1.013543000
H	2.030109000	-3.229997000	-0.178787000
H	3.654580000	-3.883428000	-0.523245000
C	5.066076000	-1.555043000	-0.591335000
H	5.570223000	-2.463672000	-0.980976000
H	5.461498000	-0.691595000	-1.158084000
H	5.344281000	-1.448159000	0.474390000
C	4.623155000	1.390194000	0.723246000
H	5.453853000	0.840581000	0.250325000
H	4.937475000	2.450001000	0.820848000
H	4.462799000	0.991405000	1.743185000
C	2.316042000	2.333670000	0.535667000
H	1.371808000	2.399777000	-0.034064000
H	2.091964000	2.061435000	1.586125000
H	2.772222000	3.344871000	0.548469000
C	-2.418527000	-2.808695000	-1.968796000
H	-2.014594000	-2.124421000	-2.740975000
H	-2.075414000	-3.833889000	-2.218459000
H	-3.524570000	-2.800395000	-2.018503000
C	-3.680725000	0.340385000	-2.266755000
H	-4.483132000	1.042353000	-2.572445000
H	-2.737641000	0.703905000	-2.720143000
H	-3.918166000	-0.648996000	-2.697249000
C	-0.350841000	-2.390168000	-0.541137000

H	0.079438000	-2.951169000	0.307537000
H	0.105005000	-2.727561000	-1.493349000
C	-2.496140000	-3.387635000	0.504557000
H	-3.602906000	-3.338007000	0.514004000
H	-2.201323000	-4.431949000	0.272927000
H	-2.124661000	-3.146828000	1.519268000
C	-4.883559000	-0.343564000	-0.131792000
H	-5.770484000	0.258622000	-0.418800000
H	-5.032466000	-1.369951000	-0.521617000
H	-4.839594000	-0.383043000	0.973556000
C	-3.424615000	1.747451000	-0.183664000
H	-3.358154000	1.762614000	0.921162000
H	-2.509938000	2.211652000	-0.604236000
H	-4.295010000	2.365330000	-0.485711000
O	0.121963000	-0.243665000	-2.749535000
C	0.064750000	1.019192000	-2.722951000
O	0.052425000	1.665731000	-1.632660000
C	0.042588000	1.786721000	-4.060983000
F	-0.856466000	1.235205000	-4.899813000
F	1.264457000	1.713613000	-4.636507000
F	-0.268680000	3.077637000	-3.882585000

1c, E = -2187.23778815058

72

Ir	-0.000368000	-0.431242000	-0.039484000
C	-0.019441000	1.597508000	-0.032802000
P	-2.324980000	-0.199253000	-0.120308000
P	2.322283000	-0.148318000	0.048005000
C	-2.476843000	1.569258000	-0.677032000
C	-3.310476000	-1.192183000	-1.412131000
C	-3.114209000	-0.248236000	1.617413000
C	2.445643000	1.629774000	0.584099000
C	3.260280000	-1.094544000	1.411785000
C	3.191197000	-0.238796000	-1.644308000
C	-1.220164000	2.326737000	-0.306616000
C	-1.236942000	3.733890000	-0.262388000
C	-0.066376000	4.456769000	0.018913000
C	1.160704000	2.354543000	0.249220000
C	1.127911000	3.762788000	0.267212000
H	-2.178901000	4.270133000	-0.463431000
H	-0.084930000	5.557355000	0.041565000
H	2.052288000	4.321439000	0.488107000
H	-2.580230000	1.529122000	-1.783506000
H	-3.398440000	2.057156000	-0.298610000
H	2.584584000	1.606077000	1.686432000
H	3.344505000	2.134373000	0.173380000
C	-3.545011000	-2.625626000	-0.905414000
C	-2.406950000	-1.250933000	-2.660767000
C	-4.646696000	-0.524436000	-1.780567000
C	-2.926801000	-1.643956000	2.241694000
C	-4.599588000	0.140479000	1.621641000
C	-2.310169000	0.770759000	2.452540000
C	2.816237000	-1.576237000	-2.309331000
C	2.627715000	0.917347000	-2.494698000

C	4.717130000	-0.091148000	-1.547674000
C	3.523853000	-2.542232000	0.963457000
C	4.574178000	-0.414440000	1.833734000
C	2.285095000	-1.110941000	2.608819000
H	-2.693695000	0.759933000	3.494548000
H	-1.230494000	0.514653000	2.481983000
H	-2.396883000	1.804691000	2.065417000
H	-4.783015000	1.121698000	1.139400000
H	-4.950675000	0.217240000	2.673009000
H	-5.228311000	-0.620339000	1.120354000
H	-3.615733000	-2.390903000	1.806742000
H	-3.144392000	-1.582229000	3.329101000
H	-1.893913000	-2.023383000	2.107006000
H	-5.341352000	-0.464192000	-0.922596000
H	-5.142630000	-1.129712000	-2.569346000
H	-4.509035000	0.496272000	-2.188664000
H	-2.149526000	-0.241890000	-3.043433000
H	-1.464284000	-1.789792000	-2.443872000
H	-2.944429000	-1.788333000	-3.470557000
H	-3.922486000	-3.246708000	-1.745589000
H	-4.306173000	-2.661352000	-0.102311000
H	-2.604770000	-3.078268000	-0.529820000
H	3.045259000	0.839062000	-3.520615000
H	1.523314000	0.875617000	-2.570334000
H	2.905416000	1.911475000	-2.093187000
H	3.214732000	-2.447376000	-1.756565000
H	3.235783000	-1.603451000	-3.337352000
H	1.716259000	-1.692095000	-2.374729000
H	5.014971000	0.840846000	-1.026170000
H	5.141051000	-0.046334000	-2.573581000
H	5.189420000	-0.949389000	-1.032671000
H	3.923114000	-3.118271000	1.825709000
H	4.277408000	-2.597586000	0.153691000
H	2.586986000	-3.029667000	0.626195000
H	1.997444000	-0.089617000	2.934362000
H	1.366752000	-1.679863000	2.361125000
H	2.776942000	-1.606828000	3.472633000
H	5.323459000	-0.393262000	1.021857000
H	5.013968000	-0.987842000	2.677823000
H	4.418140000	0.622628000	2.190630000
H	0.032771000	-0.181377000	-1.561392000
Cl	-0.032384000	-2.890221000	0.330947000

1c⁺, E = -2187.04868964158

72

Ir	0.001523000	-0.391266000	-0.075333000
C	-0.018667000	1.592866000	-0.038987000
P	-2.357807000	-0.195798000	-0.122999000
P	2.362360000	-0.147561000	0.024133000
C	-2.493161000	1.573714000	-0.665393000
C	-3.341428000	-1.179773000	-1.413896000
C	-3.082521000	-0.257912000	1.634821000
C	2.464934000	1.628291000	0.558234000
C	3.230168000	-1.099022000	1.420486000

C	3.226223000	-0.249664000	-1.660806000
C	-1.245675000	2.326470000	-0.289633000
C	-1.255126000	3.723218000	-0.229051000
C	-0.067045000	4.431730000	0.035008000
C	1.185716000	2.351650000	0.234445000
C	1.144804000	3.749497000	0.256551000
H	-2.191131000	4.273150000	-0.408740000
H	-0.085240000	5.531654000	0.065636000
H	2.062752000	4.320101000	0.463293000
H	-2.573191000	1.544539000	-1.774455000
H	-3.414090000	2.071951000	-0.302395000
H	2.597096000	1.615423000	1.661536000
H	3.357067000	2.146723000	0.153208000
C	-3.615613000	-2.603265000	-0.899672000
C	-2.437863000	-1.255502000	-2.661378000
C	-4.661003000	-0.474582000	-1.776906000
C	-2.796101000	-1.634205000	2.264480000
C	-4.589083000	0.040302000	1.651573000
C	-2.329088000	0.816315000	2.445599000
C	2.872175000	-1.600095000	-2.310784000
C	2.655310000	0.892888000	-2.523879000
C	4.749382000	-0.086355000	-1.538958000
C	3.507143000	-2.548221000	0.986247000
C	4.534241000	-0.417893000	1.871768000
C	2.214990000	-1.092096000	2.583933000
H	-2.692756000	0.784186000	3.493411000
H	-1.234534000	0.631732000	2.469145000
H	-2.496059000	1.842404000	2.063998000
H	-4.835109000	1.005894000	1.166352000
H	-4.927182000	0.104199000	2.707236000
H	-5.177300000	-0.761047000	1.165174000
H	-3.350947000	-2.451957000	1.770752000
H	-3.111676000	-1.606135000	3.328133000
H	-1.718389000	-1.888399000	2.232913000
H	-5.344068000	-0.377999000	-0.913416000
H	-5.180101000	-1.082676000	-2.547188000
H	-4.498633000	0.531466000	-2.210449000
H	-2.143430000	-0.252777000	-3.034483000
H	-1.520914000	-1.842909000	-2.461395000
H	-2.997850000	-1.758261000	-3.477073000
H	-4.038951000	-3.203355000	-1.731993000
H	-4.356363000	-2.612221000	-0.077177000
H	-2.686943000	-3.099300000	-0.555248000
H	3.092367000	0.815059000	-3.540803000
H	1.553627000	0.830895000	-2.629115000
H	2.910427000	1.895246000	-2.127966000
H	3.264935000	-2.460836000	-1.738759000
H	3.318082000	-1.635171000	-3.326413000
H	1.776526000	-1.728753000	-2.412273000
H	5.032202000	0.854634000	-1.025886000
H	5.185663000	-0.051081000	-2.559158000
H	5.219395000	-0.935557000	-1.007599000
H	3.871297000	-3.117670000	1.866902000
H	4.293440000	-2.605037000	0.208885000

H	2.59065000	-3.044491000	0.611976000
H	1.926095000	-0.065626000	2.891856000
H	1.300213000	-1.663302000	2.327859000
H	2.675214000	-1.579378000	3.468725000
H	5.299617000	-0.393988000	1.075174000
H	4.953428000	-0.998993000	2.719994000
H	4.373045000	0.615945000	2.234707000
H	0.013010000	-0.216125000	-1.616071000
Cl	-0.014980000	-2.799070000	0.090284000

2c, E = -2186.02347449488

70

Ir	0.006208000	-0.367672000	0.238763000
C	-0.072729000	1.657167000	0.138388000
P	-2.317304000	-0.228081000	-0.065162000
P	2.275590000	-0.031860000	0.345729000
C	-2.572219000	1.581424000	-0.405284000
C	-3.290345000	-1.136371000	-1.422709000
C	-3.022253000	-0.502619000	1.692335000
C	2.434066000	1.795343000	0.608045000
C	3.629051000	-0.822163000	1.407362000
C	2.330260000	-0.327308000	-1.541720000
C	-1.295546000	2.351702000	-0.134766000
C	-1.331361000	3.759296000	-0.198266000
C	-0.163978000	4.519244000	-0.032997000
C	1.107104000	2.457769000	0.298599000
C	1.052716000	3.862255000	0.204778000
H	-2.290556000	4.264831000	-0.397973000
H	-0.201057000	5.617794000	-0.095505000
H	1.978342000	4.447749000	0.329610000
H	-2.855831000	1.686058000	-1.473292000
H	-3.429987000	1.984844000	0.169475000
H	2.688004000	1.935836000	1.680621000
H	3.272979000	2.234460000	0.031068000
C	-3.080443000	-2.656125000	-1.285153000
C	-2.671084000	-0.687352000	-2.762205000
C	-4.785740000	-0.785197000	-1.392697000
C	-3.173536000	-2.007233000	1.972350000
C	-4.341998000	0.224652000	1.984283000
C	-1.908929000	0.065318000	2.602230000
C	0.782183000	-0.377571000	-1.686452000
C	2.976335000	0.812599000	-2.333988000
C	2.946594000	-1.678151000	-1.923943000
C	3.642479000	-2.350398000	1.223048000
C	4.995728000	-0.211054000	1.058079000
C	3.242294000	-0.513940000	2.868259000
H	-2.172009000	-0.105196000	3.668380000
H	-0.930617000	-0.458290000	2.437377000
H	-1.749016000	1.150777000	2.452558000
H	-4.255145000	1.323303000	1.871213000
H	-4.635792000	0.027622000	3.037596000
H	-5.167683000	-0.128338000	1.337718000
H	-4.052815000	-2.434421000	1.452824000
H	-3.330651000	-2.153444000	3.062499000

H	-2.267711000	-2.572316000	1.670683000
H	-5.281377000	-1.169107000	-0.480034000
H	-5.288612000	-1.254694000	-2.265365000
H	-4.963147000	0.307640000	-1.454301000
H	-2.799805000	0.395470000	-2.957373000
H	-1.591205000	-0.923402000	-2.810385000
H	-3.177160000	-1.232960000	-3.586125000
H	-3.426092000	-3.151839000	-2.216980000
H	-3.662251000	-3.081952000	-0.447647000
H	-2.013513000	-2.908004000	-1.117477000
H	2.865554000	0.613062000	-3.421249000
H	2.496046000	1.788569000	-2.124304000
H	4.060604000	0.898434000	-2.115452000
H	0.443689000	-1.325709000	-2.151817000
H	0.389237000	0.487481000	-2.257327000
H	4.039330000	-1.706140000	-1.741297000
H	2.783350000	-1.847019000	-3.009578000
H	2.464285000	-2.510016000	-1.374689000
H	4.261319000	-2.798540000	2.029165000
H	4.088435000	-2.649074000	0.257571000
H	2.619521000	-2.774822000	1.280267000
H	3.221685000	0.571517000	3.089608000
H	2.248917000	-0.940190000	3.114977000
H	3.992321000	-0.975926000	3.544360000
H	5.269313000	-0.398397000	0.000031000
H	5.780254000	-0.673593000	1.694809000
H	5.023584000	0.882398000	1.236540000
Cl	0.087216000	-2.863618000	0.493342000

2c⁺, E = -2185.84314527639

70

Ir	0.043563000	-0.402576000	0.221175000
C	-0.014310000	1.593523000	0.162231000
P	-2.323947000	-0.242272000	-0.067687000
P	2.349054000	-0.089414000	0.300769000
C	-2.426451000	1.508031000	-0.666913000
C	-3.228745000	-1.331535000	-1.332281000
C	-3.145056000	-0.221781000	1.658903000
C	2.466091000	1.693924000	0.769804000
C	3.677286000	-1.001573000	1.279723000
C	2.336542000	-0.198231000	-1.611745000
C	-1.240406000	2.284638000	-0.157655000
C	-1.294358000	3.683536000	-0.081626000
C	-0.150340000	4.424340000	0.262542000
C	1.152581000	2.375614000	0.478030000
C	1.069744000	3.774970000	0.517928000
H	-2.234890000	4.204334000	-0.317194000
H	-0.206502000	5.521979000	0.316770000
H	1.966709000	4.366000000	0.757676000
H	-2.357689000	1.454396000	-1.774438000
H	-3.391026000	1.999440000	-0.437674000
H	2.668510000	1.710197000	1.862040000
H	3.317086000	2.211854000	0.284275000
C	-2.868898000	-2.803553000	-1.054521000

C	-2.695876000	-0.956582000	-2.728941000
C	-4.749850000	-1.115891000	-1.290120000
C	-3.439136000	-1.661341000	2.115659000
C	-4.427736000	0.624679000	1.695762000
C	-2.101734000	0.404510000	2.609250000
C	0.819692000	-0.495095000	-1.699451000
C	2.713711000	1.133797000	-2.268683000
C	3.162079000	-1.345929000	-2.204036000
C	3.719381000	-2.489722000	0.891191000
C	5.036634000	-0.325825000	1.032949000
C	3.252033000	-0.883481000	2.757917000
H	-2.514737000	0.411894000	3.639788000
H	-1.159900000	-0.187188000	2.642794000
H	-1.851921000	1.448795000	2.338470000
H	-4.233568000	1.692612000	1.475960000
H	-4.848239000	0.575695000	2.722228000
H	-5.204935000	0.257213000	1.000821000
H	-4.259112000	-2.125211000	1.534908000
H	-3.762531000	-1.631733000	3.177267000
H	-2.540342000	-2.305624000	2.051107000
H	-5.196979000	-1.461739000	-0.339048000
H	-5.215030000	-1.705003000	-2.108335000
H	-5.025351000	-0.053664000	-1.446992000
H	-3.003677000	0.058160000	-3.047946000
H	-1.593491000	-1.031932000	-2.791933000
H	-3.118850000	-1.671808000	-3.464196000
H	-3.323014000	-3.433744000	-1.847113000
H	-3.250097000	-3.159600000	-0.080892000
H	-1.773154000	-2.964546000	-1.069802000
H	2.581451000	1.041759000	-3.366607000
H	2.077568000	1.972538000	-1.925411000
H	3.773621000	1.391837000	-2.074037000
H	0.600049000	-1.547743000	-1.982144000
H	0.267170000	0.196661000	-2.364590000
H	4.247899000	-1.193896000	-2.045630000
H	2.982620000	-1.378058000	-3.298811000
H	2.872382000	-2.328687000	-1.787411000
H	4.368413000	-3.017553000	1.620493000
H	4.151498000	-2.651208000	-0.111986000
H	2.712794000	-2.949801000	0.934337000
H	3.201243000	0.165900000	3.109830000
H	2.269713000	-1.366380000	2.929972000
H	4.007247000	-1.404319000	3.382514000
H	5.329540000	-0.363476000	-0.035433000
H	5.814343000	-0.864897000	1.613947000
H	5.047736000	0.731296000	1.364233000
Cl	0.040991000	-2.566999000	1.269048000

(^{Me4}POCOP)IrHCl, E = -1787.81800846986

32

C	-1.872427000	-0.250477000	3.440205000
C	-1.741872000	-0.353952000	2.044606000
C	-0.476726000	-0.498977000	1.428091000
C	0.664902000	-0.560747000	2.261482000

C	0.561203000	-0.459649000	3.659527000
C	-0.713095000	-0.305235000	4.235278000
H	-2.870174000	-0.129326000	3.885931000
H	1.469875000	-0.502252000	4.277086000
H	-0.804566000	-0.223473000	5.328949000
O	1.911356000	-0.724524000	1.684608000
O	-2.875725000	-0.313485000	1.253278000
P	1.926856000	-0.746123000	-0.023919000
P	-2.591305000	-0.364876000	-0.430674000
Ir	-0.301597000	-0.560746000	-0.574407000
Cl	-0.020113000	0.466470000	-2.746089000
C	2.876603000	-2.263716000	-0.353360000
H	3.827596000	-2.251235000	0.214833000
H	2.267967000	-3.139815000	-0.059767000
H	3.089656000	-2.315301000	-1.439559000
C	3.061498000	0.626785000	-0.403193000
H	4.045977000	0.474479000	0.080718000
H	3.178082000	0.676243000	-1.504418000
H	2.603342000	1.570865000	-0.051275000
C	-3.706548000	-1.710866000	-0.939487000
H	-3.726491000	-1.751535000	-2.046651000
H	-3.315660000	-2.668817000	-0.547342000
H	-4.728884000	-1.528775000	-0.553434000
C	-3.395861000	1.169319000	-0.992194000
H	-3.300222000	1.218124000	-2.095489000
H	-4.463365000	1.189960000	-0.698023000
H	-2.859681000	2.030832000	-0.550181000
H	-0.464949000	-2.049073000	-0.135308000

(^{Me}4POCOP)IrCl⁺, E = -1787.00765908448

31

C	-1.897534000	-0.578265000	3.386097000
C	-1.760493000	-0.271844000	2.030232000
C	-0.451515000	-0.274652000	1.405741000
C	0.712585000	-0.455645000	2.251612000
C	0.561586000	-0.760918000	3.606209000
C	-0.737113000	-0.813921000	4.148837000
H	-2.898388000	-0.620230000	3.836437000
H	1.449980000	-0.943067000	4.225814000
H	-0.850022000	-1.045931000	5.218725000
O	1.949357000	-0.341224000	1.718554000
O	-2.853454000	0.015447000	1.288705000
P	2.006123000	-0.198272000	0.000084000
P	-2.583614000	0.145404000	-0.410517000
Ir	-0.261538000	0.003921000	-0.483464000
Cl	-0.001605000	1.846607000	-1.848269000
C	2.909046000	-1.705903000	-0.447526000
H	3.881256000	-1.739403000	0.081792000
H	2.294576000	-2.589353000	-0.190394000
H	3.073271000	-1.684368000	-1.543785000
C	3.143079000	1.191750000	-0.217190000
H	4.088522000	0.992826000	0.323696000
H	3.343214000	1.299572000	-1.301777000
H	2.664247000	2.115885000	0.156922000

C	-3.607103000	-1.216152000	-1.033101000
H	-3.570969000	-1.183054000	-2.140656000
H	-3.185902000	-2.178307000	-0.685188000
H	-4.651548000	-1.098502000	-0.683963000
C	-3.445520000	1.685929000	-0.805552000
H	-3.427842000	1.810897000	-1.906511000
H	-4.492116000	1.634697000	-0.447805000
H	-2.911767000	2.533027000	-0.335665000

TS5⁺, E = -1866.73756034541

39

C	-1.898012000	-0.308292000	3.566588000
C	-1.768326000	-0.260535000	2.175866000
C	-0.470111000	-0.317720000	1.541271000
C	0.685409000	-0.475215000	2.396498000
C	0.556836000	-0.523317000	3.787261000
C	-0.733082000	-0.440903000	4.347397000
H	-2.892207000	-0.246728000	4.029103000
H	1.448919000	-0.626740000	4.419423000
H	-0.834825000	-0.478835000	5.442663000
O	1.915516000	-0.585589000	1.832131000
O	-2.879590000	-0.165912000	1.401602000
P	1.973768000	-0.286081000	0.138465000
P	-2.586423000	0.097494000	-0.273882000
Ir	-0.275185000	-0.082321000	-0.398668000
Cl	0.023750000	1.397473000	-2.327409000
C	2.991618000	-1.665702000	-0.445471000
H	3.939970000	-1.701935000	0.125423000
H	2.435076000	-2.613718000	-0.320018000
H	3.211741000	-1.501815000	-1.519437000
C	2.998417000	1.207807000	0.060298000
H	3.991791000	1.023484000	0.512791000
H	3.102260000	1.480487000	-1.009142000
H	2.474846000	2.027175000	0.588535000
C	-3.696695000	-1.115558000	-1.033396000
H	-3.685293000	-0.957024000	-2.130222000
H	-3.338845000	-2.136615000	-0.801843000
H	-4.726271000	-0.976497000	-0.649694000
C	-3.323180000	1.734783000	-0.527265000
H	-3.191227000	1.993388000	-1.597133000
H	-4.397290000	1.725225000	-0.259502000
H	-2.773970000	2.472319000	0.088481000
C	-0.240033000	-1.679615000	-2.258378000
H	-1.055645000	-1.197963000	-2.819792000
H	0.741288000	-1.369240000	-2.649802000
C	-0.395652000	-3.196032000	-2.145602000
H	-1.374546000	-3.493982000	-1.722207000
H	0.410609000	-3.664813000	-1.548512000
H	-0.333978000	-3.601872000	-3.178956000
H	-0.349220000	-1.623213000	-0.957412000

(^{Me4}POCOP)IrH(C₂H₅)Cl⁺, E = -1866.76402998319

39

C	-1.892148000	-0.391501000	3.473483000
C	-1.765062000	-0.368778000	2.078080000
C	-0.475925000	-0.434963000	1.479187000
C	0.679104000	-0.590881000	2.295644000
C	0.554057000	-0.613909000	3.691154000
C	-0.730603000	-0.519518000	4.256788000
H	-2.888030000	-0.308397000	3.929622000
H	1.453256000	-0.702943000	4.315870000
H	-0.829836000	-0.539567000	5.352339000
O	1.911333000	-0.717241000	1.711614000
O	-2.878905000	-0.281411000	1.286368000
P	1.994652000	-0.332849000	0.047945000
P	-2.603073000	0.063752000	-0.365182000
Ir	-0.274882000	-0.153481000	-0.500425000
Cl	0.020537000	1.524899000	-2.161088000
C	3.069399000	-1.639383000	-0.591717000
H	4.013798000	-1.662332000	-0.013583000
H	2.553315000	-2.615059000	-0.518204000
H	3.289925000	-1.414653000	-1.654405000
C	2.948285000	1.207559000	0.042624000
H	3.940766000	1.046529000	0.505899000
H	3.059459000	1.532235000	-1.011283000
H	2.381198000	1.979306000	0.597043000
C	-3.747123000	-1.072007000	-1.186102000
H	-3.733091000	-0.851958000	-2.272286000
H	-3.420204000	-2.114928000	-1.015155000
H	-4.770791000	-0.922918000	-0.790391000
C	-3.276061000	1.736402000	-0.540466000
H	-3.147439000	2.042826000	-1.597865000
H	-4.347068000	1.750333000	-0.260495000
H	-2.696293000	2.423334000	0.104898000
C	-0.249900000	-1.604234000	-2.116499000
H	-1.075153000	-1.249052000	-2.761613000
H	0.720740000	-1.394562000	-2.603509000
C	-0.403116000	-3.041852000	-1.700470000
H	-1.372409000	-3.243677000	-1.201990000
H	0.416262000	-3.387277000	-1.038542000
H	-0.370486000	-3.678182000	-2.614768000
H	-0.464783000	-1.586518000	0.168785000

(^{Me}4POCOP)Ir(C2H5)Cl, E = -1866.35665927147

38

C	-1.896407000	-0.839421000	3.176488000
C	-1.729393000	-0.504842000	1.821947000
C	-0.450705000	-0.428316000	1.216330000
C	0.669717000	-0.707683000	2.037478000
C	0.536259000	-1.045012000	3.395069000
C	-0.754115000	-1.109647000	3.952288000
H	-2.907191000	-0.887707000	3.606649000
H	1.432577000	-1.254180000	3.996688000
H	-0.871749000	-1.372523000	5.014569000
O	1.935959000	-0.667221000	1.478371000
O	-2.852014000	-0.262404000	1.048357000

P	1.984985000	-0.120186000	-0.140119000
P	-2.522276000	0.259060000	-0.545555000
Ir	-0.232310000	0.105433000	-0.712557000
Cl	0.055575000	1.164643000	-2.918285000
C	3.118627000	-1.341764000	-0.875213000
H	4.051662000	-1.399272000	-0.281356000
H	2.627136000	-2.332867000	-0.898306000
H	3.351687000	-1.026415000	-1.911520000
C	2.969388000	1.408200000	0.012714000
H	3.927365000	1.209750000	0.532150000
H	3.162196000	1.799051000	-1.006403000
H	2.378745000	2.155880000	0.576417000
C	-3.693445000	-0.771110000	-1.486449000
H	-3.683226000	-0.439634000	-2.543689000
H	-3.376416000	-1.829943000	-1.434261000
H	-4.713679000	-0.663740000	-1.069108000
C	-3.253056000	1.930664000	-0.549333000
H	-3.193568000	2.332067000	-1.580789000
H	-4.307918000	1.900122000	-0.212852000
H	-2.658209000	2.579853000	0.121781000
C	-0.324182000	-1.826871000	-1.501708000
H	-1.154558000	-1.787112000	-2.236554000
H	0.618420000	-1.937718000	-2.076471000
C	-0.509889000	-2.972523000	-0.525401000
H	-1.454968000	-2.885502000	0.046791000
H	0.318465000	-3.035945000	0.208055000
H	-0.541003000	-3.935505000	-1.083691000

TS4, E = -1866.31613524645

38

C	-1.904384000	-0.649770000	3.393676000
C	-1.745545000	-0.435821000	2.012558000
C	-0.468451000	-0.431600000	1.398829000
C	0.660508000	-0.638362000	2.229781000
C	0.533414000	-0.855007000	3.613778000
C	-0.755653000	-0.862778000	4.177981000
H	-2.909169000	-0.641376000	3.839932000
H	1.430047000	-1.006547000	4.231776000
H	-0.867609000	-1.032997000	5.259884000
O	1.919866000	-0.606751000	1.670242000
O	-2.862377000	-0.204142000	1.238622000
P	1.948122000	-0.296721000	-0.021029000
P	-2.537709000	0.081110000	-0.425840000
Ir	-0.263512000	-0.182383000	-0.639191000
Cl	0.013149000	1.927044000	-1.753784000
C	3.028713000	-1.665975000	-0.566189000
H	3.983159000	-1.658952000	-0.003957000
H	2.505181000	-2.627384000	-0.403018000
H	3.233685000	-1.544339000	-1.648746000
C	3.008948000	1.181512000	-0.105260000
H	3.938421000	1.017594000	0.474023000
H	3.252384000	1.377081000	-1.168188000
H	2.448198000	2.047780000	0.292359000
C	-3.715047000	-1.098705000	-1.175011000

H	-3.702991000	-0.959110000	-2.274606000
H	-3.393091000	-2.130787000	-0.938154000
H	-4.739496000	-0.927769000	-0.789748000
C	-3.307205000	1.713134000	-0.674783000
H	-3.320900000	1.931426000	-1.760848000
H	-4.339382000	1.713201000	-0.273590000
H	-2.691322000	2.480027000	-0.169259000
C	-0.153968000	-1.048838000	-2.648160000
H	-0.988663000	-0.690939000	-3.275718000
H	0.826966000	-0.843329000	-3.111009000
C	-0.323349000	-2.381901000	-2.015637000
H	0.548623000	-3.060410000	-2.091246000
H	-1.267915000	-2.907788000	-2.255810000
H	-0.414378000	-2.204947000	-0.846084000

(^{Me4}POCOP)IrH(C₂H₄)Cl, E = -1866.36357105032

38

C	-1.880102000	-0.304068000	3.461309000
C	-1.738225000	-0.336650000	2.061879000
C	-0.474673000	-0.453128000	1.450358000
C	0.661739000	-0.537706000	2.278233000
C	0.556163000	-0.507972000	3.680958000
C	-0.722443000	-0.391455000	4.255522000
H	-2.879208000	-0.209979000	3.910247000
H	1.461262000	-0.573008000	4.301600000
H	-0.819171000	-0.366984000	5.351757000
O	1.913021000	-0.646509000	1.699097000
O	-2.867245000	-0.246337000	1.268104000
P	1.938600000	-0.660461000	-0.008547000
P	-2.590738000	-0.279053000	-0.416999000
Ir	-0.290325000	-0.445778000	-0.588990000
Cl	-0.097446000	2.085408000	-0.350686000
C	2.845514000	-2.206310000	-0.335197000
H	3.808917000	-2.212933000	0.211333000
H	2.219830000	-3.061841000	-0.017579000
H	3.037883000	-2.282305000	-1.424242000
C	3.119580000	0.675244000	-0.366992000
H	4.025630000	0.570902000	0.261013000
H	3.397226000	0.617771000	-1.438694000
H	2.603505000	1.636238000	-0.177315000
C	-3.668481000	-1.657321000	-0.924806000
H	-3.674272000	-1.714825000	-2.031819000
H	-3.259425000	-2.600412000	-0.515452000
H	-4.701257000	-1.497044000	-0.557944000
C	-3.451290000	1.229190000	-0.957050000
H	-3.537964000	1.205498000	-2.061962000
H	-4.459741000	1.283776000	-0.502892000
H	-2.826095000	2.093593000	-0.660983000
C	-0.047035000	0.096530000	-2.782085000
H	-0.906670000	0.721308000	-3.068799000
H	0.940500000	0.567819000	-2.901063000
C	-0.171259000	-1.294868000	-2.689026000
H	0.716399000	-1.943871000	-2.753315000
H	-1.127653000	-1.790159000	-2.919927000

H -0.439061000 -2.022067000 -0.428358000

C₂H₆, E = -79.736628080489

8

C -0.296283000 -1.734219000 -2.098994000

H 0.710471000 -2.198654000 -2.148210000

H -1.021849000 -2.544570000 -1.878691000

C -0.643717000 -1.004528000 -3.396145000

H 0.081940000 -0.194320000 -3.616696000

H -1.650410000 -0.539942000 -3.347165000

H -0.641386000 -1.693730000 -4.266023000

H -0.298600000 -1.045250000 -1.228937000

C₂H₄, E = -78.505949099104

8

C -0.194855000 -1.289175000 -2.832346000

H 0.692114000 -1.933573000 -2.710533000

H -1.174052000 -1.796358000 -2.859284000

C -0.087950000 0.044151000 -2.942250000

H -0.974942000 0.688514000 -3.064068000

H 0.891270000 0.551285000 -2.915313000

(^{Me}4POCOP)IrH₂, E = -1328.31719036285

32

C -1.886558000 -0.333597000 3.463587000

C -1.747068000 -0.345361000 2.062606000

C -0.473669000 -0.450570000 1.447263000

C 0.670331000 -0.544199000 2.280212000

C 0.559071000 -0.534691000 3.683746000

C -0.724282000 -0.429100000 4.250763000

H -2.882430000 -0.251462000 3.921618000

H 1.457800000 -0.608321000 4.312387000

H -0.822287000 -0.420848000 5.347636000

O 1.913327000 -0.646250000 1.707497000

O -2.868614000 -0.252864000 1.277066000

P 1.913075000 -0.649742000 -0.023843000

P -2.561494000 -0.277156000 -0.426599000

Ir -0.289914000 -0.466720000 -0.609422000

C 2.868346000 -2.178117000 -0.322480000

H 3.807539000 -2.163564000 0.264828000

H 2.252053000 -3.050846000 -0.034852000

H 3.101073000 -2.240150000 -1.403977000

C 3.110079000 0.695934000 -0.329592000

H 4.034491000 0.527442000 0.257109000

H 3.348409000 0.712743000 -1.411542000

H 2.648764000 1.660869000 -0.046216000

C -3.687996000 -1.629048000 -0.917061000

H -3.732299000 -1.663558000 -2.023644000

H -3.285139000 -2.588620000 -0.541378000

H -4.700935000 -1.452409000 -0.504774000

C -3.445389000 1.245171000 -0.915136000

H -3.480852000 1.289455000 -2.021688000

H -4.474528000 1.239352000 -0.505308000

H -2.888649000 2.122969000 -0.536056000

H	-0.221671000	-1.208150000	-2.050838000
H	-0.101139000	0.253922000	-2.050398000

(^{Me4}POCOP)Ir, E = -1327.10462583263

30

C	-1.914015000	-0.420740000	3.490578000
C	-1.758924000	-0.300275000	2.099495000
C	-0.477755000	-0.337575000	1.480586000
C	0.649121000	-0.502588000	2.334287000
C	0.512397000	-0.624576000	3.727172000
C	-0.772943000	-0.582675000	4.296983000
H	-2.924931000	-0.386060000	3.922459000
H	1.413229000	-0.750371000	4.345533000
H	-0.887140000	-0.677482000	5.387417000
O	1.912397000	-0.544164000	1.779716000
O	-2.881578000	-0.141266000	1.312462000
P	1.934916000	-0.384567000	0.074021000
P	-2.549924000	-0.006510000	-0.363051000
Ir	-0.275044000	-0.169210000	-0.455168000
C	2.917547000	-1.860373000	-0.378198000
H	3.865249000	-1.883451000	0.196026000
H	2.322289000	-2.769157000	-0.168159000
H	3.140274000	-1.817952000	-1.463270000
C	3.128826000	0.989636000	-0.109847000
H	4.062515000	0.767580000	0.444438000
H	3.356568000	1.117931000	-1.187083000
H	2.669463000	1.920302000	0.273874000
C	-3.658021000	-1.305986000	-1.019986000
H	-3.658640000	-1.243824000	-2.126739000
H	-3.272282000	-2.297329000	-0.715371000
H	-4.688799000	-1.163553000	-0.638399000
C	-3.442247000	1.543557000	-0.748641000
H	-3.435237000	1.691408000	-1.847226000
H	-4.488423000	1.487717000	-0.387107000
H	-2.917490000	2.391056000	-0.268271000

TS6, E = -1406.84896048054

38

C	-1.920420000	-0.429429000	3.497620000
C	-1.758598000	-0.324201000	2.103364000
C	-0.482244000	-0.379304000	1.489462000
C	0.644056000	-0.526701000	2.337247000
C	0.516106000	-0.634741000	3.734818000
C	-0.772994000	-0.586643000	4.296682000
H	-2.925549000	-0.384294000	3.941132000
H	1.410984000	-0.749571000	4.363349000
H	-0.886195000	-0.669533000	5.388820000
O	1.903290000	-0.554896000	1.776968000
O	-2.874234000	-0.152172000	1.312019000
P	1.920092000	-0.396353000	0.061406000
P	-2.535636000	-0.019903000	-0.372023000
Ir	-0.272766000	-0.235324000	-0.540303000
C	2.940710000	-1.854242000	-0.369099000
H	3.891554000	-1.849824000	0.199771000

H	2.367967000	-2.773348000	-0.141276000
H	3.156452000	-1.825974000	-1.456029000
C	3.078576000	1.007064000	-0.119158000
H	4.010765000	0.818823000	0.449381000
H	3.315636000	1.131135000	-1.194812000
H	2.587393000	1.927805000	0.248418000
C	-3.680532000	-1.295798000	-1.015053000
H	-3.674552000	-1.249637000	-2.122604000
H	-3.321791000	-2.292973000	-0.696221000
H	-4.709416000	-1.125765000	-0.640576000
C	-3.389829000	1.552727000	-0.748056000
H	-3.391025000	1.698267000	-1.846898000
H	-4.432339000	1.529300000	-0.373523000
H	-2.834061000	2.385009000	-0.276295000
C	-0.094351000	-0.646860000	-2.770592000
H	-0.896660000	-0.219994000	-3.406874000
H	0.865849000	-0.359686000	-3.246527000
C	-0.216756000	-2.175838000	-2.745945000
H	-0.153172000	-2.577580000	-3.785005000
H	-1.183314000	-2.515329000	-2.322492000
H	0.593274000	-2.654341000	-2.159843000
H	-0.064810000	0.627382000	-1.903685000

(^{Me4}POCOP)IrH(C₂H₅), E = -1406.86080378473

38

C	-1.897378000	-0.559431000	3.425597000
C	-1.738311000	-0.417571000	2.034063000
C	-0.471164000	-0.451927000	1.417435000
C	0.654521000	-0.617850000	2.249566000
C	0.538541000	-0.763303000	3.644994000
C	-0.747101000	-0.735117000	4.218308000
H	-2.901680000	-0.529054000	3.873085000
H	1.438534000	-0.892170000	4.264043000
H	-0.854669000	-0.848767000	5.308093000
O	1.913478000	-0.631958000	1.668134000
O	-2.858898000	-0.232406000	1.238426000
P	1.932960000	-0.383073000	-0.030275000
P	-2.535564000	-0.008105000	-0.432631000
Ir	-0.269478000	-0.263796000	-0.648652000
C	3.000330000	-1.774586000	-0.546189000
H	3.941233000	-1.779678000	0.038633000
H	2.456612000	-2.725791000	-0.388676000
H	3.233871000	-1.665170000	-1.624191000
C	3.022281000	1.077747000	-0.143212000
H	3.958384000	0.908488000	0.424540000
H	3.259106000	1.264757000	-1.209479000
H	2.483663000	1.954180000	0.264472000
C	-3.708831000	-1.212048000	-1.150648000
H	-3.728601000	-1.078790000	-2.250858000
H	-3.363689000	-2.237424000	-0.916808000
H	-4.725704000	-1.055963000	-0.739625000
C	-3.332271000	1.610477000	-0.713747000
H	-3.342304000	1.819459000	-1.801952000
H	-4.369141000	1.605066000	-0.323678000

H	-2.738206000	2.391782000	-0.202738000
C	-0.110812000	-0.673380000	-2.770076000
H	-0.936022000	-0.328925000	-3.419849000
H	0.863340000	-0.480456000	-3.255499000
C	-0.276189000	-2.087908000	-2.264612000
H	0.596931000	-2.750364000	-2.427169000
H	-1.203434000	-2.598645000	-2.591726000
H	-0.391586000	-2.170701000	-1.080227000
H	-0.150986000	1.308810000	-0.491740000

(Me⁴POCOP)IrH(C₂H₄)H, E = -1406.87347328231

38

C	-1.882848000	-0.331240000	3.480712000
C	-1.737983000	-0.343582000	2.080811000
C	-0.475576000	-0.450472000	1.468147000
C	0.658082000	-0.545876000	2.296560000
C	0.552407000	-0.536443000	3.699981000
C	-0.726550000	-0.428590000	4.276436000
H	-2.883227000	-0.246788000	3.929131000
H	1.457342000	-0.612215000	4.319941000
H	-0.824479000	-0.419941000	5.372830000
O	1.907953000	-0.651273000	1.711501000
O	-2.864062000	-0.248036000	1.281837000
P	1.924914000	-0.652408000	0.001228000
P	-2.577522000	-0.273618000	-0.404179000
Ir	-0.291674000	-0.465482000	-0.587990000
C	2.872367000	-2.174753000	-0.335723000
H	3.834779000	-2.168184000	0.212849000
H	2.261659000	-3.045597000	-0.031737000
H	3.067933000	-2.234483000	-1.425389000
C	3.111994000	0.691643000	-0.335762000
H	4.060268000	0.526617000	0.212597000
H	3.314421000	0.717556000	-1.425558000
H	2.653833000	1.651875000	-0.032602000
C	-3.687118000	-1.625526000	-0.924204000
H	-3.692758000	-1.671380000	-2.031933000
H	-3.291482000	-2.579190000	-0.526949000
H	-4.717475000	-1.452416000	-0.555955000
C	-3.448922000	1.241301000	-0.927879000
H	-3.446679000	1.283374000	-2.035819000
H	-4.493860000	1.241716000	-0.560096000
H	-2.901352000	2.118002000	-0.533758000
C	-0.043099000	0.227466000	-2.695285000
H	-0.896438000	0.854002000	-2.999672000
H	0.942841000	0.698874000	-2.833229000
C	-0.162029000	-1.184194000	-2.697613000
H	0.731302000	-1.813203000	-2.837729000
H	-1.108252000	-1.658065000	-3.003289000
H	-0.449900000	-2.125063000	-0.414132000
H	-0.165227000	1.196496000	-0.411477000

