Supplementary Information (SI)

^{193}Ir Nuclear Forward Scattering of an Iridium(I) Complex

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Supplementary data

Gaussian Input file of the Structure optimization of $[IrCl(COD)]_2$ with CCDC 1913379

#p opt tpsstpss/qzvp EmpiricalDispersion=GD3 scf=xqc

0 1

Ir	11.640600	4.658700	3.838700
Cl	12.226100	5.576900	1.708700
C	11.023800	3.140300	5.180600
H	10.084500	2.825500	5.039500
C	12.041500	2.016000	5.354800
H	11.579200	1.143500	5.286100
H	12.443600	2.077300	6.257400
C	13.151900	2.078400	4.305500
H	13.993100	1.740200	4.705300
H	12.916900	1.483300	3.550400
C	13.388600	3.463200	3.778700
H	13.883700	3.497800	2.911300
C	13.586400	4.639900	4.643700
H	14.200600	5.334800	4.268200

C	13.611500	4.525100	6.138300
H	14.260500	5.180400	6.499700
H	13.929200	3.620200	6.385200
C	12.252000	4.766000	6.787300
H	12.186800	4.234400	7.619800
H	12.168600	5.722900	7.028500
C	11.125200	4.383900	5.859100
H	10.242600	4.781700	6.109000
Ir	10.058800	4.658700	1.255300
Cl	9.473300	5.576900	3.385300
C	10.675600	3.140300	-0.086600
H	11.614900	2.825500	0.054500
C	9.657900	2.016000	-0.260800
H	10.120200	1.143500	-0.192100
H	9.255800	2.077300	-1.163300
C	8.547600	2.078400	0.788600
H	7.706300	1.740200	0.388700
H	8.782600	1.483300	1.543600
C	8.310800	3.463200	1.315300
H	7.815800	3.497800	2.182700
C	8.113100	4.639900	0.450300
H	7.498800	5.334800	0.825800
C	8.087900	4.525100	-1.044300
H	7.438900	5.180400	-1.405700
H	7.770200	3.620200	-1.291200
C	9.447400	4.766000	-1.693300
H	9.512600	4.234400	-2.525800
H	9.530800	5.722900	-1.934500
C	10.574200	4.383900	-0.765100
H	11.456800	4.781700	-1.015000

Gaussian Input file of the Natural bond orbital (NBO) analysis with the optimized structure

#p tpsstpss empiricaldispersion=gd3 qzvp scf=xqc pop=nbo

0 1

Ir	1.43382300	-0.39779500	0.01872500
Cl	-0.02012600	-1.47585800	1.62733400
C	2.12807500	1.06112300	-1.34152500
H	1.40332300	1.14776500	-2.14944100
C	2.52040200	2.38175100	-0.68114400
H	2.10289700	3.21126600	-1.25874800
H	3.60719700	2.50128800	-0.71246400
C	2.00576200	2.45406900	0.77344900
H	2.62519700	3.13447300	1.37509400
H	0.99265300	2.86799800	0.77476800
C	1.92816200	1.08480100	1.42209600
H	1.22624600	1.02846400	2.25354300
C	2.96366600	0.09612300	1.39514700
H	2.96124900	-0.62627400	2.21029600
C	4.32610800	0.33238700	0.74105700
H	5.09667200	-0.18553700	1.31844000
H	4.57468700	1.39706200	0.78394200
C	4.34665600	-0.17514800	-0.71786000
H	5.09554000	0.36870600	-1.31184500
H	4.64653100	-1.22735800	-0.72482300
C	2.97902800	-0.09025000	-1.37403200
H	2.84530100	-0.76721100	-2.21815700
Ir	-1.43382300	-0.39779500	-0.01872500
Cl	0.02012300	-1.47585900	-1.62733300
C	-2.12807200	1.06112300	1.34152400
H	-1.40332100	1.14776600	2.14944000
C	-2.52039900	2.38175200	0.68114400

H	-2.10289500	3.21126700	1.25874700
H	-3.60719500	2.50128900	0.71246400
C	-2.00576000	2.45406900	-0.77345000
H	-2.62519500	3.13447200	-1.37509600
H	-0.99265100	2.86799800	-0.77476900
C	-1.92816000	1.08480100	-1.42209500
H	-1.22624400	1.02846400	-2.25354300
C	-2.96366400	0.09612200	-1.39514700
H	-2.96124800	-0.62627400	-2.21029600
C	-4.32610700	0.33238800	-0.74105700
H	-5.09667100	-0.18553600	-1.31844000
H	-4.57468500	1.39706400	-0.78394300
C	-4.34665500	-0.17514500	0.71786000
H	-5.09553800	0.36871100	1.31184500
H	-4.64653300	-1.22735400	0.72482500
C	-2.97902600	-0.09024900	1.37403100
H	-2.84530100	-0.76720900	2.21815700

Orca Input file of the calculations of the hyperfine parameters with the optimized structure (of the functional TPSS. To calculate with the B3LYP functional, TPSS is replaced by B3LYP)

```
! TPSS DKH-def2-TZVP SARC/J DKH2 TightSCF

%geom
        MaxIter 50
end

%basis
        basis "DKH-def2-TZVP"
        newGTO Ir "SARC-DKH-TZVP" end
end
```

```
%method
                SpecialGridAtoms 77;
                SpecialGridIntAcc 8;
                RI on
end

%scf
                MaxIter 10000
                TolE      1e-8
end

*xyz 0 1
Ir     11.640600    4.658700    3.838700
Cl     12.226100    5.576900    1.708700
C      11.023800    3.140300    5.180600
H      10.084500    2.825500    5.039500
C      12.041500    2.016000    5.354800
H      11.579200    1.143500    5.286100
H      12.443600    2.077300    6.257400
C      13.151900    2.078400    4.305500
H      13.993100    1.740200    4.705300
H      12.916900    1.483300    3.550400
C      13.388600    3.463200    3.778700
H      13.883700    3.497800    2.911300
C      13.586400    4.639900    4.643700
H      14.200600    5.334800    4.268200
C      13.611500    4.525100    6.138300
H      14.260500    5.180400    6.499700
H      13.929200    3.620200    6.385200
C      12.252000    4.766000    6.787300
```

H 12.186800 4.234400 7.619800

H 12.168600 5.722900 7.028500

C 11.125200 4.383900 5.859100

H 10.242600 4.781700 6.109000

Ir 10.058800 4.658700 1.255300

Cl 9.473300 5.576900 3.385300

C 10.675600 3.140300 -0.086600

H 11.614900 2.825500 0.054500

C 9.657900 2.016000 -0.260800

H 10.120200 1.143500 -0.192100

H 9.255800 2.077300 -1.163300

C 8.547600 2.078400 0.788600

H 7.706300 1.740200 0.388700

H 8.782600 1.483300 1.543600

C 8.310800 3.463200 1.315300

H 7.815800 3.497800 2.182700

C 8.113100 4.639900 0.450300

H 7.498800 5.334800 0.825800

C 8.087900 4.525100 -1.044300

H 7.438900 5.180400 -1.405700

H 7.770200 3.620200 -1.291200

C 9.447400 4.766000 -1.693300

H 9.512600 4.234400 -2.525800

H 9.530800 5.722900 -1.934500

C 10.574200 4.383900 -0.765100

H 11.456800 4.781700 -1.015000 *

%geom

ReducePrint false

end

%eprnmr nuclei = all Ir {rho, fgrad}

end

Supplementary figures

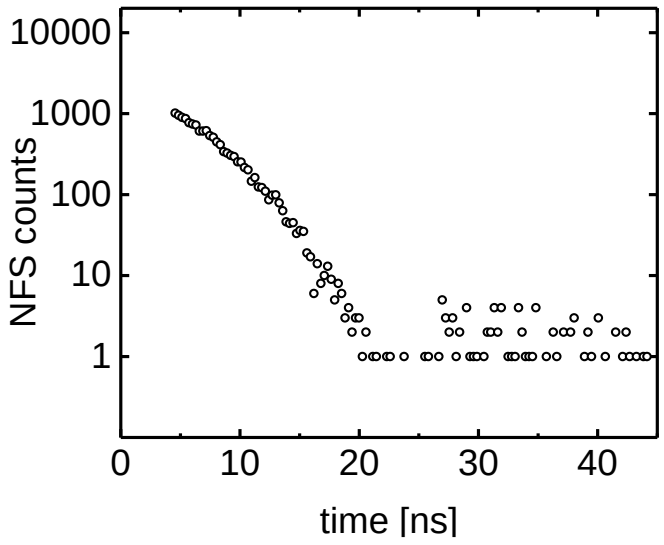

Fig. S1: ^{193}*Ir-NFS spectrum of a metallic iridium foil obtained at 10K (black circles).*