Electronic Supplementary Information for Dalton Transactions

Supplementary Information

Acetylenedithiolate as directional bridging ligand in cobalt(I) alkyne platinum dithiolato bimetallic complexes

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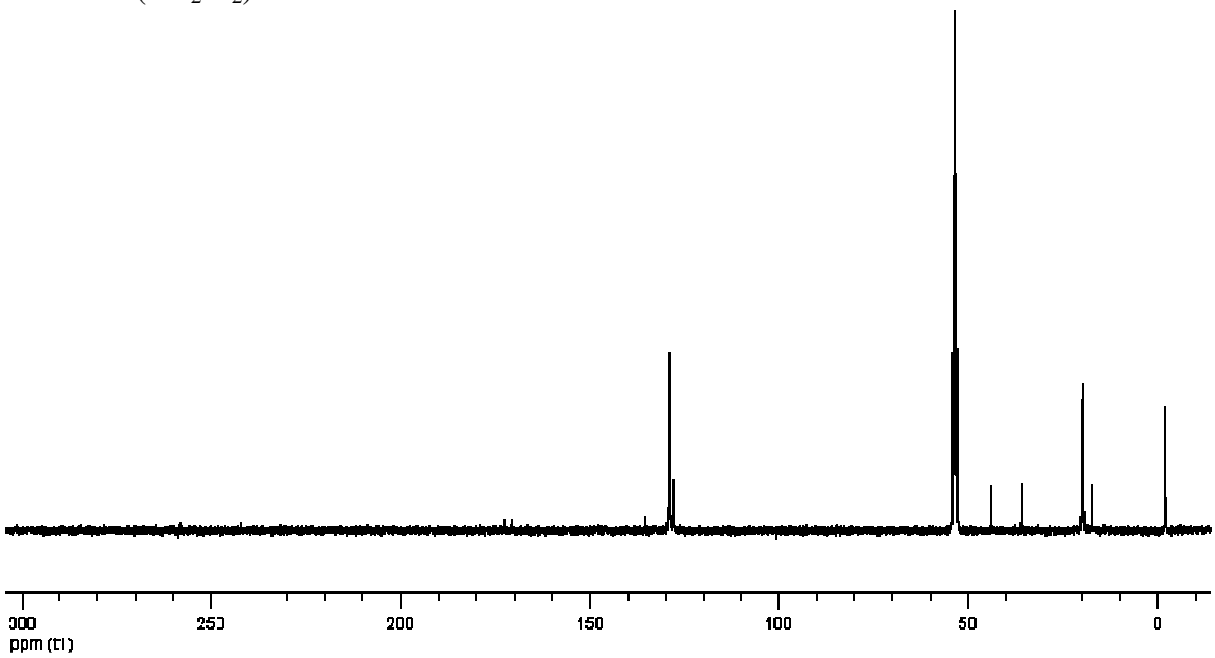
NMR and mass spectra of 2-PF_6 and 3-PF_6.

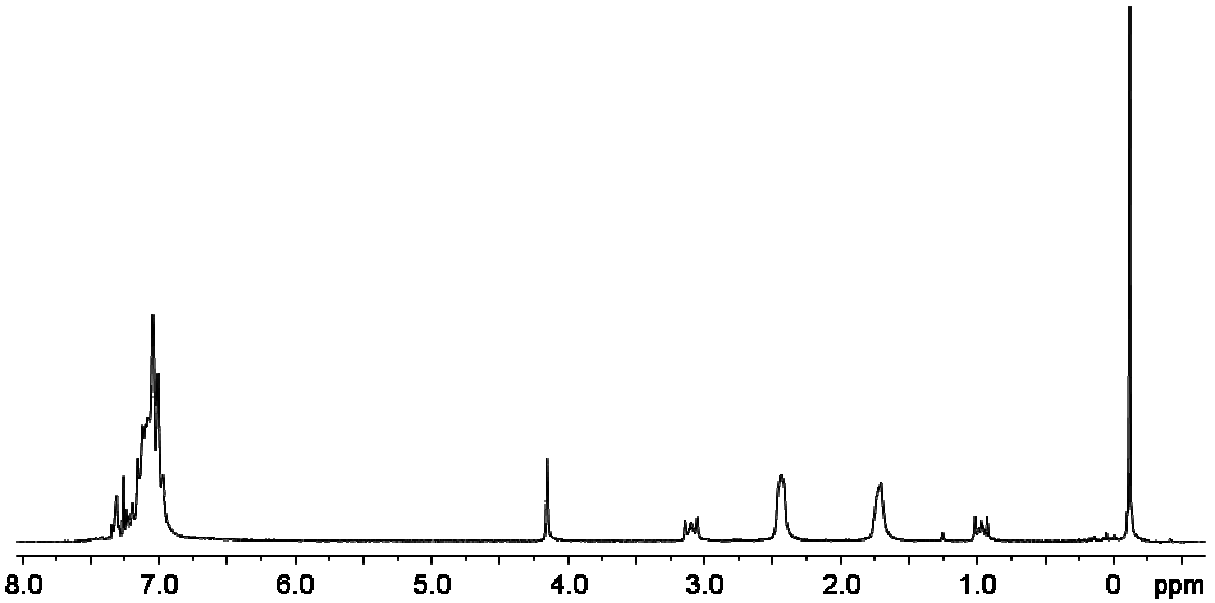
[$(PMe_3)_3$Co(**1**)], **2**-PF_6:

^{13}C NMR (CD_2Cl_2):

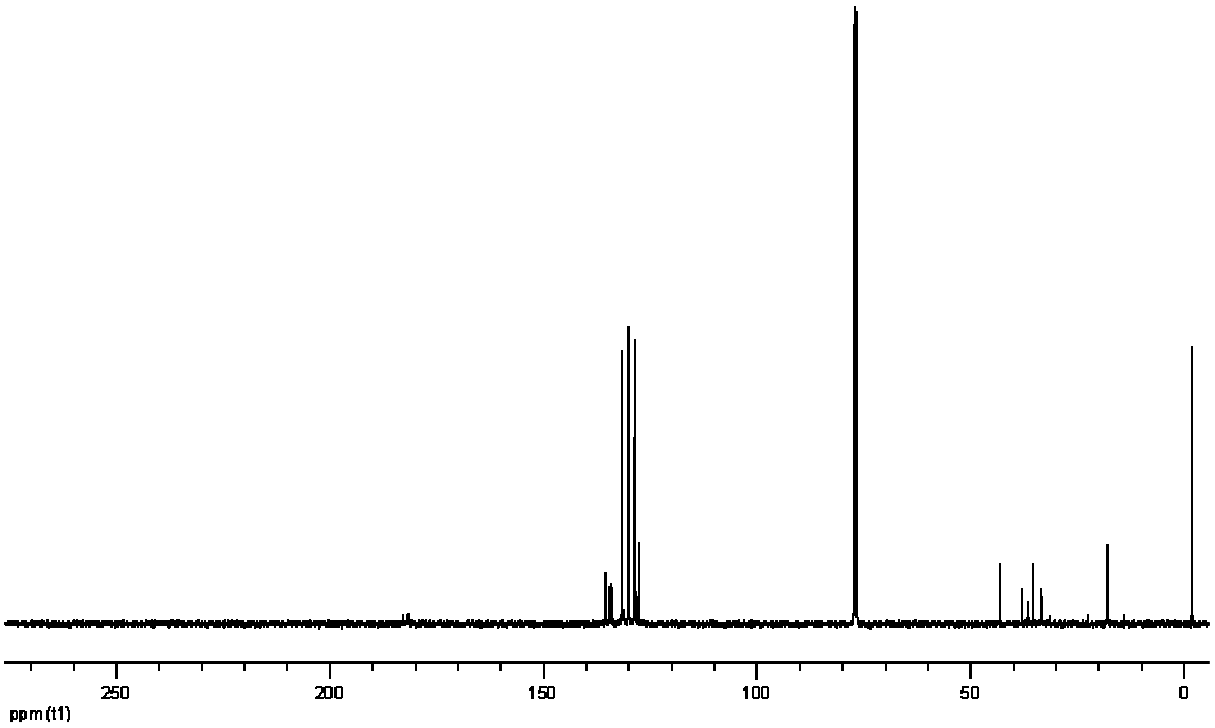


[(triphos)Co(**1**)], **3**-PF_6:

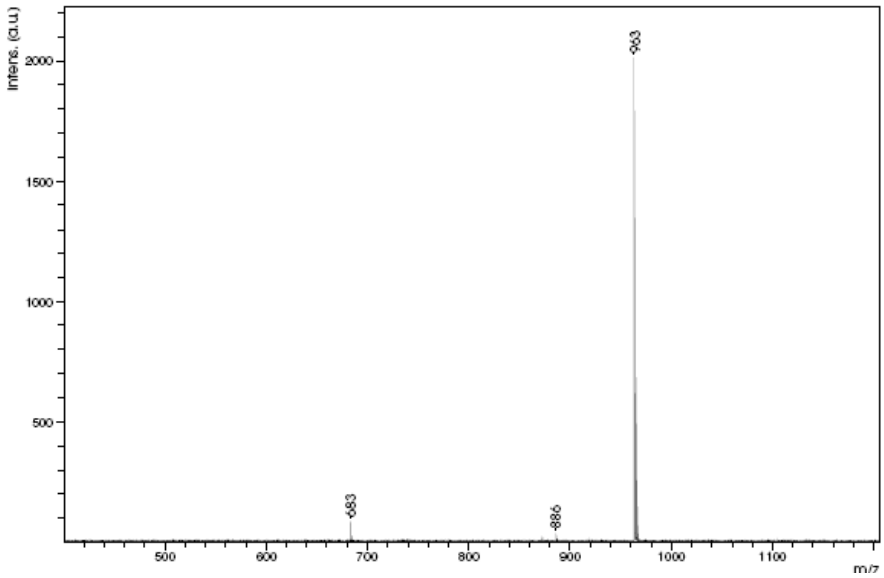
^{1}H NMR ($CDCl_3$):



^{13}C NMR ($CDCl_3$):



Mass spectrum (MALDI-TOF, Matrix DCTB:



EPR measurement of and simulation for [(triphos)Co(C_2S_2)Pt(dppe)], 7.

X-band EPR spectra were recorded on a Bruker ELEXSYS E500 spectrometer equipped with a helium flow cryostat (Oxford Instruments ESR 910) and Hewlett-Packard frequency counter HP5253B.

Measurement parameters:

m.w.-frequency	9.42830 GHz
m.w.-power	0.50 mW
sample temperat.	29.81 K
receiver gain	3162.28
time constant	0.02 s
mod. amplitude	10.00 G
mod. frequency	100.00 MHz
mod. phase	20.00 deg
harmonic	1.00 st
center field	3250.0 G
sweep	2500 G
ADC conv. time	81.92 ms
number scans	6

A simulation of the spectrum turned out to be delicate because of the superposition of couplings with a multitude of potential coupling partners. In addition, resolution of the signal is not ideal due interaction with the solvent, inadequate glass formation in frozen thf and possible intermolecular interactions. We make efforts to record a Q-band spectrum of **7** in cooperation. However, the X-band spectrum and its simulation show clearly the general coupling pattern and the platinum based SOMO. That's why the spectrum is included in the publication at the current stage. In the following two - generally similar - simulation approaches are given. Simulations were performed by the W95epr-program written by Frank Neese (MPI for Bioinorganic Chemistry, Mülheim, and University of Bonn).

Parameters of simulation **A** with large $A_x(^{195}Pt)$:

SPECIES = "platinrest" 0.662
weight = 0.662
Freq = 9.42830 GHz
Hmin = 2000.00 G
Hmax = 4500.00 G
NDATA = 1024
S = 0.5
gx = 1.934
gy = 2.031
gz = 2.222
Wx = 7
Wy = 7
Wz = 7

NUMNUCLEI = 2
Spin[31P] = 0.5
Num[31P] = 2
Abund[31P] = 1.0
AX[31P] = 120.00 MHz
AY[31P] = 250.00 MHz
AZ[31P] = 290.00 MHz
Spin[1H] = 0.5
Num[1H] = 4
Abund[1H] = 1.0
AX[1H] = 10.00 MHz
AY[1H] = 20.00 MHz
AZ[1H] = 50.00 MHz

SPECIES = "platin195"
weight = 0.338
Wx = 7
Wy = 7
Wz = 7
NUMNUCLEI = 3
Spin[195Pt] = 0.5
Num[195Pt] = 1
AX[195Pt] = 830.00 MHz
AY[195Pt] = 340.00 MHz
AZ[195Pt] = 700.00 MHz
Spin[31P] = 0.5
Num[31P] = 2
Abund[31P] = 1.0
AX[31P] = 120.00 MHz
AY[31P] = 250.00 MHz
AZ[31P] = 290.00 MHz
Spin[1H] = 0.5
Num[1H] = 4
Abund[1H] = 1.0
AX[1H] = 10.00 MHz
AY[1H] = 20.00 MHz
AZ[1H] = 50.00 MHz

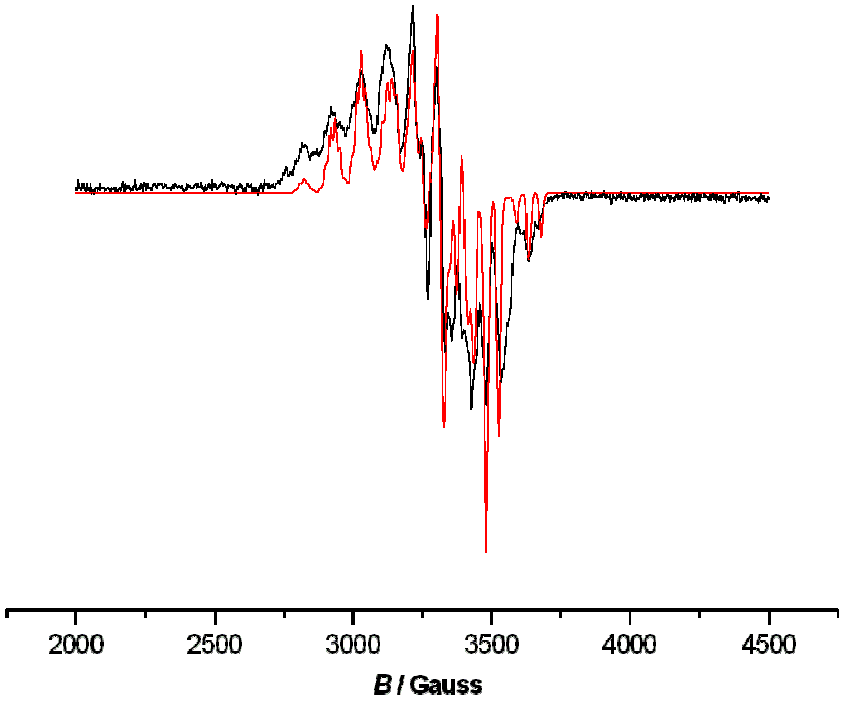


Fig. S1. EPR spectrum of [(triphos)Co(C_2S_2)Pt(dppe)], **7**, (black) and simulation **A** (red).

Parameters of simulation **B** with moderate $A_x(^{195}Pt)$:

SPECIES = "platinrest" 0.662
weight = 0.662
Freq = 9.42830 GHz
Hmin = 2000.00 G
Hmax = 4500.00 G
NDATA = 1024
S = 0.5
gx = 1.934
gy = 2.029
gz = 2.222
Wx = 7
Wy = 7
AY[1H] = 15.00 MHz
Wz = 7
NUMNUCLEI = 2
Spin[31P] = 0.5
Num[31P] = 2
Abund[31P] = 1.0
AX[31P] = 140.00 MHz
AY[31P] = 275.00 MHz
AZ[31P] = 300.00 MHz
Spin[1H] = 0.5
Num[1H] = 4
Abund[1H] = 1.0
AX[1H] = 30.00 MHz
AZ[1H] = 50.00 MHz

SPECIES = "platin195" 0.338;
weight = 0.338;
Wx = 7;
Wy = 7;
Wz = 7;
NUMNUCLEI = 3
Spin[195Pt] = 0.5
Num[195Pt] = 1
AX[195Pt] = 540.00 MHz
AY[195Pt] = 350.00 MHz
AZ[195Pt] = 700.00 MHz
Spin[31P] = 0.5
Num[31P] = 2
Abund[31P] = 1.0
AX[31P] = 140.00 MHz
AY[31P] = 275.00 MHz
AZ[31P] = 300.00 MHz
Spin[1H] = 0.5
Num[1H] = 4
Abund[1H] = 1.0
AX[1H] = 30.00 MHz
AY[1H] = 15.00 MHz
AZ[1H] = 50.00 MHz

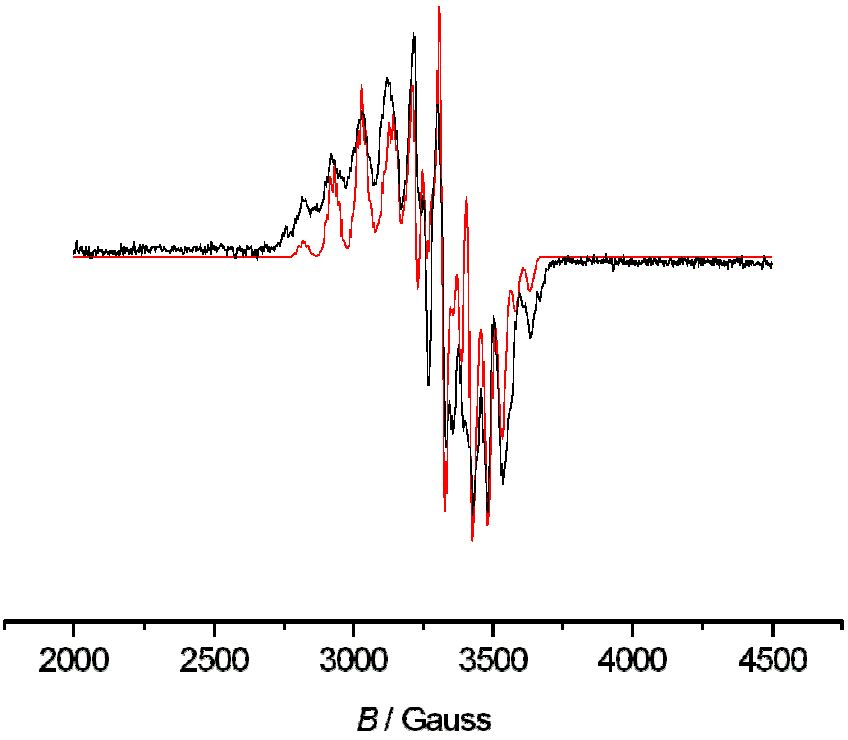


Fig. S2. EPR spectrum of [(triphos)Co(C_2S_2)Pt(dppe)], **7**, (black) and simulation **B** (red).