Supplementary Material (ESI) for Dalton Transactions

Supporting Information for

Reactivity of 17 e^- Complex $[Re^{II}Br_4(CO)_2]^{2-}$ with Bridging Aromatic Ligands. Characterization and CO-Releasing Properties.

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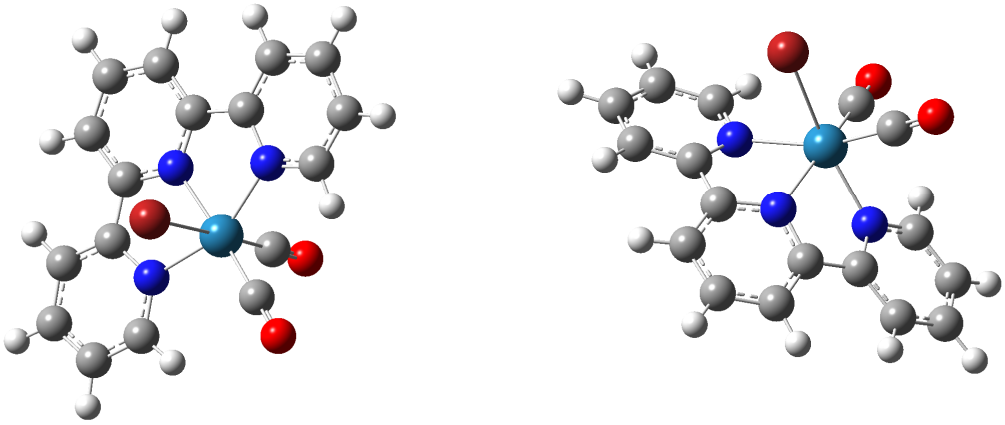


Figure S1. DFT calculated structures of meridian and facial isomers of **5**.

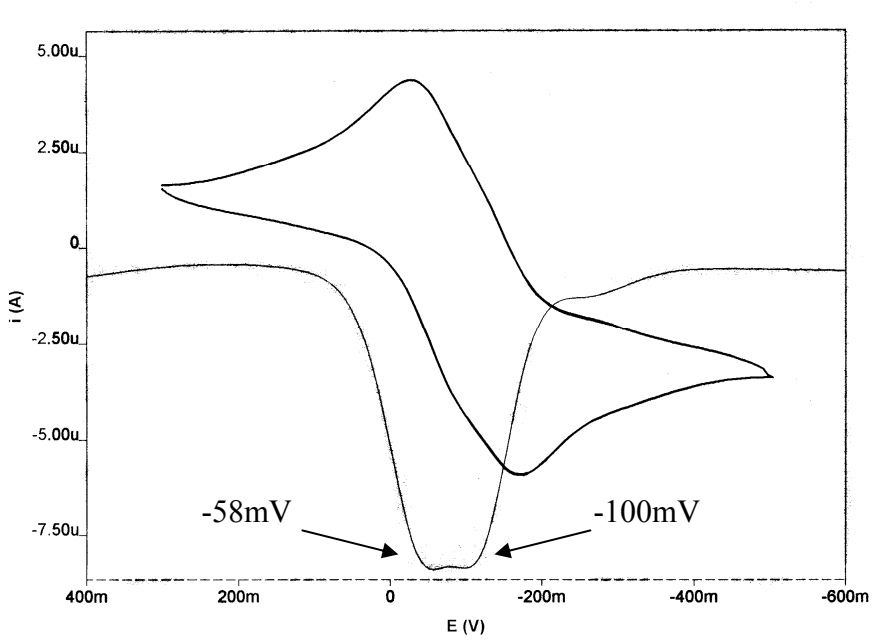
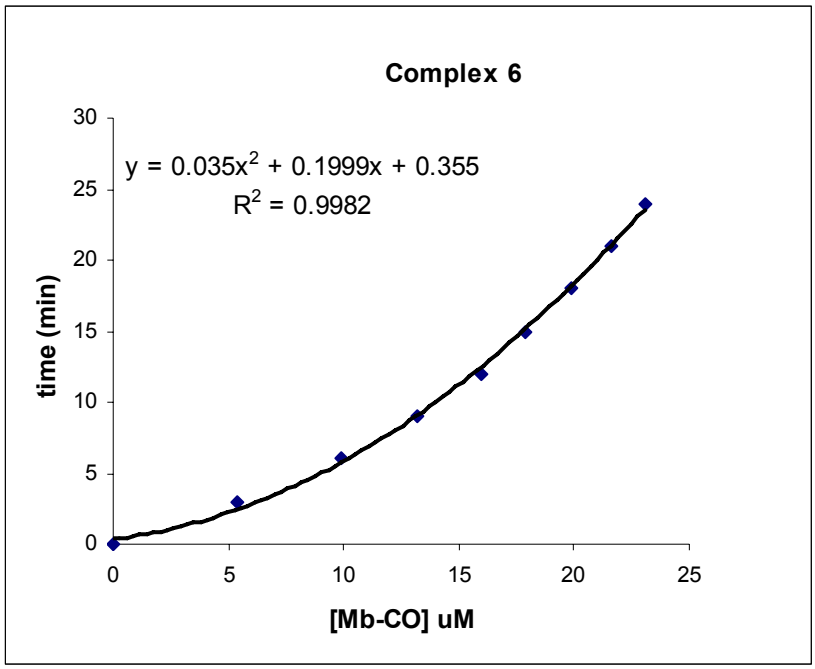


Figure S2. Differential pulse peak and CV of **7**.



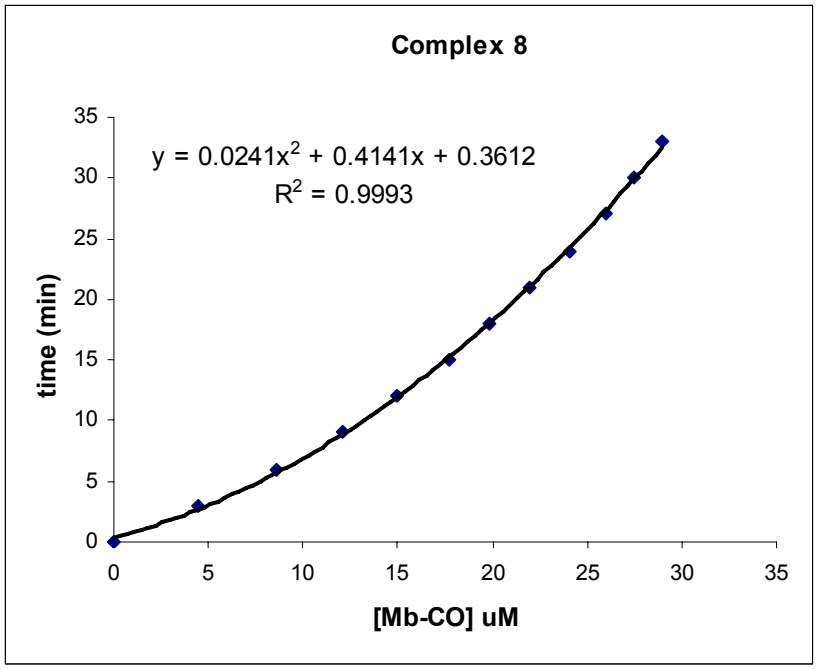


Figure S3. The amount of MbCO formed over time after addition of the Re^{II} complexes **6** and **8** to the Mb solution.

Table S1. Energies and cartesian coordinates of the optimized ground-state structure of 5-MER

Re -0.00022800 -0.69846200 -0.29686800

C -0.00178700 -2.59149000 -0.02723800

C 0.00100900 -0.97351300 -2.17133500

C 2.36202400 1.12392100 -0.21870000

C 3.09280900 -1.12676500 -0.21547200

C 3.69351000 1.57198500 -0.18154700

C 4.43346000 -0.72847300 -0.17712600

H 2.81150300 -2.17162100 -0.21934100

C 4.74517100 0.64498100 -0.16153200

H 3.90413700 2.63583500 -0.16441200

H 5.21108000 -1.48483100 -0.15483400

H 5.77692900 0.98152800 -0.13033700

C -1.19703400 2.03035100 -0.22699700

C 1.19770300 2.02993900 -0.22683200

C -1.21999000 3.43427400 -0.14414400

C 1.22116000 3.43381300 -0.14387800

C 0.00069300 4.13334900 -0.11436600

H -2.15864900 3.97340800 -0.08646700

H 2.15998600 3.97261600 -0.08586800

H 0.00089200 5.21720300 -0.04805300

C -3.09320000 -1.12569300 -0.21585800

C -2.36161600 1.12475500 -0.21902600

C -4.43367200 -0.72690800 -0.17749000

H -2.81234600 -2.17067100 -0.21969300

C -3.69296000 1.57327400 -0.18193200

C -4.74494700 0.64666800 -0.16195800

H -5.21154900 -1.48300100 -0.15507900

H -3.90318300 2.63720800 -0.16489800

H -5.77659500 0.98355500 -0.13085100

Br 0.00025300 -0.41194500 2.41880100

O 0.00246000 -1.16434900 -3.35596300

O -0.00366500 -3.77396500 0.16104500

N 2.06183500 -0.23270000 -0.24302700

N 0.00022500 1.37488500 -0.29648600

N -2.06181500 -0.23200900 -0.24351700

Zero-point correction= 0.249425 (Hartree/Particle)

Thermal correction to Energy= 0.269600

Thermal correction to Enthalpy= 0.270544

Thermal correction to Gibbs Free Energy= 0.198836

Sum of electronic and zero-point Energies= -1061.186927

Sum of electronic and thermal Energies= -1061.166752

Sum of electronic and thermal Enthalpies= -1061.165808

Sum of electronic and thermal Free Energies= -1061.237516

Table S2. Energies and cartesian coordinates of the optimized ground-state structure of 5-FAC

Re -0.10591000 -0.65323500 -0.04195000

C 0.02670700 -2.27346400 -1.01305600

C -1.05843900 -1.55593000 1.37883100

O 0.09275700 -3.22697900 -1.74205400

O -1.60826700 -2.10291300 2.27550300

Br 1.91492900 -1.14133100 1.70300300

C 1.92943800 1.54145400 -0.50668400

C 2.47695000 -0.34908900 -1.81732300

C 3.20570800 2.09199600 -0.72645400

C 3.74662200 0.16613100 -2.08740200

H 2.16878300 -1.31120000 -2.20626900

C 4.12703400 1.40334200 -1.52305600

H 3.46928800 3.04079200 -0.27053900

H 4.42686900 -0.39944200 -2.71548300

H 5.11786000 1.81110800 -1.69973200

C -2.56266800 1.05454200 -0.07598900

C -2.93320100 -0.94630700 -1.30362200

C -3.94636800 1.33001100 -0.08330600

C -4.29997300 -0.68992100 -1.36287100

H -2.50227500 -1.82760400 -1.76095300

C -4.82969600 0.45800100 -0.72298500

H -4.31323900 2.22710400 0.40549100

H -4.94354000 -1.38333200 -1.89456100

H -5.89634300 0.65906300 -0.73722900

C -1.52941100 1.95978100 0.40589800

C 0.83075700 2.21550900 0.18738700

C -1.67007600 3.31930600 0.74514000

C 0.74204800 3.57583200 0.51480000

C -0.51551000 4.11285200 0.86783700

H -2.65414000 3.76016000 0.86465900

H 1.61395100 4.21799500 0.45151800

H -0.60109800 5.15956400 1.14322700

N -2.05016400 -0.12039800 -0.64390300

N -0.27310300 1.40408900 0.31160500

N 1.56886800 0.30771900 -1.03476800

Zero-point correction= 0.248759 (Hartree/Particle)

Thermal correction to Energy= 0.268945

Thermal correction to Enthalpy= 0.269889

Thermal correction to Gibbs Free Energy= 0.198658

Sum of electronic and zero-point Energies= -1061.153431

Sum of electronic and thermal Energies= -1061.133246

Sum of electronic and thermal Enthalpies= -1061.132301

Sum of electronic and thermal Free Energies= -1061.203532

Table S3. Energies and cartesian coordinates of the optimized ground-state structure of 2

N 1.36428500 -0.95708500 -0.42646100	C -1.16338600 -2.03767800 -0.77221500
C 1.22826100 -2.21534500 -0.90396500	H -2.16998300 -2.41809500 -0.89084600
C 0.24046500 -0.27546000 -0.13576900	N -1.03506600 -0.76935300 -0.29058700
C -0.03829000 -2.80344200 -1.09510300	C 0.31332200 1.10215100 0.38918900
H 2.14678900 -2.74727700 -1.13204400	C 1.50200800 2.96085700 1.06837400
H -0.14514800 -3.81149100 -1.47780700	C -0.89898000 2.96183500 1.13300400
Re -2.66095800 0.52297600 0.24684600	C 0.30252500 3.64085800 1.36058400
C -4.02048800 1.79283000 0.76825200	H 2.47307800 3.42242200 1.21886000
C -4.14933800 -0.64023900 -0.15893900	H -1.86144800 3.41563100 1.33240000
Br -2.44977200 -0.41671900 2.68213500	H 0.30250300 4.65288300 1.74769200
Br -2.57889400 1.45091200 -2.20075700	N 1.50466800 1.69749100 0.58501400
O -4.84571500 2.57799500 1.09002300	N -0.90506600 1.68898300 0.64625600
O -5.05432000 -1.36037700 -0.41069400	

Zero-point correction= 0.155307 (Hartree/Particle)

Thermal correction to Energy= 0.173614

Thermal correction to Enthalpy= 0.174558

Thermal correction to Gibbs Free Energy= 0.104377

Sum of electronic and zero-point Energies= -859.434569

Sum of electronic and thermal Energies= -859.416262

Sum of electronic and thermal Enthalpies= -859.415318

Sum of electronic and thermal Free Energies= -859.485499

Table S4. Energies and cartesian coordinates of the optimized ground-state structure of 6

Re -3.63003800 0.00808000 0.20384900

N -1.41798700 0.02167900 0.07133100

C -0.64566000 0.88606800 0.79024400

C -0.75238700 -0.86640500 -0.72234500

C 0.75237800 0.86640400 0.72232300

H -1.15718900 1.61077600 1.40788900

C 0.64565100 -0.88606700 -0.79026900

H -1.35028900 -1.55565800 -1.29965200

H 1.35027800 1.55564200 1.29964800

H 1.15718600 -1.61078300 -1.40790100

Re 3.63003700 -0.00805700 -0.20384600

N 1.41797700 -0.02166600 -0.07137000

C 5.52401300 0.03545600 -0.19919800

C -5.52401700 -0.03543400 0.19927000

C -3.69036400 0.17916500 2.12061900

C 3.69042800 -0.17892300 -2.12063500

Br -3.64458700 -0.22583900 -2.46178400

Br -3.53738700 2.67025900 0.16226000

Br -3.41040600 -2.60986100 0.62156700

Br 3.64445500 0.22556300 2.46181100

Br 3.53743400 -2.67024700 -0.16257800

Br 3.41046500 2.60993800 -0.62129800

O -6.71792300 -0.06488700 0.19526300

O -3.77735500 0.28876600 3.30267700

O 6.71791800 0.06490900 -0.19514400

O 3.77746300 -0.28838700 -3.30270300

Zero-point correction= 0.118593 (Hartree/Particle)

Thermal correction to Energy= 0.147913

Thermal correction to Enthalpy= 0.148857

Thermal correction to Gibbs Free Energy= 0.047103

Sum of electronic and zero-point Energies= -955.150511

Sum of electronic and thermal Energies= -955.121192

Sum of electronic and thermal Enthalpies= -955.120247

Sum of electronic and thermal Free Energies= -955.222001