

Supporting Information

A Fine Tuning of Metallaborane to Bridged Boryl Complex, $[(\text{Cp}^*\text{Ru})_2(\mu\text{-CO})(\mu\text{-H})(\mu\text{-Bcat})]$ (cat = **1,2-O₂C₆H₄; Cp* = ($\eta^5\text{-C}_5\text{Me}_5$) †**

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I.1 Materials and Methods

All the manipulations were conducted under an Ar/N₂ atmosphere using standard Schlenk techniques or glove box. Solvent were distilled prior to use under Argon. [Cp*RuCl₂]₂, [Mo(CO)₆], LiBH₄ 2.0 M in THF (Aldrich) were used as received. Catechol borane (Aldrich) was purified by careful vacuum distillation prior to use. [(Cp*RuCO)₂B₂H₆] and was prepared according to literature method¹. The external reference for the ¹¹B NMR, [Bu₄N(B₃H₈)], was synthesized with the literature method². Preparative thin-layer chromatography was performed with Merck 105554 TLC Silica gel 60 F₂₅₄, layer thickness 250 µm on aluminum sheets (20 x 20 cm). NMR spectra were recorded on a 400 and 500 MHz Bruker FT-NMR spectrometer. Residual solvent protons were used as reference (δ , ppm, CDCl₃, 7.26), while a sealed tube containing [Bu₄N(B₃H₈)] in [D₆]-benzene (δ_B , ppm, -30.07) was used as an external reference for the ¹¹B NMR. Infrared spectra were recorded on a Nicolet iS10 spectrometer. The photoreactions described in this report were conducted in a Luzchem LZC-4 V photo reactor, with irradiation at 254–350 nm. Mass spectra were recorded on Bruker MicroTOF-II mass spectrometer.

I.2 Synthetic Section

*Synthesis of **2** and **3**:* Compound **1** (0.15 g, 0.27 mmol) was taken in a Flame-dried Schlenk tube. Added THF (10 cm³) and stirred at room temperature for 1 hour after the addition of catechol borane (0.02 mL, 0.12 mmol) via syringe. The solvent was evaporated under vacuum, the residue was extracted into hexane and filtration afforded an air and moisture sensitive yellow solution. After removal of solvent, the residue was subjected to chromatographic work up using silica gel TLC plates. Elution with a hexane/CH₂Cl₂ (70:30 v/v) mixture yielded yellow coloured **2** (0.105 g, 57%) and **3** (0.035 g, 23%). **2**: MS (ESI⁺) = 664. Calculated mass for ¹²C₂₈¹H₄₀¹¹B₂¹⁶O₄¹⁰¹Ru₂, 664, obsd, 663.8664. ¹¹B NMR (22 °C, 128 MHz, CDCl₃): δ 11.6 (br, 1B), 13.5 (br, 1B). ¹H NMR (22 °C, 400 MHz, CDCl₃): δ 6.90 (d, 1H; Ph),

6.86 (dd, 1H; Ph), 6.84 (dd, 1H; Ph), 6.82 (d, 1H; Ph), 5.74 (br, 1H, OH), 3.43 (partially collapsed quartet(pcq), 1H; BH_t), 4.34 (pcq, 1H; BH_t), 1.78 (s, 15H; Cp*), 1.70 (s, 15H; Cp*), 1.50 (br, 1H; B-H-B), -12.71 (br, 1H; Ru-H-B), -15.49 (s, 1H; Ru-H-Ru). ¹³C NMR (22 °C, 100 MHz, CDCl₃): δ 203.2, 198.4 (CO), 133.6, 130.2, 128.7, 127.1, 125.8, 123.06 (Ph), 100.1, 98.4 (C₅Me₅), 10.4, 9.7 ppm (C₅Me₅). IR ν̄/cm⁻¹: 1918, 1969 (CO), 2444, 2412 (B-H_t). **3**: MS (ESI⁺) = 662. Calculated mass for ¹²C₂₈¹H₃₈¹¹B₂¹⁶O₄¹⁰¹Ru₂, 662, obsd, 661.5836. ¹¹B NMR (22 °C, 128 MHz, CDCl₃): δ 23.6 (br, 1B), 8.5 (br, 1B). ¹H NMR (22 °C, 400 MHz, CDCl₃): δ 6.85 (d, 2H; Ph), 6.79 (d, 2H; Ph), 4.02 (partially collapsed quartet(pcq), 1H, BH_t), 1.83 (s, 15H; Cp*), 1.73 (s, 15H; Cp*), -12.51 (br, 2H; Ru-H-B), -15.98 ppm (s, 1H; Ru-H-Ru). ¹³C NMR (22 °C, 100 MHz, CDCl₃): δ 203.2, 198.4 (CO), 133.6, 128.7, 125.8 (Ph), 100.1, 98.7 (C₅Me₅), 11.2, 9.7 ppm (C₅Me₅). IR ν̄/cm⁻¹: 1922, 1942 (CO), 2423 (B-H_t).

*Synthesis of **4**:* In a Flame-dried Schlenk tube, a yellow solution of **3** (0.10 g, 0.15 mmol) in THF (20 mL) was irradiated for 3 h at room temperature. After this, the volatile components were removed under vacuum, and the remaining residue was extracted into hexane and passed through Celite. After removal of solvent, the residue was subjected to chromatographic work up using silica gel TLC plates. Elution with a hexane/CH₂Cl₂ (80:20 v/v) mixture yielded brown **4** (0.038 g, 41%). **4**: MS (ESI⁺) = 620. Calculated mass for ¹²C₂₇¹H₃₄¹¹B₁¹⁶O₃¹⁰¹Ru₂, 619, obsd, 618.5373. ¹¹B NMR (22 °C, 128 MHz, CDCl₃): δ 53.7 (br, 1B). ¹H NMR (22 °C, 400 MHz, CDCl₃): δ 7.71 (d, 2H; Ph), 6.92 (d, 2H; Ph), 1.62 ppm (s, 30H; Cp*), -10.73 (s, 1H; Ru-H-Ru). ¹³C NMR (22 °C, 100 MHz, CDCl₃): δ 180.3 (CO), 131.9, 130.0, 128.4 (Ph), 100.1 (C₅Me₅), 9.7 ppm (C₅Me₅). IR (hexane) ν̄/cm⁻¹: 1717 (CO).

I.3 NMR Experiment Details

❖ Experiment to confirm the release of hydrogen and formation of **3** from **2**:

The NMR experiment has been carried out by taking pure **2** in a sealed NMR tube in dry and degassed CDCl₃. The ¹H NMR spectra has been recorded at regular intervals of time that showed the gradual rise in intensity of the peak at δ = 4.62 ppm (this confirms the release of hydrogen from **2**) along with the other peaks corresponding to **3**. In addition to this, the ¹¹B NMR spectrum showed a gradual

increase in the intensity of the peaks at 8 and 23 ppm that corresponds to compound **3**.

❖ **Experiment to trap the borane released:** The NMR experiment has been carried out by recording the ^{11}B and ^{31}P NMR spectra of the reaction mixture that contains pure compound **1**, pre-distilled catechol borane and PPh_3 (added after 10 minutes of the addition of catechol borane). The reaction mixture was taken in a sealed NMR tube in dry and degassed CDCl_3 . ^{11}B and ^{31}P NMR spectra were recorded at regular intervals of time that showed an increase in intensity of the peaks at -38.5 and 20.5 ppm respectively in ^{11}B and ^{31}P NMR spectroscopy with time.

I.4 X-Ray analysis Details

The crystal data for **2** and **4** were collected and integrated using a Bruker Axs kappa apex2 CCD diffractometer, with graphite monochromated Mo-K α ($\lambda = 0.71073 \text{ \AA}$) radiation at 273 K. The structures were solved by heavy atom methods using SHELXS-97 or SIR92^{3a} and refined using SHELXL-97³. Note that, for compound **4** all non-hydrogen atoms are full matrix least squares refined with anisotropic thermal parameters. However, restraints are set on the atomic displacement parameters of light atoms to avoid abnormally shaped thermal ellipsoids for peripheral atoms. The crystal has a pseudo-merohedral twinning with ‘a’ and ‘b’ axes interchanged. The ‘a’ and ‘b’ axis are only nearly equal and hence some of the reflections are badly mixed. This leads to ‘not so good’ standard deviations for globally refined cell parameters and some of the bond distances. Apart from twinning, there are 2-fold disorders for catechol borane and Cp^* moieties. The disorders are resolved with some of the component occupancies restrained to 1. Discussions of these serious problems are mentioned in the cif file as well.

Crystal data for **2**: $\text{C}_{28}\text{H}_{40}\text{B}_2\text{O}_4\text{Ru}_2$, $M_r = 664.36 \text{ g/mol}$, orthorhombic, space group $P212121$, $a = 9.6314(3) \text{ \AA}$, $b = 13.3745(5) \text{ \AA}$, $c = 22.5647(8) \text{ \AA}$, $\alpha = 90^\circ$, $\beta = 90^\circ$, $\gamma = 90^\circ$, $V = 2906.68(17) \text{ \AA}^3$, $Z = 4$, $\rho_{\text{calcd}} = 1.518 \text{ g/cm}^3$, Final R indices [$I > 2\sigma(I)$] $R_1 = 0.0306$, $wR_2 = 0.0830$, index ranges $-10 \leq h \leq 11$, $-16 \leq k \leq 16$, $-27 \leq l \leq 27$, θ range for data collection 2.70 to

25.90°, crystal size 0.35 x 0.28 x 0.15 mm³, reflections collected 29399, independent reflections 5697, $R_{\text{int}} = 0.0342$, Goodness-of-fit on F2 1.076.

Crystal data for **4**: C₂₇H₃₄BO₃Ru₂, $M_r = 619.49$ g/mol, triclinic, space group *P-1*, $a = 10.773(4)$ Å, $b = 10.793(4)$ Å, $c = 12.098(4)$ Å, $\alpha = 73.97(2)$ °, $\beta = 73.995(19)$ °, $\gamma = 83.093(19)$ °, $V = 1298.1(8)$ Å³, $Z = 2$, $\rho_{\text{calcd}} = 1.585$ g/cm³, Final R indices [I>2σ(I)] $R_1 = 0.0694$, wR₂ = 0.1290, index ranges -12<=h<=11, -12<=k<=12, -14<=l<=13, θ range for data collection 2.31 to 25.00°, crystal size 0.15 x 0.10 x 0.05 mm³, reflections collected 11281, independent reflections 4023, $R_{\text{int}} = 0.0554$, Goodness-of-fit on F2 1.133.

I.5 Computational Details

The geometries of all ruthenium complexes were optimized using the density functional theory (DFT)⁴ method in conjunction with BP86⁵ functional and def2-SVP⁶ basis set. The 28 core electrons of ruthenium were replaced by the quasi-relativistic effective core potential, def2-ECP⁷ for ruthenium. To save computing time all the calculations were carried out with the Cp analogue model compound, instead of Cp*. The model compounds were fully optimized in gaseous state (no solvent effect) without any symmetry constraints. The nature of the optimized stationary point was confirmed by analytic computation of harmonic force constants. NMR chemical shifts were calculated using the hybrid Becke–Lee–Yang–Parr (B3LYP) functional,⁸ using the BP86/def2-SVP optimized geometries. Computation of the NMR shielding tensors employed gauge-including atomic orbitals (GIAOs),^{9–11} using the implementation of Schreckenbach, Wolff, Ziegler, and co-workers.^{12–16} The ¹¹B NMR chemical shifts were calculated relative to B₂H₆ (B3LYP B shielding constant 93.52 ppm) and converted to the usual [BF₃.OEt₂] scale using the experimental δ(¹¹B) value of B₂H₆, 16.6 ppm¹⁷. TMS (SiMe₄) was used as internal standard for the ¹H NMR chemical shift calculations. NBO analysis was carried out using the NBO routine within the Gaussian09¹⁸ package. Wiberg bond indexes (WBI)¹⁹ on some selected bonds are obtained on natural bond orbital (NBO) analysis.^{20,21}

II. Supplementary Data

II.1 Table S1. DFT calculated and experimental NMR chemical shifts δ (ppm) **1'-4'**.

	1'		2'		3'		4'		4a	
¹¹ B NMR	Exp. ^a	Cal.	Exp.	Cal.	Exp.	Cal.	Exp.	Cal.	Exp	Cal
B1	23	24.6	11.6	15.8	8.5	-6.3	53.7	54.97		52.3
B2	-3.0	-2.4	13.5	17.6	23.6	28.7	-	-	-	-
¹ H NMR										
Ru- <u>H</u> -Ru	-15.92	-12.04	-15.4	-12.12	-15.9	-11.6	-10.73	-9.94	-	-11.9, -9.7, 9.5
Ru- <u>H</u> -B	-13.15	-10.29	-12.7	-9.9	-13.5	-10.46			-	-
B- <u>H</u> -B	-3.73	-2.56	1.5	1.36	-	-	-	-	-	-

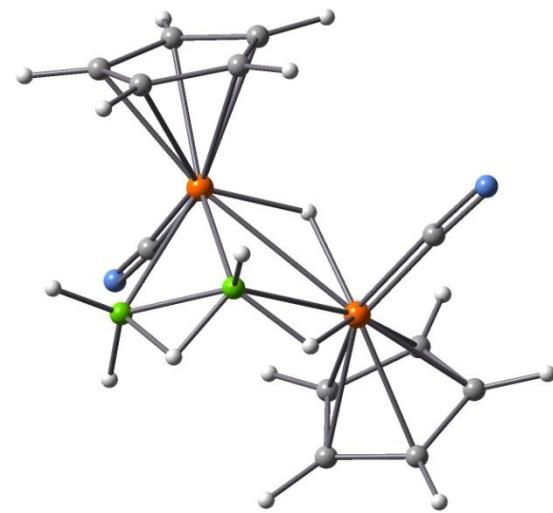
^a see reference 4 in supporting information

II.2 Table S2. Selected optimized bond lengths (\AA), Wiberg Bond Indices (WBI), HOMO-LUMO Gaps (ΔE , eV) for the model complexes **1'-4'**.

II.3 Table S3. Selected structural parameters and chemical shifts (^{11}B and ^1H NMR) of **4** and other related bridged boryl complexes.

Bridged-Boryl Complexes	d(M-M) (Å)	d _{avg} (M-B) (Å)	^{11}B NMR δ [ppm]	^1H NMR δ [ppm]	Ref.
[Pt ₂ (PPh ₃) ₂ (μ -dppm) ₂ (Bcat)(μ -Bcat)]	2.771	2.303	-		22a
[Rh(DiPPE)(μ -H) ₂ (μ -Bcat)RhH(DiPPE)]	2.574	2.250	35.0	-7.82, -8.69	22b
[(η^5 -C ₅ Me ₅)Fe(μ -CO) ₂ (μ -BCl ₂)Pd(PCy ₃)]	2.531	2.079	72.2	-	22c
[Cp [*] ₂ Ru ₂ H ₃ [B(<i>N,N</i> -diamine)]]	2.455	2.307	43.9	-13.91	22d
4	2.402	2.264	53.7	-10.32	This work

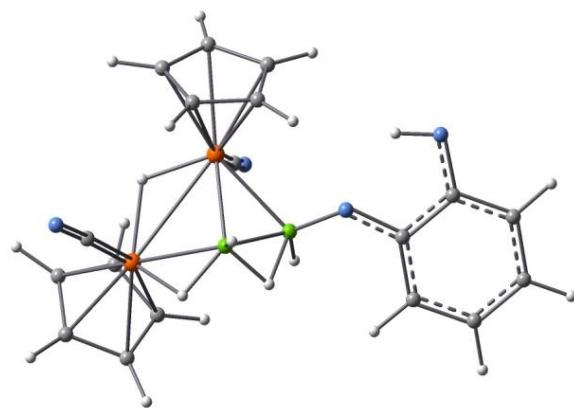
II.4 Figure S1. Optimized geometry of **1'**.



Cartesian coordinates for the calculated structure of **1'** (in Å).

C	-3.10070800	0.15845800	-1.41622700	Ru	1.46527700	0.32909300	0.15340300
C	-3.61097800	-0.19725500	-0.10943600	H	-0.10238500	-0.65216900	2.73517800
C	-3.20935800	0.83062300	0.81233900	H	-0.27710000	-2.39920600	1.87984600
C	-2.43904700	1.80334000	0.08833400	H	1.14563900	0.55467000	1.78967200
C	-2.37843700	1.38329400	-1.28839000	H	-0.61975000	1.23898200	2.38582500
C	2.66558100	-0.53408800	-1.55282100	H	-1.95285300	-1.44412300	2.64208300
C	3.51104600	0.27836500	-0.71830100	H	0.02763800	0.17585400	-0.88939100
C	3.55350800	-0.31089900	0.59414100	H	-4.23219800	-1.06988500	0.12866000
C	2.76156400	-1.52695500	0.55289500	H	-3.44079900	0.85929500	1.88423700
C	2.22380300	-1.65924700	-0.75546400	H	-1.98996100	2.71307600	0.50401300
C	-1.05074000	-1.99263700	-0.42361300	H	-1.85746900	1.91126800	-2.09740900
C	1.26790200	2.14818200	-0.05647000	H	-3.24409200	-0.41329100	-2.34199600
B	-0.20584300	0.26376000	1.78059300	H	2.58633400	-2.21327100	1.39094300
B	-0.94194900	-1.37797700	1.95818900	H	1.56223400	-2.46555400	-1.09509800
O	-0.92593600	-3.10018400	-0.79074000	H	2.45225900	-0.37256400	-2.61645800
O	1.20536100	3.30642700	-0.21965400	H	4.03299600	1.19329500	-1.02765000
Ru	-1.37184600	-0.23899800	0.03537700	H	4.13729600	0.05351600	1.44855400

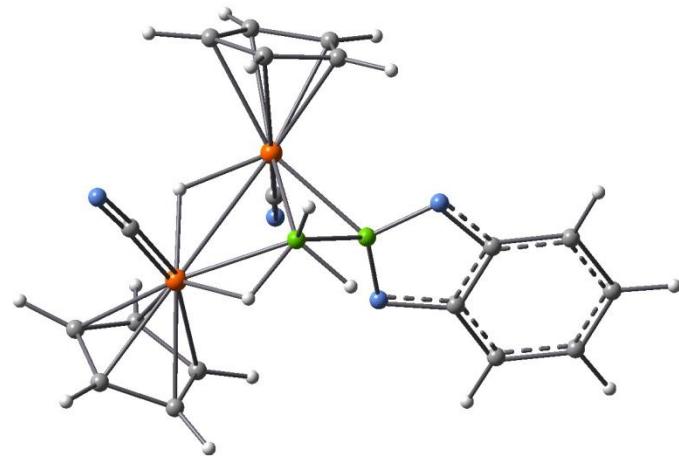
II.5 Figure S2. Optimized geometry of **2'**.



Cartesian coordinates for the calculated structure of **2'** (in Å).

C	2.61866300	-2.99196900	-0.14738200	H	-5.07257300	-3.91571800	-0.37783900
C	3.88623400	-2.31681400	-0.21098900	C	-6.16929800	-2.03636400	-0.26975900
C	3.98249800	-1.44205200	0.93522500	H	-7.15793100	-2.52051400	-0.23425100
C	2.77229300	-1.59291300	1.69519600	C	-6.08509500	-0.63105600	-0.24008500
C	1.92918100	-2.55251400	1.04285500	H	-6.98536900	-0.00046600	-0.17999200
C	0.54703000	2.90845300	-1.10188500	C	-4.82870900	-0.00757400	-0.28555600
C	1.19488100	3.26346400	0.13648700	O	-4.70609700	1.34971400	-0.25922700
C	0.20671800	3.29647600	1.16520800	H	-3.73615400	1.50277500	-0.32456800
C	-1.06797500	2.95150700	0.57405500	H	1.91160400	0.68468700	0.51567400
C	-0.85129200	2.73121800	-0.83208400	H	-0.05915800	0.21159300	-2.34336500
C	3.11514000	0.30073600	-1.61090400	H	1.18148300	-1.16862400	-1.60319400
C	-0.02153500	0.29592000	1.96481900	H	-1.18300700	-1.50865800	0.71702100
O	3.71305500	0.95830400	-2.37258200	H	-0.69390900	-1.26865400	-1.16740200
O	-0.18393400	-0.15862000	3.03289700	H	4.83762700	-0.80738700	1.19814700
Ru	2.26698400	-0.79175800	-0.38612200	H	2.52481300	-1.05669100	2.62024000
Ru	0.25118700	1.15343100	0.35495100	H	0.94391800	-2.88791300	1.38785500
B	0.16146700	-0.28950600	-1.25433900	H	2.25210800	-3.73594100	-0.86664000
O	-2.48707600	-0.06156000	-0.42167400	H	4.65482800	-2.46200300	-0.98079500
B	-1.19156000	-0.56137800	-0.05497300	H	1.03428400	2.81121500	-2.07922200
C	-3.64736500	-0.79845300	-0.36047100	H	2.26610600	3.46463100	0.26494100
C	-3.73821000	-2.19799300	-0.39718700	H	0.38161700	3.53713400	2.22172400
H	-2.82090400	-2.80140600	-0.46513700	H	-2.03288500	2.92318700	1.09611000
C	-5.00429400	-2.81701600	-0.34871500	H	-1.61630600	2.45849900	-1.56947500

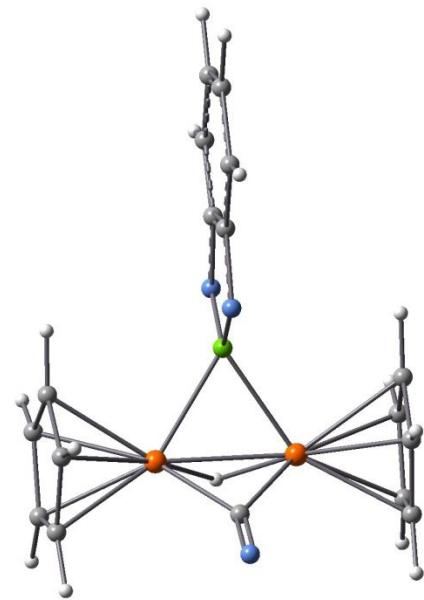
II.6 Figure S3. Optimized geometry of **3'**.



Cartesian coordinates for the calculated structure of **3'** (in Å).

C	1.86627900	-3.12009400	-0.36158100	C	-5.94680300	-0.86267500	-0.67220100
C	3.24426100	-2.72325400	-0.25074900	H	-7.01067100	-0.71874800	-0.91797000
C	3.39631800	-1.99388800	0.98816700	C	-5.54806000	-2.00550300	0.04590500
C	2.10868700	-1.94745100	1.62191800	H	-6.30464900	-2.74364600	0.35514700
C	1.15778300	-2.64631700	0.80087500	C	-4.19141900	-2.22762300	0.38026300
C	0.76716200	3.14821100	-0.85182200	H	-3.87037000	-3.11598000	0.94434400
C	1.40666000	3.24780200	0.43203600	C	-3.26710400	-1.26715900	-0.03568600
C	0.39322600	3.26839000	1.43940800	O	-1.91117000	-1.23980400	0.16438100
C	-0.89263100	3.18054600	0.78116200	H	1.75039900	0.55515800	0.59725300
C	-0.65334000	3.11294800	-0.63645900	H	-0.83226400	-0.71667100	-1.74662800
C	3.17712900	0.16723200	-1.34692300	H	0.23103000	0.76785100	-2.44599100
C	-0.35035800	0.28652300	1.82062700	H	1.04294700	-0.96377700	-1.76747000
O	3.97962300	0.78348900	-1.93537400	H	2.48964300	3.28111400	0.60811700
O	-0.67632700	-0.24333700	2.81300000	H	1.27427400	3.10783700	-1.82298100
Ru	1.99299700	-0.87936600	-0.38721900	H	0.56029600	3.34625500	2.52141100
Ru	0.17583600	1.26664800	0.35251800	H	-1.87531300	3.20810000	1.26801300
B	0.14332400	0.04034600	-1.47317400	H	-1.42636400	3.03360200	-1.41008900
O	-2.57588300	0.66682400	-1.02167700	H	4.33032800	-1.57910300	1.38670300
B	-1.42705500	-0.04096200	-0.50017000	H	1.88090400	-1.45435400	2.57538900
C	-3.66864600	-0.11911700	-0.75492500	H	0.08773300	-2.77242100	1.00662000
C	-5.00531600	0.10830300	-1.08670000	H	1.43042300	-3.69682300	-1.18796100
H	-5.30386700	1.00649800	-1.64772900	H	4.04263900	-2.96083300	-0.96511000

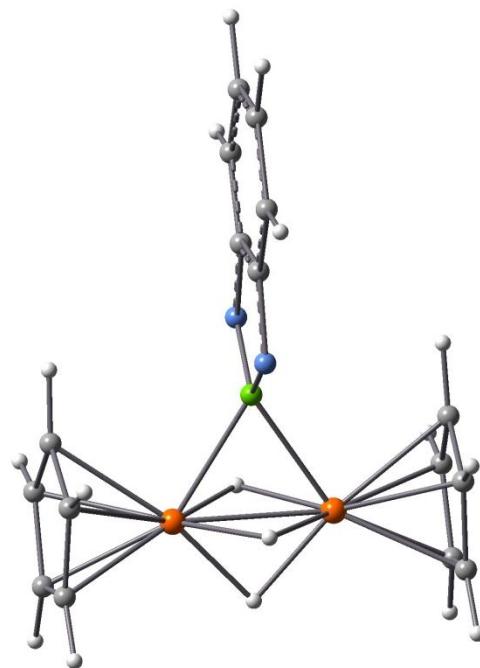
II.7 Figure S4. Optimized geometry of **4'**.



Cartesian coordinates for the calculated structure of **4'** (in Å).

C	0.53612900	3.11370200	-1.23511700	H	-6.37692600	-0.00068400	-0.92847700
C	-0.17029500	3.03084800	0.01708400	C	-5.27687800	0.00001800	0.94690100
C	0.80347600	2.98246300	1.07383800	H	-6.19382400	0.00018400	1.55705700
C	2.11403800	3.03147600	0.46817600	C	-4.01976400	0.00030500	1.59239700
C	1.95174100	3.10993800	-0.95744400	H	-3.92743900	0.00067800	2.68876200
C	1.95185700	-3.10954600	-0.95773900	C	-2.88609800	0.00008700	0.77409900
C	0.53614100	-3.11342400	-1.23489700	O	2.51247900	0.00052200	2.19198600
C	-0.16982000	-3.03092700	0.01760400	C	1.90977400	0.00009400	1.16780500
C	0.80433600	-2.98270000	1.07397600	H	1.51355700	-0.00001600	-1.46567900
C	2.11469600	-3.03147900	0.46780200	H	3.06877300	2.98881100	1.00813600
Ru	1.06338000	-1.20331400	-0.22619400	H	2.75647200	3.15975700	-1.70152300
Ru	1.06312400	1.20336600	-0.22657500	H	0.58875700	2.91162800	2.14734000
B	-0.80409600	-0.00000600	-0.08890400	H	-1.25987700	3.02017000	0.14455800
O	-1.56471100	0.00030300	1.13290600	H	0.07602700	3.14127400	-2.23135400
O	-1.73582900	-0.00051300	-1.18473600	H	0.58995700	-2.91211100	2.14756200
C	-2.99101400	-0.00039500	-0.63556000	H	3.06965200	-2.98901300	1.00738500
C	-4.23106600	-0.00068800	-1.28040500	H	-1.25936200	-3.02039900	0.14546400
H	-4.29845800	-0.00106800	-2.37862800	H	0.07571500	-3.14047600	-2.23099400
C	-5.38067100	-0.00047200	-0.45891000	H	2.75625000	-3.15929100	-1.70219500

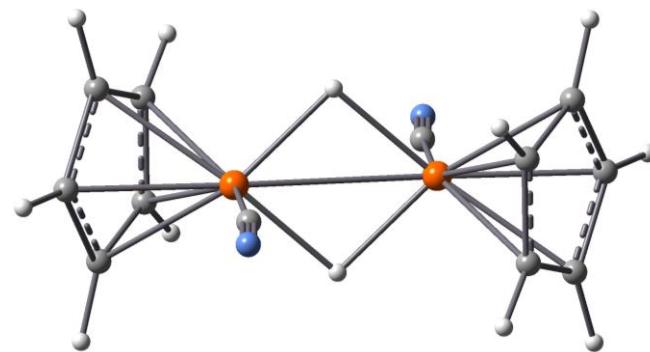
Figure S55. Optimized geometry of **4a**.



Cartesian coordinates for the calculated structure of **4a** (in Å).

C	-0.97775100	-3.07964700	-1.20060800	H	6.16805000	-0.00057600	-1.23039100
C	0.06194600	-3.01104500	-0.21062500	C	5.19771400	-0.00015000	0.71491700
C	-0.55619700	-2.97866600	1.09162700	H	6.15374800	-0.00012600	1.26175300
C	-1.98889500	-3.03578500	0.90445900	C	3.98680800	0.00004500	1.44352500
C	-2.24288700	-3.09803100	-0.51815400	H	3.96808900	0.00023400	2.54362400
C	-2.24377500	3.09873300	-0.51535600	C	2.80139900	0.00002400	0.70300700
C	-0.98044100	3.08030900	-1.20098000	H	-1.13448800	0.00056600	-1.32763000
C	0.06175900	3.01095800	-0.21369600	H	-2.74488100	-3.04923500	1.69974400
C	-0.55312800	2.97833300	1.09013600	H	-3.22928500	-3.13689700	-0.99815700
C	-1.98629400	3.03588300	0.90656500	H	-0.02804700	-2.92701500	2.05201500
Ru	-1.21816600	1.21719200	-0.00830300	H	1.13943600	-2.97907900	-0.41510900
Ru	-1.21838600	-1.21726700	-0.00826700	H	-0.82974300	-3.09237700	-2.28795000
B	0.66605000	0.00016600	-0.01594200	H	-0.02259200	2.92636100	2.04918700
O	1.50695400	0.00027400	1.15014900	H	-2.74030900	3.04935700	1.70371400
O	1.52052600	-0.00015200	-1.17200500	H	1.13871100	2.97890500	-0.42096500
C	2.80935400	-0.00018500	-0.71014100	H	-0.83524100	3.09329500	-2.28869800
C	4.00341000	-0.00040600	-1.43708900	H	-3.23137600	3.13782700	-0.99286500
H	3.99714800	-0.00059000	-2.53732500	H	-1.15872600	0.00061100	1.30075400
C	5.20579400	-0.00040400	-0.69457400	H	-2.54523300	0.00044600	-0.04615500

Figure S6. Optimized geometry of **5'** compound.



Cartesian coordinates for the calculated structure of **5'** compound (in Å).

C	1.65260000	0.46020000	2.25870000	C	2.95380000	-2.26560000	0.06660000
C	2.83480000	0.14010000	2.93710000	Ru	3.84360000	-0.97810000	-0.89700000
C	3.63350000	1.34500000	3.05320000	O	2.41610000	-3.15280000	0.57530000
C	2.88380000	2.41150000	2.48170000	H	2.61260000	0.31280000	-0.62120000
C	1.67890000	1.87410000	1.93550000	H	4.07588230	-3.44463720	-2.49698669
C	4.28390000	2.26560000	-0.06660000	H	2.70297406	-1.43939435	-3.62221803
Ru	3.39410000	0.97810000	0.89700000	H	6.36675505	-2.43860195	-1.51903128
O	4.82160000	3.15280000	-0.57530000	H	6.39464953	0.20694529	-2.04787609
H	4.62510000	-0.31280000	0.62120000	H	4.13437116	0.80788385	-3.35437555
C	5.58510000	-0.46020000	-2.25870000	H	3.16181770	3.44463720	2.49698669
C	4.40290000	-0.14010000	-2.93710000	H	4.53472594	1.43939435	3.62221803
C	3.60420000	-1.34500000	-3.05320000	H	3.10332884	-0.80788385	3.35437555
C	4.35390000	-2.41150000	-2.48170000	H	0.84305047	-0.20694529	2.04787609
C	5.55880000	-1.87410000	-1.93550000	H	0.87094495	2.43860195	1.51903128

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