Supplementary Information

Near-infrared (NIR)-responsive activation of Ru-benziphthalocyanine complexes via singlet-triplet transition

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1. General

Instrumentation.

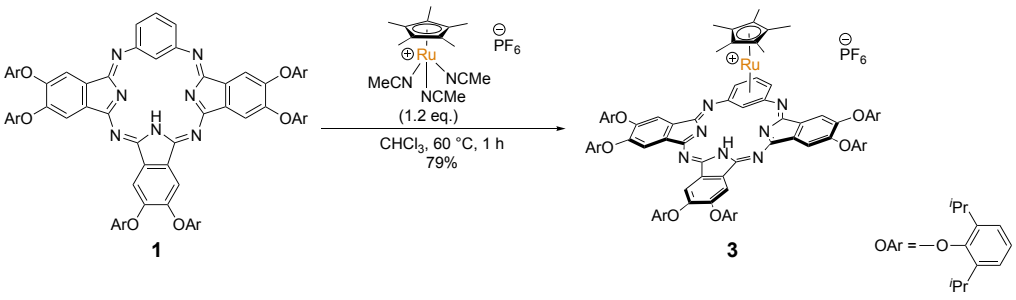
^{1}H, ^{11}B, and ^{13}C NMR spectra were obtained on a Bruker AVANCE NEO 500 spectrometer. Samples were recorded in $CDCl_3$, CD_2Cl_2, and C_6D_6 at room temperature. Chemical shifts are expressed in δ (ppm) values. ^{1}H spectra were referenced to tetramethylsilane (δ = 0.00 ppm), residual $CHCl_3$ (δ = 7.26 ppm), residual $CHDCl_2$ (δ = 5.32 ppm), or residual C_6HD_5 (δ = 7.16 ppm) as an internal standard. ^{13}C spectra were referenced to tetramethylsilane (δ = 0.00 ppm), $CDCl_3$ (δ = 77.16 ppm), or CD_2Cl_2 (δ = 53.84 ppm) as an internal standard. The following abbreviations are used: s = singlet, d = doublet, t = triplet, m = multiplet, br = broad. IR spectra were obtained on a JASCO FT/IR-4700 spectrometer. ESI mass spectra were measured on a Bruker compact spectrometer. Ultraviolet-visible-near-IR absorption spectra were recorded with a JASCO V-770 spectrophotometer. Photoreactions were performed using Kessil LEDs (427 nm and 740 nm) and CCS LEDs (850 nm and 940 nm). All the reactions were performed under an Ar atmosphere. Benziphthalocyanines **1**,[1] **2**,[2] and **5**[3] were synthesized according to the previous reports.

Materials.

Unless otherwise noted, materials were purchased from Sigma-Aldrich Corporation, FUJIFILM Wako Pure Chemical Corporation, Tokyo Chemical Industry Corporation, and Kanto Chemical Corporation. Dehydrated toluene and CH_2Cl_2 were purchased from Kanto Chemical and purified by a solvent purification system of Glass-Contour. Dehydrated $CDCl_3$ and C_6D_6 were prepared by degassing by argon bubbling and dehydration over molecular sieve 4A. All the reactions were performed under an argon atmosphere unless otherwise noted. Normal-phase column chromatographic separation was performed with silica gel 60 (230–400 mesh) from Merck or CHROMATOREXR-DIOL MB 100 neutral silica gel (75–200 μm) from Fuji Silysia Chemical. Thin-layer chromatography was carried out on 0.25 mm Merck silica gel plates (60F-254) or 0.25 mm DIOL TLC (F254) obtained from Fuji Silysia Chemical.

2. Experimental Details

2-1. Synthesis of Ru complexes



To a mixture of benziphthalocyanine **1**[1] (40 mg, 26 μmol) and [Cp*Ru(MeCN)$_3$]PF$_6$ (16 mg, 31 μmol) was added $CHCl_3$ (5 mL), and the mixture was stirred at 60 °C for 1 h. The volatiles were evaporated *in vacuo*. Column chromatography on neutral silica gel using $CHCl_3$/hexane (1:1 to $CHCl_3$ only) as an eluent gave the desired compound **3** as a red solid (39.7 mg, 79%).

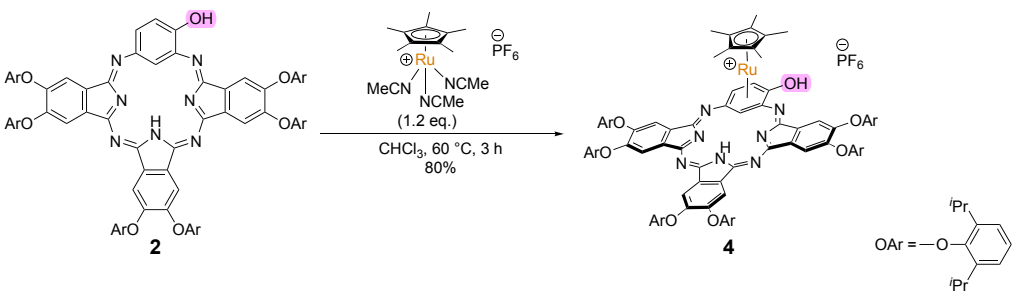
^{1}H-NMR (500 MHz, $CDCl_3$/TMS): δ 11.75 (brs, 1H), 7.46-7.27 (m, 18H), 6.89 (s, 2H), 6.88 (s, 2H), 6.64 (s, 2H), 6.09 (t, J = 6.0 Hz, 1H), 5.83-5.81 (m, 1H), 5.80 (dd, J = 6.0, 1.1 Hz, 2H), 3.28-2.80 (m, 12H), 1.72 (s, 15H), 1.40-0.95 (m, 72H).

^{13}C-NMR (126 MHz, $CDCl_3$/TMS): 179.5, 167.8, 159.8, 153.3, 152.0, 151.3, 148.42, 148.35, 148.0, 141.3, 141.1, 132.7, 132.1, 128.4, 127.1, 126.9, 126.7, 125.3, 125.0, 124.8, 113.2, 109.5, 108.6, 107.8, 96.6, 88.5, 86.4, 73.3, 27.52, 27.46, 24.5 (br), 22.9 (br), 10.0.

UV/vis/NIR (CH_2Cl_2): λ_{max} ($\varepsilon \times 10^{-4}$) = 500 (0.65) (sh), 352 (3.89) nm.

IR (ATR): 2964, 2925, 2867, 1635, 1576, 1373, 1325, 1286, 1192, 839 cm^{-1}.

HRMS (ESI): *m*/*z*: [M-PF$_6$]$^+$ Calcd for $C_{112}H_{128}N_7O_6Ru$ 1768.8964; Found 1768.8889.



To a mixture of monohydroxybenziphthalocyanine **2**[2] (72 mg, 46 μmol) and [Cp*Ru(MeCN)$_3$]PF$_6$

(28 mg, 56 µmol) was added $CHCl_3$ (5 mL), and the mixture was stirred at 60 °C for 3 h. The volatiles were evaporated *in vacuo*. Column chromatography on neutral silica gel using $CHCl_3$/EtOAc ($CHCl_3$ only to 8:2) as an eluent gave the desired compound **4** as a dark red solid (71.5 mg, 80%).

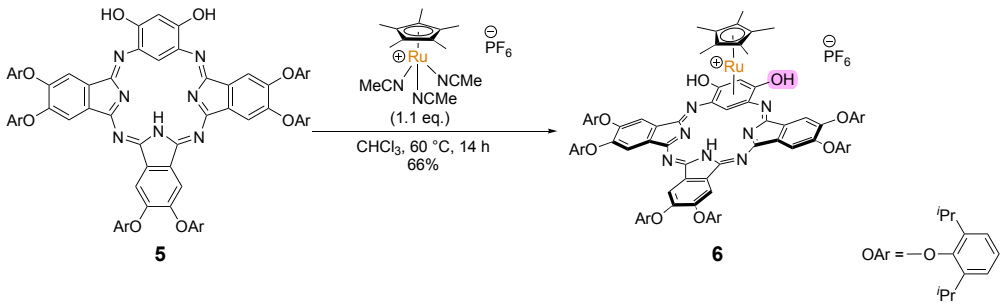
^{1}H-NMR (500 MHz, $CDCl_3$/TMS): δ 11.22 (brs, 1H), 7.50-7.39 (m, 4H), 7.39-7.27 (m, 14H), 7.00-6.95 (m, 3H), 6.93 (s, 1H), 6.75(s, 1H), 6.72 (s, 1H), 6.27 (brs, 1H), 5.82 (m, 2H), 3.32-2.93 (m, 12H), 1.54 (s, 15H), 1.42-0.87 (m, 72H).

^{13}C-NMR (126 MHz, $CDCl_3$/TMS): δ 178.8, 178.5, 167.0, 166.1, 159.9, 159.2, 153.4, 153.2, 151.9, 151.3, 151.0, 148.32, 148.26, 148.2, 147.8, 141.33, 141.28, 141.0, 132.8, 132.6, 132.31, 132.26, 128.4, 128.3, 127.0, 126.8, 126.7, 126.6, 126.5, 124.9, 124.6, 109.4, 108.3, 108.2, 108.1, 107.8, 107.4, 100.6, 95.3, 87.9, 75.1, 27.4, 27.31, 27.28, 24.2 (br), 22.7 (br), 9.5.

UV/vis/NIR (CH_2Cl_2): λ_{max} ($\varepsilon \times 10^{-4}$) = 500 (1.09) (sh), 372 (4.48) nm.

IR (ATR): 2962, 2871, 1576, 1438, 1373, 1326, 1276, 1191, 1094, 1015, 840, 749 cm^{-1}.

HRMS (ESI): *m*/*z*: $[M\text{-}PF_6]^+$ Calcd for $C_{112}H_{128}N_7O_7Ru$ 1784.8913; Found 1784.8951.



To a mixture of dihydroxybenziphthalocyanine **5**[3] (274 mg, 175 µmol) and $[Cp^*Ru(MeCN)_3]PF_6$ (96 mg, 0.19 mmol) was added $CHCl_3$ (6 mL), and the mixture was stirred at 60 °C for 14 h. The volatiles were evaporated *in vacuo*. Column chromatography on neutral silica gel using $CHCl_3$/hexane (1:1 to $CHCl_3$ only) as an eluent gave the desired compound **6** as a dark red solid (225 mg, 66%).

^{1}H-NMR (500 MHz, CD_2Cl_2): δ 10.41 (brs, 1H), 7.57-7.45 (m, 4H), 7.44-7.33 (m, 8H), 7.31-7.20 (m, 6H) 7.12 (s, 2H), 7.06 (s, 2H), 6.89 (s, 2H), 6.48 (brs, 1H), 5.89 (brs, 1H), 3.25-3.00 (m, 12H), 1.43-0.97 (m, 87H).

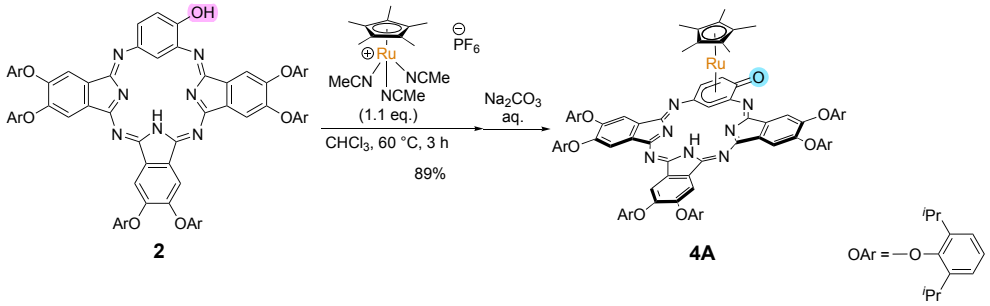
^{13}C-NMR (126 MHz, $CDCl_3$/TMS): δ 177.4, 164.7, 159.2, 153.7, 152.2, 151.4, 148.7, 148.5, 148.3, 141.7 (br), 141.5, 133.7, 132.9, 129.1, 127.5, 127.1, 127.0, 125.4, 125.1, 109.7, 108.2, 97.8, 97.6, 96.8, 93.5, 98.0, 75.5, 68.4, 27.9, 27.7, 24.5 (br), 22.9(br), 9.4.

UV/vis/NIR (CH_2Cl_2): λ_{max} ($\varepsilon \times 10^{-4}$) = 490 (1.29), 379 (5.22) nm.

UV/vis/NIR (toluene): λ_{max} ($\varepsilon \times 10^{-4}$) = 501 (1.13), 379 (4.31) nm.

IR (ATR): 2960, 2869, 1629, 1573, 1437, 1371, 1325, 1280, 1173, 1094, 1014, 841 cm^{-1}.

HRMS (ESI): *m*/*z*: $[M\text{-}PF_6]^+$ Calcd for $C_{112}H_{128}N_7O_8Ru$ 1800.8862; Found 1800.8898.



To a mixture of monohydroxybenziphthalocyanine **2**[2] (24 mg, 15 μmol) and $[Cp^*Ru(MeCN)_3]PF_6$ (8.3 mg, 16 μmol) was added $CHCl_3$ (3 mL), and the mixture was stirred at 60 °C for 3 h. After cooling to room temperature, 10% Na_2CO_3 aq. was added to the mixture, and the mixture was extracted with $CHCl_3$ three times. The combined organic layer was dried over Na_2SO_4, filtered, and evaporated *in vacuo*. Column chromatography on neutral silica gel using $CHCl_3$/hexane (1:1 to $CHCl_3$ only) as an eluent gave the desired compound **4A** as a brown solid (25 mg, 89%).

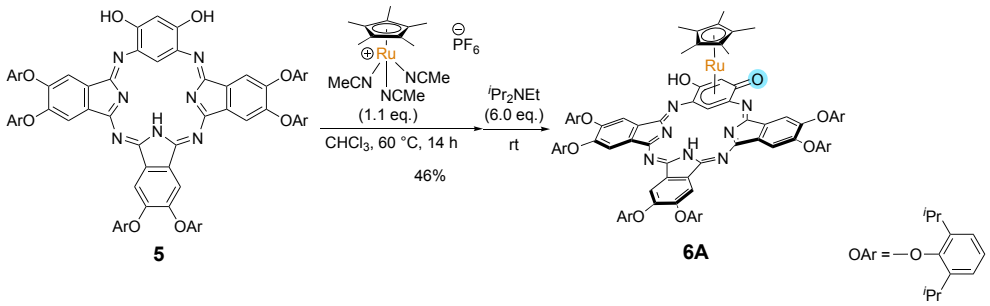
^{1}H-NMR (500 MHz, $CDCl_3$/TMS): δ 7.50-7.36 (m, 6H), 7.36-7.28 (m, 12H), 7.23 (s, 1H), 7.03 (s, 1H), 7.02 (s, 1H), 6.97 (s, 1H), 6.76 (s, 1H), 6.72 (s, 1H), 5.59 (dd, *J* = 6.6, 1.8 Hz, 1H), 5.21 (d, *J* = 1.8 Hz, 1H), 5.00 (d, *J* = 6.6 Hz, 1H), 3.35-2.89 (m, 12H), 1.53 (s, 15H), 1.44-0.90 (m, 72H).

^{13}C-NMR (126 MHz, $CDCl_3$/TMS): δ.176.3, 175.0, 163.1, 162.1, 158.3, 156.7, 152.9, 152.7, 151.3, 151.1, 150.4, 150.2, 149.0, 148.72, 148.69, 148.2, 148.1, 141.6, 141.3, 141.2, 134.4, 133.6, 132.5, 132.3, 128.8, 128.7, 127.0, 126.9, 126.5, 126.41, 126.37, 126.3, 125.0, 124.7, 124.6, 109.0, 108.9, 107.9, 107.3, 106.9, 103.1, 101.9, 91.4, 90.3, 78.0, 75.1, 27.5, 27.38, 27.35, 24.3 (br), 22.8 (br), 9.9.

UV/vis/NIR (CH_2Cl_2): λ_{max} ($\varepsilon \times 10^{-4}$) = 600 (0.41) (sh), 365 (3.25) nm.

IR (ATR): 2961, 2871, 1576, 1436, 1362, 1326, 1276, 1260, 1177, 750 cm^{-1}.

HRMS (ESI): *m*/*z*: $[M+H]^+$ Calcd for $C_{112}H_{128}N_7O_7Ru$ 1784.8913; Found 1784.8974.



To a mixture of dihydroxybenziphthalocyanine **5**[3] (282 mg, 180 μmol) and $[Cp^*Ru(MeCN)_3]PF_6$ (102 mg, 202 μmol) was added $CHCl_3$ (6 mL), and the mixture was stirred at 60 °C for 14 h. After cooling to room temperature, $^i Pr_2NEt$ (0.2 mL, 1 mmol) was added to the mixture, and the mixture was stirred for 1 min. The volatiles were evaporated *in vacuo*. Column chromatography on neutral silica gel using $CHCl_3$/hexane (1:1 to $CHCl_3$ only) as an eluent gave the desired compound **6A** as a dark brown solid (148 mg, 46%).

^{1}H-NMR (500 MHz, CD_2Cl_2): δ 9.72 (brs, 1H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.49 (t, *J* = 7.8 Hz, 2H), 7.44-7.27 (m, 14H), 7.21 (s, 2H), 7.15 (s, 2H), 6.95 (s, 2H), 5.55 (s, 1H), 5.39 (s, 1H), 3.34-2.99 (m, 12H), 1.47-0.94 (m, 87H).

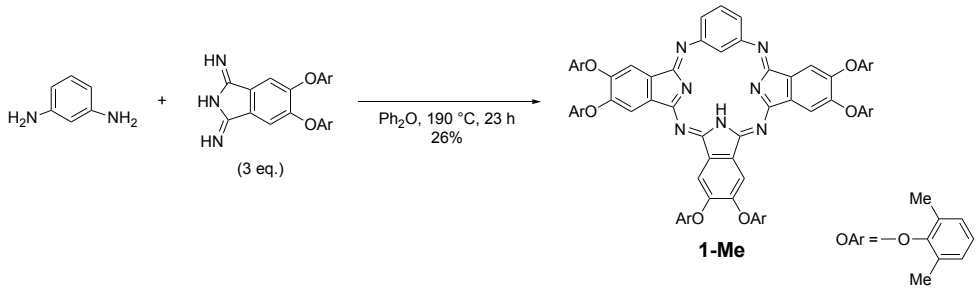
^{13}C-NMR (126 MHz, CD_2Cl_2): δ.175.3, 161.8, 157.6, 153.4, 151.9, 150.8, 149.0, 148.7, 148.4, 141.9, 141.7, 141.6, 134.6, 132.6, 131.4, 129.3, 127.4, 126.98, 126.92, 125.4, 125.1, 109.3, 108.2, 107.7, 95.9, 91.3, 76.0, 69.3, 27.9, 27.7, 24.5 (br), 22.8 (br), 9.4.

UV/vis/NIR (CH_2Cl_2): λ_{max} ($\varepsilon \times 10^{-4}$) = 600 (0.67) (sh), 367 (4.19) nm.

UV/vis/NIR (toluene): λ_{max} ($\varepsilon \times 10^{-4}$) = 529 (0.97), 362 (4.74) nm.

IR (ATR): 2962, 2870, 1576, 1457, 1437, 1362, 1277, 1193, 1175, 1094, 872, 765, 748 cm^{-1}.

HRMS (ESI): *m*/*z*: $[M+H]^+$ Calcd for $C_{112}H_{128}N_7O_8Ru$ 1800.8862; Found 1800.8922.



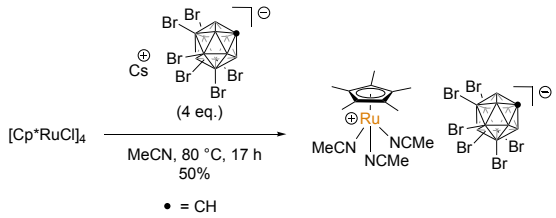
A mixture of 5,6-bis(2,6-dimethylphenyloxy)-1,3-diiminoisoindoline[4] (119.9 mg, 311 μmol) and 1,3-phenylenediamine (11.0 mg, 102 μmol) was suspended in Ph_2O (3.0 mL) and the mixture was stirred at 190 °C for 23 h. The reaction mixture was cooled to room temperature. Purification by column chromatography on neutral silica gel using toluene/hexane (hexane only to 2:1) as an eluent furnished **1-Me** as a red solid (31.9 mg, 26%).

^{1}H-NMR (500 MHz, $CDCl_3$/TMS): δ 11.75 (brs, 1H), 7.42 (t, *J* = 7.9 Hz, 1H),7.25-7.09 (m, 22H), 6.97 (s, 2H), 6.86 (t, *J* = 1.8 Hz, 1H), 6.71 (s, 2H), 2.25 (brs, 12H), 2.24 (brs, 24H).

^{13}C-NMR (126 MHz, $CDCl_3$/TMS): 177.3, 162.4, 158.5, 151.7, 151.0, 150.9, 150.5, 150.0, 149.2, 147.4, 134.2, 132.6, 131.2, 131.1, 130.9, 130.5, 129.6, 129.5, 129.3, 129.1, 126.2, 125.9, 125.7, 125.3, 109.4, 108.8, 108.2, 106.6, 16.40, 16.37, 16.3.

IR (ATR): 2916, 1577, 1474, 1365, 1272, 1179, 1087, 1008, 871, 764 cm^{-1}.

HRMS (ESI): *m*/*z*: $[M+H]^+$ Calcd for $C_{78}H_{66}N_7O_6$ 1196.5069; Found 1196.5112.



$[Cp^*Ru(MeCN)_3][CB_{11}H_6Br_6]$ was synthesized similarly to the reported procedure for $[Cp^*Ru(MeCN)_3]PF_6$.[5] To a mixture of $[Cp^*RuCl]_4$ (20.0 mg, 18.4 μmol) and $Cs[CB_{11}H_6Br_6]$[6] (55.0 mg, 73.4 μmol) were added MeCN (0.18 mL). The mixture was heated at 80 °C for 17 h and filtered through a filter paper with hot MeCN in an Ar glovebox. The filtrate was concentrated *in vacuo*. Recrystallization from MeCN/Et_2O yielded $[Cp^*Ru(MeCN)_3][CB_{11}H_6Br_6]$ as yellow crystals (36.2 mg, 50%).

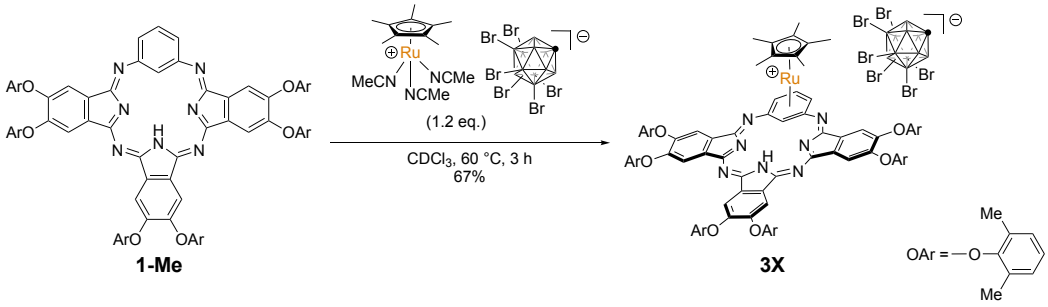
^{1}H-NMR (500 MHz, CD_2Cl_2): δ 2.63 (s, 15H), 1.97 (s, 9H).

^{13}C-NMR (126 MHz, CD_2Cl_2): δ 123.5, 80.5, 41.8, 9.8, 4.6.

^{11}B-NMR (160 MHz, CD_2Cl_2): δ –1.68, –9.83, –20.17.

IR (ATR): 3047, 2604, 2265, 1449, 1420, 1380, 1131, 1031, 992, 933, 857, 810, 746, 634 cm^{-1}.

HRMS (ESI): *m*/*z*: $[M\text{-}MeCN\text{-}CB_{11}H_6Br_6]^+$ Calcd for $C_{14}H_{21}N_2Ru$ 319.0743; Found 319.0747.



To a mixture of **1-Me** (8.5 mg, 7.1 μmol) and $[Cp^*Ru(MeCN)_3][CB_{11}H_6Br_6]$ (9.7 mg, 9.9 μmol) was added $CDCl_3$ (0.70 mL), and the mixture was heated at 60 °C for 3 h. The volatiles were evaporated *in vacuo*. Column chromatography on neutral silica gel using $CHCl_3$/hexane (1:3 to $CHCl_3$ only) as an eluent gave the desired compound **3X** as a red solid (9.7 mg, 67%).

^{1}H-NMR (500 MHz, $CDCl_3$/TMS): δ 11.76 (brs, 1H), 7.26-7.13 (m, 18H), 6.94 (s, 2H), 6.87 (s, 2H), 6.67 (s, 2H), 6.02 (s, 1H), 5.90 (t, *J* = 5.9 Hz, 1H), 5.79 (d, *J* = 5.9 Hz, 2H), 2.43 (brs, 1H), 2.25 (brs, 12H), 2.24 (brs, 12H), 2.23 (brs, 12H), 1.74 (s, 15H).

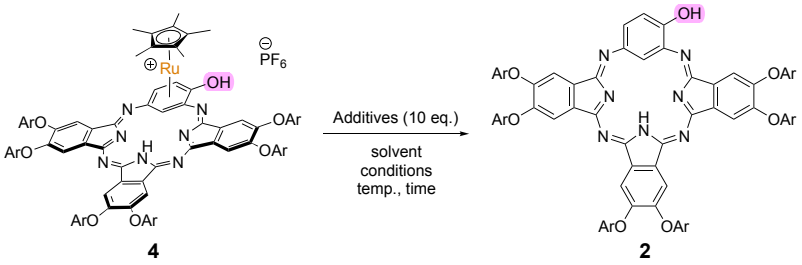
^{13}C-NMR (126 MHz, $CDCl_3$/TMS): δ 179.8, 168.0, 159.9, 152.1, 150.62, 150.59, 150.4, 150.2, 150.1, 132.9, 132.3, 131.0, 130.9, 130.7, 129.5, 129.3, 129.2, 128.7, 126.2, 126.0, 125.8, 113.1, 109.3, 108.0, 107.8, 96.7, 87.5, 85.8, 73.9, 40.8, 16.3, 16.22, 16.19, 10.2.

^{11}B-NMR (160 MHz, CD_2Cl_2/TMS): δ –1.66, –9.89, –20.28.

IR (ATR): 2920, 2605, 1634, 1574, 1478, 1449, 1368, 1283, 1174, 1087, 1011, 859 cm^{-1}.

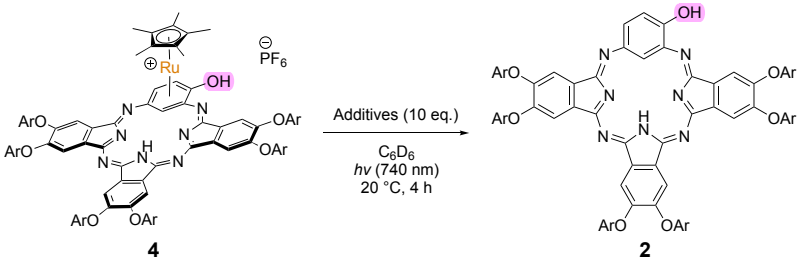
HRMS (ESI): *m*/*z*: $[M\text{-}CB_{11}H_6Br_6]^+$ Calcd for $C_{88}H_{80}N_7O_6Ru$ 1432.5208; Found 1432.5176.

2-2. Screening of reaction conditions for photochemical arene release



4 2

General procedure: In an Ar-filled glovebox, Ru complex **4** (3.0 mg, 1.6 μmol), additive (10 eq.), C_6D_6 (0.6 mL), and 1,1,2,2-tetrachloroethane (1.0 μL, 9.5 μmol) were added to a screw-cap NMR tube. The tube was capped and removed from the Ar-filled glovebox. The reaction was conducted at specified temperature in a water bath under irradiation with LEDs. The yield of **2** was determined by ^{1}H NMR analysis using 1,1,2,2-tetrachloroethane as an internal standard.



4 **2**

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2	AcOH	quant.
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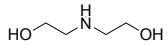
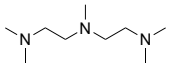
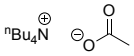
4		0
5		0
6		56
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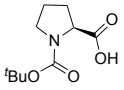
8		86
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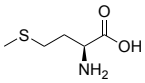
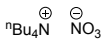
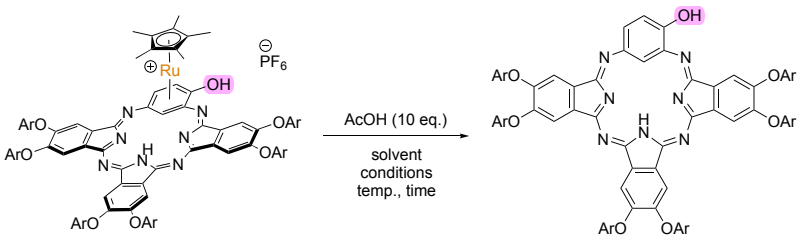
10		14
11		72

[a] Determined by ^1H NMR analysis.

Table S1. Screening of additives for photochemical arene release of **4**.



entry	AcOH	solvent	conditions	temp. (°C)	time (h)	yield (%)[a]
1	x	C_6D_6	dark	20	24	0
2	x	C_6D_6	NIR (740 nm)	20	4	14
3	o	C_6D_6	dark	20	24	0
4	o	C_6D_6	NIR (740 nm)	20	4	quant.
5	o	C_6D_6	dark	40	24	11
6	o	C_6D_6	dark	80	4	21
7	o	$CDCl_3$	NIR (740 nm)	20	4	32
8	o	C_6D_6	Blue (427 nm)	20	4	quant.
9	o	C_6D_6	NIR (850 nm)	20	4	50
10	o	C_6D_6	NIR (940 nm)	20	4	0

[a] Determined by ^{1}H NMR analysis.

Table S2. Screening of reaction conditions for photochemical arene release of **4**.

2-3. Absorption Spectra

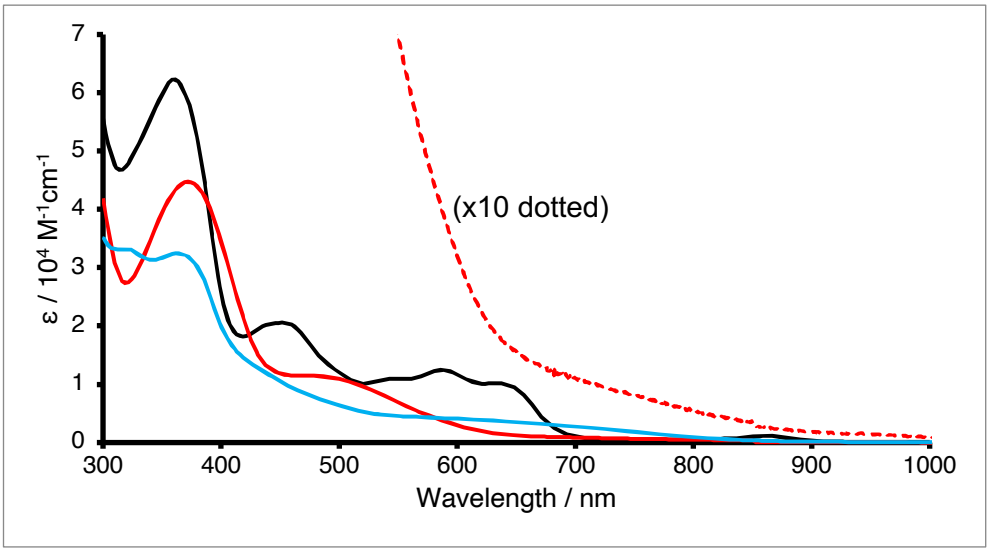


Fig. S1. Electronic absorption spectra of **2** (black), **4** (red), and **4A** (blue) measured in CH_2Cl_2.

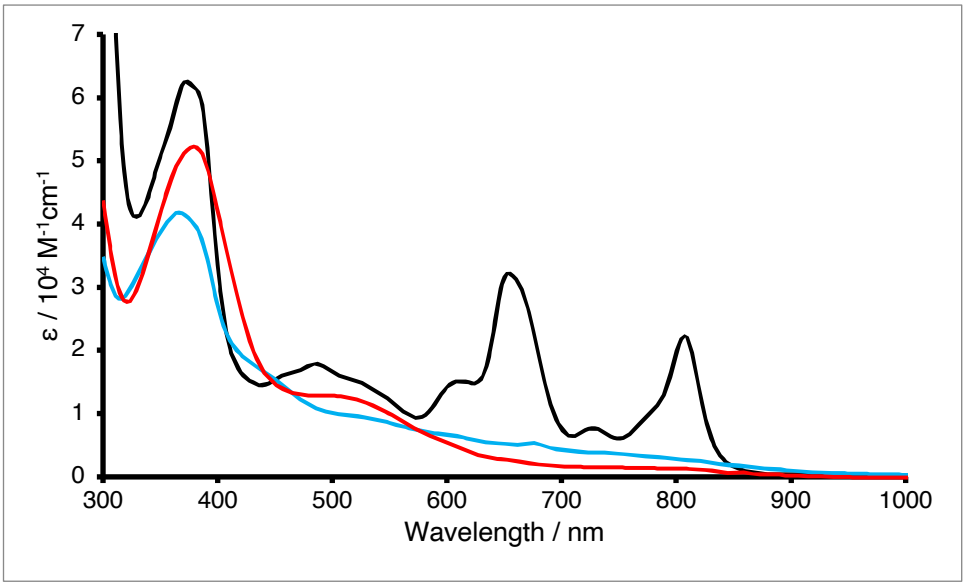


Fig. S2. Electronic absorption spectra of **5** (black), **6** (red), and **6A** (blue) measured in CH_2Cl_2.

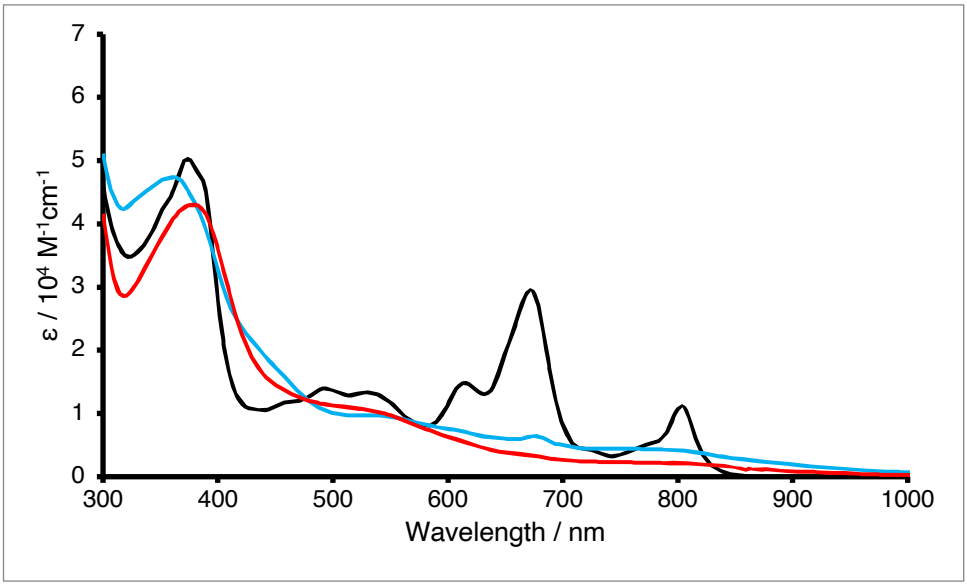


Fig. S3. Electronic absorption spectra of **5** (black), **6** (red), and **6A** (blue) measured in toluene.

2-4. X-ray Diffraction Analysis

A single crystal in immersion oil was mounted on a Rigaku XtaLAB Synergy-S diffractometer with a HyPix-6000HE HPC detector. The diffraction data were collected using Cu *K*α radiation under a cold nitrogen stream at 123 K. The images were processed with the Rigaku CrysAlis^{PRO} software. The structure was solved by a direct method and refined on F^2 by a least-squares method by the programs SHELXT2015[7] and SHELXL2015,[8] respectively. All the non-hydrogen atoms were refined anisotropically. All the hydrogen atoms were put on the calculated geometry and refined by applying riding models.

For [Cp*Ru(MeCN)$_3$][$CB_{11}H_6Br_6$], the disordered $CB_{11}H_6Br_6$ anion was fixed by using the RIGU and SIMU restriction commands available for SHELXL.

For **3X**, two molecules were included in the asymmetric unit. Solvent molecules and one of the $CB_{11}H_6Br_6$ anion, which were highly disordered, were removed by the solvent masking procedure using Olex2 software.[9] Also, disordered 2,6-diisopropylphenoxy groups and Cp* units were fixed by using the AFIX, RIGU, and SIMU restriction commands available for SHELXL.

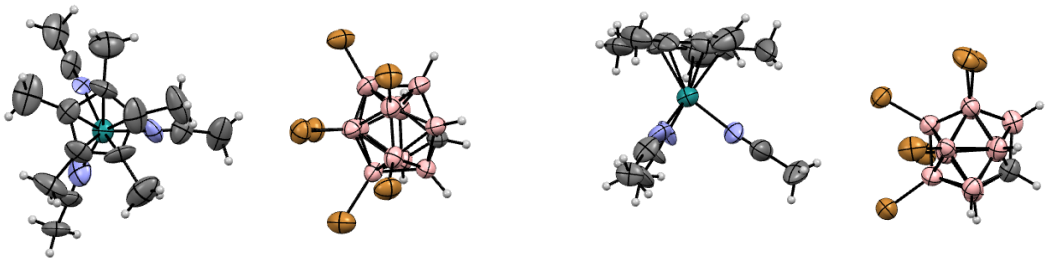


Fig. S4. X-ray structure of [Cp*Ru(MeCN)$_3$][$CB_{11}H_6Br_6$] (left: top view, right: side view). Thermal ellipsoids are set at 50% probability.

Compound	$[Cp^*Ru(MeCN)_3][CB_{11}H_6Br_6]$	**3X**
Solvent for recrystallization	MeCN/Et_2O (liquid-liquid diffusion)	acetone/*tert*-butylbenzene (vapor diffusion)
Formula	$C_{16}H_{24}N_3Ru$, $CH_6B_{11}Br_6$	$2(C_{88}H_{80}N_7O_6Ru)$, $CH_6B_{11}Br_6$, C_3H_6O
Formula weight	975.88	3539.82
Crystal system	orthorhombic	monoclinic
Space group	$Pna2_1$	$P2_1/n$
Crystal size (mm)	0.08×0.07×0.06	0.161×0.084×0.051
Crystal color and shape	Yellow block	Red plate
Wavelength (Å)	1.54184	1.54184
a (Å)	13.6340(7)	14.5575(2)
b (Å)	17.5899(10)	37.1162(5)
c (Å)	13.8373(8)	35.7361(5)
α (°)	90	90
β (°)	90	96.697(2)
γ (°)	90	90
Volume (Å)	3318.5(3)	19177.1(5)
Z	4	4
$\rho_{calcd.}$ (g cm^{-3})	1.953	1.226
μ (mm^{-1})	12.394	3.190
θ_{min}, θ_{max} (°)	4.0520, 73.8340	2.3860, 63.6070
No. of reflection (unique)	11968 (4739)	390350 (30003)
R_{int}	0.0583	0.1905
Completeness to θ (%)	99.8	95.1
Goodness-of-fit on F^2	1.028	1.227
Final R_1 and wR_2 indices [$I > 2\sigma(I)$]	0.0728, 0.1972	0.1236, 0.3336
R_1 and wR_2 indices (all data)	0.1035, 0.2221	0.1896, 0.3833
CCDC number	2472097	2472098

3. Computational Details

All DFT calculations were carried out with the Gaussian 16 program.[10] Geometry optimizations for the ground state S_0 and the excited state T_1 were performed at 298.15 K with M06[11]/6-31G(d) (C, H, N, O) & SDD (Ru). The vibrational frequencies were computed at the same level to check whether each optimized structure was an energy minimum (no imaginary frequency). Single-point energies were calculated with the same level based on the optimized structure. We used model substrates **1'–6A'** lacking any peripheral substituents and counter anions for **1–6A** (Fig. S5).

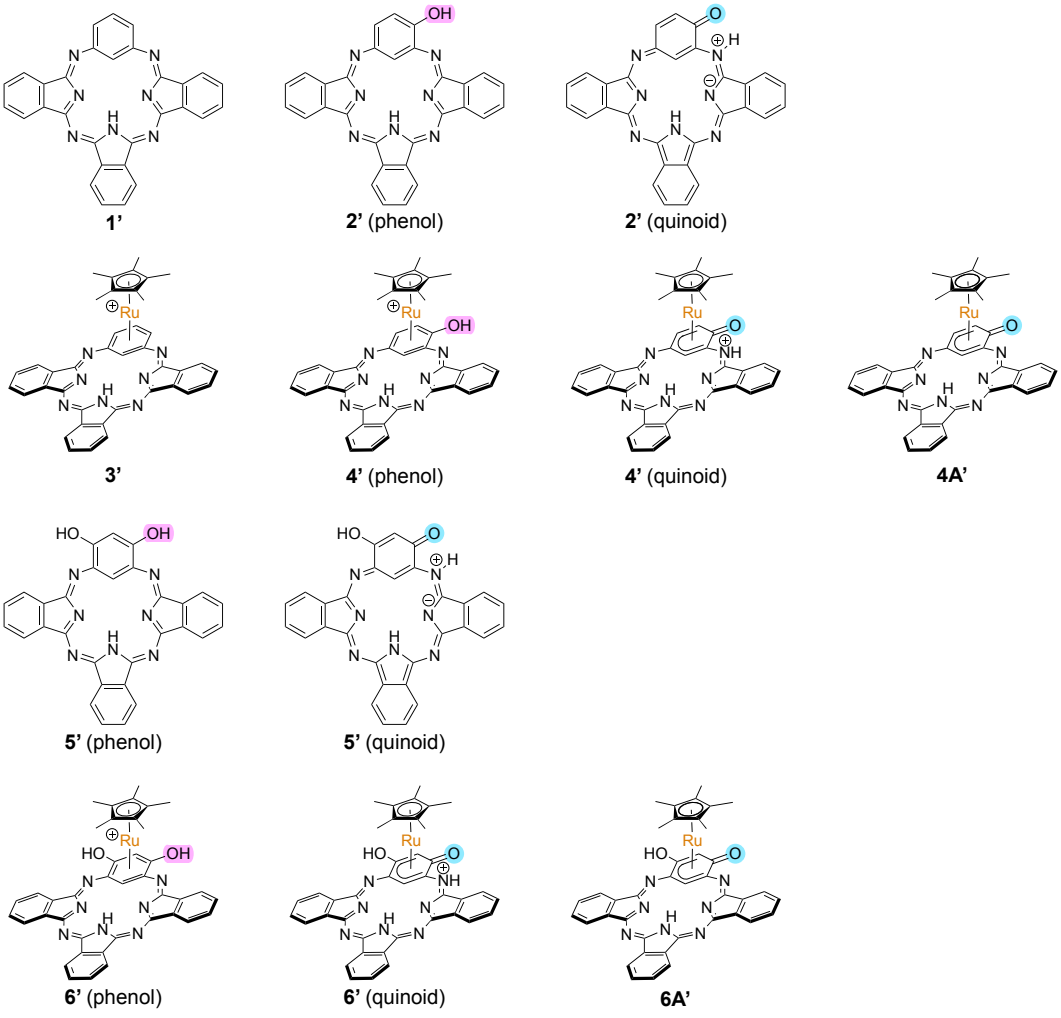


Fig. S5. Structures of model substrates **1'**–**6A'** lacking any peripheral substituents.

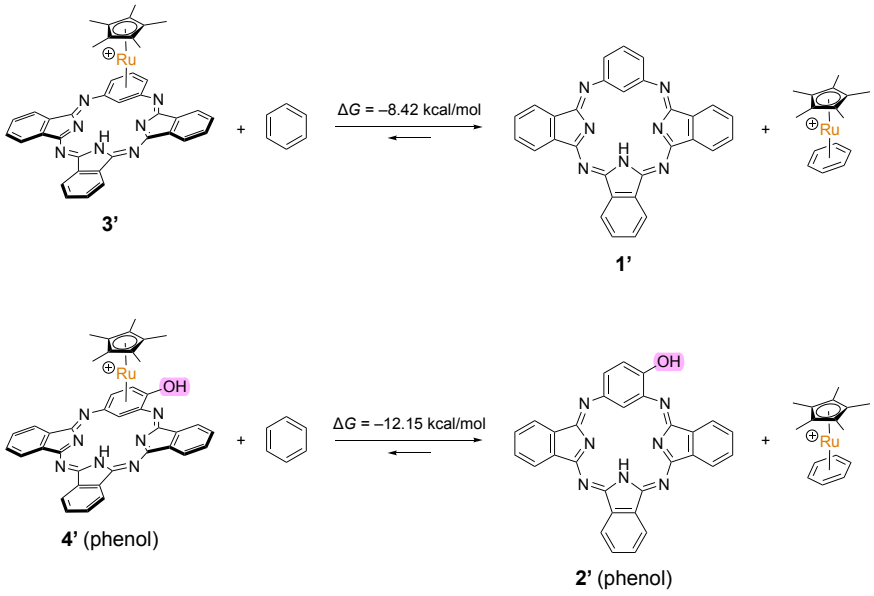


Fig. S6. Arene exchange reactions of model substrate **3'** and **4'** with benzene.

Table S3. TD-DFT calculation of **1'**.

	Energy		Oscillator Strength	Occupied MO		Unoccupied MO	Coefficient [%][a]
	[eV]	[nm]					
$S_0 \rightarrow S_1$	2.29	540.62	0.0027	HOMO-1	→	LUMO	94.8
$S_0 \rightarrow S_2$	2.35	526.52	0.1972	HOMO	→	LUMO	91.2
$S_0 \rightarrow S_3$	2.90	427.12	0.0428	HOMO–4	→	LUMO	57.2
				HOMO-3	→	LUMO	22.2
$S_0 \rightarrow S_4$	2.98	415.64	0.0812	HOMO	→	LUMO+1	66.7
				HOMO-2	→	LUMO	20.6

[a] The coefficients greater than 10 % in the CI expansion are included.

Table S4. TD-DFT calculation of **2'** (phenol form).

	Energy		Oscillator Strength	Occupied MO		Unoccupied MO	Coefficient [%][a]
	[eV]	[nm]					
$S_0 \rightarrow S_1$	2.13	583.08	0.2428	HOMO	→	LUMO	90.2
$S_0 \rightarrow S_2$	2.45	506.07	0.0949	HOMO–1	→	LUMO	60.7
				HOMO	→	LUMO+1	32.0
$S_0 \rightarrow S_3$	2.76	449.43	0.2217	HOMO	→	LUMO+1	58.8
				HOMO-1	→	LUMO	28.8

[a] The coefficients greater than 10 % in the CI expansion are included.

Table S5. TD-DFT calculation of **2'** (quinoid form).

	Energy		Oscillator Strength	Occupied MO		Unoccupied MO	Coefficient [%][a]
	[eV]	[nm]					
$S_0 \rightarrow S_1$	1.77	699.08	0.3674	HOMO	→	LUMO	97.4
$S_0 \rightarrow S_2$	2.09	593.97	0.2689	HOMO	→	LUMO+1	82.8
				HOMO–2	→	LUMO	11.2

[a] The coefficients greater than 10 % in the CI expansion are included.

Table S6. TD-DFT calculation of **3'**.

	Energy		Oscillator Strength	Occupied MO		Unoccupied MO	Coefficient [%][a]
	[eV]	[nm]					
$S_0 \rightarrow S_1$	2.43	509.81	0.0007	HOMO-1	→	LUMO	92.2
$S_0 \rightarrow S_2$	2.46	504.08	0.1370	HOMO	→	LUMO	95.3
$S_0 \rightarrow S_3$	2.61	474.34	0.0002	HOMO–2	→	LUMO	93.3
$S_0 \rightarrow T_1$	1.94	638.51	0.0000	HOMO	→	LUMO	81.5
$S_0 \rightarrow T_2$	2.03	609.64	0.0000	HOMO–1	→	LUMO	40.0
				HOMO–2	→	LUMO	18.5
$S_0 \rightarrow T_3$	2.32	534.76	0.0000	HOMO–3	→	LUMO	68.1
				HOMO-4	→	LUMO+1	13.4

[a] The coefficients greater than 10 % in the CI expansion are included.

Table S7. TD-DFT calculation of **4'** (phenol form).

	Energy		Oscillator Strength	Occupied MO		Unoccupied MO	Coefficient [%][a]
	[eV]	[nm]					
$S_0 \rightarrow S_1$	2.33	532.76	0.0094	HOMO-1	→	LUMO	78.1
				HOMO		LUMO	15.9
$S_0 \rightarrow S_2$	2.43	510.43	0.1606	HOMO	→	LUMO	79.5
				HOMO-1		LUMO	14.5
$S_0 \rightarrow S_3$	2.48	500.09	0.0001	HOMO–2	→	LUMO	76.6
				HOMO-3	→	LUMO	17.7
$S_0 \rightarrow T_1$	1.87	664.52	0.0000	HOMO	→	LUMO	82.7
$S_0 \rightarrow T_2$	1.99	622.48	0.0000	HOMO–1	→	LUMO	42.3
				HOMO–3	→	LUMO	17.8
				HOMO	→	LUMO+1	10.3
$S_0 \rightarrow T_3$	2.28	543.57	0.0000	HOMO–4	→	LUMO	25.8
				HOMO–3	→	LUMO	23.9
				HOMO–1	→	LUMO	22.2
				HOMO-4	→	LUMO+1	10.3

[a] The coefficients greater than 10 % in the CI expansion are included.

Table S8. TD-DFT calculation of **4'** (quinoid form).

	Energy		Oscillator Strength	Occupied MO		Unoccupied MO	Coefficient [%][a]
	[eV]	[nm]					
$S_0 \rightarrow S_1$	1.44	861.81	0.0488	HOMO	→	LUMO	77.9
				HOMO-1	→	LUMO	17.5
$S_0 \rightarrow S_2$	1.68	738.79	0.0237	HOMO–1	→	LUMO	62.2
				HOMO–3	→	LUMO	25.6
$S_0 \rightarrow S_3$	1.82	682.27	0.0009	HOMO–2	→	LUMO	74.2
				HOMO-3	→	LUMO	22.3

[a] The coefficients greater than 10 % in the CI expansion are included.

Table S9. TD-DFT calculation of **4A'**.

	Energy		Oscillator Strength	Occupied MO		Unoccupied MO	Coefficient [%][a]
	[eV]	[nm]					
$S_0 \rightarrow S_1$	1.60	775.57	0.0850	HOMO	→	LUMO	85.0
$S_0 \rightarrow S_2$	1.83	678.4	0.0013	HOMO–1	→	LUMO	91.3
$S_0 \rightarrow S_3$	1.89	655.34	0.0280	HOMO–2	→	LUMO	69.9
				HOMO-3	→	LUMO	15.0

[a] The coefficients greater than 10 % in the CI expansion are included.

Table S10. TD-DFT calculation of **5'** (phenol form).

	Energy		Oscillator Strength	Occupied MO		Unoccupied MO	Coefficient [%][a]
	[eV]	[nm]					
$S_0 \rightarrow S_1$	2.11	587.36	0.3458	HOMO	→	LUMO	94.8
$S_0 \rightarrow S_2$	2.35	527.22	0.1451	HOMO	→	LUMO+1	53.4
				HOMO-1	→	LUMO	42.8
$S_0 \rightarrow S_3$	2.62	472.73	0.1643	HOMO–1	→	LUMO	55.0
				HOMO	→	LUMO+1	38.3

[a] The coefficients greater than 10 % in the CI expansion are included.

Table S11. TD-DFT calculation of **5'** (quinoid form).

	Energy		Oscillator Strength	Occupied MO		Unoccupied MO	Coefficient [%][a]
	[eV]	[nm]					
$S_0 \rightarrow S_1$	1.85	669.25	0.3637	HOMO	→	LUMO	95.0
$S_0 \rightarrow S_2$	2.03	596.45	0.3255	HOMO	→	LUMO+1	84.4
$S_0 \rightarrow S_3$	2.57	483.17	0.0488	HOMO–1	→	LUMO	86.4

[a] The coefficients greater than 10 % in the CI expansion are included.

Table S12. TD-DFT calculation of **6'** (phenol form).

	Energy		Oscillator Strength	Occupied MO		Unoccupied MO	Coefficient [%][a]
	[eV]	[nm]					
$S_0 \rightarrow S_1$	2.27	545.69	0.0001	HOMO-2	→	LUMO	94.5
$S_0 \rightarrow S_2$	2.28	543.58	0.0156	HOMO–1	→	LUMO	70.6
				HOMO	→	LUMO	26.6
$S_0 \rightarrow S_3$	2.38	521.70	0.1893	HOMO	→	LUMO	71.4
				HOMO-1	→	LUMO	25.9
$S_0 \rightarrow S_4$	2.39	519.19	0.0001	HOMO-3	→	LUMO	96.0
$S_0 \rightarrow T_1$	1.80	689.21	0.0000	HOMO	→	LUMO	76.7
$S_0 \rightarrow T_2$	1.95	636.37	0.0000	HOMO–2	→	LUMO	56.8
				HOMO–4	→	LUMO	11.4
				HOMO	→	LUMO+1	10.5
$S_0 \rightarrow T_3$	2.16	575.06	0.0000	HOMO–1	→	LUMO	82.9
				HOMO	→	LUMO	10.4

[a] The coefficients greater than 10 % in the CI expansion are included.

Table S13. TD-DFT calculation of **6'** (quinoid form).

	Energy		Oscillator Strength	Occupied MO		Unoccupied MO	Coefficient [%][a]
	[eV]	[nm]					
$S_0 \rightarrow S_1$	1.35	920.76	0.0512	HOMO	→	LUMO	84.1
				HOMO-2	→	LUMO	11.5
$S_0 \rightarrow S_2$	1.61	770.05	0.0003	HOMO–1	→	LUMO	97.4
$S_0 \rightarrow S_3$	1.69	734.51	0.0103	HOMO–3	→	LUMO	49.2
				HOMO-2	→	LUMO	46.5
$S_0 \rightarrow S_4$	1.91	650.84	0.1361	HOMO-3	→	LUMO	44.7
				HOMO-2	→	LUMO	38.7
				HOMO	→	LUMO	12.4

[a] The coefficients greater than 10 % in the CI expansion are included.

Table S14. TD-DFT calculation of **6A'**.

	Energy		Oscillator Strength	Occupied MO		Unoccupied MO	Coefficient [%][a]
	[eV]	[nm]					
$S_0 \rightarrow S_1$	1.50	824.14	0.0820	HOMO	→	LUMO	85.7
$S_0 \rightarrow S_2$	1.67	741.58	0.0001	HOMO–1	→	LUMO	95.9
$S_0 \rightarrow S_3$	1.88	660.25	0.0168	HOMO–2	→	LUMO	57.2
				HOMO-3	→	LUMO	34.8
$S_0 \rightarrow S_4$	2.11	588.4	0.1433	HOMO–3	→	LUMO	56.3
				HOMO-2	→	LUMO+1	26.0

[a] The coefficients greater than 10 % in the CI expansion are included.

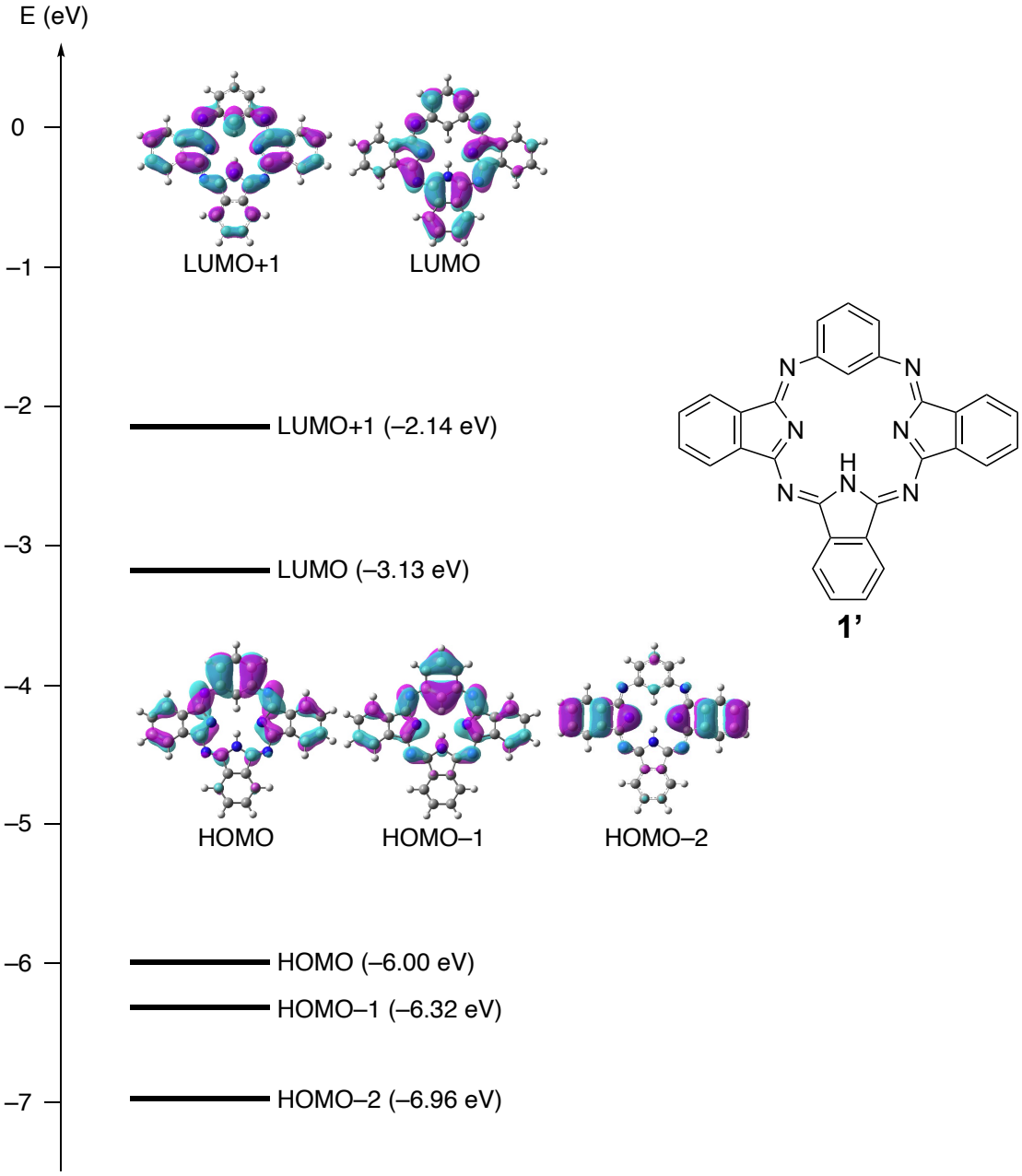


Fig. S7. Frontier molecular orbitals of **1’**. Isovalue = 0.02.

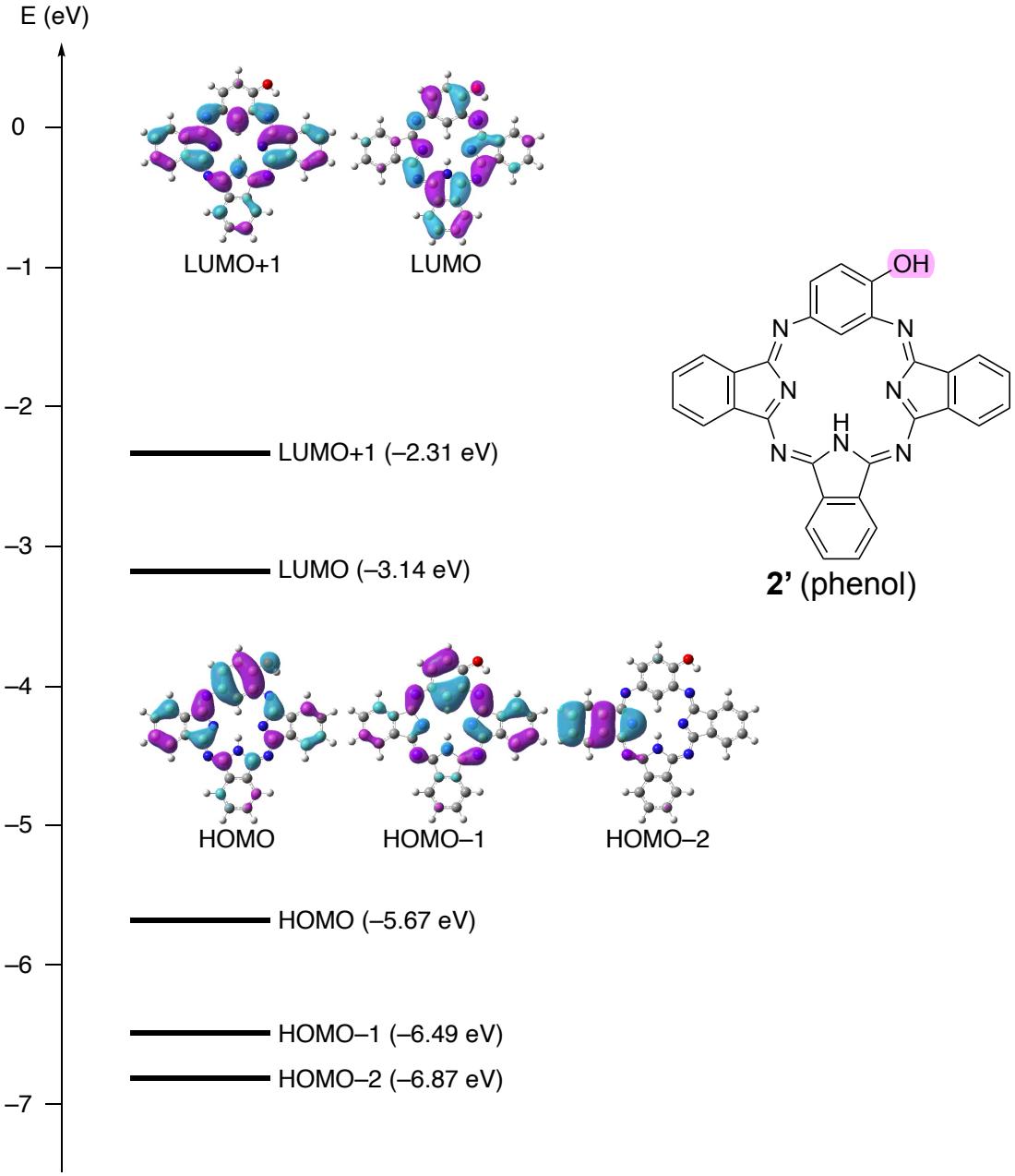


Fig. S8. Frontier molecular orbitals of **2'** (phenol form). Isovalue = 0.02.

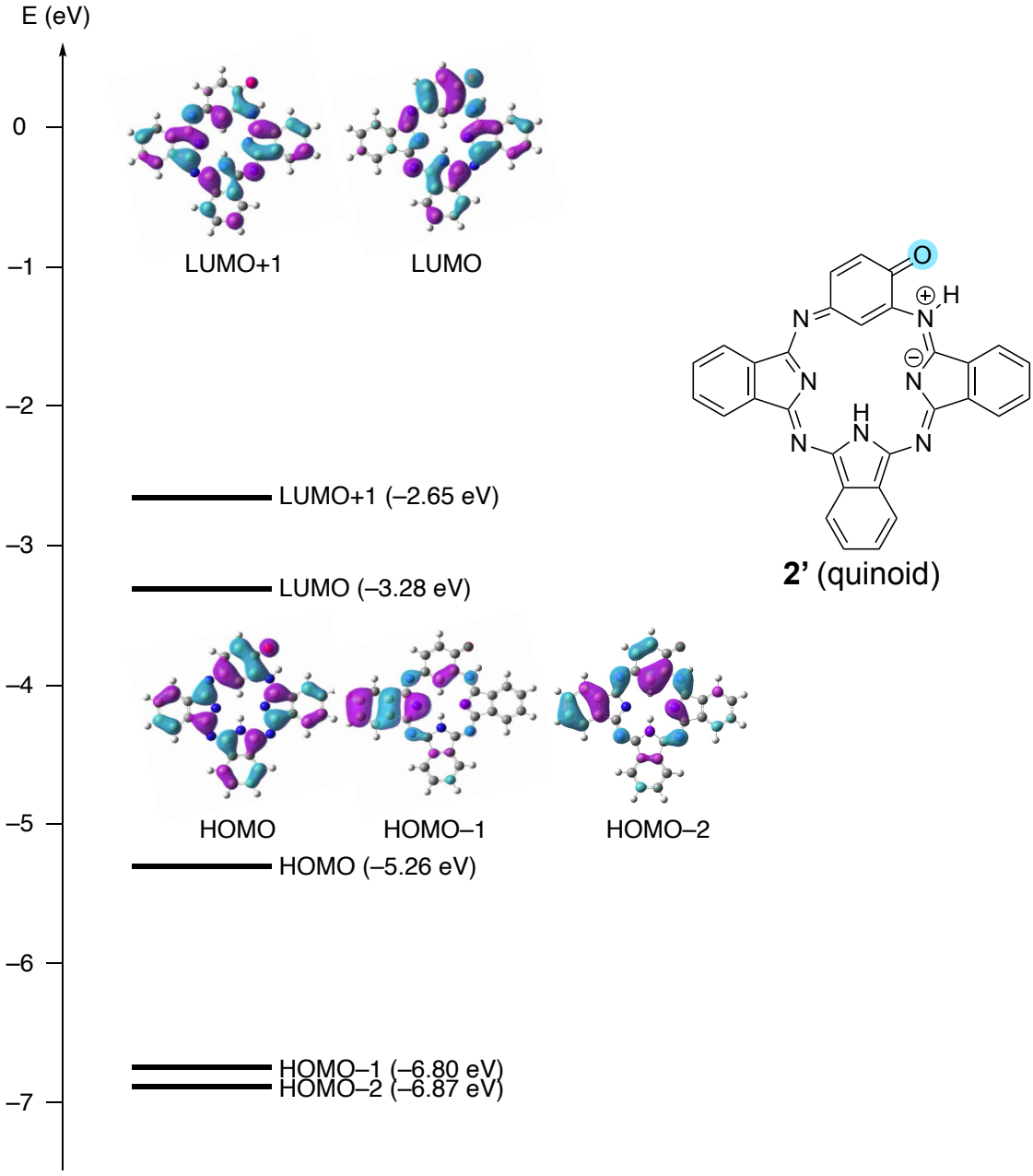


Fig. S9. Frontier molecular orbitals of **2’** (quinoid form). Isovalue = 0.02.

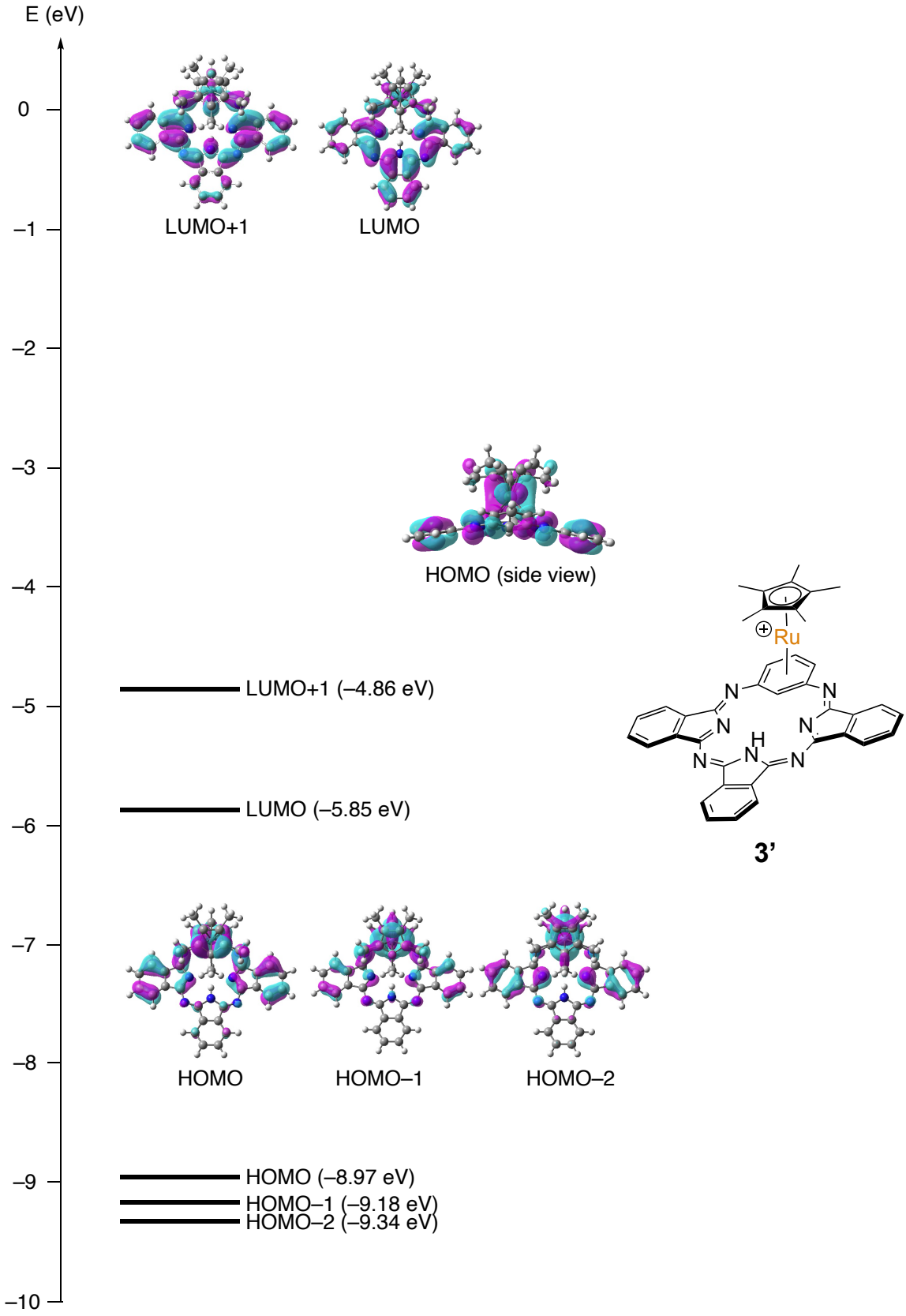


Fig. S10. Frontier molecular orbitals of **3’**. Isovalue = 0.02.

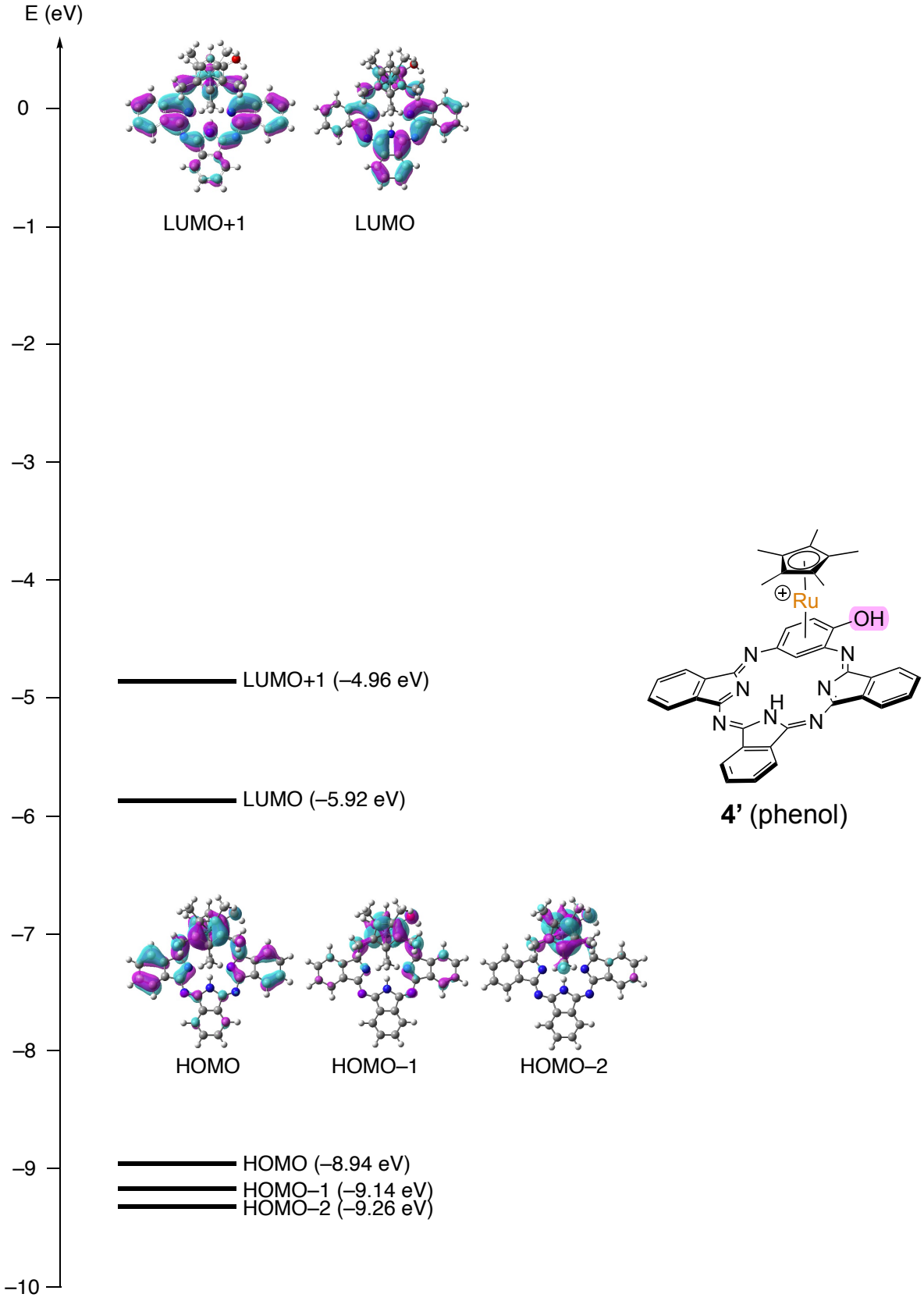


Fig. S11. Frontier molecular orbitals of **4’** (phenol form). Isovalue = 0.02.

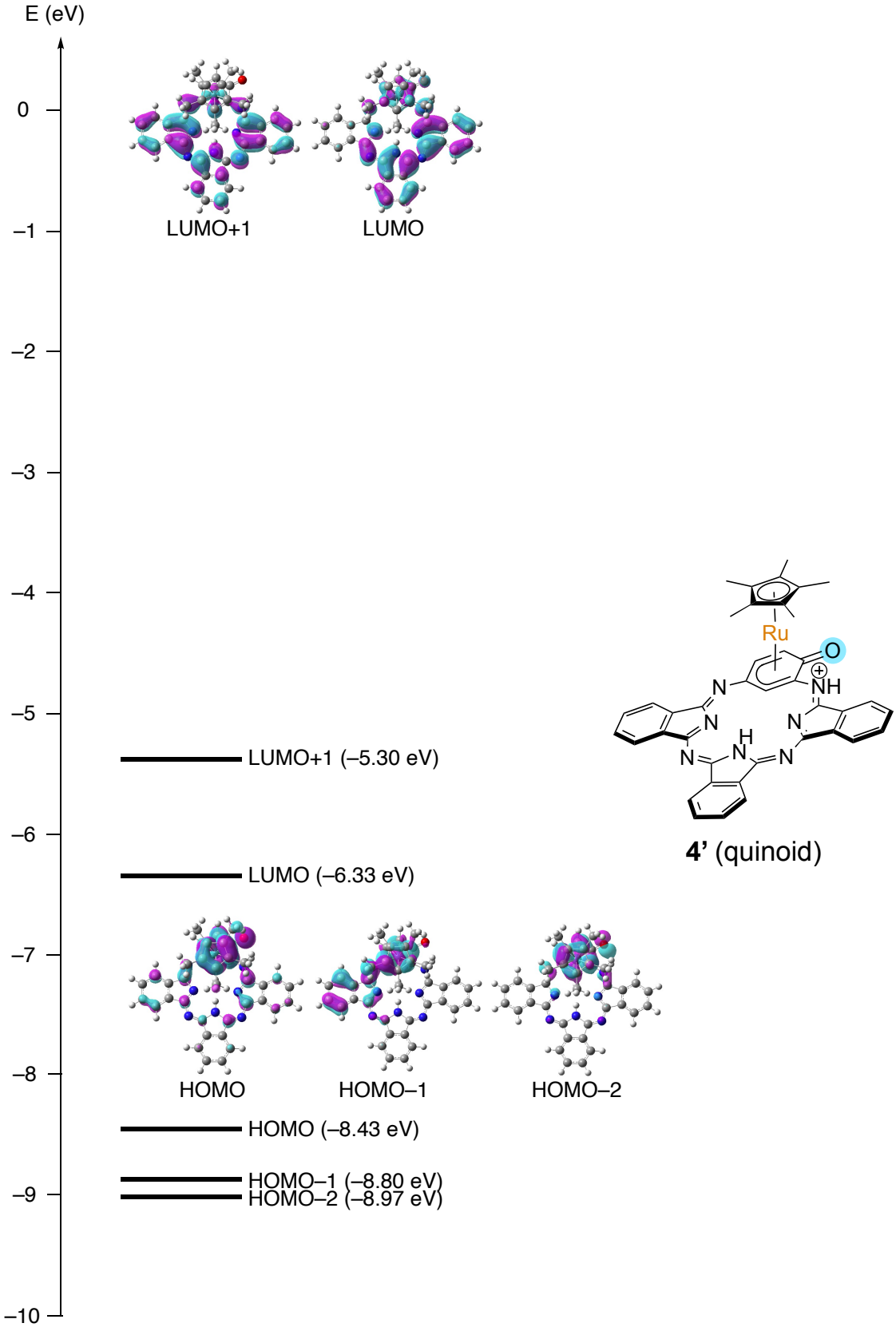


Fig. S12. Frontier molecular orbitals of **4’** (quinoid form). Isovalue = 0.02.

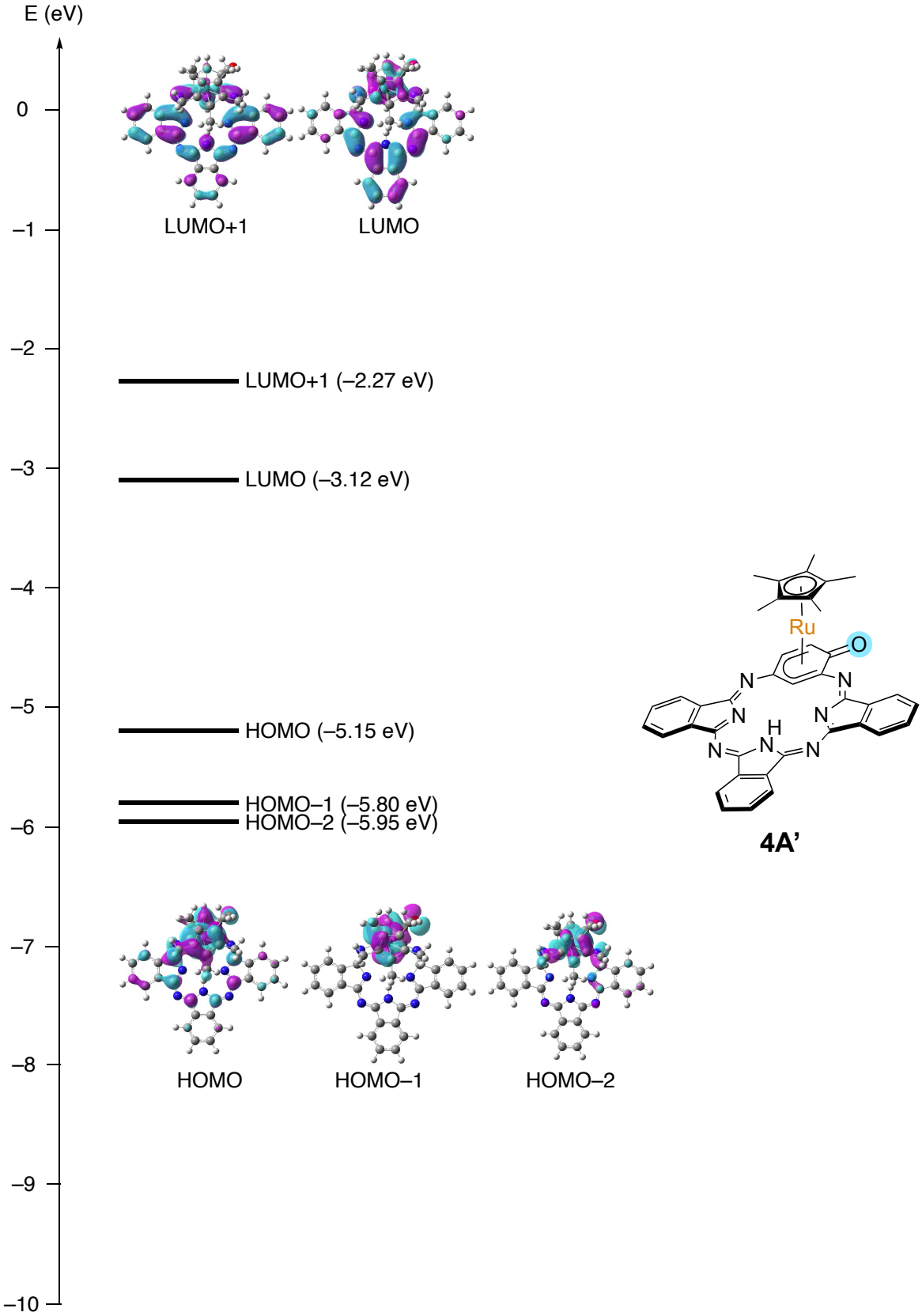


Fig. S13. Frontier molecular orbitals of **4A’**. Isovalue = 0.02.

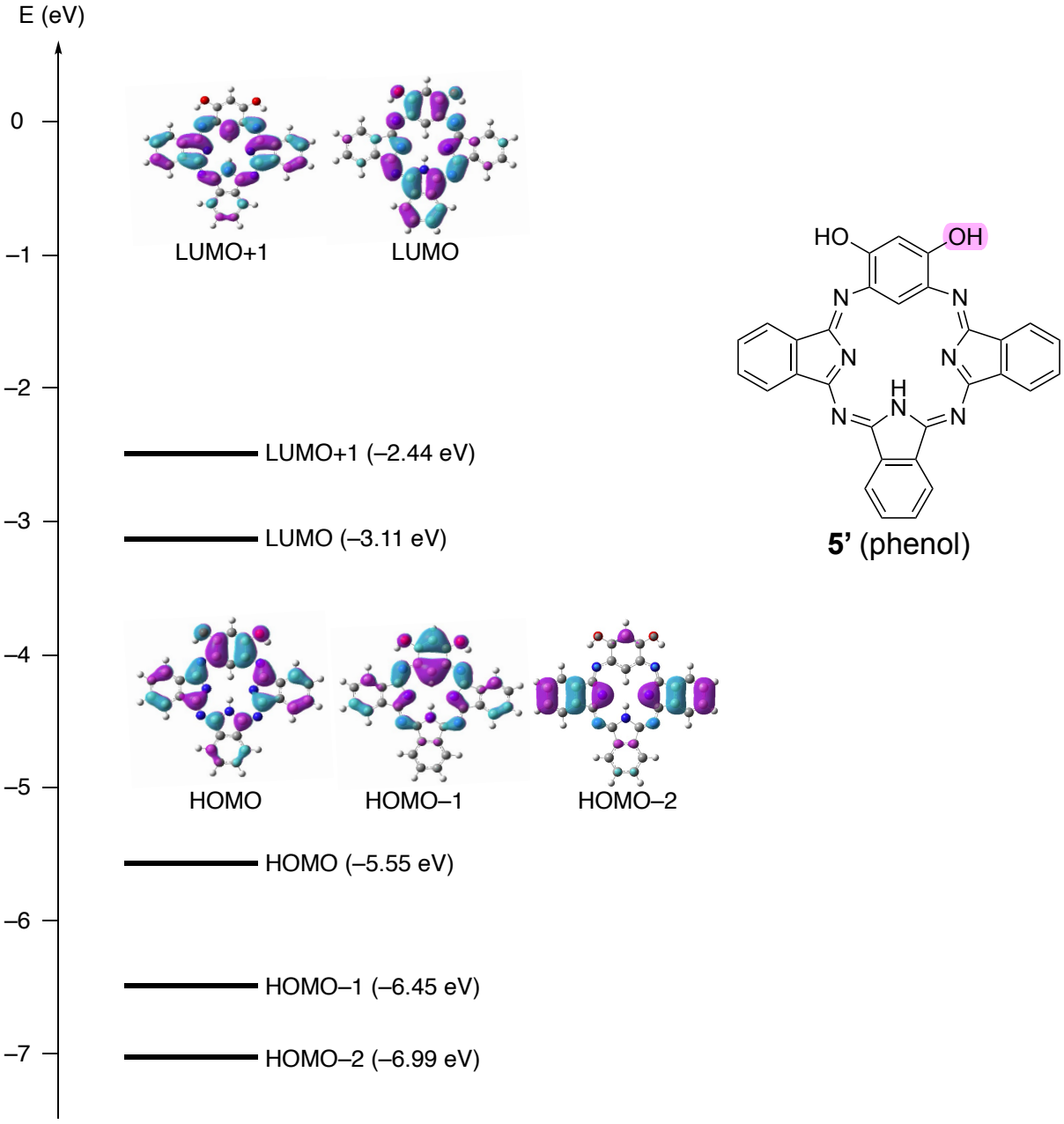


Fig. S14. Frontier molecular orbitals of **5’** (phenol form). Isovalue = 0.02.

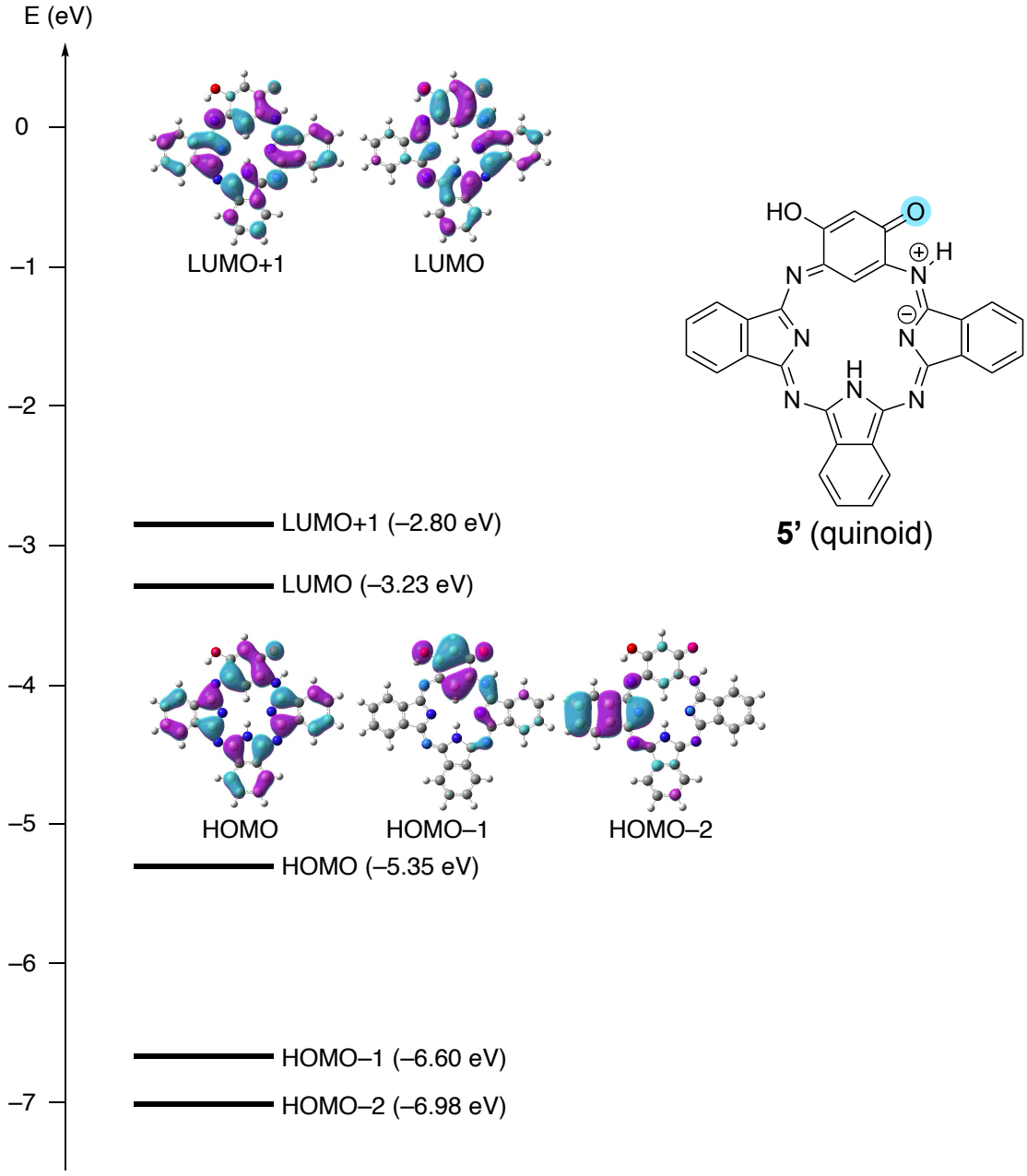


Fig. S15. Frontier molecular orbitals of **5’** (quinoid form). Isovalue = 0.02.

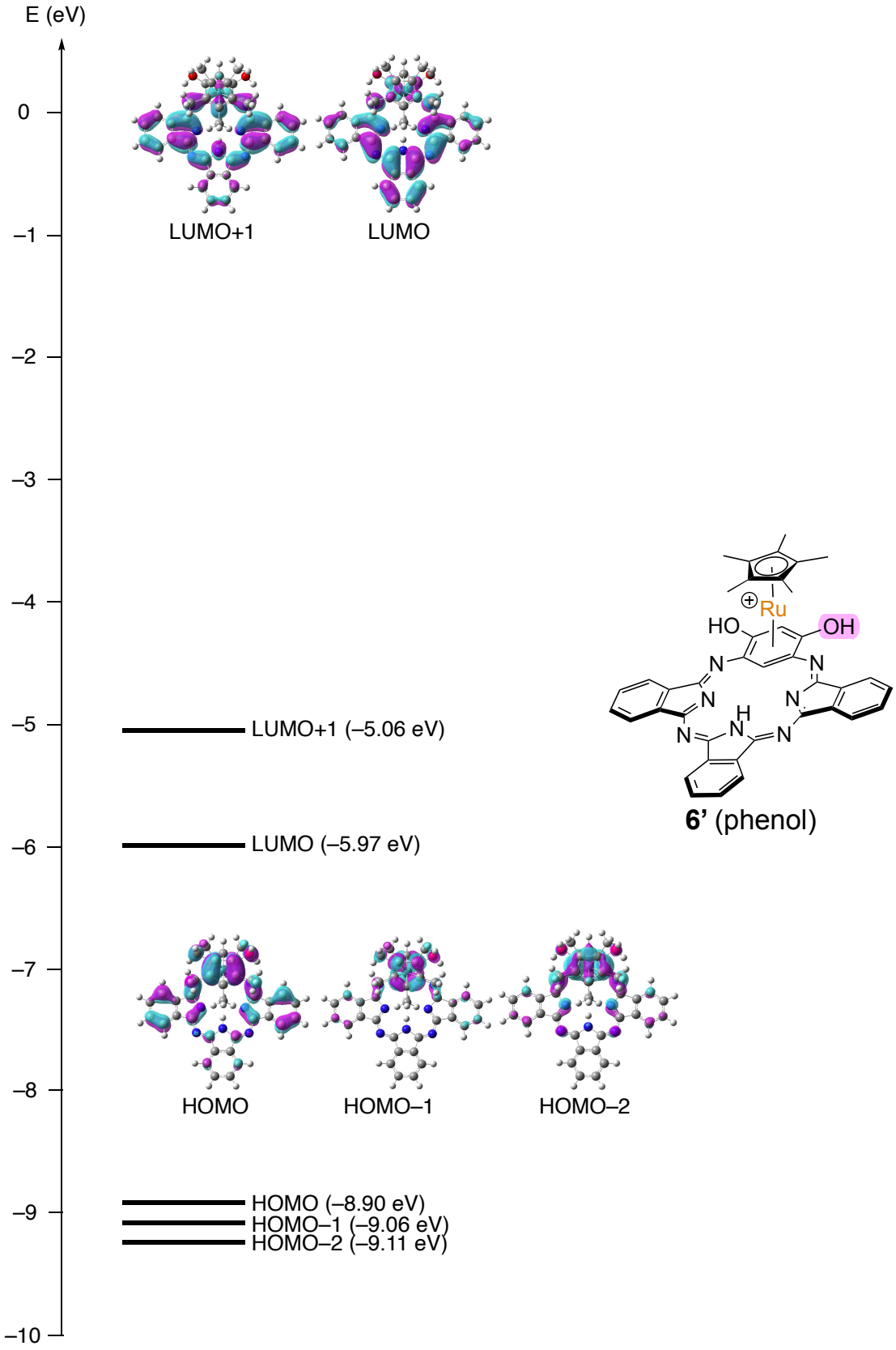


Fig. S16. Frontier molecular orbitals of **6’** (phenol form). Isovalue = 0.02.

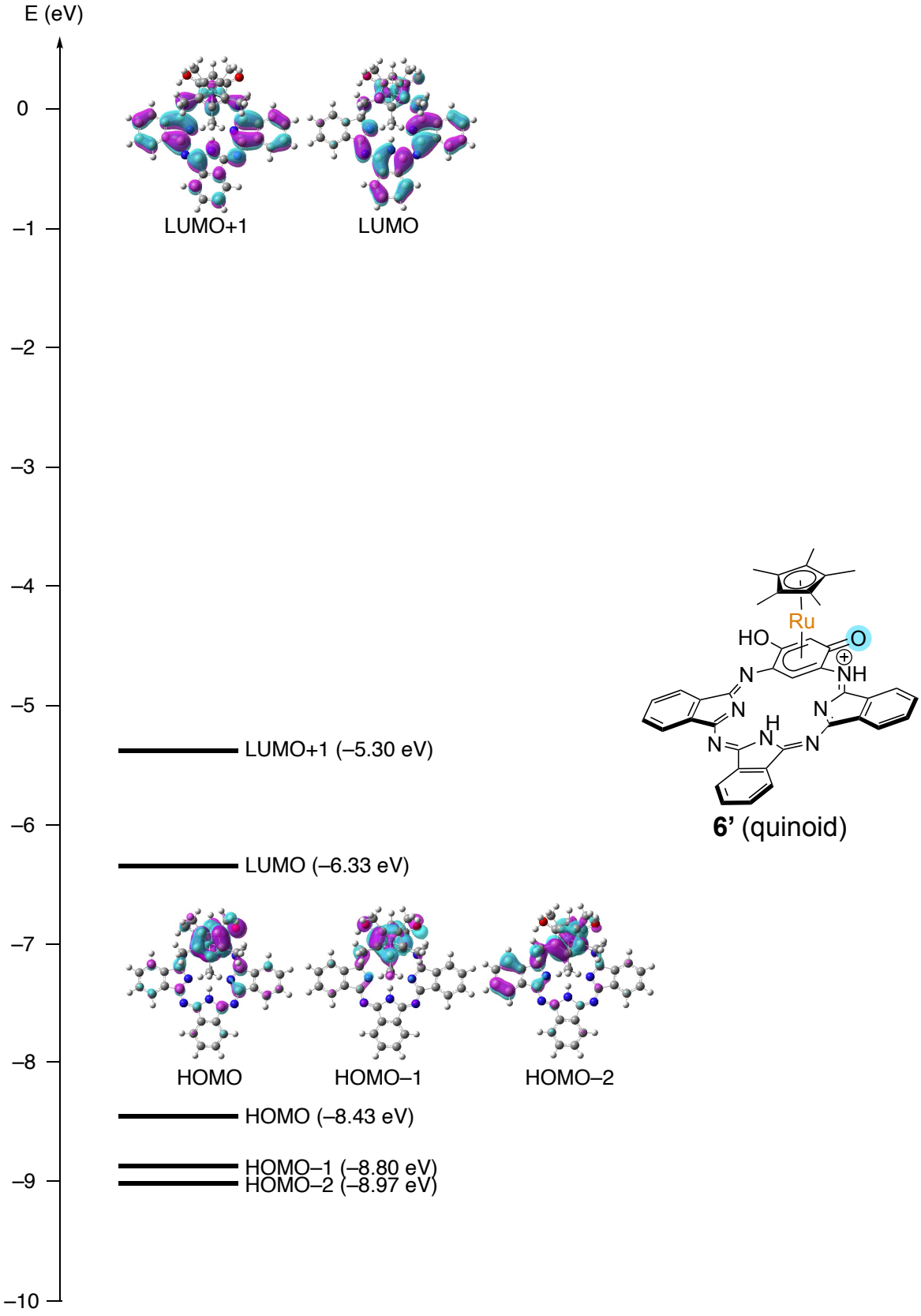


Fig. S17. Frontier molecular orbitals of **6’** (quinoid form). Isovalue = 0.02.

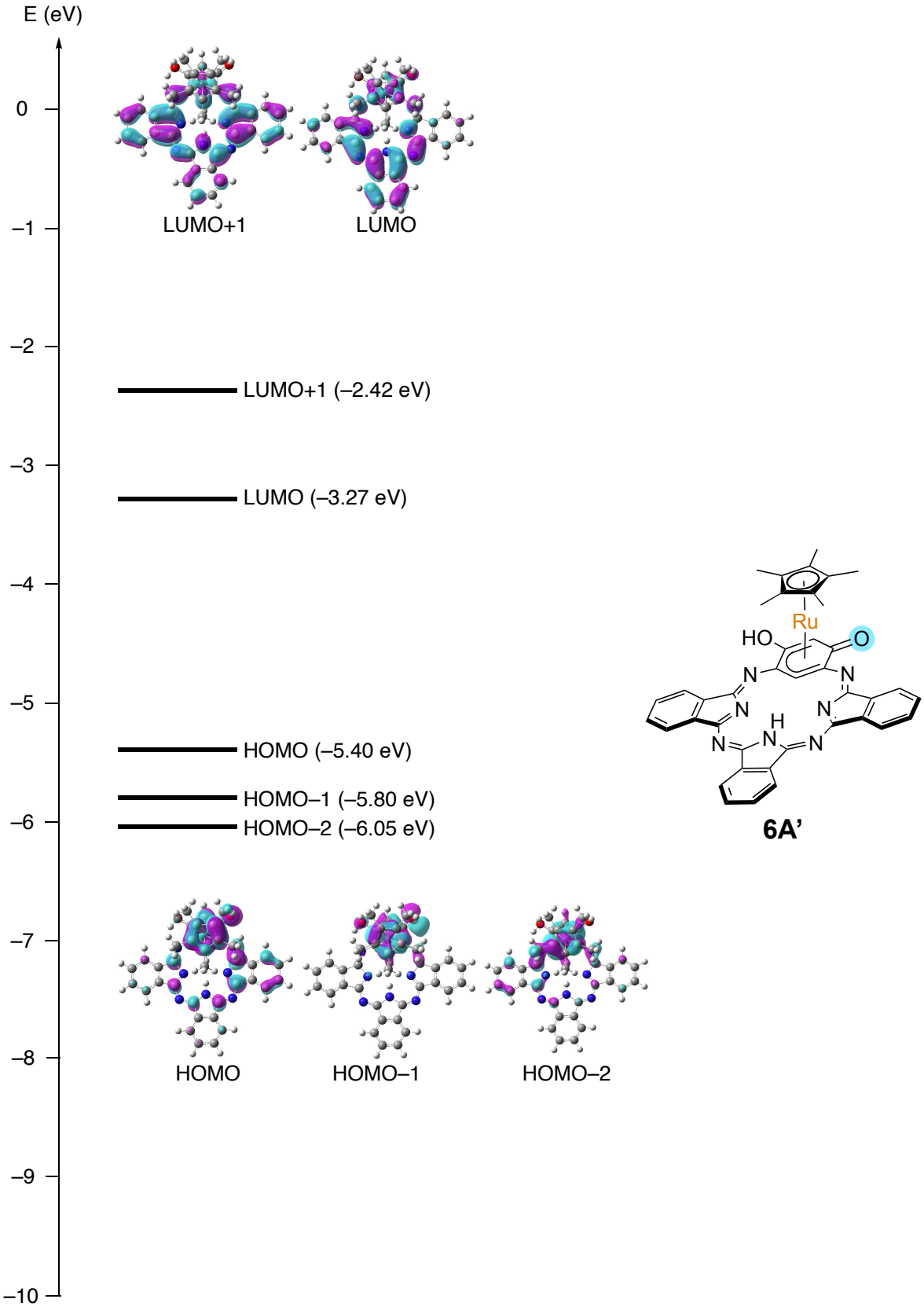


Fig. S18. Frontier molecular orbitals of **6A'**. Isovalue = 0.02.

Cartesian Coordinates (in Å) and Energies

benzene

Energy = -232.064247 A. U.

Gibbs Free Energy = -231.991627 A. U.

C	-1.39156500	-0.00460500	-0.00009000
C	-0.69966100	1.20239000	0.00003500
C	0.69169900	1.20701800	0.00000200
C	1.39168200	0.00459900	0.00002400
C	0.69967800	-1.20241300	0.00000200
C	-0.69169400	-1.20698900	0.00003400
H	-1.24633800	2.14274000	0.00004400
H	1.23178700	2.15110100	-0.00005300
H	2.47935500	0.00820300	-0.00010200
H	1.24597500	-2.14291600	-0.00005300
H	-1.23213000	-2.15094000	0.00004400
H	-2.47947500	-0.00819100	0.00007500

$[Cp^*Ru(C_6H_6)]^+$

Energy = -716.640915 A. U.

Gibbs Free Energy = -716.360575 A. U.

C	0.74951200	-0.39532300	1.66428000
C	-0.68838200	-0.40603700	1.68323200
C	-1.14818000	0.86157400	1.18641700
C	0.00365600	1.65549400	0.86007400
C	1.17714900	0.87931100	1.15530300
Ru	-0.00101800	-0.15076800	-0.38236800
C	0.32020900	0.48651000	-2.50225800
C	-1.04424100	0.13862400	-2.33759700
C	-1.39455000	-1.13548600	-1.82418100
C	-0.38014500	-2.06364300	-1.47726900
C	0.98406600	-1.71575100	-1.64228500
C	1.33446200	-0.44101400	-2.15415100
H	0.58846300	1.48233000	-2.84479800
H	-1.82078100	0.86859300	-2.55341500
H	-0.64848300	-3.01919200	-1.03377000
H	1.76202600	-2.40672100	-1.32713900
H	2.38058500	-0.15664200	-2.23168500
C	-2.57044000	1.29148200	1.07497300
H	-2.71011600	2.02805000	0.27682200
H	-3.23477500	0.44454100	0.87135200
H	-2.90828600	1.75410600	2.01117800
C	-1.55102300	-1.51670200	2.17457500
H	-1.78821500	-1.38186700	3.23718600
H	-2.50131500	-1.56215600	1.63082600
H	-1.05874300	-2.48928300	2.06998900
C	1.63639400	-1.49919300	2.12974400
H	1.82484100	-1.41632400	3.20723700
H	1.18514900	-2.48096300	1.94977400
H	2.60638500	-1.47871000	1.62314500

C	2.58827000	1.33370200	1.00376600
H	2.93536500	1.83032800	1.91814300
H	3.26441000	0.49496700	0.80762600
H	2.69643600	2.04800500	0.18025700
C	-0.01868000	3.05403400	0.34481700
H	-0.07018800	3.77126500	1.17413200
H	0.88016100	3.28648200	-0.23471500
H	-0.88799600	3.23324100	-0.29698500
H	-2.43859300	-1.38175800	-1.64759200

1'

Energy = -1535.659381 A. U.

Gibbs Free Energy = -1535.308784 A. U.

N	0.17401000	1.86672400	-2.38363700
N	-0.12824800	-2.86464600	-2.48346900
N	-0.12824800	-2.86464600	2.48346900
N	0.17401000	1.86672400	2.38363700
C	0.26192200	2.21616700	1.14372300
C	0.40702600	3.60417000	0.69719000
C	0.40702600	3.60417000	-0.69719000
C	0.26192200	2.21616700	-1.14372300
N	0.20605500	1.44225700	0.00000000
C	0.01109700	0.55847200	-2.74592800
C	-0.23166700	0.21987300	-4.15237100
C	-0.33569400	-1.16831200	-4.17888000
C	-0.14358700	-1.61912100	-2.78635600
N	0.05290100	-0.49461700	-1.95847800
C	-0.14358700	-1.61912100	2.78635600
C	-0.33569400	-1.16831200	4.17888000
C	-0.23166700	0.21987300	4.15237100
C	0.01109700	0.55847200	2.74592800
N	0.05290100	-0.49461700	1.95847800
C	-0.56560800	-1.84872400	5.36110000
C	-0.69168200	-1.08857200	6.52416100
C	-0.58674100	0.30503800	6.49627900
C	-0.35173300	0.98392900	5.30163700
C	0.51590100	4.77957400	1.42092400
C	0.63345200	5.96536800	0.69916800
C	0.63345200	5.96536800	-0.69916800
C	0.51590100	4.77957400	-1.42092400
C	-0.35173300	0.98392900	-5.30163700
C	-0.58674100	0.30503800	-6.49627900
C	-0.69168200	-1.08857200	-6.52416100
C	-0.56560800	-1.84872400	-5.36110000
C	0.51590100	-4.72581300	1.19799500
C	0.06809800	-3.39305800	1.21237900
C	-0.16993600	-2.73475300	0.00000000
C	0.06809800	-3.39305800	-1.21237900
C	0.51590100	-4.72581300	-1.19799500
C	0.75657200	-5.38028100	0.00000000

H	0.16713700	0.42042800	0.00000000
H	-0.64245200	-2.93312300	5.37048100
H	-0.87442700	-1.58704100	7.47336700
H	-0.69012700	0.86472500	7.42283200
H	-0.26544500	2.06699800	5.26395800
H	0.50946900	4.76194600	2.50745200
H	0.72530600	6.90969500	1.22973700
H	0.72530600	6.90969500	-1.22973700
H	0.50946900	4.76194600	-2.50745200
H	-0.26544500	2.06699800	-5.26395800
H	-0.69012700	0.86472500	-7.42283200
H	-0.87442700	-1.58704100	-7.47336700
H	-0.64245200	-2.93312300	-5.37048100
H	-0.55586700	-1.72461500	0.00000000
H	1.10667600	-6.40931600	0.00000000
H	0.66693300	-5.21541400	2.15660400
H	0.66693300	-5.21541400	-2.15660400

2’ (phenol form)

Energy = -1610.869293 A. U.

Gibbs Free Energy = -1610.515758 A. U.

N	2.73173900	1.68357000	-0.00005200
N	2.16444200	-3.03268800	0.00006000
N	-2.75563300	-2.31537900	0.00005000
N	-1.99491100	2.35928900	-0.00003500
C	-0.71107700	2.53770200	-0.00005200
C	-0.07383900	3.85419800	-0.00006800
C	1.30819600	3.65838600	-0.00007300
C	1.55510800	2.21647400	-0.00005600
N	0.30978600	1.61187500	-0.00002700
C	2.91638700	0.33114800	-0.00004200
C	4.27201200	-0.22026500	0.00001800
C	4.10235100	-1.60371300	0.00004900
C	2.64762100	-1.83745000	0.00002800
N	1.98145700	-0.60078400	0.00000500
C	-2.90428600	-1.03335500	0.00003200
C	-4.23815700	-0.40466600	-0.00001100
C	-4.00767200	0.97030300	-0.00003800
C	-2.54942100	1.11828400	-0.00000200
N	-1.91820500	-0.04383400	-0.00001400
C	-5.52629400	-0.91176100	-0.00002500
C	-6.57942800	0.00280800	-0.00006500
C	-6.34481100	1.38068500	-0.00009200
C	-5.04634600	1.88659800	-0.00008200
C	-0.62448000	5.12583000	-0.00007800
C	0.25655100	6.20381100	-0.00009800
C	1.64193600	6.00739400	-0.00010500
C	2.18958800	4.72737600	-0.00009100
C	5.53024400	0.36204600	0.00003600
C	6.62914500	-0.49363500	0.00007600

C	6.46056000	-1.88245200	0.00010500
C	5.19139900	-2.45889600	0.00009400
C	-1.77225300	-4.42985500	0.00007900
C	-1.56864000	-3.01814500	0.00005900
C	-0.26603200	-2.52157800	0.00005800
C	0.83165200	-3.38903600	0.00007100
C	0.59119500	-4.78487600	0.00009200
C	-0.68465200	-5.30508300	0.00009700
H	0.17026200	0.60151500	0.00003500
H	-5.70833500	-1.98380800	-0.00000400
H	-7.60431600	-0.36081500	-0.00007500
H	-7.19037600	2.06422800	-0.00012200
H	-4.84587200	2.95502500	-0.00010000
H	-1.70281600	5.26042700	-0.00007400
H	-0.13550700	7.21771400	-0.00011000
H	2.30005200	6.87264500	-0.00012000
H	3.26290400	4.55752000	-0.00009600
H	5.64446200	1.44327500	0.00001000
H	7.63489000	-0.08010200	0.00008400
H	7.34020600	-2.52222200	0.00013800
H	5.04848700	-3.53664700	0.00011900
H	-0.10823800	-1.45580600	0.00005200
H	-0.87259300	-6.37457000	0.00011000
O	-3.01288500	-4.90944800	0.00007500
H	-3.58181700	-4.11059400	0.00004800
H	1.46161800	-5.43621100	0.00010100

2’ (quinoid form)

Energy = -1610.865500 A. U.

Gibbs Free Energy = -1610.511185 A. U.

N	2.05481200	2.31703800	0.00000000
N	-2.21111300	-3.00323200	0.00003400
N	-2.69824100	1.71994200	0.00002900
C	-1.50596100	2.24938700	0.00003400
C	-1.23783300	3.67468200	-0.00000200
C	0.15386000	3.84605400	-0.00001300
C	0.75896800	2.53068300	0.00001500
N	-0.27408900	1.62411700	0.00005000
C	2.59301300	1.10164400	-0.00001300
C	4.03970100	0.90383500	-0.00001900
C	4.23634900	-0.48315400	-0.00001500
C	2.88474400	-1.03572900	-0.00003200
N	1.93677000	-0.08649200	-0.00004800
C	-2.67434800	-1.77103400	0.00002400
C	-4.12145900	-1.52761600	-0.00001500
C	-4.27551800	-0.14014400	-0.00000600
C	-2.91670800	0.39532500	0.00001900
N	-1.99242600	-0.57897500	0.00003600
C	-5.22044100	-2.37314600	-0.00004900

C	-6.48255000	-1.78495100	-0.00006800
C	-6.63595600	-0.39298800	-0.00005600
C	-5.53008300	0.45214400	-0.00002300
C	-2.09810900	4.76700400	-0.00003100
C	-1.52766500	6.03207100	-0.00006700
C	-0.13389900	6.20384700	-0.00007800
C	0.72513500	5.11470100	-0.00005300
C	5.11032200	1.78455300	-0.00001100
C	6.39161000	1.24130800	0.00000200
C	6.58959900	-0.14387200	0.00000600
C	5.51378900	-1.02808500	-0.00000300
C	-0.69364900	-4.80575600	0.00010500
C	-0.91700900	-3.37342300	0.00005600
C	0.20243500	-2.52193100	-0.00005400
C	1.46873800	-3.05862600	0.00003100
C	1.72412700	-4.51684800	0.00024600
C	0.54236000	-5.35594700	0.00013000
H	-0.16195200	0.61136800	0.00010300
H	-5.08813200	-3.45226100	-0.00005300
H	-7.36898600	-2.41521000	-0.00009200
H	-7.63763300	0.03051800	-0.00007400
H	-5.63518900	1.53434000	-0.00001800
H	-3.17471800	4.61878400	-0.00002400
H	-2.16862400	6.91023800	-0.00008900
H	0.27498000	7.21119300	-0.00010700
H	1.80558300	5.23183300	-0.00006300
H	4.94134200	2.85831700	-0.00000900
H	7.25625400	1.90029100	0.00001200
H	7.60319700	-0.53653700	0.00001600
H	5.68651600	-2.10285300	-0.00000300
H	0.06096500	-1.45354300	-0.00019600
H	0.70318300	-6.43029000	0.00008500
O	2.88617100	-4.93779900	-0.00008200
N	2.63959300	-2.34891800	-0.00001300
H	3.43498200	-2.99938100	0.00009700
H	-1.58966700	-5.42273700	0.00008300

3’

Energy = -2020.225897 A. U.

Gibbs Free Energy = -2019.664321 A. U.

N	2.99039000	2.38262800	0.04178900
N	-1.44696100	2.50914100	-1.61151200
N	-1.44867500	-2.50801800	-1.61161400
N	2.98880800	-2.38452200	0.04160500
C	3.31995200	-1.14428500	0.20293800
C	4.58248100	-0.69998700	0.79338500
C	4.58292600	0.69698100	0.79344900
C	3.32069300	1.14215800	0.20303500
N	2.62148000	-0.00081800	-0.13663800

C	1.79699100	2.74904200	-0.50062400
C	1.56630700	4.14871700	-0.87047100
C	0.26587300	4.18660100	-1.36819100
C	-0.24425300	2.80485000	-1.26962200
N	0.75140500	1.97049900	-0.73190800
C	-0.24616500	-2.80454700	-1.26975900
C	0.26301800	-4.18664800	-1.36829500
C	1.56349500	-4.14962400	-0.87061900
C	1.79514900	-2.75011200	-0.50080000
N	0.75008800	-1.97085800	-0.73208600
C	-0.30092000	-5.36265300	-1.82458100
C	0.49003400	-6.51421000	-1.76517100
C	1.79268700	-6.47644000	-1.26405600
C	2.35469200	-5.28333200	-0.80422500
C	5.65406300	-1.42510400	1.28462000
C	6.73648300	-0.70089400	1.78638500
C	6.73692700	0.69643500	1.78644600
C	5.65496600	1.42137600	1.28474400
C	2.35823500	5.28191700	-0.80409700
C	1.79701800	6.47537500	-1.26398900
C	0.49440500	6.51399100	-1.76514500
C	-0.29729800	5.36295000	-1.82453300
C	-3.43867900	-1.22085100	-1.46692400
C	-2.01562100	-1.24397200	-1.56309200
C	-1.31532100	0.00052300	-1.57905100
C	-2.01477900	1.24549500	-1.56296900
C	-3.43784000	1.22332900	-1.46671500
C	-4.14361700	0.00147300	-1.41699400
H	1.66340900	-0.00054500	-0.48631000
H	-1.31518900	-5.38474800	-2.21512000
H	0.08508400	-7.45984700	-2.11666100
H	2.37696300	-7.39242000	-1.23395300
H	3.36746900	-5.24013100	-0.41206400
H	5.64303300	-2.51166200	1.27452600
H	7.59792200	-1.23141500	2.18318000
H	7.59870300	1.22637400	2.18328800
H	5.64462400	2.50794200	1.27474400
H	3.37097200	5.23809500	-0.41190400
H	2.38189800	7.39097000	-1.23389600
H	0.09009900	7.45988700	-2.11667900
H	-1.31154200	5.38566800	-2.21509900
H	-0.23448200	0.00017600	-1.60030700
H	-5.22348500	0.00183200	-1.29109300
C	-2.23268400	-1.16221800	2.04448800
C	-3.60097800	-0.71762000	2.05728500
C	-3.60058000	0.71962600	2.05734600
C	-2.23203700	1.16347800	2.04458900
C	-1.39003100	0.00039900	2.04806700
Ru	-2.64860700	0.00082700	0.23177800
H	-3.95527000	2.17665300	-1.39297800

H	-3.95675300	-2.17383600	-1.39332600
C	0.09606300	-0.00019500	2.13171300
H	0.52012900	-0.88413700	1.64293000
H	0.52081700	0.88470500	1.64531100
H	0.41463600	-0.00170800	3.18232800
C	-1.76534100	2.57880400	2.05415000
H	-1.66839300	2.95348900	3.08115700
H	-0.78647900	2.67794700	1.56991000
H	-2.46347600	3.23573000	1.52350600
C	-4.80475700	1.59709500	2.10254800
H	-5.09984600	1.80147300	3.13946800
H	-4.61677100	2.56075700	1.61724900
H	-5.66196200	1.13278900	1.60267000
C	-4.80562000	-1.59445600	2.10237200
H	-5.10089800	-1.79872100	3.13926100
H	-5.66255000	-1.12969800	1.60244100
H	-4.61808000	-2.55819300	1.61704700
C	-1.76670400	-2.57778100	2.05407100
H	-1.67013000	-2.95252300	3.08109700
H	-2.46508600	-3.23435100	1.52330900
H	-0.78779100	-2.67741800	1.57002800

4’ (phenol form)

Energy = -2095.431900 A. U.

Gibbs Free Energy = -2094.865339 A. U.

N	3.62992800	-1.53988900	-0.02461100
N	-0.66782000	-2.81919200	-1.56243000
N	-1.96990800	2.04548500	-1.47225400
N	2.40932500	3.07256000	-0.01477700
C	3.05220400	1.95469800	0.12128100
C	4.41530600	1.85603700	0.64018500
C	4.77261900	0.50555400	0.64245500
C	3.63758600	-0.25558200	0.12099800
N	2.64911700	0.66859000	-0.17456100
C	2.55133300	-2.21111400	-0.51767400
C	2.66235200	-3.64090600	-0.81710300
C	1.40444400	-4.01687600	-1.28343200
C	0.57522500	-2.79675700	-1.23740400
N	1.34705600	-1.72026500	-0.76066300
C	-0.87820200	2.65940700	-1.16810700
C	-0.78573200	4.13242100	-1.16479200
C	0.50259000	4.42536500	-0.72118100
C	1.13737400	3.12461800	-0.48500600
N	0.33643700	2.10257800	-0.75616800
C	-1.67735800	5.13611400	-1.49326900
C	-1.23395500	6.45548400	-1.35917000
C	0.05564600	6.74634000	-0.91119900
C	0.95162400	5.72664700	-0.58188700
C	5.28931300	2.83827300	1.07309500
C	6.54533100	2.42232700	1.51664900

C	6.90275200	1.07139500	1.51895700
C	6.01768000	0.08650300	1.07765900
C	3.70594700	-4.54487200	-0.71440200
C	3.44578200	-5.86041200	-1.10317900
C	2.18588400	-6.23809000	-1.57245600
C	1.13871100	-5.31691400	-1.66990200
C	-3.53933200	0.30180600	-1.47900200
C	-2.15064700	0.67077200	-1.48614900
C	-1.16096400	-0.35375100	-1.51667000
C	-1.53011700	-1.73328000	-1.53927500
C	-2.91798500	-2.06188000	-1.46531200
C	-3.91091200	-1.05839600	-1.41117200
H	1.71597300	0.42010100	-0.50198200
H	-2.67994900	4.91115000	-1.84862400
H	-1.90490200	7.27290100	-1.61057200
H	0.36503600	7.78422800	-0.82051700
H	1.95904900	5.93829300	-0.23326500
H	4.99966300	3.88552600	1.06292100
H	7.26175500	3.16099700	1.86598200
H	7.89050300	0.78498200	1.87012100
H	6.28477300	-0.96677600	1.07111500
H	4.68192000	-4.23748400	-0.34785000
H	4.23506700	-6.60515300	-1.04224400
H	2.01907400	-7.27060100	-1.86891500
H	0.15662300	-5.60391000	-2.03718700
H	-0.11634100	-0.07935900	-1.51516100
H	-4.96450000	-1.30814300	-1.31308700
O	-4.47162300	1.24990600	-1.44410700
H	-3.98183100	2.09718400	-1.48903300
H	-3.18603600	-3.11395300	-1.40978700
C	-3.16141300	-1.74562200	2.05803700
C	-3.58818100	-0.37152400	2.09414700
C	-2.41359200	0.45492700	2.10612900
C	-1.26204100	-0.40386900	2.08189900
C	-1.72239800	-1.76475500	2.05168300
Ru	-2.45490100	-0.73803800	0.26277000
C	-2.38572300	1.94401800	2.14332600
H	-1.52496200	2.34111600	1.59112000
H	-3.29201700	2.37351500	1.70256800
H	-2.31283800	2.30958100	3.17557900
C	0.15912700	0.03530000	2.15920200
H	0.29487600	1.02456100	1.70732600
H	0.48662000	0.08936900	3.20564800
H	0.81715800	-0.66340700	1.62987600
C	-0.85481500	-2.97592200	2.03982100
H	0.09876600	-2.77548500	1.53679100
H	-0.62872200	-3.30594200	3.06183500
H	-1.33372200	-3.81113900	1.51693600
C	-4.05308800	-2.94028800	2.07131100
H	-3.57775300	-3.80022000	1.58757000

H	-4.29987800	-3.23349000	3.09946900
H	-4.99650600	-2.74477700	1.54973500
C	-4.99774800	0.11146500	2.13326300
H	-5.68436400	-0.61736300	1.68995900
H	-5.32336600	0.28658100	3.16638000
H	-5.11725500	1.05051400	1.58241200

4' (quinoid form)

Energy = -2095.417887 A. U.

Gibbs Free Energy = --2094.851716 A. U.

N	3.60770400	-1.62204900	-0.06171300
N	-0.74512200	-2.82041100	-1.52074700
N	-1.85274900	2.04557900	-1.45318700
N	2.51246600	3.03115400	-0.06649200
C	3.12964800	1.88151800	0.05078300
C	4.50715700	1.75994400	0.50766900
C	4.83280600	0.40040400	0.51930000
C	3.65878900	-0.34092000	0.06278300
N	2.67577500	0.61306400	-0.20017400
C	2.49850100	-2.28465100	-0.50808500
C	2.54811200	-3.73210700	-0.70564700
C	1.27400400	-4.08401200	-1.14979900
C	0.49936400	-2.83053700	-1.19534000
N	1.32012400	-1.75766000	-0.79060800
C	-0.76634500	2.70981500	-1.13051500
C	-0.71431600	4.17248000	-1.02192500
C	0.59097400	4.43740800	-0.59681200
C	1.24488000	3.12937600	-0.48132700
N	0.41778300	2.12351000	-0.81608500
C	-1.62601400	5.19192000	-1.23324500
C	-1.18417700	6.49916400	-1.00292800
C	0.11802100	6.76212300	-0.57798800
C	1.03255700	5.72649400	-0.36553400
C	5.42154600	2.73026800	0.88615900
C	6.68488000	2.29317000	1.28242900
C	7.01016500	0.93350700	1.29429500
C	6.08535300	-0.03892400	0.91009500
C	3.55020900	-4.67354600	-0.53279800
C	3.23147200	-5.99967500	-0.82517400
C	1.95510000	-6.35351500	-1.27124200
C	0.95121300	-5.39690500	-1.44094300
C	-3.56980600	0.45642000	-1.64598400
C	-2.11583400	0.67834100	-1.52621200
C	-1.14001800	-0.34326600	-1.53331400
C	-1.56571300	-1.70683300	-1.56165600
C	-2.97472400	-1.97019500	-1.52574600
C	-3.92963800	-0.93570200	-1.47209900
H	1.73446400	0.37537000	-0.51255900
H	-2.64429200	5.00713400	-1.56958200
H	-1.86976700	7.32724900	-1.16066500

H	0.42388500	7.79136200	-0.41117900
H	2.04956500	5.91802100	-0.03396000
H	5.15521200	3.78355600	0.87037000
H	7.43278900	3.02007300	1.58732000
H	8.00523600	0.63001400	1.60857700
H	6.32862900	-1.09791000	0.91355100
H	4.53886600	-4.38503500	-0.18530200
H	3.98576600	-6.77313400	-0.70635300
H	1.74229300	-7.39660700	-1.49161300
H	-0.04223400	-5.66571300	-1.79105000
H	-0.08725400	-0.10550200	-1.50962000
H	-4.98722900	-1.16905900	-1.36998000
O	-4.34277800	1.42720000	-1.68823400
H	-3.27980100	-3.01238400	-1.45495200
C	-3.23128800	-1.67939400	1.99310300
C	-3.63170900	-0.29595700	2.01639100
C	-2.44068400	0.50473800	2.06212200
C	-1.30431000	-0.37283500	2.06678000
C	-1.79148400	-1.72620200	2.02631100
Ru	-2.45577700	-0.69453300	0.22259400
C	-2.39860800	1.99381200	2.08603700
H	-1.47749700	2.37728200	1.62815200
H	-3.25107400	2.42538900	1.54822600
H	-2.43130800	2.37271900	3.11571900
C	0.12612600	0.03345300	2.16903900
H	0.29094900	1.02614500	1.73318000
H	0.44990800	0.06584900	3.21755000
H	0.77369100	-0.67219400	1.63473300
C	-0.94318400	-2.95079400	2.04020900
H	0.01173200	-2.77998000	1.52676500
H	-0.71510600	-3.25931300	3.06867200
H	-1.43757600	-3.79082200	1.54016300
C	-4.14816700	-2.85499500	1.98063700
H	-3.66794700	-3.73156300	1.53278200
H	-4.45508700	-3.12778700	2.99817100
H	-5.05763100	-2.64737800	1.40586700
C	-5.02792800	0.22731400	2.00448100
H	-5.73481700	-0.52933700	1.64959700
H	-5.34467000	0.53067900	3.01048500
H	-5.12447800	1.09678700	1.34381600
H	-2.75222800	2.54141600	-1.58799000

4A’

Energy = -2094.990914 A. U.

Gibbs Free Energy = -2094.440896 A. U.

N	3.72767500	-1.40957100	-0.10090900
N	-0.57408800	-2.84707000	-1.49126900
N	-2.04006600	1.93415700	-1.46994100
N	2.32788400	3.15277800	-0.05256100
C	3.01909500	2.06716800	0.05584300

C	4.40952100	2.02015900	0.50918700
C	4.81653500	0.68481900	0.49464900
C	3.68634900	-0.12123800	0.03257000
N	2.65417700	0.75848100	-0.21253800
C	2.65225900	-2.12219600	-0.53477600
C	2.77100000	-3.57132000	-0.72101500
C	1.51228800	-3.99001400	-1.14605900
C	0.67455800	-2.77639000	-1.19346400
N	1.44361800	-1.66369500	-0.81590000
C	-0.97121400	2.57170000	-1.15107300
C	-0.97110900	4.04185100	-1.05762500
C	0.30404900	4.40562900	-0.62907800
C	1.03093600	3.14442500	-0.48264300
N	0.30036900	2.08598700	-0.78840000
C	-1.95387900	4.98996500	-1.28951900
C	-1.61168800	6.32575300	-1.08268600
C	-0.32985900	6.69244000	-0.65522200
C	0.65165300	5.73241300	-0.41864900
C	5.26871600	3.03337800	0.90367500
C	6.55663100	2.66625900	1.28708100
C	6.96460800	1.32762900	1.27213300
C	6.09693100	0.31361800	0.87337800
C	3.81892300	-4.46262800	-0.55044600
C	3.56446300	-5.80526700	-0.82540000
C	2.30103800	-6.22676600	-1.25289100
C	1.25216500	-5.32201300	-1.41929200
C	-3.67123800	0.18731200	-1.69014500
C	-2.23641000	0.57599900	-1.54790300
C	-1.18984300	-0.39953900	-1.54540600
C	-1.47944400	-1.79966900	-1.53474700
C	-2.85521200	-2.19163800	-1.45438200
C	-3.88000200	-1.23616000	-1.40653400
H	1.72086300	0.48282900	-0.52394300
H	-2.94498900	4.68699600	-1.61928800
H	-2.35360200	7.10229300	-1.25561200
H	-0.10089500	7.74507500	-0.50505200
H	1.64998900	6.00256100	-0.08264000
H	4.93682300	4.06833700	0.90839700
H	7.26077900	3.43176100	1.60384300
H	7.97787500	1.07831300	1.57741800
H	6.39757100	-0.73070400	0.85479000
H	4.79494600	-4.11909300	-0.21634600
H	4.35797700	-6.53950500	-0.70719000
H	2.13680900	-7.28199600	-1.45956400
H	0.26674300	-5.63885800	-1.75238900
H	-0.15976500	-0.06899900	-1.52950600
H	-4.91287800	-1.55100400	-1.26518900
O	-4.59569500	0.98402000	-1.81506900
H	-3.06218600	-3.25441400	-1.33807500
C	-3.48660006	-1.43781562	2.04828834

C	-3.91223006	-0.06112562	2.00201334
C	-2.73442806	0.76330538	2.00435134
C	-1.58404706	-0.09195062	2.04957534
C	-2.04597306	-1.45476762	2.07000234
Ru	-2.41348300	-0.82179900	0.24482300
C	-0.16019306	0.34203938	2.12859034
H	-0.02107406	1.32983938	1.67484034
H	0.17676994	0.39402038	3.17302534
H	0.49588394	-0.35586562	1.59383034
C	-2.72150406	2.25217238	1.94680134
H	-2.79451606	2.68661438	2.95273834
H	-1.79826906	2.62711238	1.48810034
H	-3.55743606	2.63282638	1.34845934
C	-5.31638206	0.44077038	1.96313234
H	-5.64163006	0.80140338	2.94824034
H	-5.42166206	1.26474538	1.24745034
H	-6.01101106	-0.34597662	1.64999134
C	-4.38071606	-2.63072862	2.09954034
H	-4.66734906	-2.87518862	3.13101334
H	-5.30209406	-2.46178562	1.53044034
H	-3.89004606	-3.51273762	1.67258534
C	-1.16884706	-2.65915262	2.11969934
H	-0.89165206	-2.91239462	3.15200234
H	-1.66192406	-3.53261262	1.67829834
H	-0.23986206	-2.49418662	1.55804134

5’ (phenol form)

Energy = -1686.081259 A. U.

Gibbs Free Energy = -1685.722347 A. U.

N	-2.38965900	-2.20450500	-0.00014100
N	-2.48191000	2.53033300	-0.00001900
N	2.48181700	2.53037600	-0.00001000
N	2.38971900	-2.20442500	0.00043100
C	1.14452200	-2.56538200	-0.00004900
C	0.69853800	-3.95590500	-0.00019900
C	-0.69841200	-3.95592600	-0.00034000
C	-1.14445100	-2.56541800	-0.00026100
N	0.00000700	-1.79238200	-0.00017900
C	-2.76988600	-0.90177200	-0.00023000
C	-4.19011000	-0.54936100	0.00018800
C	-4.22391900	0.84601400	0.00035400
C	-2.81750500	1.27745100	0.00009600
N	-1.98217400	0.16486200	-0.00004800
C	2.81745900	1.27752000	0.00025200
C	4.22389900	0.84611900	0.00029100
C	4.19013300	-0.54925400	0.00050900
C	2.76991500	-0.90169300	0.00052100
N	1.98216300	0.16489400	0.00014100
C	5.42930500	1.52941900	0.00020200
C	6.60008400	0.77312800	0.00036900

C	6.56260800	-0.62506100	0.00059100
C	5.34953800	-1.30885200	0.00059700
C	1.42132200	-5.13920200	-0.00030800
C	0.70019000	-6.32903500	-0.00060000
C	-0.69999300	-6.32905600	-0.00074900
C	-1.42116200	-5.13924600	-0.00061100
C	-5.34949100	-1.30900000	0.00035600
C	-6.56258200	-0.62524600	0.00068900
C	-6.60010000	0.77294200	0.00079900
C	-5.42934800	1.52927300	0.00068400
C	1.19221000	4.48104900	-0.00047900
C	1.21288900	3.04252500	-0.00016100
C	-0.00003300	2.35775800	0.00008100
C	-1.21299500	3.04255100	-0.00004800
C	-1.19235900	4.48106000	-0.00042400
C	-0.00006700	5.18959100	-0.00060900
H	-0.00002900	-0.77337000	0.00042100
H	5.45902400	2.61646800	0.00006100
H	7.56342900	1.27776900	0.00032200
H	7.49643300	-1.18202100	0.00072100
H	5.30227000	-2.39497600	0.00077300
H	2.50788200	-5.12165900	-0.00023400
H	1.23033400	-7.27808500	-0.00067100
H	-1.23010700	-7.27812400	-0.00094800
H	-2.50772100	-5.12172700	-0.00077500
H	-5.30218600	-2.39512300	0.00031600
H	-7.49638900	-1.18223500	0.00088800
H	-7.56345800	1.27755700	0.00104200
H	-5.45912600	2.61632000	0.00082900
H	-0.00005200	1.28073500	0.00026500
H	-0.00001900	6.27435100	-0.00090100
O	-2.35053000	5.12796200	-0.00063800
H	-3.02674000	4.41566200	-0.00060600
O	2.35039900	5.12789400	-0.00076100
H	3.02658600	4.41559800	-0.00062100

5' (quinoid form)

Energy = -1686.077156 A. U.

Gibbs Free Energy = -1685.718408 A. U.

N	2.45569000	2.14476600	0.00033300
N	-2.53113700	-2.48682000	-0.00012600
N	-2.33742600	2.24660300	0.00001000
C	-1.07711000	2.59600500	0.00004600
C	-0.60580100	3.96580500	-0.00011800
C	0.79679000	3.93361700	-0.00000900
C	1.20500200	2.54588000	0.00020600
N	0.04919300	1.79875500	0.00019700
C	2.81530500	0.86574300	0.00017000
C	4.21674400	0.45831600	0.00022500
C	4.20789400	-0.94338000	0.00001900

C	2.79184900	-1.29177700	-0.00028400
N	1.99293200	-0.21578000	-0.00021800
C	-2.83571300	-1.19957900	-0.00003300
C	-4.23131000	-0.75135700	0.00012200
C	-4.17532800	0.64531100	0.00013700
C	-2.75273500	0.97514800	-0.00005300
N	-1.98557100	-0.13261900	-0.00008600
C	-5.44769500	-1.41843600	0.00025000
C	-6.60651000	-0.64651200	0.00041500
C	-6.54762000	0.75217100	0.00040800
C	-5.32625200	1.41934500	0.00026900
C	-1.29830900	5.17240600	-0.00036100
C	-0.55051400	6.34072700	-0.00050100
C	0.85402000	6.30832500	-0.00040300
C	1.54582400	5.10667600	-0.00015600
C	5.40615800	1.17135200	0.00052000
C	6.59310500	0.44529400	0.00061900
C	6.58528700	-0.95438100	0.00040900
C	5.39172100	-1.67051800	0.00009700
C	-1.30726800	-4.49091000	-0.00005500
C	-1.30220800	-3.01731800	-0.00027200
C	-0.07219300	-2.34946900	-0.00054000
C	1.09377700	-3.07665700	-0.00042300
C	1.11819100	-4.57031900	-0.00023200
C	-0.15731500	-5.22269000	-0.00001800
H	0.01792300	0.78095700	0.00028900
H	-5.49284100	-2.50495600	0.00025500
H	-7.57725600	-1.13663200	0.00054900
H	-7.47347200	1.32240500	0.00048300
H	-5.26541600	2.50483100	0.00024200
H	-2.38502700	5.18255400	-0.00044000
H	-1.05720400	7.30261000	-0.00066400
H	1.40459200	7.24574700	-0.00049700
H	2.63180700	5.06589300	-0.00009000
H	5.39783500	2.25833300	0.00064900
H	7.54529200	0.96986400	0.00080600
H	7.53019700	-1.49164800	0.00048900
H	5.40386700	-2.75897300	-0.00004200
H	-0.05278200	-1.27264900	-0.00088900
H	-0.18905900	-6.30723300	0.00018600
O	2.21677800	-5.13885900	-0.00028200
O	-2.50095300	-5.07189900	0.00022000
H	-3.14048400	-4.32654300	0.00016900
N	2.35244500	-2.55696200	-0.00054500
H	3.03581800	-3.32700700	-0.00068500

6’ (phenol form)

Energy = -2170.637646 A. U.

Gibbs Free Energy = -2170.067217 A. U.

N	3.20720800	2.38803200	-0.06042700
N	-1.31387000	2.52358000	-1.44362200
N	-1.31277800	-2.52431400	-1.44355100
N	3.20825100	-2.38680300	-0.06034600
C	3.54694700	-1.14285900	0.06427300
C	4.86048200	-0.69751500	0.52623000
C	4.86015900	0.69949200	0.52620400
C	3.54642100	1.14422500	0.06422400
N	2.81410900	0.00052300	-0.19602300
C	1.97780800	2.76985900	-0.49522500
C	1.68787900	4.19210400	-0.69938800
C	0.36034000	4.24146300	-1.12235400
C	-0.10049200	2.84031600	-1.14650700
N	0.94148100	1.98809000	-0.76230100
C	-0.09929200	-2.84053500	-1.14638400
C	0.36217000	-4.24147600	-1.12225000
C	1.68969000	-4.19152500	-0.69929300
C	1.97901300	-2.76915600	-0.49520100
N	0.94233900	-1.98784100	-0.76221000
C	-0.25189400	-5.44430200	-1.41758800
C	0.51199000	-6.60610600	-1.27205500
C	1.84031200	-6.55372900	-0.84558500
C	2.45472300	-5.33509600	-0.54986000
C	5.97512100	-1.42211000	0.91153200
C	7.10128900	-0.69723800	1.30372600
C	7.10096700	0.70026000	1.30370300
C	5.97446800	1.42460500	0.91148600
C	2.45240100	5.33602200	-0.55000400
C	1.83744100	6.55437300	-0.84575200
C	0.50909400	6.60615400	-1.27221500
C	-0.25427200	5.44400400	-1.41771200
C	-3.26914000	-1.22251300	-1.44882500
C	-1.83059000	-1.23886500	-1.45992600
C	-1.12654500	-0.00032400	-1.46075500
C	-1.83111200	1.23791400	-1.45992400
C	-3.26965100	1.22091100	-1.44869700
C	-3.97302400	-0.00095400	-1.36499200
H	1.84144200	0.00021800	-0.49977300
H	-1.28395900	-5.48652500	-1.75696800
H	0.06522000	-7.57106100	-1.49754600
H	2.40297400	-7.47815200	-0.74546300
H	3.48834400	-5.27924600	-0.21853900
H	5.96315600	-2.50863500	0.90413300
H	7.99779600	-1.22718700	1.61420200
H	7.99723100	1.23063500	1.61415400
H	5.96201900	2.51112400	0.90404700
H	3.48604200	5.28065900	-0.21866300
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C	-1.22209600	0.00002900	2.12733700
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H	0.59876900	0.00075000	3.24819100
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C	-1.59807400	2.57681300	2.13291000
H	-1.46097300	2.94015300	3.15941000
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H	-4.93588600	-1.83589300	3.17029800
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H	-4.45426900	-2.54527800	1.62090900
C	-1.59721700	-2.57690500	2.13385400
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6’ (quinoid form)

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Gibbs Free Energy = -2170.054109 A. U.

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C	-7.19294800	-0.49699100	1.10316400
C	-6.07230400	-1.25024500	0.75561400
C	-2.57449100	-5.29429600	-0.36119900
C	-1.95942200	-6.53286000	-0.56278300
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C	0.13988200	-5.47425500	-1.20167700
C	3.30233400	1.10773400	-1.50903900
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C	1.09954400	-0.00648100	-1.46248700
C	1.78182000	-1.24207500	-1.49556600
C	3.24827100	-1.38819900	-1.61619700
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H	-0.18147000	-7.59876100	-1.12322500
H	1.17438600	-5.56250000	-1.52765900
H	0.02198800	0.03710600	-1.43699800
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O	3.75001900	-2.52132500	-1.67767000
O	4.01811000	2.23065700	-1.49084000
H	3.36727600	2.96087700	-1.49471600
C	2.13446300	1.09664000	2.10779500
C	3.49683100	0.63207300	2.05889700
C	3.47160400	-0.80927900	2.04843700
C	2.09533400	-1.22464600	2.09443700
C	1.26846000	-0.05189500	2.12813700
Ru	2.46072500	-0.05135300	0.28283200
C	-0.21867700	-0.02175600	2.23238000
H	-0.66996400	-0.90224500	1.75857000
H	-0.53852600	-0.00236200	3.28245500

H	-0.63177000	0.86556500	1.73702700
C	1.61685800	-2.63539300	2.09696400
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H	0.61686900	-2.72346600	1.65246200
H	2.29775300	-3.28823400	1.53764700
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C	4.71546800	1.48993500	2.05124100
H	5.06098200	1.69594500	3.07218900
H	5.53906500	1.01040500	1.51146000
H	4.52569700	2.45092400	1.56181200
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6A'

Energy = -2170.197465 A. U.

Gibbs Free Energy = -2169.641528 A. U.

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N	3.39362900	-2.18521800	-0.11829300
C	3.65059400	-0.91762100	-0.00433300
C	4.94655600	-0.38903600	0.41694300
C	4.85523800	1.00428300	0.42799200
C	3.50112300	1.36560800	0.01160400
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C	1.80268000	2.87288600	-0.49522300
C	1.38129700	4.26662700	-0.63002200
C	0.04996500	4.20546800	-1.03951200
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C	6.11971100	-1.04082800	0.76502200
C	7.20676400	-0.24992800	1.12789200
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H	-4.88894600	-1.94624100	3.20592600
H	-5.44169400	-1.31243800	1.64612400
H	-4.35427400	-2.69636200	1.68998300
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H	-2.20861900	-3.31765400	1.80638700
H	-0.55916900	-2.69691900	1.66043800

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5. NMR Spectra

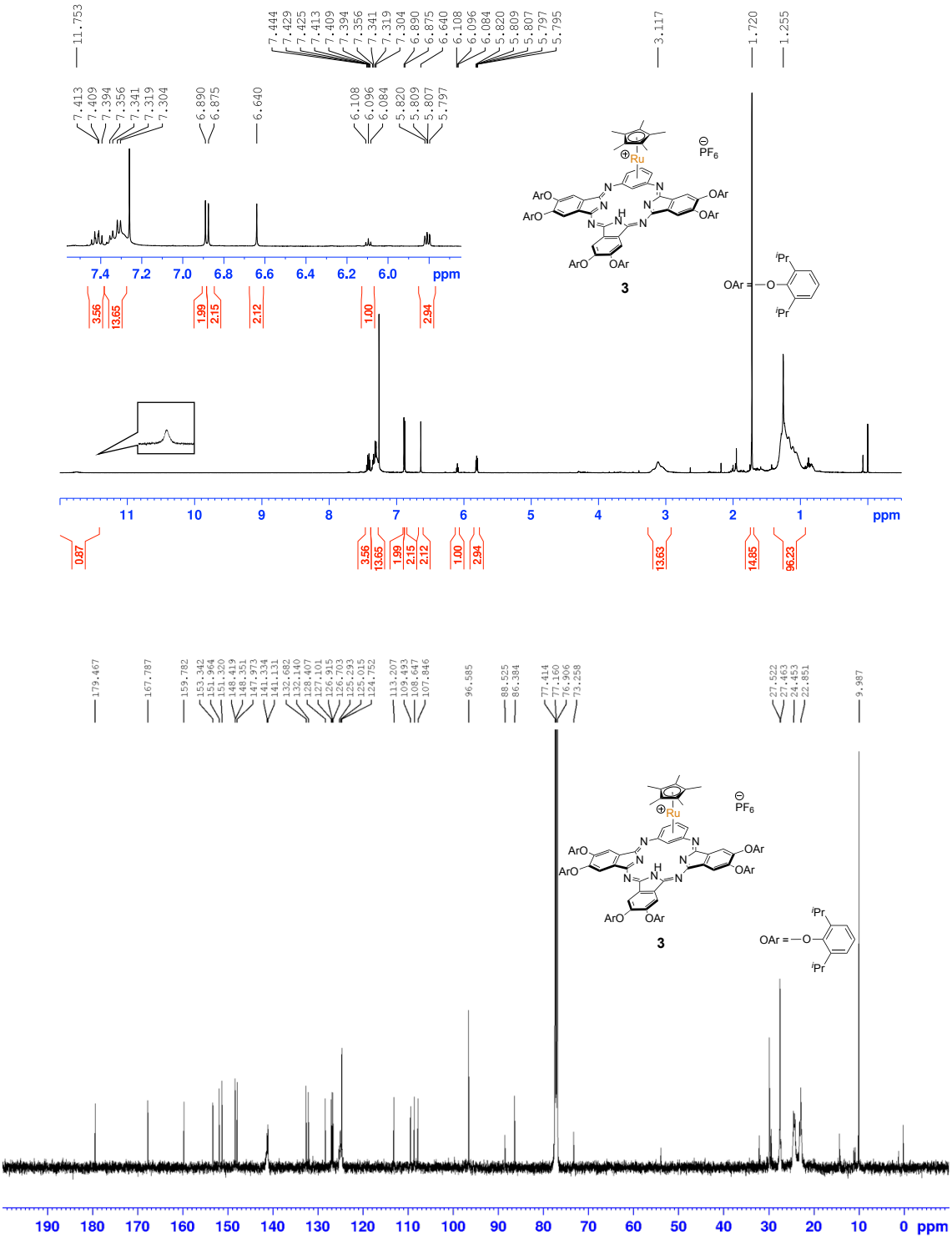

Fig. S19. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **3** in $CDCl_3$.

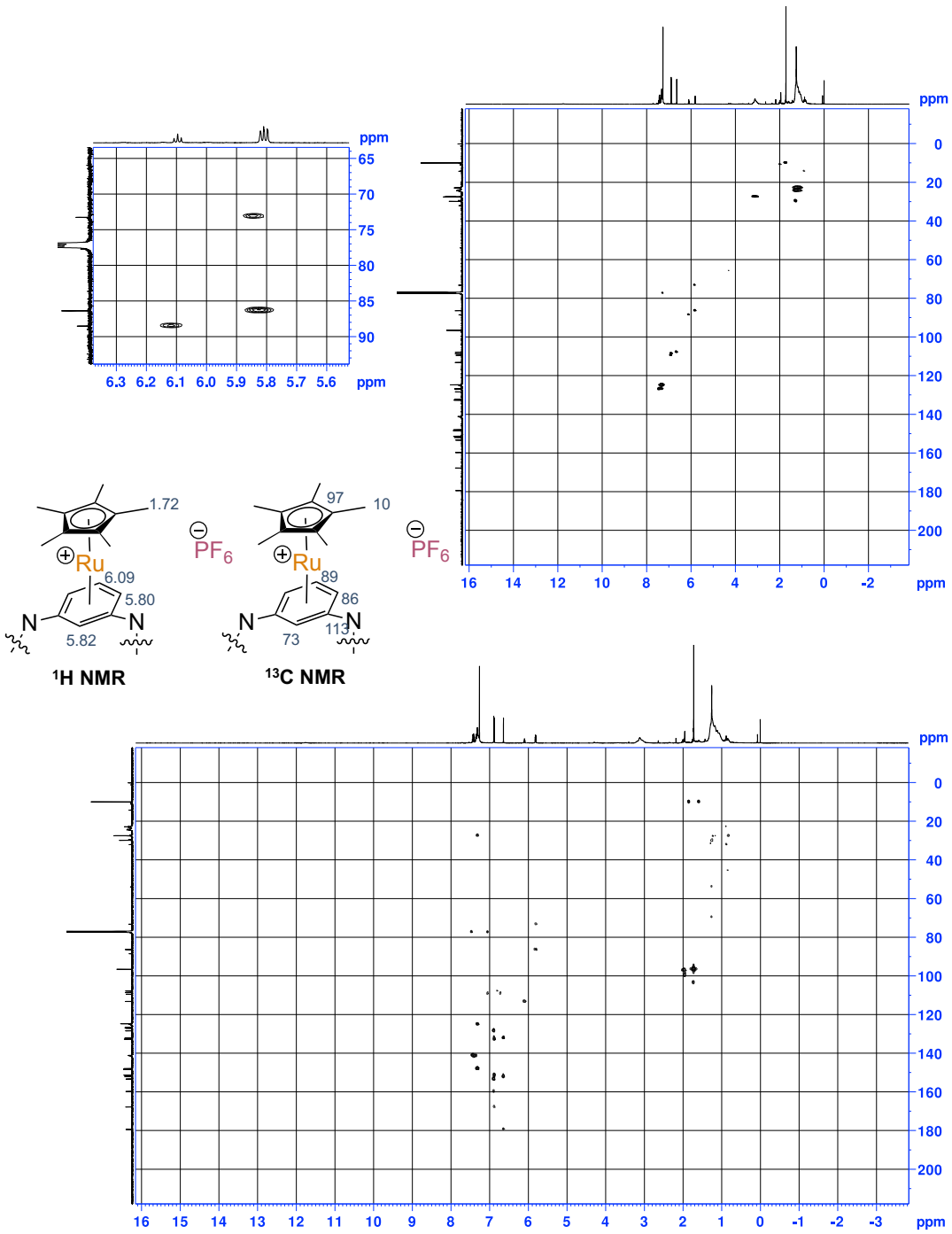

Fig. S20. ^{1}H-^{13}C HMQC (top) and HMBC (bottom) NMR spectra of **3** in $CDCl_3$.

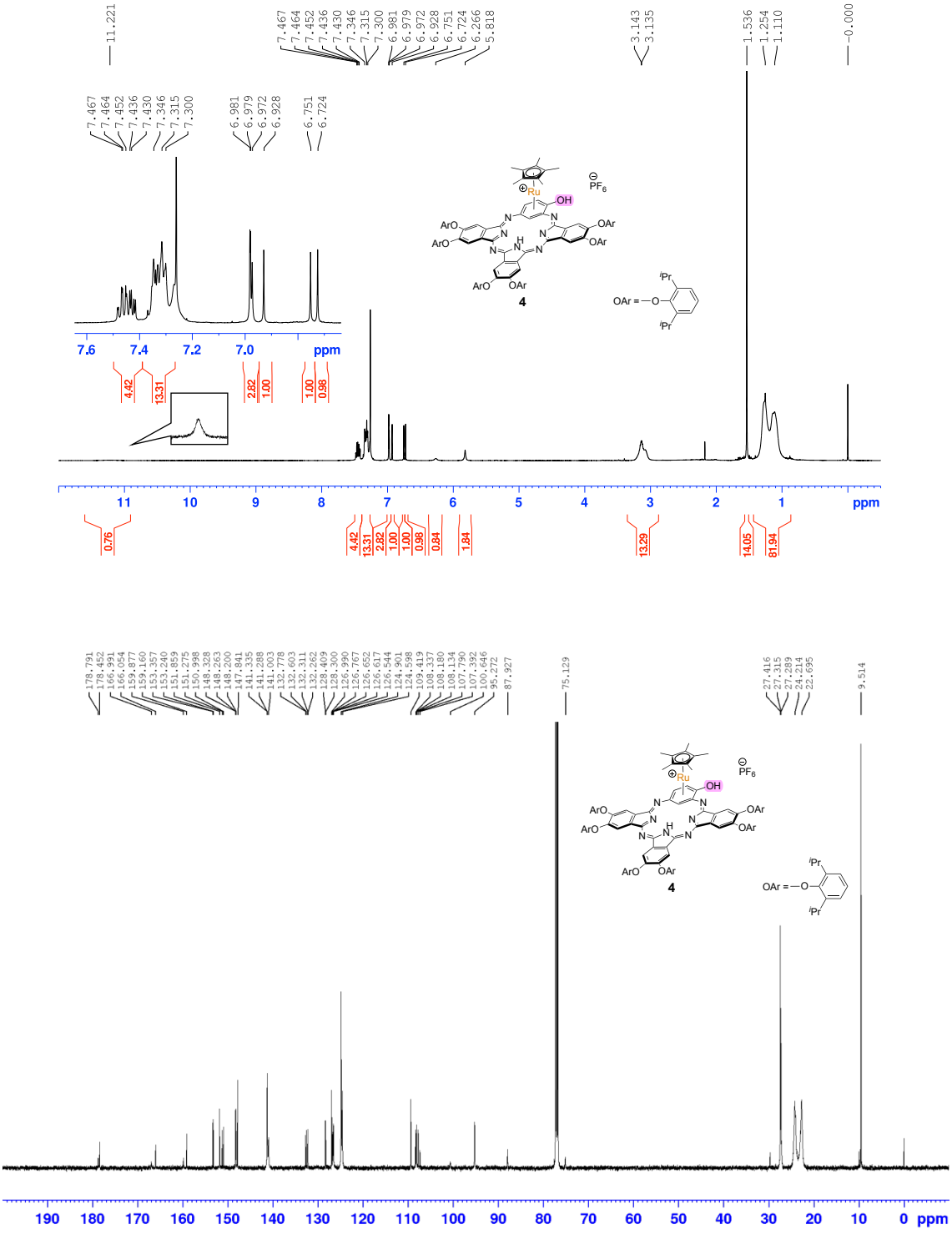

Fig. S21. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **4** in $CDCl_3$.

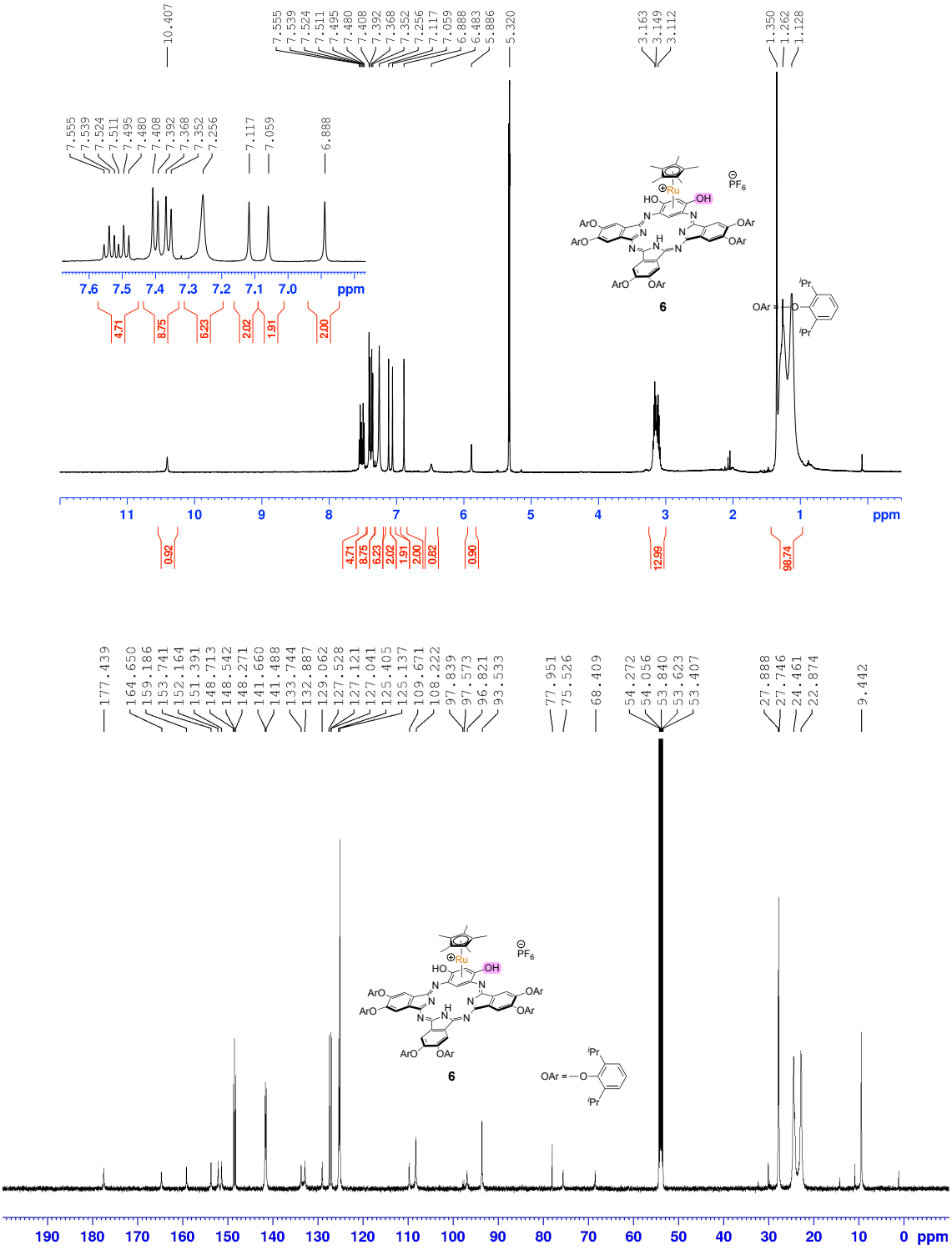

Fig. S22. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **6** in CD_2Cl_2.

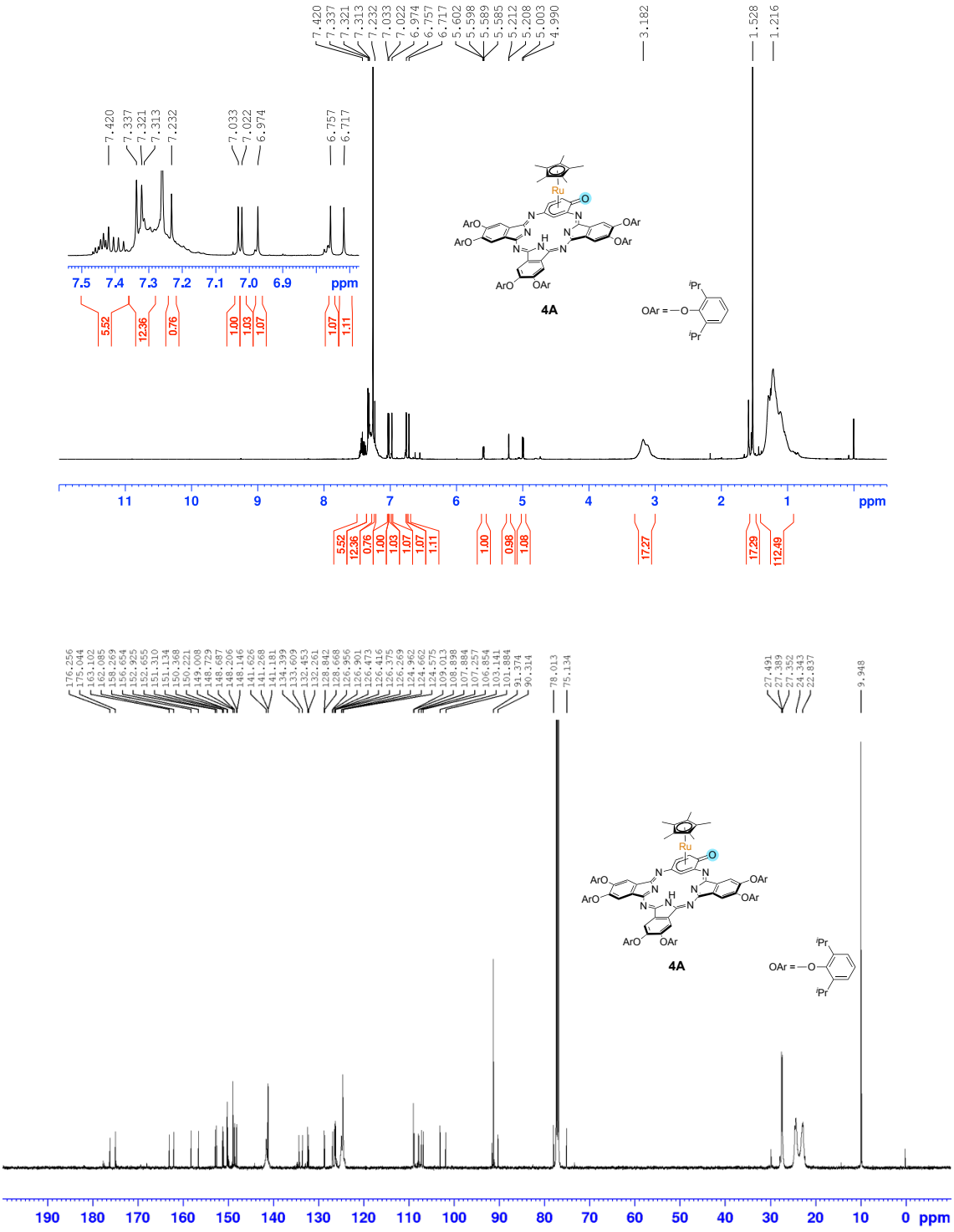

Fig. S23. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **4A** in $CDCl_3$.

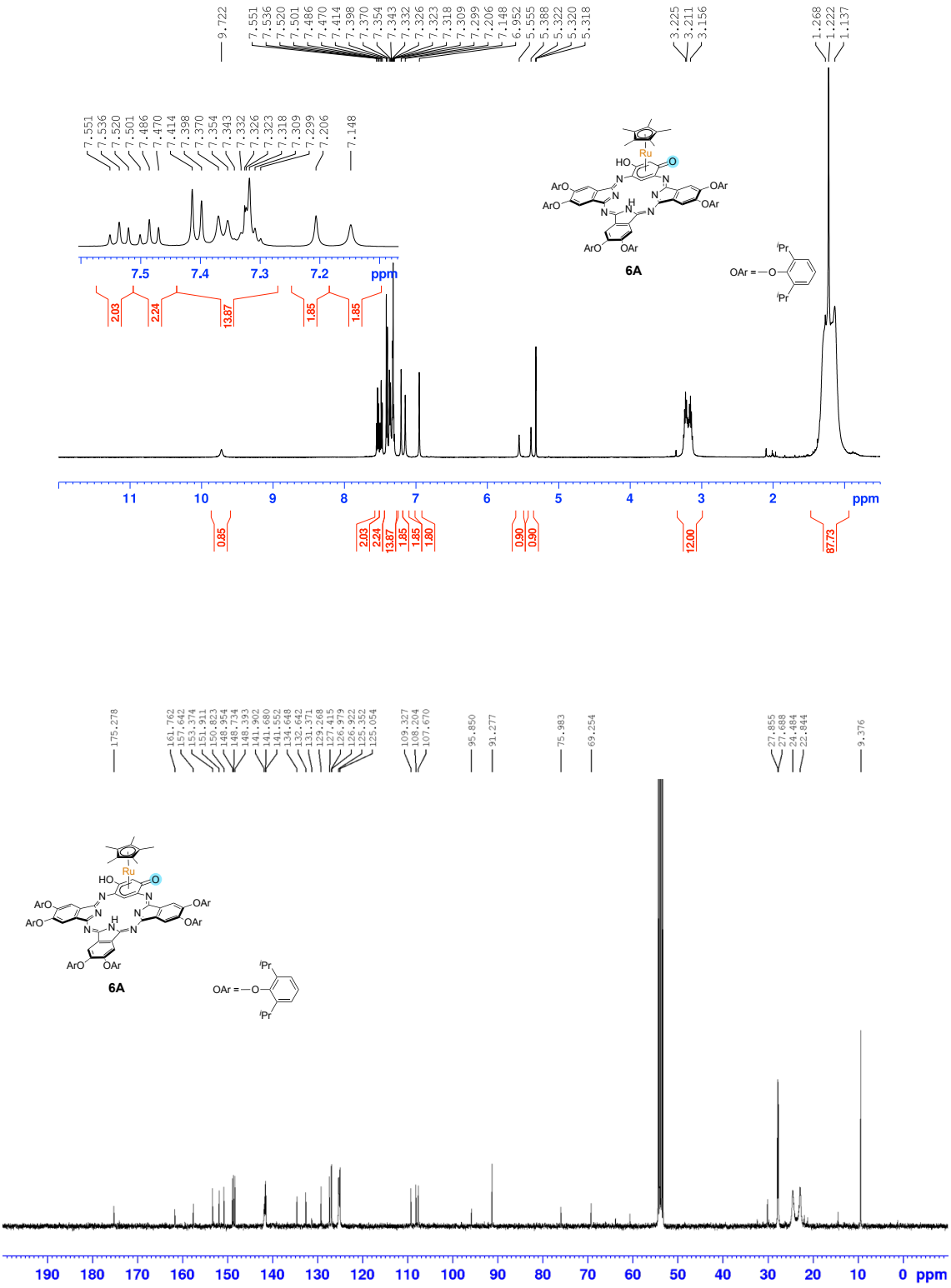

Fig. S24. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **6A** in CD_2Cl_2.

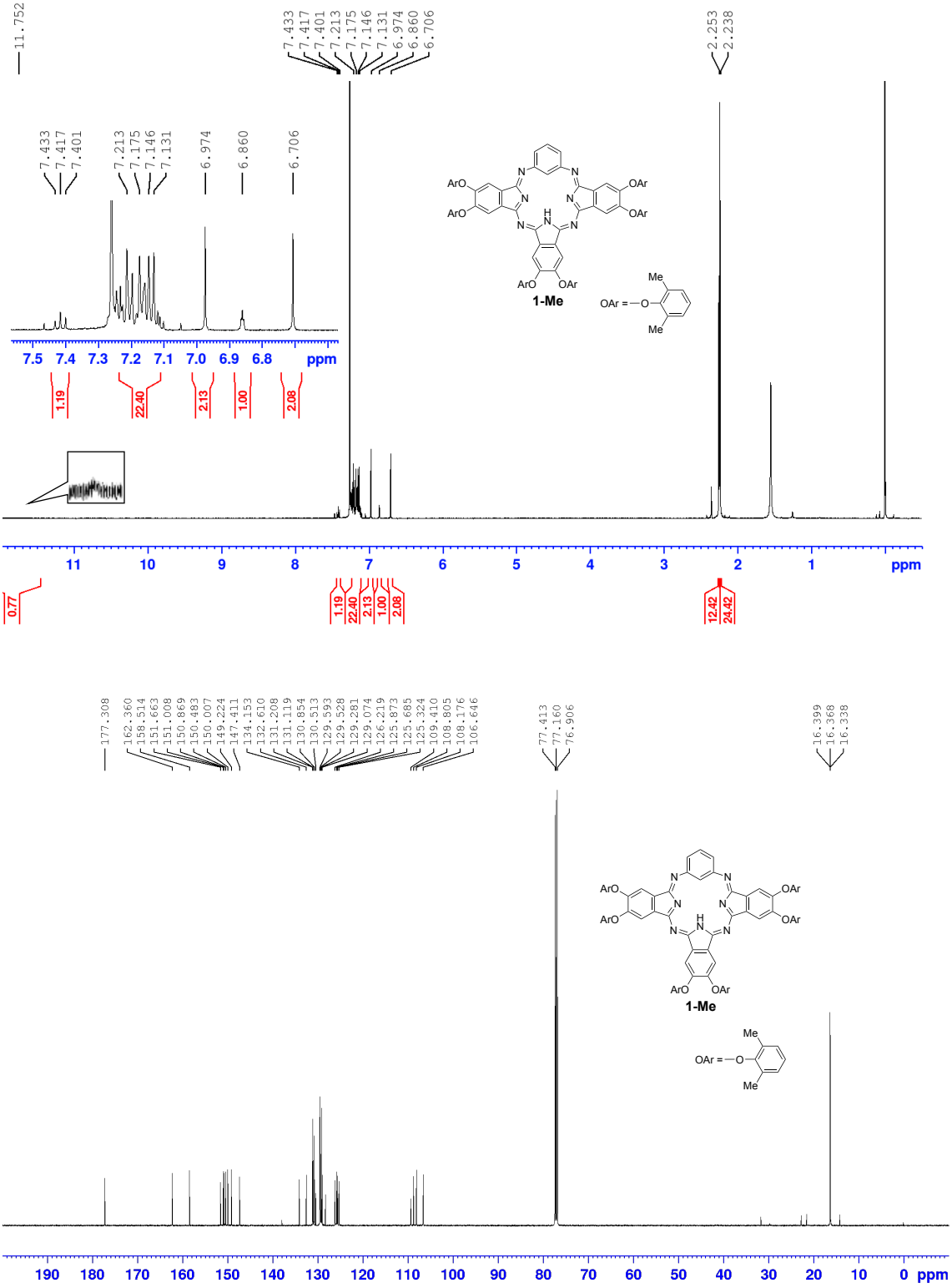

Fig. S25. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **1-Me** in $CDCl_3$.

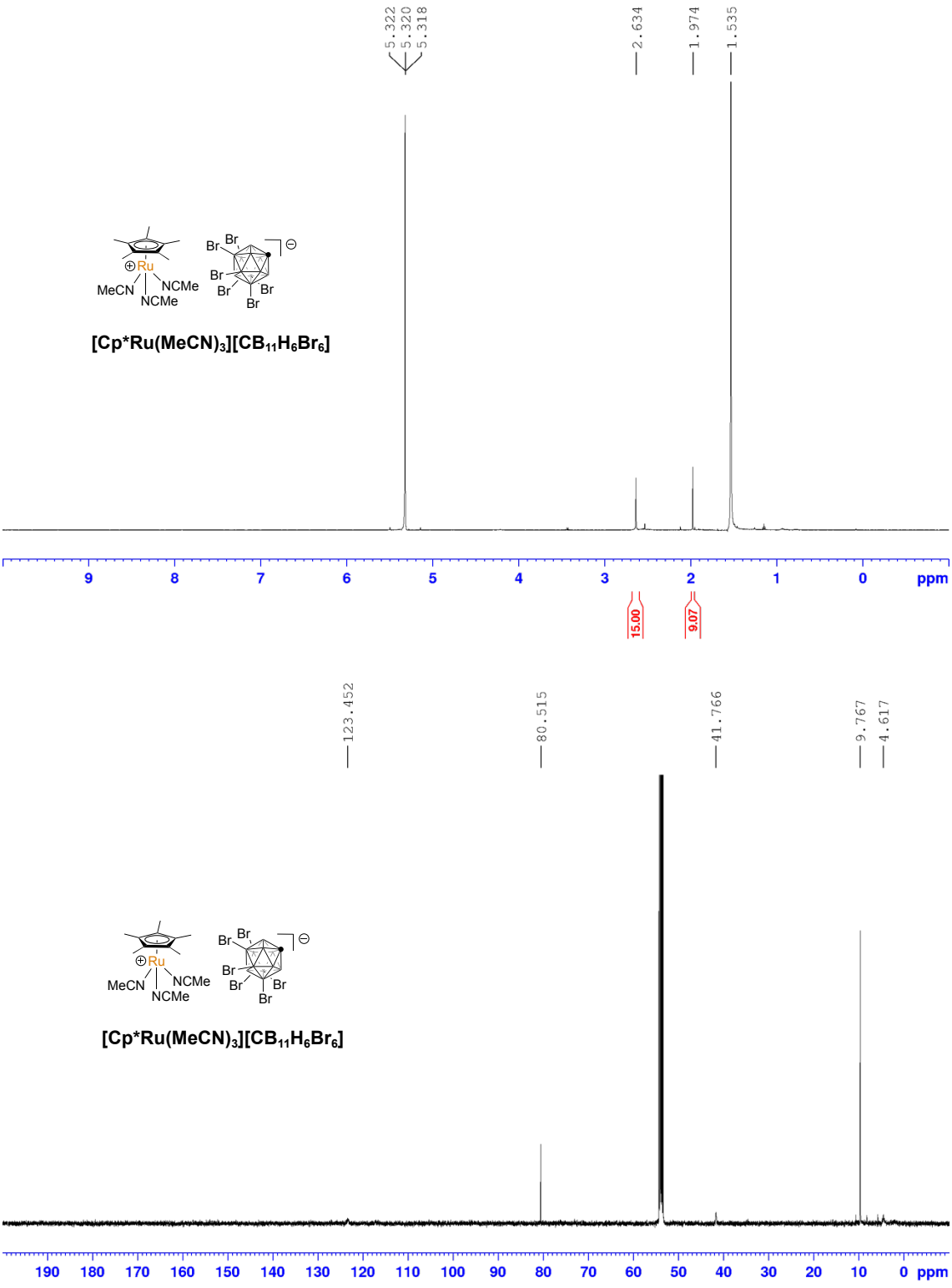

Fig. S26. ^{1}H (top) and ^{13}C (bottom) NMR spectra of $[Cp^*Ru(MeCN)_3][CB_{11}H_6Br_6]$ in CD_2Cl_2.

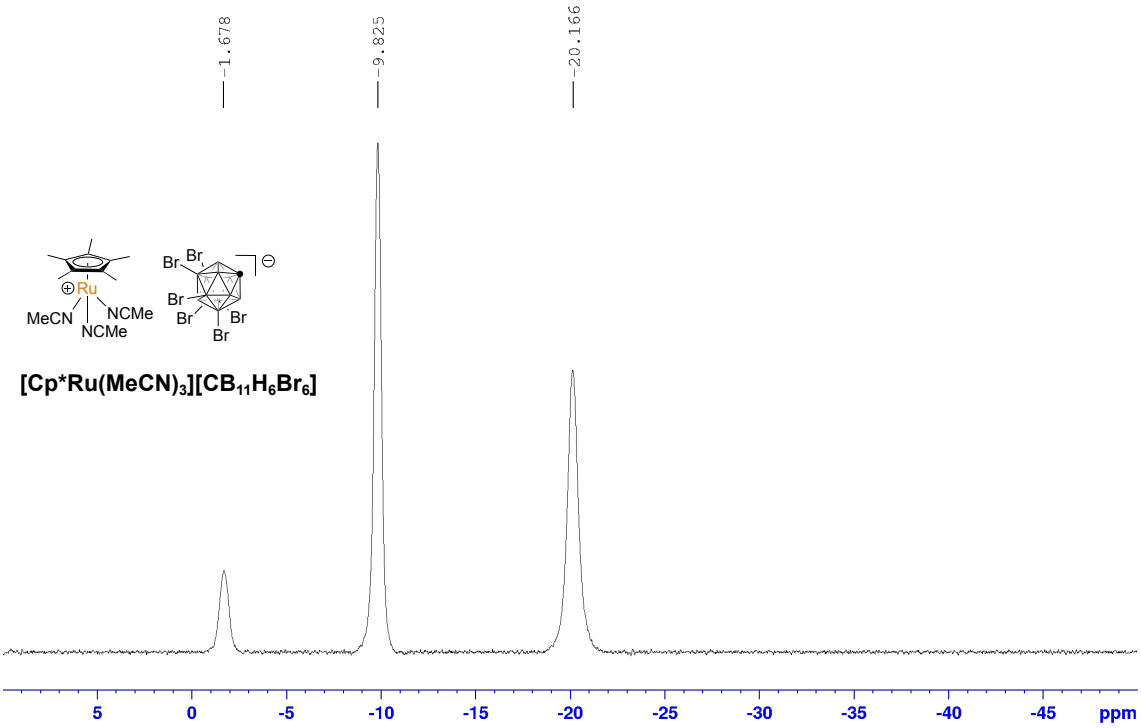

Fig. S27. ^{11}B NMR spectrum of $[Cp^*Ru(MeCN)_3][CB_{11}H_6Br_6]$ in CD_2Cl_2.

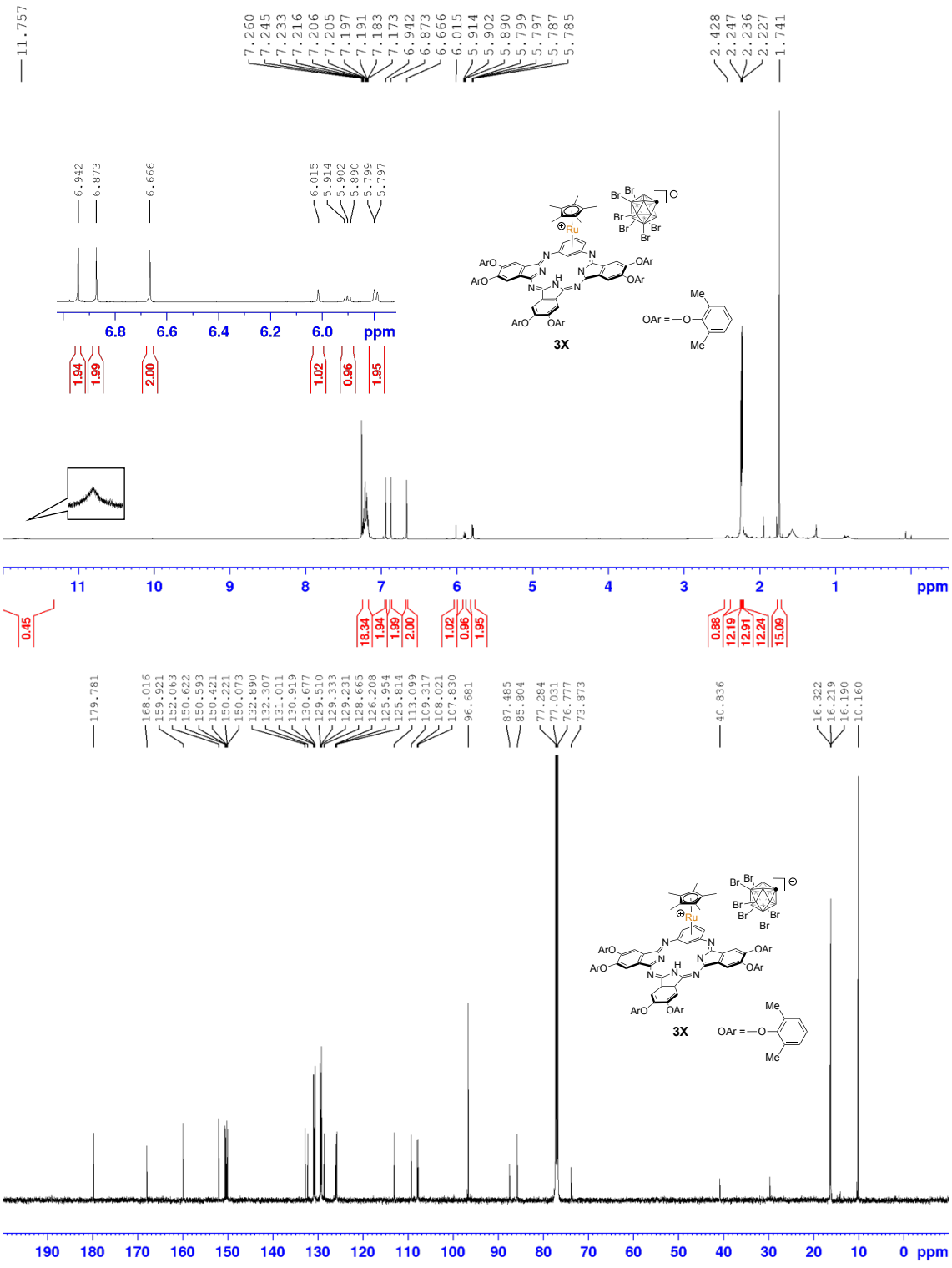

Fig. S28. ^{1}H (top) and ^{13}C (bottom) NMR spectra of **3X** in $CDCl_3$.

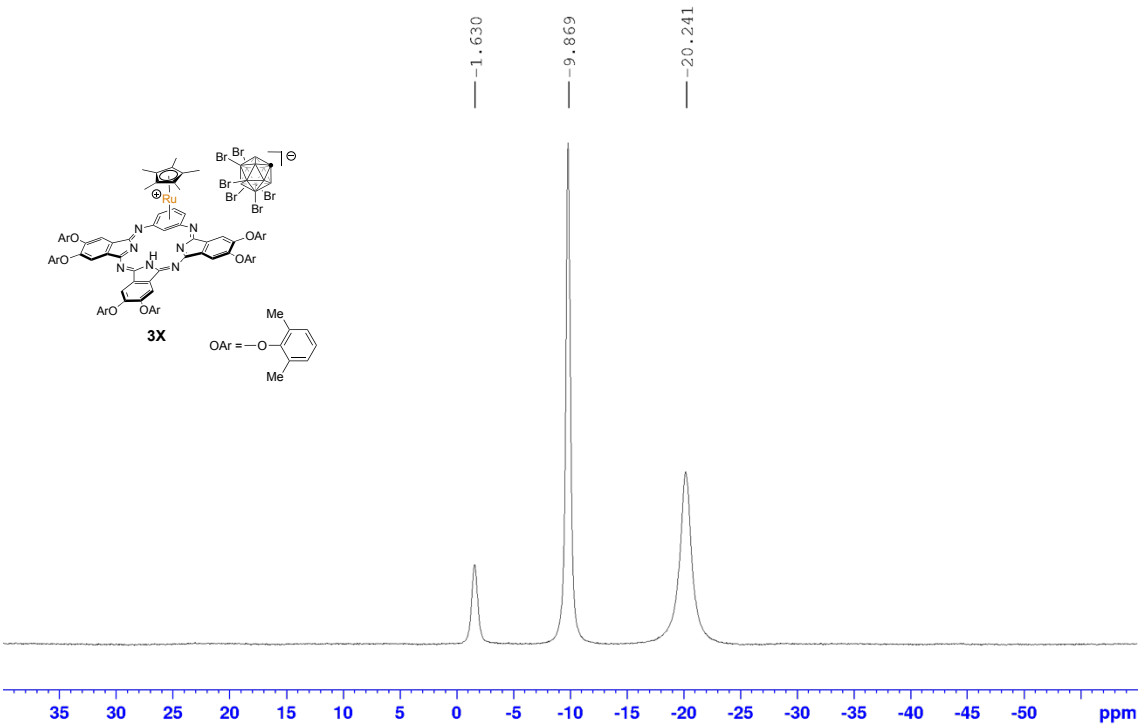

Fig. S29. ^{11}B NMR spectrum of **3X** in $CDCl_3$.