Supporting Information For:

Cyclometalated Ruthenium(II) Complexes with a Bis-Carbene CCC-Pincer Ligand

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Experimental Section

Spectroscopic Measurement. All optical ultraviolet-visible (UV/vis) absorption spectra were obtained using a TU-1810DSPC spectrometer of Beijing Purkinje General Instrument Co. Ltd. at room temperature in acetonitrile, with a conventional 1.0 cm quartz cell. Emission spectra were recorded using a F-380 spectrofluorimeter of Tianjin Gangdong Sci & Tech Development Co. Ltd., with a red-sensitive photomultiplier tube R928F.

Electrochemical Measurement. All cyclic voltammetry (CV) measurements were taken using a CHI620D potentiostat with one-compartment electrochemical cell under an atmosphere of nitrogen. All measurements were carried out in 0.1 M of Bu_4NClO_4/acetonitrile at a scan rate of 100 mV/s. The working electrode was a glassy carbon with a diameter of 0.3 mm. The electrode was polished prior to use with 0.05 μm alumina and rinsed thoroughly with water and acetone. A large area platinum wire coil was used as the counter electrode. All potentials are referenced to a Ag/AgCl electrode in saturated aqueous NaCl without regard for the liquid junction potential.

Computational Methods. DFT and TDDFT calculations are carried out using the B3LYP exchange correlation functional[1] and implemented in the *Gaussian* 03 program package.[2] The electronic structures of complexes were determined using a general basis set with the Los Alamos effective core potential LanL2DZ basis set for ruthenium, and 6-31G* for other atoms in vacuum.[3]

Synthesis of Complex 2. To 15 mL of dry acetone were added Ru(daatpy)Cl_3 (67 mg, 0.1 mmol) and AgOTf (82 mg, 0.3 mmol). The mixture was refluxed for 2 h before cooling to room temperature. After removing the white AgCl precipitate by filtering, the filtrate was concentrated to dryness. To the residue were added the carbene precursor **1** (48.8 mg, 0.1 mmol), *t*-BuOK (56 mg, 0.5 mmol), 10 mL DMF, and 10 mL *t*-BuOH. The resulting system was refluxed for 24 h. After cooling to room temperature, the solvent was removed under reduced pressure. The residue was dissolved in proper amount of methanol. After adding an excess of KPF_6, the resulting precipitate was collected by filtering and washing with water and Et_2O. The obtained solid was subjected to flash column chromatography on silica gel using acetonitrile, saturated aqueous KNO_3 and water (200/1/20) as the eluent. The desired complex **2** was

obtained as a reddish violet solid (44 mg, 43%). ^{1}HNMR (400 MHz, CD_3CN): δ 0.61 (m, 10H), 0.77 (m, 4H), 2.82 (t, *J* = 8 Hz, 4H), 3.87 (s, 6H), 6.79 (s, 2H), 6.83 (t, *J* = 6.4 Hz, 2H), 7.09 (d, *J* = 8.8 Hz, 4H), 7.14 (d, *J* = 4.8 Hz, 2H), 7.28 (t, *J* = 7.6 Hz, 1H), 7.37 (d, *J* = 8.8 Hz, 4H), 7.48 (d, *J* = 7.6 Hz, 2H), 7.52 (t, *J* = 7.8 Hz, 2H), 7.79 (s, 2H), 7.95 (s, 2H), 8.01 (d, *J* = 8.4 Hz, 2H). MALDI-MS: 833.1 for $[M - PF_6]^+$. Anal. Calcd for $C_{41}H_{42}F_6N_9PRu\cdot 2.5H_2O$: C, 54.85; H, 5.07; N, 10.62. Found: C, 54.60; H, 4.63; N, 10.62.

Synthesis of Complex 3. According the similar synthetic procedure for **2**, complex **3** was prepared from $Ru(Mebip)Cl_3$ and **1** as a reddish violet solid in a yield of 22%. ^{1}HNMR (400 MHz, CD_3CN): δ 0.52 (m, 14H), 2.66 (s, 4H), 4.38 (s, 6H), 6.08 (d, *J* = 8.4 Hz, 2H), 6.61 (d, *J* = 2.0 Hz, 2H), 6.86 (t, *J* = 7.6 Hz, 2H), 7.28 (t, *J* = 8.0 Hz, 2H), 7.50 (t, *J* = 8.4 Hz, 1H), 7.52 (d, *J* = 8.4 Hz, 2H), 7.59 (d, *J* = 7.6 Hz, 2H), 7.73 (d, *J* = 1.6 Hz, 2H), 8.03 (t, *J* = 8.0 Hz, 1H), 8.69 (d, *J* = 8.0 Hz, 2H). MALDI-MS: 762.1 for $[M - PF_6]^+$. Anal. Calcd for $C_{41}H_{42}F_6N_9PRu\cdot 3H_2O$: C, 51.25; H, 5.03; N, 13.12. Found: C, 51.64; H, 4.83; N, 13.26.

Synthesis of Complex 4. According the similar synthetic procedure for **2**, complex **4** was prepared from $Ru(ttpy)Cl_3$ and **1** as a reddish violet solid in a yield of 49%. ^{1}HNMR (400 MHz, CD_3CN): δ 0.52 (m, 14H), 2.49 (s, 3H), 2.65 (m, 4H), 6.75 (d, *J* = 2.0 Hz, 2H), 6.95 (m, 2H), 7.28 (d, *J* = 5.6 Hz, 2H), 7.36 (t, *J* = 8.0 Hz, 1H), 7.52 (m, 4H), 7.70 (m, 2H), 7.80 (d, *J* = 2.0 Hz, 2H), 8.02 (d, *J* = 8.0 Hz, 2H), 8.58 (d, *J* = 8.0 Hz, 2H), 8.93 (s, 2H). MALDI-MS: 746.1 for $[M - PF_6]^+$. Anal. Calcd for $C_{42}H_{42}F_6N_7PRu\cdot 2H_2O$: C, 54.42; H, 5.00; N, 10.58 Found: C, 54.04; H, 4.75; N, 10.33.

Synthesis of Complex 5. According the similar synthetic procedure for **2**, complex **5** was prepared from $Ru(Me_3tcbtpy)Cl_3$ and **1** as a green solid in a yield of 21%. ^{1}HNMR (400 MHz, CD_3CN): δ 0.45 (m, 14H), 2.44 (m, 4H), 3.92 (s, 6H), 4.15 (s, 3H), 6.73 (d, *J* = 2.0 Hz, 2H), 7.46 (t, *J* = 8.0 Hz, 1H), 7.49 (d, *J* = 8.0 Hz, 2H), 7.57 (m, 4H), 7.80 (d, *J* = 1.6 Hz, 2H), 9.06 (s, 2H), 9.37 (s, 2H). MALDI-MS: 830.0 for $[M - PF_6]^+$. Anal. Calcd for $C_{41}H_{42}F_6N_7O_6PRu\cdot 2H_2O$: C, 48.71; H, 4.59; N, 9.70. Found: C, 49.08; H, 4.42; N, 9.43.

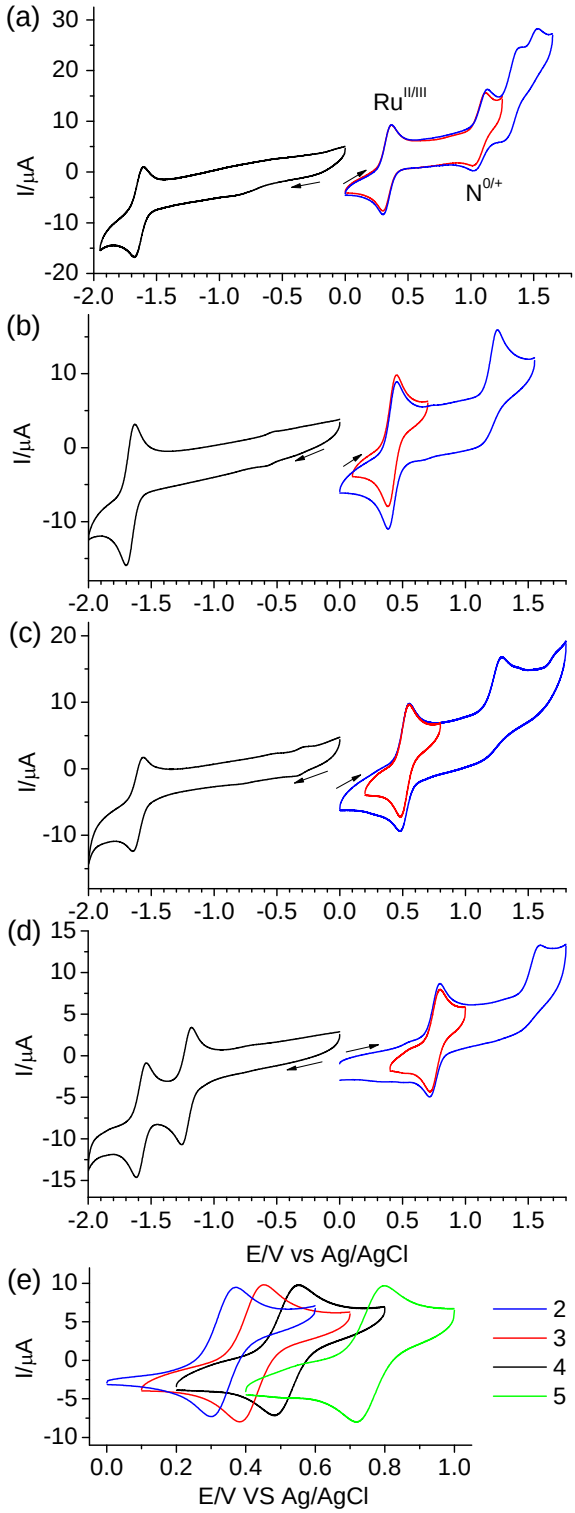


Figure S1. Cyclic voltammograms of (a-d) **2-5** in acetonitrile containing 0.1 M $^{n}Bu_4NClO_4$ as the supporting electrolyte at a scan rate of 100 mV/s. (e): A comparison of the $Ru^{II/III}$ processes of four complexes. The working electrode was a glassy carbon and the counter electrode was a platinum wire. The reference electrode was Ag/AgCl in saturated aqueous NaCl solution.

Table S1. Electrochemical data of **2-5** and related complexes.

complex	$E_{1/2}$ [a] anodic	$E_{1/2}$ [a] cathodic	ΔE[b] (eV)
2	+0.33, +1.07, +1.33, +1.52[c]	-1.64	1.97
3	+0.42, +1.26[c]	-1.67	2.09
4	+0.51, +1.28[c]	-1.61	2.12
5	+0.75, +1.59[c]	-1.22, -1.58	1.97
$[Ru(Mebip)(dpb)]^+$	+0.43, +1.49[c]	-1.56	1.92
$[Ru(tpy)(dpb)]^+$	+0.56, +1.60[c]	-1.51	2.07

[a]The potential is reported as the $E_{1/2}$ value vs Ag/AgCl. [b]The electrochemical energy gap is determined by the potential difference between the first oxidation and first reduction wave. [c]$E_{p,anodic}$, irreversible.

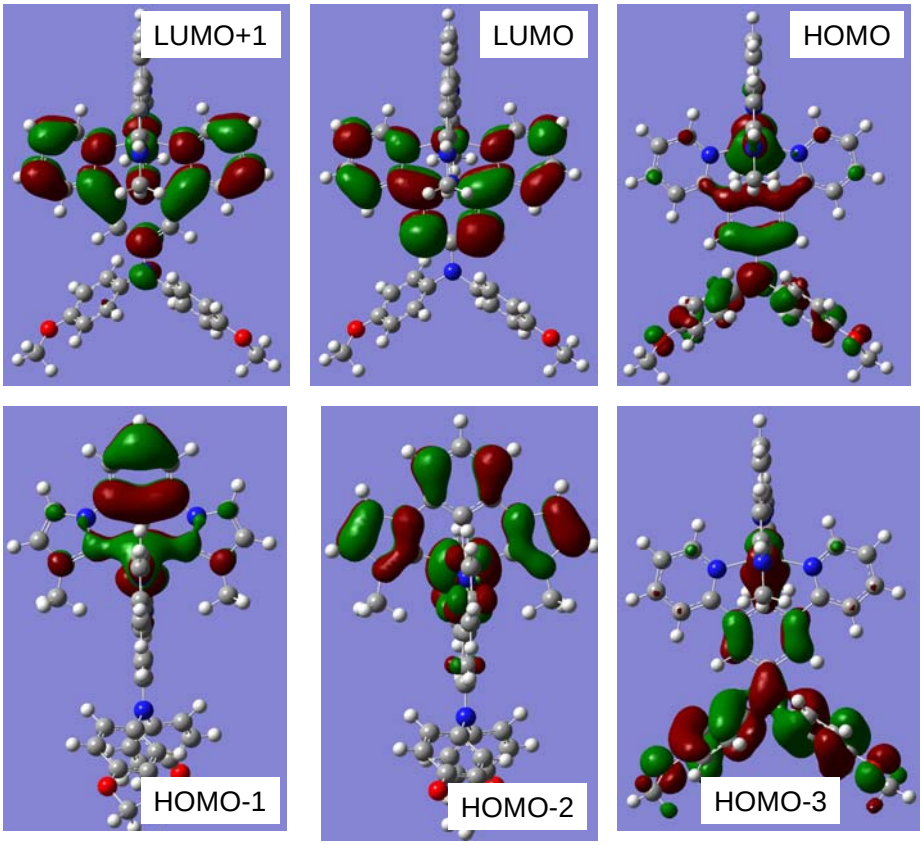


Figure S2. Isodensity plots of frontiers orbitals of complex **2**. All orbitals have been computed at an isovalue of 0.02.

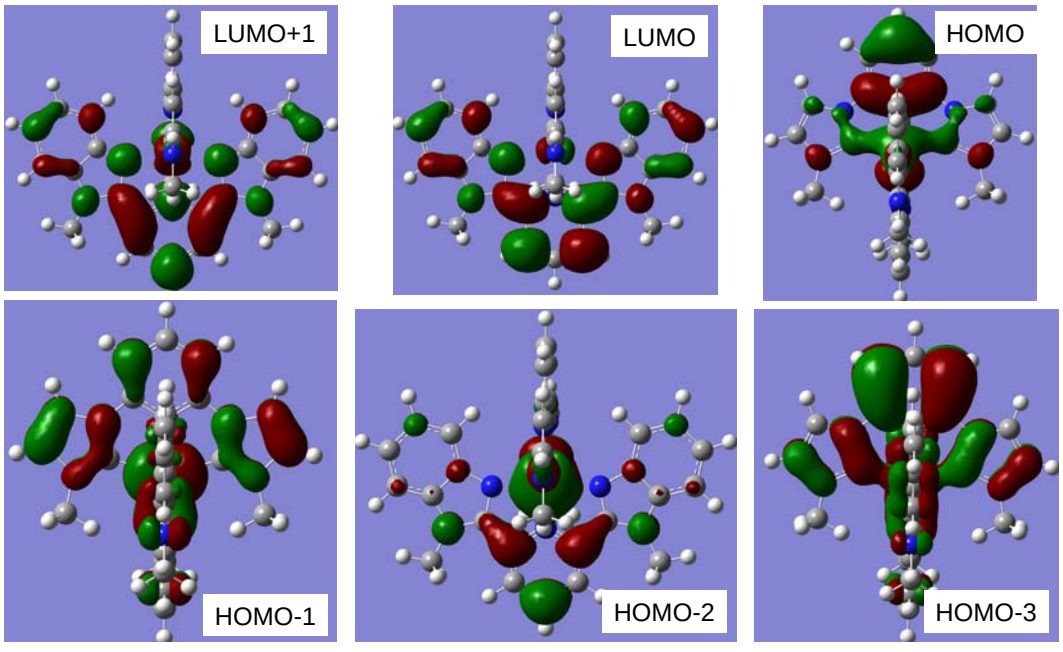


Figure S3. Isodensity plots of frontiers orbitals of complex **3**. All orbitals have been computed at an isovalue of 0.02.

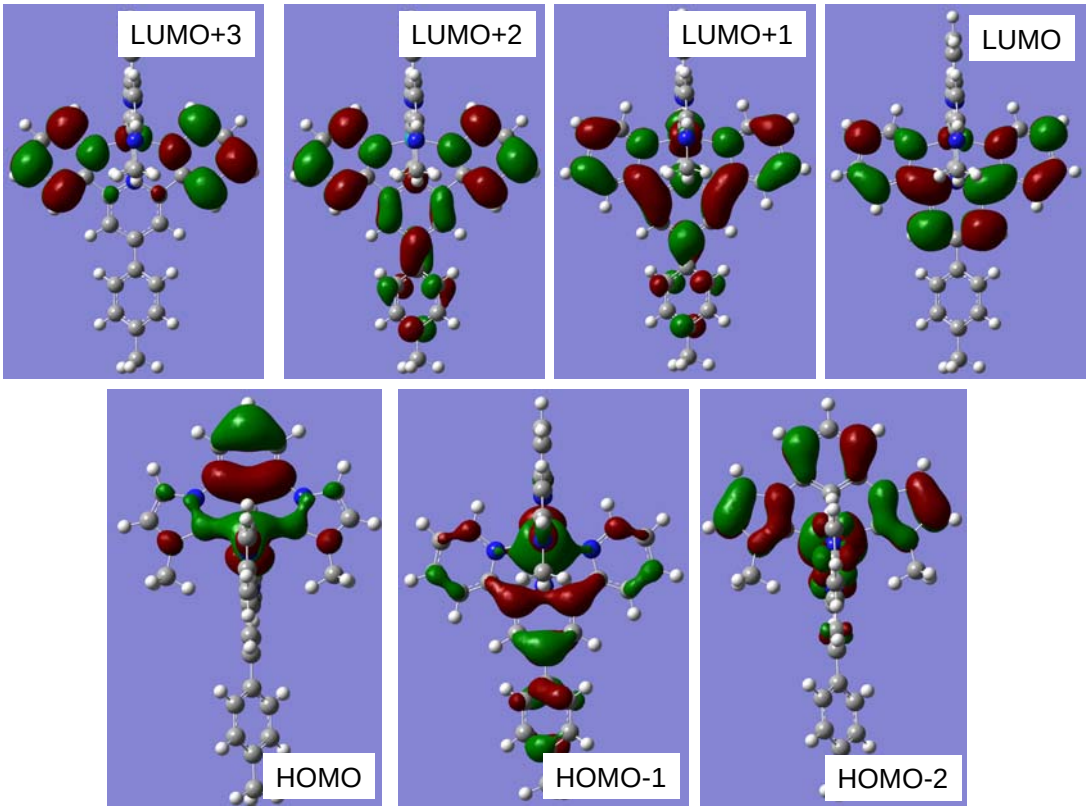


Figure S4. Isodensity plots of frontiers orbitals of complex **4**. All orbitals have been computed at an isovalue of 0.02.

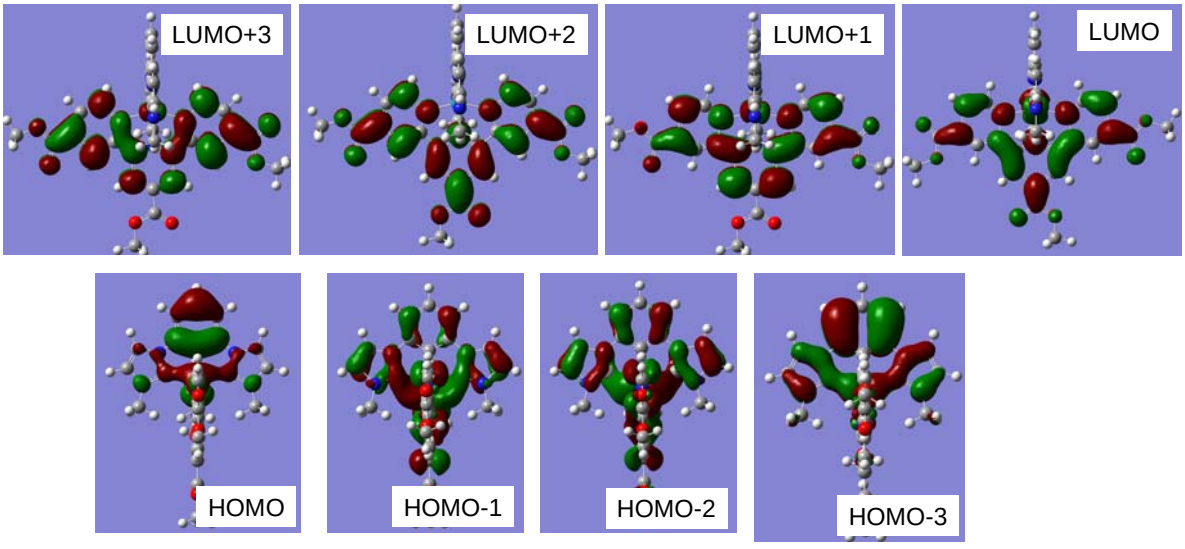


Figure S5. Isodensity plots of frontiers orbitals of complex **5**. All orbitals have been computed at an isovalue of 0.02.

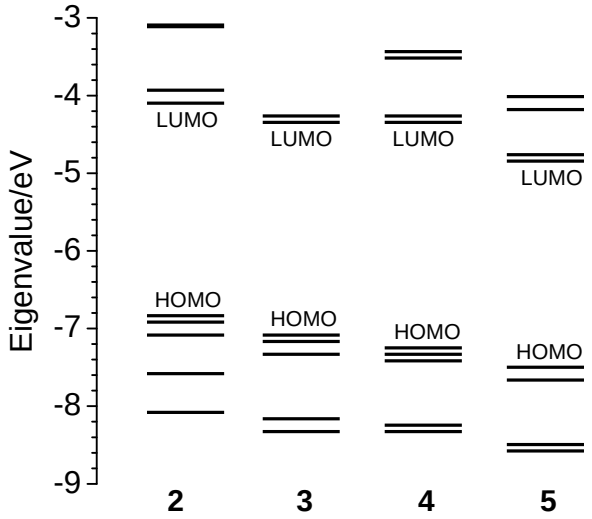


Figure S6. Frontier orbital energy level alignment of complexes **2-5**.

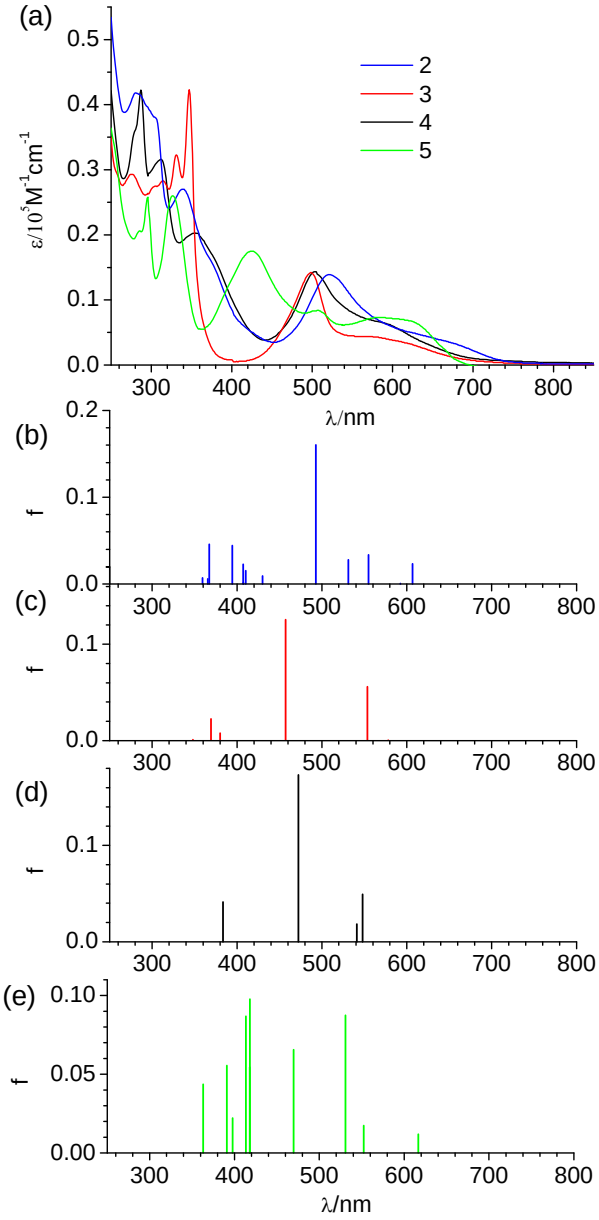


Figure S7. (a) UV/vis spectra of **2-5** in acetonitrile. (b-e) TDDFT-predicted low-energy excitations of **2-5**, respectively.

Table S2. Observed absorption data and calculated excitation energy (E), oscillator strength (f), dominant contributing transitions and the associated percent contribution and assignment of complexes **2-5**.[a]

complex	S_n	E/eV	E/nm	f	λ_{max}/nm observed	ε ($\times10^5 M^{-1}cm^{-1}$)	dominant transitions (percent contribution[b])
2	1	2.04	606.8	0.0233			HOMO → LUMO (89%)
	4	2.23	554.9	0.0337			HOMO-2 → LUMO (42%)
							HOMO → LUMO+1 (51%)
	5	2.33	351.1	0.0278			HOMO-2 → LUMO+1 (91%)
	6	2.52	492.7	0.160	520	0.139	HOMO-2 → LUMO (53%)
							HOMO → LUMO+1 (32%)
	7	2.88	430.1	0.0092			HOMO-3 → LUMO (94%)
3	4	2.14	578.1	0.0004			HOMO-2 → LUMO+1 (23%)
							HOMO-1 → LUMO (76%)
	5	2.24	553.6	0.056			HOMO-2 → LUMO (94%)
	6	2.71	457.1	0.1255	498	0.142	HOMO-2 → LUMO+1 (55%)
	7	3.26	380.1	0.0078			HOMO-3 → LUMO+1 (97%)
	9	3.36	369.4	0.0225			HOMO-3 → LUMO (93%)
4	4	2.26	548.0	0.0493			HOMO-1 → LUMO (67%)
	5	2.29	541.1	0.0184			HOMO-2 → LUMO (60%)
							HOMO-1 → LUMO+1 (36%)
	6	2.63	472.3	0.1732	502	0.143	HOMO-2 → LUMO (36%)
							HOMO-1 → LUMO+1 (42%)
	9	3.23	383.3	0.0413			HOMO-1 → LUMO+2 (94%)
	10	3.26	380.7	0.0117			HOMO-1 → LUMO+3 (92%)
5	2	2.01	616.6	0.0119			HOMO-2 → LUMO (53%)
							HOMO-1 → LUMO (35%)
	4	2.24	552	0.0174	625	0.067	HOMO-2 → LUMO (20%)
							HOMO-2 → LUMO+1 (29%)
							HOMO-1 → LUMO (26%)
							HOMO-1 → LUMO+1 (20%)
	5	2.33	530.8	0.0874	577	0.073	HOMO-2 → LUMO+1 (34%)
							HOMO-1 → LUMO+1 (56%)
	6	2.64	469.6	0.0656	508	0.084	HOMO-2 → LUMO+1 (27%)
							HOMO-1 → LUMO (17%)
							HOMO-1 → LUMO+1 (14%)
	9	2.96	418.1	0.0976	424	0.175	HOMO-1 → LUMO+2 (65%)
	10	2.97	417.8	0.0545			HOMO-2 → LUMO+2 (56%)
	11	3.00	413.4	0.0868			HOMO-2 → LUMO+2 (20%)
							HOMO-2 → LUMO+3 (38%)
							HOMO-1 → LUMO+3 (32%)
	13	3.12	397.6	0.0222			HOMO-3 → LUMO (91%)
	14	3.17	390.9	0.0555			HOMO-2 → LUMO+3 (44%)
							HOMO-1 → LUMO+3 (31%)
	16	3.42	362.9	0.0436			HOMO-3 → LUMO+1 (86%)

[a]Computed at the TDDFT/B3LYP/LANL2DZ/6-31G*/vacuum level of theory. [b]The actual percent contribution = $(\text{configuration coefficient})^2 \times 2 \times 100\%$.

Cartesian coordinates of DFT-optimized structure of complex **2**:

Charge = 1; multiplicity=1

Ru	-0.00282600	-0.06759100	0.02095000
C	-4.24250300	0.84992600	-0.73185200
C	-1.17566800	2.67773400	-0.27911700
C	1.17708800	2.68978300	0.11536000
C	1.20946300	4.08440900	0.06445800
C	0.00387300	4.76234600	-0.16474700
C	-1.20383100	4.07208300	-0.33949300
C	4.23763700	0.89480000	0.71771100
H	2.12999800	4.64658000	0.19620100
H	0.00555900	5.84708800	-0.20779000
H	-2.12274000	4.62464900	-0.51565900
H	0.87748400	0.50875900	-5.13984900
C	0.74539900	-0.21474600	-4.34228800
H	0.97312500	-1.96955300	-5.58823600
C	0.79773500	-1.58778000	-4.58736000
C	0.51939200	0.22674400	-3.04380900
H	0.47204500	1.28229400	-2.80148900
C	0.62122100	-2.46348200	-3.52135100
N	0.34579300	-0.61132600	-2.00288600
H	0.65968200	-3.53468400	-3.68497400
C	0.39502900	-1.96527400	-2.23392900
C	0.19938800	-2.83118400	-1.05095800
H	0.35189900	-4.78420200	-1.95143100
C	0.20499300	-4.22249600	-1.03870300
N	-0.35072200	-0.47982100	2.07716700
H	-0.47975900	1.46108400	2.75154000
C	-0.19689400	-2.75637300	1.27118400
C	0.01283800	-4.91722300	0.18042900
C	-0.52570900	0.42341300	3.06170900
C	-0.39650700	-1.81610700	2.39536500
C	-0.18883500	-4.14543900	1.35073100
C	-0.75036900	0.06649100	4.38618100
C	-0.62188300	-2.23050400	3.71236200
H	-0.88359600	0.83980700	5.13534100
H	-0.33014200	-4.64766200	2.29835200
C	-0.80014000	-1.28797200	4.71951500
H	-0.65884700	-3.28899500	3.94463500
H	-0.97500800	-1.60451700	5.74298500
N	-0.00186600	-2.12712600	0.08817200
N	-2.28416200	1.79715300	-0.43271200
N	-3.26332300	-0.12064400	-0.53436300
N	2.28323300	1.82080000	0.33708200
N	3.25674100	-0.08571900	0.59031300
C	3.62258500	2.09451900	0.55833000
C	2.03143900	0.46178800	0.35212100
C	-2.03560000	0.44029200	-0.34381200
C	-3.62390100	2.05666000	-0.66822800
H	4.02006300	3.09664100	0.58529100
H	5.27220900	0.65365100	0.90869300
H	-4.01913900	3.05473600	-0.77126300
H	-5.27847400	0.59763900	-0.89943300
C	-3.53844200	-1.54988600	-0.52354500
H	-4.03501000	-1.84595700	-1.45289100
H	-2.59225200	-2.08120700	-0.43522200
H	-4.18219600	-1.81059800	0.32308100
C	3.52562200	-1.51208900	0.69667400
H	2.58098200	-2.04603300	0.60760600

H	4.20256500	-1.83473900	-0.10116700
H	3.98164700	-1.74088100	1.66513200
C	-0.00044500	1.96012000	-0.05288500
C	-0.50604900	-7.01393100	1.35799900
C	0.30823000	-7.88569500	2.08404700
C	-1.85393900	-6.87395300	1.72723700
C	-0.20067800	-8.61130000	3.16297700
H	1.34852000	-8.00814400	1.79774200
C	-2.36439200	-7.57763000	2.80900500
H	-2.50049400	-6.21205400	1.15786800
C	-1.54302100	-8.45669900	3.53610400
H	0.45451300	-9.28496100	3.70264600
H	-3.40484200	-7.48062900	3.10210800
C	0.56626300	-7.08155700	-0.85120800
C	-0.22675300	-8.02464100	-1.50836700
C	1.91011200	-6.93699400	-1.23346500
C	0.29886300	-8.81584300	-2.53179500
H	-1.26336600	-8.15143100	-1.21086300
C	2.43666900	-7.70632300	-2.26138600
H	2.54121600	-6.21940400	-0.71668400
C	1.63654500	-8.65658000	-2.91942200
H	-0.34023300	-9.54357600	-3.01788800
H	3.47421700	-7.60588700	-2.56354900
N	0.02210000	-6.30263900	0.22661800
O	2.24986500	-9.36218700	-3.90343700
O	-2.14175800	-9.10250800	4.56885100
C	1.50478700	-10.35782900	-4.59442200
H	0.64809400	-9.92174800	-5.12397900
H	2.19329800	-10.79472800	-5.31882800
H	1.15140700	-11.13972000	-3.91049900
C	-1.37548200	-10.02805200	5.33058200
H	-0.53143800	-9.53483400	5.82948100
H	-2.05600700	-10.42871400	6.08293400
H	-1.00079000	-10.84798300	4.70501800

Cartesian coordinates of DFT-optimized structure of complex **3**:

Charge = 1; multiplicity=1

Ru	0.00452000	-0.11239100	0.02131400
C	-4.29540100	0.81891200	0.03763800
C	-1.19665000	2.64044300	-0.06207600
C	1.18775400	2.64724400	-0.08813000
C	1.21368300	4.04223500	-0.13574100
C	-0.01111000	4.72382200	-0.14555000
C	-1.23149700	4.03525500	-0.10908100
C	4.29839900	0.84374000	-0.05769900
H	2.14516000	4.60078500	-0.16447800
H	-0.01460700	5.80872500	-0.18196100
H	-2.16650800	4.58856000	-0.11748700
C	0.00292500	-2.89883300	-1.07429100
H	0.00709500	-4.87960100	-1.95838400
C	0.01283300	-4.29860700	-1.04626300
C	0.03082900	-2.81745600	1.30743000
C	0.03144900	-4.95098000	0.18759600
C	0.04026700	-4.21590300	1.37419300
H	0.05496100	-4.73361700	2.32349400
N	0.01314700	-2.18501100	0.09367300
N	-2.31573000	1.76497000	-0.01890800
N	-3.29639200	-0.15192700	0.06180100
N	2.31249200	1.77820700	-0.06972400
N	3.30587100	-0.13297500	-0.01265200
C	3.67086400	2.04650200	-0.09361400
C	2.06155900	0.42252600	-0.01899300
C	-2.05584800	0.41081000	0.02713300
C	-3.67585000	2.02530300	-0.01291900
H	4.07072200	3.04715200	-0.13308300
H	5.34908700	0.59700400	-0.06008300
H	-4.08226800	3.02361200	-0.04363200
H	-5.34441900	0.56605200	0.05877700
C	-3.56927600	-1.58015200	0.11333000
H	-4.12696100	-1.89492700	-0.77475900
H	-2.61935100	-2.11068300	0.14973700
H	-4.15493400	-1.82321300	1.00568500
C	3.58876200	-1.55941800	0.03431200
H	2.64266200	-2.09705300	0.06407500
H	4.15215100	-1.86560600	-0.85306900
H	4.17269300	-1.80282000	0.92781200
C	-0.00210000	1.91962000	-0.05053700
H	0.03934300	-6.03532500	0.22461200
C	0.03780000	-1.84661200	2.39455800
C	0.03758500	0.14465100	3.29970200
C	0.05182300	-0.79545300	4.35452200
C	0.03387200	1.52227600	3.56180800
C	0.06255900	-0.39451200	5.69525800
C	0.04447100	1.91894600	4.89130300
H	0.02315400	2.23516700	2.74444000
C	0.05854100	0.97361900	5.94111700
H	0.07355000	-1.10557400	6.51503300
H	0.04197000	2.97694700	5.13462800
H	0.06652600	1.32398500	6.96878400
C	-0.01589500	-2.00512500	-2.22548900
C	-0.03229400	-0.08039800	-3.26480700
C	-0.04199000	-1.09050400	-4.25287500
C	-0.03831900	1.27587800	-3.62066800
C	-0.05760300	-0.78196400	-5.61804900

C	-0.05372400	1.58091800	-4.97403800
H	-0.03074800	2.04337100	-2.85475200
C	-0.06320800	0.56611700	-5.95677200
H	-0.06429500	-1.54728000	-6.38748300
H	-0.05845400	2.61989800	-5.28881300
H	-0.07489300	0.84551200	-7.00593700
N	0.02900500	-0.53500800	2.09877100
N	0.05176600	-2.05077000	3.75895800
N	-0.01670100	-0.67633700	-2.02014500
N	-0.03224400	-2.30203900	-3.57277100
C	0.06297900	-3.31600300	4.47918000
H	-0.83043900	-3.90587700	4.25252000
H	0.95909600	-3.89711200	4.24070000
H	0.06900500	-3.10500700	5.54826000
C	-0.04254800	-3.61357800	-4.20465600
H	0.86211900	-4.17767600	-3.95749100
H	-0.92672500	-4.18583100	-3.90783900
H	-0.07378600	-3.47620200	-5.28524500

Cartesian coordinates of DFT-optimized structure of complex **4**:

Charge = 1; multiplicity=1

Ru	0.00510100	-0.02744700	0.01944200
C	-4.30015700	0.89971500	0.02435400
C	-1.20077300	2.72425600	-0.07785000
C	1.18329600	2.73523800	-0.09753100
C	1.20752000	4.12988400	-0.15170400
C	-0.01891000	4.80836000	-0.16808300
C	-1.23861600	4.11861200	-0.13167600
C	4.30045600	0.93915300	-0.04308000
H	2.13743500	4.69106300	-0.18024500
H	-0.02425800	5.89307100	-0.20961900
H	-2.17394900	4.67130100	-0.14492600
H	-0.05170700	0.56256200	-5.21362600
C	-0.04081800	-0.16091500	-4.40533100
H	-0.04977200	-1.91511700	-5.67282000
C	-0.03959200	-1.53427800	-4.65646100
C	-0.02766800	0.28049500	-3.08763100
H	-0.02824100	1.33582700	-2.84031600
C	-0.02494400	-2.41072500	-3.57699900
N	-0.01382200	-0.55867100	-2.03334900
H	-0.02343700	-3.48182600	-3.74548700
C	-0.01227700	-1.91194700	-2.26950500
C	0.00457700	-2.77380800	-1.07151600
H	-0.03685100	-4.73363500	-1.97090000
C	0.00154300	-4.16786200	-1.04718000
N	0.02881000	-0.42124700	2.10699400
H	0.03232700	1.52295600	2.78427100
C	0.02293700	-2.69652300	1.29530700
C	0.01344900	-4.85664900	0.18058900
C	0.03888500	0.48671300	3.10239500
C	0.03625700	-1.75601800	2.43306500
C	0.02604400	-4.08980300	1.36133000
C	0.05668200	0.13480400	4.44691800
C	0.05417200	-2.16568300	3.77093000
H	0.06412100	0.91063200	5.20511600
H	0.06252300	-4.59482500	2.31977100
C	0.06469300	-1.21862700	4.78907300
H	0.06041800	-3.22302900	4.01134700
H	0.07896000	-1.53072400	5.82857800
N	0.01341000	-2.07120300	0.09029000
N	-2.31988300	1.84529000	-0.03241100
N	-3.30217000	-0.07133900	0.05454800
N	2.31099500	1.86658900	-0.07061800
N	3.31196200	-0.04110200	-0.00032100
C	3.66843000	2.13965400	-0.08744400
C	2.06551000	0.50895300	-0.01596700
C	-2.06117000	0.49005800	0.02011300
C	-3.67985900	2.10590300	-0.03021000
H	4.06501400	3.14160100	-0.12846600
H	5.35212100	0.69650900	-0.03812300
H	-4.08607600	3.10418100	-0.06594200
H	-5.34936600	0.64742700	0.04451000
C	-3.57731500	-1.50020500	0.11102900
H	-4.13600600	-1.81605600	-0.77574000
H	-2.62923700	-2.03355300	0.14814400
H	-4.16240000	-1.73861200	1.00477200
C	3.60119100	-1.46715700	0.05743400
H	2.65839300	-2.01093100	0.06977200

H	4.18380000	-1.77200200	-0.81758100
H	4.16786900	-1.70420800	0.96343500
C	0.00986500	-6.33629200	0.22519800
C	-0.68905100	-7.03007600	1.22915700
C	0.70308700	-7.09140700	-0.73482300
C	-0.69458500	-8.42075900	1.26497000
H	-1.26024200	-6.47783000	1.97067300
C	0.69613500	-8.48383100	-0.69098400
H	1.28329900	-6.58837500	-1.50381600
C	-0.00399500	-9.17670100	0.30528900
H	-1.25219200	-8.93069100	2.04687300
H	1.25241300	-9.04265400	-1.43924100
C	-0.03184000	-10.68548800	0.34085600
H	0.15332300	-11.06546800	1.35184100
H	-1.01130500	-11.06899400	0.02718300
H	0.72048300	-11.11653300	-0.32636100
C	-0.00519000	2.00622100	-0.06010200

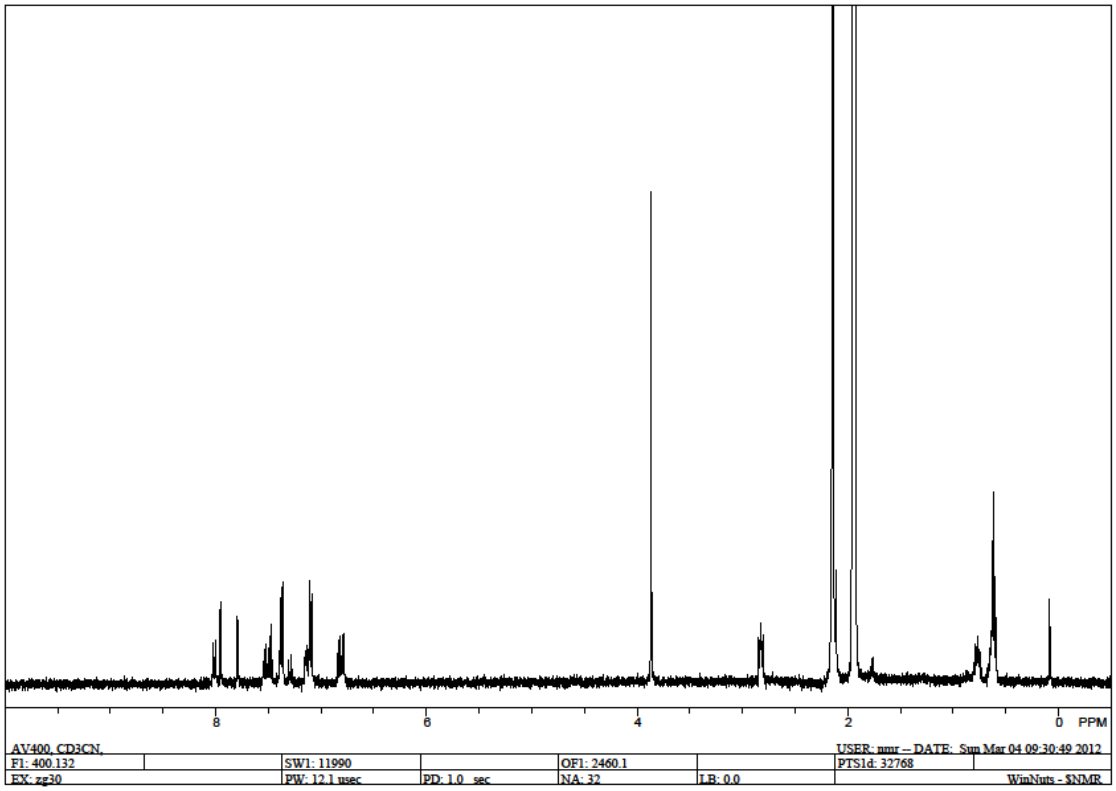
Cartesian coordinates of DFT-optimized structure of complex 5:

Charge = 1; multiplicity=1

Ru	0.00376300	-0.04661300	0.01385500
C	-4.29782200	0.89176700	0.04905900
C	-1.19774200	2.71368500	-0.06935000
C	1.18494700	2.72131700	-0.09743100
C	1.21134500	4.11599800	-0.14755800
C	-0.01386900	4.79617200	-0.15782600
C	-1.23413800	4.10816400	-0.11896800
C	4.29849700	0.91924600	-0.05453300
H	2.14208000	4.67546500	-0.17692700
H	-0.01779300	5.88092800	-0.19570100
H	-2.16881500	4.66175600	-0.12649000
H	-0.05623100	0.58174000	-5.21650800
C	-0.04556300	-0.13872200	-4.40767700
C	-0.04299400	-1.51404000	-4.66855500
C	-0.03384000	0.29214200	-3.08774500
H	-0.03545800	1.34609100	-2.83536100
C	-0.02928900	-2.39654600	-3.59036300
N	-0.01951500	-0.55350200	-2.03744800
H	-0.02747300	-3.46128500	-3.79328700
C	-0.01752500	-1.90672200	-2.28392700
C	-0.00145600	-2.77573000	-1.09443600
H	-0.00794700	-4.74586300	-1.99765200
C	0.00168700	-4.17063900	-1.08025600
N	0.03036300	-0.43464300	2.09606000
H	0.03504700	1.50900300	2.78204600
C	0.02597200	-2.70705800	1.28321800
C	0.01726600	-4.83650000	0.15271100
C	0.03978500	0.47155000	3.09534700
C	0.03650200	-1.77004200	2.42053300
C	0.02952900	-4.09838800	1.34412800
C	0.05409300	0.11487800	4.43567100
C	0.05084300	-2.18797800	3.75385100
H	0.06082600	0.86860500	5.21483300
H	0.04143700	-4.63930200	2.28339300
C	0.05934100	-1.24223900	4.77748600
H	0.05499100	-3.24281900	3.99868300
N	0.01070700	-2.08005700	0.07477700
N	-2.31833000	1.83691900	-0.02080900
N	-3.30023500	-0.07980600	0.06933500
N	2.31191900	1.85173000	-0.07605500
N	3.30793300	-0.05880100	-0.01274600
C	3.66981900	2.12169900	-0.09443800
C	2.06493600	0.49635500	-0.02460500
C	-2.06152500	0.48323800	0.02664700
C	-3.67799500	2.09816200	-0.00742700
H	4.06878100	3.12276600	-0.13265500
H	5.34939500	0.67340000	-0.05169100
H	-4.08410300	3.09664800	-0.03676200
H	-5.34674400	0.63919700	0.07732400
C	-3.57810000	-1.50893800	0.12665700
H	-4.14384200	-1.82177900	-0.75644500
H	-2.63169800	-2.04545200	0.15677200
H	-4.15702900	-1.74580400	1.02449800
C	3.59674800	-1.48592300	0.04056700
H	2.65462400	-2.03057600	0.05214100
H	4.17825000	-1.78743200	-0.83605800
H	4.16415300	-1.72470600	0.94538300

C	-0.00378500	1.99422900	-0.05838400
C	-0.05361800	-2.09537600	-6.04960000
O	-0.05273800	-3.28969000	-6.26764800
O	-0.06343800	-1.14540700	-6.99591100
C	0.07334400	-1.61478800	6.22911900
O	0.08122200	-0.79684100	7.12442000
O	0.07554400	-2.94575700	6.40893400
C	0.02121600	-6.32826800	0.26322700
O	0.03402700	-6.91809400	1.32466700
O	0.00889800	-6.92533800	-0.93989100
C	-0.07319200	-1.62143000	-8.35864100
H	-0.07964600	-0.72506800	-8.97752800
H	0.81763700	-2.22287900	-8.55367200
H	-0.96472600	-2.22614800	-8.53983400
C	0.01139100	-8.36850900	-0.92062100
H	0.00092400	-8.67127000	-1.96702300
H	0.90829800	-8.73747100	-0.41784700
H	-0.87368400	-8.74025000	-0.39925200
C	0.08791500	-3.38774700	7.78314200
H	-0.79867300	-3.02017600	8.30483900
H	0.08788900	-4.47610700	7.73666000
H	0.98331000	-3.01951300	8.28907700

^{1}H NMR of **2**: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LB: 0.0
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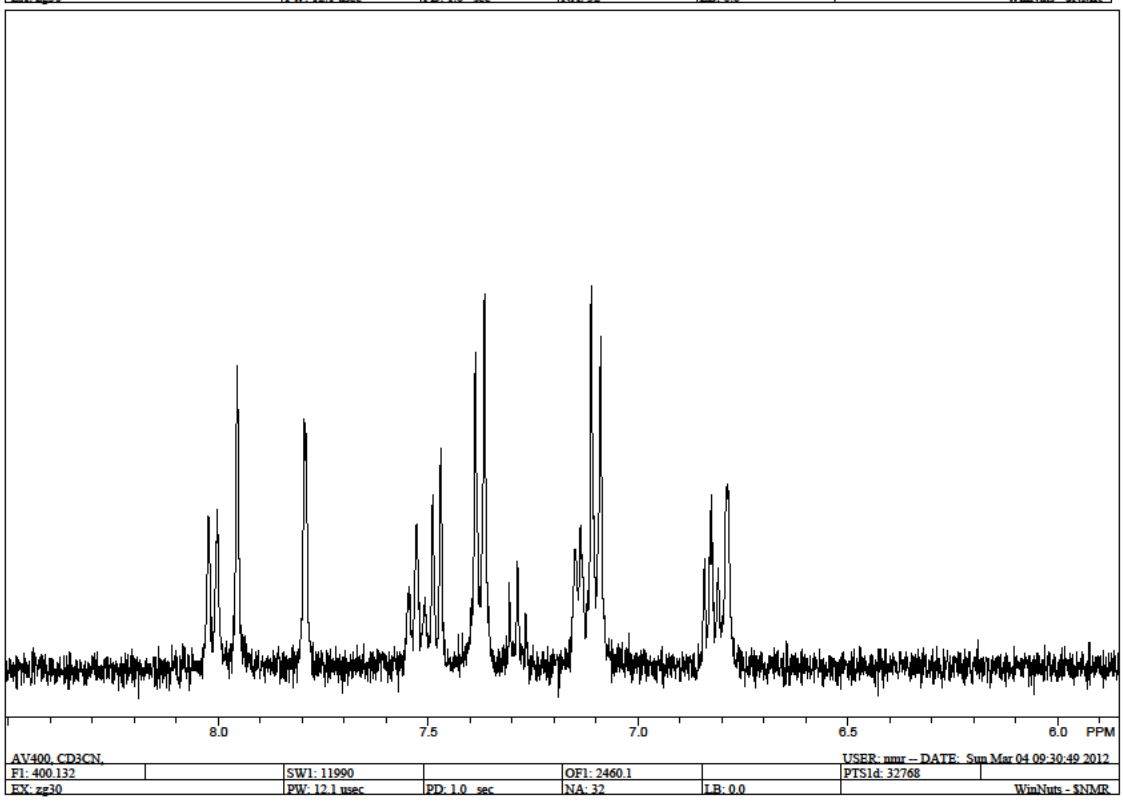
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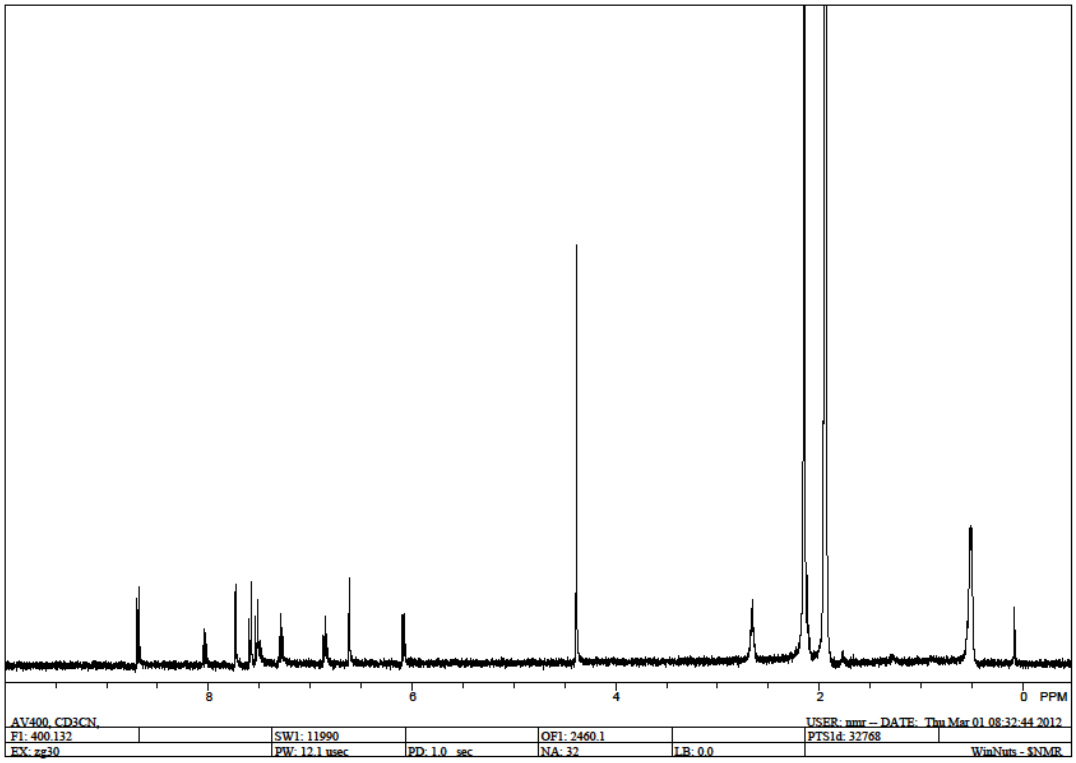
PD: 1.0 sec
NA: 32
LB: 0.0
WinNuts - $NMR

H NMR of **3**: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LB: 0.0
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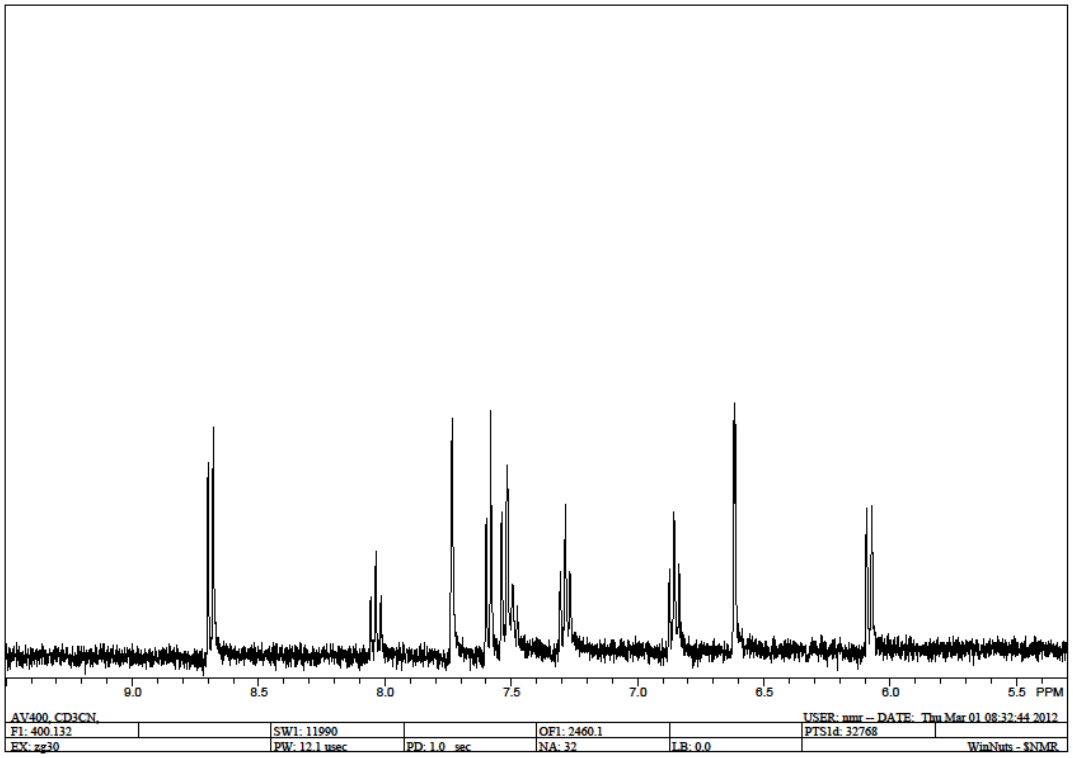
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6.5
6.0
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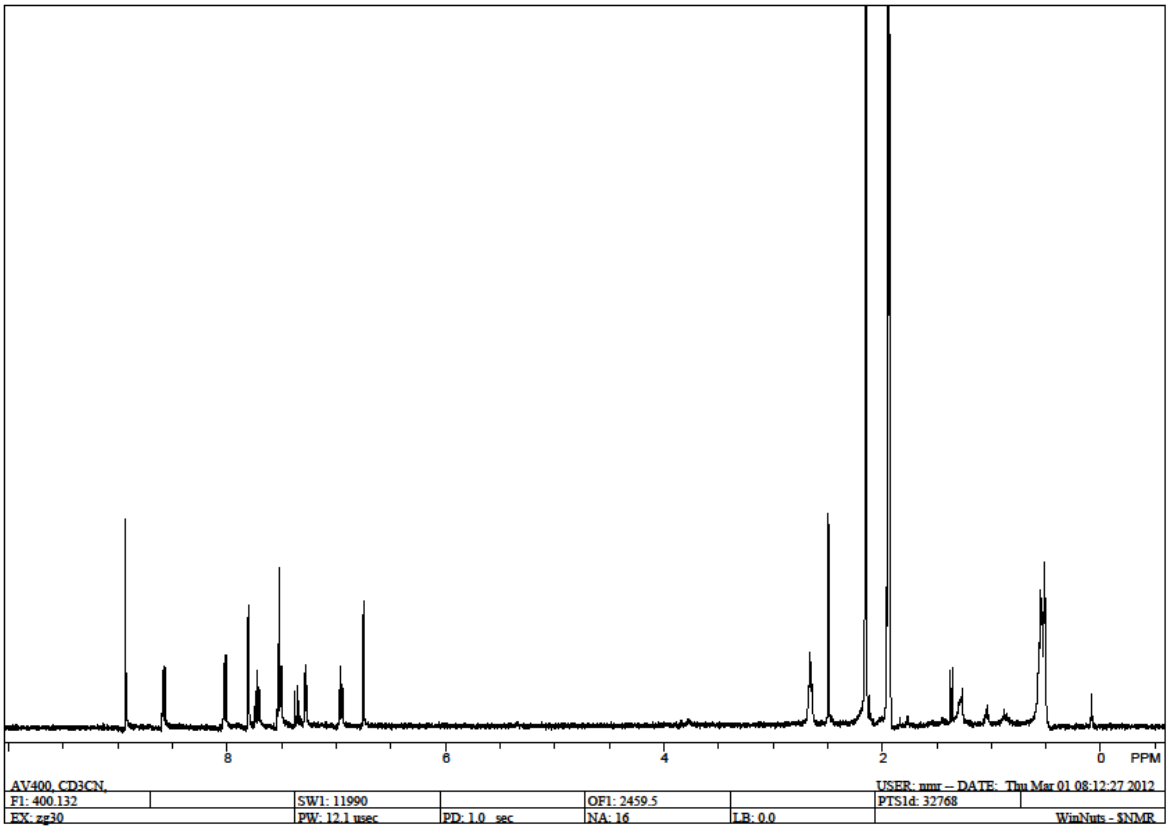
SW1: 11990
OF1: 2460.1
PTS1d: 32768
EX: zg30
PW: 12.1 usec
PD: 1.0 sec
NA: 32
LB: 0.0
WinNuts - $NMR

^{1}H NMR of **4**: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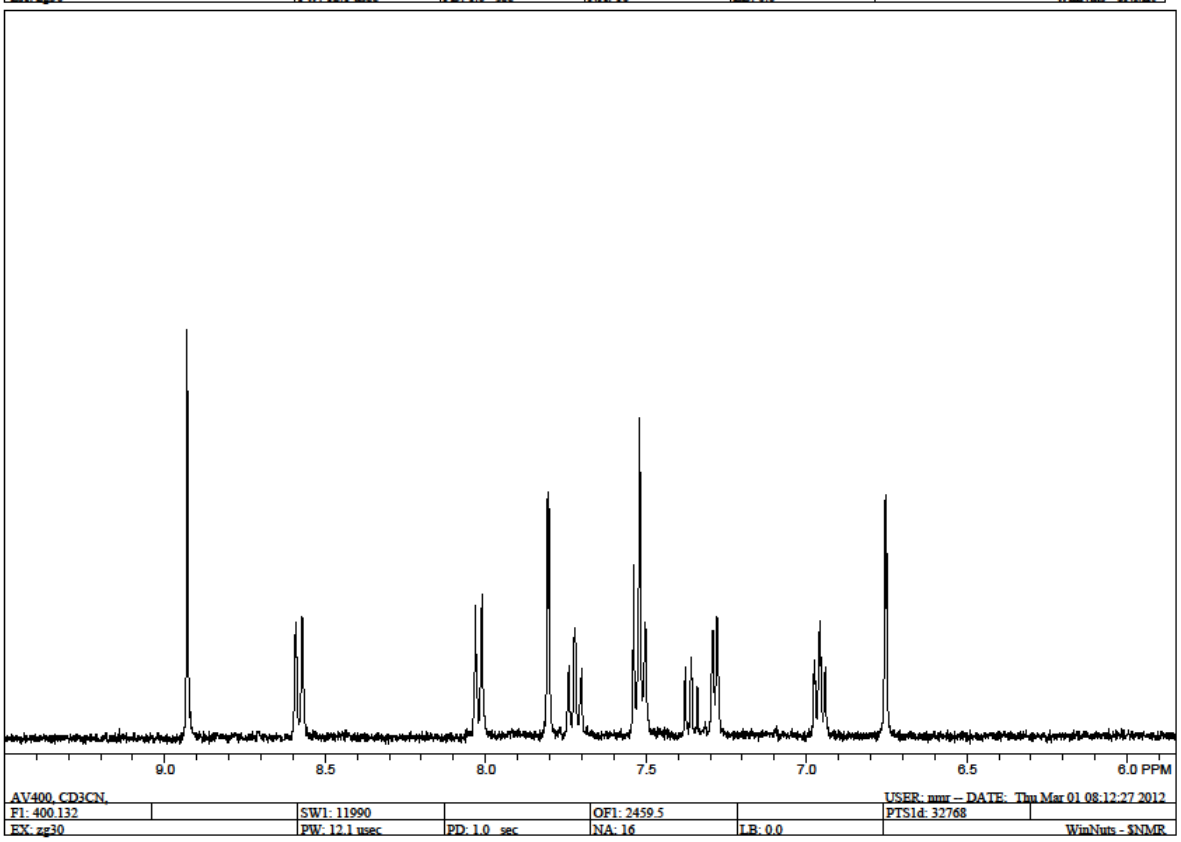
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7.0
6.5
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SW1: 11990
OF1: 2459.5
PTS1d: 32768
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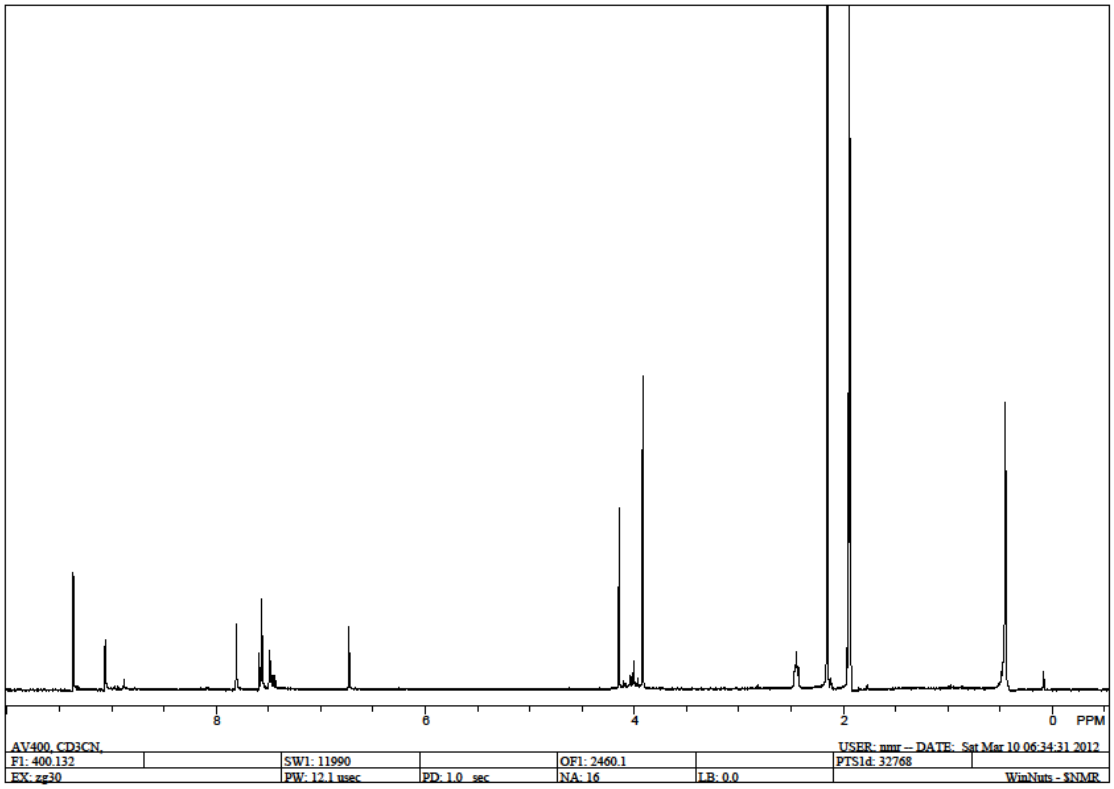
LB: 0.0
WinNuts - $NMR

^{1}H NMR of **5**: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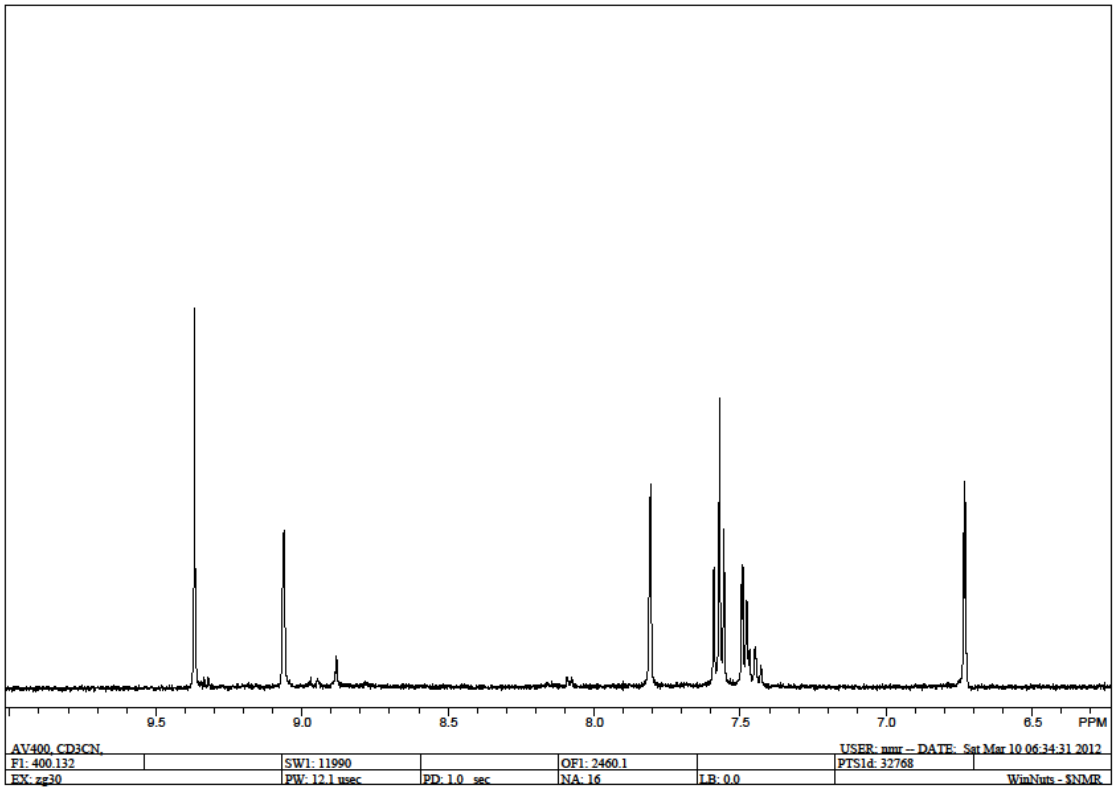
LB: 0.0
WinNuts - $NMR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8.0
7.5
7.0
6.5
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PTS1d: 32768
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WinNuts - $NMR

Reference:

(1) (a) Becke, A. D. *J. Chem. Phys.* **1993**, *98*, 5648. (b) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785.

(2) Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J. A.; Vreven, Jr. T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A. Gaussian 03, revision E.01; Gaussian Inc.: Pittsburgh PA, 2007.

(3) (a) Dunning, T. H.; Hay, P. J. In *Modern Theoretical Chemistry*; Schaefer, H. F., Ed.; Plenum: New York, 1976; Vol. 3, p 1. (b) Hay, P. J.; Wadt, W. R. *J. Chem. Phys*. **1985**, *82*, 270. (c) Wadt, W. R.; Hay, P. J. *J. Chem. Phys*. **1985**, *82*, 284. (d) Hay, P. J.; Wadt, W. R. *J. Chem. Phys*. **1985**, *82*, 299.