Cyaphide-alkynyls: Metal-ligand conjugations and the influence of remote substituents.

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Supporting Information

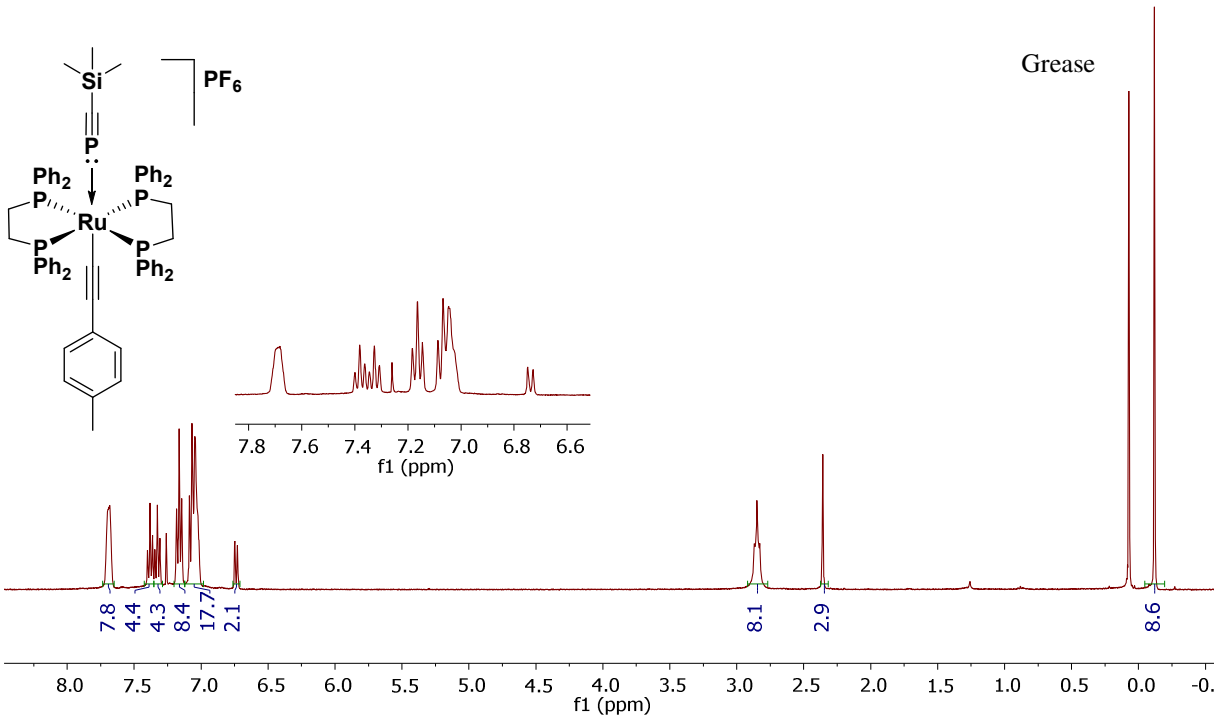


Figure S1: ^{1}H NMR Spectrum ($CDCl_3$, 303 K, 399 MHz) for complex **7a·[PF$_6$]**

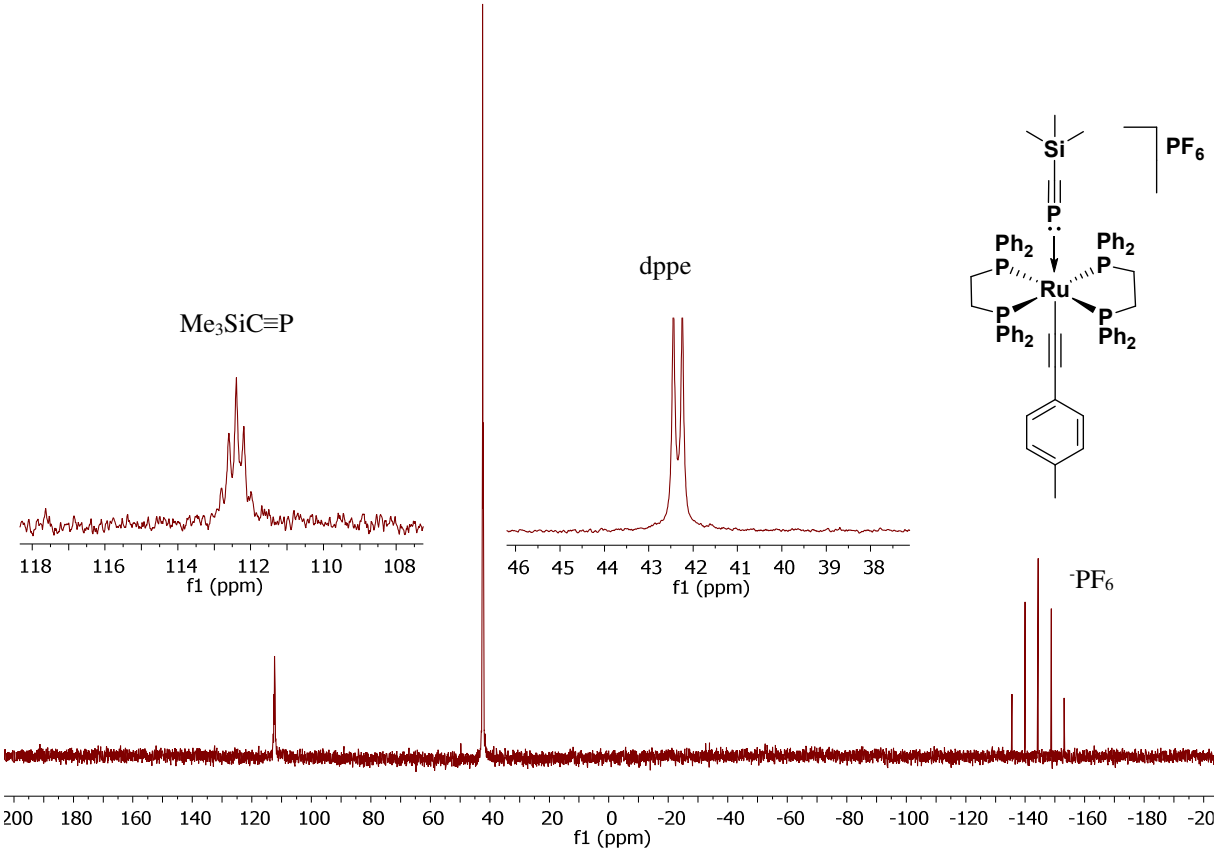


Figure S2: $^{31}P\{^{1}H\}$ NMR Spectrum ($CDCl_3$, 303 K, 162 MHz) for complex **7a·[PF$_6$]**

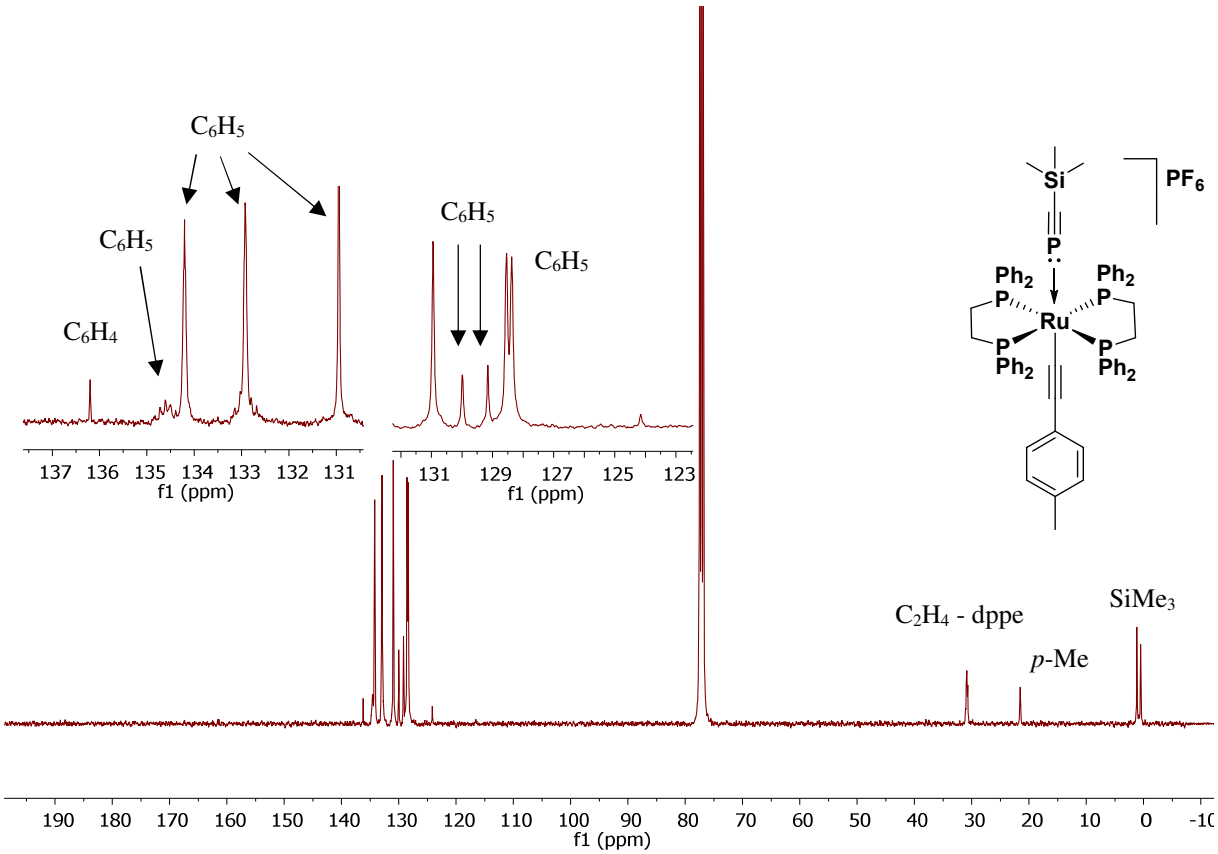


Figure S3: $^{13}C\{^{1}H\}$ NMR Spectrum ($CDCl_3$, 303 K, 100 MHz) for complex **7a·[PF$_6$]**

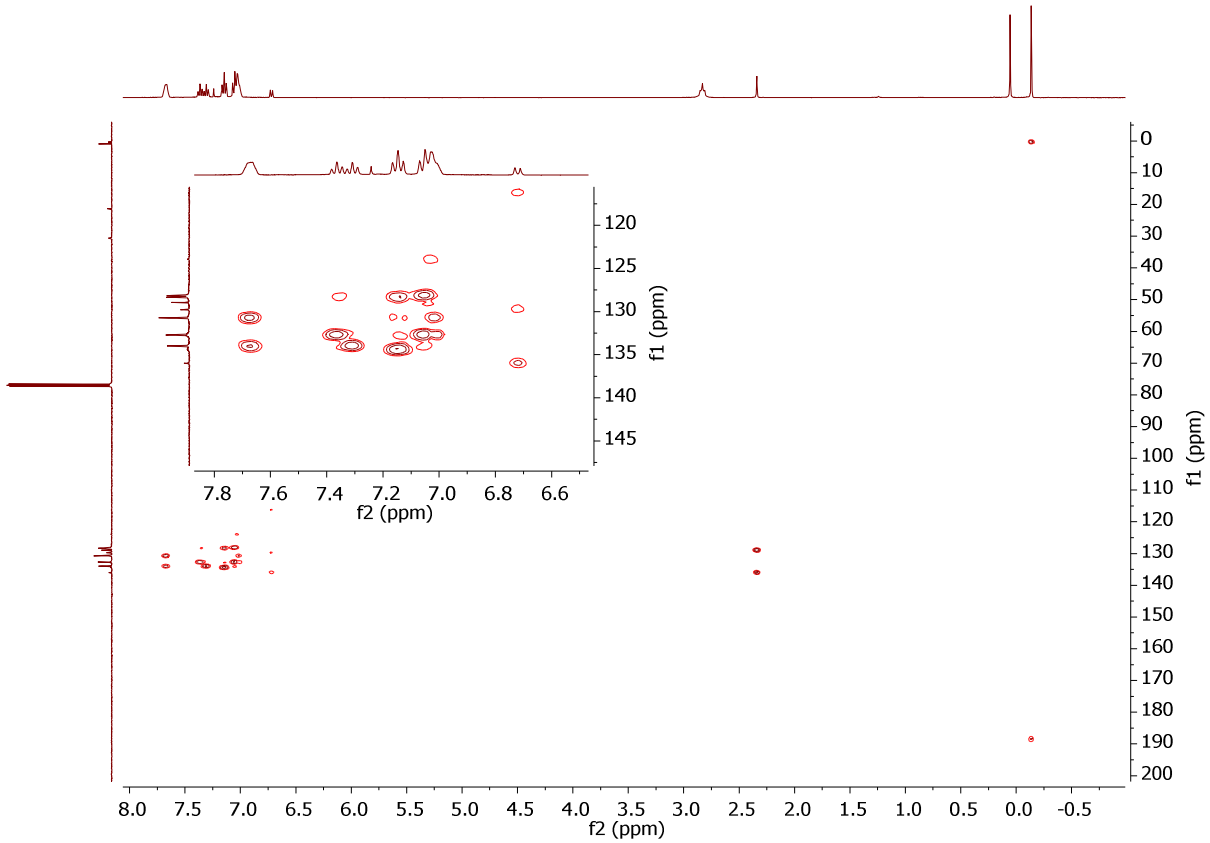


Figure S4: ^{1}H-^{13}C HMBC trace ($CDCl_3$, 303 K, 399, 100 MHz) for complex **7a·[PF$_6$]**

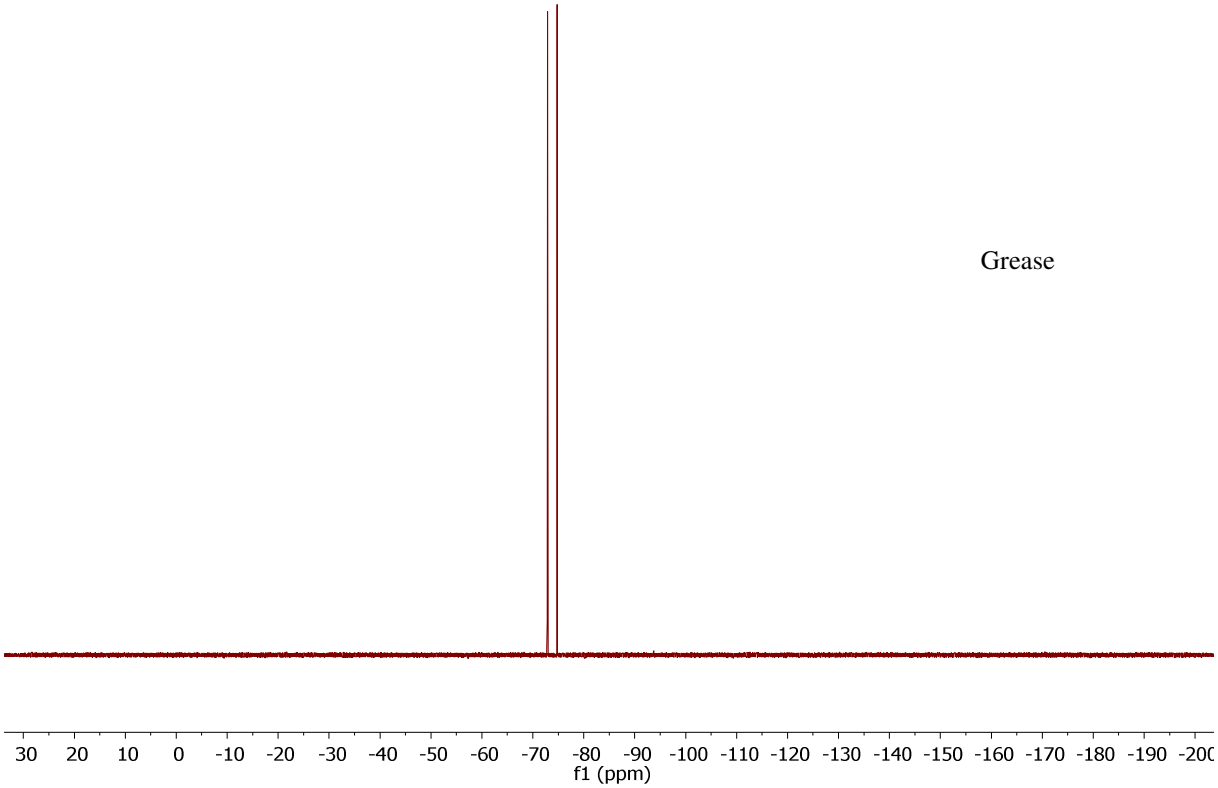


Figure S5: ^{19}F NMR Spectrum ($CDCl_3$, 303 K, 376 MHz) for complex **7a·[PF_6]**

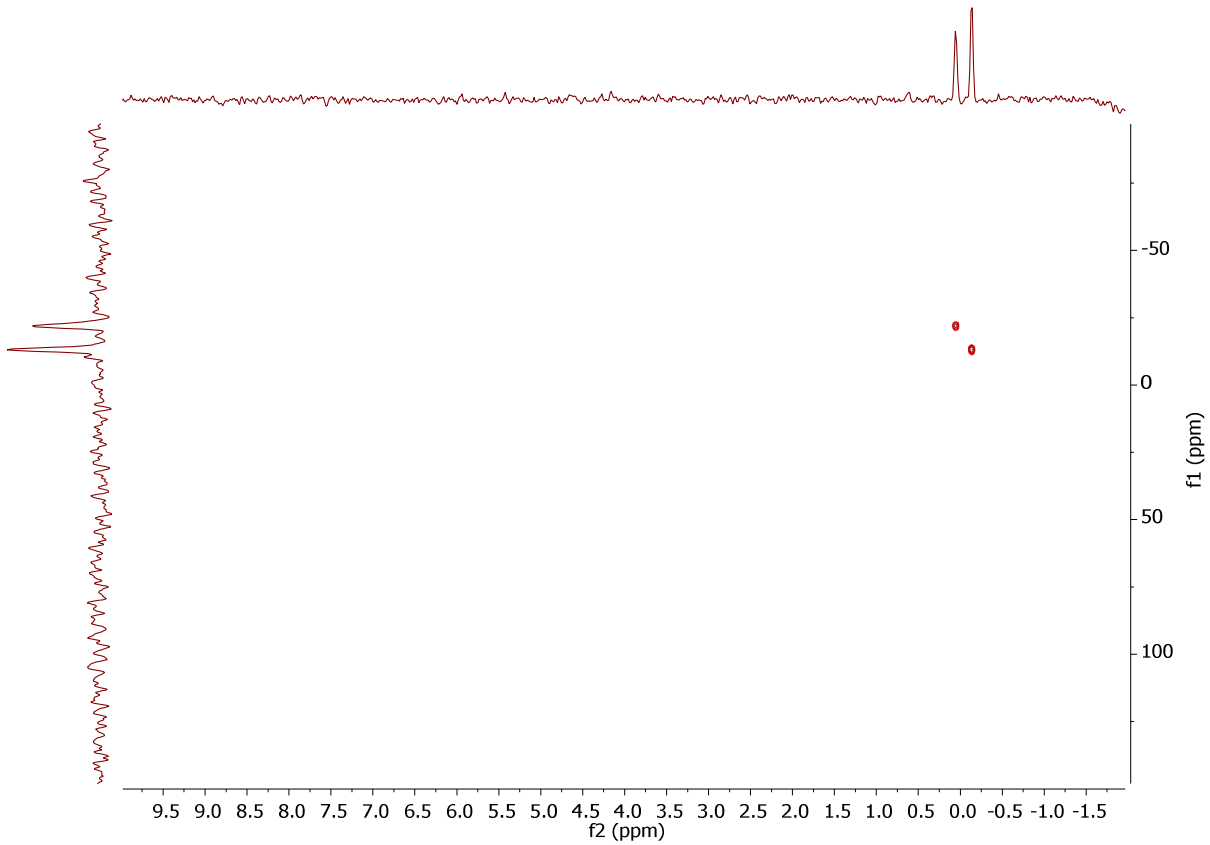


Figure S6: ^{1}H-^{29}Si HMBC trace ($CDCl_3$, 303 K, 399, 79 MHz) for complex **7a·[PF_6]**

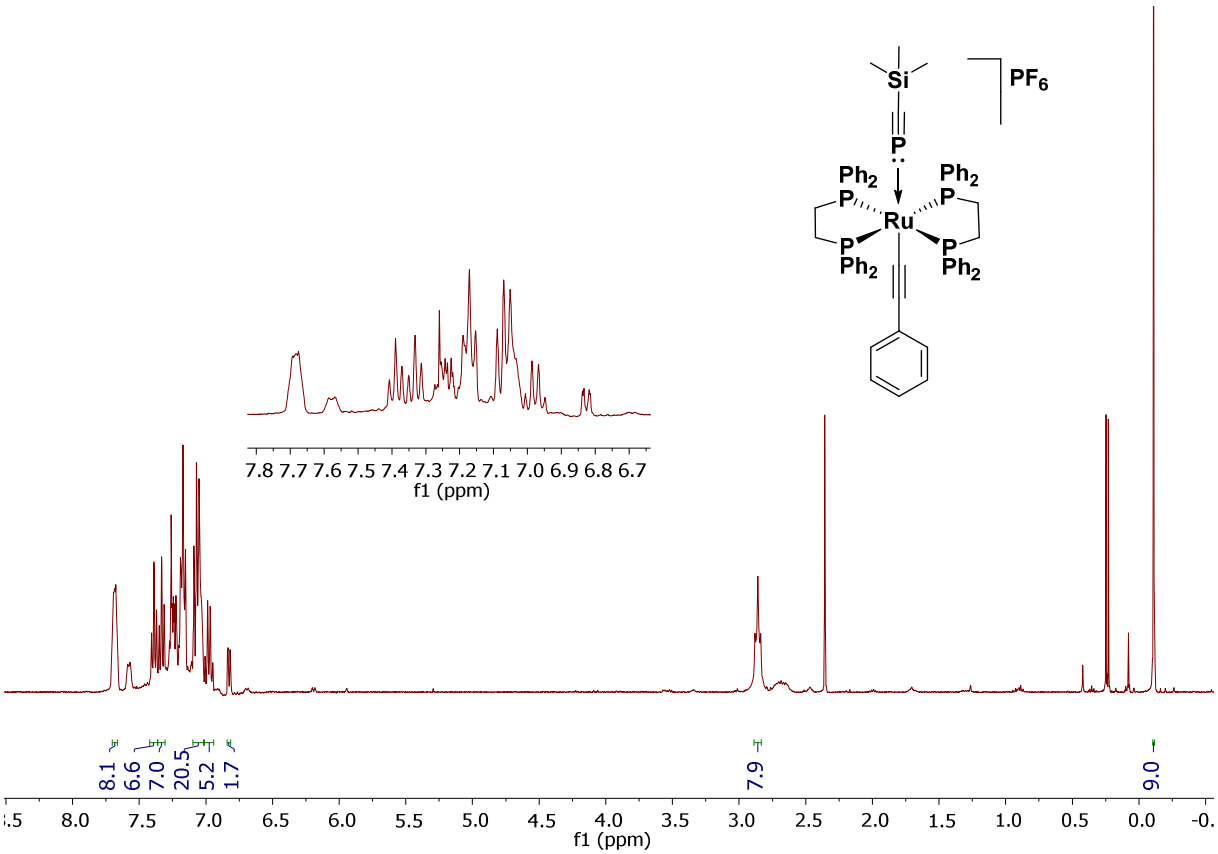


Figure S7: ^{1}H NMR Spectrum ($CDCl_3$, 303 K, 399 MHz) for complex **7b·[PF$_6$]**

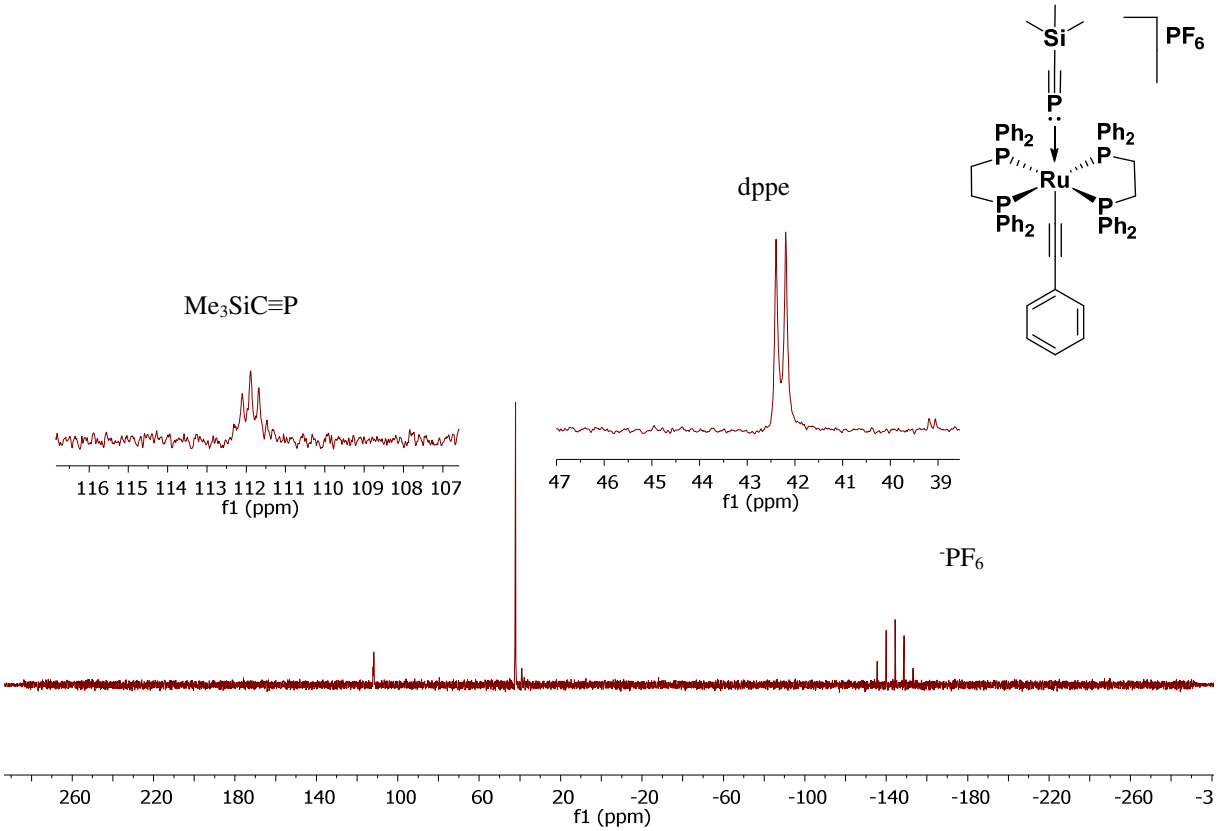


Figure S8: $^{31}P\{^{1}H\}$ NMR Spectrum ($CDCl_3$, 303 K, 162 MHz) for complex **7b·[PF$_6$]**

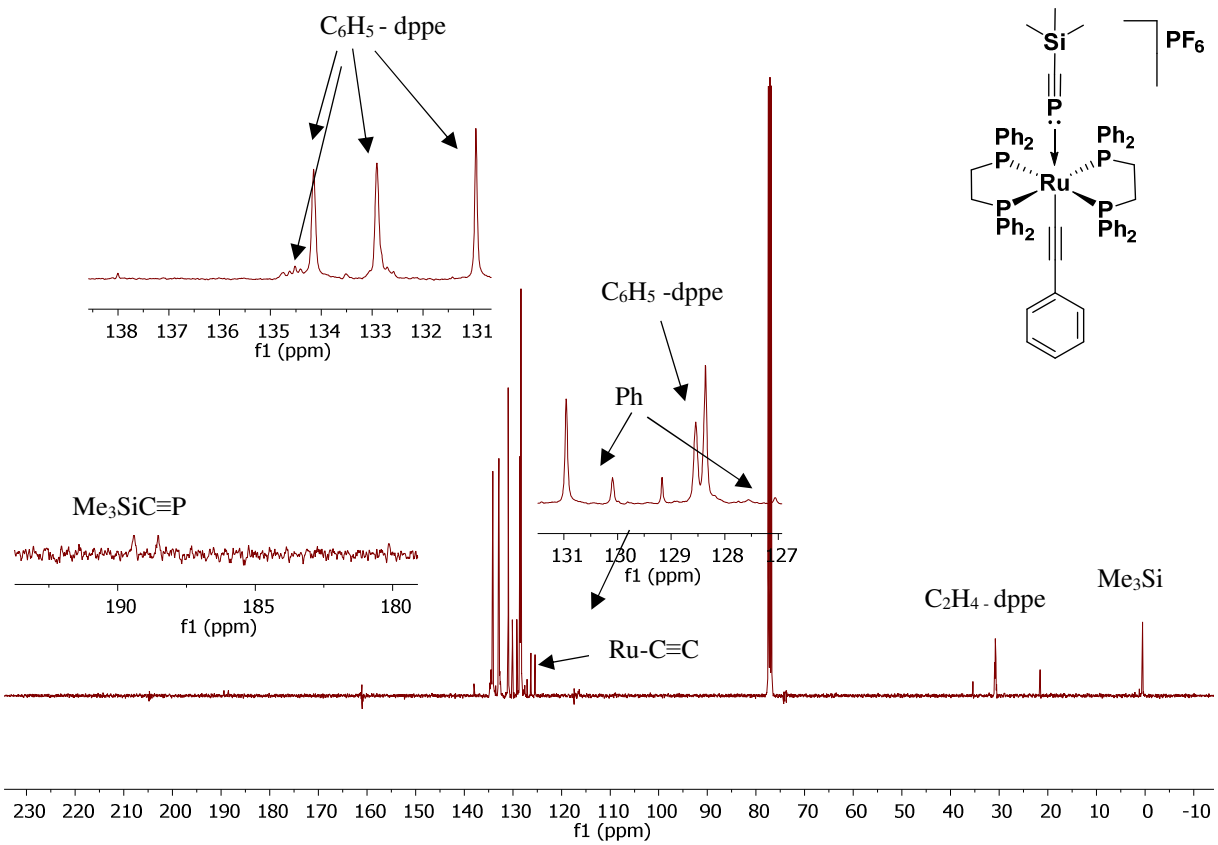


Figure S9: $^{13}C\{^{1}H\}$ NMR Spectrum ($CDCl_3$, 303 K, 100 MHz) complex **7b·[PF_6]**

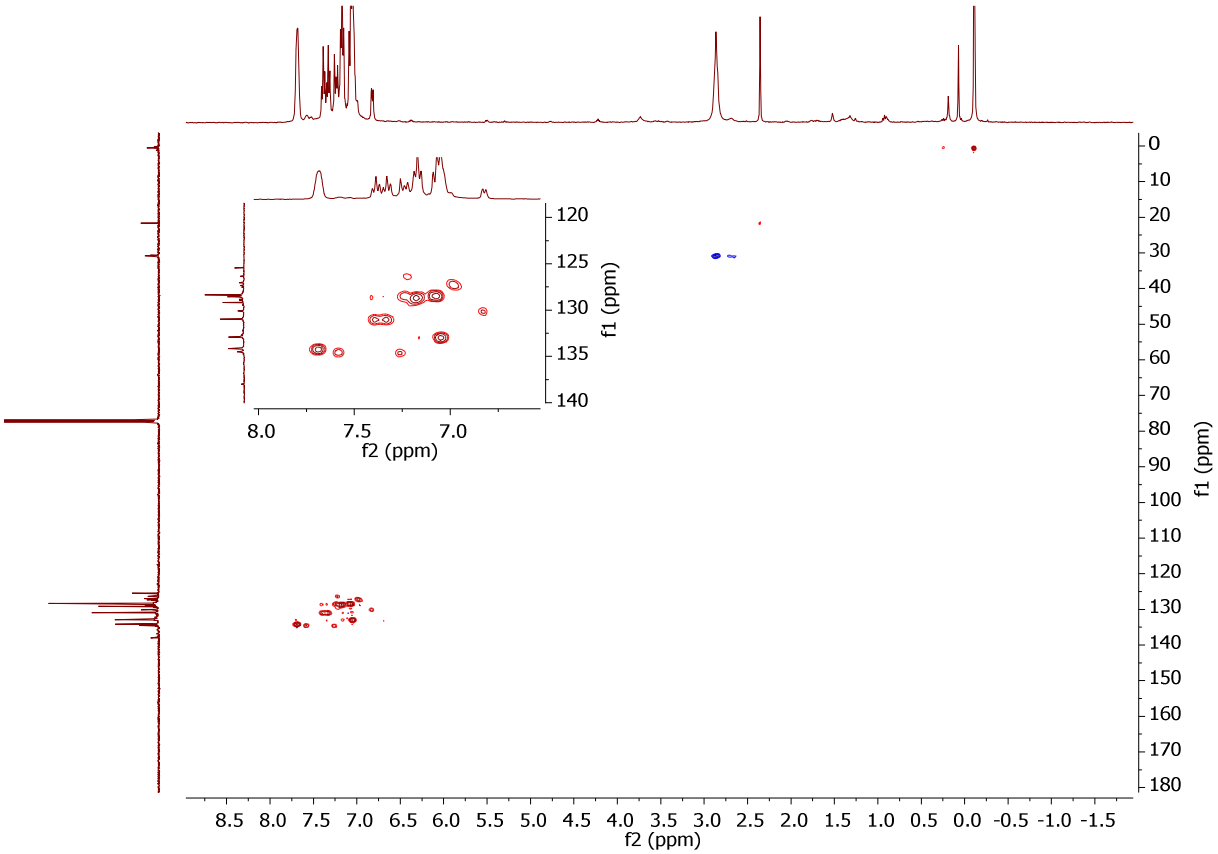


Figure S7: ^{1}H-^{13}C HSQC trace ($CDCl_3$, 303 K, 399, 100 MHz) for complex **7b·[PF_6]**

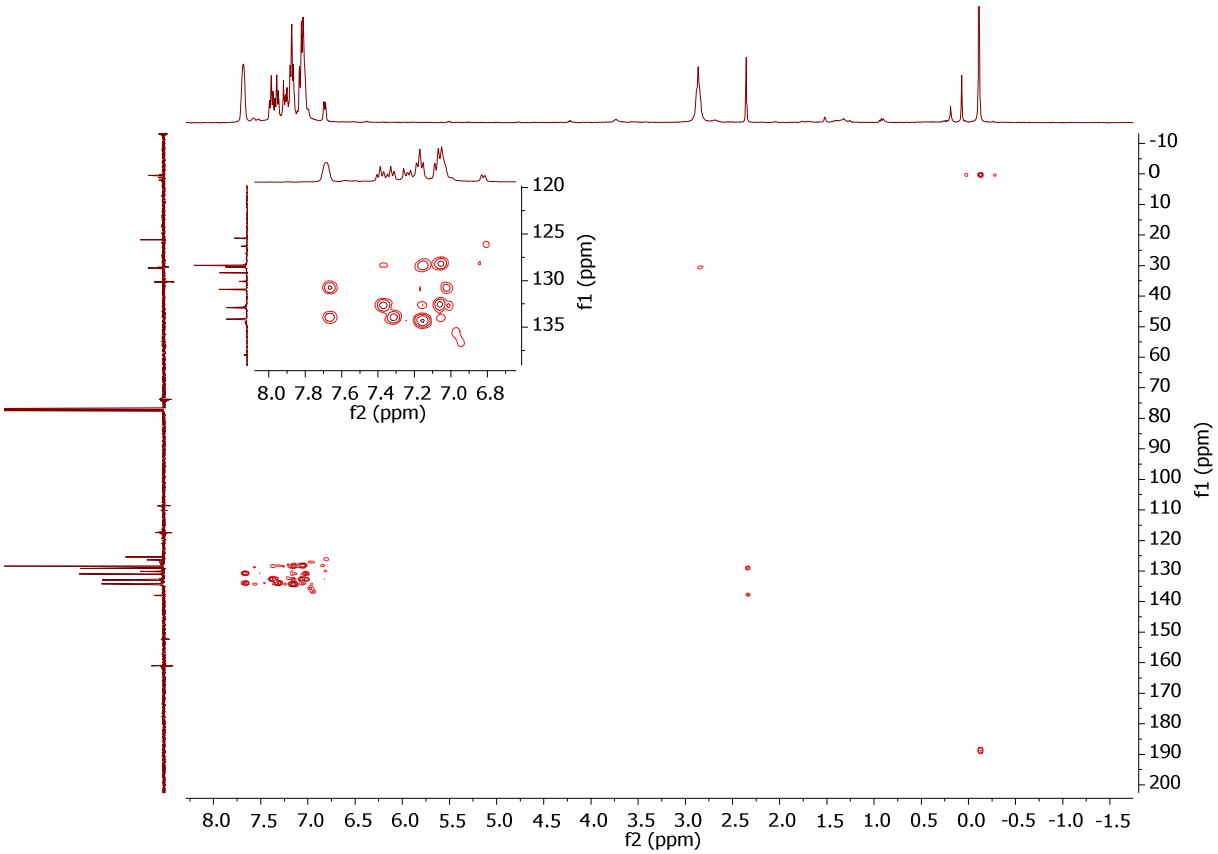


Figure S8: ^{1}H-^{13}C HMBC trace ($CDCl_3$, 303 K, 399, 100 MHz) for complex **7b·[PF_6]**

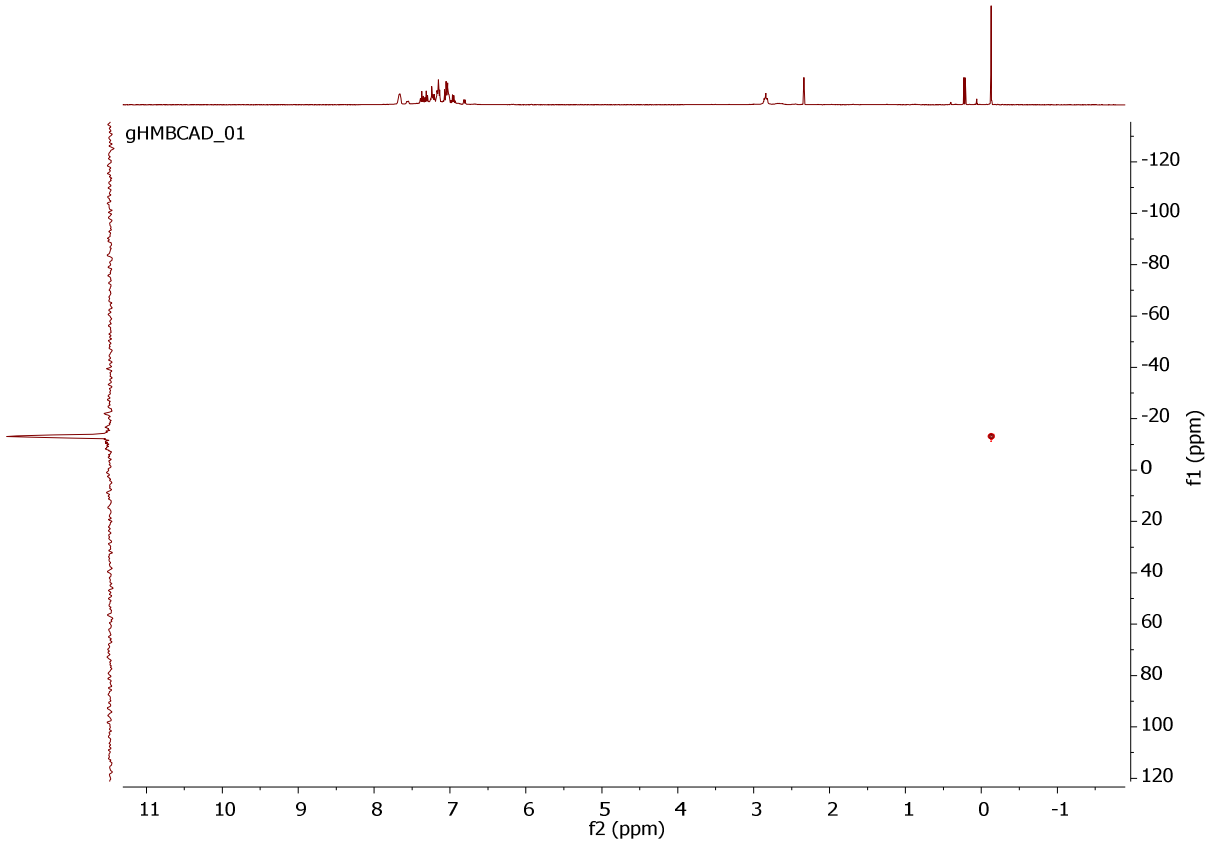


Figure S9: ^{1}H-^{29}Si HMBC trace ($CDCl_3$, 303 K, 399, 79 MHz) for complex **7b·[PF_6]**

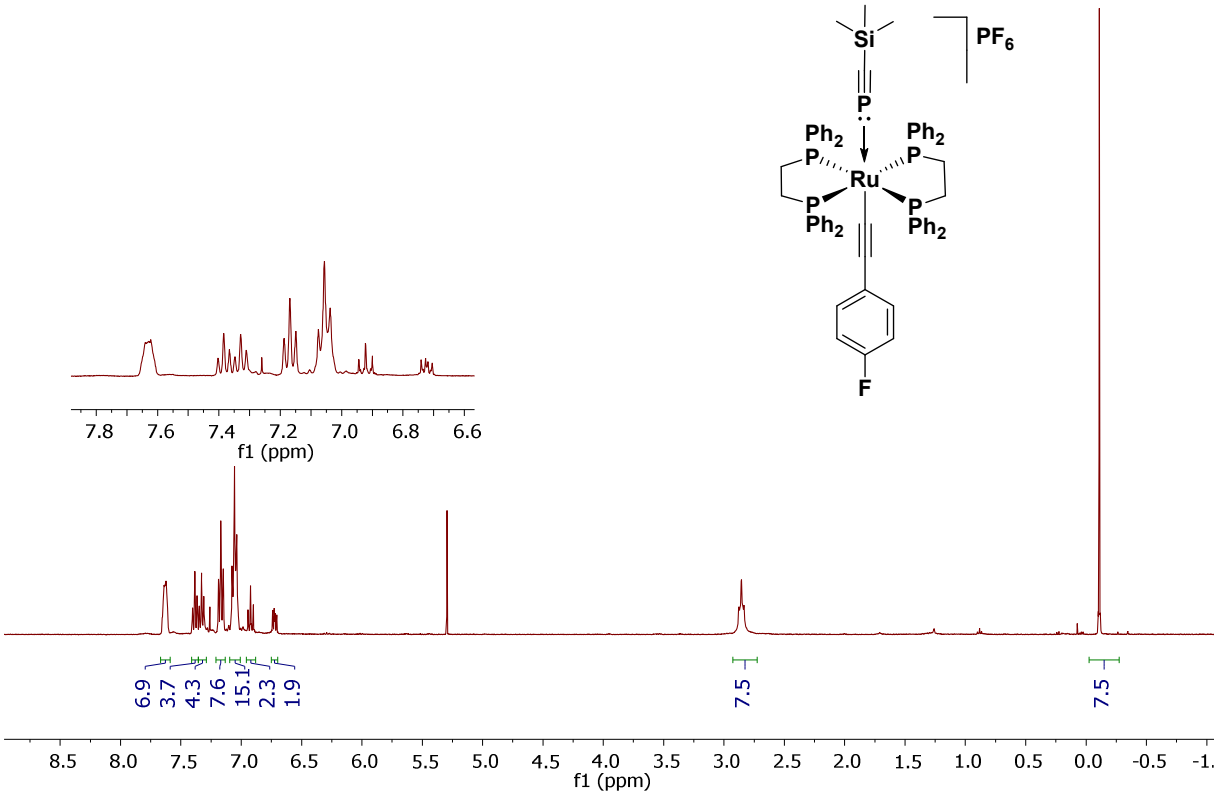


Figure S10: ^{1}H NMR Spectrum ($CDCl_3$, 303 K, 399 MHz) for complex **7c·[PF$_6$]**

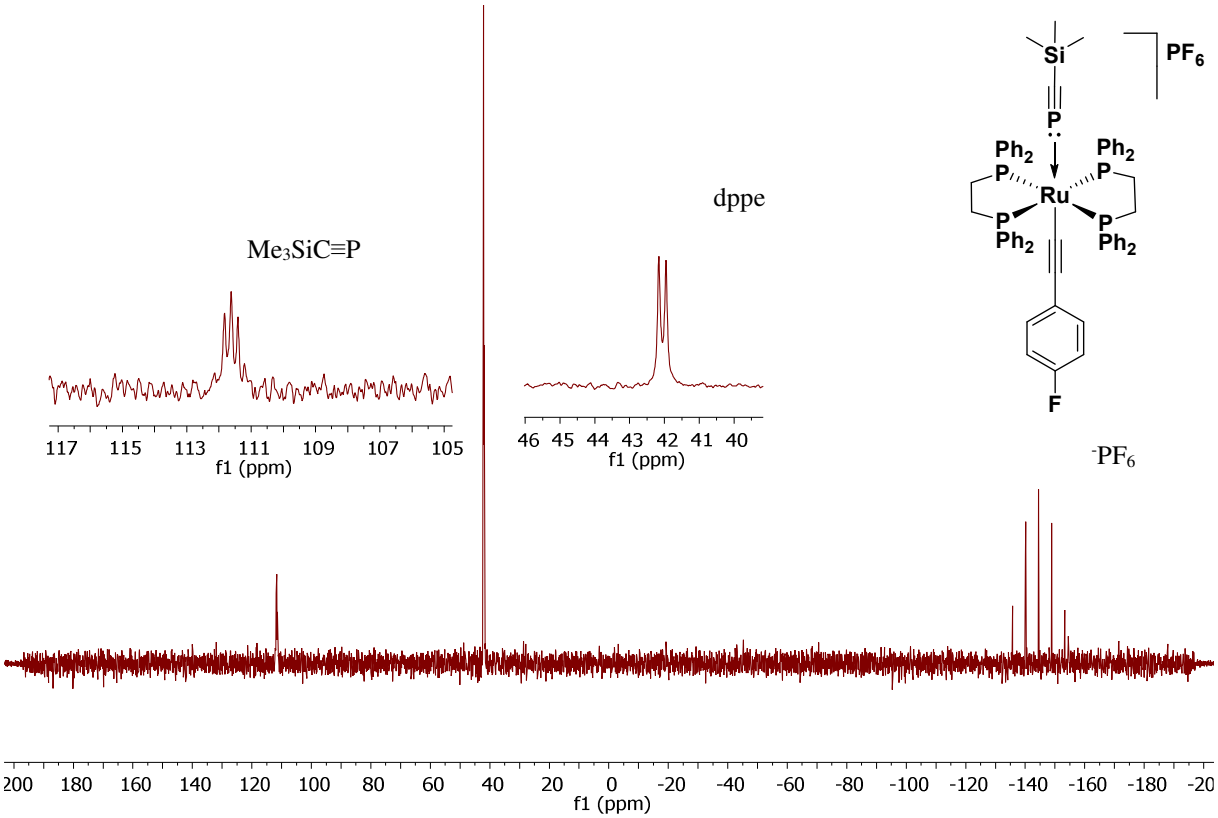


Figure S11: $^{31}P\{^{1}H\}$ NMR Spectrum ($CDCl_3$, 303 K, 162 MHz) for complex **7c·[PF$_6$]**

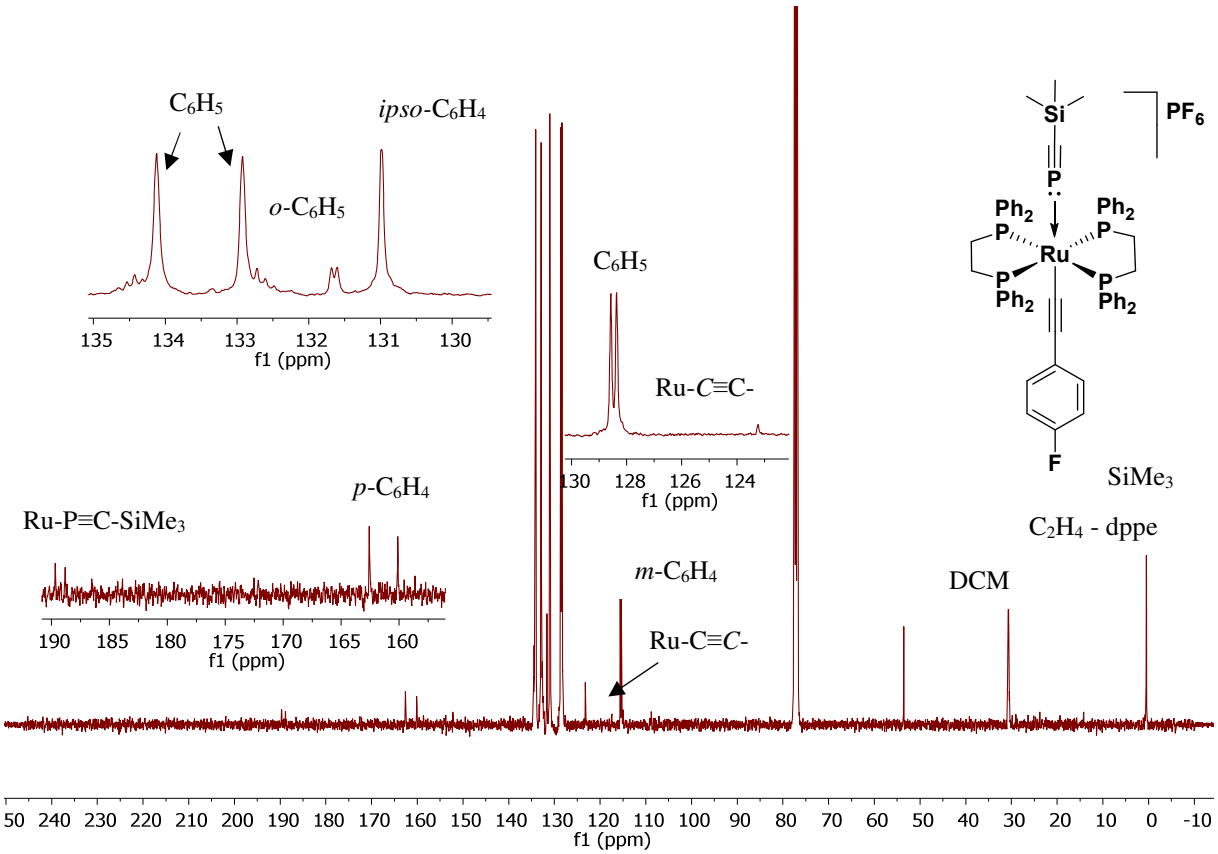


Figure S12: $^{13}C\{^{1}H\}$ NMR Spectrum ($CDCl_3$, 303 K, 100 MHz) for complex **7c·[PF$_6$]**

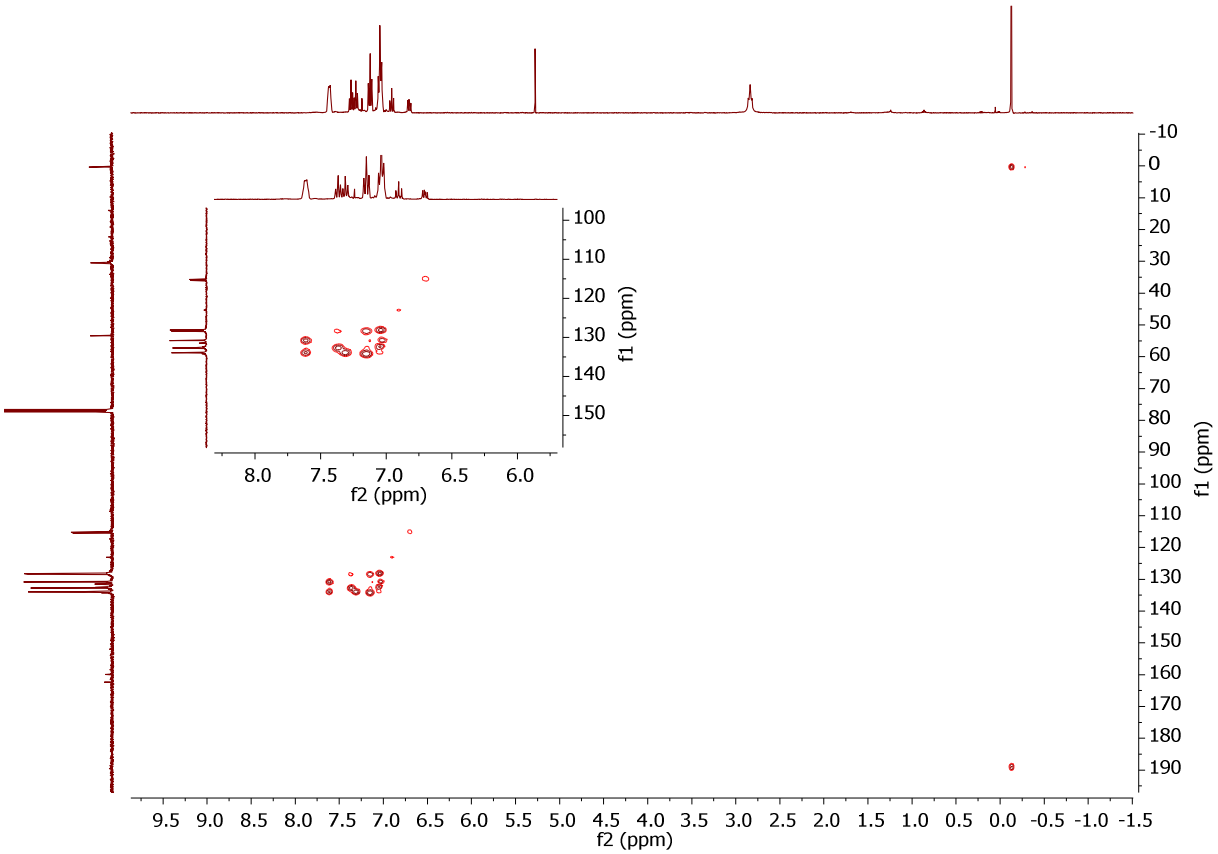


Figure S13: ^{1}H-^{13}C HMBC trace ($CDCl_3$, 303 K, 399, 100 MHz) for complex **7c·[PF$_6$]**

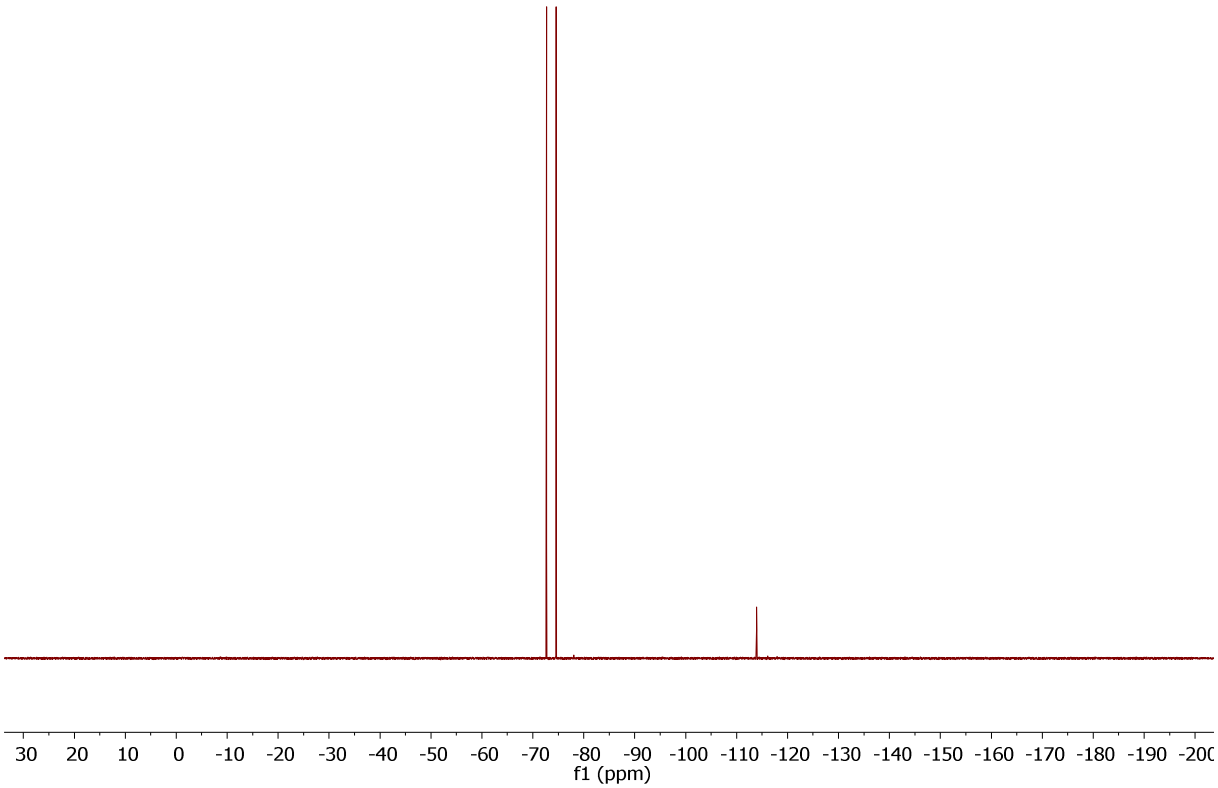


Figure S14: ^{19}F NMR Spectrum ($CDCl_3$, 303 K, 376 MHz) for complex **7c·[PF_6]**

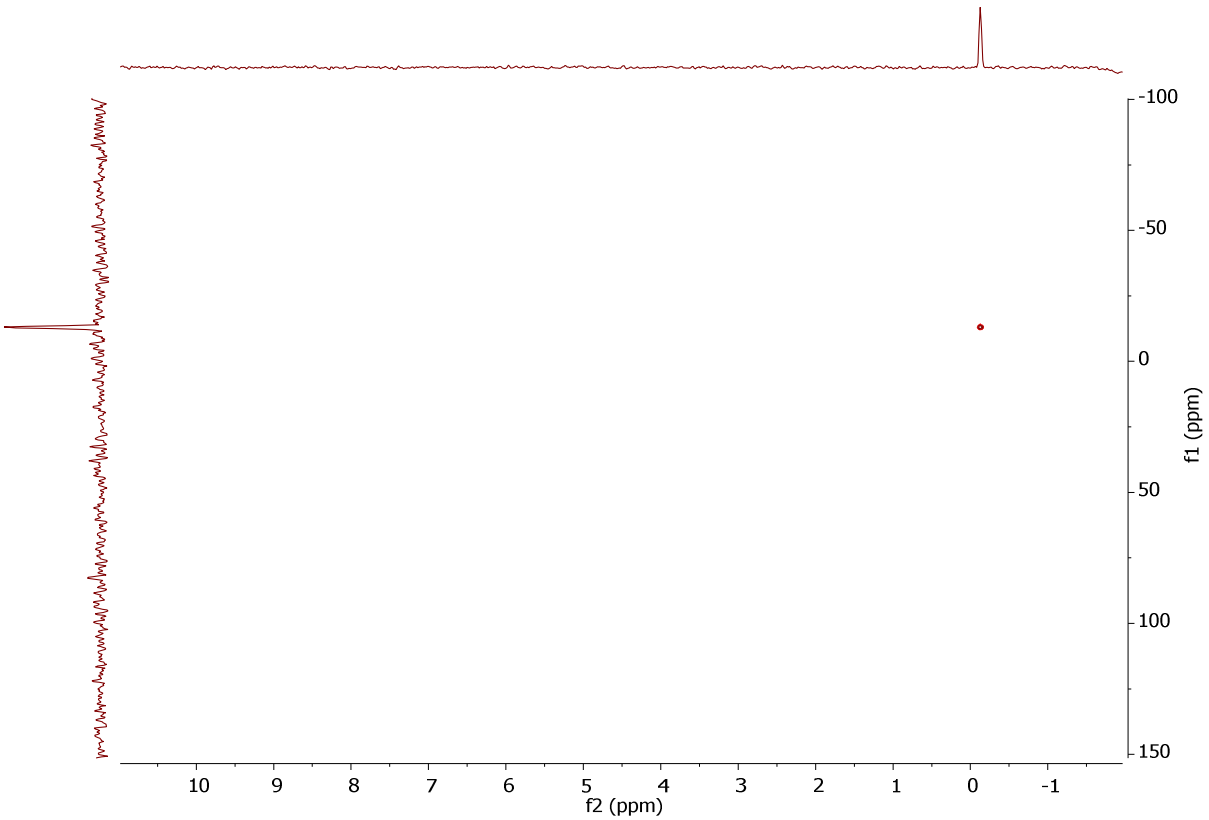


Figure S15: ^{1}H-^{29}Si HMBC trace ($CDCl_3$, 303 K, 399, 79 MHz) for complex **7c·[PF_6]**

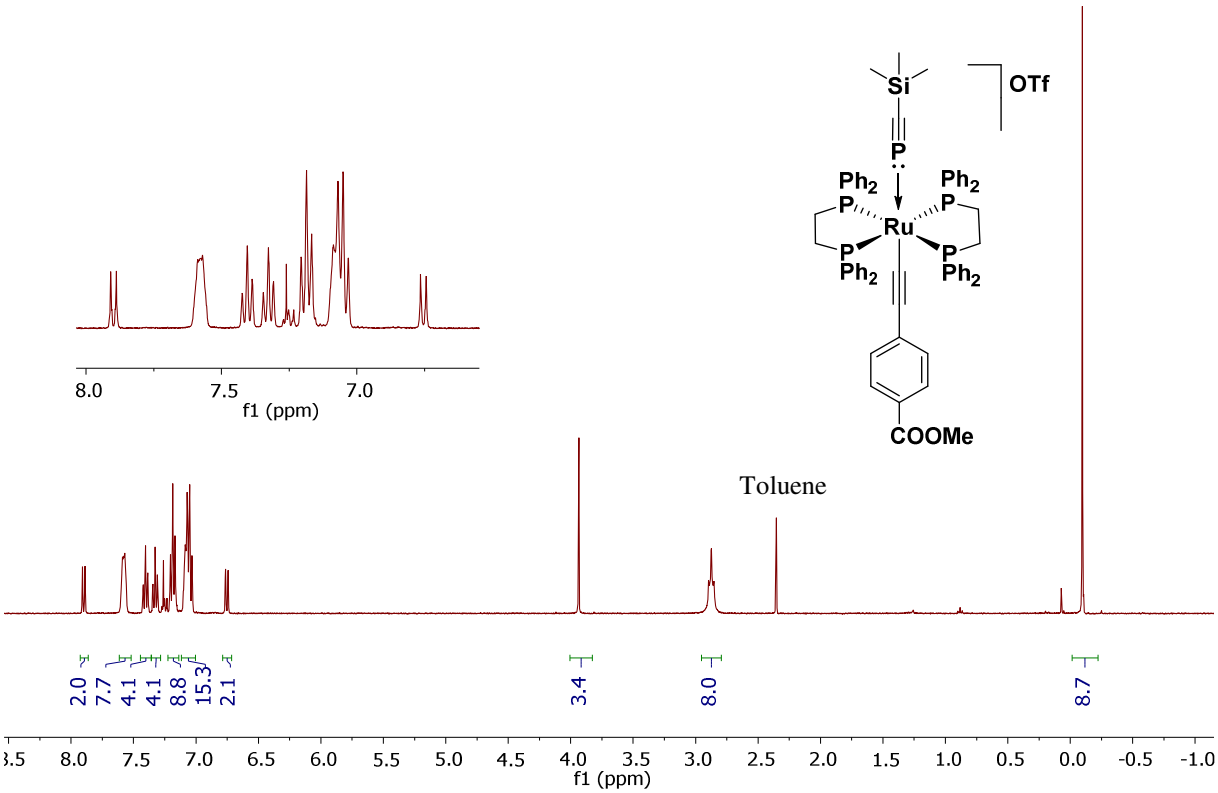


Figure S19: ^{1}H NMR Spectrum ($CDCl_3$, 303 K, 399 MHz) for complex **7d·[OTf]**

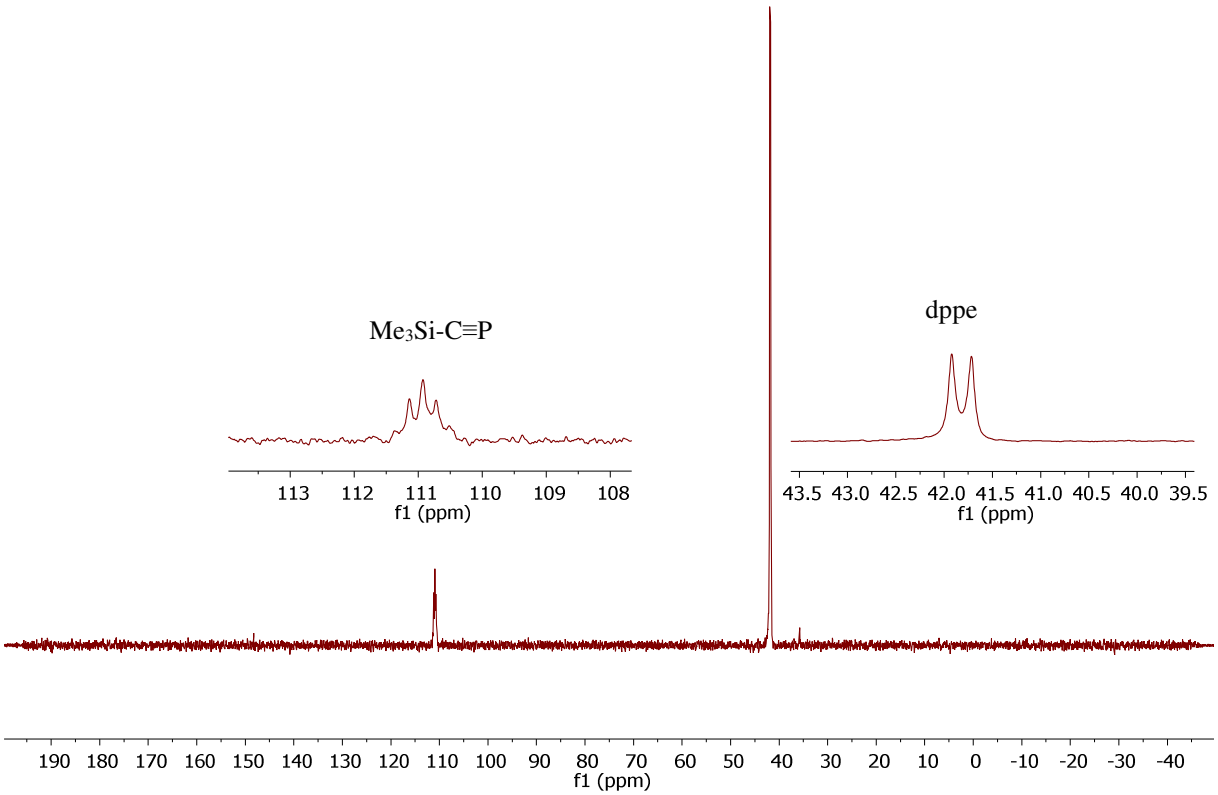


Figure S16: $^{31}P\{^{1}H\}$ NMR Spectrum ($CDCl_3$, 303 K, 162 MHz) for complex **7d·[OTf]**

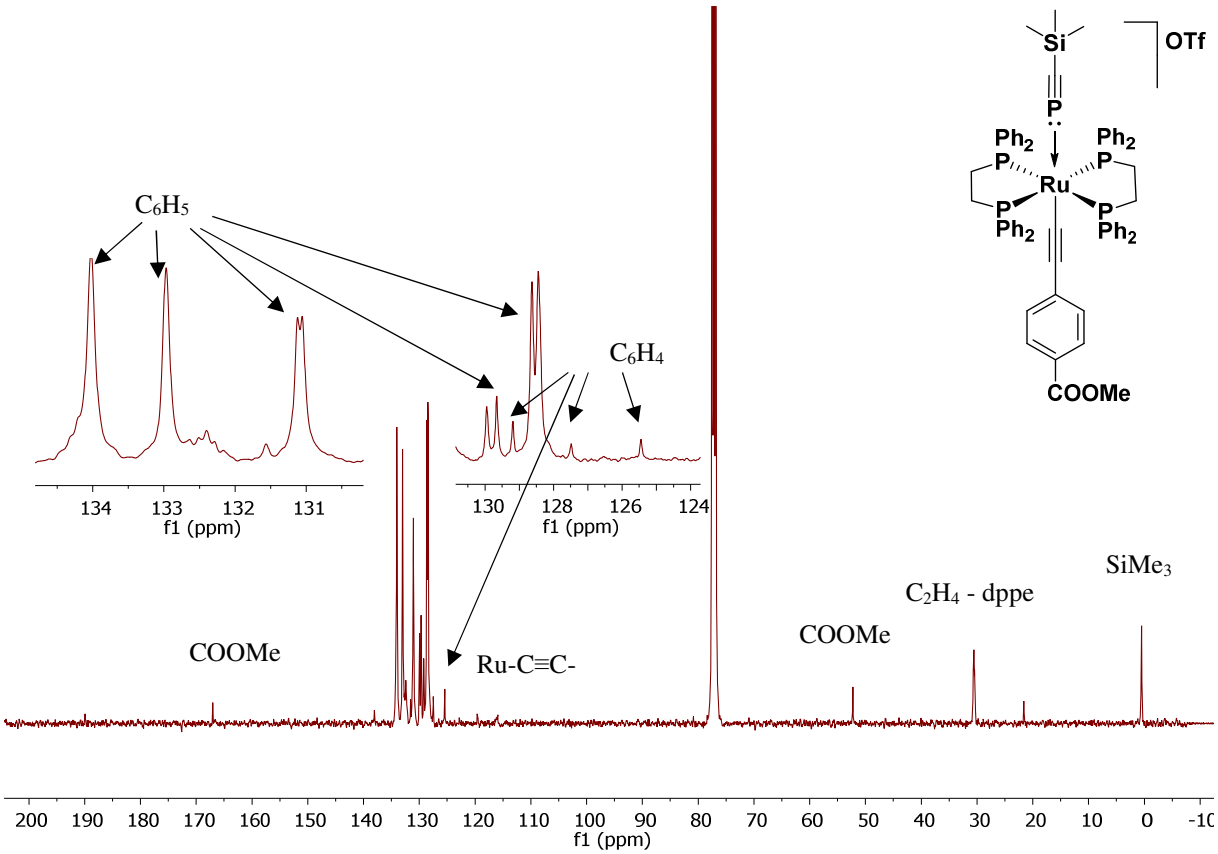


Figure S17: $^{13}C\{^{1}H\}$ NMR Spectrum ($CDCl_3$, 303 K, 100 MHz) for complex **7d·[OTf]**

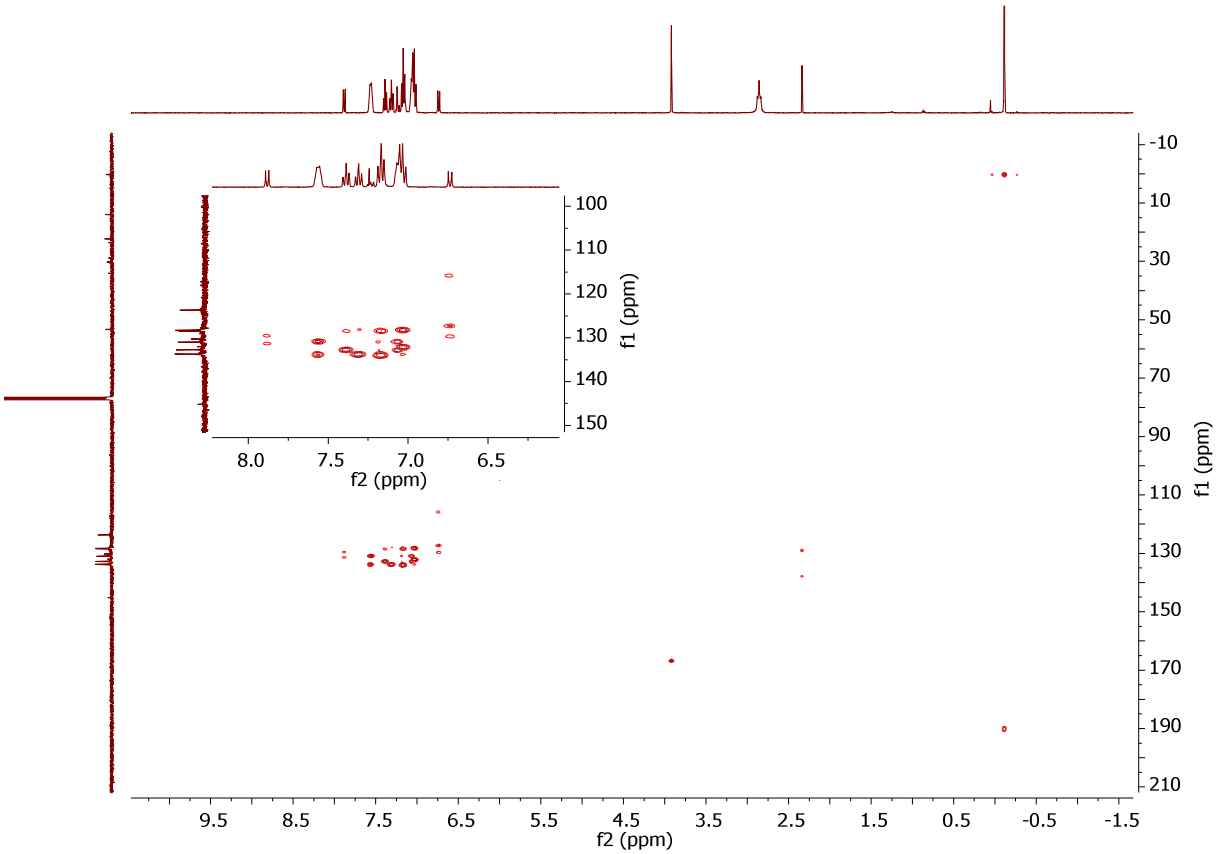


Figure S18: ^{1}H-^{13}C HMBC trace ($CDCl_3$, 303 K, 399, 100 MHz) for **7d·[OTf]**

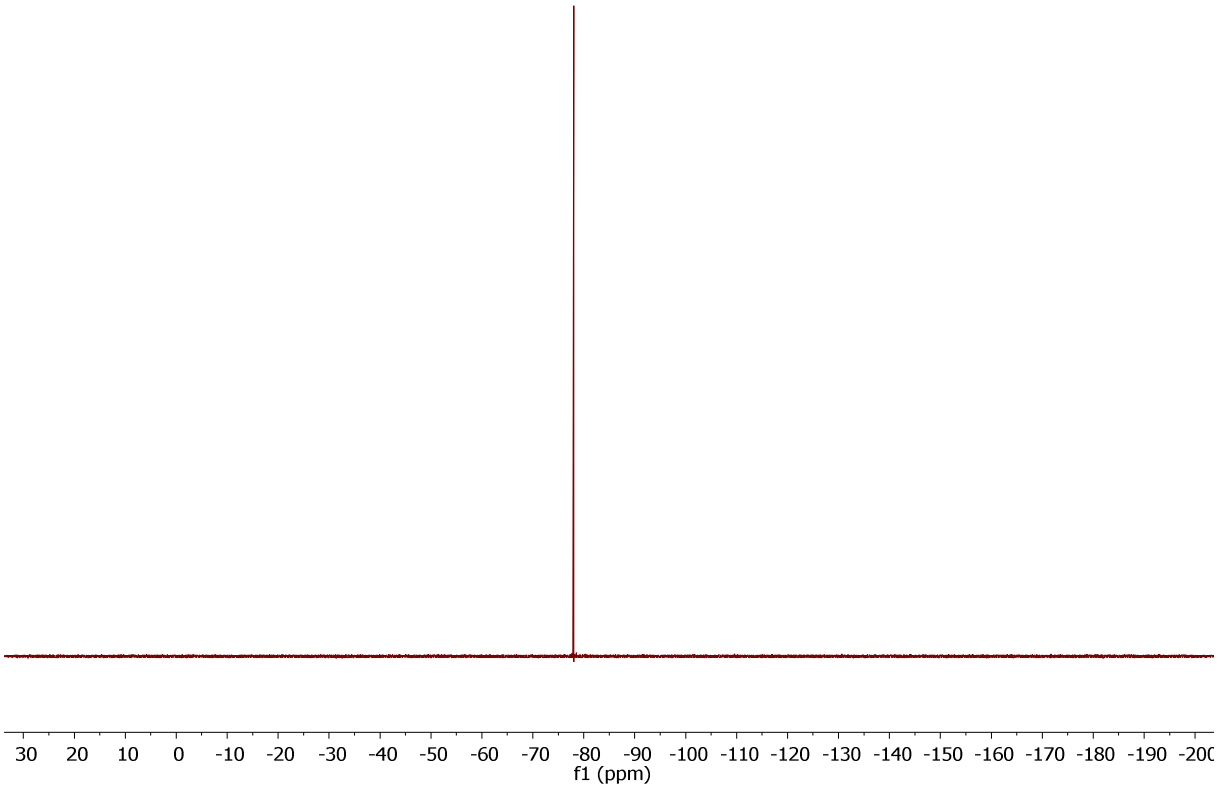


Figure S19: ^{19}F NMR Spectrum ($CDCl_3$, 303 K, 276 MHz) for complex **7d·[OTf]**

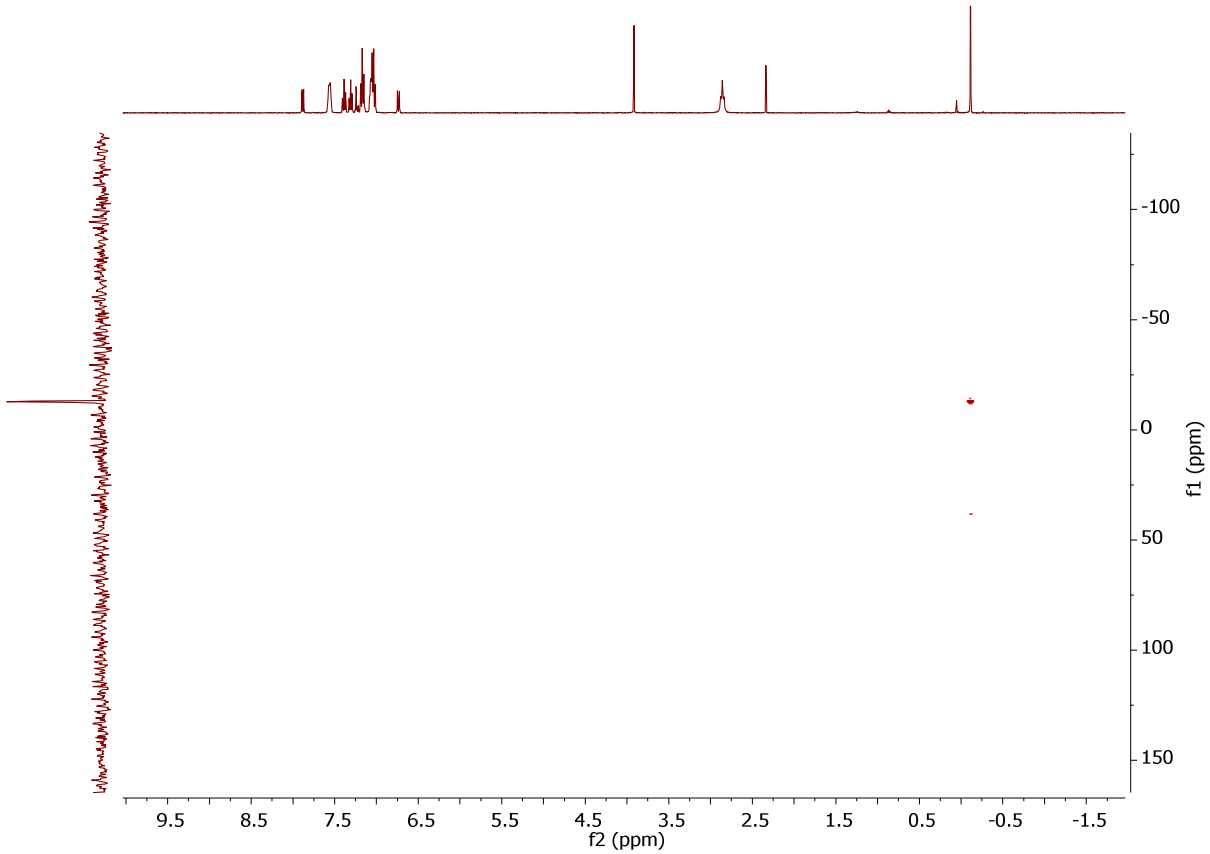


Figure S20: ^{1}H-^{29}Si HMBC trace ($CDCl_3$, 303 K, 399, 79 MHz) for complex **7d·[OTf]**

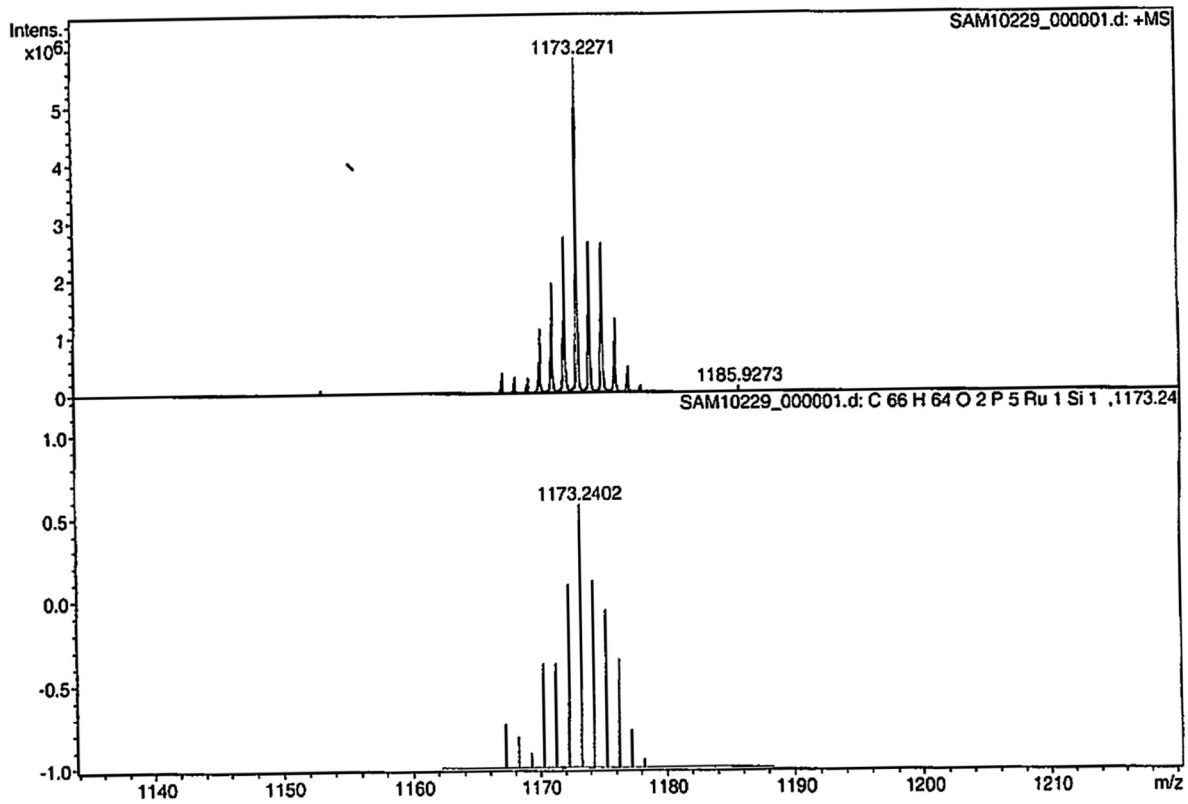


Figure S21: HR-ESI$^+$ complex **7d·[OTf]** (top, observed for $[M]^+$ and bottom, simulated for $[M]^+$**)**

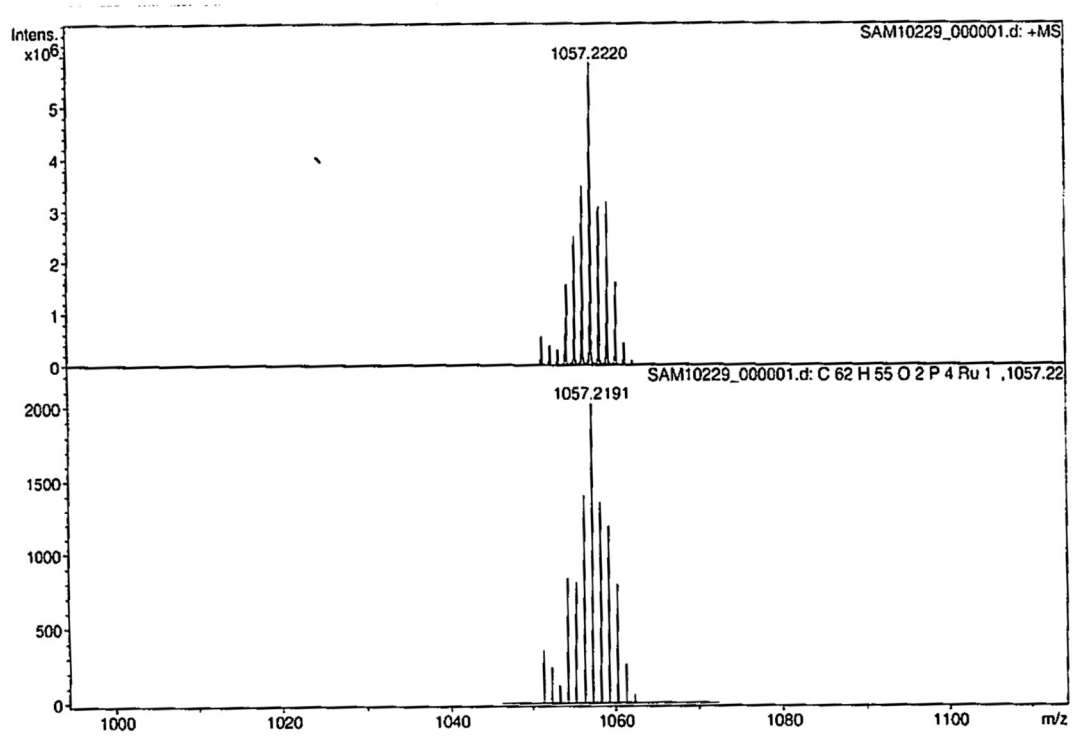


Figure S22: HR-ESI$^+$ complex **7d·[OTf]** (top, observed for $[M - Me_3SiC{\equiv}P]^+$ and bottom, simulated for $[M - Me_3SiC{\equiv}P]^+$**)**

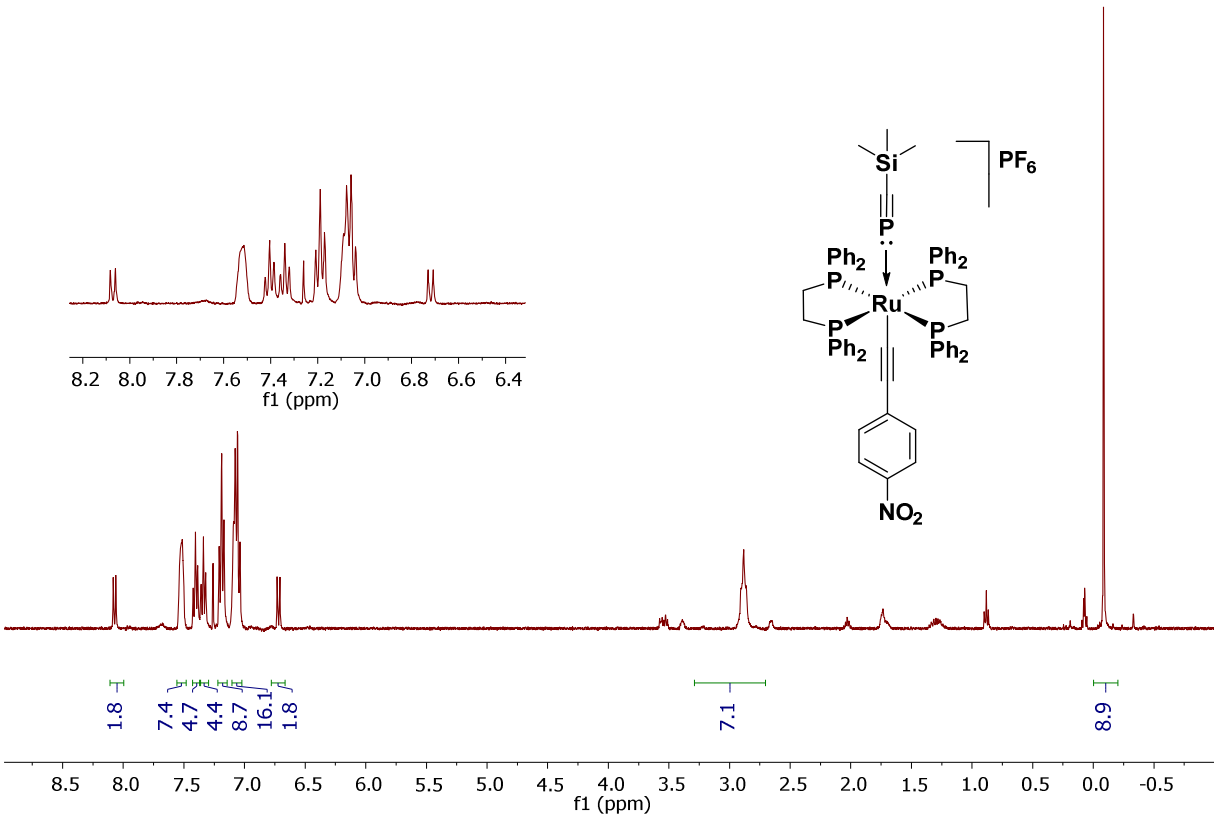


Figure S23: ^{1}H NMR Spectrum ($CDCl_3$, 303 K, 399 MHz) for complex **7e·[PF$_6$]**

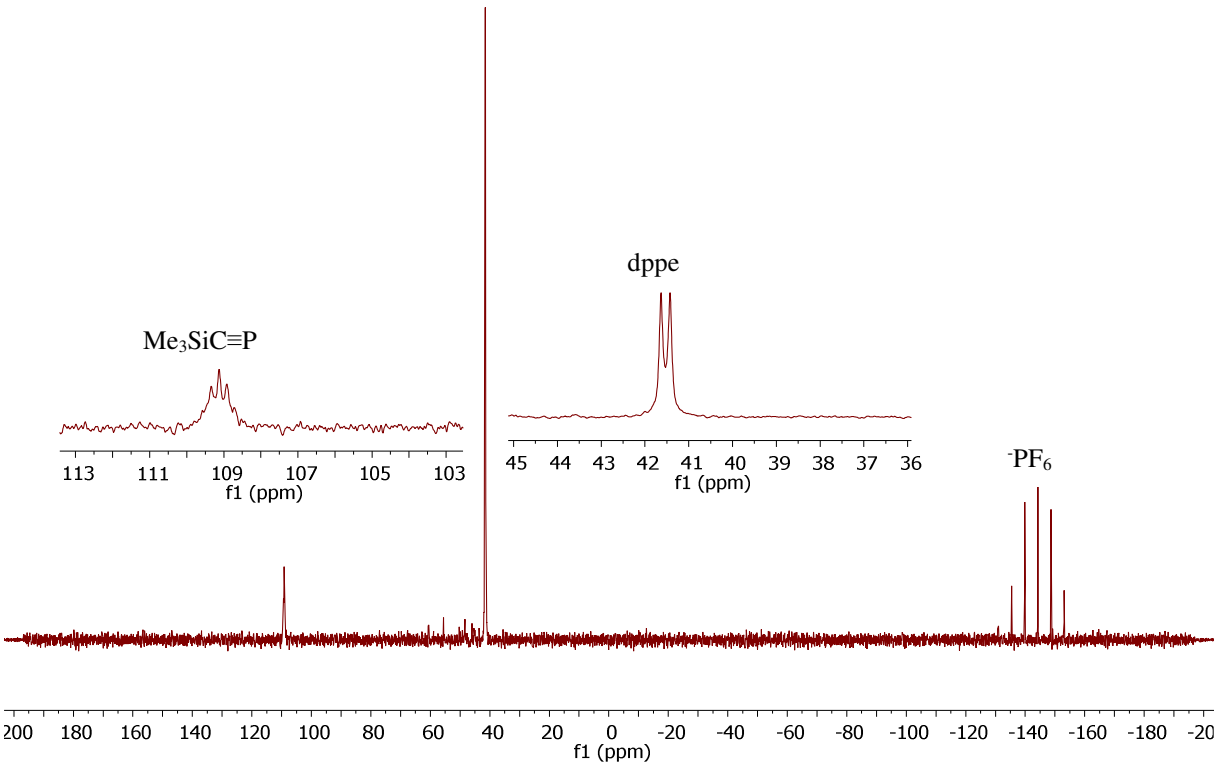


Figure S28: $^{31}P\{^{1}H\}$ NMR Spectrum ($CDCl_3$, 303 K, 162 MHz) for complex **7e·[PF$_6$]**

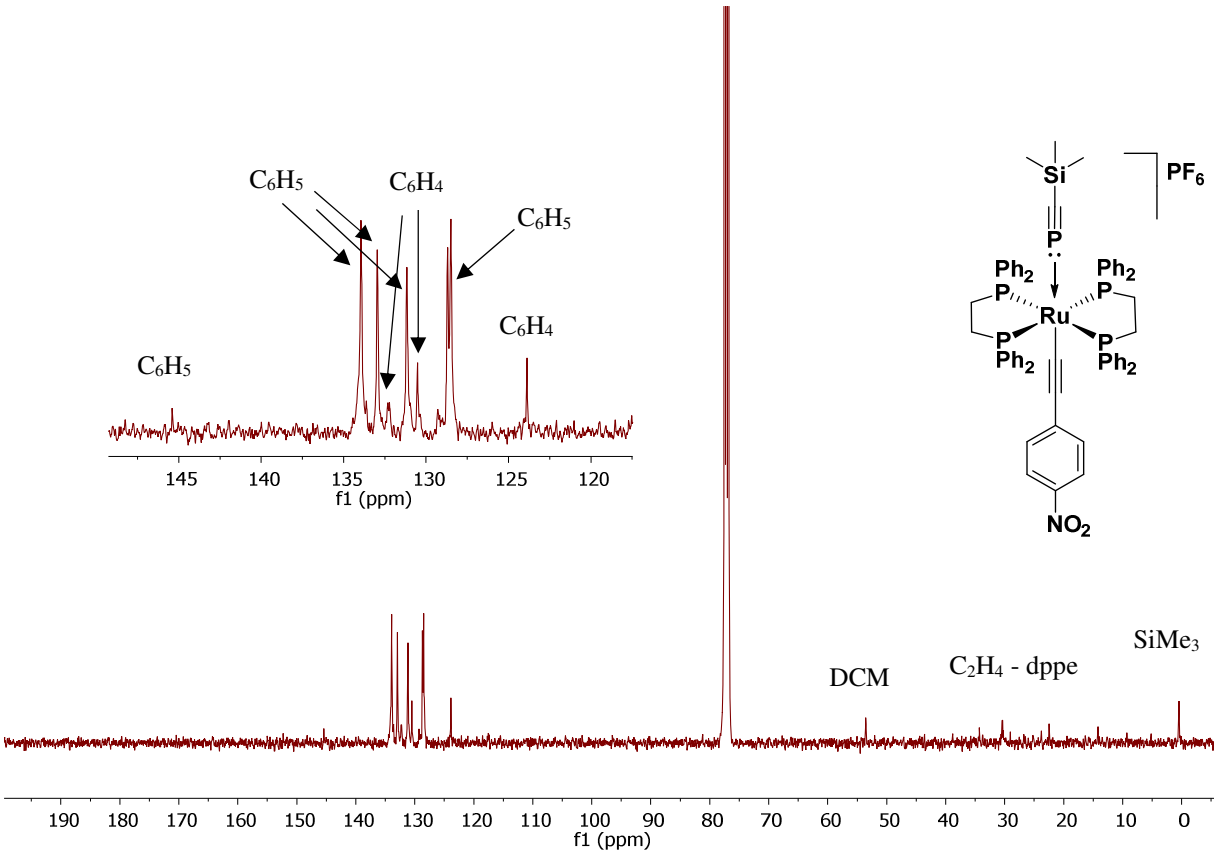


Figure S29: $^{13}C\{^{1}H\}$ NMR Spectrum ($CDCl_3$, 303 K, 162 MHz) for **7e·[PF$_6$]**

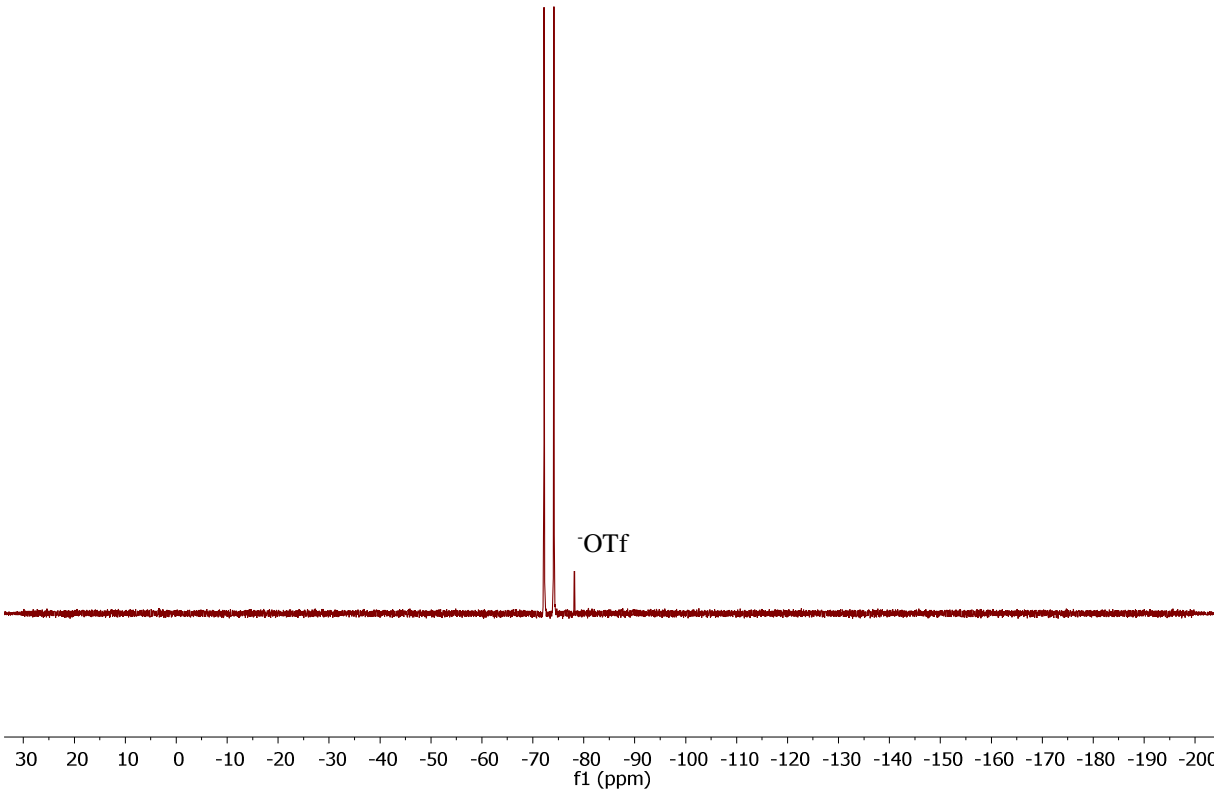


Figure S30: ^{13}F NMR Spectrum ($CDCl_3$, 303 K, 376 MHz) for complex **7e·[PF$_6$]**

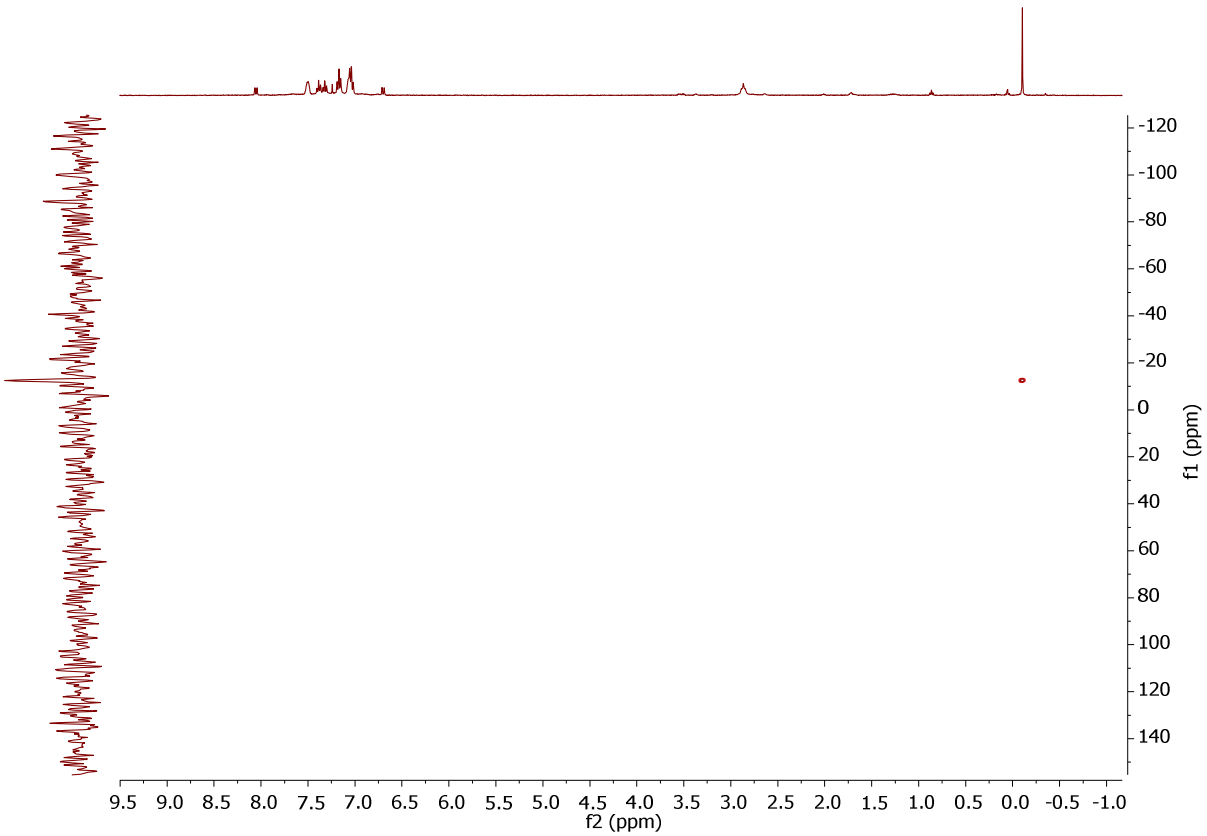


Figure S31: ^{1}H-^{29}Si HMBC trace ($CDCl_3$, 303 K, 399, 79 MHz) for complex **7e·[PF_6]**

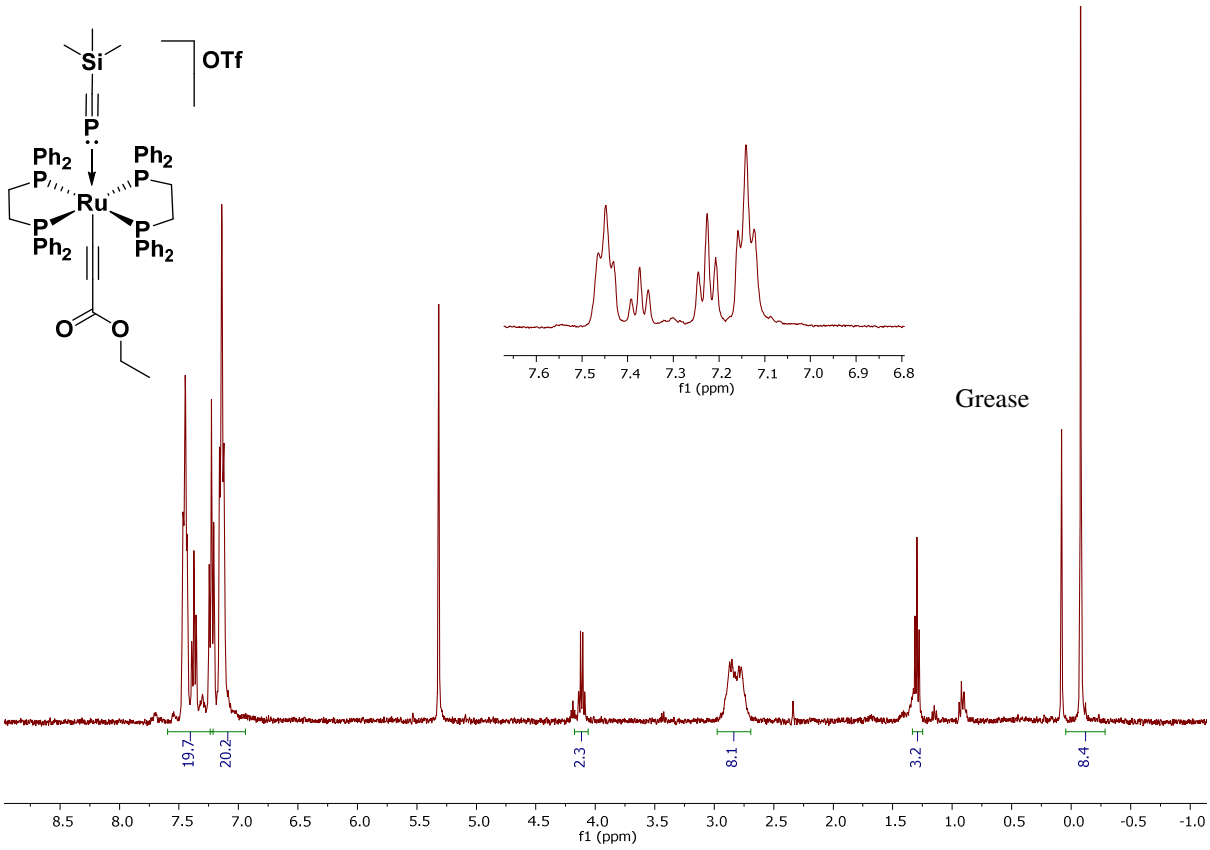


Figure S24: ^{1}H NMR Spectrum (CD_2Cl_2, 303 K, 399 MHz) for complex **7f·[OTf]**

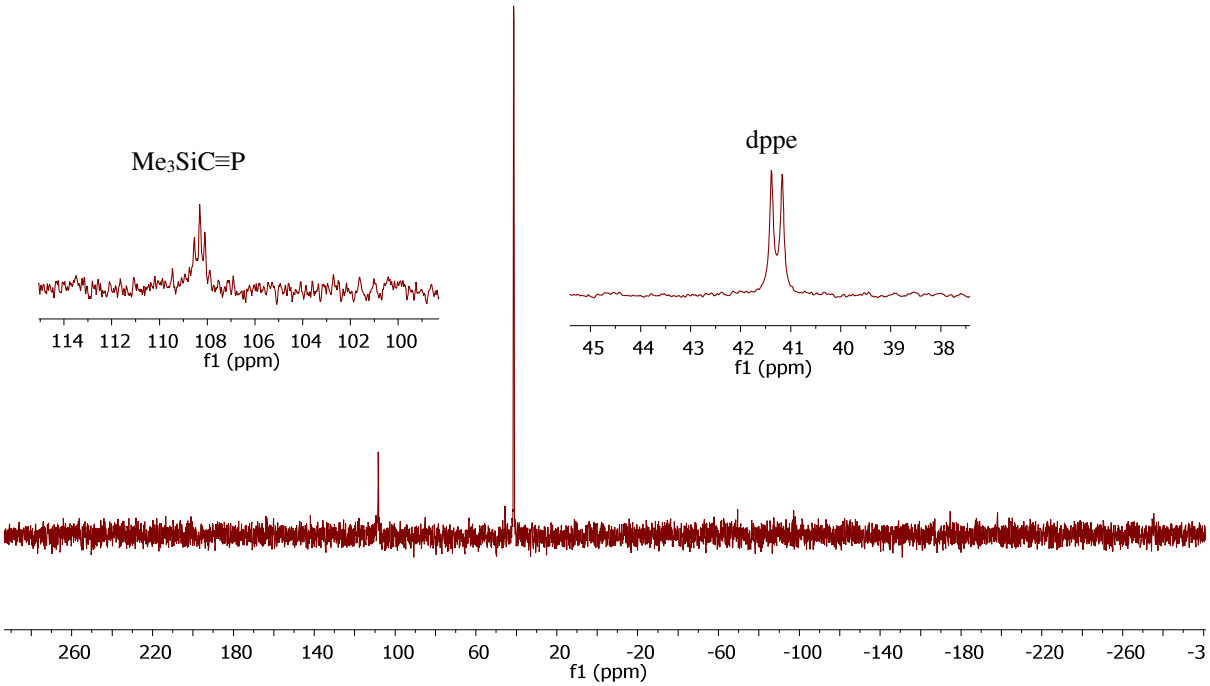


Figure S25: $^{31}P\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 162 MHz) for complex **7f·[OTf]**

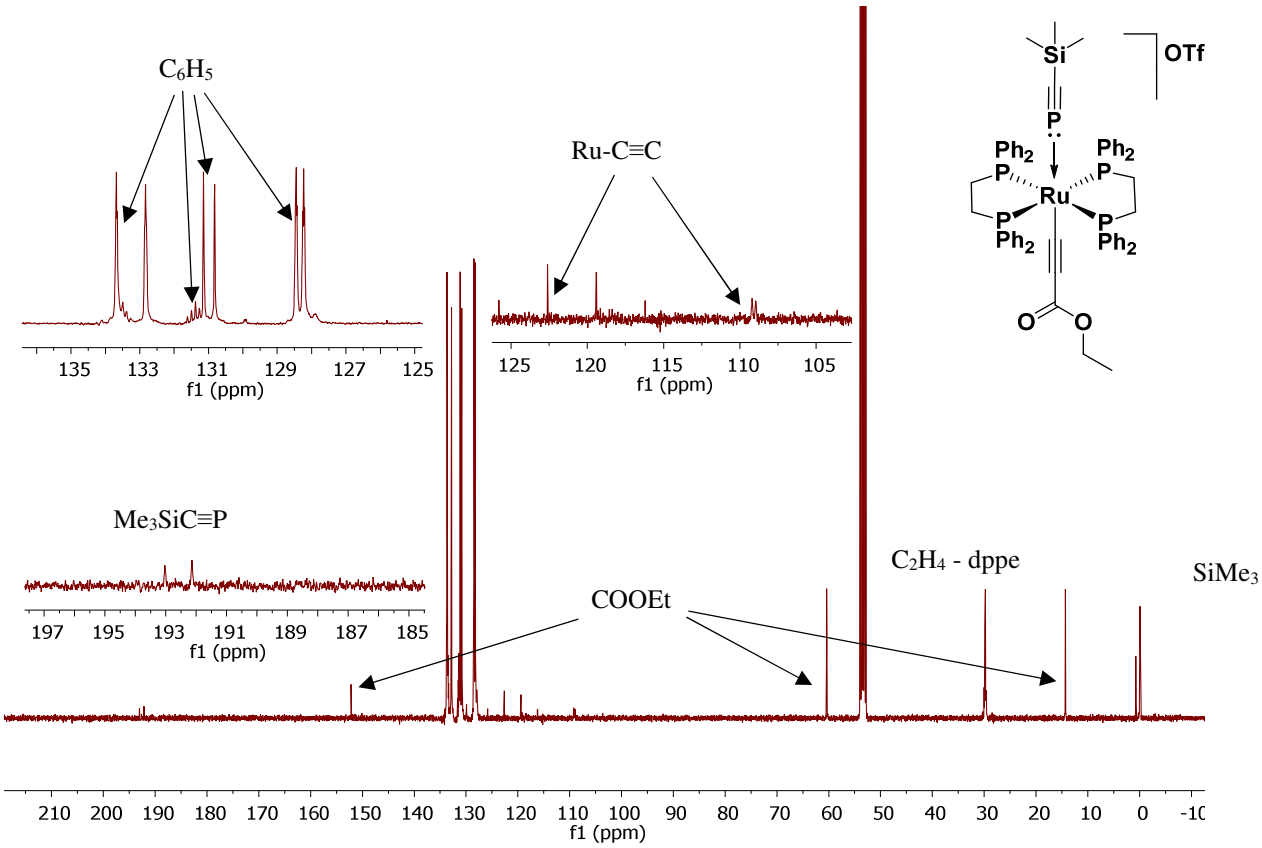


Figure S26: $^{13}C\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 100 MHz) for complex **7f·[OTf]**

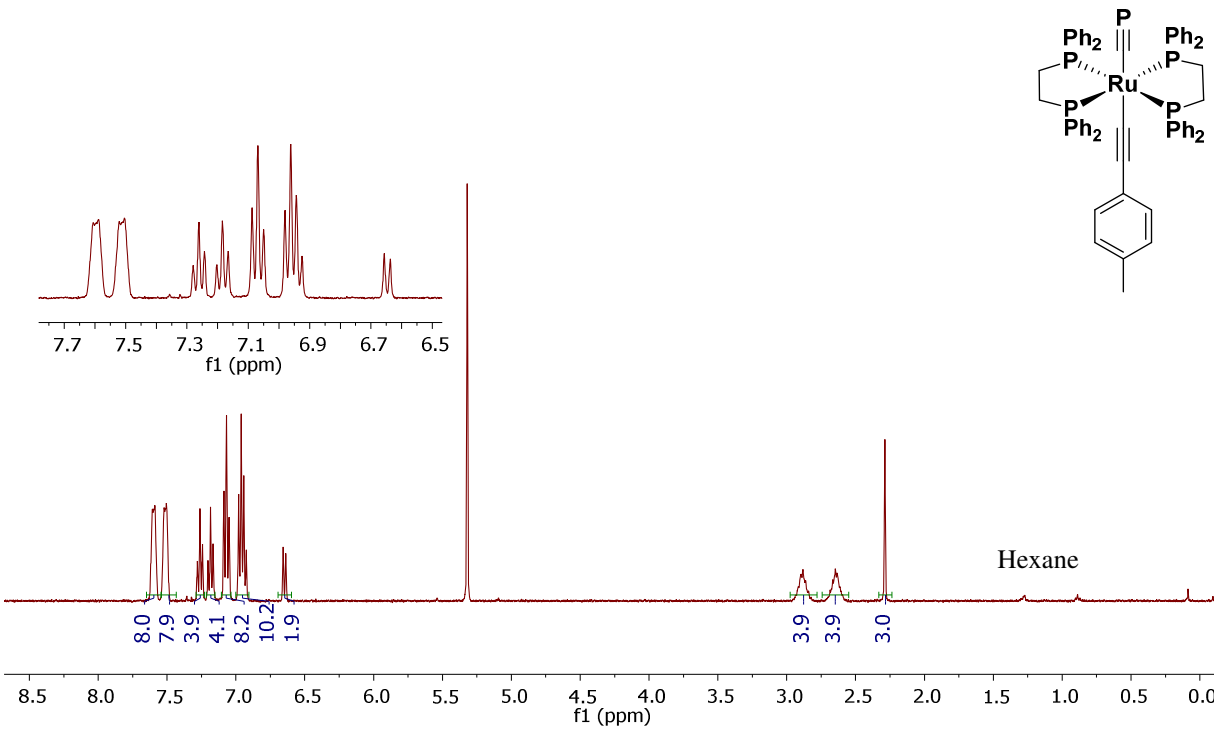


Figure S27: ^{1}H NMR Spectrum (CD_2Cl_2, 303 K, 399 MHz) for complex **8a**

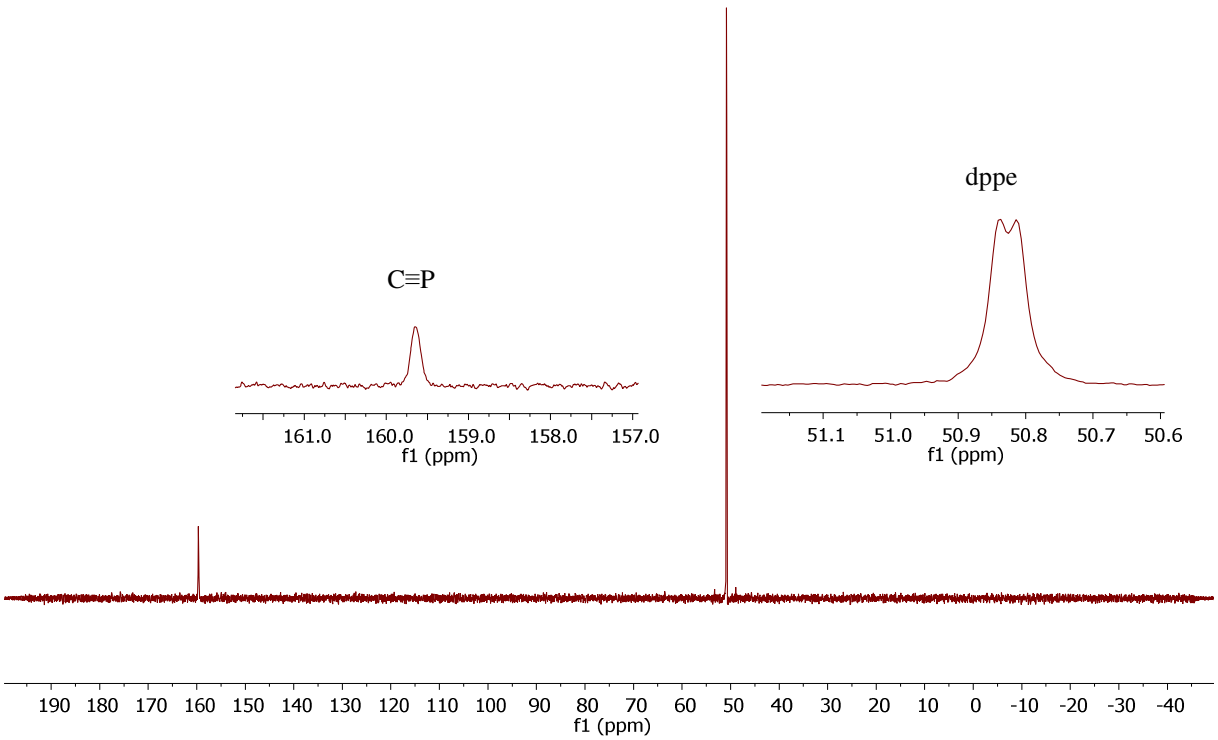


Figure S28: $^{31}P\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 162 MHz) for complex **8a**

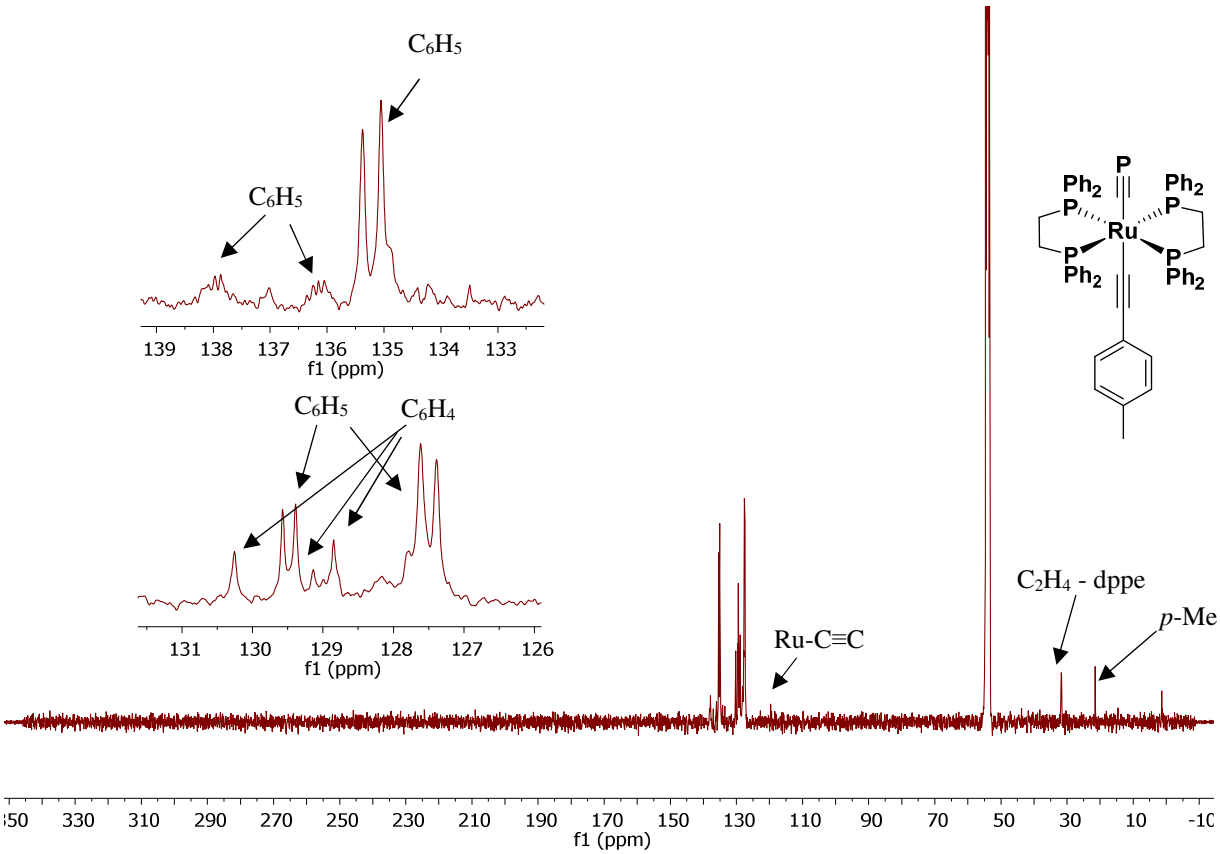


Figure S29: $^{13}C\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 100 MHz) for complex **8a**

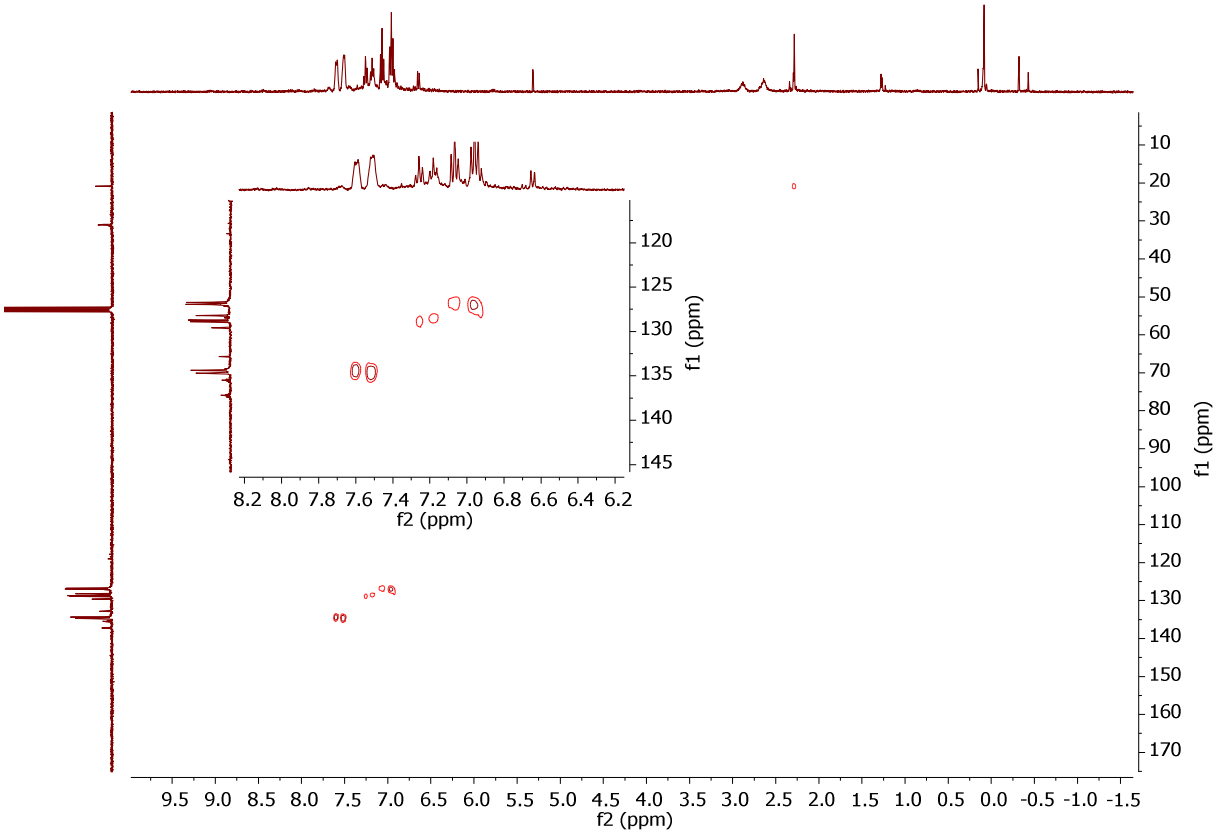


Figure S38: ^{1}H-^{13}C HSQC trace (CD_2Cl_2, 303 K, 399, 100 MHz) for complex **8a**

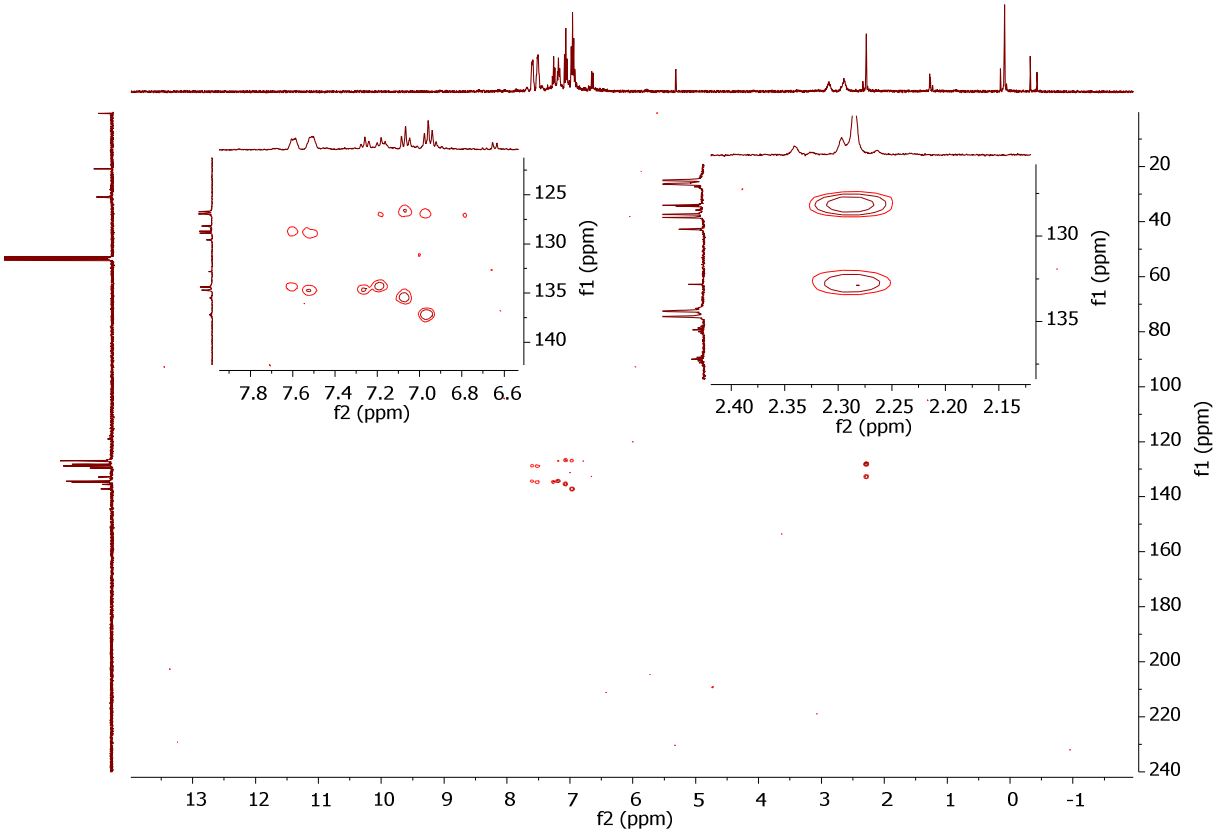


Figure S39: ^{1}H-^{13}C HMBC trace (CD_2Cl_2, 303 K, 399, 100 MHz) for complex **8a**

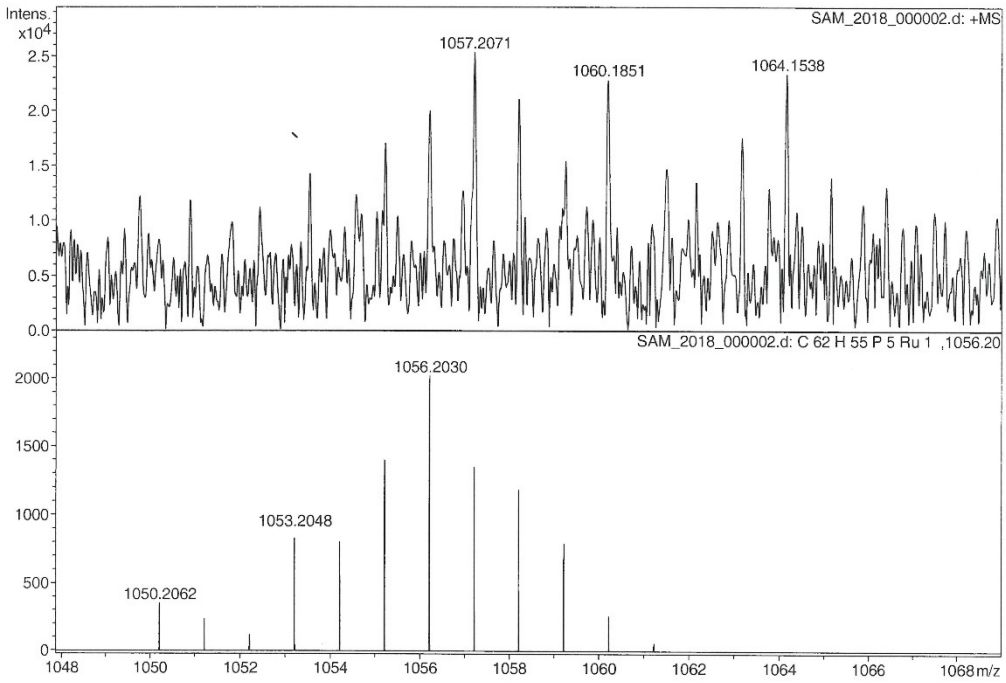


Figure S30: HR-ESI^{+} complex **8a** (top, observed for $[MH]^{+}$ and bottom, simulated for $[M]^{+}$)

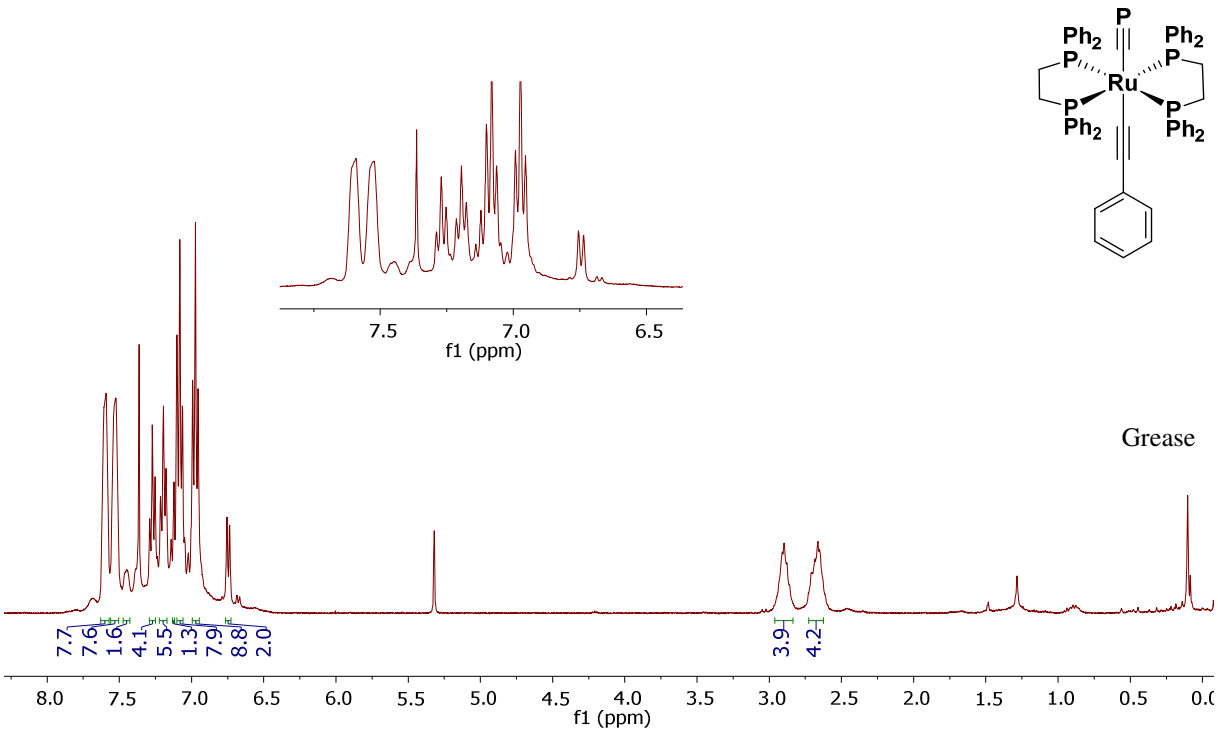


Figure S31: ^{1}H NMR Spectrum (CD_2Cl_2, 303 K, 399 MHz) for complex **8b**

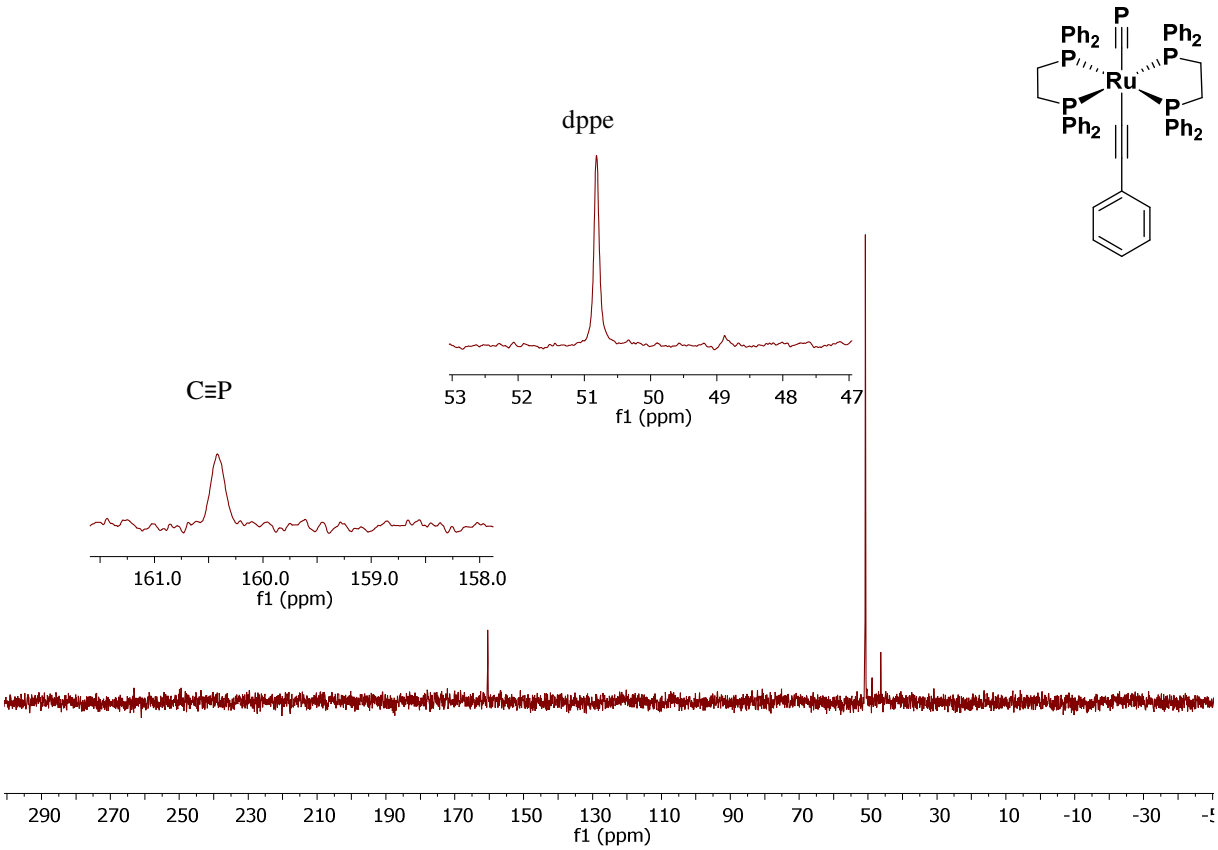


Figure S32: $^{31}P\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 162 MHz) for complex **8b**

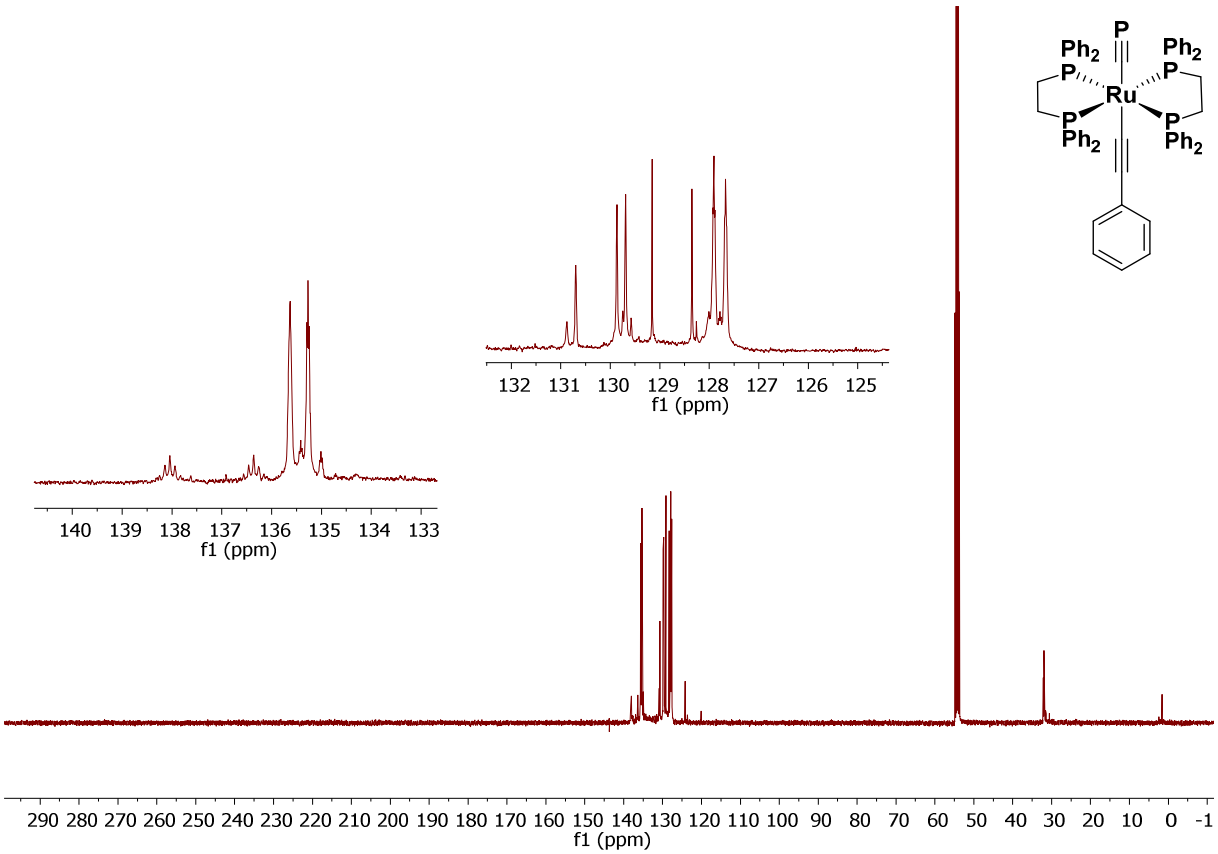


Figure S33: $^{13}C\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 100 MHz) for complex **8b**

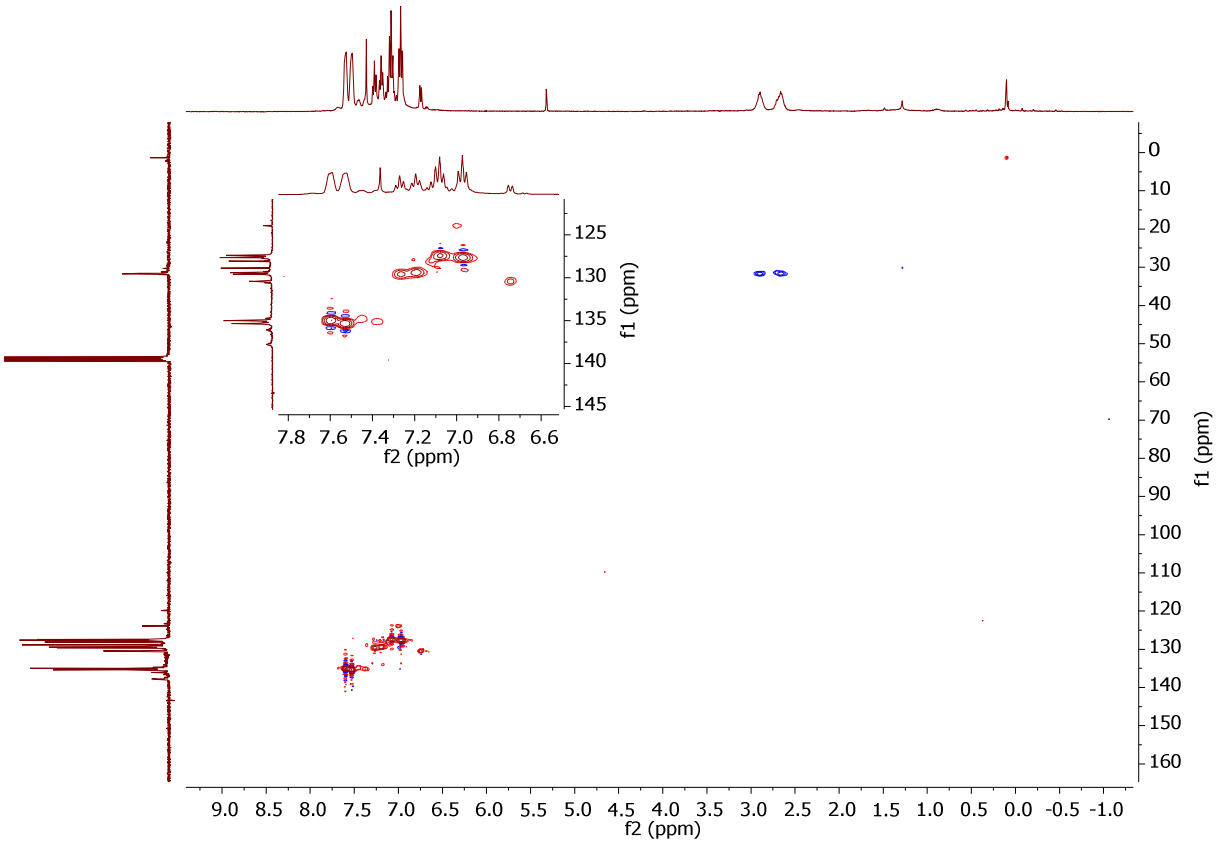


Figure S34: ^{1}H-^{13}C HSQC trace (CD_2Cl_2, 303 K, 399, 100 MHz) for complex **8b**

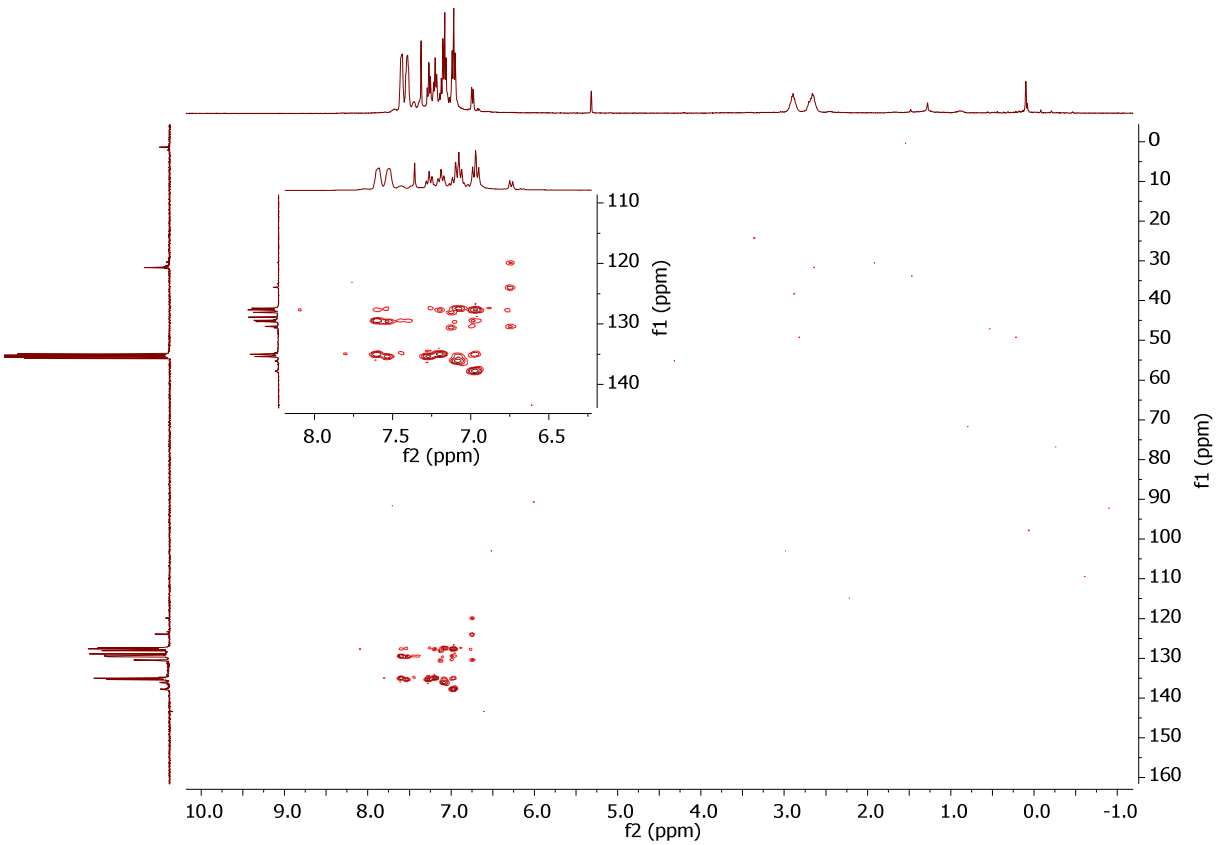


Figure S35: ^{1}H-^{13}C HMBC trace (CD_2Cl_2, 303 K, 399, 100 MHz) for complex **8b**

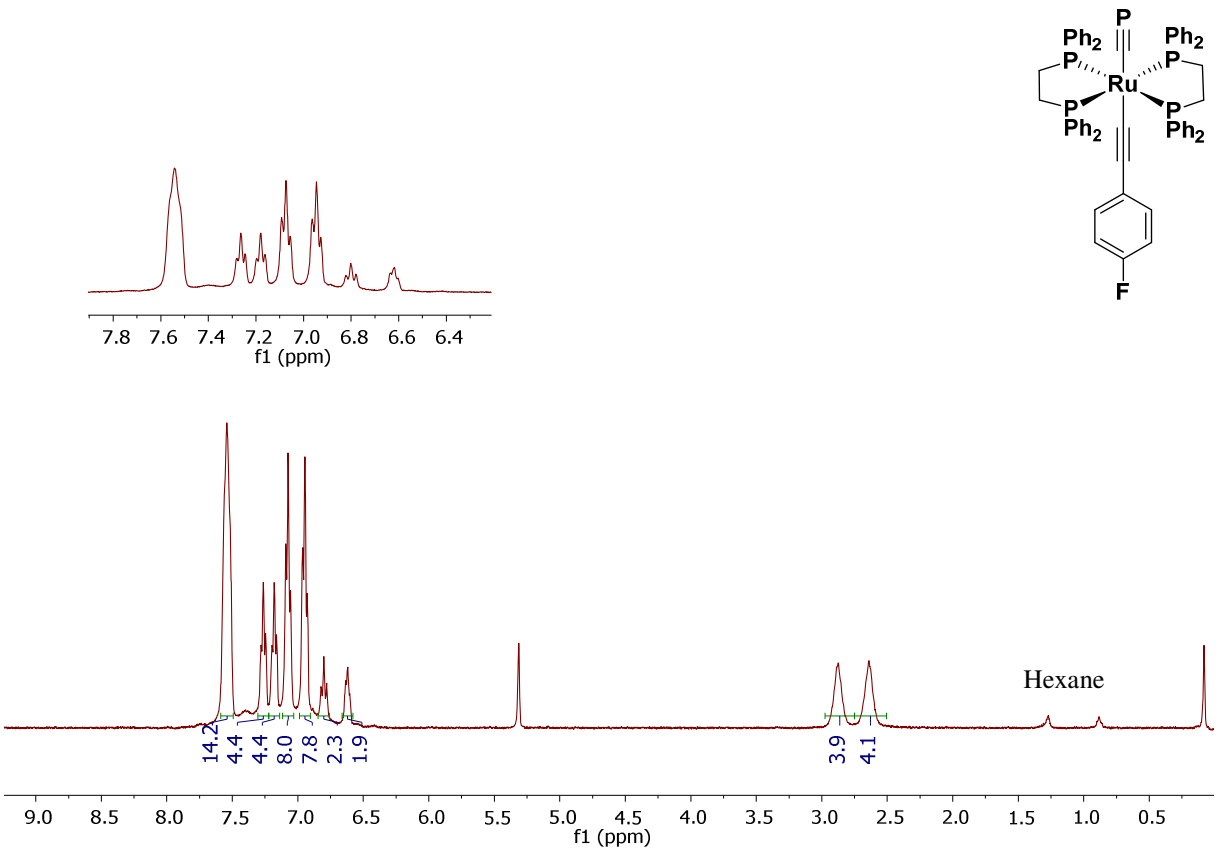


Figure S36: ^{1}H NMR Spectrum (CD_2Cl_2, 303 K, 399 MHz) for complex **8c**

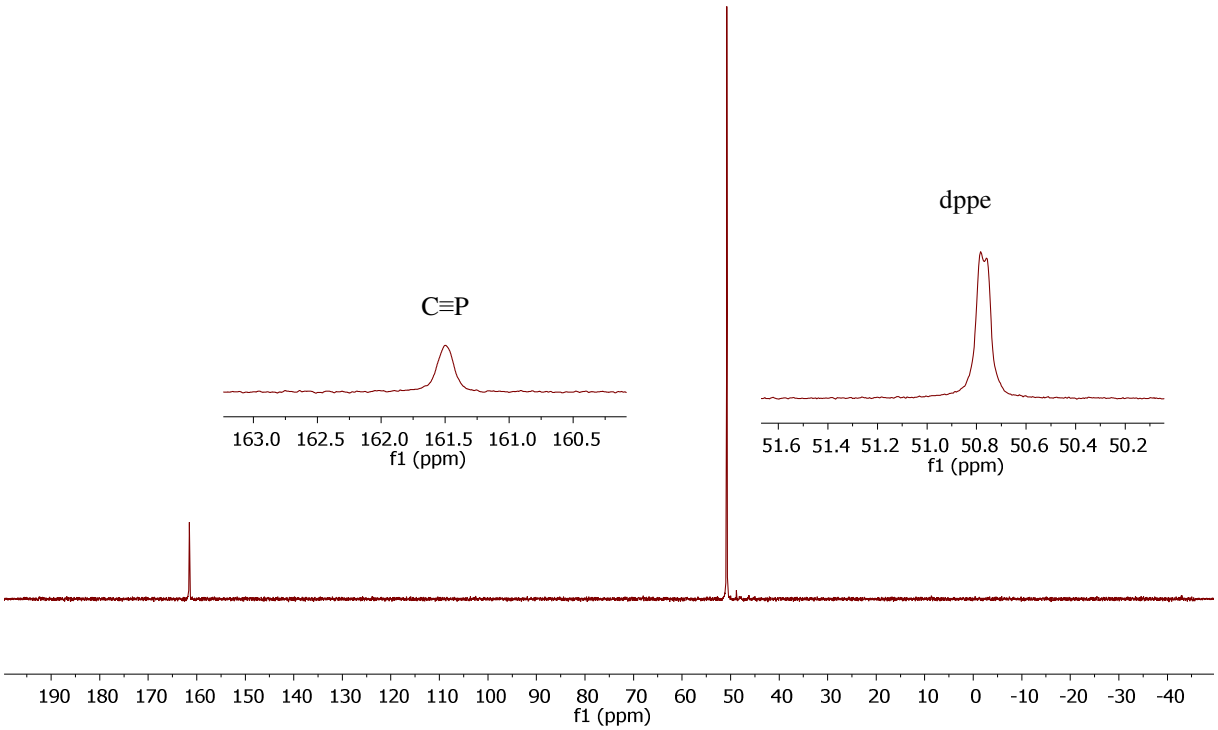


Figure S37: $^{31}P\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 162 MHz) for complex **8c**

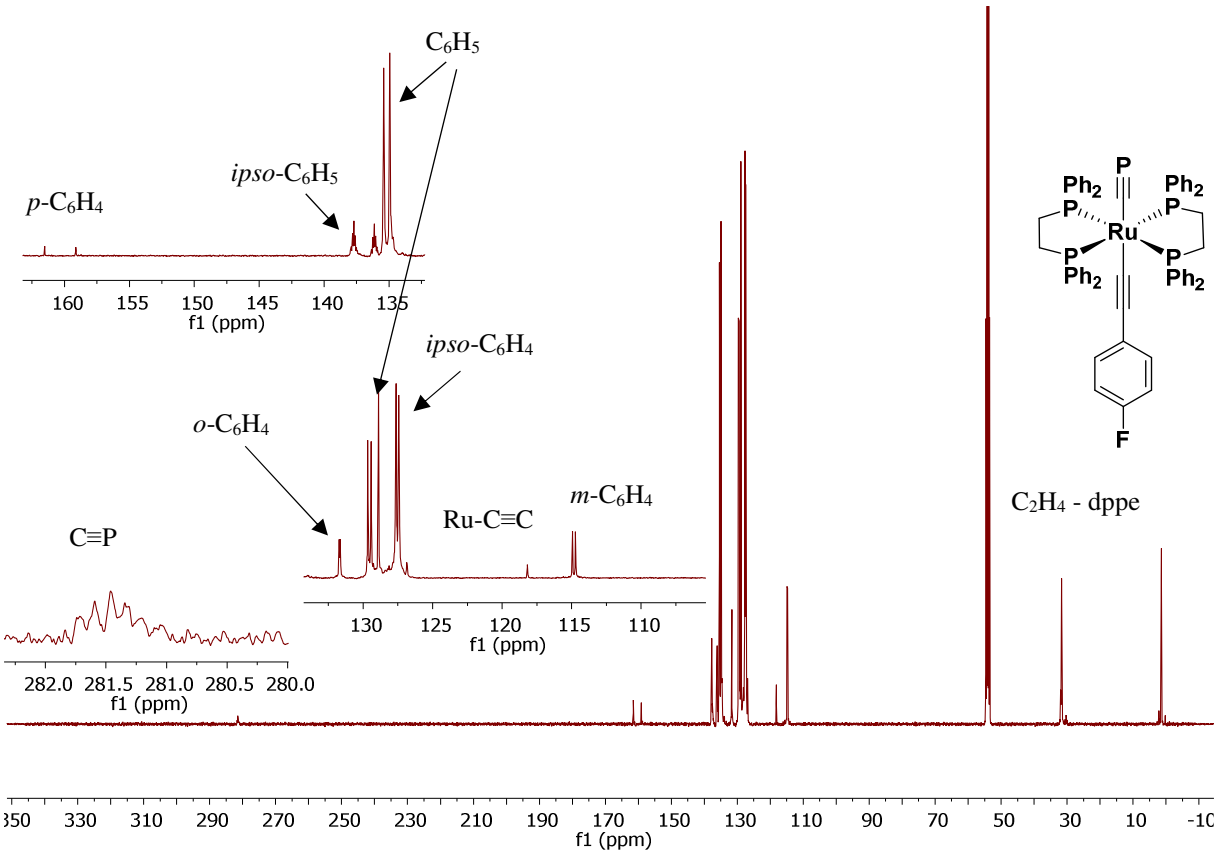


Figure S48: $^{13}C\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 100 MHz) for complex **8c**

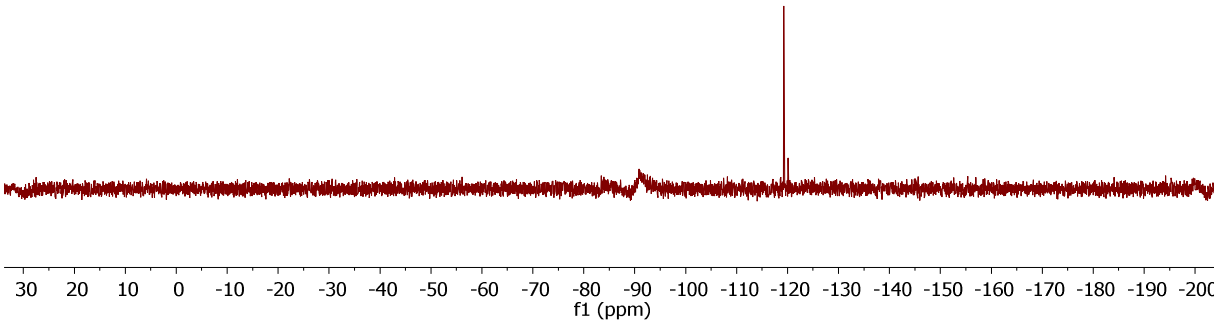


Figure S49: ^{19}F NMR Spectrum (CD_2Cl_2, 303 K, 376 MHz) for complex **8c**

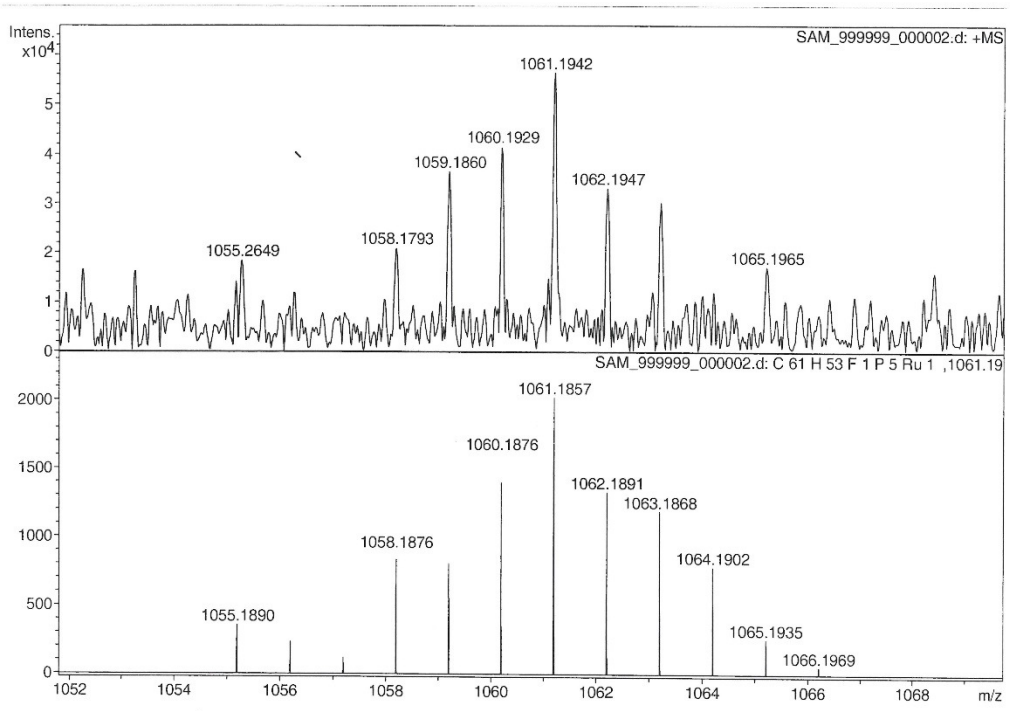


Figure S38: HR-ESI$^+$ complex **8c** (top, observed for $[M]^+$ and bottom, simulated for $[M]^+$**)**

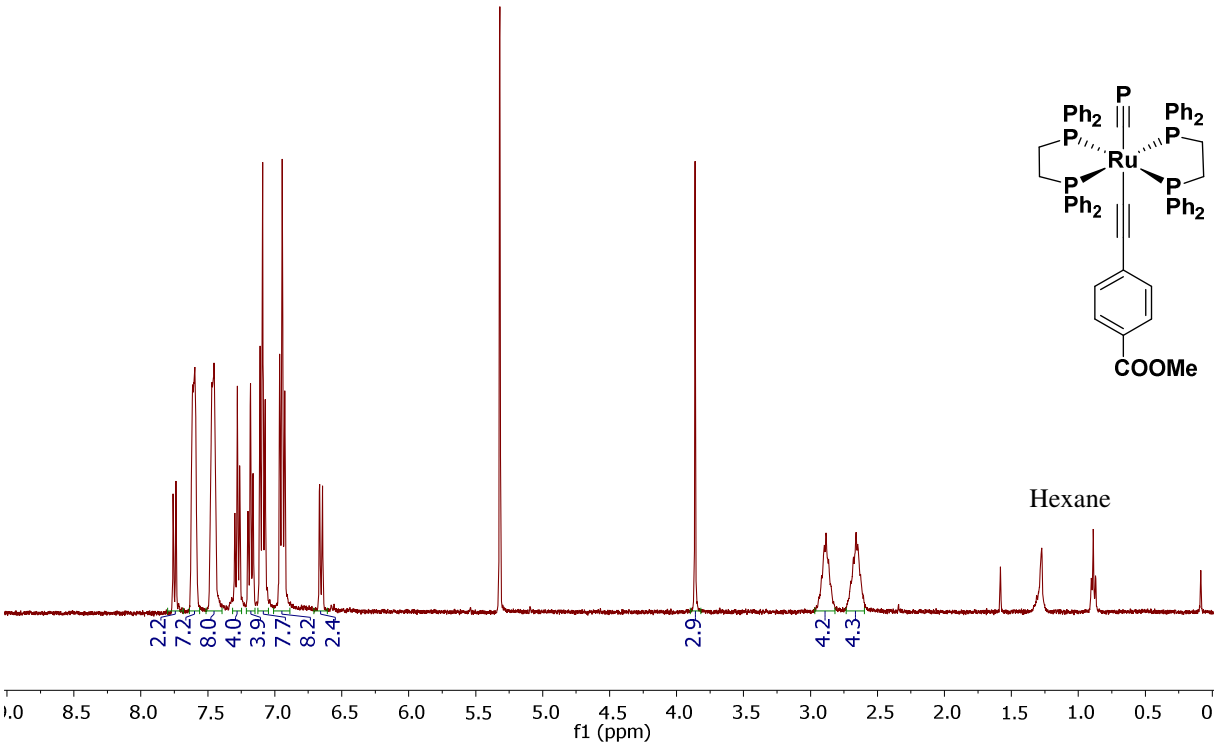


Figure S39: ^{1}H NMR Spectrum (CD_2Cl_2, 303 K, 399 MHz) for complex **8d**

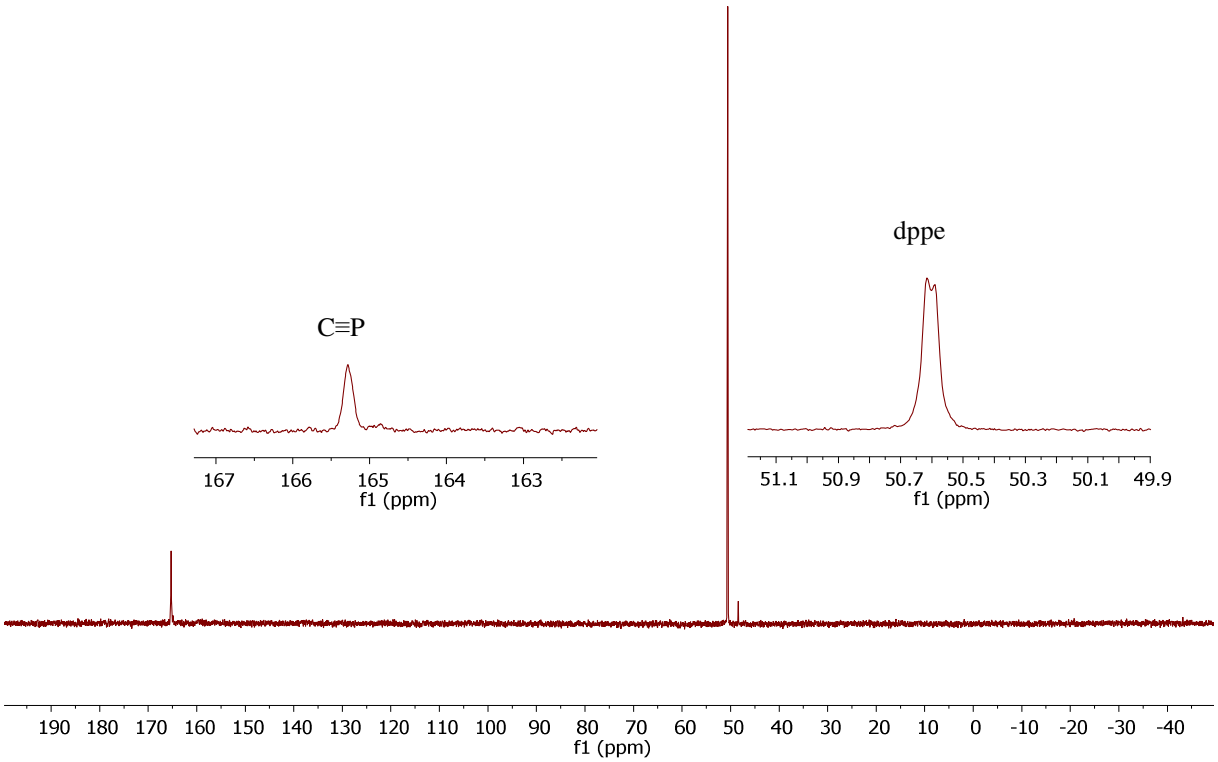


Figure S40: $^{31}P\{1H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 162 MHz) for complex **8d**

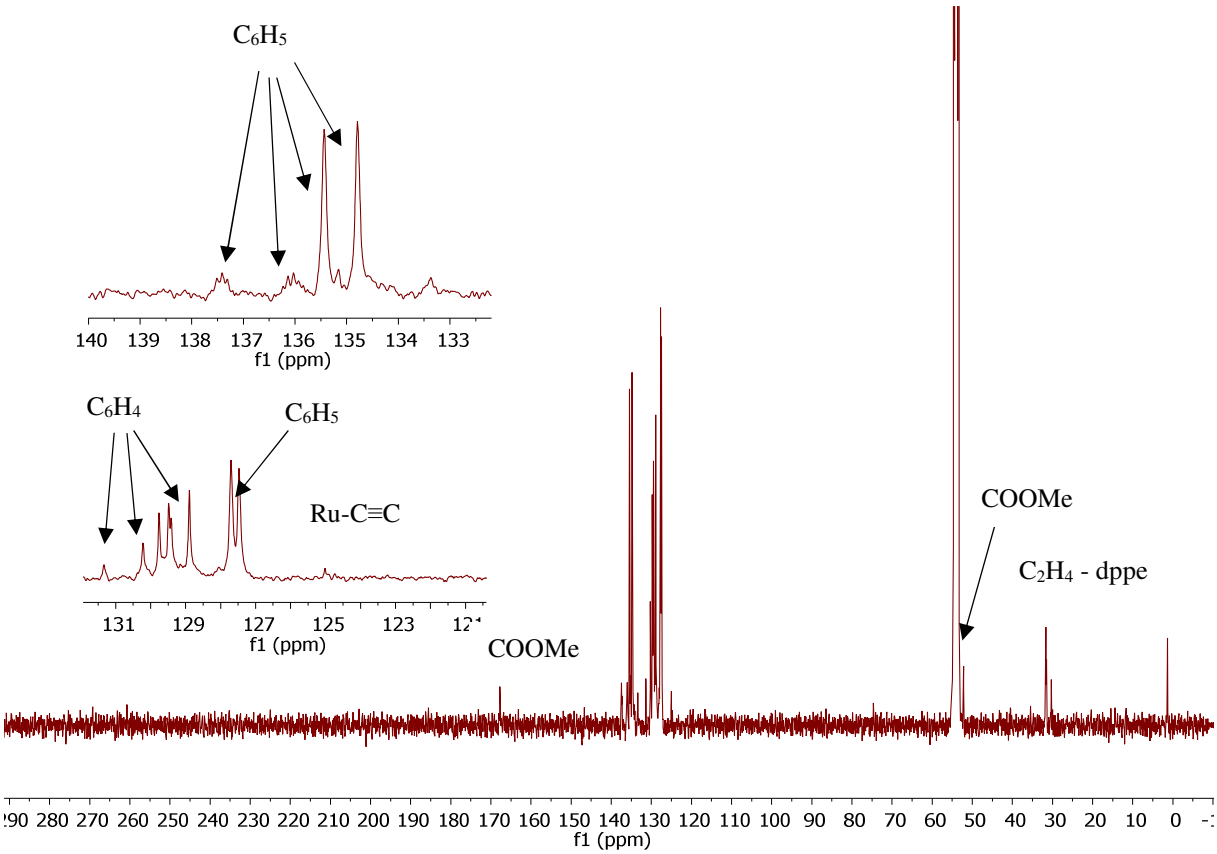


Figure S41: $^{13}C\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 100 MHz) for complex **8d**

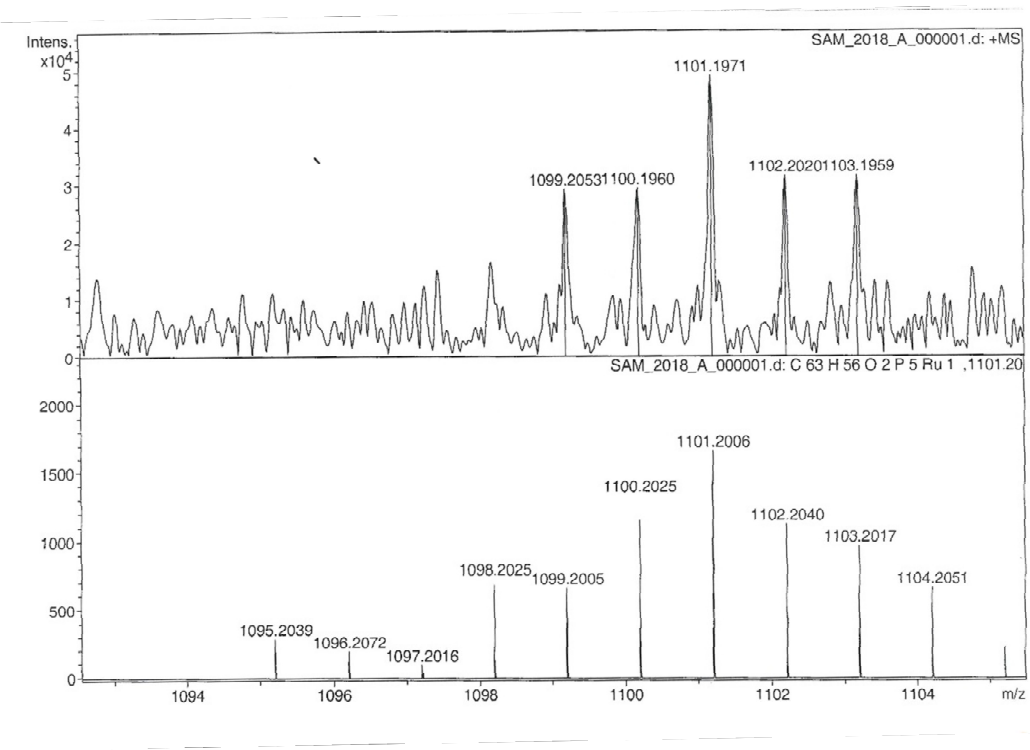


Figure S42: HR-ESI^{+} complex **8d** (top, observed for $[M]^{+}$ and bottom, simulated for $[M]^{+}$)

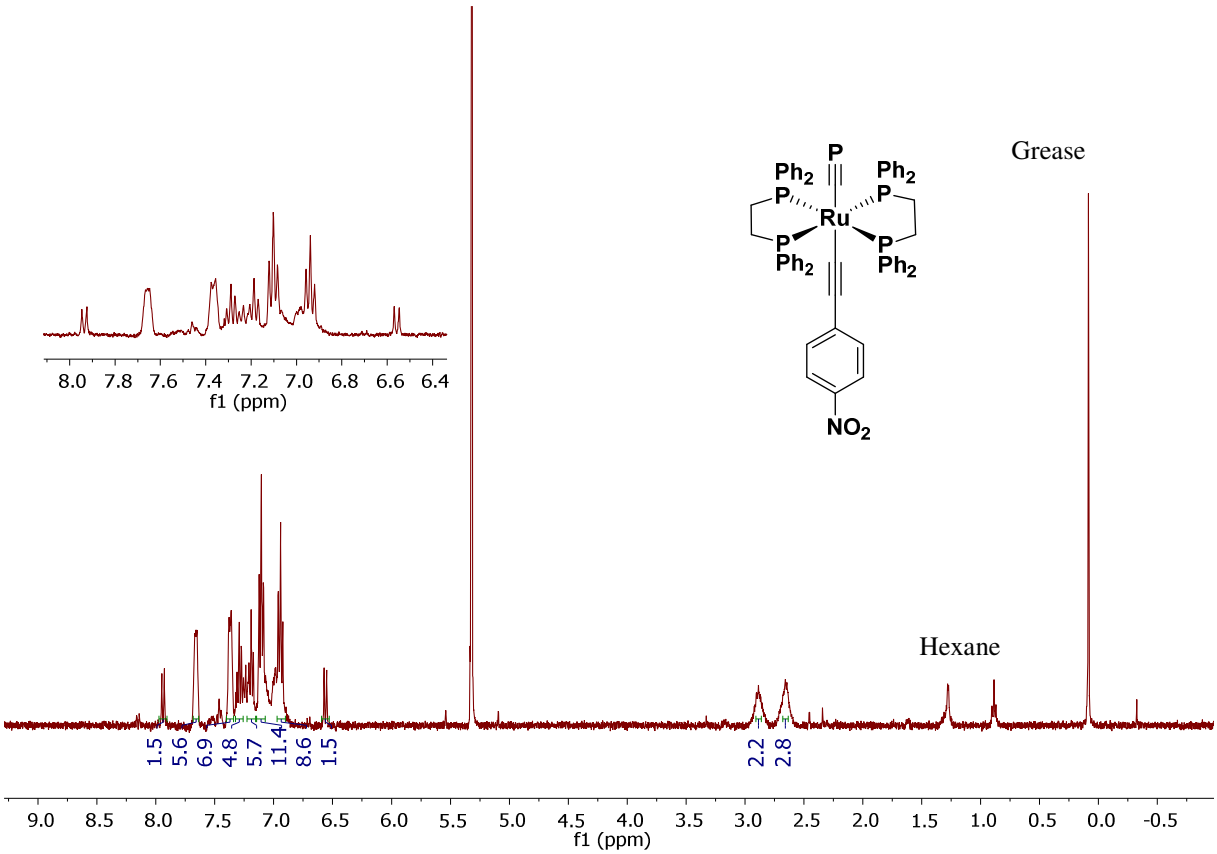


Figure S43: ^{1}H NMR Spectrum (CD_2Cl_2, 303 K, 399 MHz) for complex **8e**

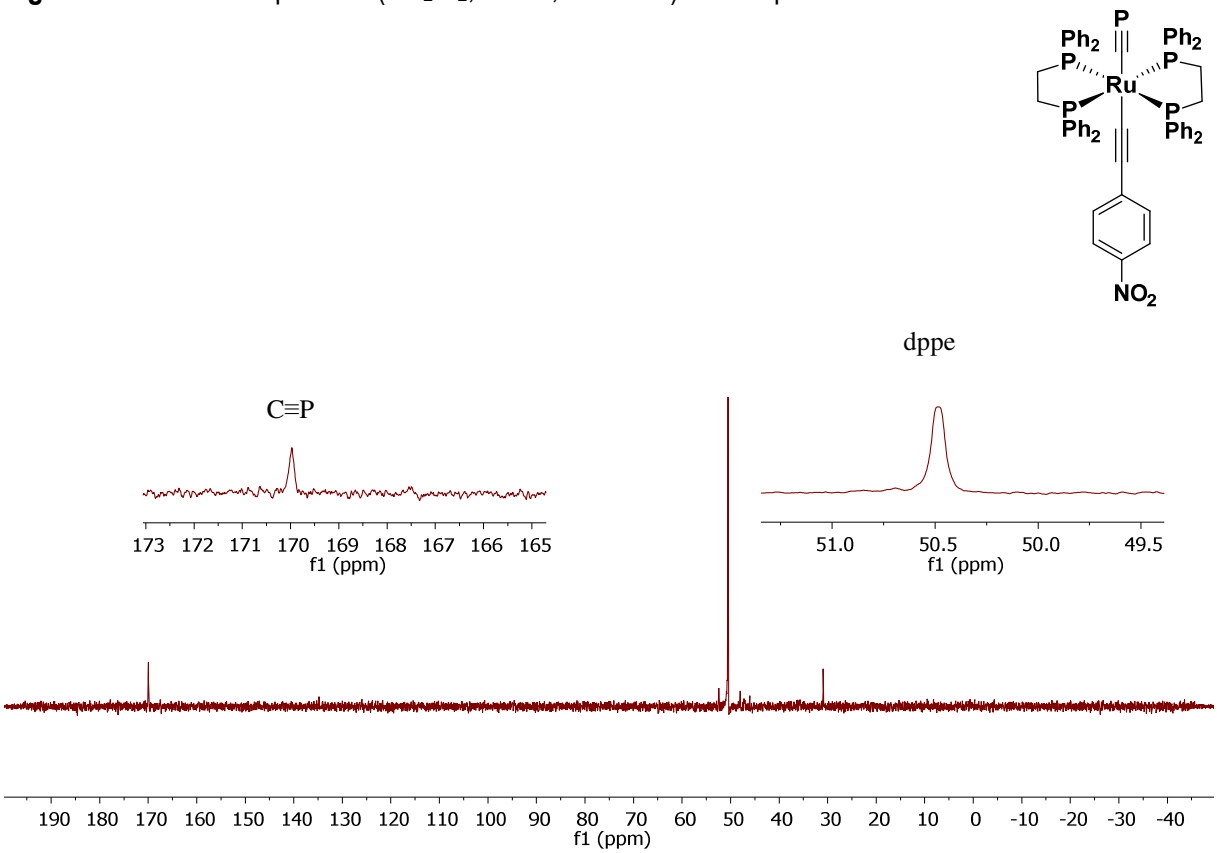


Figure S56: $^{31}P\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 162 MHz) for complex **8e**

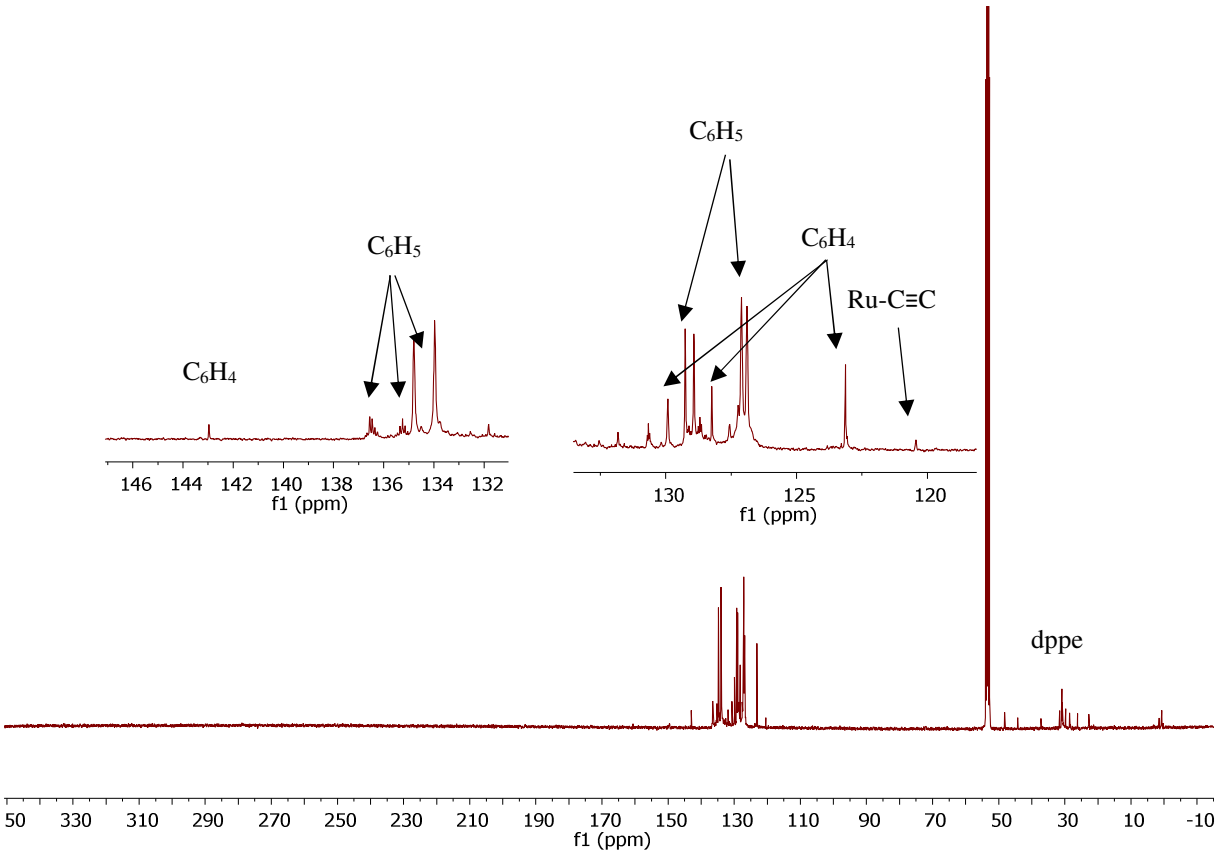


Figure S57: $^{13}C\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 100 MHz) for complex **8e**

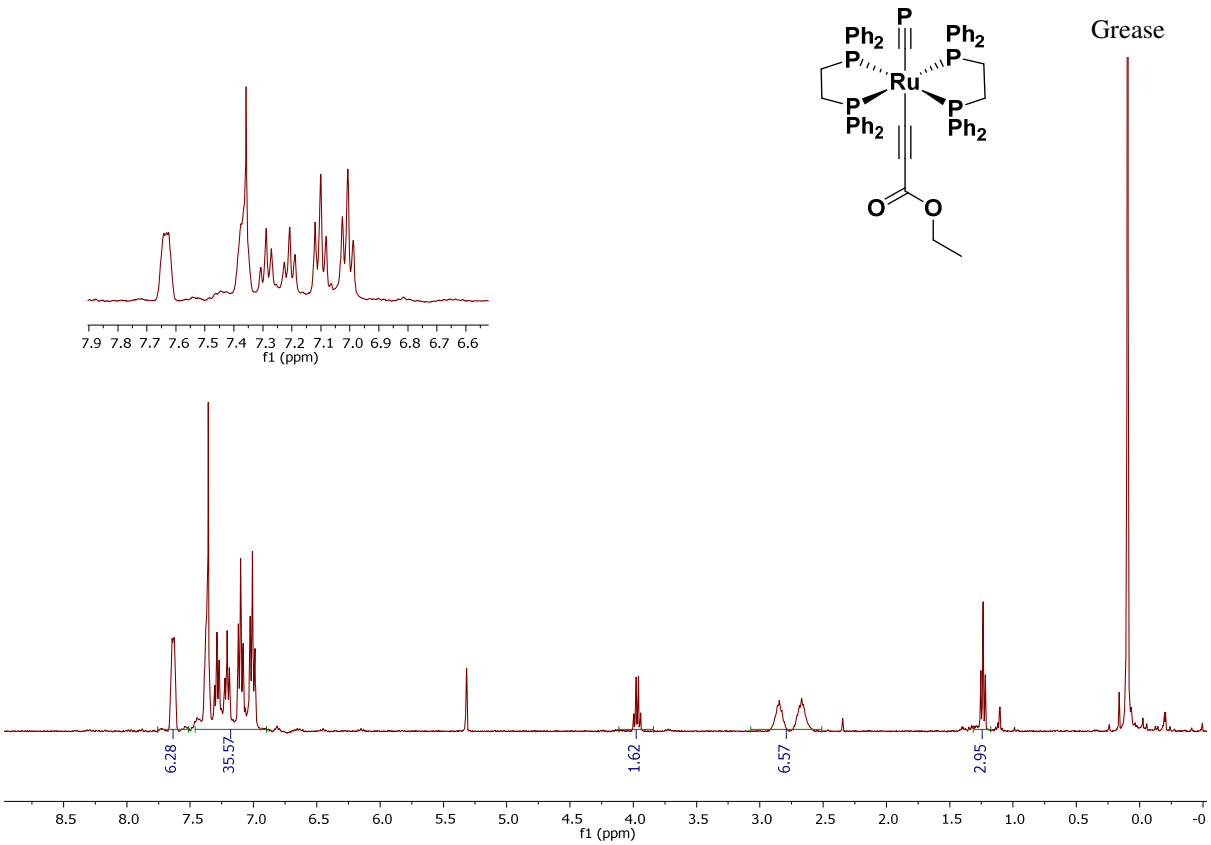


Figure S58: ^{1}H NMR Spectrum (CD_2Cl_2, 303 K, 399 MHz) for complex **8f**

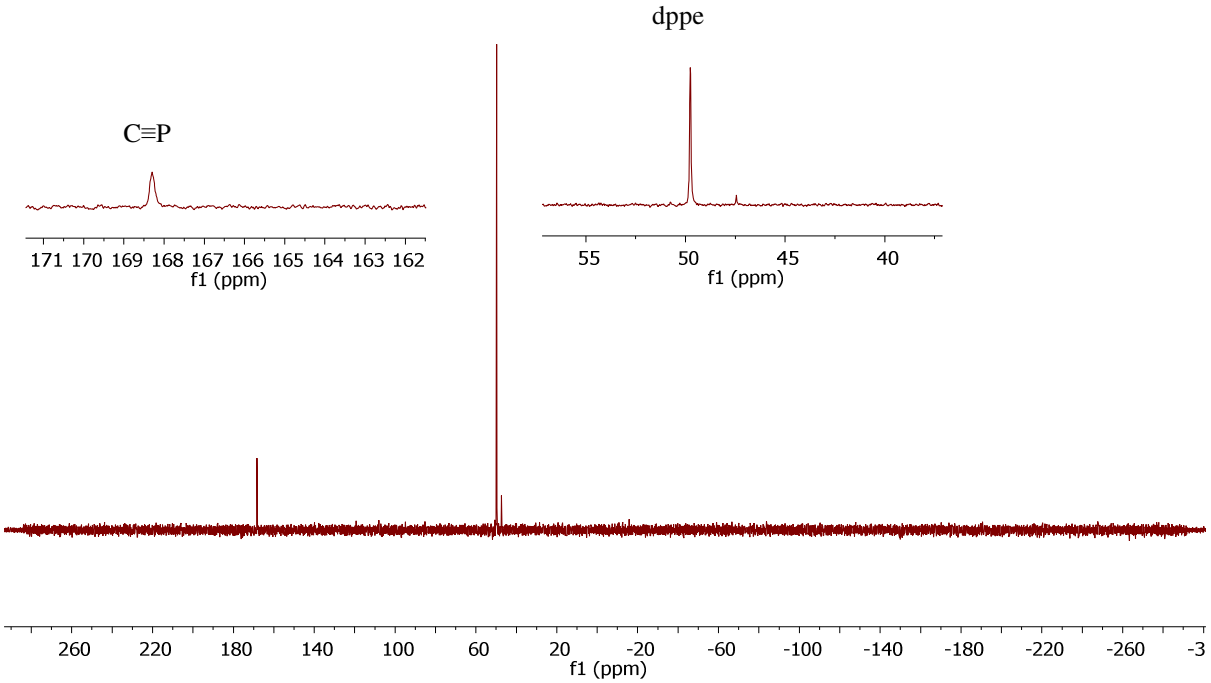


Figure S59: $^{31}P\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 162 MHz) for complex **8f**

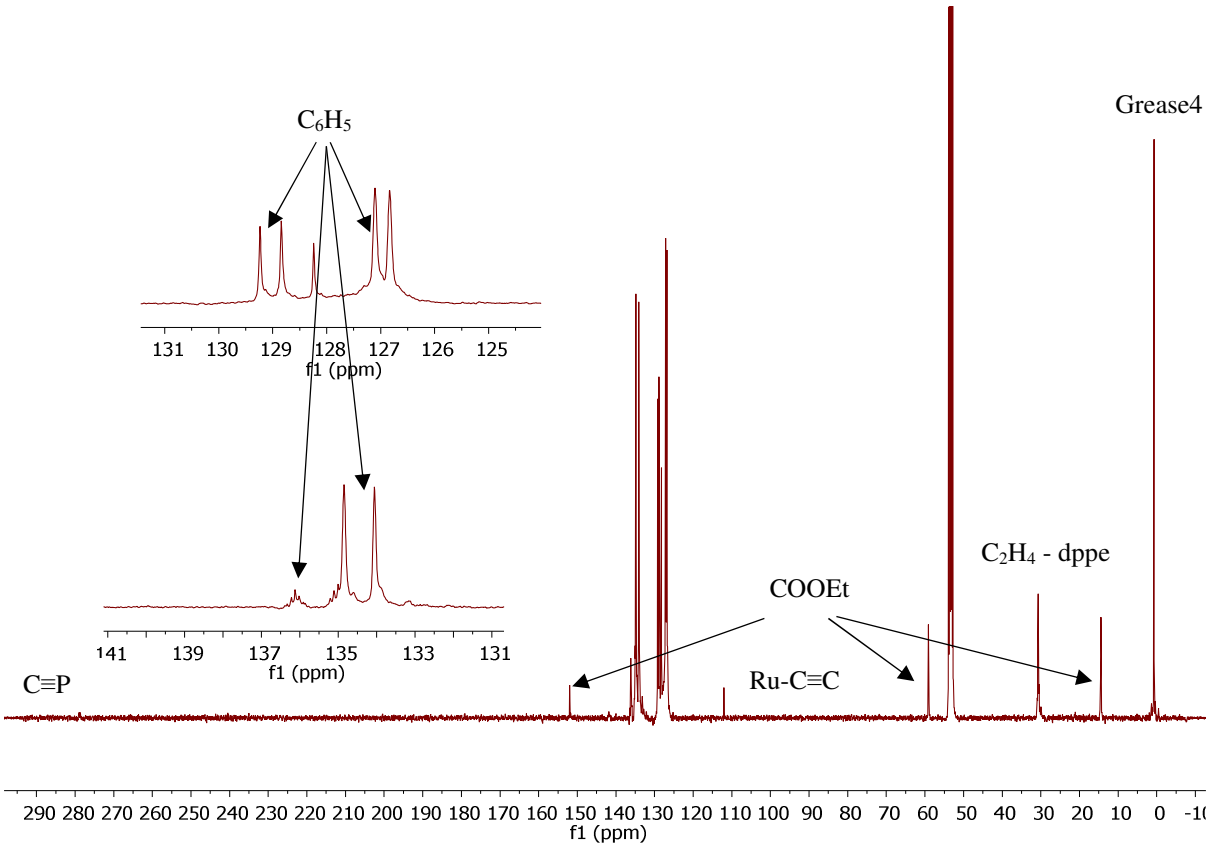


Figure S44: $^{13}C\{^{1}H\}$ NMR Spectrum (CD_2Cl_2, 303 K, 100 MHz) for complex **8f**

Crystallographic and Computational Details

X-ray diffraction data for Compounds **3** (1902215) **7a.PF$_6$** (1902212), **7c.PF$_6$** (1902216), **8c** (1902214) and **8d** (1902213) have been deposited in the CCDC with the submission numbers shown and are available in cif format free of charge from the Cambridge Crystallographic Data centre (http://www.ccdc.cam.ac.uk).

Computational Data

The supplemental file cyaphides.xyz contains the computed Cartesian coordinates of compounds **8a- 8e** inclusive. This file may be opened as a text file to read the coordinates, or directly by a molecular modelling program such as Mercury (Version 3.3. or later, http://www.ccdc.cam.ac.uk/pages/Home.aspx) for visualisation and analysis.

Table S1. Composition of selected molecular orbitals for **8a** (Ar = C_6H_4Me).

Orbital	Energy / eV	% Ru	%C≡P	%C≡C	%Ar	%dppe
L+20	0.77	8	65	1	5	21
L+19	0.59	7	70	3	2	18
L+18	0.42	16	9	0	2	72
L+17	0.35	0	0	0	93	7
L+16	0.29	1	1	0	0	98
L+15	0.24	1	0	0	2	98
L+14	0.19	2	1	0	1	97
L+13	0.16	1	1	1	1	97
L+12	0.08	0	2	3	10	85
L+11	-0.04	1	4	10	46	39
L+10	-0.07	1	1	1	4	92
L+9	-0.13	1	0	1	5	92
L+8	-0.18	1	3	0	1	95
L+7	-0.21	1	0	0	2	96
L+6	-0.26	1	1	1	1	95
L+5	-0.33	0	1	0	2	97
L+4	-0.4	2	1	1	1	96
L+3	-0.42	1	1	0	0	98
L+2	-0.5	3	1	1	0	95
L+1	-0.53	3	0	0	0	97
LUMO	-0.93	24	0	0	0	76
HOMO	-4.43	33	29	20	14	4
H-1	-4.61	35	43	14	2	5
H-2	-5.19	2	38	23	23	14
H-3	-5.58	3	27	44	3	23
H-4	-5.94	81	1	0	0	18
H-5	-6.19	11	4	1	4	80
H-6	-6.26	15	12	3	5	65
H-7	-6.3	10	48	15	1	25
H-8	-6.4	0	0	0	97	3
H-9	-6.44	14	9	2	5	70
H-10	-6.49	6	2	0	4	88

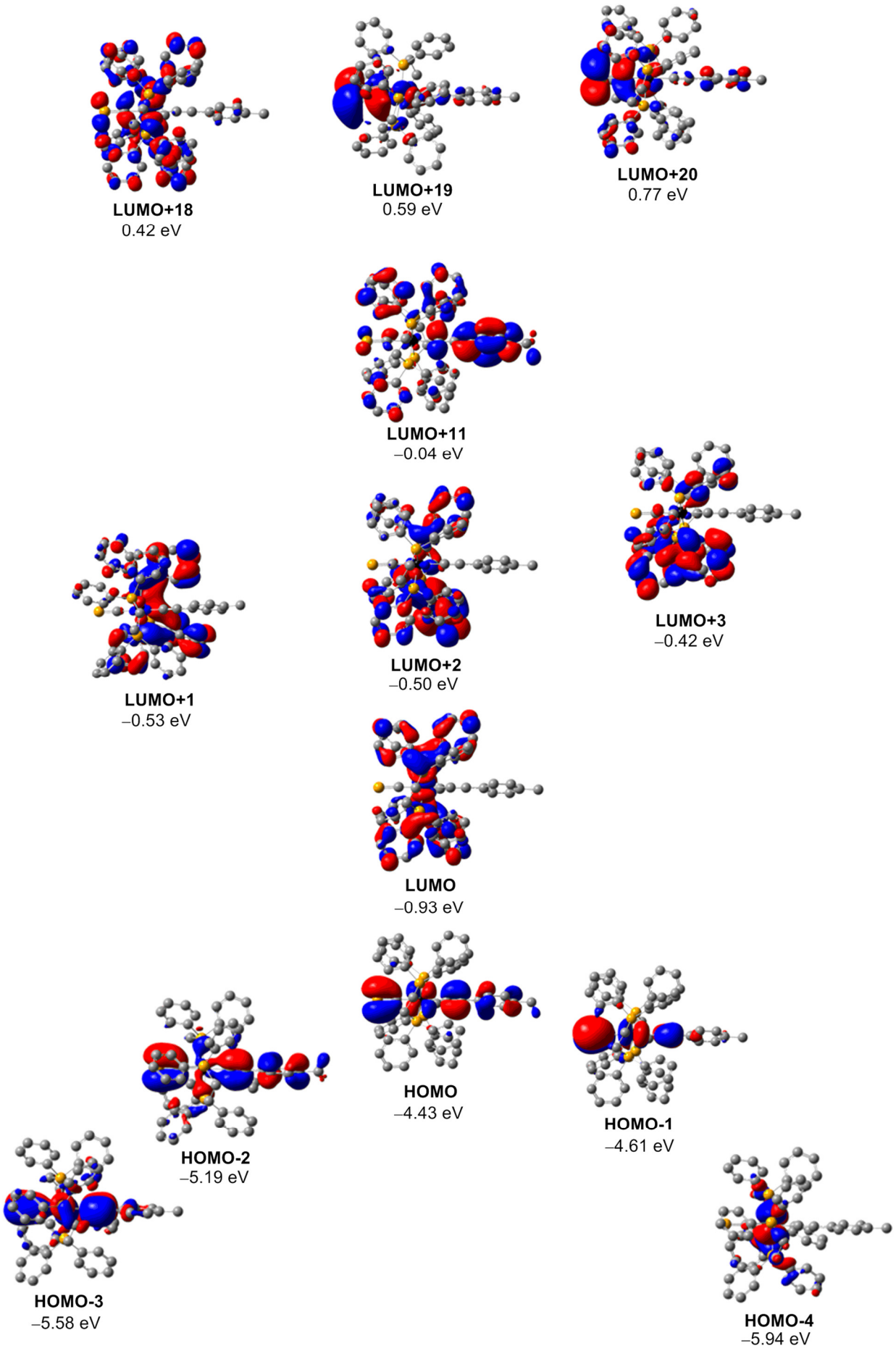


Figure S61 Selected molecular orbitals of compound **8a**

Table S2. Composition of selected molecular orbitals for **8b** (Ar = Ph).

Orbital	Energy / eV	% Ru	%C≡P	%C≡C	%Ar	%dppe
L+20	0.66	9	65	1	7	18
L+19	0.54	11	41	2	2	44
L+18	0.4	11	35	1	8	45
L+17	0.34	1	1	0	70	27
L+16	0.27	1	1	0	16	82
L+15	0.22	1	1	0	0	98
L+14	0.19	0	2	0	0	97
L+13	0.17	2	1	1	2	95
L+12	-0.01	1	2	8	32	57
L+11	-0.05	0	1	2	11	86
L+10	-0.1	0	1	0	1	98
L+9	-0.14	1	0	0	1	98
L+8	-0.15	1	3	2	7	87
L+7	-0.22	2	2	2	9	85
L+6	-0.34	2	1	1	2	95
L+5	-0.37	2	2	1	2	94
L+4	-0.38	1	2	2	5	91
L+3	-0.39	4	3	1	1	90
L+2	-0.5	4	1	0	1	95
L+1	-0.55	1	2	0	0	97
LUMO	-0.99	23	0	0	0	77
HOMO	-4.49	34	29	20	13	4
H-1	-4.7	36	42	14	1	6
H-2	-5.26	2	34	26	21	17
H-3	-5.63	3	27	43	3	24
H-4	-5.96	82	0	0	0	17
H-5	-6.16	9	3	2	4	83
H-6	-6.27	7	23	8	0	61
H-7	-6.41	10	30	12	5	42
H-8	-6.45	1	1	0	92	6
H-9	-6.46	24	19	5	6	47
H-10	-6.52	9	3	2	3	83

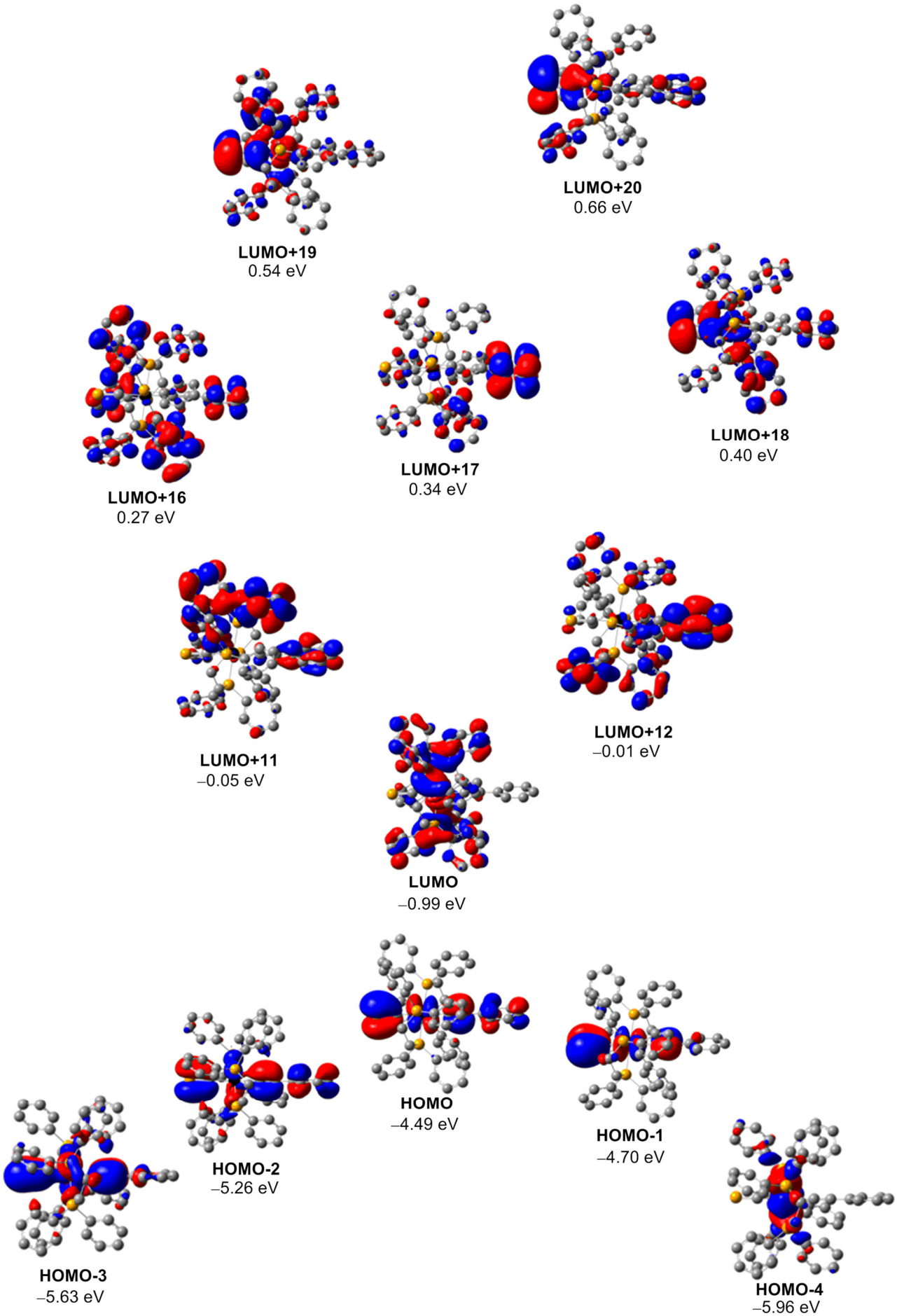


Figure S62 Selected molecular orbitals of compound **8b**

Table S3. Composition of selected molecular orbitals for **8c** (Ar = C_6H_4F).

Orbital	Energy / eV	% Ru	%C≡P	%C≡C	%Ar	%dppe
L+20	0.77	9	73	1	6	12
L+19	0.53	6	70	2	0	21
L+18	0.41	16	0	0	2	82
L+17	0.31	1	3	0	1	95
L+16	0.19	2	1	0	2	95
L+15	0.13	0	1	0	64	34
L+14	0.1	0	1	0	29	70
L+13	0.07	1	2	1	4	92
L+12	0	1	2	4	17	74
L+11	-0.02	1	2	11	44	42
L+10	-0.15	1	1	0	1	97
L+9	-0.22	1	0	0	0	98
L+8	-0.24	2	1	0	1	95
L+7	-0.27	1	1	0	0	98
L+6	-0.36	3	1	1	3	93
L+5	-0.43	2	1	0	0	96
L+4	-0.51	0	2	0	1	97
L+3	-0.53	1	1	0	1	96
L+2	-0.59	0	1	0	1	98
L+1	-0.67	4	1	0	0	94
LUMO	-0.98	25	0	0	0	75
HOMO	-4.46	33	33	18	12	4
H-1	-4.67	36	44	14	1	5
H-2	-5.21	1	33	26	25	14
H-3	-5.64	3	29	42	3	23
H-4	-5.99	82	1	1	0	17
H-5	-6.26	11	21	7	3	58
H-6	-6.28	8	22	8	3	59
H-7	-6.38	21	15	4	7	53
H-8	-6.49	14	10	2	4	70
H-9	-6.53	5	3	1	7	84
H-10	-6.57	5	4	3	0	88

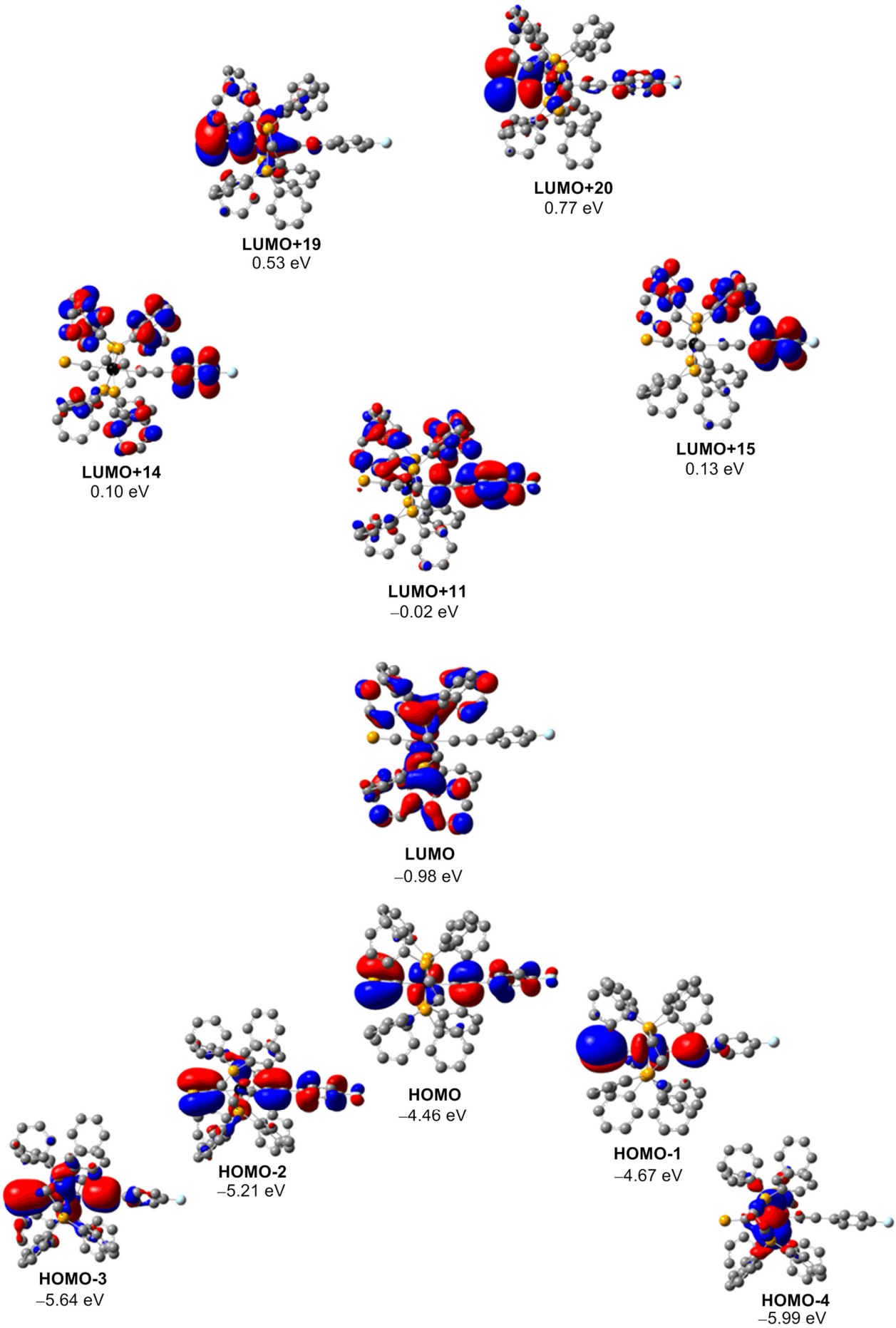


Figure S63. Selected molecular orbitals of compound **8c**

Table S4. Composition of selected molecular orbitals for **8d** (Ar = $C_6H_4CO_2Me$).

Orbital	Energy / eV	% Ru	%C≡P	%C≡C	%Ar	%CO_2Me	%dppe
L+20	0.53	11	31	1	8	3	46
L+19	0.37	1	16	0	58	0	25
L+18	0.31	6	43	1	2	0	48
L+17	0.28	9	44	1	2	2	43
L+16	0.23	2	7	0	23	1	67
L+15	0.17	2	7	0	3	6	82
L+14	0.11	2	7	0	3	4	85
L+13	0.05	1	0	0	0	0	98
L+12	-0.11	0	1	0	1	1	97
L+11	-0.15	1	1	0	0	6	92
L+10	-0.23	1	0	0	0	1	97
L+9	-0.26	2	1	0	0	0	97
L+8	-0.27	0	0	0	0	0	99
L+7	-0.34	4	3	1	0	2	90
L+6	-0.47	0	1	0	1	2	96
L+5	-0.47	3	1	1	1	0	93
L+4	-0.58	2	0	0	1	2	95
L+3	-0.61	1	2	0	0	0	96
L+2	-0.65	1	0	0	0	0	97
L+1	-0.95	2	2	11	52	13	20
LUMO	-1	23	0	0	2	1	73
HOMO	-4.68	36	31	19	8	1	5
H-1	-4.73	35	32	20	7	1	5
H-2	-5.42	3	35	25	20	2	16
H-3	-5.66	3	28	41	3	0	25
H-4	-6.07	81	0	1	0	0	17
H-5	-6.28	10	2	8	1	0	79
H-6	-6.36	8	4	3	3	1	82
H-7	-6.46	1	5	2	50	0	43
H-8	-6.49	10	51	18	6	0	16
H-9	-6.58	6	2	1	22	1	69
H-10	-6.6	3	1	0	14	2	80

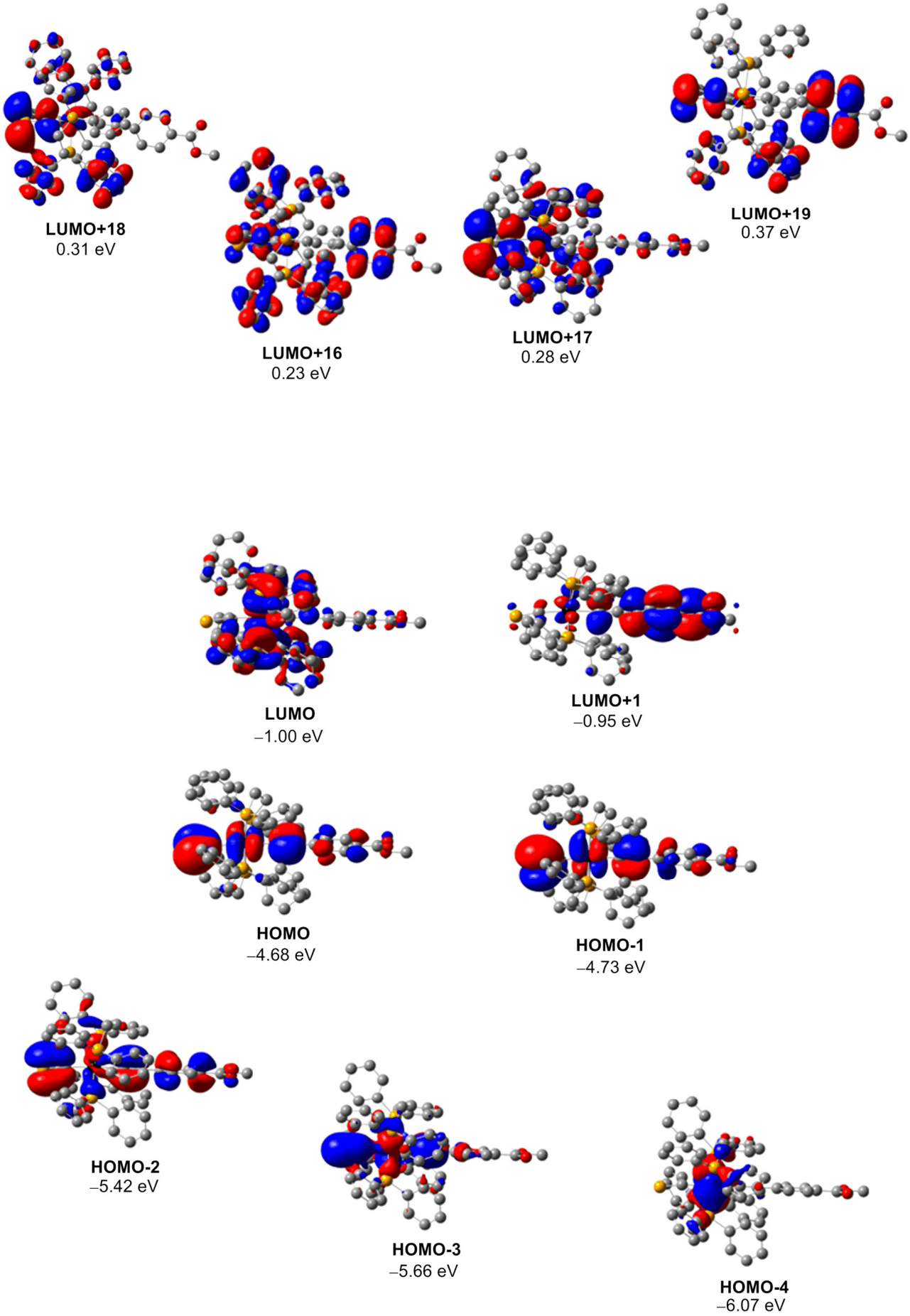


Figure S64. Selected molecular orbitals of compound **8d**

Table S5. Composition of selected molecular orbitals for **8e** (Ar = $C_6H_4NO_2$).

Orbital	Energy / eV	% Ru	%C≡P	%C≡C	%Ar	%NO_2	%dppe
L+20	0.32	7	66	3	2	1	22
L+19	0.21	1	3	3	9	5	79
L+18	0.16	17	4	0	1	0	78
L+17	0.14	2	14	10	29	18	27
L+16	-0.04	0	1	0	1	0	97
L+15	-0.06	0	1	0	4	0	95
L+14	-0.1	0	0	0	21	1	77
L+13	-0.11	0	0	0	62	0	37
L+12	-0.16	0	1	0	0	0	99
L+11	-0.19	1	1	0	5	0	94
L+10	-0.38	2	1	0	0	0	97
L+9	-0.41	1	1	0	0	0	98
L+8	-0.44	1	1	0	1	0	97
L+7	-0.48	3	1	0	1	0	95
L+6	-0.57	1	2	0	0	0	97
L+5	-0.61	1	2	1	0	0	96
L+4	-0.64	1	1	0	2	0	95
L+3	-0.68	2	1	1	1	0	95
L+2	-0.84	5	1	1	0	0	93
L+1	-1.21	25	0	0	0	0	75
LUMO	-1.91	1	1	7	33	57	1
HOMO	-4.72	34	39	13	8	1	5
H-1	-4.88	36	43	14	1	0	5
H-2	-5.55	1	30	32	19	2	16
H-3	-5.85	3	28	41	3	0	24
H-4	-6.19	84	0	0	0	0	16
H-5	-6.45	9	19	8	2	0	62
H-6	-6.47	8	18	5	0	0	67
H-7	-6.6	11	24	8	1	0	57
H-8	-6.65	6	1	1	2	0	91
H-9	-6.71	16	9	4	4	0	67
H-10	-6.76	5	1	1	0	0	92

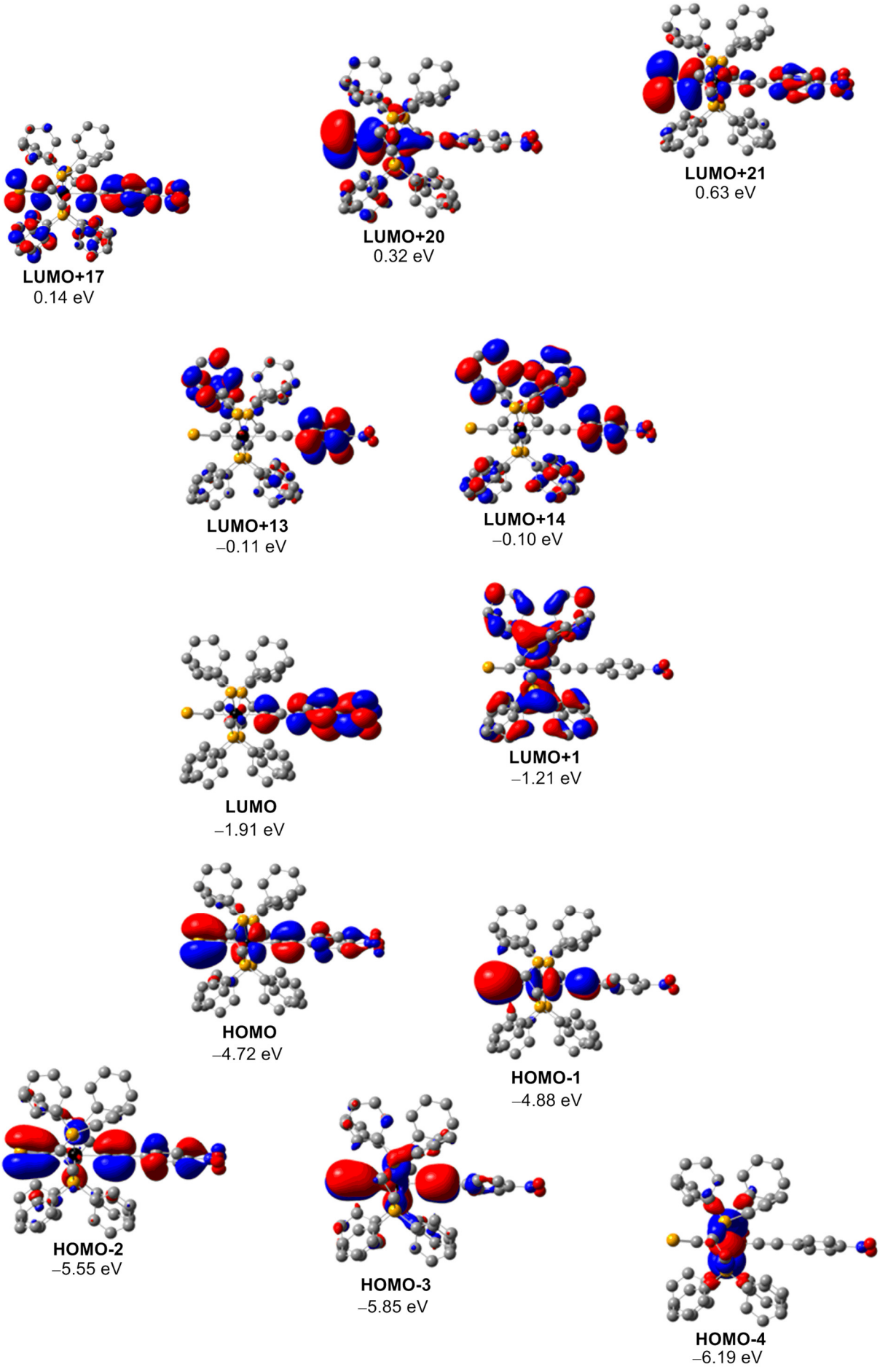


Figure S65. Selected molecular orbitals of compound **8e**

Table S6. First 100 excited states for compound **8a** derived from TD-DFT.

No.	E /cm^{-1}	λ / nm	Osc. Strength	Major contributions
1	21883.59	456.9635	0.0009	HOMO->LUMO (92%)
2	23349.91	428.2671	0.0018	H-1->LUMO (93%)
3	26945.56	371.1187	0.003	HOMO->L+1 (25%), HOMO->L+2 (64%)
4	27288.34	366.4568	0.0011	HOMO->L+1 (66%), HOMO->L+2 (28%)
5	28273.15	353.6924	0.0025	HOMO->L+3 (54%), HOMO->L+4 (32%)
6	28501.41	350.8598	0.0006	HOMO->L+3 (39%), HOMO->L+4 (55%)
7	28638.53	349.18	0.0046	H-1->L+1 (29%), H-1->L+2 (54%)
8	28864.36	346.448	0.0013	H-1->L+1 (48%), H-1->L+2 (26%), HOMO->L+5 (13%)
9	29157.14	342.9691	0.011	HOMO->L+5 (78%)
10	29603.17	337.8016	0.0113	HOMO->L+6 (89%)
11	29712.06	336.5637	0.001	H-1->L+3 (61%), H-1->L+4 (15%)
12	29971.77	333.6473	0.0002	H-1->L+4 (62%), H-1->L+5 (12%)
13	30250.84	330.5693	0.0121	H-2->LUMO (18%), HOMO->L+7 (16%), HOMO->L+8 (40%)
14	30356.5	329.4188	0.0014	H-1->L+3 (16%), H-1->L+5 (36%), HOMO->L+8 (12%)
15	30371.02	329.2613	0.0051	H-4->LUMO (41%), H-2->LUMO (15%), HOMO->L+8 (13%)
16	30616.21	326.6243	0.0016	HOMO->L+7 (57%), HOMO->L+8 (24%)
17	30858.18	324.0632	0.0195	H-4->LUMO (18%), H-2->LUMO (53%), HOMO->L+7 (15%)
18	30967.87	322.9153	0.0081	H-1->L+5 (17%), H-1->L+6 (41%)
19	31235.65	320.147	0.0556	H-1->L+6 (33%), HOMO->L+9 (45%)
20	31294.53	319.5447	0.0032	H-1->L+6 (12%), HOMO->L+9 (41%), HOMO->L+10 (28%)
21	31636.51	316.0905	0.0286	H-1->L+8 (51%), HOMO->L+10 (19%)
22	31942.2	313.0655	0.005	H-1->L+8 (14%), HOMO->L+11 (55%)
23	32071.25	311.8058	0.0173	H-1->L+7 (64%), HOMO->L+11 (13%)
24	32309.18	309.5096	0.0319	H-1->L+7 (23%), H-1->L+9 (33%), HOMO->L+11 (11%)
25	32686.65	305.9353	0.0734	HOMO->L+10 (18%), HOMO->L+19 (34%)
26	32899.58	303.9552	0.0154	H-1->L+9 (14%), HOMO->L+12 (44%)
27	33068.15	302.4058	0.0321	H-1->L+9 (19%), H-1->L+10 (10%), H-1->L+11 (19%), HOMO->L+12 (35%)
28	33277.05	300.5074	0.0063	H-1->L+11 (29%), HOMO->L+18 (20%)
29	33369.81	299.6721	0.0603	H-3->LUMO (49%), H-1->L+10 (22%), H-1->L+11 (14%)
30	33458.53	298.8775	0.0145	H-3->LUMO (29%), H-1->L+10 (20%), H-1->L+11 (14%), HOMO->L+14 (11%), HOMO->L+18 (11%)
31	33787.6	295.9665	0.0251	HOMO->L+13 (74%), HOMO->L+14 (11%)
32	33969.08	294.3854	0.0006	H-1->L+18 (15%), HOMO->L+14 (35%)
33	34167.49	292.6758	0.0399	H-1->L+12 (12%), H-1->L+18 (16%), HOMO->L+14 (20%)
34	34336.87	291.2321	0.0073	HOMO->L+15 (81%)
35	34453.82	290.2435	0.0192	H-2->L+1 (69%)
36	34651.43	288.5884	0.031	H-2->L+2 (62%), H-1->L+12 (13%)
37	34715.96	288.052	0.0176	H-2->L+2 (14%), H-1->L+12 (54%), H-1->L+18 (12%)
38	34800.64	287.351	0.0496	H-1->L+19 (12%), HOMO->L+16 (31%), HOMO->L+20 (17%)
39	34965.99	285.9922	0.0044	HOMO->L+16 (49%), HOMO->L+18 (17%)
40	35307.16	283.2286	0.0188	H-1->L+13 (65%)
41	35373.3	282.6991	0.0109	H-2->L+3 (80%)
42	35487.03	281.7931	0.0082	HOMO->L+17 (71%)
43	35519.29	281.5372	0.0012	H-1->L+13 (14%), H-1->L+14 (66%)
44	35627.37	280.6831	0.0108	H-2->L+4 (84%)

45	35824.98	279.1349	0.0014	H-1->L+15 (94%)
46	36185.51	276.3537	0.0018	H-2->L+5 (66%)
47	36308.91	275.4145	0.0023	H-2->L+5 (14%), H-1->L+16 (68%)
48	36505.71	273.9297	0.0022	H-2->L+6 (10%), H-1->L+16 (18%), H-1->L+18 (14%), H-1->L+20 (26%)
49	36755.75	272.0663	0.0094	H-2->L+6 (84%)
50	37229.2	268.6064	0.0053	H-3->L+1 (88%)
51	37402.61	267.361	0.0069	H-3->L+2 (83%)
52	37450.19	267.0213	0.0017	H-1->L+17 (84%)
53	37536.5	266.4074	0.0062	H-2->L+7 (61%), H-2->L+8 (31%)
54	37644.57	265.6425	0.0066	H-2->L+7 (33%), H-2->L+8 (62%)
55	37937.36	263.5924	0.0088	H-7->LUMO (20%), H-6->LUMO (55%), H-5->LUMO (15%)
56	38122.86	262.3098	0.0048	H-2->L+9 (58%), HOMO->L+21 (13%)
57	38204.33	261.7505	0.0126	H-3->L+3 (55%), HOMO->L+21 (21%)
58	38274.5	261.2706	0.0311	H-3->L+3 (12%), H-3->L+4 (27%), H-2->L+9 (29%), HOMO->L+21 (14%)
59	38431.78	260.2013	0.0114	H-3->L+3 (18%), H-3->L+4 (54%)
60	38760.85	257.9923	0.0661	H-5->LUMO (15%), H-2->L+10 (47%)
61	38816.51	257.6224	0.062	H-5->LUMO (38%), H-2->L+10 (22%), H-2->L+11 (22%)
62	38903.62	257.0455	0.0838	H-7->LUMO (22%), H-5->LUMO (18%), H-2->L+11 (33%)
63	39044.76	256.1163	0.055	H-7->LUMO (21%), H-3->L+5 (17%), H-2->L+11 (11%)
64	39132.68	255.5409	0.0352	H-3->L+5 (61%)
65	39383.52	253.9133	0.0052	H-4->L+1 (31%), H-4->L+2 (14%), H-2->L+11 (15%)
66	39495.63	253.1926	0.005	H-3->L+6 (58%)
67	39731.15	251.6917	0.0269	H-4->L+1 (23%), H-4->L+2 (46%), H-3->L+6 (10%)
68	39926.33	250.4613	0.036	H-4->L+1 (28%), H-1->L+21 (27%)
69	39972.31	250.1732	0.0161	H-2->L+12 (70%)
70	40168.3	248.9525	0.0139	H-3->L+6 (10%), H-3->L+7 (16%), H-3->L+8 (14%), H-1->L+21 (15%)
71	40428.82	247.3483	0.0012	H-3->L+8 (63%)
72	40537.71	246.6839	0.006	H-2->L+13 (56%)
73	40555.45	246.576	0.0082	H-3->L+7 (47%)
74	40665.14	245.9109	0.0253	H-4->L+3 (14%), H-4->L+4 (12%), H-3->L+9 (10%)
75	40699.02	245.7062	0.0036	H-4->L+3 (45%), H-2->L+14 (13%)
76	40820.81	244.9731	0.038	H-9->LUMO (19%), H-4->L+3 (11%), H-4->L+4 (19%), H-2->L+14 (14%)
77	40857.91	244.7506	0.0395	H-9->LUMO (16%), H-4->L+3 (18%), H-4->L+4 (34%)
78	40897.43	244.5141	0.0094	H-2->L+13 (14%), H-2->L+14 (28%), H-2->L+19 (25%)
79	41084.55	243.4005	0.001	H-2->L+13 (13%), H-2->L+14 (26%)
80	41232.15	242.5292	0.008	H-3->L+9 (30%), H-3->L+10 (32%), H-2->L+15 (14%)
81	41366.04	241.7442	0.0031	H-2->L+15 (68%)
82	41419.28	241.4335	0.0227	H-4->L+5 (79%)
83	41662.86	240.0219	0.0008	H-3->L+10 (11%), H-3->L+11 (56%), H-2->L+16 (11%)
84	41805.62	239.2023	0.005	H-10->LUMO (40%), H-4->L+6 (11%)
85	41837.88	239.0178	0.0012	H-2->L+16 (70%)
86	41911.28	238.5993	0.0035	H-2->L+17 (52%)
87	41954.83	238.3516	0.001	H-11->LUMO (16%), H-4->L+6 (22%), H-2->L+17 (22%)
88	42045.97	237.8349	0.0804	H-4->L+6 (35%)
89	42140.34	237.3023	0.0191	H-5->L+1 (24%), H-5->L+2 (34%)
90	42181.47	237.0709	0.0068	H-5->L+1 (24%), H-5->L+2 (12%), H-4->L+6 (13%)
91	42266.97	236.5914	0.0498	H-2->L+18 (35%)
92	42339.56	236.1857	0.0013	H-8->LUMO (76%)

93	42473.45	235.4412	0.0102	H-12->LUMO (20%), H-2->L+18 (11%)
94	42591.21	234.7902	0.0325	H-4->L+8 (12%), HOMO->L+21 (10%), HOMO->L+22 (37%)
95	42643.63	234.5016	0.0042	H-4->L+8 (47%)
96	42675.9	234.3243	0.0037	H-6->L+1 (31%)
97	42729.94	234.028	0.0048	H-13->LUMO (16%)
98	42772.68	233.7941	0.0018	H-6->L+2 (24%), H-3->L+12 (11%)
99	42826.72	233.4991	0.0046	H-3->L+12 (61%)
100	42942.06	232.8719	0.0051	H-15->LUMO (21%), H-4->L+7 (13%)

Table S7. First 150 excited states for compound **8c** derived from TD-DFT.

No.	E /cm^{-1}	λ / nm	Osc. Strength	Major contributions
1	20859.92	479.3883	0.0001	HOMO->LUMO (88%)
2	22290.74	448.6167	0.0004	H-1->LUMO (88%)
3	26311.42	380.0631	0.0004	HOMO->L+1 (81%)
4	26741.31	373.9532	0.002	H-4->LUMO (75%)
5	27660.78	361.5227	0.0024	HOMO->L+2 (73%), HOMO->L+3 (22%)
6	27901.94	358.398	0.0021	HOMO->L+2 (17%), HOMO->L+3 (69%)
7	28071.32	356.2355	0.0024	H-1->L+1 (79%)
8	28324.58	353.0503	0.0045	HOMO->L+4 (93%)
9	28928.69	345.6776	0.0028	HOMO->L+5 (90%)
10	29241.63	341.9782	0.001	H-1->L+2 (65%), H-1->L+3 (22%)
11	29419.07	339.9155	0.0077	H-1->L+2 (12%), H-1->L+3 (14%), HOMO->L+6 (60%)
12	29623.13	337.574	0.0043	H-1->L+3 (58%), HOMO->L+6 (24%)
13	29911.07	334.3244	0.0015	H-1->L+4 (87%)
14	30199.82	331.1278	0.0002	HOMO->L+7 (71%), HOMO->L+9 (19%)
15	30358.71	329.3948	0.0038	HOMO->L+7 (14%), HOMO->L+8 (38%), HOMO->L+9 (31%)
16	30490.98	327.9658	0.0001	H-1->L+5 (82%)
17	30579.7	327.0143	0.011	HOMO->L+7 (10%), HOMO->L+8 (52%), HOMO->L+9 (25%)
18	30804.73	324.6254	0.0032	H-2->LUMO (11%), H-1->L+6 (43%), HOMO->L+10 (18%)
19	30858.77	324.057	0.0092	H-2->LUMO (57%), H-1->L+6 (19%)
20	31070.09	321.8529	0.0135	H-2->LUMO (11%), H-1->L+6 (10%), HOMO->L+10 (63%)
21	31778.24	314.6807	0.0023	H-1->L+7 (70%), H-1->L+9 (11%)
22	32009.73	312.4051	0.0338	H-1->L+7 (13%), H-1->L+8 (14%), HOMO->L+11 (14%), HOMO->L+12 (14%), HOMO->L+13 (10%)
23	32049.25	312.0198	0.0075	H-1->L+8 (44%)
24	32171.84	310.8308	0.001	H-1->L+8 (18%), H-1->L+9 (57%)
25	32331.54	309.2955	0.0149	H-1->L+8 (11%), H-1->L+10 (10%), H-1->L+11 (14%), HOMO->L+11 (20%), HOMO->L+12 (35%)
26	32416.23	308.4875	0.0008	H-1->L+10 (20%), H-1->L+11 (12%), HOMO->L+12 (26%), HOMO->L+13 (12%)
27	32679.97	305.9978	0.0552	H-1->L+10 (35%), H-1->L+11 (12%), HOMO->L+11 (14%), HOMO->L+13 (11%)
28	32765.47	305.1994	0.0874	H-1->L+11 (13%), HOMO->L+11 (21%), HOMO->L+13 (22%), HOMO->L+19 (13%)
29	33041.31	302.6515	0.0209	H-1->L+11 (17%), HOMO->L+14 (11%), HOMO->L+15 (10%), HOMO->L+19 (25%)
30	33183.26	301.3567	0.0096	HOMO->L+13 (21%), HOMO->L+14 (37%), HOMO->L+16 (18%), HOMO->L+18 (11%)
31	33336.51	299.9714	0.0115	HOMO->L+14 (28%), HOMO->L+15 (11%), HOMO->L+19 (20%)
32	33532.5	298.2181	0.0259	H-3->LUMO (33%), H-1->L+13 (15%), H-1->L+18 (10%)
33	33850.28	295.4185	0.0108	HOMO->L+15 (65%), HOMO->L+16 (18%)
34	33962.39	294.4433	0.0019	H-1->L+12 (78%)
35	34076.12	293.4607	0.0152	H-3->LUMO (36%), H-1->L+13 (47%)
36	34147.09	292.8507	0.0223	H-2->L+1 (64%), HOMO->L+16 (16%)
37	34288.24	291.6452	0.011	H-2->L+1 (20%), HOMO->L+16 (22%), HOMO->L+18 (32%)
38	34757.66	287.7064	0.0011	H-1->L+13 (15%), H-1->L+16 (19%), H-1->L+18 (14%)
39	34785.08	287.4796	0.0063	H-2->L+2 (69%)
40	34848.8	286.9539	0.0038	H-2->L+2 (14%), H-1->L+14 (19%), HOMO->L+17 (40%)

41	34937.52	286.2253	0.0032	H-1->L+14 (55%), H-1->L+15 (10%), HOMO->L+17 (24%)
42	35146.42	284.524	0.0224	H-2->L+3 (34%), H-2->L+4 (15%), HOMO->L+20 (10%)
43	35352.89	282.8623	0.0051	H-2->L+3 (57%), HOMO->L+21 (12%)
44	35453.71	282.0579	0.0005	H-2->L+4 (62%), HOMO->L+21 (17%)
45	35569.86	281.1369	0.0006	H-1->L+14 (10%), H-1->L+15 (61%), H-1->L+16 (18%)
46	35740.85	279.7919	0.0128	H-5->LUMO (36%), H-1->L+19 (13%), HOMO->L+20 (10%), HOMO->L+21 (11%)
47	35893.29	278.6036	0.015	H-5->LUMO (43%), HOMO->L+21 (14%)
48	35926.35	278.3472	0.0033	H-5->LUMO (12%), H-1->L+16 (28%), H-1->L+18 (34%)
49	36270.75	275.7042	0.0087	H-1->L+20 (53%)
50	36307.05	275.4286	0.0165	H-2->L+5 (87%)
51	36555.47	273.5569	0.0041	H-1->L+17 (74%)
52	36632.9	272.9787	0.0041	H-2->L+6 (88%)
53	36985.36	270.3773	0.0031	H-1->L+21 (55%)
54	37279.75	268.2421	0.0038	H-2->L+7 (87%)
55	37371.7	267.5822	0.0085	H-4->L+1 (16%), H-3->L+1 (66%)
56	37566.08	266.1976	0.0031	H-2->L+8 (37%), H-2->L+9 (53%)
57	37698.35	265.2636	0.0037	H-2->L+8 (44%), H-2->L+9 (39%)
58	37735.46	265.0028	0.0095	H-4->L+1 (53%), H-3->L+1 (18%)
59	38024.2	262.9904	0.0146	H-3->L+2 (73%)
60	38221	261.6363	0.0093	H-7->LUMO (25%), H-3->L+2 (15%), H-2->L+10 (14%)
61	38252.46	261.4211	0.0131	H-2->L+10 (81%)
62	38573.47	259.2456	0.0032	H-3->L+3 (70%)
63	38618.63	258.9424	0.0023	H-4->L+2 (69%)
64	38758.97	258.0048	0.0019	H-4->L+4 (10%), H-3->L+4 (79%)
65	38972.71	256.5898	0.005	H-4->L+3 (71%)
66	39278.39	254.5929	0.023	H-6->LUMO (12%), H-4->L+4 (58%)
67	39325.17	254.29	0.008	H-2->L+11 (11%), H-2->L+12 (68%)
68	39479.23	253.2978	0.0959	H-7->LUMO (14%), H-6->LUMO (33%), H-4->L+4 (16%), H-2->L+12 (16%)
69	39552.62	252.8277	0.004	H-4->L+5 (11%), H-3->L+5 (81%)
70	39675.22	252.0465	0.1085	H-2->L+11 (54%), H-2->L+13 (20%)
71	39830.88	251.0615	0.0051	H-3->L+6 (74%)
72	39979.29	250.1295	0.041	H-4->L+5 (58%), H-2->L+13 (12%)
73	40052.69	249.6711	0.0701	H-4->L+5 (18%), H-2->L+11 (11%), H-2->L+13 (37%)
74	40120.44	249.2495	0.0085	H-2->L+13 (11%), H-2->L+14 (64%), H-2->L+15 (13%)
75	40265.62	248.3508	0.0156	H-2->L+14 (19%), H-2->L+15 (49%)
76	40332.56	247.9386	0.0152	H-5->L+1 (20%), H-4->L+6 (42%), H-2->L+15 (13%)
77	40424.51	247.3747	0.0251	H-5->L+1 (36%), H-4->L+6 (16%)
78	40466.45	247.1183	0.1109	H-8->LUMO (38%), H-4->L+6 (17%)
79	40632.6	246.1078	0.0041	H-3->L+7 (18%), H-2->L+16 (63%)
80	40664.05	245.9174	0.0098	H-3->L+7 (59%), H-2->L+16 (19%)
81	40871.34	244.6702	0.0047	H-3->L+8 (62%), H-3->L+11 (13%)
82	40950.38	244.198	0.0127	H-3->L+8 (20%), H-3->L+9 (50%), H-3->L+11 (10%)
83	41076.2	243.45	0.0027	H-5->L+2 (28%), H-5->L+3 (44%)
84	41171.38	242.8872	0.0024	H-3->L+9 (19%), H-3->L+11 (34%)
85	41252.84	242.4076	0.0047	H-4->L+7 (59%), H-4->L+9 (18%)
86	41415.76	241.454	0.0196	H-2->L+18 (21%)
87	41491.58	241.0128	0.0405	H-9->LUMO (10%), H-8->LUMO (10%)

88	41526.26	240.8115	0.0036	H-4->L+7 (17%), H-4->L+8 (48%), H-4->L+9 (13%)
89	41559.33	240.6199	0.0044	H-5->L+2 (19%), H-2->L+17 (27%), H-2->L+19 (10%)
90	41642.41	240.1398	0.0077	H-5->L+2 (23%), H-5->L+3 (21%), H-2->L+17 (14%), H-2->L+18 (12%)
91	41680.31	239.9214	0.0119	H-3->L+10 (31%), H-2->L+17 (10%), H-2->L+18 (21%)
92	41689.99	239.8657	0.01	H-4->L+8 (18%), H-4->L+9 (32%), H-3->L+10 (12%)
93	41820.65	239.1163	0.0073	H-5->L+4 (58%)
94	41892.44	238.7066	0.0046	H-5->L+4 (21%)
95	41967.45	238.2799	0.0059	H-4->L+10 (30%), H-3->L+10 (16%), H-2->L+18 (17%)
96	42196.51	236.9864	0.0041	H-2->L+17 (10%), H-2->L+19 (19%)
97	42262.65	236.6156	0.044	H-6->L+1 (18%), H-2->L+19 (12%)
98	42332.01	236.2279	0.053	H-9->LUMO (15%), H-6->L+1 (42%)
99	42455.41	235.5412	0.0012	H-10->LUMO (14%), HOMO->L+22 (23%)
100	42492.51	235.3356	0.0028	H-5->L+5 (45%), HOMO->L+22 (11%)
101	42562.68	234.9476	0.006	H-4->L+10 (12%), H-4->L+11 (20%), HOMO->L+22 (10%)
102	42643.34	234.5032	0.012	H-3->L+12 (12%)
103	42695.77	234.2153	0.0101	H-11->LUMO (10%), H-4->L+11 (24%)
104	42796.58	233.6635	0.0043	H-6->L+2 (14%), H-3->L+12 (46%)
105	42869.17	233.2678	0.0033	H-7->L+1 (31%), H-6->L+2 (15%)
106	42990.16	232.6114	0.0055	H-5->L+6 (18%), H-3->L+13 (18%)
107	43053.07	232.2715	0.0041	H-6->L+2 (14%), H-5->L+6 (33%)
108	43099.04	232.0237	0.0122	H-6->L+2 (10%), H-6->L+3 (12%)
109	43123.24	231.8935	0.001	H-3->L+13 (11%)
110	43190.18	231.5341	0.0234	HOMO->L+23 (21%)
111	43249.87	231.2146	0.0112	H-6->L+4 (15%)
112	43314.39	230.8701	0.0007	H-3->L+13 (19%)
113	43341.82	230.7241	0.012	H-6->L+3 (16%), HOMO->L+23 (13%)
114	43495.06	229.9112	0	H-3->L+14 (15%), HOMO->L+23 (10%)
115	43532.16	229.7152	0.0127	
116	43553.94	229.6004	0.0008	H-4->L+12 (41%), H-3->L+14 (25%), H-3->L+15 (10%)
117	43578.94	229.4686	0.0013	H-4->L+12 (18%), H-3->L+15 (31%)
118	43623.3	229.2353	0.0036	H-3->L+15 (11%)
119	43649.11	229.0997	0.0066	H-6->L+3 (27%)
120	43703.96	228.8122	0.0313	H-7->L+2 (13%)
121	43806.39	228.2772	0.001	H-5->L+7 (13%), H-1->L+22 (16%)
122	43838.65	228.1092	0.0203	H-3->L+15 (11%), H-1->L+22 (20%)
123	43899.14	227.7949	0.0048	H-13->LUMO (10%), H-5->L+7 (34%), H-1->L+22 (13%)
124	43928.99	227.6401	0.0057	H-6->L+4 (17%)
125	43957.22	227.4939	0.0004	H-7->L+2 (25%), H-6->L+4 (12%)
126	43999.16	227.2771	0.0058	H-13->LUMO (10%), H-5->L+8 (15%), H-5->L+9 (12%), H-5->L+10 (15%)
127	44095.14	226.7824	0.0037	H-4->L+13 (13%), H-3->L+16 (38%)
128	44142.72	226.5379	0.0146	H-8->L+1 (10%), H-7->L+3 (23%)
129	44195.15	226.2692	0.0026	H-7->L+3 (13%), H-5->L+8 (32%)
130	44233.06	226.0753	0.0085	H-16->LUMO (11%), H-8->L+1 (10%)
131	44262.9	225.9228	0.013	H-8->L+1 (23%), H-5->L+9 (13%)
132	44323.39	225.6145	0.0137	H-17->LUMO (12%)
133	44352.43	225.4668	0.0027	H-16->LUMO (13%), H-4->L+13 (15%), H-4->L+14 (19%), H-3->L+16 (15%)
134	44450.83	224.9677	0.0133	H-16->LUMO (20%)
135	44471.8	224.8616	0.0032	H-4->L+14 (40%), H-4->L+15 (18%)

136	44557.29	224.4302	0.0009	H-7->L+4 (24%)
137	44611.33	224.1583	0.0287	H-6->L+5 (23%), H-5->L+9 (10%), H-5->L+10 (21%)
138	44633.11	224.0489	0.0127	H-6->L+5 (20%), H-5->L+9 (10%), H-5->L+10 (22%)
139	44707.31	223.6771	0.0047	H-7->L+4 (11%), H-6->L+6 (11%)
140	44755.71	223.4352	0.0039	H-8->L+2 (13%), H-6->L+6 (15%)
141	44784.74	223.2903	0.01	H-8->L+2 (16%), H-1->L+23 (18%)
142	44858.94	222.921	0.0092	H-8->L+2 (19%), H-8->L+3 (12%)
143	44952.5	222.457	0.0008	H-19->LUMO (15%), H-17->LUMO (18%), H-3->L+18 (13%)
144	44983.96	222.3015	0.0063	H-3->L+18 (12%), H-1->L+23 (15%)
145	45039.61	222.0268	0.0072	H-3->L+17 (13%), H-3->L+18 (23%)
146	45121.07	221.6259	0.0038	H-18->LUMO (43%)
147	45164.63	221.4122	0.0162	H-4->L+18 (13%), H-4->L+19 (37%)
148	45255.77	220.9663	0.0026	H-7->L+5 (19%), H-4->L+16 (11%)
149	45314.65	220.6792	0.0336	H-7->L+5 (15%), H-6->L+6 (15%)
150	45336.42	220.5732	0.0075	H-8->L+3 (12%), H-5->L+11 (22%)

Table S8. First 150 excited states for compound **8d** derived from TD-DFT.

No.	E /cm^{-1}	λ / nm	Osc. Strength	Major contributions
1	22087.65	452.7418	0.0002	H-1->LUMO (15%), HOMO->LUMO (57%), HOMO->L+1 (13%)
2	22974.06	435.2736	0.0001	H-1->LUMO (57%), H-1->L+1 (13%), HOMO->LUMO (15%)
3	26082.54	383.3983	0.0018	H-1->L+1 (34%), HOMO->LUMO (11%), HOMO->L+1 (43%)
4	27548.06	363.002	0.0006	H-4->LUMO (64%), H-4->L+1 (16%)
5	27959.4	357.6614	0.192	H-1->L+1 (25%), HOMO->L+1 (15%), HOMO->L+2 (29%)
6	28058.61	356.3969	0.1718	H-1->L+1 (17%), H-1->L+2 (14%), HOMO->L+1 (16%), HOMO->L+2 (21%)
7	28728.05	348.0918	0.0161	H-1->L+2 (10%), H-1->L+3 (13%), HOMO->L+2 (34%), HOMO->L+3 (31%)
8	28847.42	346.6514	0.0133	H-1->L+2 (43%), HOMO->L+3 (41%)
9	29167.63	342.8458	0.0014	HOMO->L+4 (72%)
10	29355.56	340.651	0.0005	H-1->L+2 (17%), H-1->L+3 (68%)
11	29674.96	336.9845	0.013	H-1->L+4 (81%)
12	29962.09	333.7551	0.0042	HOMO->L+6 (66%)
13	30312.94	329.8921	0.0005	HOMO->L+5 (76%)
14	30520.23	327.6515	0.0019	H-1->L+5 (37%), H-1->L+6 (41%)
15	30603.31	326.7621	0.0109	H-1->L+5 (18%), H-1->L+6 (12%), H-1->L+7 (13%), HOMO->L+5 (15%), HOMO->L+7 (20%)
16	30769.46	324.9976	0.0012	H-1->L+5 (31%), H-1->L+6 (11%), H-1->L+7 (28%), HOMO->L+7 (10%)
17	31136.44	321.1671	0.0016	H-1->L+6 (10%), H-1->L+7 (23%), HOMO->L+7 (47%)
18	31707.49	315.3829	0.0016	HOMO->L+8 (82%)
19	31789.76	314.5667	0.0044	HOMO->L+9 (36%), HOMO->L+10 (38%)
20	31880.9	313.6675	0.0185	H-2->LUMO (45%), H-2->L+1 (10%), H-1->L+10 (15%)
21	31985.75	312.6392	0.0033	H-1->L+10 (10%), HOMO->L+9 (42%), HOMO->L+10 (21%)
22	32111.57	311.4142	0.0019	H-1->L+8 (46%), H-1->L+9 (12%), H-1->L+10 (12%), HOMO->L+10 (11%)
23	32148.68	311.0548	0.006	H-2->LUMO (12%), H-1->L+8 (37%), H-1->L+9 (22%), HOMO->L+10 (11%)
24	32410.81	308.5391	0.0018	H-1->L+9 (49%), H-1->L+10 (25%)
25	32518.08	307.5212	0.0026	H-1->L+10 (15%), HOMO->L+11 (13%), HOMO->L+18 (22%)
26	32869.74	304.2312	0.0084	HOMO->L+11 (70%)
27	33085.9	302.2436	0.0017	HOMO->L+12 (73%)
28	33208.49	301.1278	0.0012	H-1->L+11 (85%)
29	33364.16	299.7228	0.0069	H-1->L+12 (67%)
30	33605.32	297.5719	0.0056	H-1->L+18 (13%), HOMO->L+14 (14%), HOMO->L+16 (13%), HOMO->L+17 (14%)
31	33781.96	296.016	0.0344	H-3->LUMO (71%), H-3->L+1 (15%)
32	33825.51	295.6348	0.0288	H-1->L+12 (11%), H-1->L+14 (12%), H-1->L+16 (12%), H-1->L+17 (13%)
33	34269.12	291.8079	0.0156	HOMO->L+13 (63%)
34	34389.3	290.7881	0.0558	H-3->L+1 (47%), H-2->L+1 (19%)
35	34596.58	289.0459	0.0075	H-1->L+13 (26%), HOMO->L+13 (21%)
36	34708.7	288.1122	0.0129	H-1->L+13 (39%), HOMO->L+20 (10%)
37	34865.98	286.8126	0.1412	H-3->L+1 (11%), H-2->L+1 (44%), H-1->L+13 (10%)
38	34995.83	285.7483	0.0188	HOMO->L+14 (58%)
39	35203.92	284.0592	0.0036	H-1->L+14 (17%), H-1->L+16 (13%), H-1->L+17 (10%), HOMO->L+15 (15%)
40	35416.05	282.3579	0.0026	H-1->L+14 (46%), HOMO->L+15 (24%)
41	35515.26	281.5691	0.0074	H-1->L+15 (25%), HOMO->L+15 (28%)
42	35679.79	280.2707	0.0178	H-2->L+2 (83%)
43	35962.9	278.0644	0.0014	H-1->L+15 (20%), HOMO->L+16 (30%), HOMO->L+17 (16%)

44	36010.48	277.6969	0.001	H-2->L+3 (19%), H-1->L+15 (18%), HOMO->L+16 (10%), HOMO->L+17 (15%)
45	36133.08	276.7547	0.0034	H-2->L+3 (64%)
46	36289.55	275.5614	0.005	H-1->L+16 (29%), H-1->L+17 (47%)
47	36464.58	274.2387	0.002	H-2->L+4 (76%)
48	36697.67	272.4968	0.0003	H-1->L+21 (23%), HOMO->L+17 (12%), HOMO->L+21 (29%)
49	36798.49	271.7503	0.0138	H-4->LUMO (18%), H-4->L+1 (72%)
50	37101.76	269.529	0.0001	H-1->L+19 (16%), HOMO->L+19 (30%), HOMO->L+20 (11%)
51	37134.83	269.289	0.0021	H-6->LUMO (20%), H-5->LUMO (48%), H-5->L+1 (11%)
52	37209.03	268.7519	0.0085	H-2->L+6 (23%), H-1->L+21 (18%), HOMO->L+21 (13%)
53	37342.11	267.7942	0.0039	H-2->L+5 (51%), H-2->L+6 (24%)
54	37481.65	266.7972	0.0047	H-2->L+5 (35%), H-2->L+6 (40%)
55	37593.76	266.0016	0.0257	H-3->L+2 (80%)
56	37836.54	264.2948	0.0036	H-3->L+3 (31%), H-1->L+19 (27%), HOMO->L+19 (17%)
57	37879.28	263.9965	0.009	H-3->L+3 (56%), H-1->L+19 (14%)
58	38125.28	262.2931	0.0062	H-3->L+4 (39%), H-2->L+7 (45%)
59	38222.88	261.6234	0.0033	H-3->L+4 (50%), H-2->L+7 (38%)
60	38309.99	261.0285	0.0108	H-4->L+2 (58%), H-4->L+3 (13%)
61	38706.01	258.3578	0.002	H-16->L+1 (15%), H-2->L+8 (61%)
62	38707.62	258.3471	0.0008	H-16->LUMO (11%), H-16->L+1 (44%), H-2->L+8 (20%)
63	38766.5	257.9547	0.0055	H-4->L+2 (16%), H-4->L+3 (68%)
64	38879.42	257.2055	0.0151	H-2->L+9 (37%), H-2->L+10 (20%)
65	38935.07	256.8379	0.0824	H-6->LUMO (34%), H-5->LUMO (11%), H-2->L+9 (13%)
66	39014.92	256.3122	0.0089	H-3->L+5 (41%), H-3->L+6 (35%), H-2->L+10 (12%)
67	39060.89	256.0105	0.002	H-2->L+9 (37%), H-2->L+10 (49%)
68	39153.65	255.404	0.0127	H-4->L+4 (35%), H-3->L+5 (27%), H-3->L+6 (24%)
69	39194.78	255.136	0.0042	H-4->L+4 (35%), H-3->L+5 (12%), H-3->L+6 (29%)
70	39672.27	252.0653	0.1148	H-7->LUMO (48%)
71	39786.8	251.3397	0.0091	H-2->L+11 (75%)
72	39831.97	251.0546	0.0264	H-3->L+7 (73%)
73	39915.04	250.5321	0.0019	H-6->L+1 (21%), H-5->LUMO (11%), H-5->L+1 (43%)
74	40036.03	249.775	0.0106	H-4->L+5 (10%), H-4->L+6 (21%), H-2->L+11 (11%), H-2->L+12 (31%)
75	40092.48	249.4233	0.0157	H-4->L+5 (12%), H-4->L+6 (31%), H-2->L+12 (35%)
76	40234.44	248.5433	0.0148	H-4->L+5 (43%), H-4->L+6 (24%)
77	40265.89	248.3491	0.0376	H-4->L+5 (23%), H-2->L+12 (13%)
78	40386.88	247.6052	0.0151	H-6->L+1 (38%), H-5->L+1 (23%)
79	40534.48	246.7036	0.0052	H-3->L+8 (83%)
80	40553.84	246.5858	0.0046	H-4->L+7 (65%)
81	40674.01	245.8572	0.0068	H-3->L+9 (51%), H-3->L+10 (33%)
82	40830.49	244.915	0.0034	H-3->L+9 (35%), H-3->L+10 (46%)
83	40970.83	244.0761	0.018	H-9->LUMO (11%), H-8->LUMO (25%)
84	40995.83	243.9272	0.01	H-8->L+1 (25%), H-2->L+14 (12%), H-2->L+16 (15%)
85	41241.83	242.4723	0.0037	H-7->L+1 (11%), H-2->L+13 (73%)
86	41393.47	241.584	0.0107	H-7->L+1 (19%), H-2->L+13 (15%), H-2->L+14 (24%)
87	41485.41	241.0486	0.0062	H-7->L+1 (17%), H-3->L+11 (24%)
88	41516.06	240.8706	0.0087	H-7->L+1 (23%), H-3->L+11 (29%)
89	41562.04	240.6042	0.0081	H-13->LUMO (14%), H-8->LUMO (19%)
90	41587.04	240.4595	0.0212	H-4->L+9 (20%), H-4->L+10 (23%), H-3->L+11 (22%)

91	41774.97	239.3778	0.0019	H-5->L+2 (17%), H-3->L+12 (45%)
92	41808.04	239.1885	0.0038	H-4->L+8 (72%)
93	41837.88	239.0178	0.0023	H-6->L+2 (16%), H-5->L+2 (40%), H-3->L+12 (15%)
94	41944.35	238.4112	0.0106	H-5->L+3 (13%), H-2->L+14 (11%), H-2->L+15 (11%)
95	41997.58	238.109	0.0505	H-10->LUMO (10%), H-5->L+3 (19%)
96	42020.97	237.9764	0.001	H-5->L+3 (30%), H-4->L+9 (29%), H-4->L+10 (15%)
97	42060.49	237.7528	0.0054	H-5->L+3 (10%), H-4->L+9 (13%), H-2->L+14 (15%)
98	42249.23	236.6907	0.0168	H-2->L+15 (44%)
99	42431.51	235.6739	0.0188	H-6->L+3 (40%)
100	42471.84	235.4501	0.0203	H-9->L+1 (22%), H-6->L+3 (14%)
101	42568.62	234.9148	0.003	H-6->L+4 (12%), H-2->L+18 (10%)
102	42592.01	234.7858	0.0118	H-7->L+2 (19%), H-6->L+2 (11%)
103	42615.4	234.6569	0.0084	
104	42693.64	234.2269	0.0038	H-10->LUMO (11%), H-9->LUMO (12%), H-4->L+11 (13%)
105	42748.49	233.9264	0.012	H-6->L+4 (11%), H-5->L+4 (41%)
106	42815.43	233.5607	0.0107	H-6->L+2 (19%), H-5->L+4 (23%)
107	42842.05	233.4155	0.0101	H-4->L+11 (15%), H-3->L+18 (17%)
108	42904.96	233.0733	0.0039	H-9->LUMO (10%), H-6->L+4 (12%), H-4->L+11 (16%)
109	42963.84	232.7539	0.0045	H-11->LUMO (12%), H-3->L+13 (10%), HOMO->L+22 (25%)
110	43011.43	232.4964	0.005	H-4->L+12 (29%), H-3->L+13 (13%)
111	43068.69	232.1872	0.0038	H-4->L+12 (34%), H-3->L+13 (16%)
112	43085.63	232.096	0.0057	H-3->L+13 (17%), HOMO->L+22 (24%)
113	43159.03	231.7012	0.0091	H-2->L+16 (12%), H-2->L+17 (33%)
114	43196.93	231.4979	0.0003	
115	43317.92	230.8514	0.0134	H-7->L+4 (10%)
116	43334.86	230.7611	0.0066	
117	43378.41	230.5294	0.0036	H-7->L+2 (12%), H-2->L+20 (10%)
118	43439.71	230.2041	0.0042	H-5->L+5 (12%), H-5->L+6 (17%), H-1->L+22 (12%)
119	43484.07	229.9693	0.0023	
120	43548.59	229.6285	0.0228	
121	43566.34	229.535	0.0077	H-5->L+5 (13%), H-2->L+20 (10%)
122	43599.41	229.3609	0.0045	H-10->L+1 (11%), H-1->L+22 (12%)
123	43649.41	229.0981	0.0097	H-2->L+20 (10%), H-1->L+22 (10%)
124	43728.46	228.684	0.0042	H-10->L+1 (23%)
125	43756.69	228.5365	0.0028	
126	43778.46	228.4228	0.004	H-7->L+3 (11%), H-5->L+6 (18%)
127	43804.27	228.2882	0.008	H-4->L+18 (20%), H-3->L+14 (14%)
128	43836.54	228.1202	0.0455	H-7->L+3 (22%)
129	43872.02	227.9357	0.0119	H-4->L+18 (10%), H-3->L+14 (26%)
130	43915.58	227.7096	0.0143	
131	44047.05	227.03	0.0071	H-7->L+3 (10%), H-6->L+6 (12%)
132	44109.15	226.7103	0.0028	H-5->L+7 (20%), H-3->L+15 (12%)
133	44169.65	226.3998	0.0234	H-11->L+1 (11%), H-7->L+4 (21%), H-6->L+6 (13%)
134	44227.72	226.1026	0.0041	H-11->L+1 (18%), H-6->L+5 (12%)
135	44234.17	226.0696	0.0051	HOMO->L+23 (32%)
136	44261.59	225.9295	0.007	H-6->L+6 (19%), H-5->L+7 (10%), H-3->L+15 (18%)
137	44359.19	225.4324	0.0124	H-6->L+5 (22%)
138	44418.87	225.1295	0.0019	H-4->L+13 (52%)

139	44432.58	225.0601	0.0054	
140	44550.34	224.4652	0.0041	H-15->LUMO (15%), H-15->L+1 (14%), H-14->L+1 (14%)
141	44634.22	224.0433	0.0145	
142	44697.94	223.7239	0.0066	H-3->L+16 (24%)
143	44746.34	223.482	0.0241	H-14->L+1 (18%)
144	44760.85	223.4095	0.0089	H-3->L+16 (15%), H-3->L+17 (24%)
145	44811.67	223.1562	0.0031	H-4->L+14 (12%), H-4->L+20 (10%)
146	44829.41	223.0678	0.0058	
147	44875.39	222.8393	0.0077	H-8->L+2 (10%)
148	44938.3	222.5273	0.0059	H-5->L+8 (16%)
149	44959.27	222.4236	0.0044	H-6->L+8 (10%), H-5->L+8 (44%)
150	45022.18	222.1127	0.0033	H-8->L+2 (17%)

Table S9. First 150 excited states for compound **8e** derived from TD-DFT.

No.	E /cm^{-1}	λ / nm	Osc. Strength	Major contributions
1	21020.42	475.7279	0.036	H-1->LUMO (76%), HOMO->LUMO (20%)
2	21155.92	472.6809	0.0011	HOMO->L+1 (87%)
3	21546.3	464.1169	0.2186	H-1->LUMO (19%), HOMO->LUMO (79%)
4	22213.32	450.1804	0.0005	H-1->L+1 (89%)
5	26713.89	374.3371	0.0005	H-4->L+1 (83%), H-4->L+17 (13%)
6	26825.19	372.7839	0.0008	HOMO->L+2 (84%)
7	28256.83	353.8968	0.0016	H-1->L+2 (84%)
8	28716.56	348.2311	0.239	H-2->LUMO (85%)
9	28839.16	346.7507	0.0058	HOMO->L+4 (74%)
10	29028.7	344.4867	0.0357	H-16->LUMO (39%), H-3->LUMO (35%)
11	29244.86	341.9405	0.0015	HOMO->L+3 (91%)
12	29311.8	341.1595	0.0017	HOMO->L+5 (73%)
13	29631.2	337.4822	0.0061	HOMO->L+5 (12%), HOMO->L+6 (85%)
14	29784.44	335.7458	0.0062	H-16->LUMO (32%), H-3->LUMO (51%)
15	30130.45	331.8901	0.0002	H-1->L+4 (69%)
16	30447.43	328.4349	0.001	H-1->L+3 (15%), HOMO->L+7 (71%)
17	30524.05	327.6105	0.0015	H-1->L+3 (76%), H-1->L+4 (10%)
18	30594.22	326.8591	0.0021	H-1->L+5 (63%), H-1->L+6 (16%)
19	30887.81	323.7523	0.0005	H-1->L+5 (18%), H-1->L+6 (76%)
20	30957.17	323.0269	0.0021	HOMO->L+8 (25%), HOMO->L+9 (45%), HOMO->L+10 (13%)
21	30962.01	322.9764	0.0024	H-4->LUMO (92%)
22	31097.51	321.5691	0.003	HOMO->L+8 (65%), HOMO->L+9 (28%)
23	31318.51	319.3	0.0018	HOMO->L+9 (14%), HOMO->L+10 (74%)
24	31565.31	316.8034	0.0009	H-1->L+7 (77%)
25	31690.33	315.5537	0.0283	H-2->L+1 (92%)
26	32326.7	309.3418	0.0018	H-1->L+7 (10%), H-1->L+8 (18%), H-1->L+9 (43%), H-1->L+10 (14%)
27	32381.55	308.8179	0.0002	H-1->L+8 (77%), H-1->L+9 (18%)
28	32555.76	307.1653	0.0001	HOMO->L+11 (51%), HOMO->L+17 (20%)
29	32563.83	307.0892	0.0007	H-1->L+9 (22%), H-1->L+10 (65%)
30	32833.22	304.5696	0.0014	HOMO->L+11 (13%), HOMO->L+17 (24%), HOMO->L+20 (21%)
31	32918.71	303.7786	0	H-25->LUMO (93%)
32	33115.51	301.9733	0.0017	HOMO->L+12 (93%)
33	33381.67	299.5656	0.0028	HOMO->L+11 (22%), HOMO->L+20 (33%)
34	33491.37	298.5844	0.0016	HOMO->L+13 (71%)
35	33546.21	298.0963	0.0385	H-3->L+1 (42%), H-1->L+11 (10%), H-1->L+17 (19%)
36	33691.39	296.8117	0.0026	H-5->LUMO (95%)
37	33808.34	295.785	0.0115	HOMO->L+15 (67%)
38	33908.35	294.9126	0.0004	HOMO->L+14 (48%), HOMO->L+15 (15%), HOMO->L+17 (17%)
39	34041.44	293.7596	0.0485	H-3->L+1 (31%), H-1->L+11 (48%)
40	34177.74	292.5881	0.0044	HOMO->L+16 (91%)
41	34362.44	291.0154	0.0011	H-1->L+12 (73%)
42	34516.5	289.7165	0.0078	H-3->L+1 (10%), H-1->L+11 (20%), H-1->L+12 (17%), H-1->L+14 (11%), H-1->L+17 (29%)
43	34760.88	287.6797	0.0027	H-1->L+13 (78%)
44	34991.56	285.7832	0.0022	H-1->L+15 (14%), H-1->L+20 (24%), HOMO->L+18 (20%), HOMO->L+21

				(14%)
45	35111.73	284.8051	0.0102	H-6->LUMO (23%), H-1->L+14 (12%), H-1->L+15 (39%)
46	35127.87	284.6743	0.0115	H-6->LUMO (67%), H-1->L+15 (16%)
47	35327.08	283.0689	0.0012	H-1->L+16 (37%), H-1->L+18 (26%), H-1->L+21 (13%)
48	35369.83	282.7268	0.0003	H-1->L+14 (50%), H-1->L+15 (21%), H-1->L+17 (10%)
49	35514.2	281.5775	0.004	H-1->L+16 (55%), H-1->L+18 (13%)
50	35552.92	281.2709	0.028	H-2->L+2 (85%)
51	35739.23	279.8045	0.0198	H-5->L+1 (82%)
52	35834.41	279.0614	0.0013	HOMO->L+18 (13%), HOMO->L+19 (56%), HOMO->L+22 (10%)
53	36242.52	275.919	0.0012	H-7->LUMO (77%)
54	36437.71	274.441	0.0005	HOMO->L+22 (62%)
55	36714.36	272.373	0.0018	H-2->L+3 (57%)
56	36762.75	272.0145	0.0088	H-4->L+2 (11%), H-2->L+4 (22%), HOMO->L+19 (11%)
57	36966.81	270.5129	0.0029	H-9->LUMO (13%), H-8->LUMO (38%), H-2->L+3 (17%)
58	37017.62	270.1416	0.0143	H-2->L+4 (67%)
59	37107.15	269.4898	0.0035	H-2->L+5 (23%), H-1->L+19 (29%), H-1->L+22 (18%)
60	37186.19	268.917	0.0057	H-9->LUMO (12%), H-8->LUMO (17%), H-2->L+5 (39%)
61	37350.73	267.7324	0.0084	H-19->LUMO (13%), H-15->LUMO (11%), H-8->LUMO (17%)
62	37373.31	267.5706	0.0441	H-9->LUMO (13%), H-2->L+5 (11%)
63	37508.01	266.6097	0.0031	H-1->L+19 (17%), H-1->L+22 (27%)
64	37653.19	265.5818	0.0102	H-4->L+2 (15%), H-1->L+19 (15%), H-1->L+21 (10%)
65	37667.7	265.4794	0.0021	H-2->L+6 (81%)
66	37729.81	265.0424	0.0165	H-10->LUMO (40%), H-9->LUMO (14%)
67	37928.22	263.6559	0.011	H-3->L+2 (65%)
68	38083.89	262.5782	0.0053	H-4->L+2 (33%), H-1->L+21 (25%)
69	38119.38	262.3338	0.0003	H-11->LUMO (66%), H-10->LUMO (16%)
70	38381.51	260.5422	0.0134	H-2->L+7 (83%)
71	38589.6	259.1372	0.004	H-13->LUMO (67%), H-12->LUMO (17%)
72	38662.19	258.6507	0.01	H-8->L+1 (10%), H-7->L+1 (12%), H-2->L+8 (18%), H-2->L+9 (10%)
73	38667.03	258.6183	0.0062	H-19->LUMO (11%), H-15->LUMO (12%), H-14->LUMO (36%)
74	38800.11	257.7312	0.0144	H-2->L+8 (68%)
75	38908.99	257.01	0.0026	H-2->L+9 (83%)
76	38999.33	256.4147	0.0006	H-14->LUMO (30%), H-12->LUMO (26%)
77	39121.92	255.6112	0.0017	H-3->L+3 (62%), H-2->L+10 (12%)
78	39147.73	255.4426	0.0006	H-3->L+3 (18%), H-2->L+10 (47%)
79	39150.15	255.4269	0.0013	H-15->LUMO (24%), H-12->LUMO (17%), H-2->L+10 (28%)
80	39238.87	254.8493	0.0605	H-6->L+1 (54%), H-3->L+4 (21%)
81	39354.21	254.1024	0.0189	H-4->L+4 (18%), H-3->L+3 (11%), H-3->L+4 (45%)
82	39400.18	253.8059	0.0031	H-18->LUMO (33%), H-17->LUMO (29%), H-15->LUMO (10%)
83	39503.42	253.1426	0.0298	H-6->L+1 (10%), H-4->L+4 (55%), H-3->L+4 (13%)
84	39616.34	252.4211	0.0077	H-3->L+5 (78%)
85	39757.49	251.5249	0.002	H-4->L+3 (85%)
86	39891.38	250.6808	0.0598	H-4->L+5 (70%)
87	39989.78	250.0639	0.0149	H-20->LUMO (54%), H-19->LUMO (13%)
88	40047.04	249.7063	0.0035	H-3->L+6 (87%)
89	40065.59	249.5907	0.0094	H-21->LUMO (22%), H-20->LUMO (16%), H-18->LUMO (29%), H-17->LUMO (12%)
90	40258.36	248.3956	0.076	H-10->L+1 (18%), H-8->L+1 (27%), H-7->L+1 (11%), H-4->L+5 (11%)

91	40327.72	247.9684	0.0106	H-2->L+11 (84%)
92	40369.66	247.7108	0.0064	H-4->L+6 (81%)
93	40389.02	247.592	0.0021	H-23->LUMO (11%), H-21->LUMO (38%), H-19->LUMO (13%), H-18->LUMO (18%), H-17->LUMO (12%)
94	40609.21	246.2496	0.0063	H-5->L+2 (61%), H-3->L+7 (13%)
95	40751.16	245.3918	0.0133	H-5->L+2 (12%), H-3->L+7 (64%), H-2->L+12 (12%)
96	40773.75	245.2559	0.0122	H-22->LUMO (70%)
97	40812.46	245.0232	0.0233	H-22->LUMO (14%), H-3->L+7 (11%), H-2->L+12 (56%)
98	40887.47	244.5737	0.1382	H-10->L+1 (13%), H-9->L+1 (18%), H-7->L+1 (28%), H-2->L+12 (14%)
99	41039.1	243.67	0.0026	H-4->L+7 (84%)
100	41174.6	242.8682	0.0036	H-3->L+8 (57%), H-3->L+9 (12%), H-2->L+13 (18%)
101	41265.74	242.3317	0.0034	H-3->L+8 (10%), H-3->L+10 (19%), H-2->L+13 (35%), H-2->L+14 (18%)
102	41282.68	242.2323	0.0016	H-23->LUMO (71%), H-21->LUMO (15%)
103	41319.78	242.0148	0.0062	H-3->L+8 (12%), H-3->L+9 (68%)
104	41411.73	241.4775	0.0113	H-2->L+13 (32%), H-2->L+14 (14%), H-2->L+15 (17%)
105	41477.06	241.0971	0.0006	H-3->L+10 (57%)
106	41578.69	240.5078	0.004	H-4->L+8 (35%), H-4->L+9 (31%), H-4->L+10 (12%)
107	41614.98	240.2981	0.0208	H-2->L+14 (10%), H-2->L+16 (17%)
108	41695.64	239.8332	0.0131	H-2->L+14 (15%), H-2->L+15 (60%)
109	41790.81	239.2871	0.0126	H-10->L+1 (11%), H-9->L+1 (25%), H-8->L+1 (18%), H-2->L+16 (15%)
110	41802.91	239.2178	0.0006	H-4->L+8 (46%), H-4->L+9 (37%)
111	41911.79	238.5963	0.0048	H-24->LUMO (39%), H-2->L+16 (19%)
112	41939.22	238.4403	0.0088	H-24->LUMO (21%), H-4->L+10 (36%)
113	41966.64	238.2845	0.0091	H-24->LUMO (21%), H-5->L+4 (24%), H-2->L+16 (15%)
114	42027.13	237.9415	0.0006	H-27->LUMO (72%)
115	42090.04	237.5859	0.0072	H-4->L+10 (12%), H-2->L+17 (38%)
116	42101.33	237.5222	0.0068	H-6->L+2 (17%), H-4->L+10 (11%), H-2->L+17 (18%)
117	42237.64	236.7556	0.0247	H-5->L+5 (12%), H-5->L+6 (12%), H-2->L+16 (12%), H-2->L+17 (13%)
118	42377.18	235.9761	0.0182	H-13->L+1 (14%), H-11->L+1 (22%)
119	42578.01	234.863	0.005	H-5->L+3 (21%), H-5->L+4 (13%), H-5->L+5 (24%), H-2->L+20 (14%)
120	42609.46	234.6896	0.0002	H-5->L+3 (18%), H-5->L+6 (48%)
121	42695.77	234.2153	0.007	H-5->L+4 (13%), H-5->L+5 (14%), H-3->L+11 (49%)
122	42744.16	233.9501	0.0086	H-5->L+3 (16%), H-4->L+11 (10%), H-4->L+17 (27%)
123	42761.9	233.853	0.0088	H-5->L+3 (16%), H-4->L+17 (17%)
124	42802.23	233.6327	0.0364	H-6->L+2 (14%), H-5->L+3 (12%), H-3->L+11 (22%)
125	42902.24	233.088	0.0162	H-2->L+20 (19%)
126	43028.07	232.4065	0.0023	H-14->L+1 (20%), H-12->L+1 (10%)
127	43103.08	232.002	0.0098	H-15->L+1 (15%), H-7->L+2 (13%)
128	43232.93	231.3052	0.013	H-13->L+1 (22%), H-3->L+12 (14%)
129	43278.9	231.0595	0.005	H-12->L+1 (27%), H-3->L+12 (15%), H-2->L+18 (13%)
130	43370.85	230.5696	0.0054	H-2->L+18 (54%)
131	43383.76	230.501	0.0049	H-8->L+2 (11%), H-3->L+13 (18%)
132	43391.02	230.4625	0.0033	H-5->L+7 (28%), H-3->L+14 (19%)
133	43422.47	230.2955	0.0265	H-5->L+7 (10%), H-3->L+12 (23%)
134	43482.96	229.9751	0.0233	H-3->L+14 (11%)
135	43514.42	229.8089	0.0087	H-17->L+1 (11%), H-13->L+1 (11%), H-3->L+14 (15%)
136	43562	229.5578	0.0022	H-15->L+1 (19%), H-4->L+11 (13%)
137	43607.17	229.3201	0.0032	H-4->L+11 (31%)

138	43638.63	229.1548	0.0214	H-15->L+1 (15%), H-7->L+2 (17%), H-4->L+11 (10%)
139	43694.28	228.8629	0.0014	H-3->L+13 (10%)
140	43788.65	228.3697	0.0065	H-7->L+2 (13%), H-3->L+13 (10%), H-2->L+19 (12%)
141	43848.33	228.0588	0.0123	H-2->L+19 (49%)
142	43887.85	227.8535	0.0023	H-4->L+12 (41%), H-3->L+13 (12%)
143	43929.79	227.6359	0.0025	H-4->L+12 (38%)
144	44005.61	227.2438	0.0036	H-6->L+3 (16%), H-3->L+15 (24%), HOMO->L+23 (12%)
145	44027.39	227.1314	0.0091	H-3->L+15 (27%)
146	44088.68	226.8156	0.0062	HOMO->L+23 (39%)
147	44125.79	226.6249	0.004	H-6->L+3 (16%), H-3->L+15 (23%)
148	44255.64	225.9599	0.0301	H-18->L+1 (24%), H-6->L+3 (12%)
149	44287.1	225.7994	0.0017	H-8->L+2 (12%), H-5->L+8 (35%)
150	44300	225.7336	0.0171	H-4->L+13 (34%), H-3->L+16 (25%)

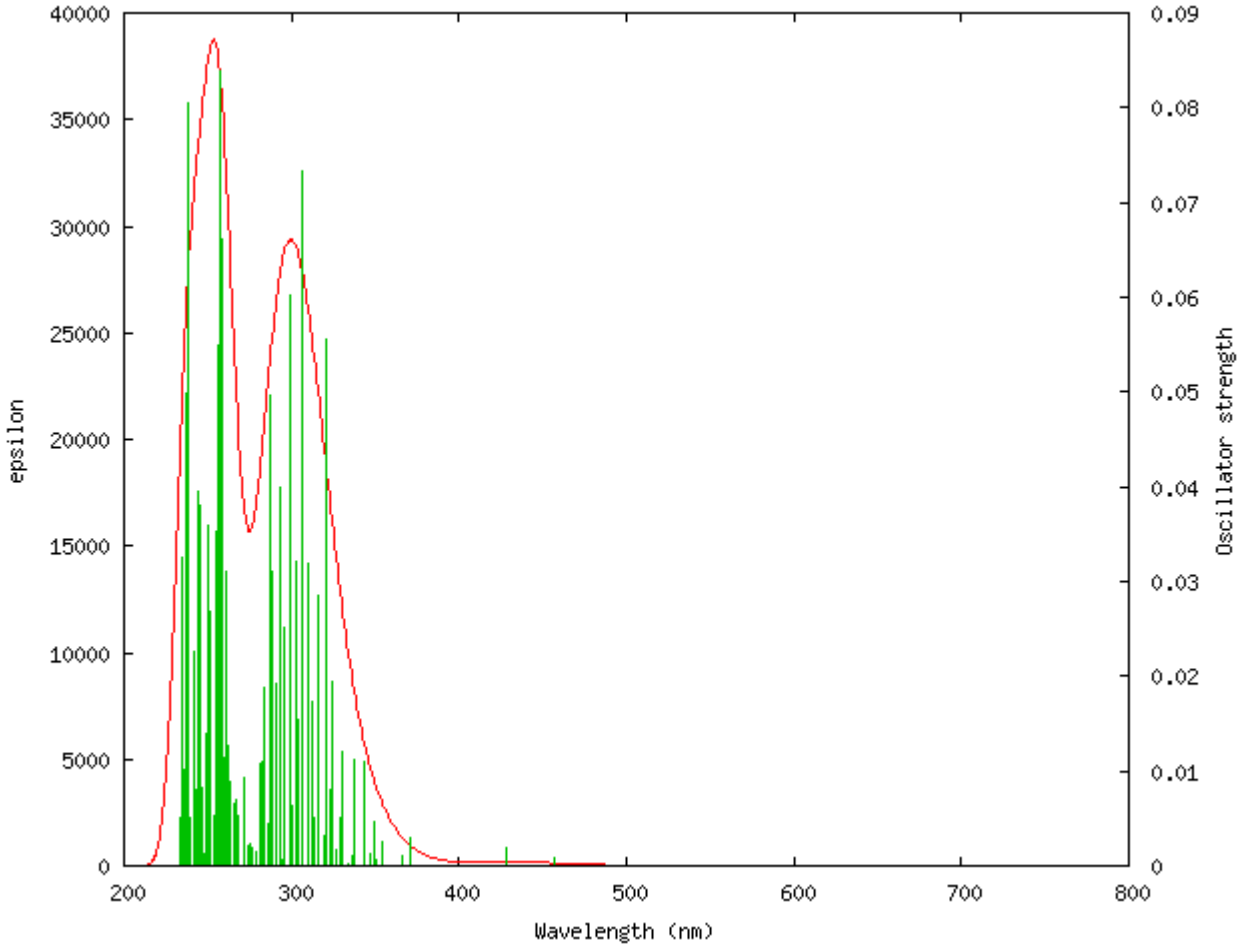


Figure S66: Simulated UV/Vis spectrum for **8a**, showing calculated transitions, derived from TD-DFT.

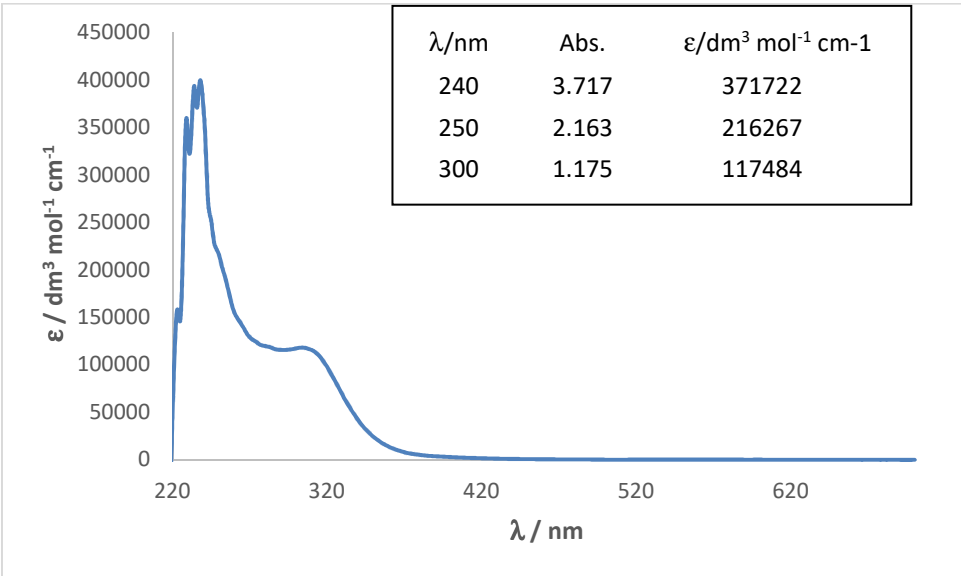
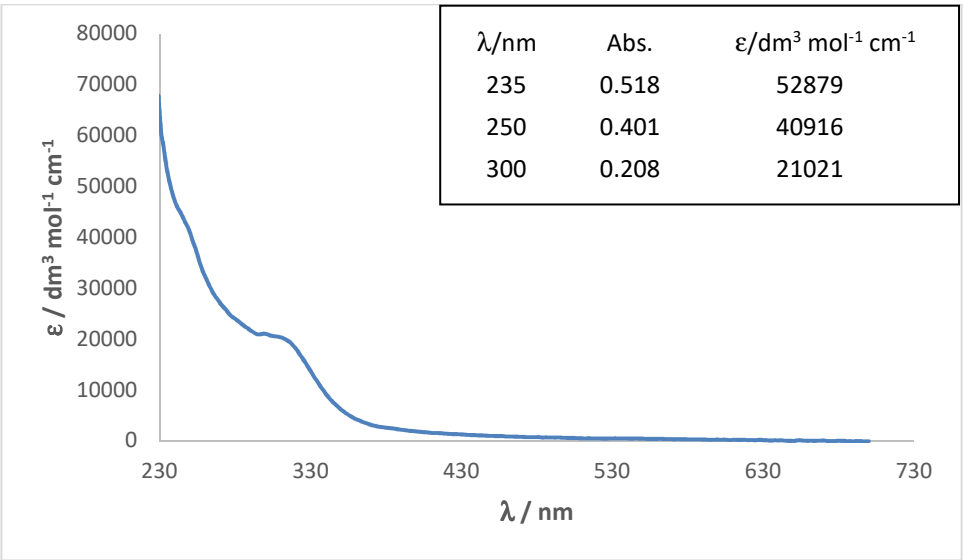


Figure S67: Experimental UV/Vis spectrum for **8a**, 1.0 x 10^{-5} mol dm^{-3} in CH_2Cl_2, 1 cm path.



λ/nm	Abs.	ε/dm³ mol⁻¹ cm⁻¹
235	0.518	52879
250	0.401	40916
300	0.208	21021

Figure S68: Experimental UV/Vis spectrum for **8b**, 9.8 x 10^{-6} mol dm^{-3} in CH_2Cl_2, 1 cm path.

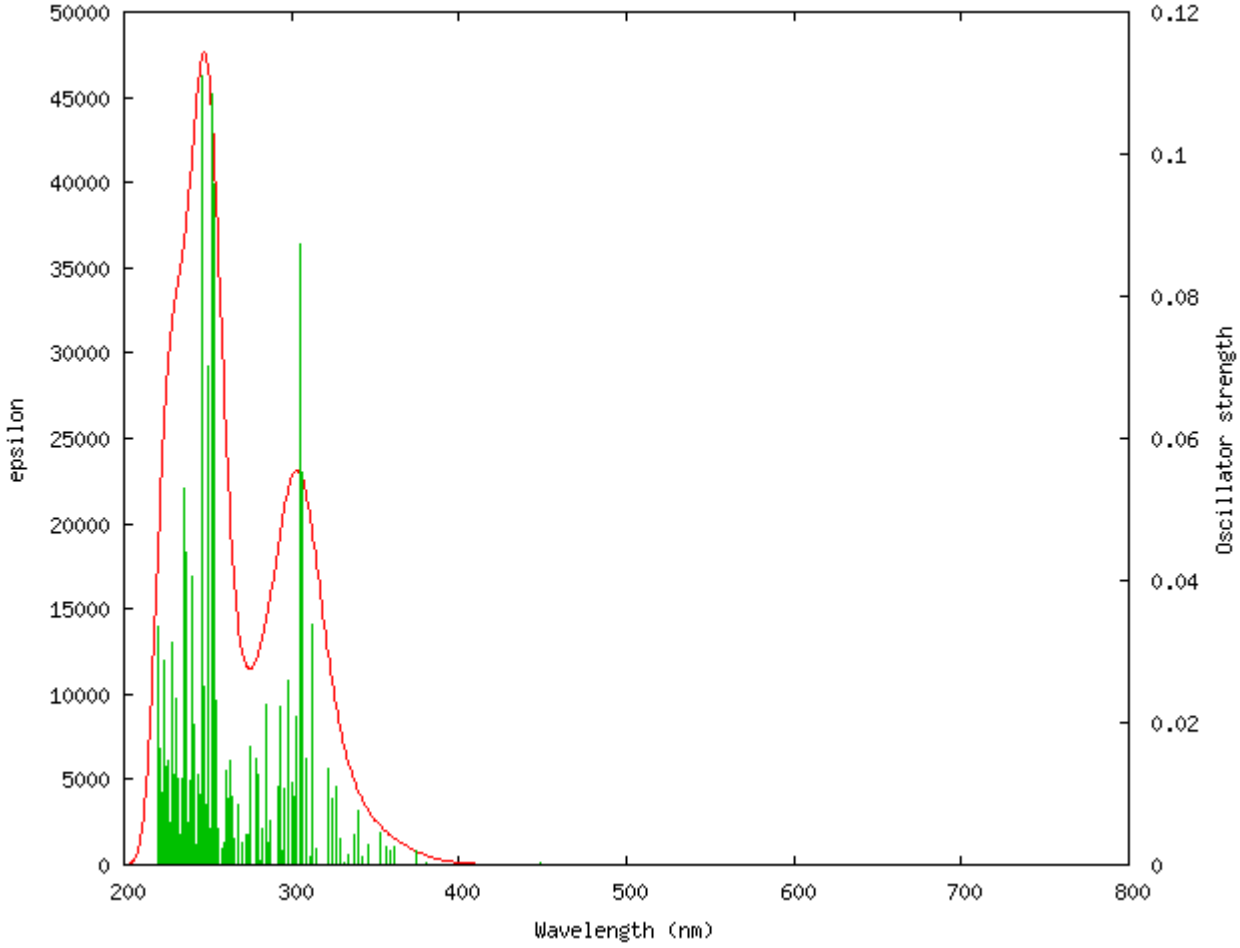
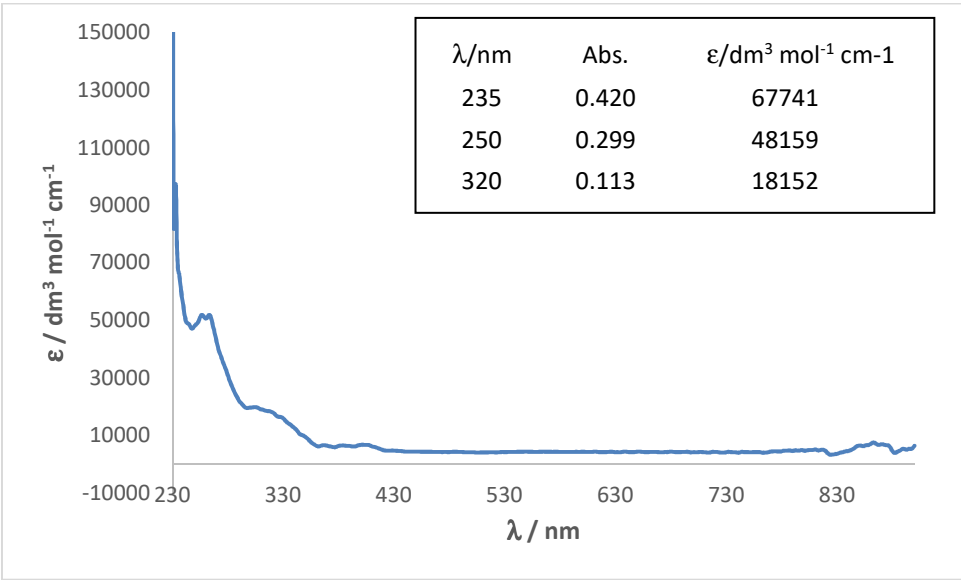


Figure S69: Simulated UV/Vis spectrum for **8c**, showing electronic transitions, derived from TD-DFT.



λ/nm	Abs.	ε/dm³ mol⁻¹ cm-1
235	0.420	67741
250	0.299	48159
320	0.113	18152

Figure S70: Experimental UV/Vis spectrum for **8c**, 6.2 x 10^{-6} mol dm^{-3} in CH_2Cl_2, 1 cm path.

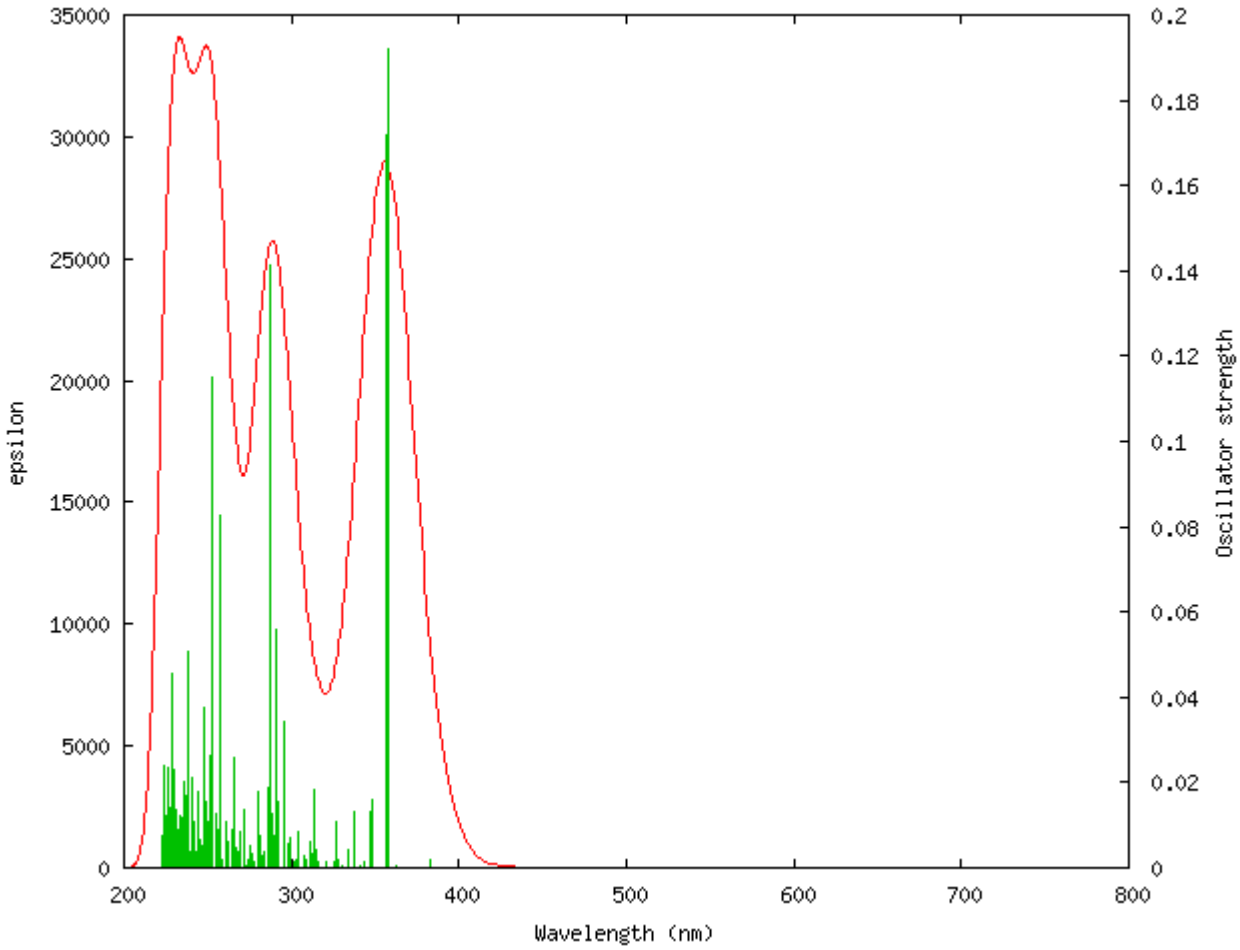


Figure S71: Simulated UV/Vis spectrum for **8d**, showing electronic transitions, derived from TD-DFT.

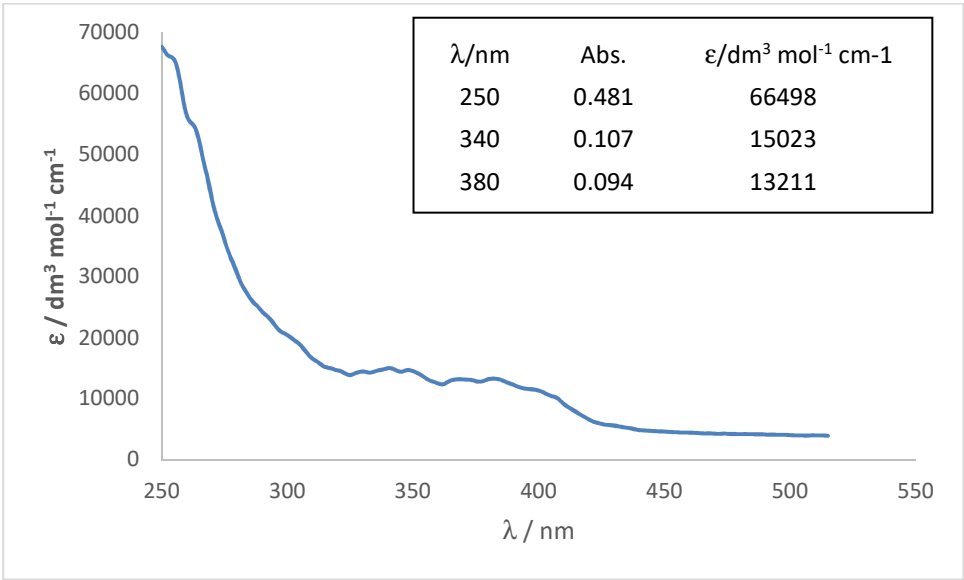


Figure S72: Experimental UV/Vis spectrum for **8d**, 8.0 x 10^{-6} mol dm^{-3} in CH_2Cl_2, 1 cm path.

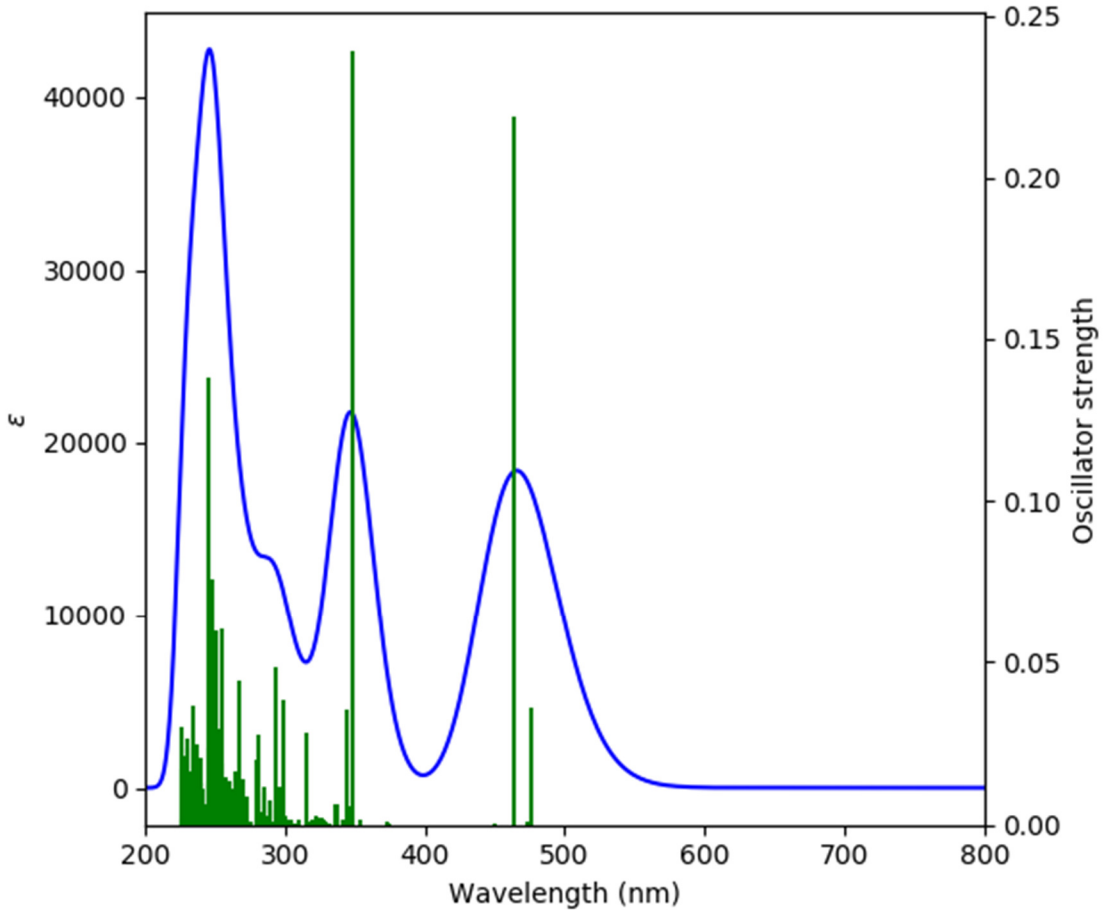


Figure S73: Simulated UV/Vis spectrum for **8e**, showing electronic transitions, derived from TD-DFT.

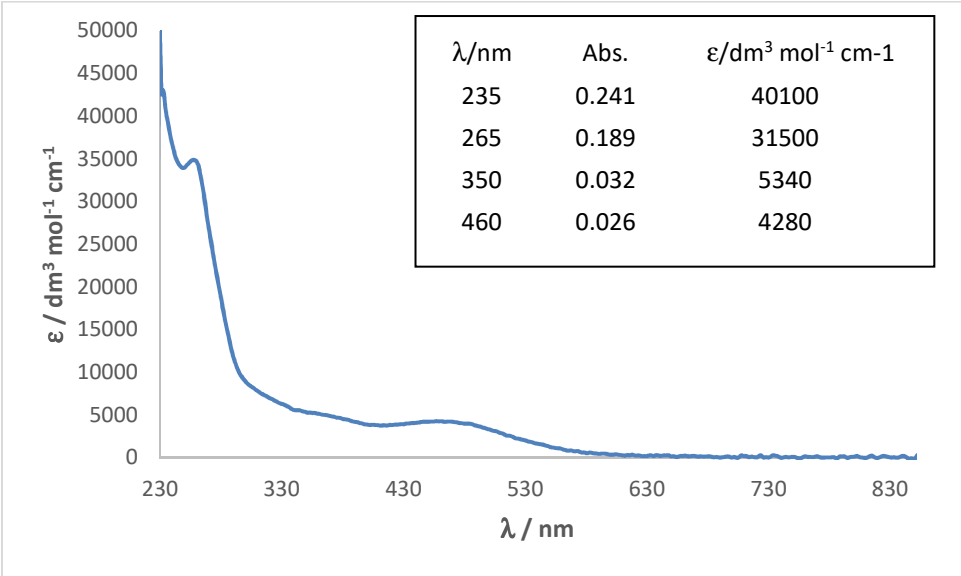


Figure S74: Experimental UV/Vis spectrum for **8e**, 6.0 x 10^{-6} mol dm^{-3} in CH_2Cl_2, 1 cm path.

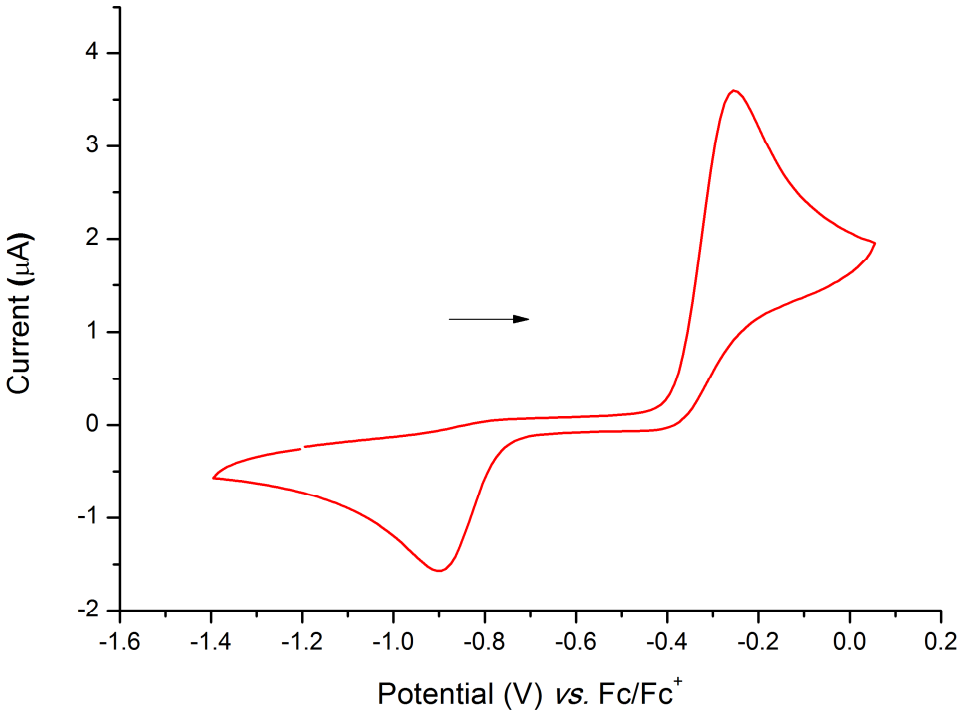


Figure S75: Cyclic Voltammagram for **4**, as solution in CH_2Cl_2 (1 mM) with $^nBu_4NPF_6$ (0.1 M) supporting electrolyte; recorded at 100 mV s^{-1}.

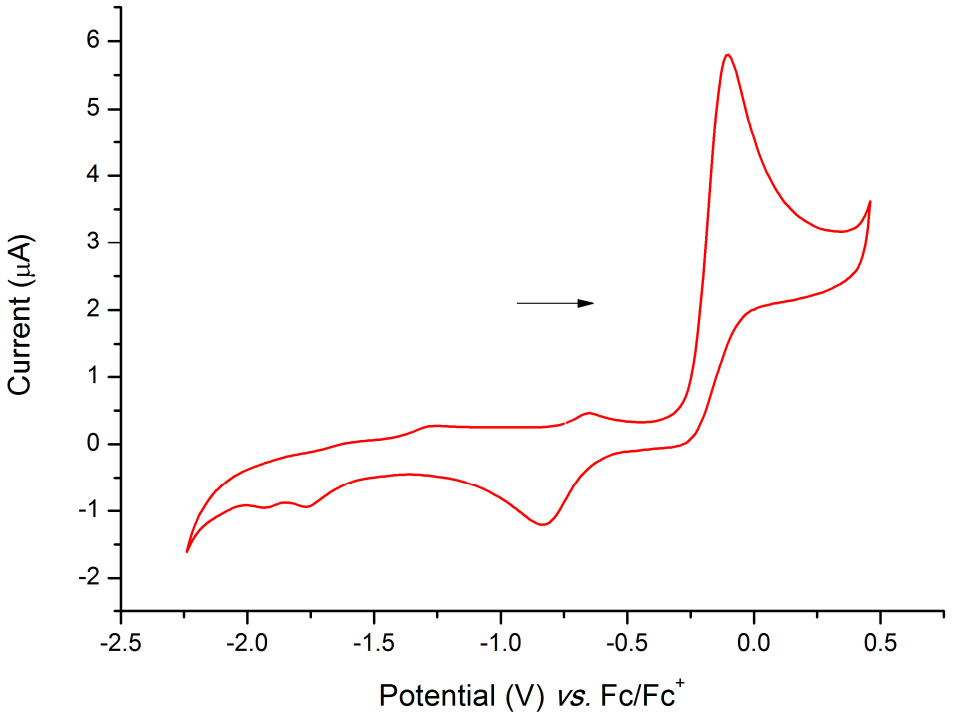


Figure S76: Cyclic Voltammagram for **8a** as solution in CH_2Cl_2 (1 mM) with $^nBu_4NPF_6$ (0.1 M) supporting electrolyte; recorded at 100 mV s^{-1}. Weak events arise from trace contaminants in the electrolyte.

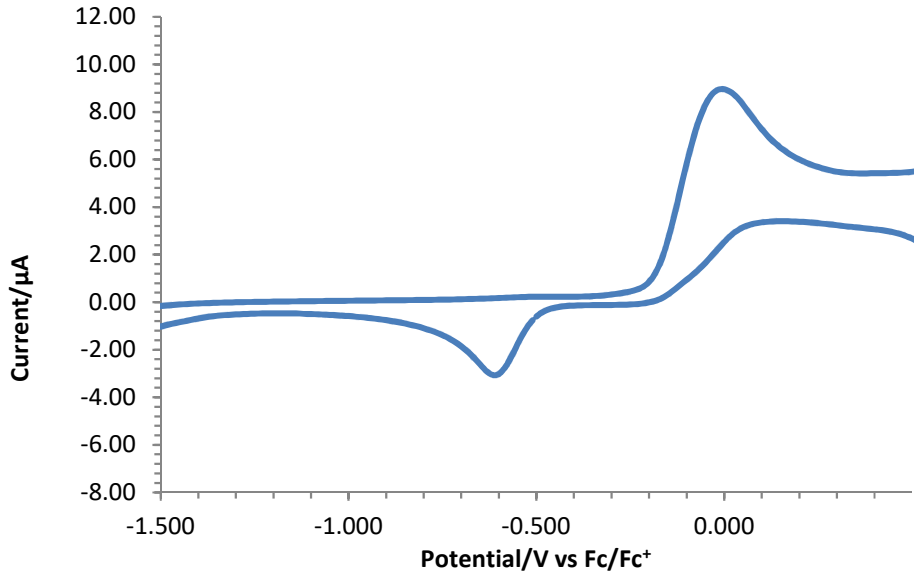


Figure S77: Cyclic Voltammagram for **8b** as solution in CH_2Cl_2 (3.4 mM) with $^nBu_4NPF_6$ (0.1 M) supporting electrolyte; recorded at 100 mV s^{-1}.

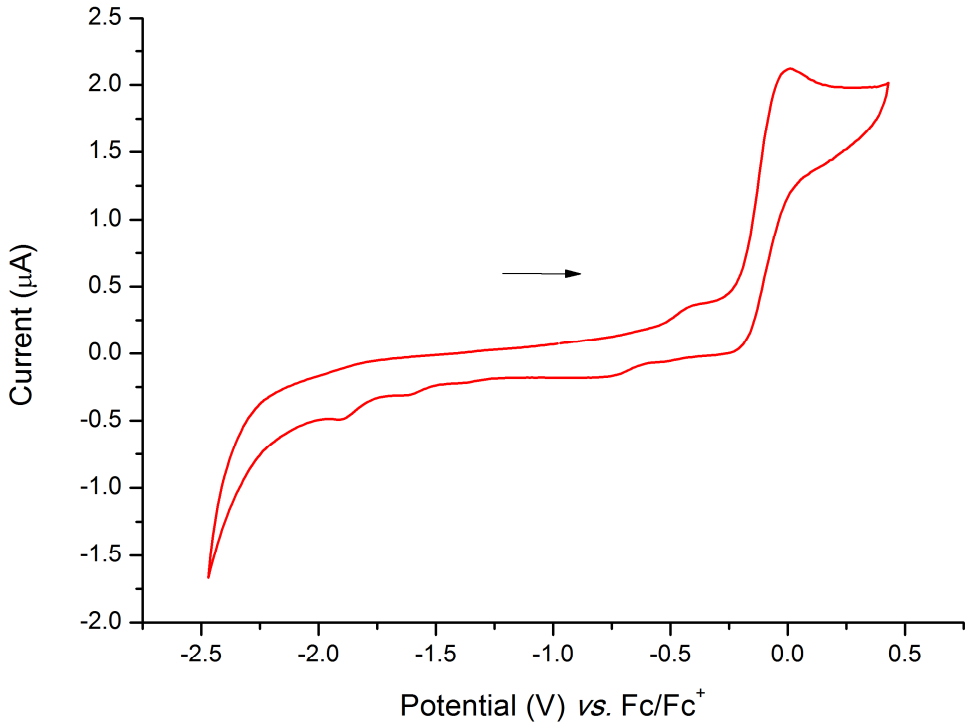


Figure S78: Cyclic Voltammagram for **8c** as solution in CH_2Cl_2 (2 mM) with $^nBu_4NPF_6$ (0.1 M) supporting electrolyte; recorded at 100 mV s^{-1}.

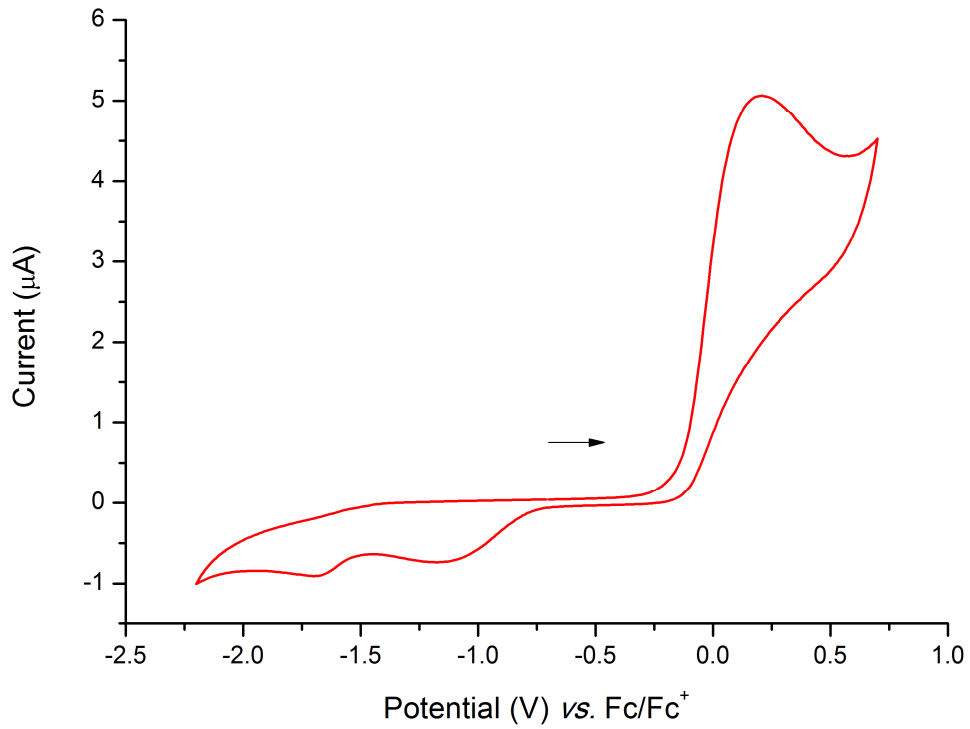


Figure S79: Cyclic Voltammagram for **8d** as solution in CH_2Cl_2 (4.6 mM) with $^nBu_4NPF_6$ (0.1 M) supporting electrolyte; recorded at 100 mV s^{-1}.

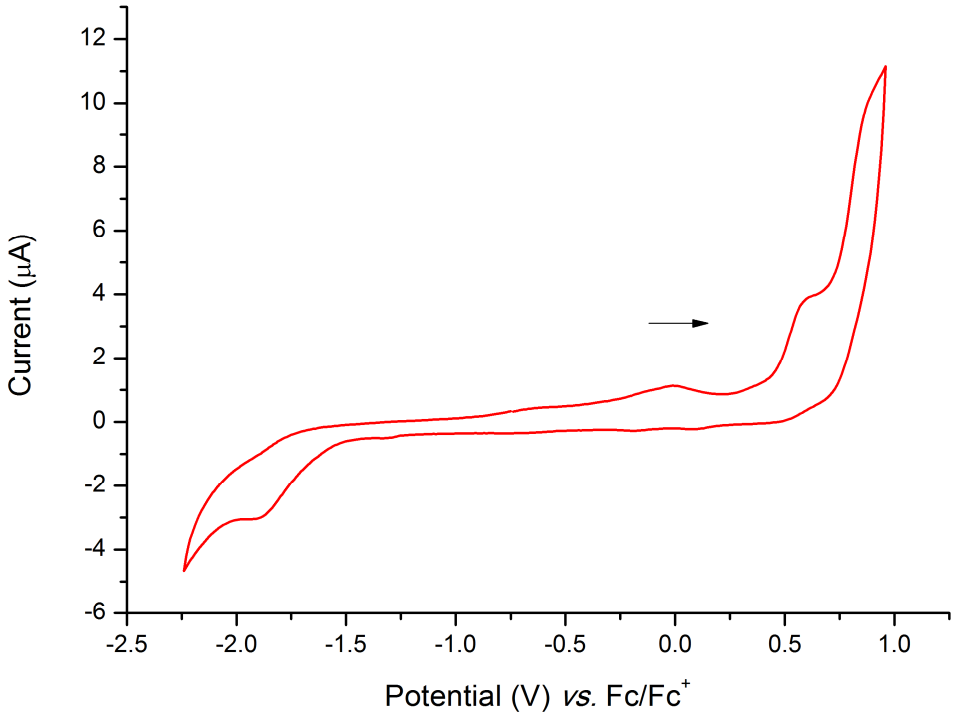


Figure S80: Cyclic Voltammagram for **8e** as solution in CH_2Cl_2 (1.9 mM) with $^nBu_4NPF_6$ (0.1 M) supporting electrolyte; recorded at 100 mV s^{-1}. The event around 0 V is attributable to a residual trace of **7e**$^+$, which consistently contaminates samples of **8e**.

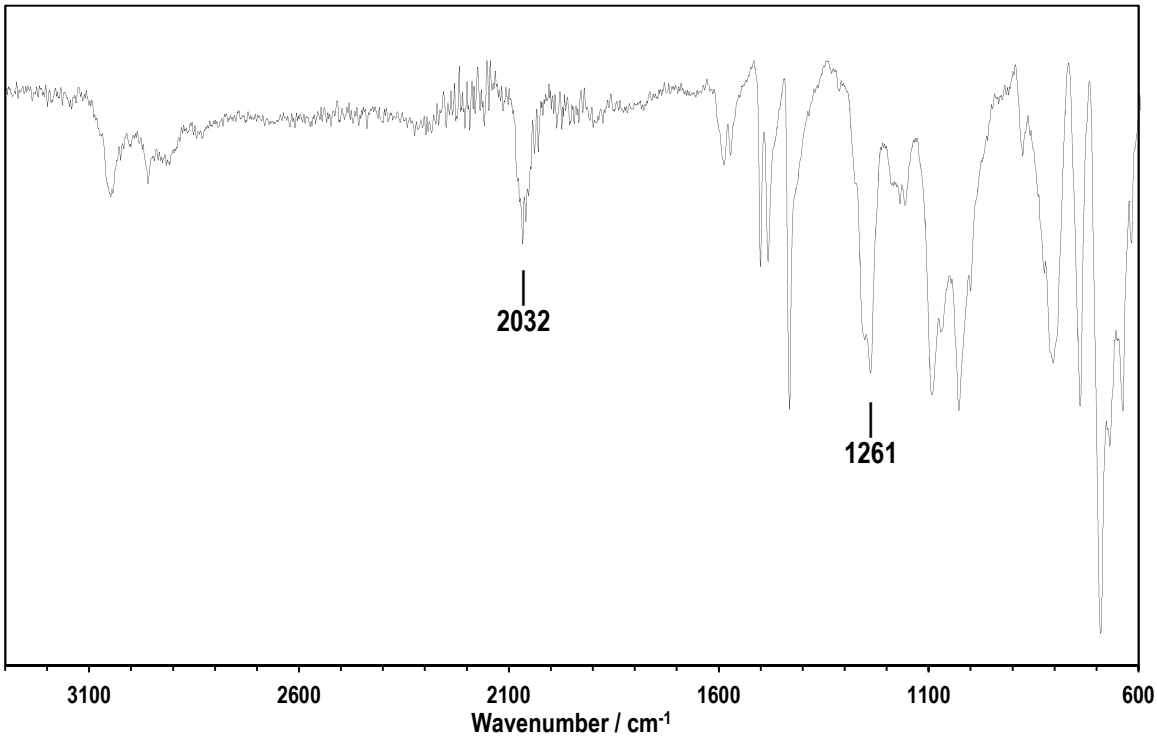


Figure S81: IR Spectrum for compound **4**

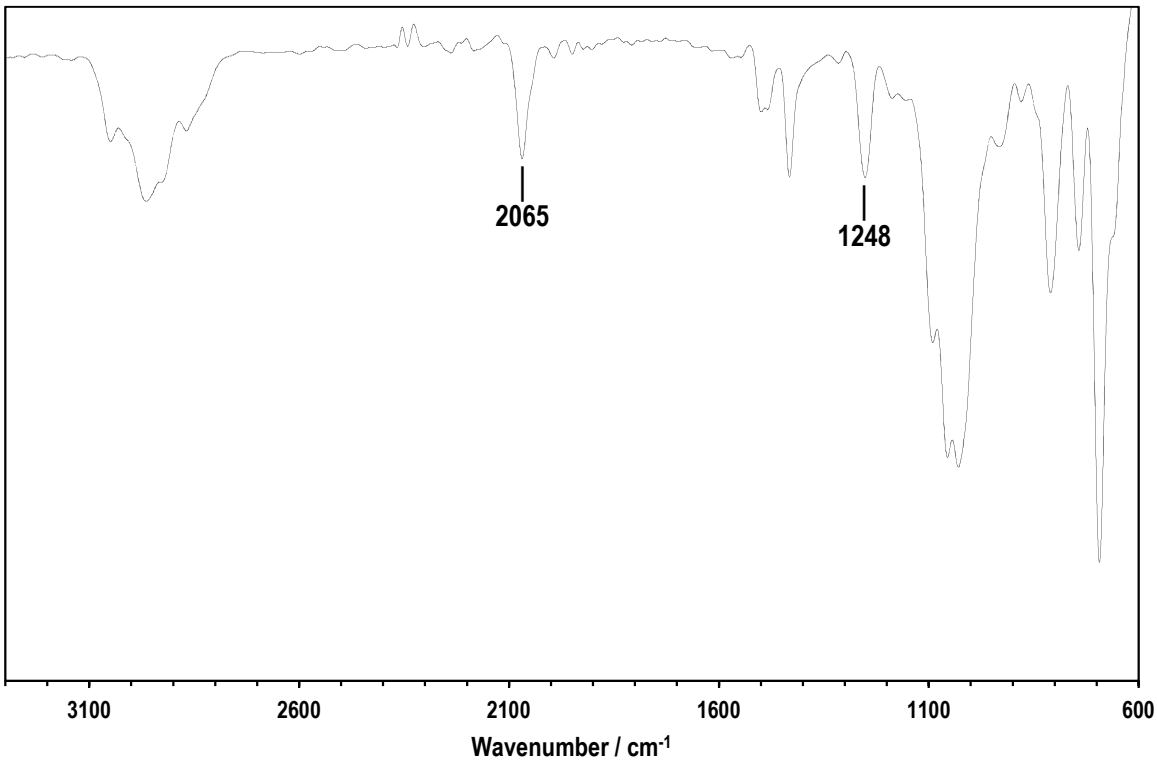


Figure S82: IR Spectrum for compound **8a**

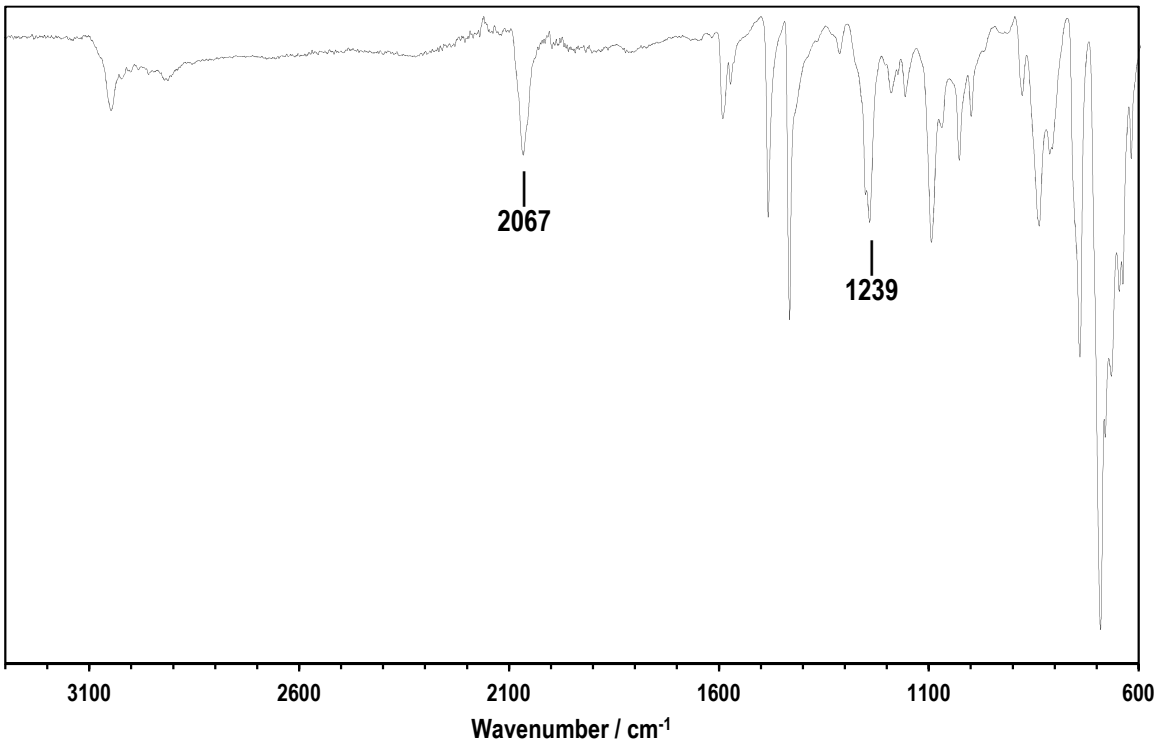


Figure S83: IR Spectrum for compound **8b**

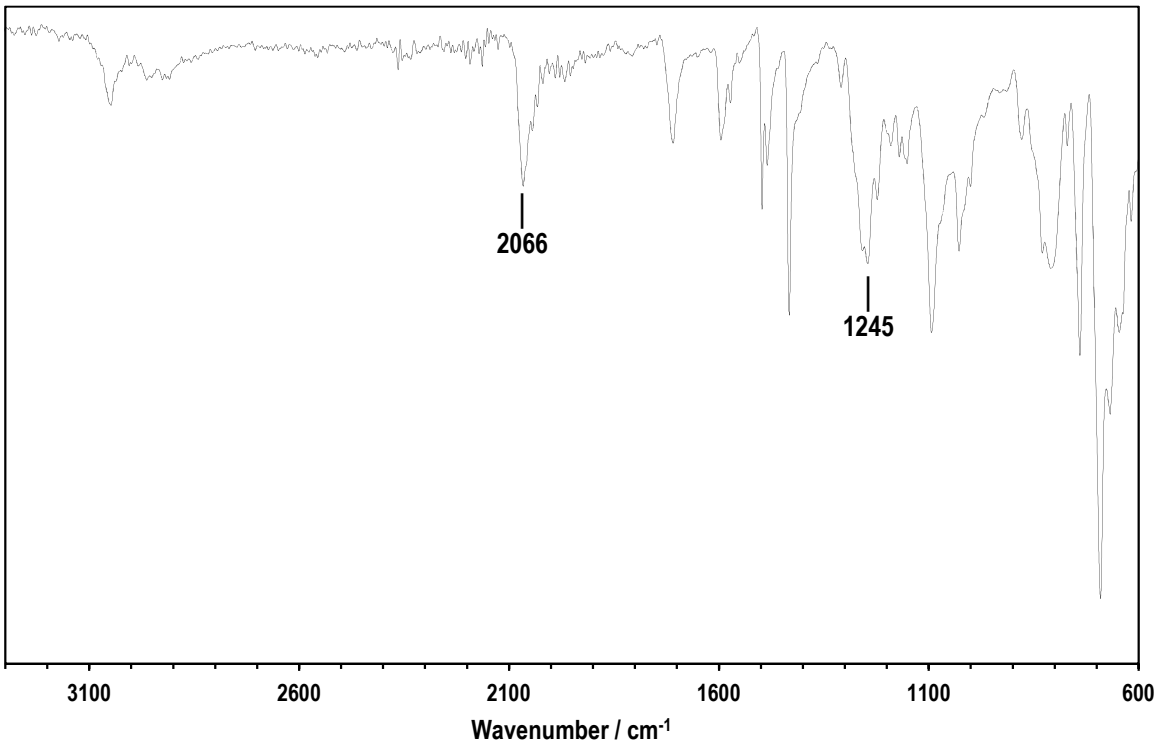


Figure S84: IR Spectrum for compound **8c**

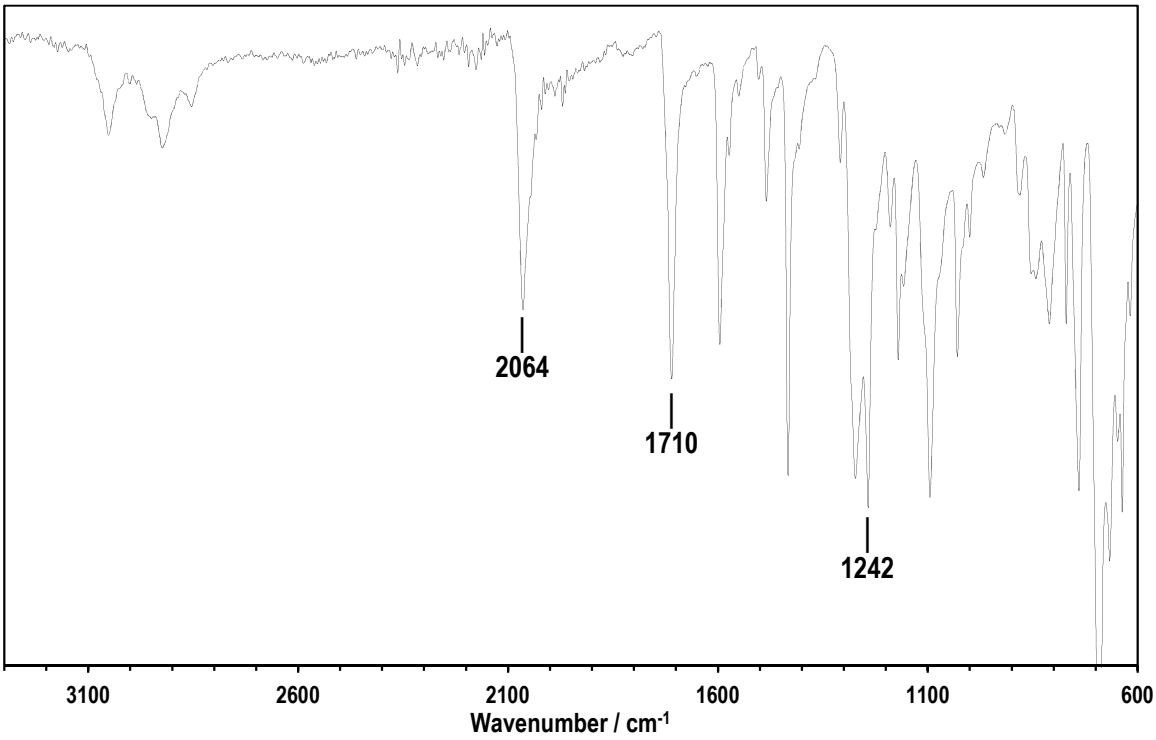


Figure S85: IR Spectrum for compound **8d**

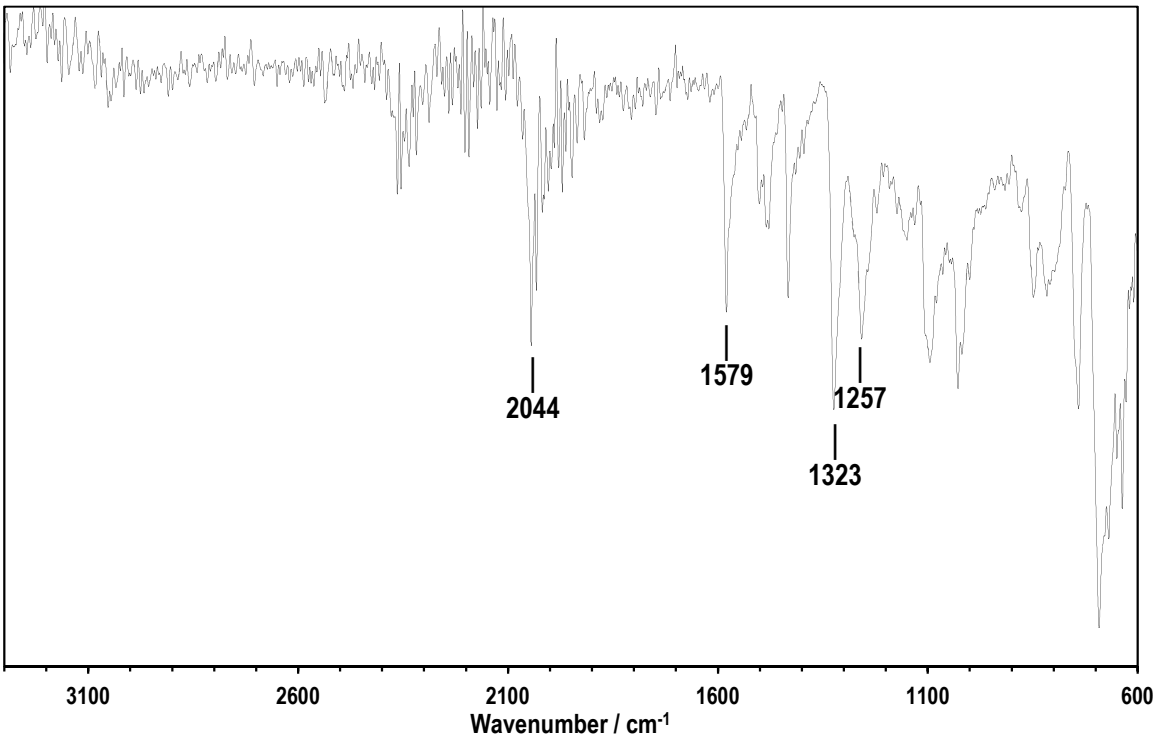


Figure S86: IR Spectrum for compound **8e**

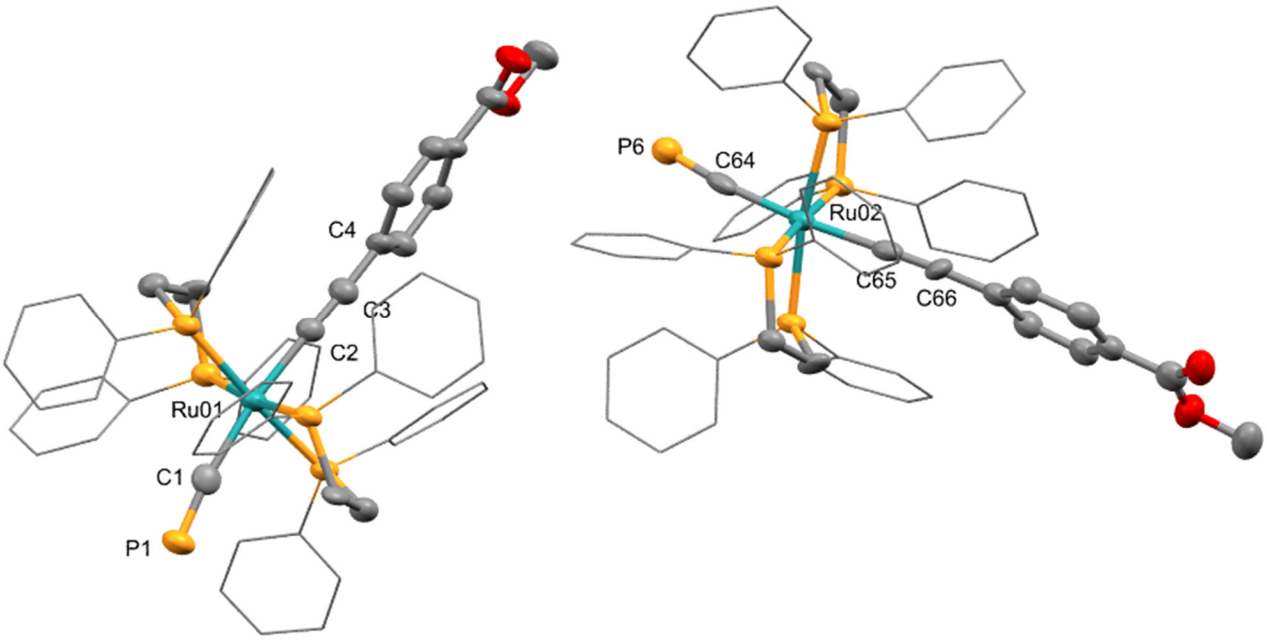


Figure S87: Plot of both independent molecules in the asymmetric unit of **8d**, with solvent molecules and hydrogen atoms removed for clarity. Displacement ellipsoids at 50%