Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information for:

Pyrene Fluorescence in 2,7-Di(4-phenylethynyl)pyrene-Bridged Bis(alkenylruthenium) Complexes

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Table of Contents

Synthetic Route for the Synthesis of PyrDPE-Ru$_{Cl}$ and PyrDPE-Ru$_{acac}$

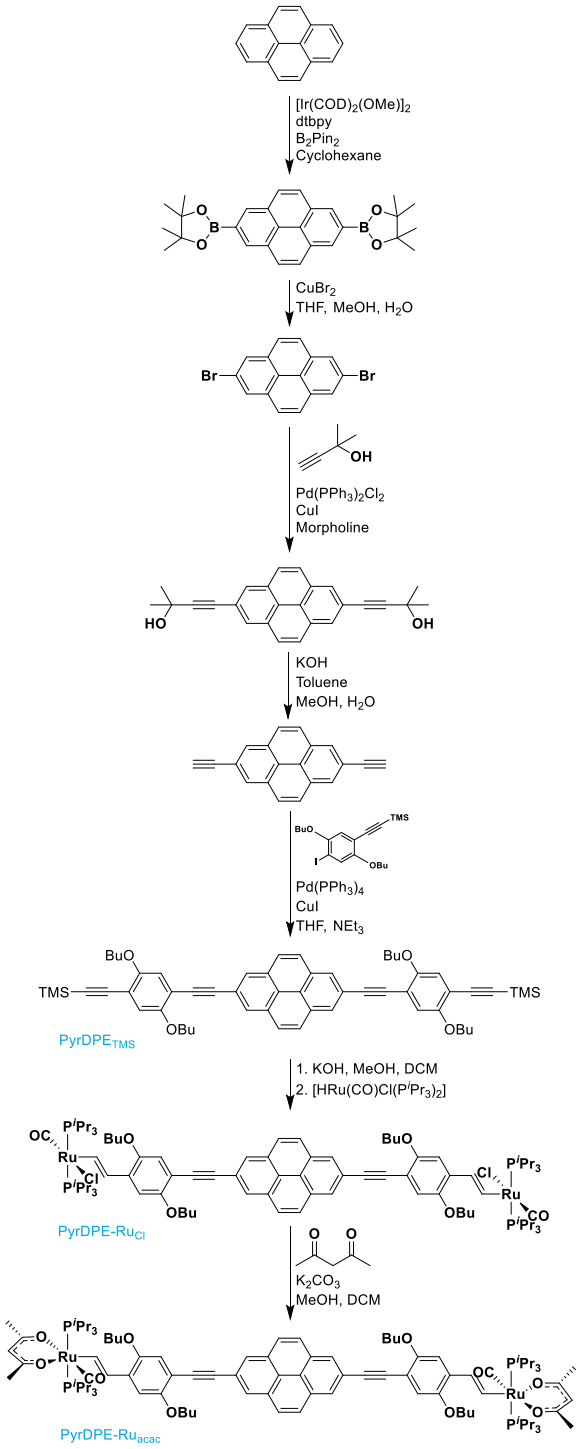

Figure S1 | Reaction scheme for the synthesis of **PyrDPE-Ru$_{Cl}$** and **PyrDPE-Ru$_{acac}$**.

NMR Spectroscopy

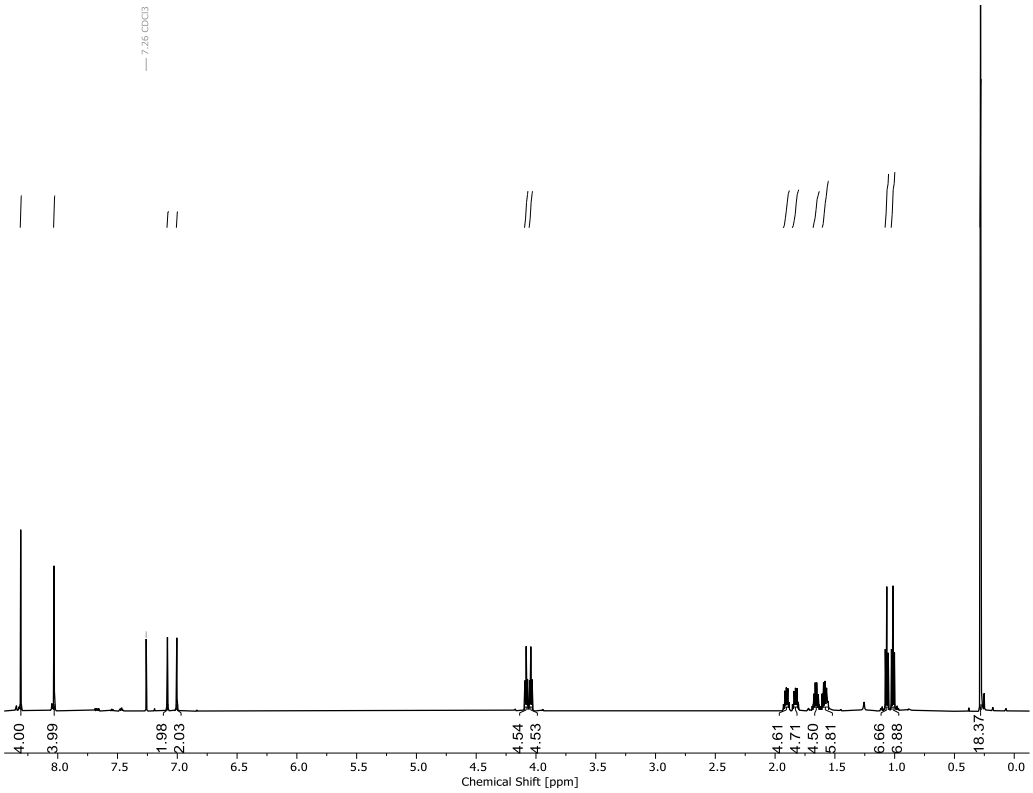

Figure S2 | ^{1}H-NMR spectrum of **PyrDPE$_{TMS}$**; measured in $CDCl_3$ at 298 K.

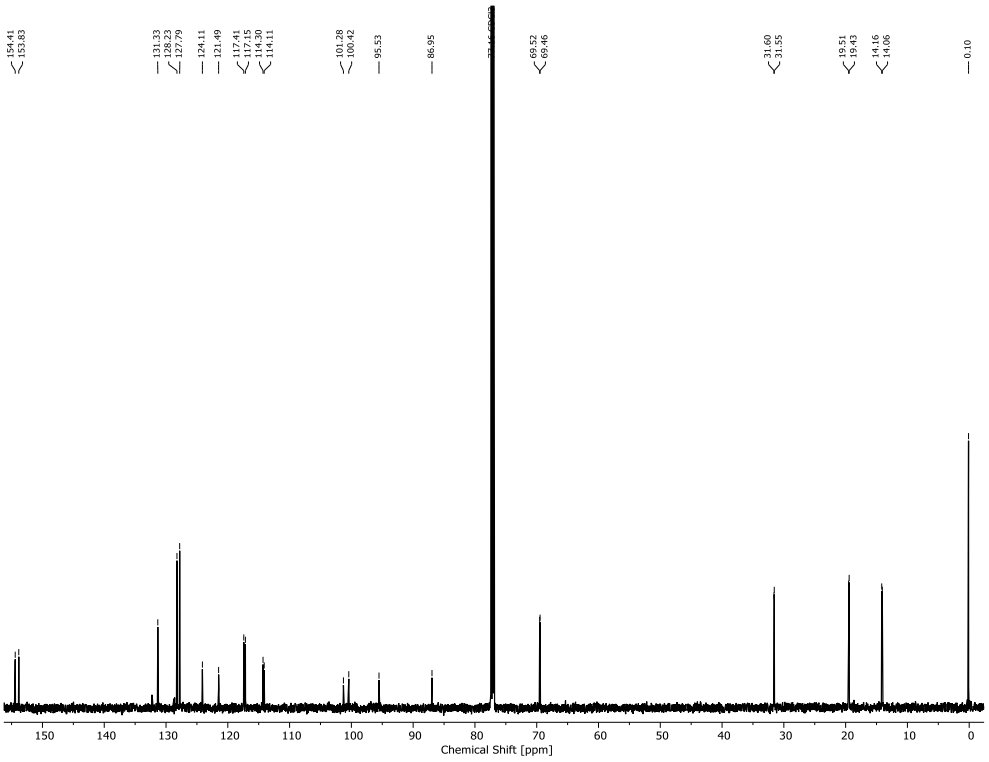

Figure S3 | $^{13}C\{^{1}H\}$-NMR spectrum of **PyrDPE$_{TMS}$**; measured in $CDCl_3$ at 298 K.

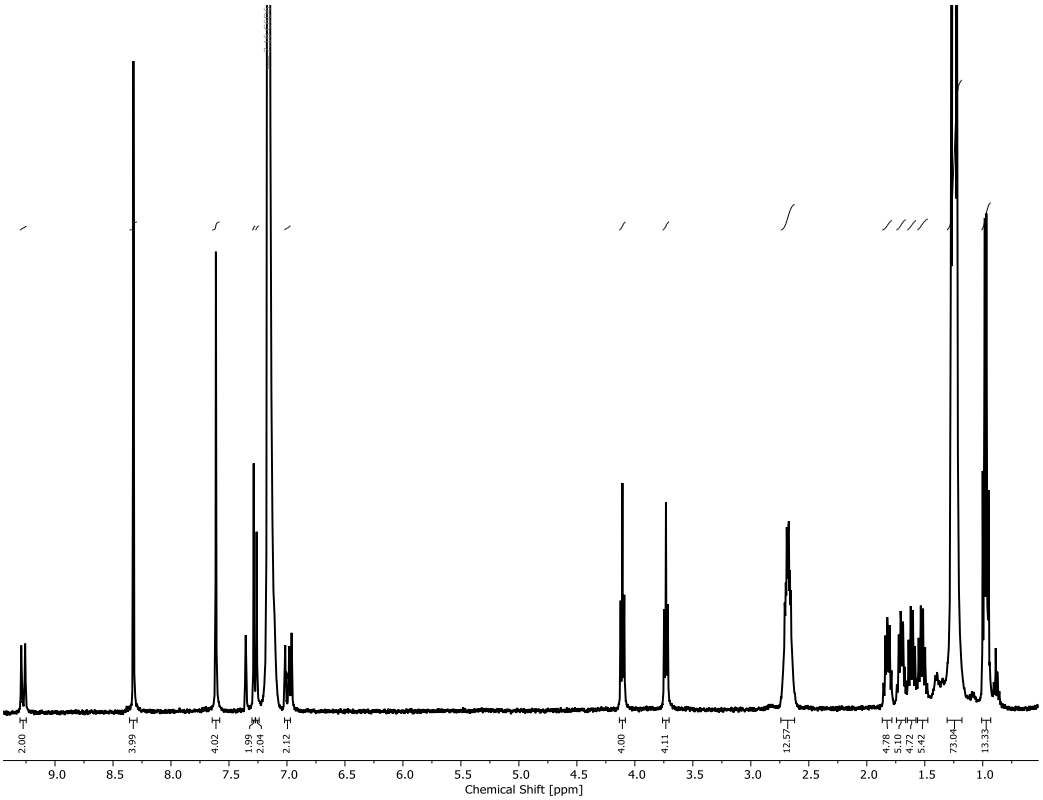

Figure S4 | ^{1}H-NMR spectrum of **PyrDPE-Ru$_{Cl}$**; measured in C_6D_6 at 298 K.

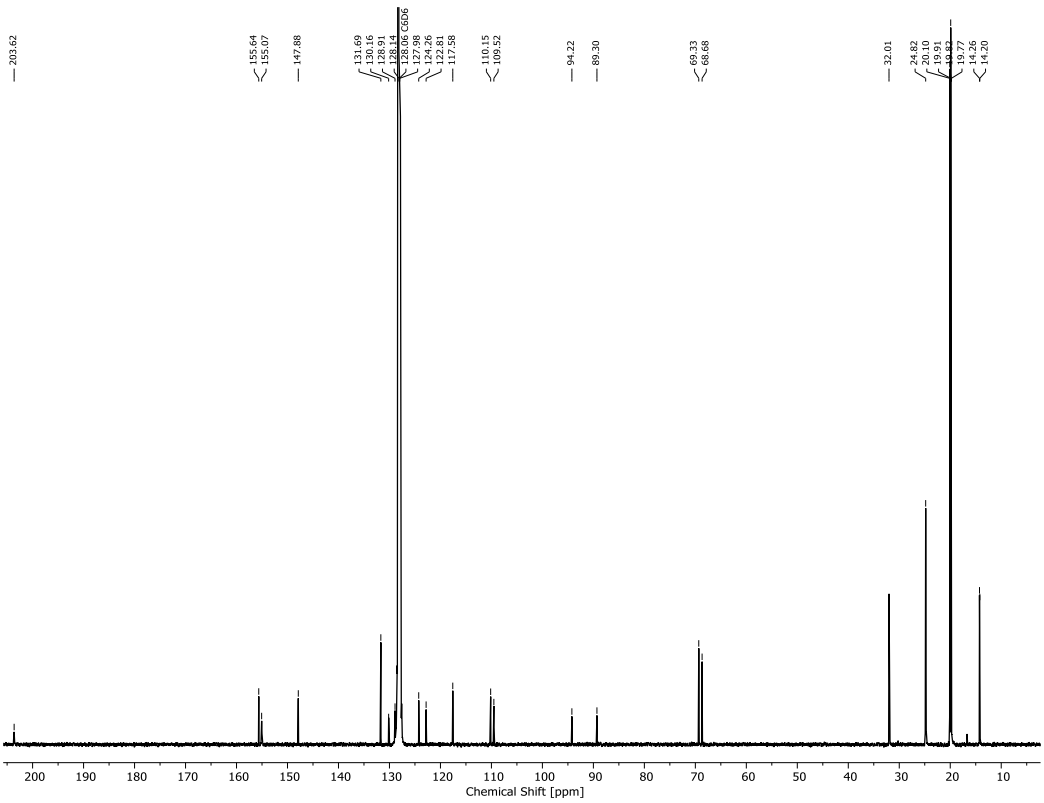

Figure S5 | ^{13}C{^{1}H}-NMR spectrum of **PyrDPE-Ru$_{Cl}$**; measured in C_6D_6 at 298 K.

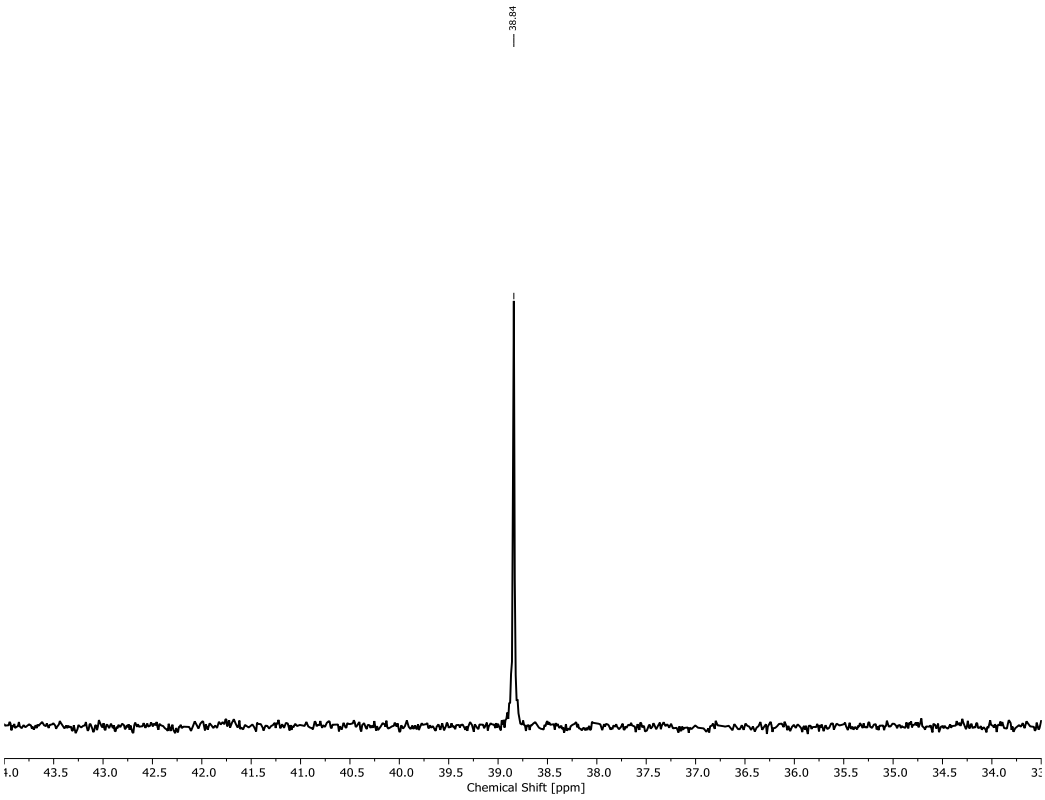

Figure S6 | ^{31}P-{^{1}H}-NMR spectrum of **PyrDPE-Ru$_{Cl}$**; measured in C_6D_6 at 298 K.

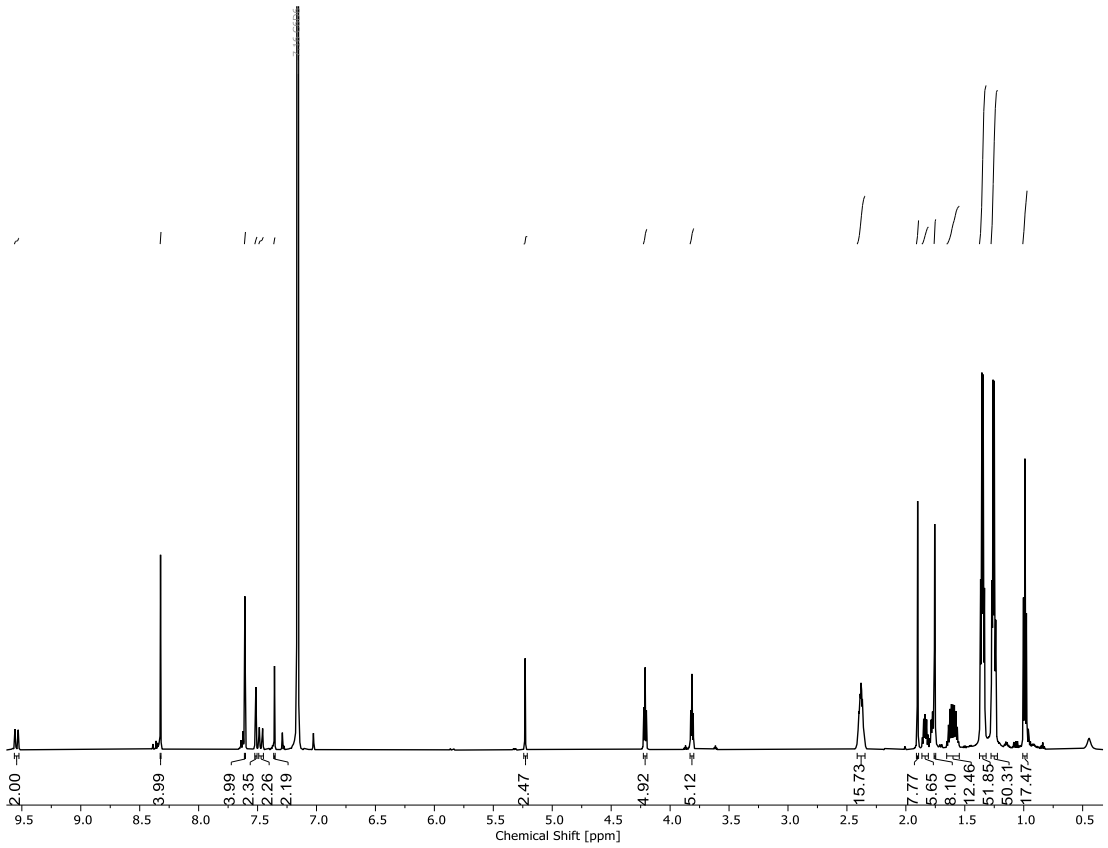

Figure S7 | ^{1}H-NMR spectrum of **PyrDPE-Ru$_{acac}$**; measured in C_6D_6 at 298 K.

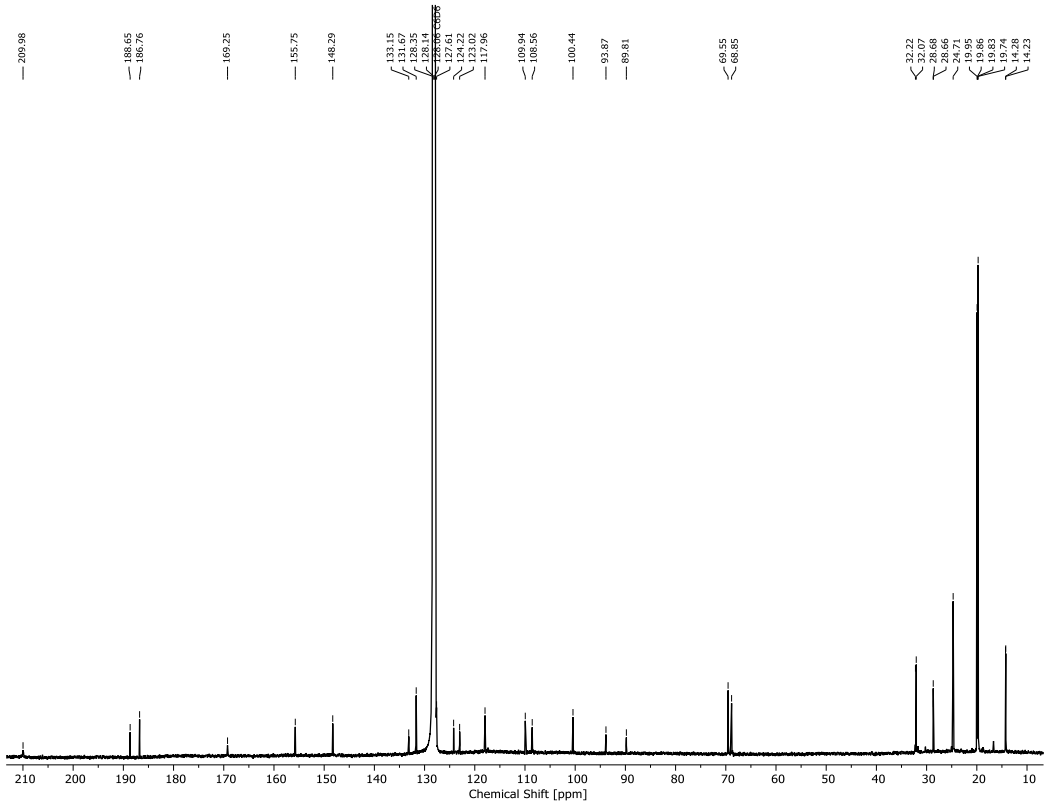

Figure S8 | $^{13}C\{^{1}H\}$-NMR spectrum of **PyrDPE-Ru$_{acac}$**; measured in C_6D_6 at 298 K.

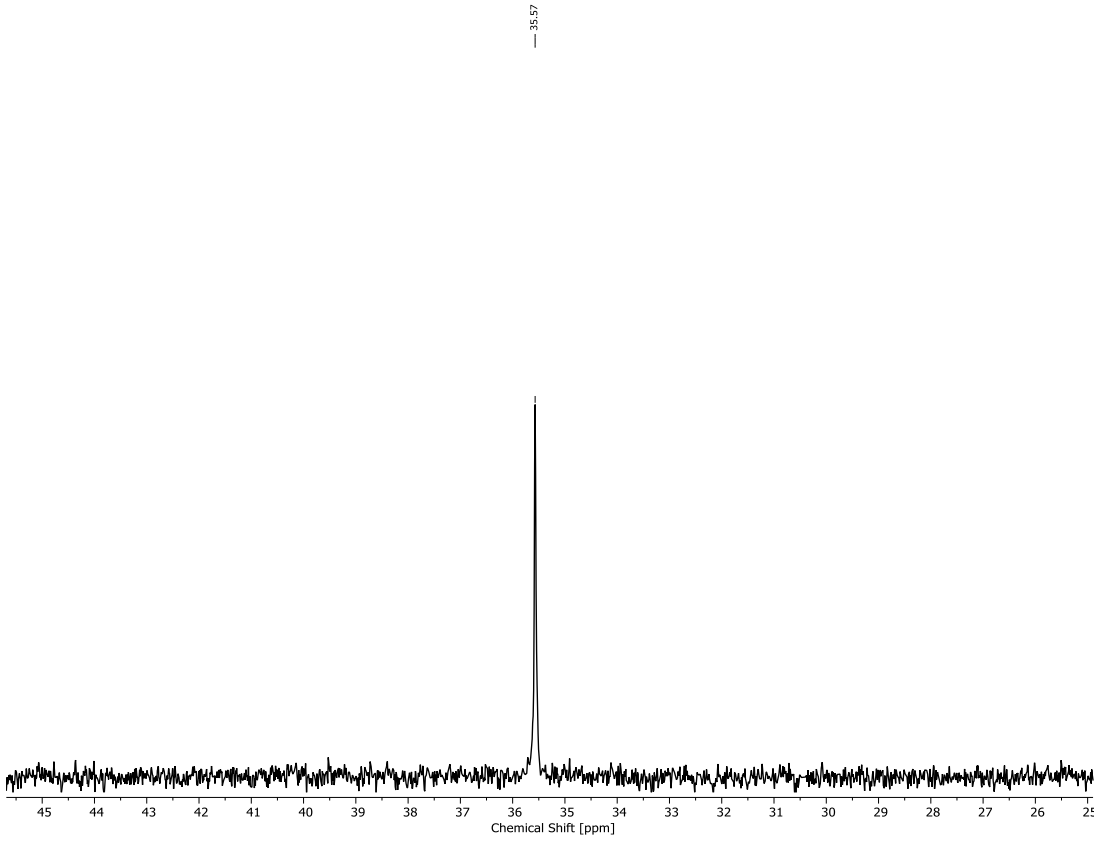

Figure S9 | $^{31}P\{^{1}H\}$-NMR spectrum of **PyrDPE-Ru$_{acac}$**; measured in C_6D_6 at 298 K.

Mass Spectrometry

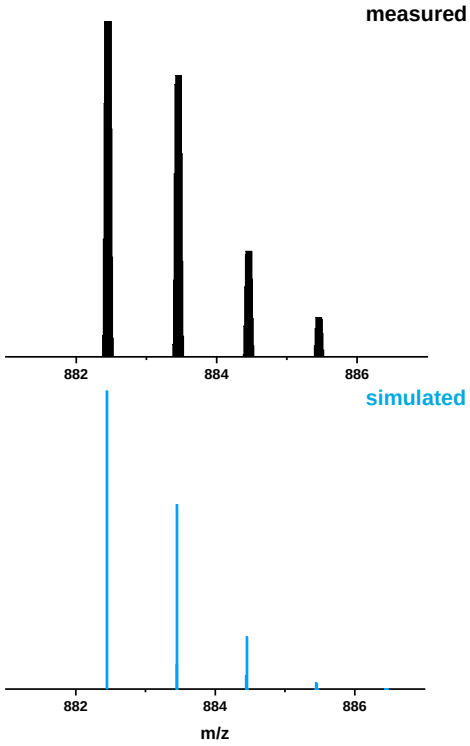

Figure S10 | Experimental (black) and simulated (blue) ESI MS for the molecule ion peak M^+ of **PyrDPE$_{TMS}$**, measured in CH_2Cl_2.

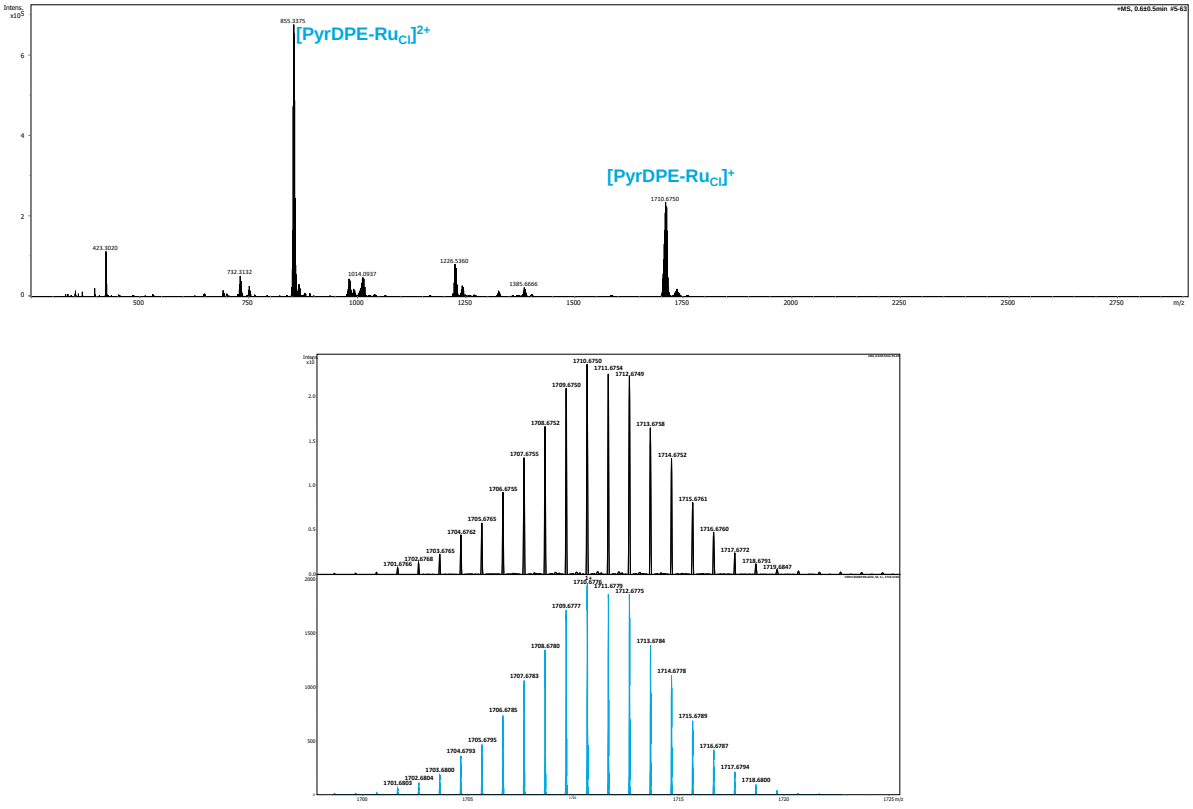

Figure S11 | Top: Experimental ESI mass spectrum of **PyrDPE-Ru$_{Cl}$** measured in CH_2Cl_2; bottom: experimental (black) and simulated molecule ion peak M^+.

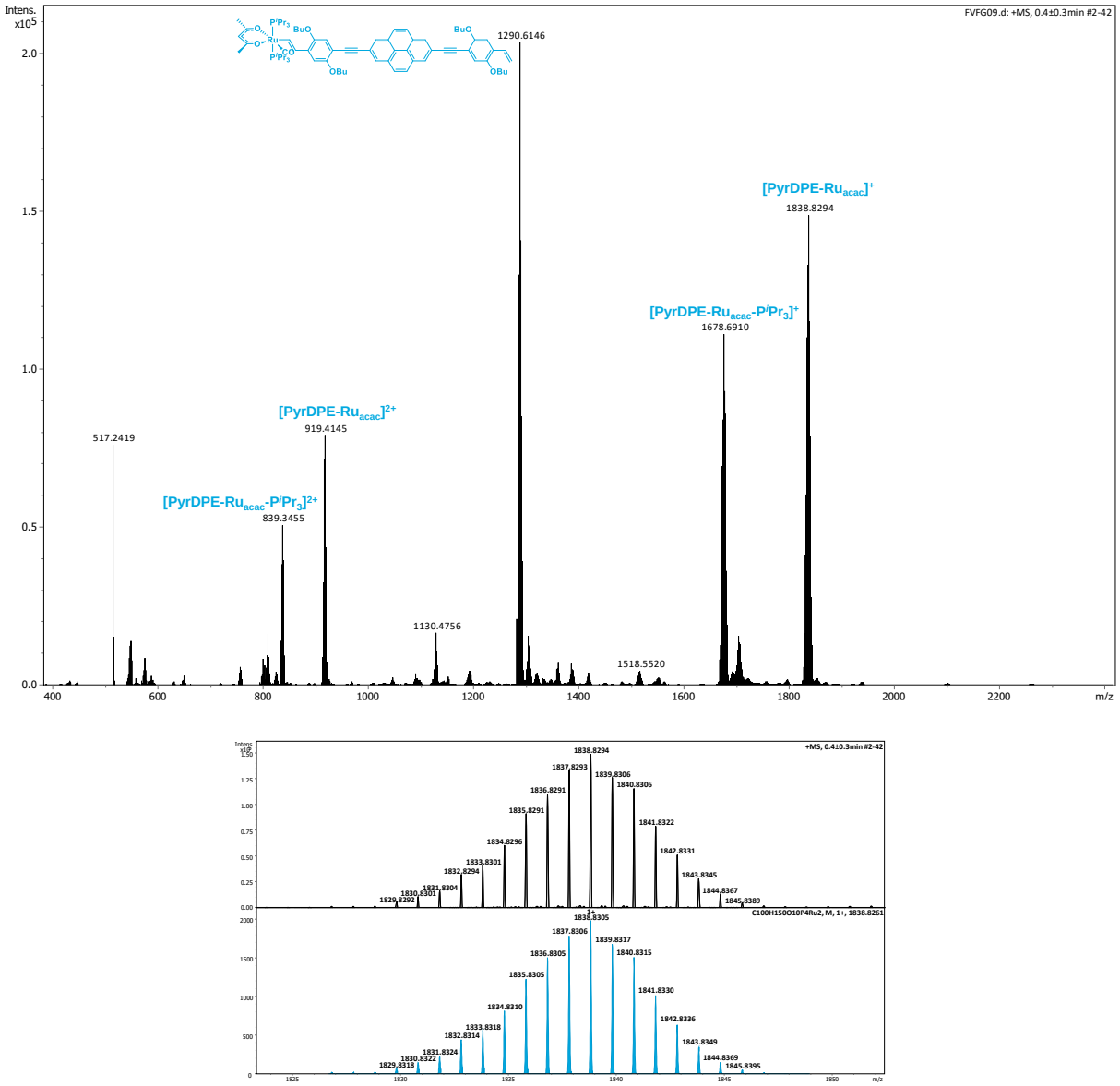

Figure S12 | Top: Experimental ESI mass spectrum of **PyrDPE-Ru$_{acac}$** measured in CH_2Cl_2 with peak assignments; bottom: experimental (black) and simulated molecule ion peak M^+.

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Cyclic Voltammetry

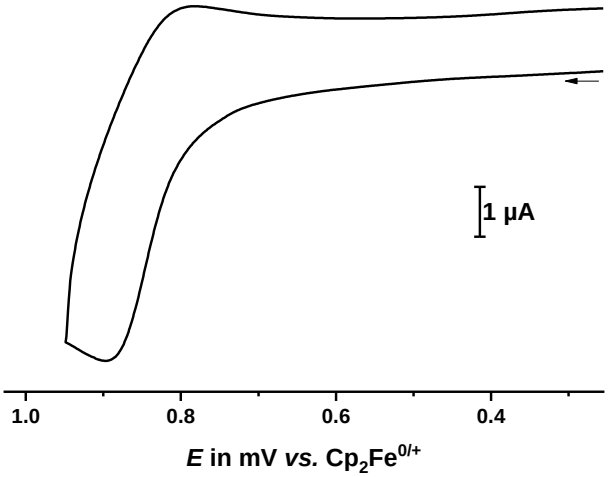

Figure S13 | Cyclic voltammogram of **PyrDPE$_{TMS}$** at a scan rate of v = 100 mVs^{-1}, measured in 0.1 M $^{n}Bu_4^{+}NPF_6^{-}$ / CH_2Cl_2.

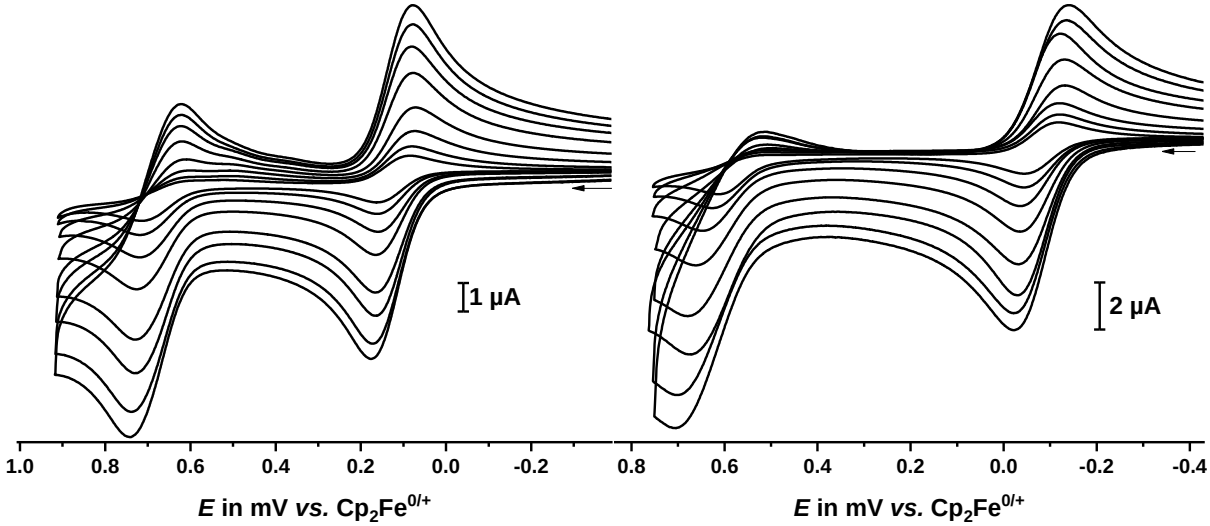

Figure S14 | Cyclic voltammograms of **PyrDPE-Ru$_{Cl}$** (left) and **PyrDPE-Ru$_{acac}$** (right) at different scan rates ranging from v = 25 to 1000 mVs^{-1}, measured in 0.1 M $^{n}Bu_4N^{+}$ PF_6^{-} / CH_2Cl_2.

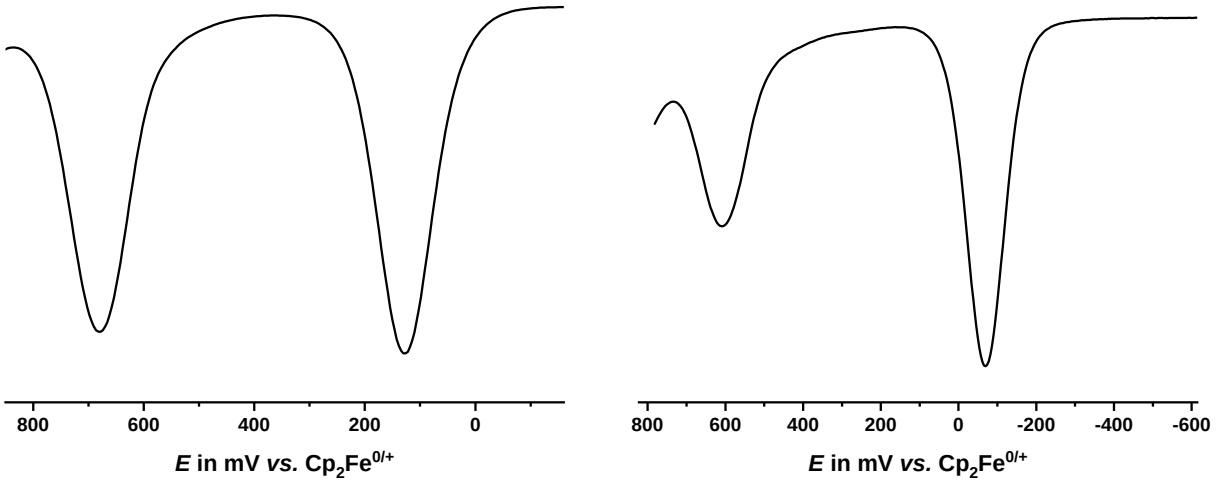

Figure S15 | Square wave voltammograms of **PyrDPE-Ru$_{Cl}$** (left) and **PyrDPE-Ru$_{acac}$** (right); measured in 0.1 M $^{n}Bu_4N^+$ PF_6^- / CH_2Cl_2.

IR Spectroscopy

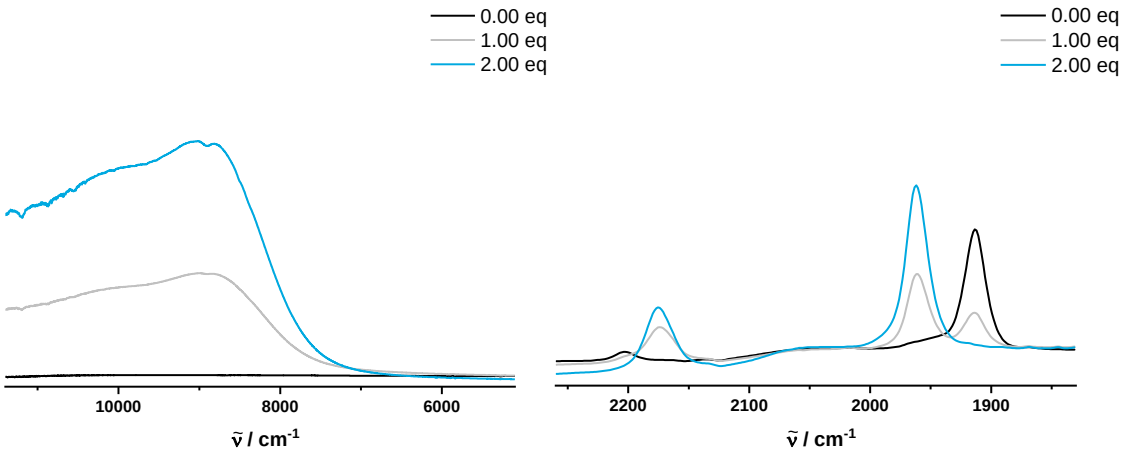

Figure S16 | NIR (left) and IR (right) spectra of neutral **PyrDPE-Ru$_{Cl}$** (black line) and after chemical oxidation with 1.00 and 2.00 equiv. of acetylferrocenium hexafluoroantimonate

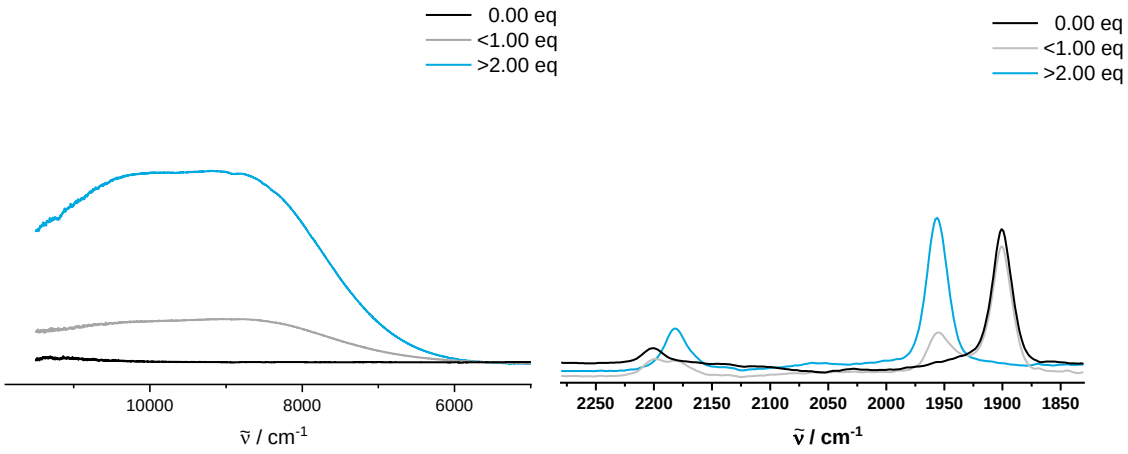

Figure S17 | NIR (left) and IR (right) spectra of of neutral **PyrDPE-Ru$_{acac}$** (black line) and after chemical oxidation with 0.60 and 2.00 equiv. of 1,1'-diacetylferrocenium hexafluoroantimonate.

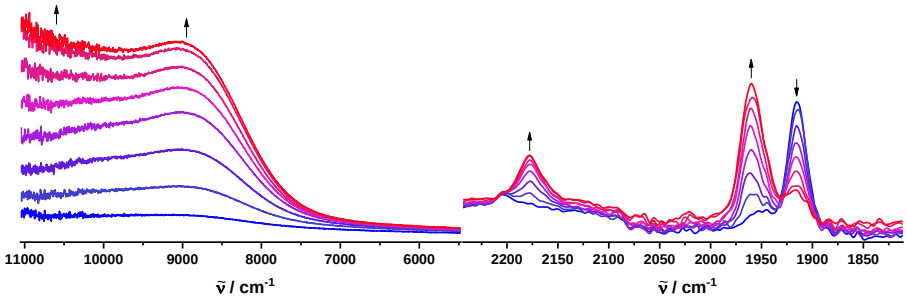

Figure S18 | Changes in IR (right) and in the NIR (left) during electrochemical oxidation of **PyrDPE-Ru$_{Cl}$** past the first redox wave, measured in 1,2-$C_2H_4Cl_2$ / $^nBu_4N^+PF_6^-$ (0.2 M) at r. t.

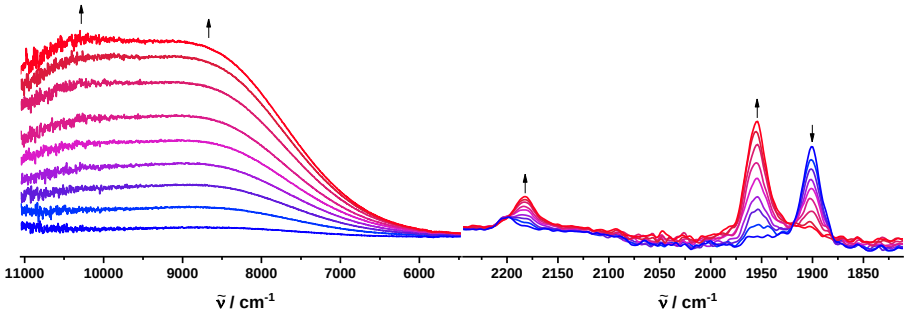

Figure S19 | Changes in IR (right) and in the NIR (left) during electrochemical oxidation of **PyrDPE-Ru$_{acac}$** past the first redox wave, measured in 1,2-$C_2H_4Cl_2$ / $^nBu_4N^+PF_6^-$ (0.2 M) at r. t.

UV/Vis/NIR Spectroscopy

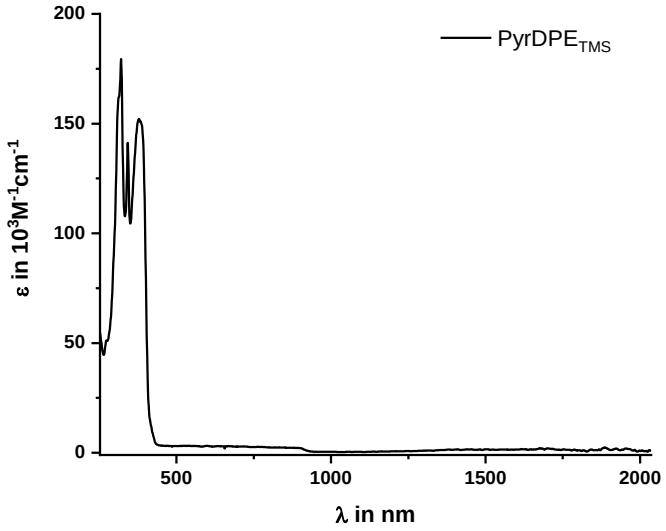

Figure S20 | UV/Vis/NIR spectrum of **PyrDPE$_{TMS}$**, measured in CH_2Cl_2.

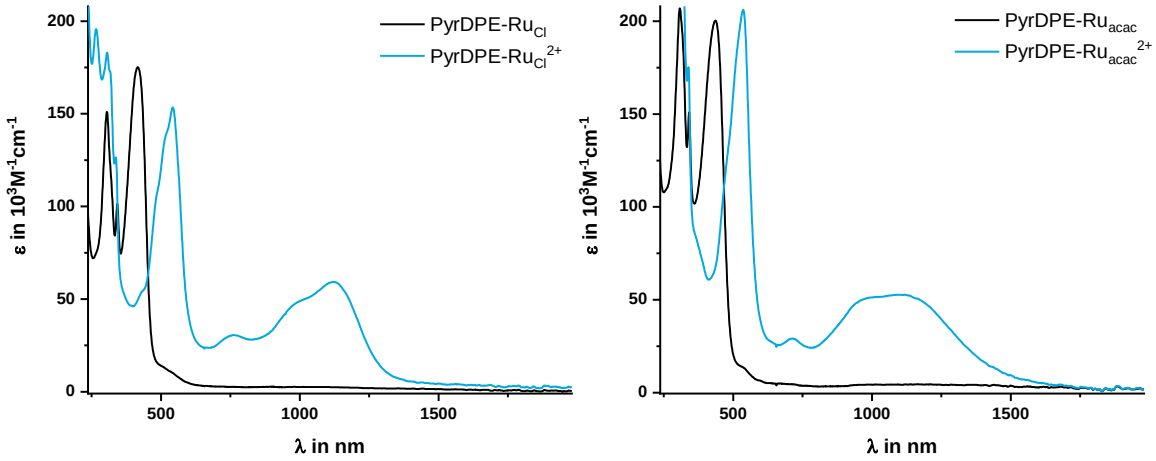

Figure S21 | UV/Vis/NIR spectra of **PyrDPE-Ru$_{Cl}$** and chemically generated **PyrDPE-Ru$_{Cl}^{2+}$** (left) and of **PyrDPE-Ru$_{acac}$** and chemically generated **PyrDPE-Ru$_{acac}^{2+}$** (right), measured in CH_2Cl_2.

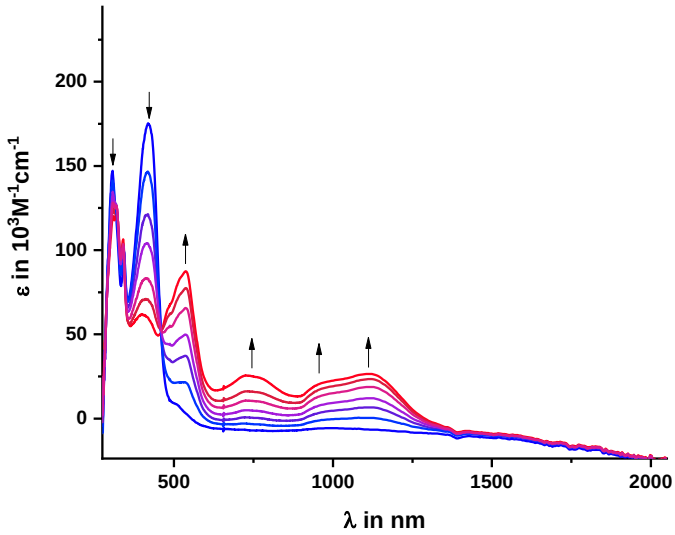

Figure S22 | Changes in UV/Vis/NIR spectra during the electrochemical oxidation of **PyrDPE-Ru$_{Cl}$** past the first redox wave, measured in 1,2-$C_2H_4Cl_2$ / $^nBu_4N^+PF_6^-$ (0.2 M) at r. t.

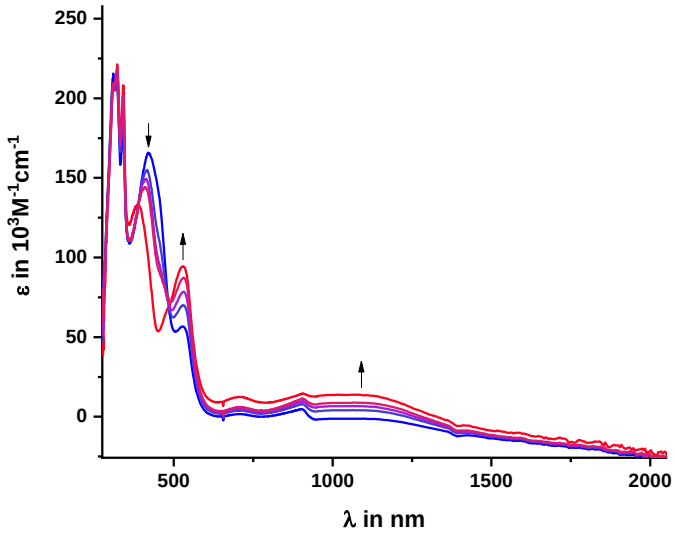

Figure S23 | Changes in UV/Vis/NIR spectra during the electrochemical oxidation of **PyrDPE-Ru$_{acac}$** past the first redox wave, measured in 1,2-$C_2H_4Cl_2$ / $^nBu_4N^+PF_6^-$ (0.2 M) at r. t..

EPR Spectroscopy

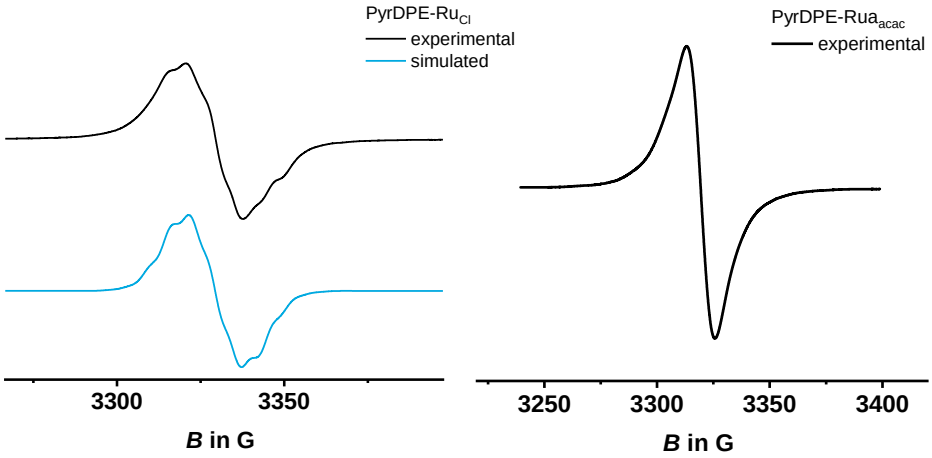

Figure S24 | EPR spectra of **PyrDPE-Ru$_{Cl}^{2+}$** with its simulation (left) and of **PyrDPE-Ru$_{acac}^{2+}$** (right), measured in CH_2Cl_2.

Table S1 | EPR spectroscopic data for **PyrDPE-Ru$_{Cl}^{2+}$** and **PyrDPE-Ru$_{acac}^{2+}$**; hyperfine coupling constants *A* are given in *Gauss*.

	g_{iso} (20 °C)	*A* (^{31}P)	*A* ($^{99/101}$Ru)	*A* (^{1}H)
PyrDPE-Ru$_{Cl}$	2.017	7.3 (2)	5.0 (1)	6.1 (2) 4.6 (1) 3.6 (1)
PyrDPE-Ru$_{acac}$	2.023	-	-	-

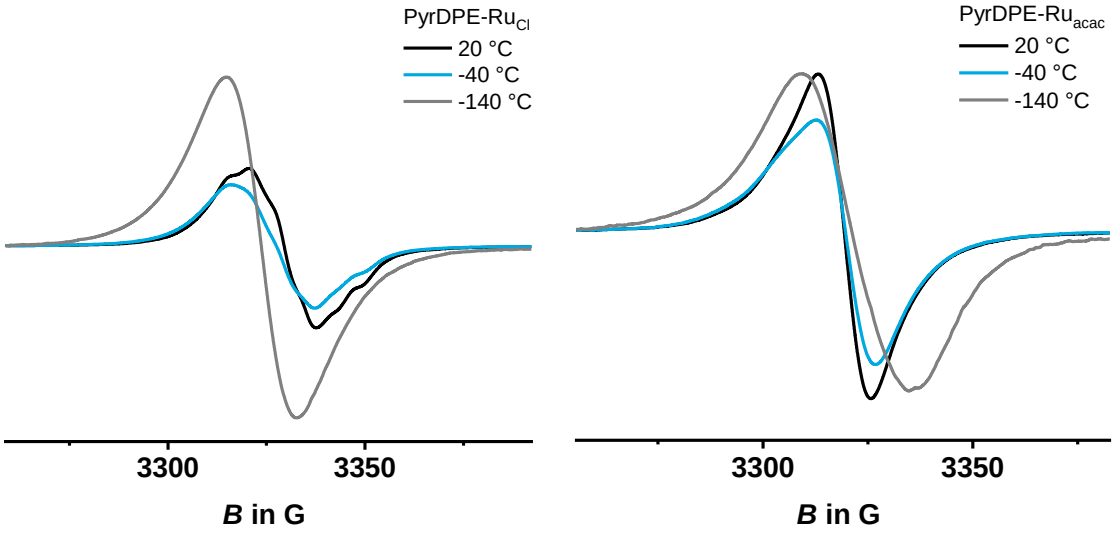

Figure S25 | Temperature-dependent EPR spectra of **PyrDPE-Ru$_{Cl}^{2+}$** (left) and of **PyrDPE-Ru$_{acac}^{2+}$** (right), measured in CH_2Cl_2.

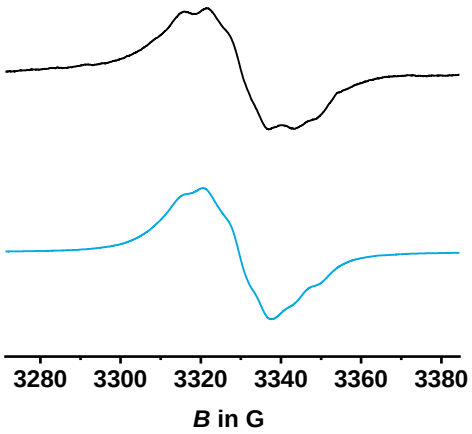

Figure S 26 I EPR spectra of **PyrDPE-Ru$_{Cl}^{\bullet+}$** (black) and **PyrDPE-Ru$_{Cl}^{2+}$** (blue), measured in CH_2Cl_2.

Luminescence Studies

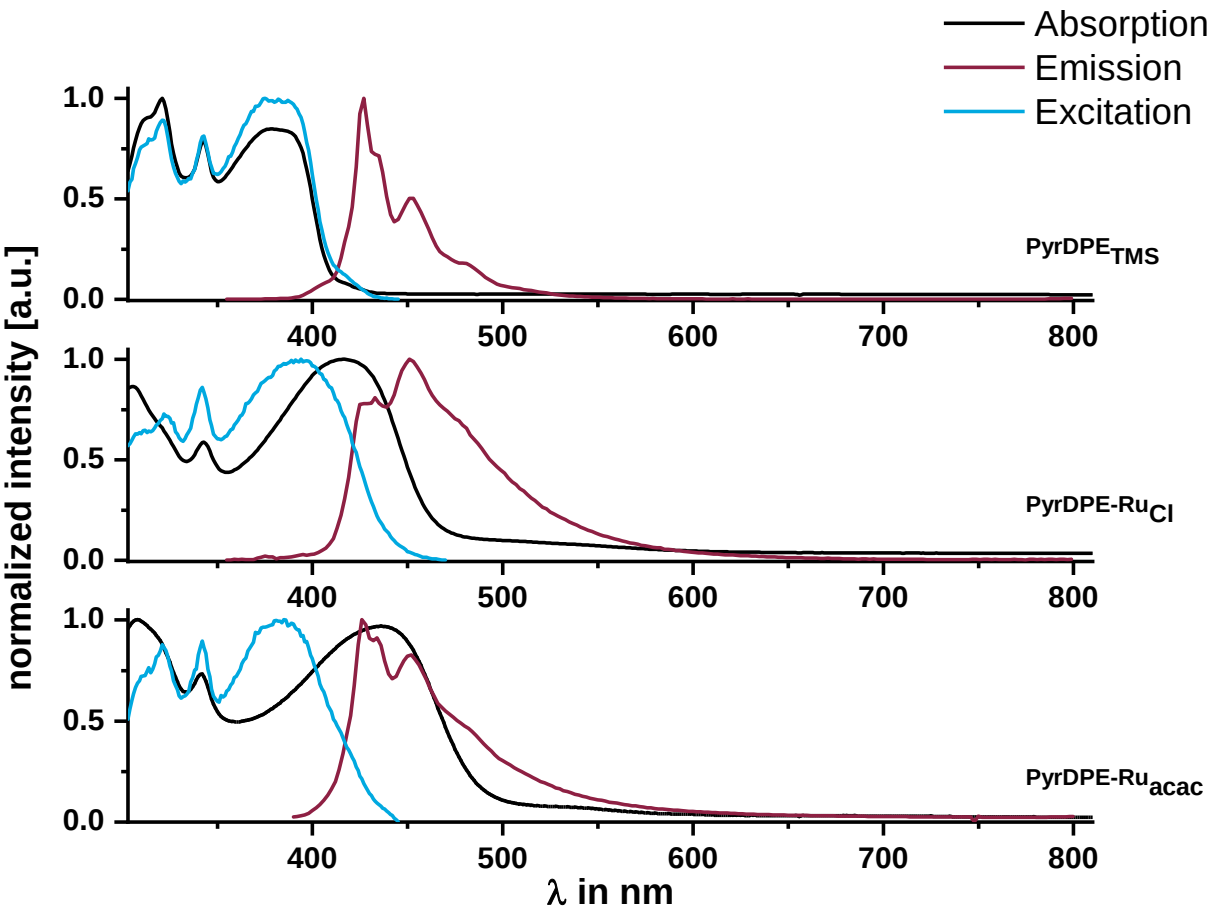

Figure S27 | Absorption, emission and excitation spectra of **PyrDPE$_{TMS}$** (top), and of **PyrDPE-Ru$_{Cl}$** (middle) and **PyrDPE-Ru$_{acac}$** (bottom) in CH_2Cl_2 at at r.t.

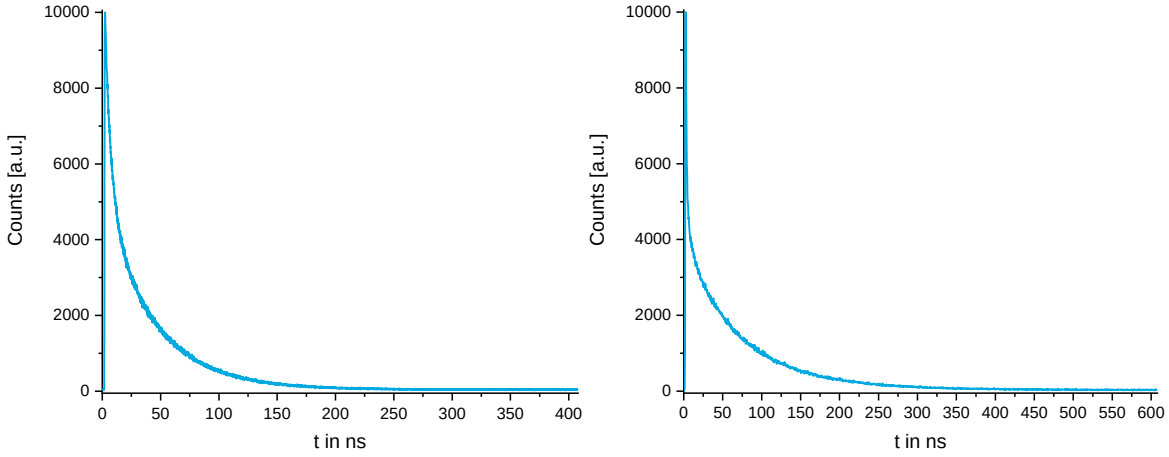

Figure S28 | Emission decay of **PyrDPE$_{TMS}$** in CH_2Cl_2 at r.t. (left) and in methylcyclohexane at 77 K (right).

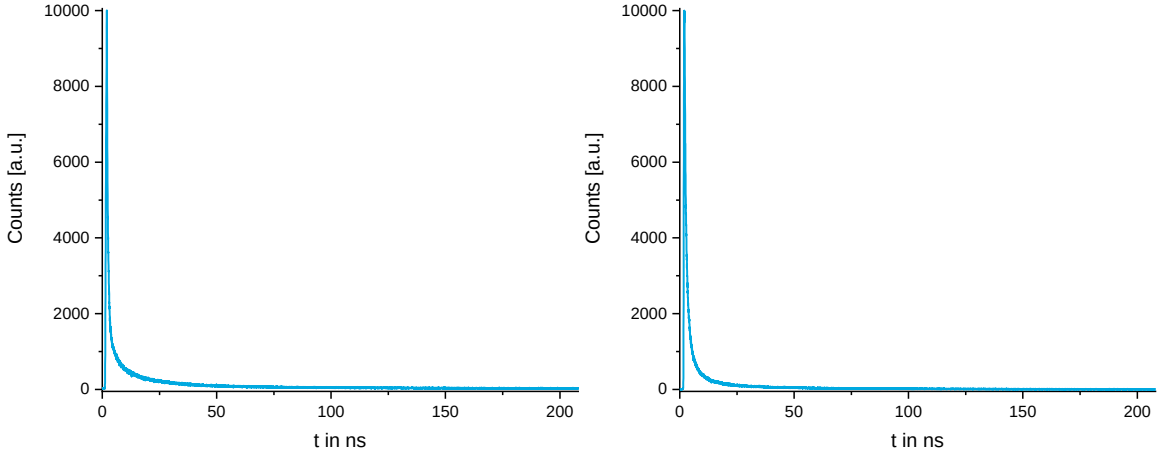

Figure S29 | Emission decays of **PyrDPE-Ru$_{Cl}$** (left) and of **PyrDPE-Ru$_{acac}$** in methylcyclohexane at 77 K.

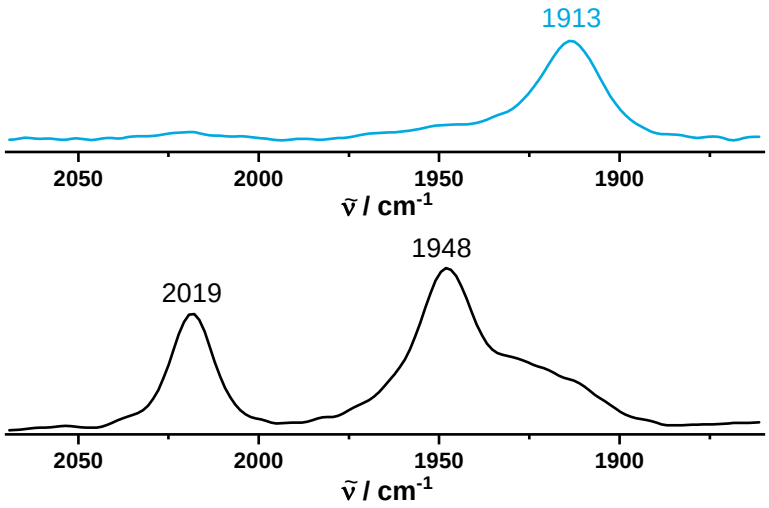

Figure S30 | IR spectra of **PyrDPE-Ru$_{Cl}$** before (top, blue curve) and after (bottom, black curve) irradiation with a 275 nm LED.

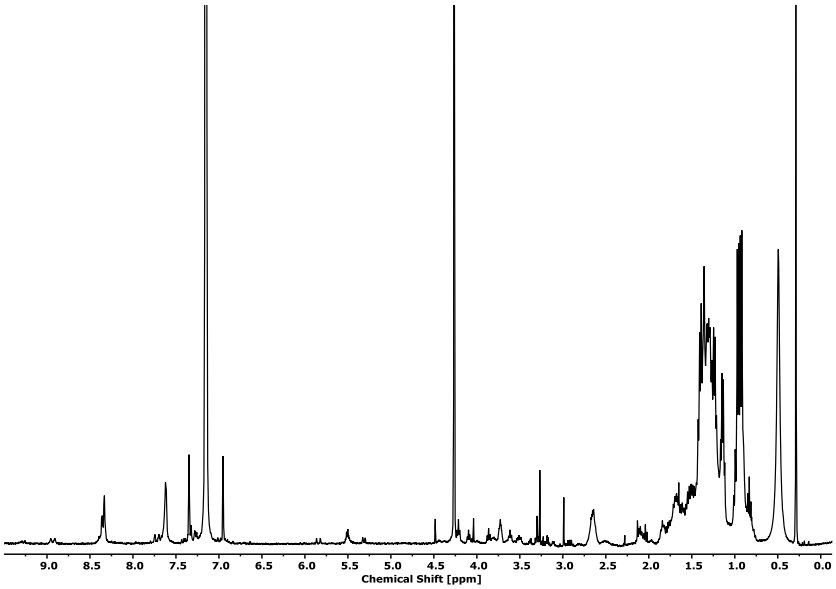

Figure S31 | ^{1}H NMR spectrum of **PyrDPE-Ru$_{Cl}$** after irradiation with a 275 nm LED.

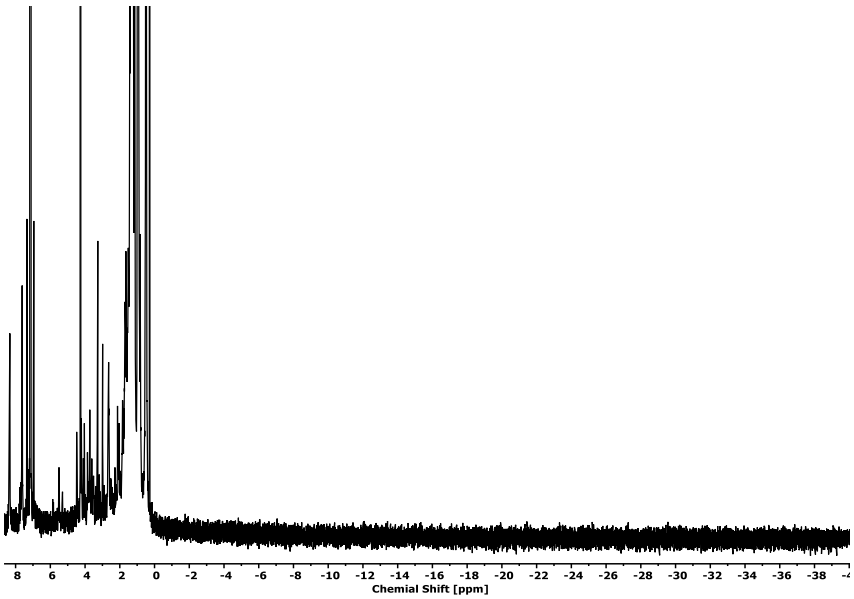

Figure S32 | ^{1}H NMR spectrum of **PyrDPE-Ru$_{Cl}$** after irradiation with a 275 nm LED.

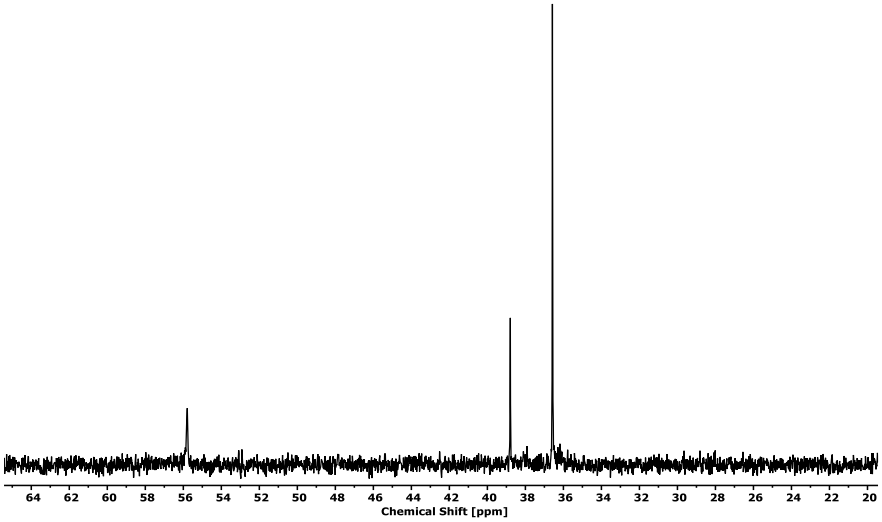

Figure S33 | $^{31}P\{^{1}H\}$ NMR spectrum of **PyrDPE-Ru$_{Cl}$** after irradiation with a 275 nm LED.

The ^{1}H NMR spectrum of the crude reaction mixture obtained after photoexcitation of a CH_2Cl_2 solution of the complex **PyrDPE-Ru$_{Cl}$** with a 275 nm LED indicate a substantial loss of intensity for the original vinyl -CH=CH- resonances and the formation of several new CH and butoxy resonances in the aromatic and aliphatic regions. At ca. 0.90 ppm two equally integrating doublets of aliphatic protons appear, which can be assigned to diastereotopic methyl protons of $P^{i}Pr_3$ ligands. No hydride resonance is found in the negative shift region (see Figure S32). The ^{31}P NMR spectrum shows a dominant singlet resonance at 36.6 ppm besides the resonance of remaining alkenyl-ruthenium end groups at 38.8 ppm. The IR spectrum shows a pair similarly intense CO bands at 2019 and 1948 cm^{-1}. The main spectroscopic features agree with the formation of a dicarbonyl ruthenium complex $[Ru(CO)_2(P^{i}Pr_3)_2(Cl)(X)]$ with *trans*-coordinated phosphine and mutually *cis*-disposed, ligands Cl and X, assuming that the chloro ligand is retained. We cannot make any definite statement on the identity of ligand X apart from that it is neither chloride (owing to the diastereotopic methyl groups at the $P^{i}Pr_3$ ligands) nor hydride (lack of a hydride resonance).

Quantum Chemical Calculations

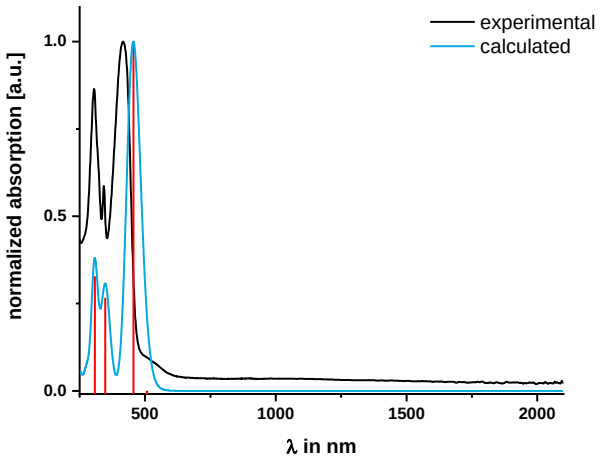

Figure S34 | Comparison of the experimental and TD-DFT computed absorption spectrum of model complex **PyrDPE-Ru$_{Cl}^{Me}$**.

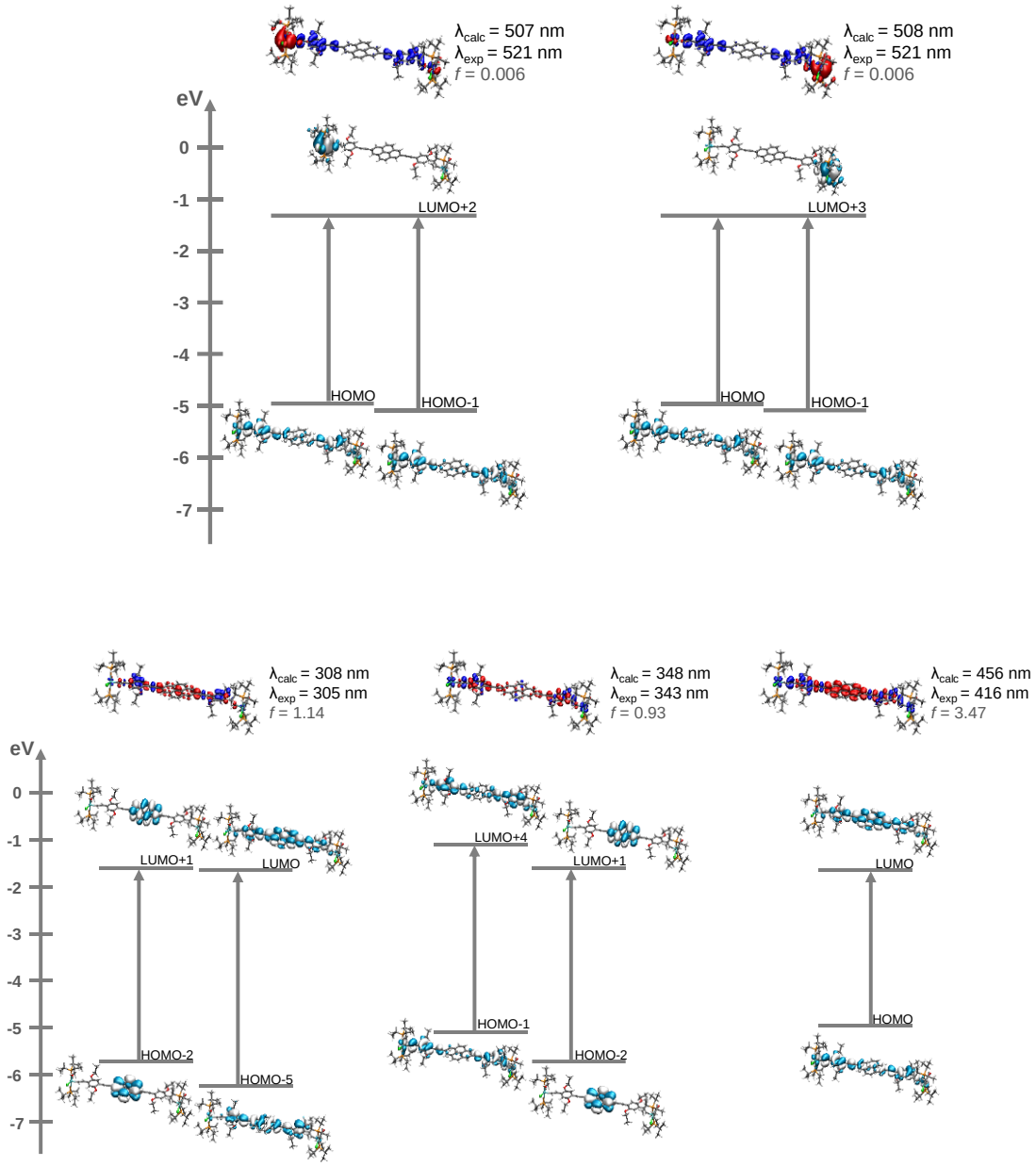

Figure S35 | pbe1pbe/6-31G(d)PCM (CH_2Cl-CH_2Cl)-calculated electronic transitions of **PyrDPE-Ru$_{Cl}^{Me}$** with the respective acceptor and donor molecular orbitals and the corresponding electron density difference maps (EDDMs) for the corresponding transition (top; blue colour = electron density decrease, red colour = electron density increase).

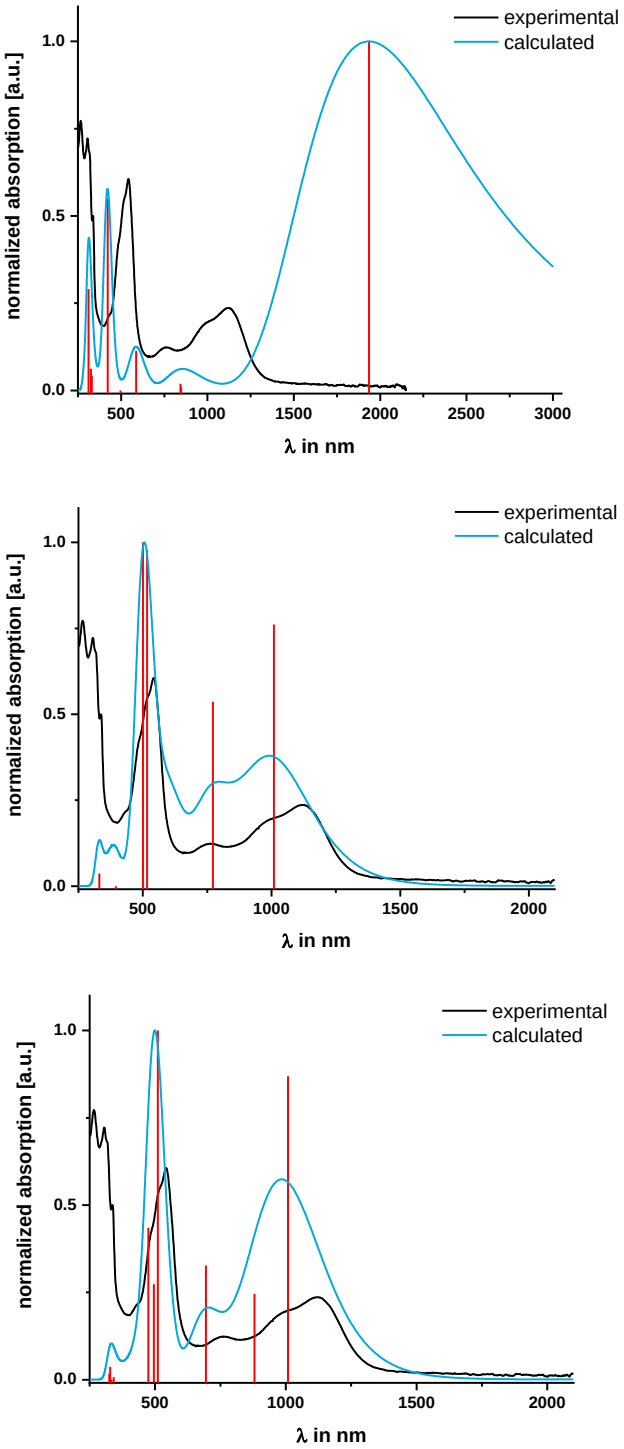

Figure S36 | Comparison of the experimental and the TD-DFT computed absorption spectrum of model complex [**PyrDPE-Ru**$_{Cl}^{Me}$**]**$^{2+}$ in the electronic singlet state (top), triplet state (middle) and open-shell singlet state (bottom).

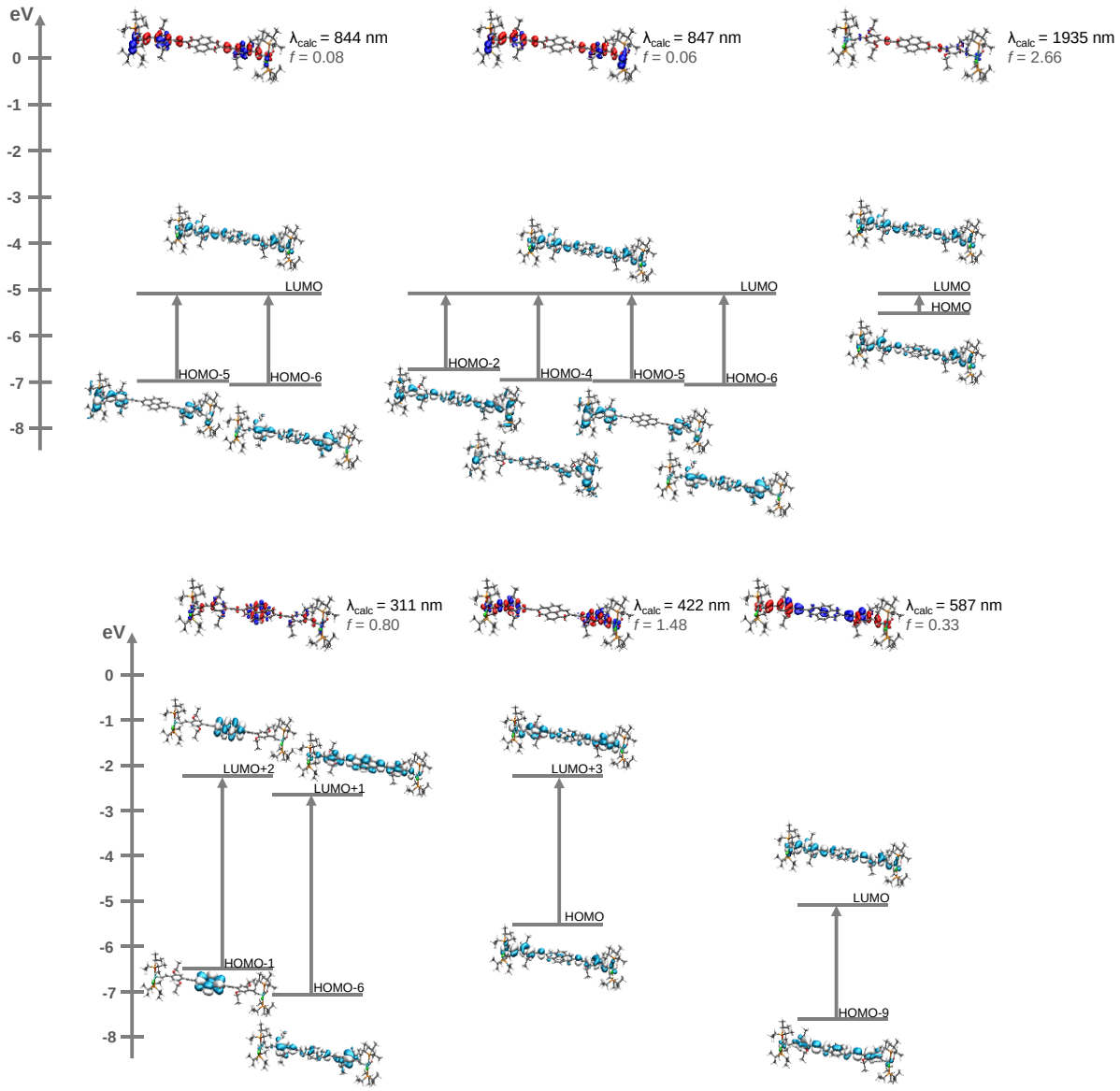

Figure S37 | pbe1pbe/6-31G(d)PCM (CH_2Cl-CH_2Cl)-calculated electronic transitions of **[PyrDPE-Ru$_{Cl}^{Me}$]$^{2+}$** in the electronic singlet state) with the respective acceptor and donor molecular orbitals and the corresponding electron density difference maps (EDDMs) for the corresponding transition (top; blue colour = electron density decrease, red colour = electron density increase).

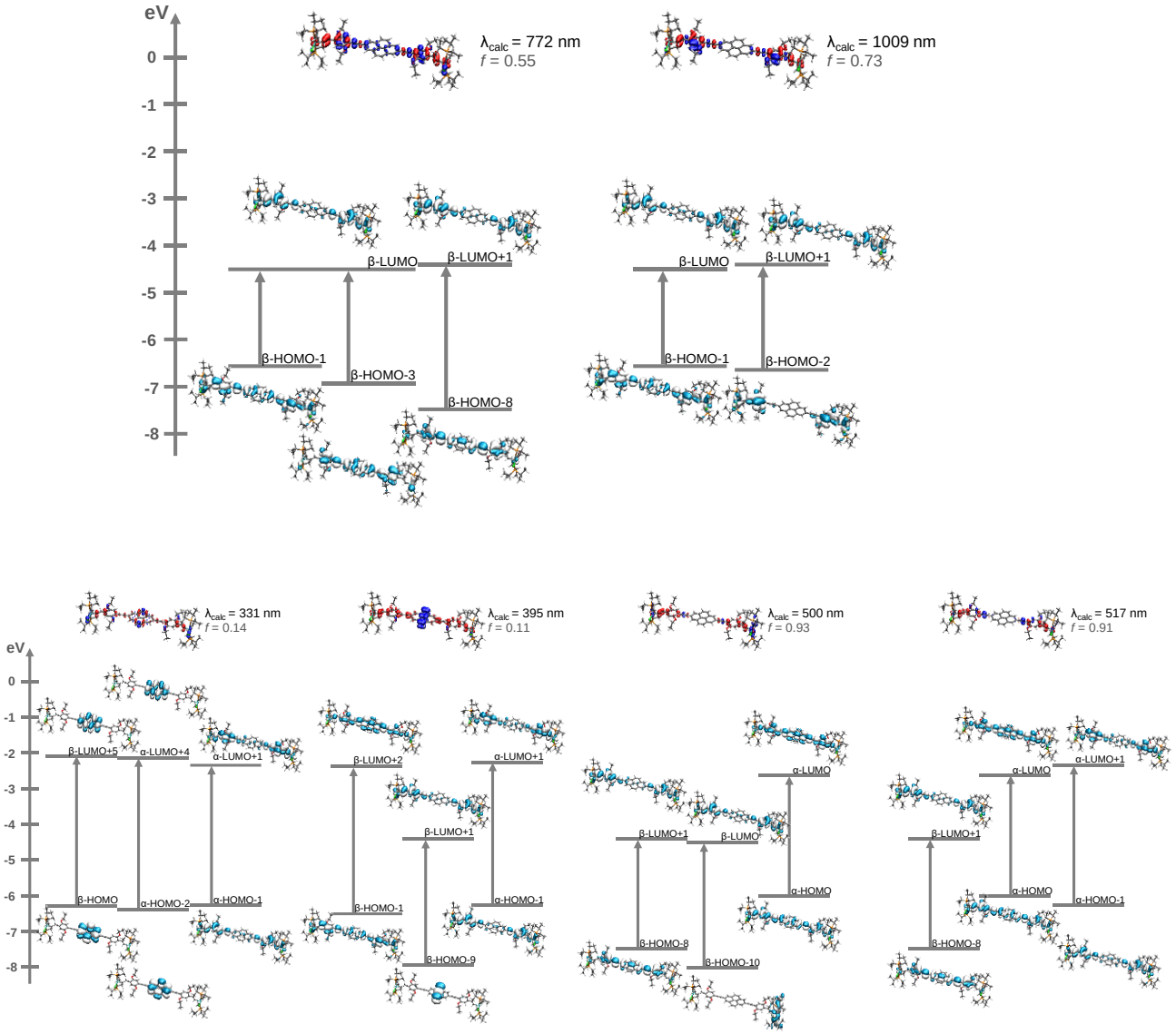

Figure S38 | pbe1pbe/6-31G(d)PCM (CH_2Cl-CH_2Cl)-calculated electronic transitions of **[PyrDPE-Ru$_{Cl}^{Me}$]$^{2+}$** in the electronic triplet state with the respective acceptor and donor molecular orbitals and the corresponding electron density difference maps (EDDMs) for the corresponding transition (top; blue colour = electron density decrease, red colour = electron density increase).

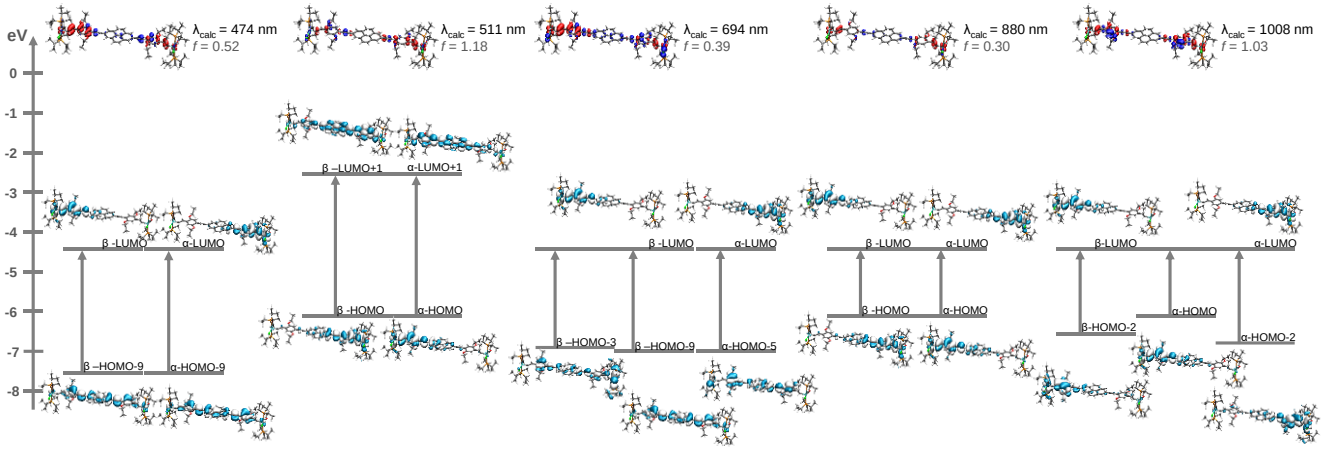

Figure S39 | pbe1pbe/6-31G(d)PCM (CH_2Cl-CH_2Cl)-calculated electronic transitions of **[PyrDPE-Ru$_{Cl}^{Me}$]$^{2+}$** in the electronic open-shell singlet state with the respective acceptor and donor molecular orbitals and the corresponding electron density difference maps (EDDMs) for the corresponding transition (top; blue colour = electron density decrease, red colour = electron density increase).

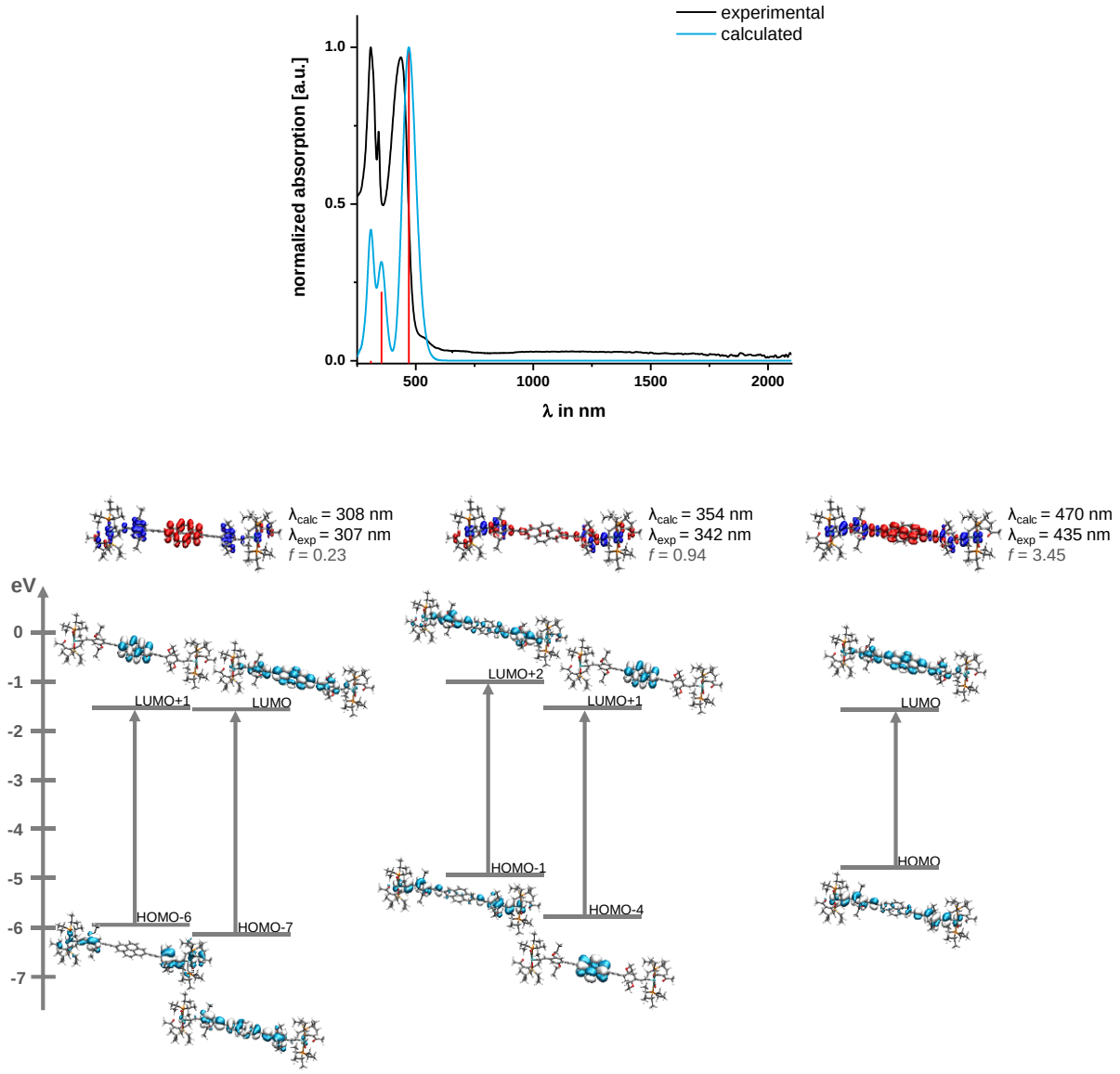

Figure S40 | pbe1pbe/6-31G(d)PCM (CH_2Cl-CH_2Cl) calculated electronic transitions of **PyrDPE-Ru$_{acac}^{Me}$** with the respective acceptor and donor molecular orbitals and the corresponding electron density difference maps (EDDMs) for the corresponding transition (top; blue colour = electron density decrease, red colour = electron density increase).

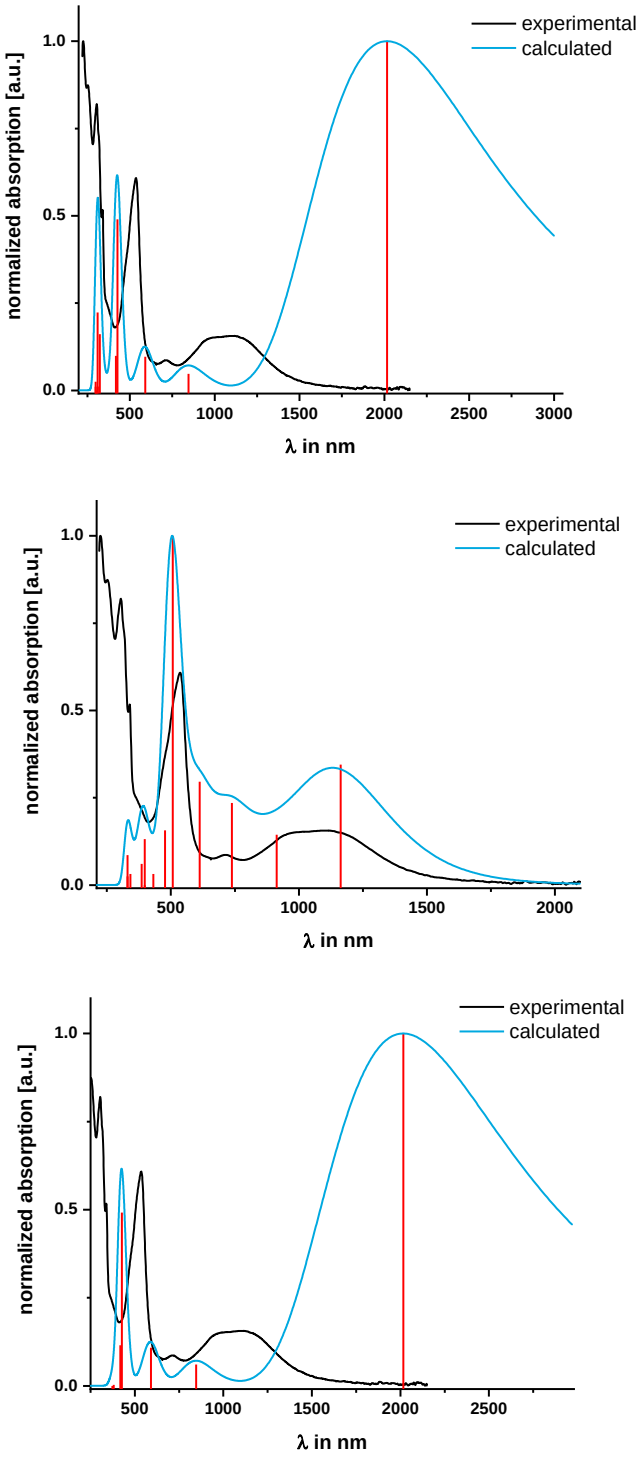

Figure S41 | Comparison of the experimental and the TD-DFT computed absorption spectrum of model complex [**PyrDPE-Ru$_{acac}^{Me}$**]$^{2+}$ in the electronic singlet state (top), triplet state (middle) and open-shell singlet state (bottom).

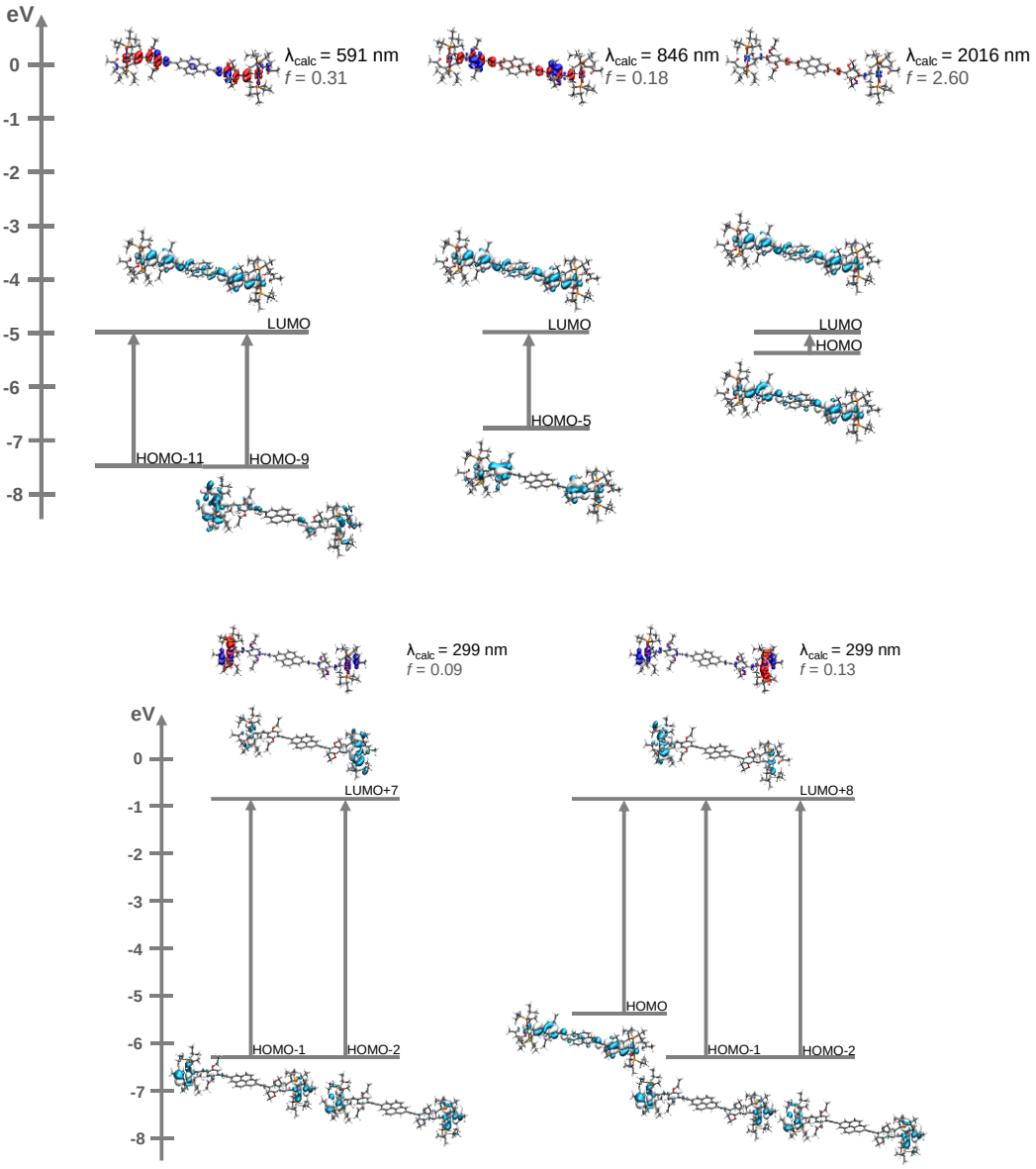

Figure S42 | pbe1pbe/6-31G(d)PCM (CH_2Cl-CH_2Cl) calculated electronic transitions of **[PyrDPE-Ru$_{acac}^{Me}$]$^{2+}$** in the electronic singlet state with the respective acceptor and donor molecular orbitals and the corresponding electron density difference maps (EDDMs) for the corresponding transition (top; blue colour = electron density decrease, red colour = electron density increase).

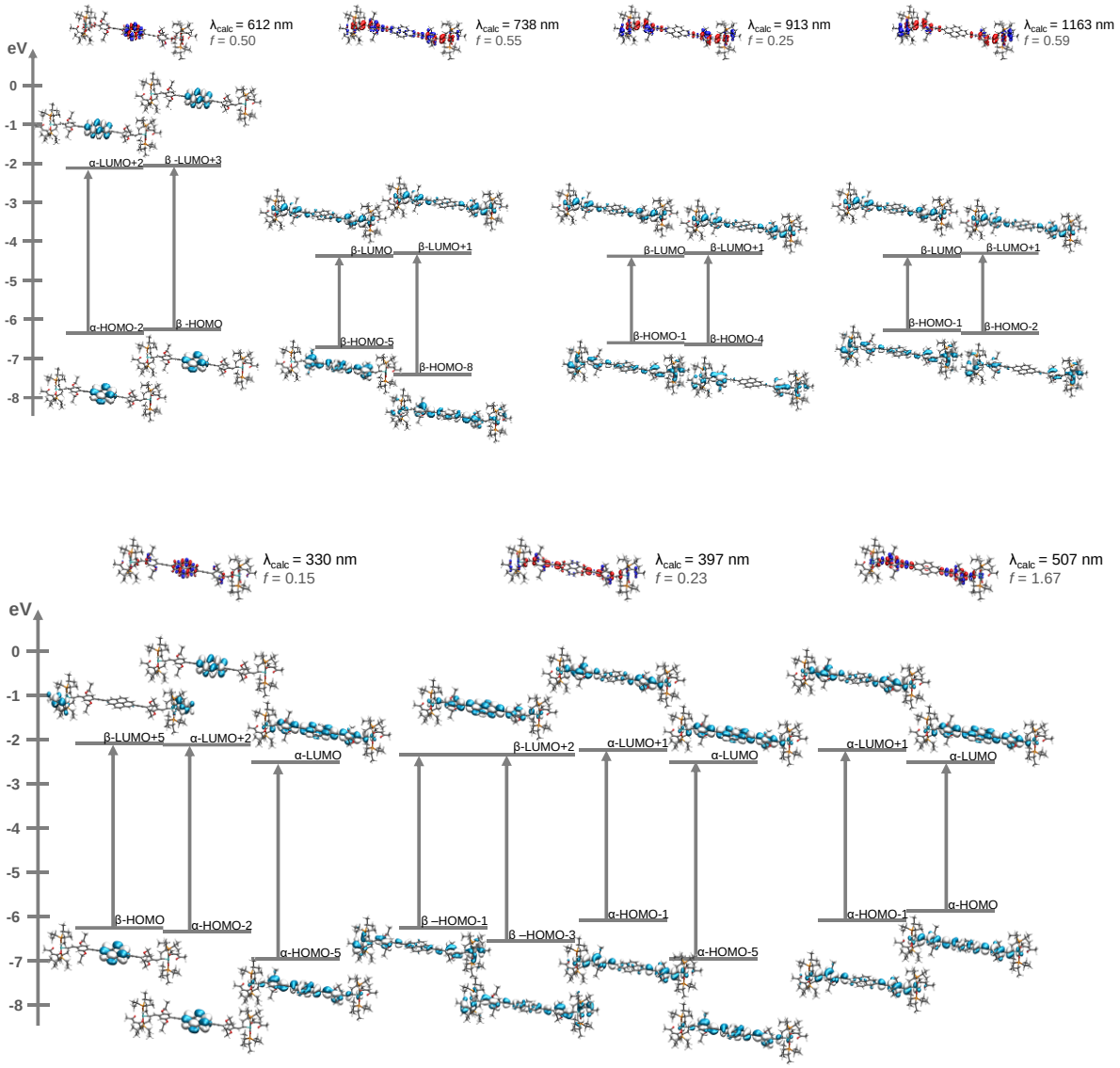

Figure S43 | pbe1pbe/6-31G(d)PCM (CH_2Cl-CH_2Cl) calculated electronic transitions of **[PyrDPE-Ru$_{acac}^{Me}$]$^{2+}$** in the electronic triplet state with the respective acceptor and donor molecular orbitals and the corresponding electron density difference maps (EDDMs) for the corresponding transition (top; blue colour = electron density decrease, red colour = electron density increase).

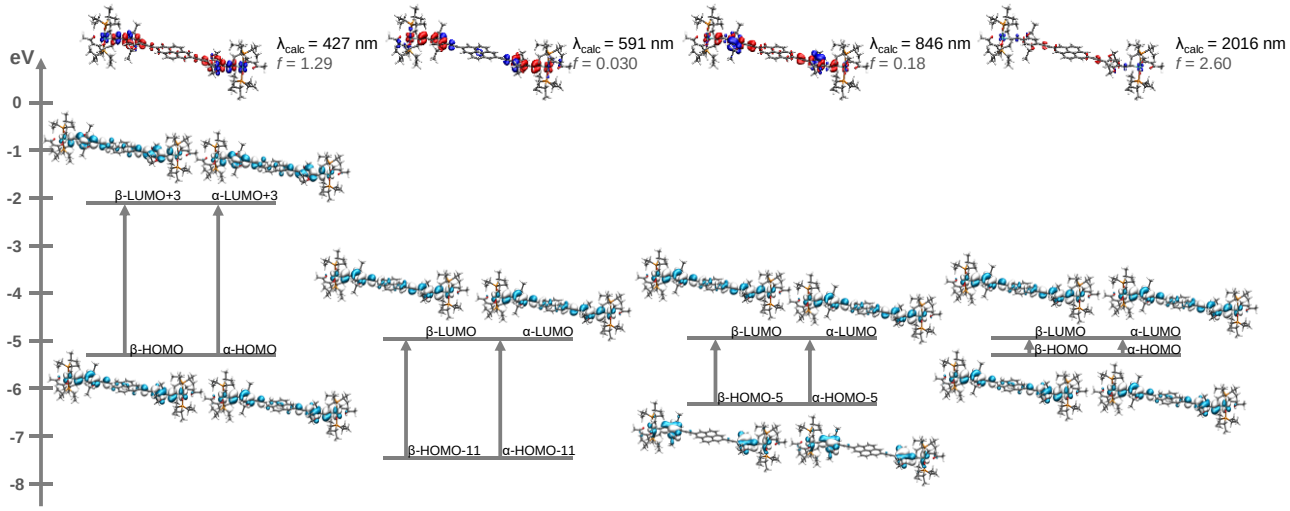

Figure S44 | pbe1pbe/6-31G(d)PCM (CH_2Cl-CH_2Cl) calculated electronic transitions of **[PyrDPE-Ru$_{acac}^{Me}$]$^{2+}$** in the open-shell singlet state with the respective acceptor and donor molecular orbitals and the corresponding electron density difference maps (EDDMs) for the corresponding transition (top; blue colour = electron density decrease, red colour = electron density increase).

Table S2 I Atomic coordinates of **PyrDPE-Ru$_{Cl}$** from its DFT structure.

C	**-33.07598**	**28.89899**	**22.92028**
C	**-34.03475**	**29.56720**	**22.57723**
C	**-35.13935**	**30.34880**	**22.15994**
C	**-36.36148**	**30.30537**	**22.86626**
C	**-35.03396**	**31.17887**	**21.02912**
C	**-37.42876**	**31.07927**	**22.42266**
C	**-36.10152**	**31.95390**	**20.59949**
H	**-34.08358**	**31.19715**	**20.50873**
H	**-38.38205**	**31.02755**	**22.93584**
C	**-25.37438**	**23.34285**	**25.72147**
C	**-24.44073**	**22.64272**	**26.07025**
C	**-23.34499**	**21.83203**	**26.45382**
C	**-22.14431**	**21.86854**	**25.72053**
C	**-23.43422**	**20.98067**	**27.57693**
C	**-21.05938**	**21.07998**	**26.07485**
H	**-22.09662**	**22.52924**	**24.86287**
C	**-22.33690**	**20.20083**	**27.92730**
H	**-22.38801**	**19.56378**	**28.80257**
O	**-36.06863**	**32.76669**	**19.50612**
C	**-34.85679**	**32.92108**	**18.78021**
C	**-33.88845**	**33.87350**	**19.45710**
H	**-34.39946**	**31.94143**	**18.59014**
H	**-33.56590**	**33.50241**	**20.43466**
H	**-32.99904**	**34.00684**	**18.83185**
H	**-34.35914**	**34.85160**	**19.60005**
O	**-36.38410**	**29.49310**	**23.95112**
C	**-37.59080**	**29.33779**	**24.68898**
C	**-38.55282**	**28.36729**	**24.02996**
H	**-38.05524**	**30.31583**	**24.86776**
H	**-38.87955**	**28.72273**	**23.04774**
H	**-38.07617**	**27.39062**	**23.89966**
H	**-39.43967**	**28.23751**	**24.65965**
O	**-24.60761**	**21.01970**	**28.25456**
C	**-24.81180**	**20.14457**	**29.35828**
C	**-25.14137**	**18.72713**	**28.92888**
H	**-23.94653**	**20.17583**	**30.03296**
H	**-24.31571**	**18.26325**	**28.38027**
H	**-25.35284**	**18.11285**	**29.81070**

H	**-26.02654**	**18.72253**	**28.28505**
O	**-19.88160**	**21.06377**	**25.39265**
C	**-19.74048**	**21.91648**	**24.26853**
C	**-18.35130**	**21.71044**	**23.70987**
H	**-20.50451**	**21.67157**	**23.51703**
H	**-18.20790**	**20.66866**	**23.40591**
H	**-18.20157**	**22.35057**	**22.83479**
H	**-17.59237**	**21.96222**	**24.45731**
C	**-37.33024**	**31.92288**	**21.30543**
C	**-38.44026**	**32.75686**	**20.84275**
C	**-39.53041**	**33.09576**	**21.56362**
H	**-38.31531**	**33.15767**	**19.84037**
H	**-39.60513**	**32.72782**	**22.59656**
C	**-40.57949**	**34.71269**	**19.61564**
P	**-40.13672**	**36.17235**	**22.23474**
P	**-42.34212**	**32.31219**	**20.24106**
O	**-40.29095**	**35.09871**	**18.55081**
C	**-41.49348**	**37.44832**	**22.51034**
C	**-39.16923**	**36.07881**	**23.83939**
C	**-39.04331**	**37.16797**	**21.06693**
C	**-41.82991**	**30.62778**	**20.87437**
C	**-44.21090**	**32.41945**	**20.29248**
C	**-42.02916**	**32.24079**	**18.37863**
H	**-41.00346**	**38.41993**	**22.38103**
C	**-42.54909**	**37.30455**	**21.41203**
C	**-42.14928**	**37.45089**	**23.88883**
H	**-39.13598**	**37.11671**	**24.20171**
C	**-37.73333**	**35.59078**	**23.62644**
C	**-39.82755**	**35.20699**	**24.90835**
H	**-39.76456**	**37.43735**	**20.28127**
C	**-38.48260**	**38.46862**	**21.65074**
C	**-37.91007**	**36.38539**	**20.39368**
H	**-40.77409**	**30.58814**	**20.57243**
C	**-41.85999**	**30.51137**	**22.39928**
C	**-42.56217**	**29.44744**	**20.23355**
H	**-44.55127**	**31.72340**	**19.51676**
C	**-44.88874**	**32.00904**	**21.59834**
C	**-44.62788**	**33.83537**	**19.88809**
H	**-41.97317**	**33.29930**	**18.10108**

C	**-43.11187**	**31.62127**	**17.49126**
C	**-40.66238**	**31.62349**	**18.07417**
H	**-43.11192**	**36.37139**	**21.53589**
H	**-43.26678**	**38.13209**	**21.47411**
H	**-42.11863**	**37.31632**	**20.40416**
H	**-42.65125**	**36.50130**	**24.09454**
H	**-41.43044**	**37.65134**	**24.68926**
H	**-42.90281**	**38.24804**	**23.91892**
H	**-37.25922**	**35.44901**	**24.60530**
H	**-37.70928**	**34.62990**	**23.10144**
H	**-37.11927**	**36.29999**	**23.06872**
H	**-40.86172**	**35.47926**	**25.11814**
H	**-39.82450**	**34.15588**	**24.60494**
H	**-39.24909**	**35.29556**	**25.83660**
H	**-37.95119**	**39.01148**	**20.85964**
H	**-39.24792**	**39.14327**	**22.04429**
H	**-37.76070**	**38.27516**	**22.45099**
H	**-37.01713**	**36.35185**	**21.02377**
H	**-38.17840**	**35.35629**	**20.15620**
H	**-37.63086**	**36.88878**	**19.46054**
H	**-41.36692**	**31.35305**	**22.88882**
H	**-42.88132**	**30.46087**	**22.78646**
H	**-41.34811**	**29.58667**	**22.69334**
H	**-42.39612**	**29.38166**	**19.15572**
H	**-42.19577**	**28.51336**	**20.67728**
H	**-43.64254**	**29.48965**	**20.41029**
H	**-44.73873**	**30.94990**	**21.82552**
H	**-44.53040**	**32.60021**	**22.44375**
H	**-45.96982**	**32.16958**	**21.49604**
H	**-44.17381**	**34.16064**	**18.94489**
H	**-45.71690**	**33.88428**	**19.76727**
H	**-44.34624**	**34.55478**	**20.66536**
H	**-42.75818**	**31.63761**	**16.45283**
H	**-43.33266**	**30.57984**	**17.74228**
H	**-44.04949**	**32.18429**	**17.51777**
H	**-39.87149**	**32.02276**	**18.71515**
H	**-40.67621**	**30.53475**	**18.19641**
H	**-40.39134**	**31.83229**	**17.03261**
C	**-21.14043**	**20.21633**	**27.19531**

C	-19.98796	19.38537	27.54500
C	-20.01242	18.30914	28.35981
H	-19.05976	19.66969	27.05609
H	-20.97749	18.00797	28.79043
C	-17.36256	17.69267	28.00903
P	-19.20782	15.39793	27.28828
P	-18.03632	18.48244	30.87193
O	-16.45036	18.07203	27.38464
C	-18.41083	13.75723	27.75528
C	-20.98121	15.01043	26.81366
C	-18.32125	15.68906	25.65178
C	-19.38022	19.65347	31.44068
C	-17.30842	17.63949	32.37726
C	-16.60750	19.60516	30.35408
H	-18.14347	13.28542	26.80292
C	-17.11625	14.03100	28.52371
C	-19.29184	12.77242	28.51927
H	-20.91920	14.05387	26.27432
C	-21.57401	16.06299	25.87219
C	-21.92135	14.84020	28.00694
H	-17.26972	15.60774	25.96470
C	-18.57262	14.62470	24.57912
C	-18.50587	17.08146	25.03802
H	-19.55556	20.24632	30.53237
C	-20.70072	18.95724	31.77668
C	-18.97517	20.60249	32.57008
H	-16.76789	18.43378	32.90551
C	-18.29534	17.02690	33.36913
C	-16.29348	16.59473	31.90746
H	-16.01277	18.95545	29.70209
C	-15.65641	20.10648	31.44383
C	-17.10646	20.76941	29.49541
H	-17.33475	14.45134	29.51306
H	-16.56898	13.09284	28.67901
H	-16.44650	14.71998	27.99639
H	-19.60927	13.18410	29.48141
H	-20.17951	12.48239	27.94880
H	-18.71465	11.85952	28.71311
H	-22.63735	15.84164	25.71923

H	**-21.50047**	**17.06952**	**26.29783**
H	**-21.10035**	**16.07265**	**24.88900**
H	**-21.57143**	**14.11316**	**28.73961**
H	**-22.05509**	**15.79053**	**28.53231**
H	**-22.90138**	**14.51533**	**27.63526**
H	**-17.92835**	**14.83202**	**23.71609**
H	**-18.35163**	**13.60527**	**24.90745**
H	**-19.60769**	**14.64634**	**24.22253**
H	**-19.41562**	**17.13531**	**24.43417**
H	**-18.56199**	**17.87601**	**25.78185**
H	**-17.66099**	**17.29618**	**24.37298**
H	**-20.99260**	**18.23048**	**31.01651**
H	**-20.65265**	**18.42858**	**32.73273**
H	**-21.48942**	**19.71587**	**31.85707**
H	**-18.15780**	**21.27065**	**32.28864**
H	**-19.83358**	**21.23190**	**32.83585**
H	**-18.67670**	**20.06051**	**33.47422**
H	**-18.92904**	**17.78331**	**33.84048**
H	**-18.93701**	**16.28213**	**32.89369**
H	**-17.72652**	**16.53502**	**34.16882**
H	**-15.55944**	**17.00079**	**31.20180**
H	**-15.74243**	**16.19569**	**32.76775**
H	**-16.80375**	**15.75614**	**31.42034**
H	**-14.91099**	**20.76234**	**30.97705**
H	**-16.15935**	**20.68844**	**32.22147**
H	**-15.10742**	**19.29354**	**31.92812**
H	**-17.81788**	**20.44911**	**28.72935**
H	**-17.59345**	**21.53879**	**30.10471**
H	**-16.25572**	**21.24159**	**28.99032**
Ru	**-18.68660**	**17.01265**	**29.02794**
Ru	**-41.14137**	**34.18922**	**21.24715**
H	**-37.26613**	**28.94959**	**25.65824**
H	**-35.17001**	**33.32534**	**17.81362**
H	**-25.65742**	**20.58349**	**29.89465**
H	**-19.88985**	**22.96241**	**24.57241**
C	**-31.96583**	**28.11035**	**23.32565**
C	**-32.07173**	**27.26180**	**24.44033**
C	**-30.75499**	**28.16811**	**22.61590**
C	**-30.99515**	**26.47443**	**24.85168**

H	**-33.00902**	**27.21929**	**24.98809**
C	**-29.65744**	**27.39503**	**22.99861**
H	**-30.67429**	**28.82514**	**21.75435**
C	**-29.76945**	**26.53405**	**24.12803**
C	**-31.08112**	**25.59817**	**25.98659**
C	**-28.41025**	**27.43600**	**22.28730**
C	**-28.66524**	**25.73762**	**24.52967**
C	**-30.02439**	**24.83605**	**26.37098**
H	**-32.01822**	**25.55673**	**26.53614**
C	**-27.35348**	**26.67384**	**22.67174**
H	**-28.32868**	**28.09502**	**21.42648**
C	**-28.77800**	**24.87529**	**25.65804**
C	**-27.44010**	**25.79571**	**23.80507**
H	**-30.10556**	**24.17729**	**27.23200**
H	**-26.41630**	**26.71574**	**22.12229**
C	**-27.68324**	**24.09637**	**26.03610**
C	**-26.36589**	**25.00249**	**24.21204**
C	**-26.47408**	**24.14920**	**25.32262**
H	**-27.76423**	**23.43589**	**26.89491**
H	**-25.43025**	**25.04297**	**23.66119**
Cl	**-42.45307**	**33.89684**	**23.28901**
Cl	**-19.97463**	**15.65974**	**30.60466**

Table S3 I Atomic coordinates of **PyrDPE-Ru$_{Cl}^{+}$** from its DFT structure.

C	**-32.97457**	**28.95732**	**22.75773**
C	**-33.92484**	**29.65121**	**22.43259**
C	**-35.01706**	**30.44778**	**22.06017**
C	**-36.15995**	**30.53484**	**22.92788**
C	**-35.00543**	**31.16274**	**20.85464**
C	**-37.23093**	**31.31744**	**22.55816**
C	**-36.08574**	**31.95183**	**20.48480**
H	**-34.12819**	**31.08036**	**20.22549**
H	**-38.09784**	**31.37941**	**23.20306**
C	**-25.40246**	**23.28694**	**25.61518**
C	**-24.47511**	**22.58359**	**25.97554**
C	**-23.38433**	**21.77329**	**26.36837**
C	**-22.21995**	**21.72305**	**25.57814**
C	**-23.43883**	**21.01186**	**27.55709**
C	**-21.13704**	**20.93750**	**25.94193**
H	**-22.19963**	**22.31565**	**24.67109**
C	**-22.34354**	**20.23252**	**27.91469**
H	**-22.36582**	**19.66508**	**28.83771**
O	**-36.16090**	**32.64932**	**19.34633**
C	**-35.05396**	**32.68389**	**18.43582**
C	**-33.98367**	**33.65825**	**18.88196**
H	**-34.66452**	**31.67038**	**18.29089**
H	**-33.52829**	**33.36370**	**19.83225**
H	**-33.19410**	**33.70136**	**18.12486**
H	**-34.40618**	**34.66110**	**18.99598**
O	**-36.05534**	**29.82764**	**24.05949**
C	**-37.13038**	**29.82719**	**25.00412**
C	**-38.24053**	**28.87346**	**24.61124**
H	**-37.49329**	**30.85136**	**25.15128**
H	**-38.72943**	**29.16899**	**23.67783**
H	**-37.84516**	**27.86075**	**24.48820**
H	**-38.99901**	**28.85379**	**25.40060**
O	**-24.57616**	**21.13269**	**28.28305**
C	**-24.74613**	**20.35035**	**29.46056**
C	**-25.12778**	**18.91331**	**29.15903**
H	**-23.84854**	**20.41091**	**30.08929**
H	**-24.33942**	**18.38602**	**28.61286**
H	**-25.31206**	**18.37563**	**30.09528**

H	-26.04186	18.88208	28.55780
O	-19.99369	20.83940	25.21126
C	-19.88729	21.59848	24.01799
C	-18.53082	21.31472	23.41503
H	-20.69121	21.31484	23.32397
H	-18.42410	20.24905	23.18891
H	-18.40911	21.88018	22.48587
H	-17.73231	21.60547	24.10478
C	-37.23806	32.04886	21.34650
C	-38.32011	32.87625	20.93426
C	-39.49275	33.08606	21.63961
H	-38.18509	33.37856	19.98155
H	-39.60931	32.57908	22.60442
C	-40.41156	34.85530	19.79063
P	-40.31997	36.04332	22.61417
P	-42.17835	32.34434	19.98536
O	-40.06979	35.37662	18.81070
C	-41.81368	37.14440	22.89560
C	-39.46390	35.81918	24.26503
C	-39.23242	37.23022	21.64221
C	-41.57173	30.61647	20.36830
C	-44.04693	32.35399	20.01796
C	-41.81239	32.60467	18.15242
H	-41.40892	38.16248	22.91973
C	-42.74921	37.03462	21.69034
C	-42.57777	36.92294	24.19801
H	-39.52292	36.81667	24.72448
C	-37.98875	35.44455	24.10256
C	-40.12690	34.80951	25.20129
H	-39.91406	37.53031	20.83306
C	-38.83153	38.49510	22.40855
C	-37.98720	36.61666	20.99041
H	-40.51174	30.67775	20.08454
C	-41.62021	30.24998	21.85237
C	-42.23325	29.52309	19.52599
H	-44.32542	31.77770	19.12765
C	-44.72297	31.69253	21.21720
C	-44.54162	33.79054	19.83835
H	-41.81177	33.69594	18.05228

C	-42.84185	32.08304	17.14620
C	-40.40831	32.11174	17.79448
H	-43.22336	36.04593	21.65619
H	-43.55378	37.77460	21.77633
H	-42.24133	37.21299	20.73578
H	-42.99471	35.91344	24.25361
H	-41.95386	37.09878	25.07923
H	-43.40964	37.63646	24.23872
H	-37.56962	35.23106	25.09275
H	-37.86483	34.54306	23.49188
H	-37.38931	36.24203	23.66137
H	-41.19151	34.98407	25.35331
H	-40.01371	33.79107	24.81855
H	-39.62468	34.86381	26.17480
H	-38.29745	39.16488	21.72448
H	-39.68003	39.05548	22.81001
H	-38.15213	38.26887	23.23677
H	-37.13687	36.61385	21.67693
H	-38.13307	35.59127	20.64817
H	-37.70242	37.22196	20.12271
H	-41.16811	31.01317	22.48800
H	-42.64332	30.09557	22.20419
H	-41.07361	29.31025	21.99685
H	-42.04852	29.64195	18.45605
H	-41.82200	28.55053	19.82166
H	-43.31589	29.48034	19.68447
H	-44.51434	30.62082	21.27158
H	-44.42431	32.15570	22.15961
H	-45.80841	31.80630	21.10517
H	-44.06996	34.30524	18.99344
H	-45.62375	33.78930	19.66355
H	-44.35468	34.37598	20.74493
H	-42.46888	32.29037	16.13604
H	-43.00680	31.00443	17.21673
H	-43.80926	32.58473	17.23851
H	-39.64759	32.43690	18.51040
H	-40.36832	31.01895	17.73566
H	-40.12656	32.50414	16.81109
C	-21.18360	20.16308	27.12898

C	**-20.03365**	**19.33455**	**27.48710**
C	**-20.04367**	**18.31495**	**28.37317**
H	**-19.12210**	**19.56486**	**26.94194**
H	**-20.99573**	**18.06396**	**28.86118**
C	**-17.41742**	**17.64309**	**27.96592**
P	**-19.31191**	**15.33374**	**27.43976**
P	**-17.98309**	**18.59973**	**30.80253**
O	**-16.52360**	**17.97528**	**27.29055**
C	**-18.51656**	**13.71306**	**27.97452**
C	**-21.10471**	**14.94406**	**27.04755**
C	**-18.47950**	**15.51388**	**25.75893**
C	**-19.29856**	**19.80804**	**31.36101**
C	**-17.20184**	**17.83104**	**32.32068**
C	**-16.57111**	**19.68465**	**30.17113**
H	**-18.28461**	**13.18552**	**27.04235**
C	**-17.19474**	**14.01441**	**28.68399**
C	**-19.38136**	**12.78278**	**28.82091**
H	**-21.07158**	**13.95946**	**26.55856**
C	**-21.71686**	**15.95288**	**26.07127**
C	**-22.00614**	**14.85023**	**28.27838**
H	**-17.41917**	**15.43080**	**26.03981**
C	**-18.78700**	**14.39276**	**24.76123**
C	**-18.66207**	**16.87007**	**25.06846**
H	**-19.50518**	**20.35535**	**30.43090**
C	**-20.60924**	**19.14053**	**31.78235**
C	**-18.84489**	**20.81037**	**32.42388**
H	**-16.63904**	**18.64816**	**32.78731**
C	**-18.15461**	**17.27573**	**33.37740**
C	**-16.20903**	**16.75776**	**31.86822**
H	**-16.00389**	**18.99749**	**29.53325**
C	**-15.57797**	**20.23800**	**31.19616**
C	**-17.09894**	**20.80337**	**29.27019**
H	**-17.37602**	**14.49175**	**29.65478**
H	**-16.65219**	**13.07995**	**28.87406**
H	**-16.53573**	**14.66450**	**28.09716**
H	**-19.66255**	**13.25096**	**29.76843**
H	**-20.29014**	**12.47138**	**28.29681**
H	**-18.80681**	**11.87561**	**29.04677**
H	**-22.78654**	**15.73567**	**25.96310**

H	**-21.62037**	**16.97904**	**26.44185**
H	**-21.27440**	**15.90705**	**25.07472**
H	**-21.64112**	**14.15748**	**29.03640**
H	**-22.10960**	**15.82874**	**28.75661**
H	**-23.00215**	**14.52045**	**27.95691**
H	**-18.16630**	**14.53312**	**23.86799**
H	**-18.57741**	**13.39005**	**25.14394**
H	**-19.83217**	**14.41673**	**24.43564**
H	**-19.59129**	**16.90454**	**24.49344**
H	**-18.67839**	**17.70963**	**25.76307**
H	**-17.83748**	**17.02803**	**24.36323**
H	**-20.93624**	**18.38037**	**31.07077**
H	**-20.52678**	**18.65811**	**32.76029**
H	**-21.38867**	**19.90939**	**31.85678**
H	**-18.03581**	**21.45756**	**32.07719**
H	**-19.68906**	**21.45852**	**32.69018**
H	**-18.51421**	**20.31312**	**33.34238**
H	**-18.76550**	**18.05949**	**33.83391**
H	**-18.81850**	**16.51417**	**32.96299**
H	**-17.55965**	**16.81889**	**34.17882**
H	**-15.50020**	**17.12252**	**31.11581**
H	**-15.62791**	**16.40067**	**32.72710**
H	**-16.73994**	**15.89771**	**31.44473**
H	**-14.84848**	**20.86423**	**30.66764**
H	**-16.04942**	**20.86287**	**31.96004**
H	**-15.01398**	**19.44885**	**31.70210**
H	**-17.83979**	**20.44538**	**28.54988**
H	**-17.56048**	**21.60675**	**29.85498**
H	**-16.26663**	**21.24356**	**28.70869**
Ru	**-18.71348**	**17.03882**	**29.06615**
Ru	**-41.06873**	**34.10514**	**21.31709**
H	**-36.66040**	**29.50600**	**25.93615**
H	**-35.50229**	**33.00537**	**17.49369**
H	**-25.55460**	**20.85154**	**29.99951**
H	**-19.99978**	**22.66816**	**24.24524**
C	**-31.88638**	**28.14732**	**23.15861**
C	**-31.95197**	**27.44884**	**24.37740**
C	**-30.74336**	**28.03859**	**22.34744**
C	**-30.89317**	**26.64485**	**24.79614**

H	**-32.84007**	**27.54033**	**24.99591**
C	**-29.66646**	**27.24311**	**22.73715**
H	**-30.70204**	**28.58176**	**21.40778**
C	**-29.73328**	**26.53471**	**23.97348**
C	**-30.93268**	**25.92015**	**26.03564**
C	**-28.48523**	**27.11275**	**21.93037**
C	**-28.64711**	**25.72106**	**24.38495**
C	**-29.89208**	**25.14101**	**26.42758**
H	**-31.81963**	**26.00937**	**26.65745**
C	**-27.44586**	**26.33375**	**22.32626**
H	**-28.44019**	**27.65483**	**20.98938**
C	**-28.71176**	**25.01142**	**25.61917**
C	**-27.48636**	**25.60942**	**23.56603**
H	**-29.93542**	**24.59776**	**27.36801**
H	**-26.55801**	**26.24441**	**21.70559**
C	**-27.63438**	**24.21504**	**26.00757**
C	**-26.42728**	**24.80472**	**23.98661**
C	**-26.48767**	**24.10262**	**25.20261**
H	**-27.67815**	**23.67153**	**26.94706**
H	**-25.54043**	**24.71664**	**23.36545**
Cl	**-42.40899**	**33.42781**	**23.20968**
Cl	**-19.96453**	**15.79395**	**30.75649**

Table S4 I Atomic coordinates of **PyrDPE-Ru$_{Cl}^{2+}$ (S)** from its DFT structure.

C	**-4.93103**	**0.31623**	**-0.78320**
C	**-6.15605**	**0.31747**	**-0.76915**
C	**-7.54815**	**0.32145**	**-0.77192**
C	**-8.26789**	**-0.05038**	**0.41719**
C	**-8.26117**	**0.68804**	**-1.92890**
C	**-9.64586**	**-0.04506**	**0.40243**
C	**-9.64285**	**0.69113**	**-1.93930**
H	**-7.69049**	**0.96807**	**-2.80522**
H	**-10.19087**	**-0.33143**	**1.29253**
C	**4.90715**	**0.25553**	**-0.80479**
C	**6.13207**	**0.24307**	**-0.79313**
C	**7.52444**	**0.23320**	**-0.79548**
C	**8.24297**	**0.56845**	**-1.95971**
C	**8.23999**	**-0.12076**	**0.40044**
C	**9.62425**	**0.55879**	**-1.96520**
H	**7.68039**	**0.83379**	**-2.84599**
C	**9.61875**	**-0.12898**	**0.38708**
H	**10.16001**	**-0.40721**	**1.28186**
O	**-10.39628**	**1.00416**	**-2.99944**
C	**-9.78812**	**1.42284**	**-4.22757**
C	**-9.38143**	**2.88170**	**-4.19228**
H	**-8.94928**	**0.75994**	**-4.46707**
H	**-8.61131**	**3.07760**	**-3.44022**
H	**-8.98399**	**3.17066**	**-5.17059**
H	**-10.24809**	**3.51257**	**-3.97318**
O	**-7.49487**	**-0.36332**	**1.46170**
C	**-8.08980**	**-0.77385**	**2.69827**
C	**-8.50324**	**-2.23144**	**2.67783**
H	**-8.92368**	**-0.10703**	**2.94629**
H	**-9.28481**	**-2.42889**	**1.93777**
H	**-7.64275**	**-2.86739**	**2.44962**
H	**-8.88857**	**-2.51320**	**3.66310**
O	**7.46524**	**-0.41038**	**1.45104**
C	**8.05941**	**-0.79686**	**2.69551**
C	**8.47152**	**-2.25522**	**2.70619**
H	**8.89381**	**-0.12585**	**2.93027**
H	**9.25596**	**-2.46961**	**1.97376**
H	**8.85185**	**-2.51697**	**3.69896**

H	7.61111	-2.89469	2.48753
O	10.37448	0.86635	-3.02963
C	9.73454	1.21717	-4.25909
C	10.81932	1.50305	-5.26875
H	9.09762	0.38378	-4.58133
H	11.44664	0.62045	-5.42559
H	10.36577	1.77937	-6.22533
H	11.45245	2.33045	-4.93441
C	-10.37946	0.32211	-0.74973
C	-11.80066	0.34851	-0.80651
C	-12.65676	0.01497	0.22752
H	-12.22202	0.66161	-1.75637
H	-12.21309	-0.29379	1.18109
C	-14.85608	0.64899	-1.23975
P	-14.76132	2.15745	1.41821
P	-14.75167	-2.33961	-0.52048
O	-15.13504	1.09763	-2.27435
C	-16.49785	2.28725	2.11801
C	-13.56913	2.73152	2.74442
C	-14.82575	3.55883	0.16591
C	-13.18189	-3.34697	-0.37750
C	-16.18764	-3.35932	0.10542
C	-15.11340	-2.24003	-2.36942
H	-16.76125	3.34648	2.01975
C	-17.45085	1.47906	1.23547
C	-16.66170	1.90686	3.58678
H	-14.07823	3.59693	3.19331
C	-12.23769	3.20231	2.15388
C	-13.28430	1.70745	3.84237
H	-15.72935	3.29522	-0.40253
C	-15.04858	4.94529	0.77909
C	-13.66004	3.62335	-0.82829
H	-12.47698	-2.75400	-0.97702
C	-12.61430	-3.42342	1.04072
C	-13.27830	-4.74611	-0.99012
H	-16.31078	-4.13243	-0.66238
C	-16.00025	-4.07340	1.44245
C	-17.44794	-2.49208	0.12449
H	-15.76786	-1.36432	-2.44548

C	**-15.88072**	**-3.40377**	**-3.00278**
C	**-13.84200**	**-1.93315**	**-3.16428**
H	**-17.26303**	**0.40348**	**1.34256**
H	**-18.48688**	**1.65671**	**1.54762**
H	**-17.37917**	**1.74216**	**0.17413**
H	**-16.39072**	**0.86244**	**3.76544**
H	**-16.06849**	**2.54554**	**4.24783**
H	**-17.71453**	**2.03674**	**3.86519**
H	**-11.55034**	**3.43229**	**2.97632**
H	**-11.76888**	**2.42370**	**1.54133**
H	**-12.33104**	**4.10433**	**1.54755**
H	**-14.18180**	**1.29553**	**4.30263**
H	**-12.70373**	**0.86768**	**3.44979**
H	**-12.68890**	**2.19730**	**4.62249**
H	**-15.18306**	**5.67014**	**-0.03220**
H	**-15.93427**	**5.00860**	**1.41693**
H	**-14.18446**	**5.27241**	**1.36624**
H	**-12.82441**	**4.20312**	**-0.42804**
H	**-13.27206**	**2.64335**	**-1.10970**
H	**-13.99585**	**4.12604**	**-1.74208**
H	**-12.56287**	**-2.44744**	**1.52621**
H	**-13.20773**	**-4.07744**	**1.68476**
H	**-11.60093**	**-3.83959**	**0.98905**
H	**-13.49780**	**-4.72682**	**-2.05989**
H	**-12.31549**	**-5.25561**	**-0.86365**
H	**-14.03824**	**-5.35998**	**-0.49535**
H	**-15.20438**	**-4.82175**	**1.40449**
H	**-15.78371**	**-3.37242**	**2.25087**
H	**-16.93114**	**-4.60181**	**1.68321**
H	**-17.60677**	**-1.94171**	**-0.81011**
H	**-18.32826**	**-3.12362**	**0.29112**
H	**-17.40083**	**-1.76852**	**0.94528**
H	**-15.98260**	**-3.20315**	**-4.07605**
H	**-15.37097**	**-4.36564**	**-2.89869**
H	**-16.89228**	**-3.50601**	**-2.59983**
H	**-13.24717**	**-1.12856**	**-2.72187**
H	**-13.19961**	**-2.81578**	**-3.25135**
H	**-14.11480**	**-1.62393**	**-4.17935**
C	**10.35688**	**0.20258**	**-0.77185**

C	11.77944	0.19220	-0.83420
C	12.63039	-0.08717	0.21807
H	12.20379	0.42604	-1.80548
H	12.18288	-0.30699	1.19452
C	14.83641	0.08820	-1.36367
P	14.64077	-2.60215	0.08248
P	14.79731	2.23799	0.82782
O	15.11999	0.25456	-2.47811
C	16.33959	-3.17190	0.64173
C	13.38013	-3.73988	0.87446
C	14.71395	-3.11298	-1.72584
C	13.27152	3.05439	1.53984
C	16.28228	2.72597	1.85213
C	15.12866	3.13989	-0.79653
H	16.57949	-4.01810	-0.01173
C	17.35380	-2.05967	0.37005
C	16.44525	-3.66163	2.08334
H	13.85162	-4.73162	0.81524
C	12.06397	-3.77904	0.09416
C	13.07293	-3.43023	2.33896
H	15.63608	-2.61087	-2.05273
C	14.89406	-4.61687	-1.95687
C	13.57108	-2.59721	-2.60944
H	12.53707	2.90094	0.73675
C	12.71874	2.37117	2.79162
C	13.42115	4.55898	1.77650
H	16.41430	3.79157	1.62952
C	16.15090	2.59070	3.36761
C	17.51081	1.97045	1.34126
H	15.74813	2.42763	-1.35283
C	15.93043	4.44275	-0.73003
C	13.83616	3.34081	-1.59118
H	17.19267	-1.21567	1.05185
H	18.36977	-2.43088	0.55013
H	17.31825	-1.68938	-0.66091
H	16.20352	-2.86809	2.79584
H	15.79893	-4.52281	2.27736
H	17.47839	-3.98009	2.26783
H	11.33921	-4.37782	0.65830

H	11.63690	-2.77734	-0.02944
H	12.16253	-4.23352	-0.89270
H	13.95937	-3.35380	2.96782
H	12.52603	-2.48707	2.42846
H	12.43542	-4.23068	2.73389
H	15.01142	-4.79446	-3.03232
H	15.77512	-5.03657	-1.46414
H	14.01814	-5.18551	-1.62792
H	12.72624	-3.29064	-2.61272
H	13.19060	-1.62089	-2.30559
H	13.92596	-2.51271	-3.64245
H	12.62320	1.29066	2.67366
H	13.34836	2.54933	3.66717
H	11.72666	2.78645	3.00565
H	13.62362	5.11513	0.85853
H	12.48397	4.94733	2.19301
H	14.21495	4.78452	2.49639
H	15.38004	3.24941	3.77624
H	15.92780	1.56470	3.66689
H	17.10453	2.88473	3.82353
H	17.63596	2.03797	0.25449
H	18.41543	2.38010	1.80541
H	17.45168	0.91119	1.61356
H	16.01488	4.84487	-1.74677
H	15.45554	5.21186	-0.11475
H	16.94874	4.28967	-0.36174
H	13.21820	2.43914	-1.63309
H	13.22574	4.14622	-1.16901
H	14.08354	3.62169	-2.62102
Ru	14.52727	-0.17886	0.41149
Ru	-14.55327	-0.06285	0.41064
H	-7.30177	-0.60714	3.43564
H	-10.56721	1.25660	-4.97422
H	7.27149	-0.61466	3.42934
H	9.10015	2.09723	-4.09459
C	-3.52886	0.31021	-0.78896
C	-2.82144	-0.05417	0.37708
C	-2.82248	0.66666	-1.95789
C	-1.43304	-0.06689	0.39004

H	**-3.37644**	**-0.32619**	**1.26983**
C	**-1.43402**	**0.66259**	**-1.97710**
H	**-3.37704**	**0.94552**	**-2.84884**
C	**-0.71711**	**0.29337**	**-0.79523**
C	**-0.68907**	**-0.43333**	**1.56455**
C	**-0.69091**	**1.01974**	**-3.15499**
C	**0.69276**	**0.28435**	**-0.79860**
C	**0.66668**	**-0.44105**	**1.56154**
H	**-1.24090**	**-0.70552**	**2.45999**
C	**0.66485**	**1.01013**	**-3.15842**
H	**-1.24335**	**1.29900**	**-4.04789**
C	**1.40963**	**-0.08373**	**0.38359**
C	**1.40887**	**0.64311**	**-1.98413**
H	**1.21935**	**-0.71945**	**2.45456**
H	**1.21657**	**1.28158**	**-4.05417**
C	**2.79802**	**-0.08715**	**0.36456**
C	**2.79741**	**0.62829**	**-1.97173**
C	**3.50480**	**0.26590**	**-0.80532**
H	**3.35355**	**-0.36438**	**1.25537**
H	**3.35131**	**0.89831**	**-2.86582**
Cl	**-14.72086**	**-1.02572**	**2.62128**
Cl	**14.69642**	**-0.55374**	**2.79482**

Table S5 I Atomic coordinates of **PyrDPE-Ru$_{Cl}^{2+}$ (T)** from its DFT structure.

C	**-33.00739**	**29.03135**	**23.03314**
C	**-33.94691**	**29.73782**	**22.70828**
C	**-35.02141**	**30.55217**	**22.31365**
C	**-36.24657**	**30.53047**	**23.06366**
C	**-34.90684**	**31.38449**	**21.19340**
C	**-37.29656**	**31.32662**	**22.66387**
C	**-35.96701**	**32.18707**	**20.79137**
H	**-33.96799**	**31.38294**	**20.65433**
H	**-38.22597**	**31.30628**	**23.21771**
C	**-25.47385**	**23.21816**	**25.66393**
C	**-24.54823**	**22.49269**	**25.98741**
C	**-23.46794**	**21.66701**	**26.33902**
C	**-22.26883**	**21.72331**	**25.61610**
C	**-23.58981**	**20.76022**	**27.44649**
C	**-21.19543**	**20.91249**	**25.95821**
H	**-22.20340**	**22.41720**	**24.78779**
C	**-22.52447**	**19.95289**	**27.77963**
H	**-22.61617**	**19.25896**	**28.60510**
O	**-35.94537**	**32.99103**	**19.72410**
C	**-34.76152**	**33.11426**	**18.92398**
C	**-33.74923**	**34.05163**	**19.54866**
H	**-34.34710**	**32.11965**	**18.72669**
H	**-33.37197**	**33.67467**	**20.50399**
H	**-32.89876**	**34.17047**	**18.86972**
H	**-34.19581**	**35.03629**	**19.71637**
O	**-36.23659**	**29.71345**	**24.12435**
C	**-37.40342**	**29.59396**	**24.94452**
C	**-38.43721**	**28.66373**	**24.34235**
H	**-37.81128**	**30.58993**	**25.15432**
H	**-38.83758**	**29.04477**	**23.39784**
H	**-37.99968**	**27.67780**	**24.15917**
H	**-39.27137**	**28.54621**	**25.04166**
O	**-24.77239**	**20.79984**	**28.07320**
C	**-25.02068**	**19.92854**	**29.18134**
C	**-25.38420**	**18.52513**	**28.73915**
H	**-24.16073**	**19.94206**	**29.86160**
H	**-24.56513**	**18.03302**	**28.20541**
H	**-25.63026**	**17.91968**	**29.61756**

H	-26.25847	18.54909	28.08179
O	-20.02207	20.91748	25.31964
C	-19.82558	21.80090	24.21015
C	-18.42028	21.58437	23.70470
H	-20.56873	21.57326	23.43627
H	-18.28061	20.55065	23.37459
H	-18.23149	22.24717	22.85492
H	-17.68772	21.80719	24.48629
C	-37.20249	32.17463	21.53412
C	-38.26298	33.01063	21.08721
C	-39.51570	33.11813	21.67133
H	-38.04514	33.60484	20.20522
H	-39.71777	32.52280	22.56937
C	-40.28473	34.99868	19.87014
P	-40.58880	35.96754	22.76031
P	-41.96531	32.42791	19.65655
O	-39.85187	35.60843	18.98219
C	-42.15666	36.98642	22.91946
C	-39.93750	35.65073	24.48781
C	-39.44541	37.26333	22.01874
C	-41.33456	30.69497	19.97197
C	-43.82387	32.37560	19.46804
C	-41.40056	32.85304	17.90745
H	-41.80644	38.01357	23.07185
C	-42.92186	36.93775	21.59579
C	-43.07134	36.63462	24.08943
H	-40.10202	36.60718	25.00531
C	-38.43687	35.34863	24.49113
C	-40.66395	34.54765	25.25633
H	-40.03518	37.59787	21.15308
C	-39.20298	38.48143	22.91632
C	-38.10205	36.74835	21.48819
H	-40.25251	30.81637	19.82285
C	-41.53978	30.20104	21.40473
C	-41.84517	29.65551	18.97121
H	-43.97139	31.86176	18.51051
C	-44.60601	31.60034	20.52610
C	-44.35635	33.80392	19.33732
H	-41.43353	33.94833	17.89657

C	**-42.28537**	**32.38772**	**16.74772**
C	**-39.94562**	**32.43590**	**17.67987**
H	**-43.34511**	**35.93975**	**21.42819**
H	**-43.76241**	**37.64102**	**21.62773**
H	**-42.30418**	**37.20621**	**20.73127**
H	**-43.44225**	**35.60833**	**24.01661**
H	**-42.57571**	**36.76592**	**25.05583**
H	**-43.93519**	**37.31006**	**24.07081**
H	**-38.13552**	**35.08042**	**25.51041**
H	**-38.19167**	**34.50008**	**23.84227**
H	**-37.82696**	**36.20006**	**24.18623**
H	**-41.74574**	**34.67335**	**25.28717**
H	**-40.46122**	**33.56737**	**24.81557**
H	**-40.28694**	**34.54235**	**26.28621**
H	**-38.61810**	**39.21931**	**22.35488**
H	**-40.12022**	**38.97925**	**23.24184**
H	**-38.62447**	**38.21959**	**23.80811**
H	**-37.34496**	**36.71869**	**22.27578**
H	**-38.15825**	**35.75033**	**21.05163**
H	**-37.73818**	**37.43181**	**20.71306**
H	**-41.21156**	**30.92575**	**22.15140**
H	**-42.58772**	**29.97082**	**21.61297**
H	**-40.96362**	**29.27784**	**21.54022**
H	**-41.54825**	**29.87440**	**17.94323**
H	**-41.42373**	**28.67713**	**19.23107**
H	**-42.93547**	**29.55776**	**18.99999**
H	**-44.35464**	**30.53652**	**20.53191**
H	**-44.44443**	**32.00366**	**21.52761**
H	**-45.67436**	**31.68028**	**20.28990**
H	**-43.80829**	**34.40297**	**18.60108**
H	**-45.40758**	**33.77855**	**19.02790**
H	**-44.30974**	**34.31900**	**20.30270**
H	**-41.80811**	**32.69372**	**15.80910**
H	**-42.41264**	**31.30246**	**16.70897**
H	**-43.27673**	**32.84889**	**16.76674**
H	**-39.28704**	**32.71901**	**18.50638**
H	**-39.85517**	**31.35424**	**17.53470**
H	**-39.56696**	**32.92177**	**16.77384**
C	**-21.30437**	**19.99409**	**27.06321**

C	-20.18315	19.17351	27.36607
C	-20.09925	18.26122	28.40635
H	-19.32834	19.29478	26.70828
H	-20.96594	18.15605	29.06918
C	-17.63123	17.44428	27.60548
P	-19.62438	15.12758	27.82426
P	-17.57305	18.77776	30.37835
O	-16.86786	17.61599	26.74793
C	-18.72510	13.62290	28.49314
C	-21.45877	14.74734	27.82943
C	-19.10026	15.02623	26.02109
C	-18.68068	20.18798	30.91035
C	-16.64440	18.13589	31.86749
C	-16.19651	19.57903	29.36658
H	-18.66628	12.93228	27.64411
C	-17.29931	14.02470	28.87540
C	-19.40866	12.88564	29.64112
H	-21.50316	13.70314	27.48676
C	-22.22940	15.62020	26.83527
C	-22.13860	14.84301	29.19482
H	-18.00738	14.95369	26.11966
C	-19.58701	13.76738	25.29529
C	-19.40262	16.25827	25.16169
H	-18.97431	20.62264	29.94459
C	-19.96436	19.74646	31.61509
C	-17.96741	21.26724	31.72818
H	-15.94236	18.94502	32.10148
C	-17.46180	17.86407	33.12852
C	-15.83985	16.89938	31.46257
H	-15.81337	18.74627	28.76616
C	-14.99684	20.14169	30.13393
C	-16.75555	20.62350	28.39722
H	-17.30120	14.67552	29.75879
H	-16.71955	13.13153	29.13682
H	-16.76595	14.53529	28.06565
H	-19.52273	13.52649	30.52010
H	-20.39011	12.49543	29.35592
H	-18.78575	12.02874	29.92463
H	-23.30166	15.42708	26.95692

H	**-22.06574**	**16.68800**	**27.02123**
H	**-21.97852**	**15.41156**	**25.79423**
H	**-21.63721**	**14.27434**	**29.97723**
H	**-22.19402**	**15.88246**	**29.53034**
H	**-23.16273**	**14.46359**	**29.09372**
H	**-19.12571**	**13.73493**	**24.30146**
H	**-19.32274**	**12.83587**	**25.80315**
H	**-20.67185**	**13.77718**	**25.14908**
H	**-20.42599**	**16.24163**	**24.77914**
H	**-19.26668**	**17.20227**	**25.69049**
H	**-18.73126**	**16.26137**	**24.29571**
H	**-20.48715**	**18.95326**	**31.07834**
H	**-19.77148**	**19.38338**	**32.62777**
H	**-20.63377**	**20.61128**	**31.69395**
H	**-17.14959**	**21.74269**	**31.18226**
H	**-18.68899**	**22.05243**	**31.98354**
H	**-17.56878**	**20.87359**	**32.66908**
H	**-17.92022**	**18.77194**	**33.52902**
H	**-18.24508**	**17.12405**	**32.95383**
H	**-16.78479**	**17.47519**	**33.89920**
H	**-15.25131**	**17.04866**	**30.54997**
H	**-15.14354**	**16.63295**	**32.26609**
H	**-16.50569**	**16.04387**	**31.30651**
H	**-14.30843**	**20.59347**	**29.40983**
H	**-15.26988**	**20.91959**	**30.85224**
H	**-14.43791**	**19.36577**	**30.66450**
H	**-17.63562**	**20.27138**	**27.85113**
H	**-17.03060**	**21.54815**	**28.91554**
H	**-15.98808**	**20.87744**	**27.65764**
Ru	**-18.73788**	**17.07987**	**29.01004**
Ru	**-41.08373**	**34.10524**	**21.24588**
H	**-37.02292**	**29.18795**	**25.88429**
H	**-35.12861**	**33.51583**	**17.97746**
H	**-25.85961**	**20.39684**	**29.70048**
H	**-19.97461**	**22.83429**	**24.54627**
C	**-31.92234**	**28.20343**	**23.41392**
C	**-32.04321**	**27.35946**	**24.53072**
C	**-30.72809**	**28.22290**	**22.67421**
C	**-30.98782**	**26.53347**	**24.91723**

H	**-32.97058**	**27.35219**	**25.09581**
C	**-29.65335**	**27.40973**	**23.03382**
H	**-30.64446**	**28.87890**	**21.81282**
C	**-29.77675**	**26.55227**	**24.16578**
C	**-31.08462**	**25.65993**	**26.05302**
C	**-28.42170**	**27.40852**	**22.29513**
C	**-28.69412**	**25.71608**	**24.54409**
C	**-30.04928**	**24.85967**	**26.41455**
H	**-32.01132**	**25.65254**	**26.62055**
C	**-27.38590**	**26.60923**	**22.65738**
H	**-28.33524**	**28.06533**	**21.43368**
C	**-28.81818**	**24.85703**	**25.67485**
C	**-27.48325**	**25.73477**	**23.79236**
H	**-30.13581**	**24.20267**	**27.27584**
H	**-26.45892**	**26.61725**	**22.09030**
C	**-27.74562**	**24.03937**	**26.03079**
C	**-26.42930**	**24.90591**	**24.17638**
C	**-26.55213**	**24.05744**	**25.28948**
H	**-27.82930**	**23.37986**	**26.88945**
H	**-25.50283**	**24.91318**	**23.60970**
Cl	**-42.59758**	**33.22664**	**22.90755**
Cl	**-19.76475**	**16.24866**	**31.02997**

Table S6 I Atomic coordinates of **PyrDPE-Ru$_{Cl}^{2+}$ (OSS)** from its DFT structure.

C	**-4.95499**	**-0.30741**	**0.54824**
C	**-6.17497**	**-0.29786**	**0.56246**
C	**-7.57795**	**-0.29400**	**0.60962**
C	**-8.33369**	**0.10704**	**-0.54481**
C	**-8.24694**	**-0.68100**	**1.77823**
C	**-9.70953**	**0.10514**	**-0.48474**
C	**-9.63391**	**-0.67961**	**1.83809**
H	**-7.64846**	**-0.98187**	**2.62868**
H	**-10.28436**	**0.41289**	**-1.34858**
C	**4.91509**	**-0.32114**	**0.49800**
C	**6.13524**	**-0.31008**	**0.50633**
C	**7.53778**	**-0.29900**	**0.55505**
C	**8.20575**	**-0.62895**	**1.74279**
C	**8.29537**	**0.05430**	**-0.61342**
C	**9.59145**	**-0.61092**	**1.80526**
H	**7.61078**	**-0.89578**	**2.60710**
C	**9.67135**	**0.07277**	**-0.54707**
H	**10.24710**	**0.34748**	**-1.42134**
O	**-10.34579**	**-1.01134**	**2.91962**
C	**-9.69470**	**-1.46144**	**4.11551**
C	**-9.30001**	**-2.92110**	**4.03066**
H	**-8.84394**	**-0.80853**	**4.33890**
H	**-8.55734**	**-3.10307**	**3.24807**
H	**-8.87137**	**-3.23683**	**4.98724**
H	**-10.17809**	**-3.54101**	**3.82611**
O	**-7.59188**	**0.44141**	**-1.60789**
C	**-8.22747**	**0.88306**	**-2.81198**
C	**-8.64145**	**2.33912**	**-2.74124**
H	**-9.06885**	**0.22161**	**-3.05051**
H	**-9.39965**	**2.51712**	**-1.97240**
H	**-7.77450**	**2.96996**	**-2.52338**
H	**-9.05735**	**2.64629**	**-3.70632**
O	**7.55542**	**0.33212**	**-1.69406**
C	**8.19212**	**0.72822**	**-2.91330**
C	**8.58986**	**2.19062**	**-2.90454**
H	**9.04170**	**0.06648**	**-3.11930**
H	**9.34148**	**2.41123**	**-2.14024**
H	**9.00765**	**2.45924**	**-3.88030**

H	7.71483	2.82080	-2.71946
O	10.29391	-0.91278	2.90109
C	9.60464	-1.26725	4.10462
C	10.64917	-1.54330	5.15827
H	8.94962	-0.43778	4.39817
H	11.26298	-0.65578	5.33893
H	10.15827	-1.82096	6.09579
H	11.30133	-2.36690	4.85234
C	-10.40505	-0.28704	0.68448
C	-11.82326	-0.31885	0.78475
C	-12.71951	0.02247	-0.21612
H	-12.21238	-0.64882	1.74276
H	-12.31551	0.34997	-1.18091
C	-14.83830	-0.66303	1.33866
P	-14.83780	-2.14038	-1.34533
P	-14.82102	2.33841	0.65233
O	-15.06458	-1.12721	2.37835
C	-16.60215	-2.28562	-1.96705
C	-13.70019	-2.67481	-2.73453
C	-14.82170	-3.55749	-0.10926
C	-13.27642	3.37535	0.45691
C	-16.30035	3.33638	0.09718
C	-15.10431	2.20926	2.51297
H	-16.84246	-3.35144	-1.88167
C	-17.52756	-1.51398	-1.02450
C	-16.83939	-1.87560	-3.41780
H	-14.22133	-3.53676	-3.17632
C	-12.33780	-3.14294	-2.21667
C	-13.47722	-1.62702	-3.82444
H	-15.70073	-3.31558	0.50555
C	-15.05337	-4.93905	-0.73013
C	-13.60977	-3.61717	0.82756
H	-12.53716	2.79153	1.02309
C	-12.76561	3.47643	-0.98130
C	-13.37702	4.76635	1.08752
H	-16.40497	4.09831	0.87871
C	-16.18187	4.06911	-1.23758
C	-17.54433	2.44598	0.12091
H	-15.73902	1.32058	2.60510

C	-15.86644	3.35098	3.19116
C	-13.79595	1.91855	3.25204
H	-17.36141	-0.43317	-1.11389
H	-18.57327	-1.70081	-1.29620
H	-17.40676	-1.80051	0.02618
H	-16.59449	-0.82286	-3.58468
H	-16.26707	-2.48897	-4.11983
H	-17.90164	-2.01804	-3.65030
H	-11.68776	-3.34779	-3.07525
H	-11.84758	-2.37255	-1.61054
H	-12.39346	-4.05871	-1.62664
H	-14.39902	-1.21423	-4.23299
H	-12.88446	-0.79012	-3.44394
H	-12.91642	-2.09682	-4.64151
H	-15.14026	-5.67576	0.07689
H	-15.96704	-5.00654	-1.32655
H	-14.21337	-5.24680	-1.36102
H	-12.77442	-4.15340	0.37056
H	-13.24252	-2.63511	1.12815
H	-13.88804	-4.16241	1.73633
H	-12.70680	2.50576	-1.47641
H	-13.39941	4.11946	-1.59723
H	-11.76179	3.91772	-0.96431
H	-13.54903	4.73144	2.16555
H	-12.43194	5.29814	0.92502
H	-14.17097	5.36789	0.63272
H	-15.39603	4.82885	-1.22501
H	-15.99105	3.38149	-2.06367
H	-17.13016	4.58607	-1.43032
H	-17.65200	1.87973	1.05334
H	-18.44211	3.06348	0.00222
H	-17.52071	1.73522	-0.71204
H	-15.92160	3.13512	4.26484
H	-15.37812	4.32304	3.07960
H	-16.89496	3.43967	2.83024
H	-13.20213	1.13295	2.77543
H	-13.16934	2.81352	3.32705
H	-14.02169	1.58937	4.27231
C	10.36493	-0.24881	0.64436

C	11.78112	-0.22090	0.76684
C	12.68242	0.08775	-0.24029
H	12.16517	-0.46503	1.75236
H	12.28411	0.32213	-1.23435
C	14.77013	-0.06339	1.48913
P	14.67416	2.61997	0.02315
P	14.92365	-2.22263	-0.70074
O	14.97715	-0.21746	2.62091
C	16.44034	3.14399	-0.33255
C	13.53336	3.77386	-0.91367
C	14.54716	3.14844	1.82355
C	13.43316	-3.07561	-1.44089
C	16.44297	-2.68221	-1.68781
C	15.23618	-3.09278	0.94407
H	16.61243	4.01368	0.31194
C	17.38818	2.02859	0.11304
C	16.73717	3.56795	-1.76815
H	14.00075	4.76037	-0.77901
C	12.13056	3.81148	-0.30128
C	13.40775	3.49381	-2.41093
H	15.43429	2.66139	2.25312
C	14.68991	4.65747	2.04812
C	13.32616	2.63132	2.59137
H	12.67367	-2.92474	-0.66113
C	12.90668	-2.41678	-2.71705
C	13.61573	-4.58053	-1.65091
H	16.61183	-3.73334	-1.42566
C	16.33177	-2.60695	-3.20938
C	17.63372	-1.86172	-1.18837
H	15.81778	-2.35472	1.50813
C	16.07834	-4.37112	0.91554
C	13.92754	-3.32413	1.70368
H	17.28722	1.14702	-0.53293
H	18.42688	2.36928	0.02799
H	17.22978	1.71877	1.15195
H	16.54929	2.75571	-2.47628
H	16.15352	4.44295	-2.06842
H	17.79676	3.84171	-1.83858
H	11.48162	4.41642	-0.94530

H	11.68802	2.81057	-0.23847
H	12.10760	4.25838	0.69363
H	14.36452	3.41668	-2.92630
H	12.86497	2.56145	-2.58900
H	12.83623	4.31275	-2.86448
H	14.73076	4.84895	3.12666
H	15.59686	5.08376	1.61104
H	13.83133	5.21003	1.65322
H	12.45030	3.26459	2.43056
H	13.04557	1.61140	2.32568
H	13.54766	2.64826	3.66439
H	12.79663	-1.33560	-2.61722
H	13.56120	-2.60078	-3.57270
H	11.92487	-2.84510	-2.95105
H	13.80955	-5.11846	-0.72022
H	12.69459	-4.99237	-2.08024
H	14.42829	-4.80247	-2.35041
H	15.59626	-3.31114	-3.60681
H	16.07522	-1.60192	-3.54959
H	17.30472	-2.87836	-3.63759
H	17.73553	-1.86935	-0.09679
H	18.56186	-2.26439	-1.61017
H	17.54500	-0.82155	-1.51964
H	16.14147	-4.76279	1.93781
H	15.64693	-5.15885	0.29154
H	17.10316	-4.18928	0.57960
H	13.27827	-2.44373	1.71343
H	13.35708	-4.15584	1.27722
H	14.15306	-3.57965	2.74493
Ru	14.57972	0.19303	-0.30788
Ru	-14.61743	0.07387	-0.31626
H	-7.46473	0.73715	-3.57988
H	-10.44523	-1.30758	4.89332
H	7.43484	0.54071	-3.67754
H	8.98507	-2.15210	3.91407
C	-3.53942	-0.31673	0.53569
C	-2.84250	0.05734	-0.62617
C	-2.83052	-0.69854	1.68776
C	-1.44813	0.05643	-0.65185

H	**-3.40001**	**0.35021**	**-1.51094**
C	**-1.43627**	**-0.70971**	**1.69587**
H	**-3.37850**	**-0.98623**	**2.58023**
C	**-0.72924**	**-0.32883**	**0.51771**
C	**-0.71006**	**0.43458**	**-1.82444**
C	**-0.68741**	**-1.09337**	**2.85969**
C	**0.68930**	**-0.33167**	**0.50991**
C	**0.64755**	**0.43105**	**-1.83215**
H	**-1.26510**	**0.72636**	**-2.71195**
C	**0.67002**	**-1.09531**	**2.85252**
H	**-1.23400**	**-1.38359**	**3.75294**
C	**1.39696**	**0.04969**	**-0.66781**
C	**1.40758**	**-0.71425**	**1.68066**
H	**1.19391**	**0.71999**	**-2.72594**
H	**1.22527**	**-1.38702**	**3.73994**
C	**2.79156**	**0.04453**	**-0.65761**
C	**2.80161**	**-0.70659**	**1.65793**
C	**3.49956**	**-0.32909**	**0.49769**
H	**3.34056**	**0.33404**	**-1.54880**
H	**3.35813**	**-0.99414**	**2.54512**
Cl	**-14.89262**	**1.06273**	**-2.50065**
Cl	**14.89179**	**0.54724**	**-2.67360**

Table S7 I Atomic coordinates of **PyrDPE-Ru$_{acac}$** from its DFT structure.

C	**-32.87827**	**28.95948**	**22.47045**
C	**-25.12972**	**23.42431**	**25.18743**
C	**-31.76376**	**28.16597**	**22.85284**
C	**-31.74499**	**26.78767**	**22.58098**
C	**-30.66879**	**28.75294**	**23.50918**
C	**-30.65866**	**25.99370**	**22.95231**
H	**-32.59147**	**26.33445**	**22.07247**
C	**-29.56624**	**27.98972**	**23.89677**
H	**-30.68502**	**29.81889**	**23.71867**
C	**-29.55161**	**26.59231**	**23.61985**
C	**-30.61741**	**24.58327**	**22.68339**
C	**-28.43784**	**28.56740**	**24.57232**
C	**-28.44002**	**25.79989**	**24.00859**
C	**-29.55251**	**23.82526**	**23.05328**
H	**-31.46393**	**24.13059**	**22.17298**
C	**-27.37498**	**27.80852**	**24.94643**
H	**-28.45241**	**29.63428**	**24.78098**
C	**-28.42486**	**24.40278**	**23.73021**
C	**-27.33512**	**26.39745**	**24.68060**
H	**-29.53675**	**22.75883**	**22.84245**
H	**-26.52915**	**28.26102**	**25.45814**
C	**-27.32477**	**23.63858**	**24.12252**
C	**-26.25286**	**25.60167**	**25.06025**
C	**-26.23474**	**24.22328**	**24.78913**
H	**-27.30885**	**22.57251**	**23.91370**
H	**-25.40924**	**26.05366**	**25.57459**
C	**-33.83108**	**29.64672**	**22.14773**
C	**-34.95272**	**30.42240**	**21.76839**
C	**-34.95007**	**31.82615**	**21.92145**
C	**-36.09166**	**29.80269**	**21.22109**
C	**-36.06727**	**32.55428**	**21.52991**
O	**-33.81080**	**32.36019**	**22.42914**
C	**-37.20305**	**30.53833**	**20.83756**
H	**-36.06919**	**28.72469**	**21.11133**
H	**-36.06827**	**33.63254**	**21.63729**
C	**-37.21252**	**31.94999**	**20.98609**
C	**-33.72506**	**33.76451**	**22.63769**
O	**-38.34570**	**29.98753**	**20.33485**

C	-38.39293	32.70886	20.56957
C	-34.42004	34.21079	23.91061
H	-34.10104	34.30238	21.75787
H	-32.65150	33.96148	22.70530
C	-38.38703	28.59837	20.04228
C	-38.61989	34.02778	20.77821
H	-39.13081	32.10613	20.04905
H	-35.49746	34.02201	23.87569
H	-34.00633	33.67980	24.77373
H	-34.26596	35.28495	24.06047
C	-37.66646	28.24739	18.75346
H	-38.00512	28.01809	20.89247
H	-39.45340	28.37369	19.95104
H	-37.83077	34.55871	21.32833
Ru	-40.06324	35.39029	20.41040
H	-36.59696	28.47189	18.80887
H	-37.78051	27.17863	18.54234
H	-38.09245	28.81110	17.91726
C	-41.14037	34.30972	19.45039
P	-38.89914	35.93991	18.29586
P	-41.22674	34.60746	22.46748
O	-41.34808	37.17108	20.24505
O	-38.80815	36.69651	21.56630
O	-41.88043	33.65950	18.81992
C	-39.39841	37.51592	17.39106
C	-37.02399	36.13553	18.29442
C	-39.29324	34.71402	16.91058
C	-40.04685	33.87340	23.73073
C	-42.37484	35.74785	23.41344
C	-42.42439	33.19429	22.07541
C	-41.14318	38.33078	20.70916
C	-38.96703	37.91835	21.86775
H	-38.85494	37.45236	16.44020
C	-40.89585	37.53692	17.07859
C	-38.94062	38.81463	18.05314
H	-36.82321	36.74114	17.39833
C	-36.24164	34.82762	18.16740
C	-36.51124	36.90240	19.51479
H	-40.38550	34.80464	16.84724

C	**-38.71883**	**35.07882**	**15.53700**
C	**-39.00760**	**33.24233**	**17.21244**
H	**-39.59367**	**33.06059**	**23.14796**
C	**-38.90654**	**34.81212**	**24.13584**
C	**-40.68978**	**33.27707**	**24.98354**
H	**-42.81930**	**35.10392**	**24.18355**
C	**-41.69230**	**36.90942**	**24.13095**
C	**-43.50056**	**36.25655**	**22.50897**
H	**-42.89876**	**33.53219**	**21.14615**
C	**-43.55675**	**32.90571**	**23.06777**
C	**-41.68308**	**31.89474**	**21.76109**
C	**-40.04012**	**38.73683**	**21.48372**
C	**-42.19588**	**39.36082**	**20.37419**
C	**-37.88112**	**38.50876**	**22.73306**
H	**-41.49169**	**37.47778**	**17.99335**
H	**-41.14711**	**38.47058**	**16.55969**
H	**-41.19573**	**36.71376**	**16.42173**
H	**-39.27604**	**38.90795**	**19.08924**
H	**-37.85121**	**38.91473**	**18.03719**
H	**-39.34856**	**39.66349**	**17.48965**
H	**-35.17115**	**35.04348**	**18.27662**
H	**-36.52196**	**34.11237**	**18.94677**
H	**-36.37716**	**34.34833**	**17.19525**
H	**-37.03045**	**37.84828**	**19.68137**
H	**-36.62463**	**36.30587**	**20.42328**
H	**-35.44504**	**37.12116**	**19.37392**
H	**-38.94564**	**34.26874**	**14.83321**
H	**-39.14860**	**35.99296**	**15.11894**
H	**-37.62944**	**35.19279**	**15.55760**
H	**-37.94434**	**33.00265**	**17.13960**
H	**-39.34458**	**32.94617**	**18.20327**
H	**-39.53546**	**32.62650**	**16.47368**
H	**-38.49121**	**35.35724**	**23.28672**
H	**-39.23254**	**35.54433**	**24.88182**
H	**-38.10782**	**34.21773**	**24.59747**
H	**-41.33325**	**32.42138**	**24.76774**
H	**-39.89707**	**32.92386**	**25.65523**
H	**-41.27670**	**34.01798**	**25.53881**
H	**-41.00102**	**36.56773**	**24.90545**

H	**-41.14563**	**37.55574**	**23.43822**
H	**-42.45753**	**37.52266**	**24.62438**
H	**-44.06117**	**35.44845**	**22.02932**
H	**-44.21118**	**36.84297**	**23.10482**
H	**-43.10532**	**36.89137**	**21.71433**
H	**-44.16732**	**32.09113**	**22.65813**
H	**-43.19287**	**32.57504**	**24.04364**
H	**-44.22442**	**33.75532**	**23.22774**
H	**-40.85911**	**32.04156**	**21.06245**
H	**-41.27320**	**31.43767**	**22.66888**
H	**-42.38172**	**31.17445**	**21.31861**
H	**-40.02038**	**39.76888**	**21.81633**
H	**-42.22656**	**39.50626**	**19.28793**
H	**-43.18377**	**38.99593**	**20.67606**
H	**-42.00926**	**40.32493**	**20.85310**
H	**-36.90798**	**38.36703**	**22.25013**
H	**-38.03202**	**39.57238**	**22.93142**
H	**-37.84792**	**37.97099**	**23.68794**
C	**-24.19180**	**22.72621**	**25.52982**
C	**-23.09755**	**21.93064**	**25.94624**
C	**-23.00182**	**20.57404**	**25.56595**
C	**-22.08012**	**22.48348**	**26.74616**
C	**-21.91227**	**19.82418**	**25.99248**
O	**-24.00087**	**20.11436**	**24.77136**
C	**-20.99918**	**21.72488**	**27.17025**
H	**-22.17393**	**23.52725**	**27.02253**
H	**-21.82921**	**18.78470**	**25.69799**
C	**-20.89315**	**20.35955**	**26.79704**
C	**-23.99974**	**18.75396**	**24.35632**
O	**-20.00421**	**22.19798**	**27.97525**
C	**-19.74496**	**19.57525**	**27.25503**
C	**-24.51575**	**17.81404**	**25.43000**
H	**-23.00020**	**18.46450**	**24.00717**
H	**-24.66505**	**18.73680**	**23.48855**
C	**-19.96234**	**23.57898**	**28.30410**
C	**-19.57520**	**18.23871**	**27.11572**
H	**-18.98690**	**20.17124**	**27.75392**
H	**-23.87318**	**17.81394**	**26.31586**
H	**-25.52440**	**18.10767**	**25.73753**

H	-24.55855	16.79171	25.03882
C	-19.43526	24.43772	27.16908
H	-20.94806	23.91946	28.64744
H	-19.28597	23.63144	29.16185
H	-20.39853	17.71071	26.61521
Ru	-18.22317	16.82353	27.60694
H	-20.08554	24.39726	26.28998
H	-19.36439	25.48145	27.49376
H	-18.43677	24.10041	26.87286
C	-17.00068	17.93529	28.32642
P	-17.13129	17.20622	25.41648
P	-19.30036	16.67985	29.84833
O	-17.06577	14.97783	27.93832
O	-19.67194	15.47579	26.76809
O	-16.17035	18.60541	28.80560
C	-15.88890	15.92688	24.80771
C	-18.19451	17.39464	23.87116
C	-15.97231	18.70044	25.43650
C	-21.11889	17.14708	29.81309
C	-19.16856	15.11354	30.86852
C	-18.52717	17.91772	31.05573
C	-17.37714	13.79013	27.63057
C	-19.63237	14.21434	26.64117
H	-15.45939	16.38950	23.91041
C	-14.75887	15.71152	25.81610
C	-16.49838	14.60245	24.35098
H	-17.50927	17.14370	23.04808
C	-18.73259	18.80484	23.62550
C	-19.36249	16.40725	23.83983
H	-15.27829	18.42361	26.24077
C	-15.14633	18.89964	24.16074
C	-16.59800	20.03170	25.85541
H	-21.06595	18.17128	29.42043
C	-21.95158	16.33602	28.81620
C	-21.82841	17.17929	31.16715
H	-19.62018	15.37902	31.83327
C	-19.93841	13.91478	30.32065
C	-17.70022	14.75320	31.10993
H	-17.45636	17.82914	30.83703

C	**-18.69008**	**17.66514**	**32.55917**
C	**-18.93924**	**19.35468**	**30.73598**
C	**-18.57510**	**13.37333**	**27.02027**
C	**-16.34072**	**12.74089**	**27.95616**
C	**-20.86444**	**13.59540**	**26.02862**
H	**-15.14747**	**15.36439**	**26.77730**
H	**-14.06371**	**14.95594**	**25.42885**
H	**-14.17774**	**16.62284**	**25.99153**
H	**-17.10812**	**14.12515**	**25.12242**
H	**-17.11601**	**14.72775**	**23.45656**
H	**-15.68811**	**13.91092**	**24.08680**
H	**-19.41048**	**18.77908**	**22.76277**
H	**-19.29715**	**19.17678**	**24.48601**
H	**-17.94258**	**19.52287**	**23.39432**
H	**-19.06071**	**15.37407**	**24.02231**
H	**-20.10799**	**16.66558**	**24.59590**
H	**-19.83950**	**16.45254**	**22.85246**
H	**-14.57117**	**19.82889**	**24.25414**
H	**-14.42648**	**18.09619**	**23.98348**
H	**-15.77491**	**18.99726**	**23.26877**
H	**-17.17548**	**20.48946**	**25.04897**
H	**-17.25533**	**19.93263**	**26.71643**
H	**-15.79229**	**20.72796**	**26.11927**
H	**-21.43944**	**16.19068**	**27.86371**
H	**-22.21118**	**15.35003**	**29.21535**
H	**-22.89470**	**16.86598**	**28.63174**
H	**-21.41842**	**17.93007**	**31.84591**
H	**-22.88519**	**17.42895**	**31.00854**
H	**-21.79882**	**16.20636**	**31.67134**
H	**-21.01693**	**14.09127**	**30.30072**
H	**-19.61342**	**13.64266**	**29.31229**
H	**-19.76186**	**13.04923**	**30.97239**
H	**-17.13615**	**15.56083**	**31.58631**
H	**-17.64175**	**13.87730**	**31.76821**
H	**-17.19790**	**14.51829**	**30.16996**
H	**-18.14320**	**18.45077**	**33.09570**
H	**-19.73060**	**17.71550**	**32.88921**
H	**-18.27859**	**16.70841**	**32.88876**
H	**-18.84954**	**19.58987**	**29.67514**

H	**-19.97565**	**19.54978**	**31.03412**
H	**-18.30156**	**20.04977**	**31.29539**
H	**-18.69354**	**12.31186**	**26.83231**
H	**-15.41661**	**12.96145**	**27.40942**
H	**-16.09761**	**12.77824**	**29.02396**
H	**-16.66959**	**11.73067**	**27.70129**
H	**-21.07074**	**14.06656**	**25.06130**
H	**-20.76900**	**12.51604**	**25.88957**
H	**-21.72789**	**13.79472**	**26.67429**

Table S8 I Atomic coordinates of **PyrDPE-Ru$_{acac}^{+}$** from its DFT structure.

C	**-32.92946**	**28.90452**	**22.51574**
C	**-25.22339**	**23.38164**	**25.28980**
C	**-31.82455**	**28.11309**	**22.90643**
C	**-31.81354**	**26.73038**	**22.64688**
C	**-30.72863**	**28.70576**	**23.56036**
C	**-30.73302**	**25.93792**	**23.02884**
H	**-32.66126**	**26.27752**	**22.14077**
C	**-29.63257**	**27.94269**	**23.95734**
H	**-30.74295**	**29.77374**	**23.75794**
C	**-29.62402**	**26.54060**	**23.69377**
C	**-30.69859**	**24.52420**	**22.77446**
C	**-28.50341**	**28.52434**	**24.62907**
C	**-28.51889**	**25.74956**	**24.09178**
C	**-29.63843**	**23.76622**	**23.15439**
H	**-31.54638**	**24.07067**	**22.26747**
C	**-27.44489**	**27.76571**	**25.01226**
H	**-28.51497**	**29.59319**	**24.82616**
C	**-28.50966**	**24.34774**	**23.82689**
C	**-27.41152**	**26.35158**	**24.76000**
H	**-29.62602**	**22.69768**	**22.95561**
H	**-26.59765**	**28.21903**	**25.52035**
C	**-27.41465**	**23.58426**	**24.22599**
C	**-26.33419**	**25.55787**	**25.14837**
C	**-26.32274**	**24.17532**	**24.88802**
H	**-27.39997**	**22.51643**	**24.02762**
H	**-25.48897**	**26.00979**	**25.65948**
C	**-33.87961**	**29.59559**	**22.18480**
C	**-34.98580**	**30.37409**	**21.80108**
C	**-34.98926**	**31.78057**	**22.02451**
C	**-36.10093**	**29.77473**	**21.18802**
C	**-36.08987**	**32.52490**	**21.63930**
O	**-33.87058**	**32.27303**	**22.59270**
C	**-37.19955**	**30.52642**	**20.80443**
H	**-36.06943**	**28.70408**	**21.02663**
H	**-36.09938**	**33.59480**	**21.80668**
C	**-37.21612**	**31.94113**	**21.02332**
C	**-33.77188**	**33.66861**	**22.87033**
O	**-38.31320**	**30.01208**	**20.23688**

C	-38.37065	32.69698	20.60244
C	-34.48901	34.05683	24.14880
H	-34.12396	34.24789	22.00785
H	-32.69780	33.84538	22.96791
C	-38.37429	28.62571	19.90882
C	-38.57951	34.03906	20.78976
H	-39.12107	32.10443	20.09067
H	-35.56778	33.88501	24.08305
H	-34.09937	33.47879	24.99238
H	-34.32485	35.11990	24.35449
C	-37.63226	28.30150	18.62676
H	-38.01945	28.02429	20.75455
H	-39.44246	28.42739	19.79152
H	-37.77877	34.56434	21.32704
Ru	-39.98880	35.37668	20.39652
H	-36.55973	28.50109	18.71083
H	-37.76405	27.24202	18.38329
H	-38.02960	28.89702	17.79888
C	-41.07019	34.28870	19.43541
P	-38.81624	35.91276	18.26359
P	-41.20311	34.64069	22.46010
O	-41.26495	37.14274	20.18728
O	-38.74216	36.68250	21.54428
O	-41.80769	33.64108	18.80621
C	-39.34555	37.45847	17.32811
C	-36.94672	36.13732	18.28618
C	-39.17337	34.64696	16.90486
C	-40.03928	33.90952	23.73943
C	-42.34089	35.81581	23.37114
C	-42.41274	33.24012	22.06629
C	-41.05626	38.31314	20.62869
C	-38.89639	37.91227	21.82036
H	-38.80082	37.37751	16.37954
C	-40.84283	37.44459	17.01338
C	-38.90613	38.78177	17.95316
H	-36.74287	36.71095	17.37021
C	-36.14463	34.83716	18.21979
C	-36.46259	36.95712	19.48365
H	-40.26425	34.72688	16.81138

C	**-38.56697**	**34.98687**	**15.53806**
C	**-38.88426**	**33.18513**	**17.24734**
H	**-39.59119**	**33.08197**	**23.17284**
C	**-38.89309**	**34.84067**	**24.14545**
C	**-40.70242**	**33.33602**	**24.99258**
H	**-42.79663**	**35.18934**	**24.14911**
C	**-41.64881**	**36.98106**	**24.07321**
C	**-43.45590**	**36.31924**	**22.45049**
H	**-42.87636**	**33.57618**	**21.13086**
C	**-43.55505**	**32.97778**	**23.05486**
C	**-41.68819**	**31.92661**	**21.77165**
C	**-39.95874**	**38.72832**	**21.40416**
C	**-42.09878**	**39.33982**	**20.26018**
C	**-37.82041**	**38.50982**	**22.69056**
H	**-41.44163**	**37.40197**	**17.92695**
H	**-41.10664**	**38.35896**	**16.46776**
H	**-41.12719**	**36.59944**	**16.37816**
H	**-39.23590**	**38.89920**	**18.98832**
H	**-37.81895**	**38.90033**	**17.92650**
H	**-39.33244**	**39.60662**	**17.36874**
H	**-35.07971**	**35.07365**	**18.33670**
H	**-36.42224**	**34.14677**	**19.02262**
H	**-36.25792**	**34.31808**	**17.26567**
H	**-37.00637**	**37.89443**	**19.61639**
H	**-36.56417**	**36.38718**	**20.41055**
H	**-35.40206**	**37.19888**	**19.34046**
H	**-38.77475**	**34.16173**	**14.84651**
H	**-38.99153**	**35.88959**	**15.09145**
H	**-37.47899**	**35.10611**	**15.58057**
H	**-37.81574**	**32.95935**	**17.25598**
H	**-39.29275**	**32.89338**	**18.21232**
H	**-39.34900**	**32.55209**	**16.48160**
H	**-38.46089**	**35.37328**	**23.29682**
H	**-39.21962**	**35.58408**	**24.87951**
H	**-38.10718**	**34.24246**	**24.62320**
H	**-41.35310**	**32.48502**	**24.78071**
H	**-39.92012**	**32.98277**	**25.67595**
H	**-41.28558**	**34.09063**	**25.53260**
H	**-40.96382**	**36.64525**	**24.85556**

H	-41.09443	37.61234	23.37324
H	-42.41074	37.60761	24.55407
H	-44.02585	35.50917	21.98593
H	-44.16004	36.92669	23.03216
H	-43.05087	36.93283	21.64464
H	-44.17836	32.17346	22.64493
H	-43.20182	32.64419	24.03341
H	-44.20732	33.84021	23.20767
H	-40.87038	32.04787	21.06092
H	-41.27663	31.48084	22.68402
H	-42.39881	31.20764	21.34739
H	-39.93692	39.76665	21.71569
H	-42.10867	39.46933	19.17152
H	-43.09318	38.98241	20.54862
H	-41.91685	40.30991	20.72809
H	-36.84030	38.34665	22.22926
H	-37.96377	39.57897	22.86136
H	-37.81150	37.99406	23.65802
C	-24.28068	22.68746	25.63513
C	-23.18818	21.90322	26.04581
C	-23.13924	20.51499	25.73232
C	-22.12805	22.48051	26.76790
C	-22.05468	19.76431	26.14959
O	-24.18377	20.05216	25.01691
C	-21.04416	21.72304	27.18092
H	-22.18986	23.53913	26.98887
H	-22.01392	18.70675	25.92015
C	-20.98229	20.32649	26.87259
C	-24.23543	18.67603	24.64565
O	-20.00567	22.20772	27.89786
C	-19.83411	19.56787	27.30678
C	-24.73641	17.79096	25.77041
H	-23.25661	18.35204	24.27085
H	-24.93280	18.65300	23.80445
C	-19.92446	23.60147	28.18758
C	-19.62536	18.22603	27.11905
H	-19.08528	20.15981	27.82161
H	-24.06045	17.79862	26.63091
H	-25.72317	18.12534	26.10517

H	-24.82456	16.75882	25.41500
C	-19.42828	24.40996	27.00449
H	-20.89013	23.96470	28.55979
H	-19.21251	23.65967	29.01452
H	-20.43121	17.69870	26.59151
Ru	-18.24515	16.87411	27.56453
H	-20.11722	24.36147	26.15581
H	-19.31930	25.45989	27.29590
H	-18.45154	24.04032	26.67692
C	-17.03637	18.01358	28.28299
P	-17.18005	17.31558	25.35356
P	-19.26443	16.63638	29.83970
O	-17.01329	15.08954	27.85109
O	-19.66098	15.49895	26.73901
O	-16.21581	18.69443	28.75465
C	-15.87226	16.10441	24.74776
C	-18.27590	17.44046	23.82703
C	-16.11387	18.87718	25.35977
C	-21.09007	17.07527	29.84548
C	-19.08863	15.04543	30.81137
C	-18.48204	17.85833	31.05524
C	-17.28218	13.89417	27.52442
C	-19.57464	14.24074	26.59186
H	-15.46936	16.59347	23.85247
C	-14.73077	15.95244	25.75523
C	-16.40711	14.75043	24.28336
H	-17.58326	17.24997	22.99425
C	-18.91660	18.81095	23.60479
C	-19.37034	16.37212	23.79566
H	-15.37487	18.63664	26.13509
C	-15.34855	19.13207	24.05571
C	-16.80039	20.16543	25.81496
H	-21.06204	18.11233	29.48447
C	-21.92814	16.27846	28.84172
C	-21.77332	17.05650	31.21345
H	-19.53153	15.28642	31.78660
C	-19.85037	13.84815	30.24921
C	-17.61385	14.69816	31.03068
H	-17.41457	17.78995	30.81369

C	**-18.61222**	**17.56666**	**32.55495**
C	**-18.92206**	**19.29613**	**30.77943**
C	**-18.47518**	**13.43963**	**26.93420**
C	**-16.19103**	**12.88749**	**27.79420**
C	**-20.79461**	**13.58329**	**25.99899**
H	**-15.09438**	**15.57906**	**26.71617**
H	**-13.99413**	**15.24055**	**25.36288**
H	**-14.20263**	**16.89503**	**25.93200**
H	**-17.00300**	**14.24041**	**25.04427**
H	**-17.01643**	**14.84429**	**23.37959**
H	**-15.55802**	**14.10303**	**24.03115**
H	**-19.59724**	**18.74600**	**22.74675**
H	**-19.50362**	**19.13118**	**24.47145**
H	**-18.18443**	**19.58896**	**23.37858**
H	**-18.99633**	**15.36257**	**23.97619**
H	**-20.13372**	**16.57673**	**24.55052**
H	**-19.84841**	**16.38484**	**22.80826**
H	**-14.81873**	**20.08835**	**24.13975**
H	**-14.59506**	**18.36943**	**23.84309**
H	**-16.01315**	**19.20610**	**23.18833**
H	**-17.49170**	**20.56052**	**25.06750**
H	**-17.35220**	**20.03873**	**26.74365**
H	**-16.02903**	**20.92630**	**25.98591**
H	**-21.43611**	**16.16907**	**27.87396**
H	**-22.16124**	**15.27685**	**29.21659**
H	**-22.88435**	**16.79593**	**28.69448**
H	**-21.36088**	**17.79226**	**31.90682**
H	**-22.83587**	**17.29577**	**31.08139**
H	**-21.72134**	**16.06927**	**31.68639**
H	**-20.93097**	**14.01078**	**30.24263**
H	**-19.53021**	**13.59648**	**29.23425**
H	**-19.65641**	**12.97498**	**30.88508**
H	**-17.04603**	**15.51178**	**31.49175**
H	**-17.54107**	**13.82756**	**31.69391**
H	**-17.12423**	**14.45689**	**30.08641**
H	**-18.06156**	**18.34413**	**33.09885**
H	**-19.64611**	**17.59900**	**32.90692**
H	**-18.18483**	**16.60648**	**32.85191**
H	**-18.84264**	**19.56520**	**29.72575**

H	**-19.95840**	**19.46605**	**31.09192**
H	**-18.29003**	**19.98531**	**31.35165**
H	**-18.55385**	**12.37755**	**26.73085**
H	**-15.32333**	**13.11990**	**27.16536**
H	**-15.86052**	**12.96352**	**28.83557**
H	**-16.50655**	**11.86165**	**27.59102**
H	**-21.03850**	**14.05560**	**25.04109**
H	**-20.66134**	**12.50999**	**25.84675**
H	**-21.65061**	**13.74377**	**26.66493**

Table S9 I Atomic coordinates of **PyrDPE-Ru$_{acac}^{2+}$ (S)** from its DFT structure.

C	**-33.00514**	**28.81162**	**22.56020**
C	**-25.26707**	**23.37776**	**25.30061**
C	**-31.90222**	**28.03348**	**22.94631**
C	**-31.87882**	**26.64860**	**22.67852**
C	**-30.81148**	**28.63912**	**23.60562**
C	**-30.79293**	**25.86924**	**23.05760**
H	**-32.72218**	**26.19195**	**22.16941**
C	**-29.71075**	**27.88761**	**23.99716**
H	**-30.84026**	**29.70583**	**23.80660**
C	**-29.68818**	**26.48353**	**23.72650**
C	**-30.74547**	**24.45609**	**22.79739**
C	**-28.58749**	**28.48108**	**24.67021**
C	**-28.57850**	**25.70594**	**24.11911**
C	**-29.67851**	**23.70874**	**23.17424**
H	**-31.58913**	**23.99693**	**22.28933**
C	**-27.52134**	**27.73346**	**25.04864**
H	**-28.61190**	**29.54879**	**24.87040**
C	**-28.55554**	**24.30191**	**23.84806**
C	**-27.47473**	**26.32006**	**24.78978**
H	**-29.65377**	**22.64122**	**22.97306**
H	**-26.67784**	**28.19246**	**25.55712**
C	**-27.45560**	**23.55003**	**24.24144**
C	**-26.39097**	**25.53997**	**25.17303**
C	**-26.36748**	**24.15494**	**24.90563**
H	**-27.42677**	**22.48333**	**24.04036**
H	**-25.54916**	**25.99603**	**25.68520**
C	**-33.95981**	**29.50336**	**22.22931**
C	**-35.05128**	**30.28262**	**21.84924**
C	**-35.05212**	**31.69338**	**22.12271**
C	**-36.15449**	**29.70324**	**21.19435**
C	**-36.13487**	**32.45503**	**21.74156**
O	**-33.94746**	**32.14501**	**22.73044**
C	**-37.23787**	**30.47198**	**20.81236**
H	**-36.12231**	**28.63877**	**20.99905**
H	**-36.14492**	**33.51725**	**21.94921**
C	**-37.25039**	**31.89372**	**21.07546**
C	**-33.82929**	**33.53166**	**23.06219**
O	**-38.33276**	**29.99532**	**20.20537**

C	-38.37433	32.65272	20.64286
C	-34.56033	33.87858	24.34358
H	-34.15962	34.14440	22.21508
H	-32.75408	33.68308	23.18050
C	-38.42133	28.61229	19.84588
C	-38.55825	34.01584	20.82377
H	-39.13153	32.07825	20.12215
H	-35.64065	33.72789	24.25604
H	-34.19193	33.26277	25.16949
H	-34.38212	34.93000	24.59174
C	-37.67012	28.30706	18.56590
H	-38.08838	27.99077	20.68478
H	-39.49222	28.44470	19.71372
H	-37.75098	34.51992	21.37069
Ru	-39.91269	35.35828	20.40394
H	-36.59441	28.47934	18.66730
H	-37.82335	27.25709	18.29635
H	-38.04491	28.93034	17.74836
C	-41.01117	34.29238	19.42471
P	-38.70875	35.87543	18.26949
P	-41.19840	34.67750	22.45708
O	-41.15167	37.12972	20.15943
O	-38.66163	36.63678	21.56347
O	-41.75566	33.66953	18.78467
C	-39.22946	37.41075	17.31565
C	-36.84104	36.09254	18.32804
C	-39.04317	34.59037	16.92385
C	-40.07168	33.91313	23.75024
C	-42.30887	35.89141	23.34791
C	-42.44103	33.31546	22.03720
C	-40.92690	38.30262	20.59199
C	-38.79792	37.87239	21.82788
H	-38.67926	37.31182	16.37217
C	-40.72457	37.39756	16.99002
C	-38.78467	38.74127	17.92182
H	-36.61833	36.64222	17.40201
C	-36.04508	34.78732	18.30801
C	-36.37486	36.93791	19.51467
H	-40.12839	34.68452	16.78811

C	**-38.38233**	**34.90076**	**15.57487**
C	**-38.78875**	**33.13068**	**17.30104**
H	**-39.64225**	**33.07060**	**23.19062**
C	**-38.90435**	**34.80867**	**24.17589**
C	**-40.77214**	**33.35943**	**24.99188**
H	**-42.78768**	**35.27516**	**24.12035**
C	**-41.59244**	**37.03655**	**24.05858**
C	**-43.40291**	**36.42529**	**22.41964**
H	**-42.88000**	**33.66824**	**21.09595**
C	**-43.60629**	**33.08754**	**23.00773**
C	**-41.75216**	**31.98072**	**21.75224**
C	**-39.83602**	**38.70366**	**21.38236**
C	**-41.93823**	**39.34514**	**20.18780**
C	**-37.73211**	**38.45373**	**22.71910**
H	**-41.33229**	**37.37590**	**17.89818**
H	**-40.97772**	**38.30282**	**16.42507**
H	**-41.00820**	**36.54294**	**16.36756**
H	**-39.11373**	**38.87735**	**18.95479**
H	**-37.69717**	**38.85541**	**17.89304**
H	**-39.20787**	**39.55775**	**17.32412**
H	**-34.98142**	**35.02281**	**18.43542**
H	**-36.33512**	**34.11970**	**19.12591**
H	**-36.14565**	**34.24167**	**17.36767**
H	**-36.92456**	**37.87465**	**19.62458**
H	**-36.48132**	**36.38370**	**20.45058**
H	**-35.31466**	**37.18297**	**19.37721**
H	**-38.59683**	**34.07794**	**14.88306**
H	**-38.76298**	**35.81307**	**15.10915**
H	**-37.29305**	**34.98405**	**15.64951**
H	**-37.72723**	**32.89918**	**17.41086**
H	**-39.29061**	**32.84504**	**18.22322**
H	**-39.18476**	**32.49411**	**16.50070**
H	**-38.44127**	**35.33176**	**23.33772**
H	**-39.22022**	**35.55906**	**24.90704**
H	**-38.14538**	**34.18547**	**24.66470**
H	**-41.45018**	**32.53365**	**24.76758**
H	**-40.01177**	**32.97581**	**25.68329**
H	**-41.33394**	**34.13264**	**25.52768**
H	**-40.92212**	**36.68277**	**24.84543**

H	**-41.01852**	**37.65645**	**23.36445**
H	**-42.34311**	**37.67941**	**24.53492**
H	**-43.97488**	**35.63306**	**21.92798**
H	**-44.10837**	**37.02802**	**23.00402**
H	**-42.97980**	**37.05296**	**21.63497**
H	**-44.25197**	**32.31039**	**22.58105**
H	**-43.28012**	**32.73269**	**23.98810**
H	**-44.22875**	**33.97192**	**23.15818**
H	**-40.92718**	**32.07412**	**21.04510**
H	**-41.36089**	**31.52514**	**22.66850**
H	**-42.48008**	**31.28231**	**21.32372**
H	**-39.80059**	**39.74410**	**21.68495**
H	**-41.87755**	**39.50315**	**19.10429**
H	**-42.95114**	**38.98913**	**20.40231**
H	**-41.77751**	**40.30159**	**20.68989**
H	**-36.74312**	**38.24669**	**22.29646**
H	**-37.84561**	**39.53048**	**22.86066**
H	**-37.77490**	**37.96155**	**23.69799**
C	**-24.31314**	**22.69158**	**25.64503**
C	**-23.22304**	**21.92261**	**26.04899**
C	**-23.19337**	**20.51489**	**25.76124**
C	**-22.14671**	**22.51219**	**26.73846**
C	**-22.11456**	**19.76356**	**26.17307**
O	**-24.25524**	**20.06245**	**25.08222**
C	**-21.06505**	**21.75499**	**27.14708**
H	**-22.19723**	**23.57567**	**26.93545**
H	**-22.09130**	**18.70012**	**25.97333**
C	**-21.01988**	**20.33762**	**26.86309**
C	**-24.34560**	**18.67825**	**24.73230**
O	**-20.01321**	**22.23408**	**27.82392**
C	**-19.87845**	**19.60048**	**27.28627**
C	**-24.85221**	**17.82912**	**25.88066**
H	**-23.37899**	**18.32903**	**24.35034**
H	**-25.05463**	**18.66264**	**23.90159**
C	**-19.90676**	**23.63299**	**28.10951**
C	**-19.65589**	**18.24573**	**27.08521**
H	**-19.12947**	**20.18949**	**27.80226**
H	**-24.16354**	**17.83289**	**26.73098**
H	**-25.82509**	**18.19459**	**26.22276**

H	-24.97197	16.79425	25.54371
C	-19.40880	24.42031	26.91456
H	-20.86463	24.00737	28.48787
H	-19.18639	23.67820	28.92889
H	-20.45537	17.72104	26.54609
Ru	-18.28248	16.93204	27.53195
H	-20.10836	24.38043	26.07420
H	-19.27708	25.46917	27.19924
H	-18.44264	24.03049	26.57990
C	-17.08921	18.08072	28.27848
P	-17.15950	17.38582	25.33832
P	-19.31756	16.64321	29.80623
O	-17.03226	15.17822	27.83167
O	-19.66698	15.55008	26.68269
O	-16.28068	18.76091	28.76386
C	-15.77806	16.22357	24.80857
C	-18.22563	17.43780	23.78934
C	-16.17237	18.99980	25.33517
C	-21.14807	17.06094	29.78977
C	-19.12891	15.04043	30.75236
C	-18.55944	17.86216	31.03779
C	-17.27003	13.98118	27.47969
C	-19.55424	14.29500	26.51769
H	-15.34905	16.73056	23.93633
C	-14.68318	16.11905	25.87279
C	-16.22971	14.85014	24.31312
H	-17.49953	17.30505	22.97414
C	-18.95747	18.76118	23.56383
C	-19.24313	16.29739	23.72281
H	-15.40287	18.79751	26.09150
C	-15.45033	19.29345	24.01383
C	-16.91348	20.25056	25.80841
H	-21.12840	18.10321	29.44225
C	-21.96672	16.26421	28.76996
C	-21.84540	17.01983	31.15032
H	-19.59099	15.26518	31.72266
C	-19.86608	13.84034	30.16410
C	-17.65331	14.71136	30.99353
H	-17.48841	17.80499	30.80930

C	**-18.70649**	**17.55262**	**32.53260**
C	**-19.01036**	**19.29837**	**30.77162**
C	**-18.44106**	**13.51329**	**26.85942**
C	**-16.16425**	**12.99462**	**27.75684**
C	**-20.75568**	**13.62238**	**25.90758**
H	**-15.07288**	**15.71510**	**26.81043**
H	**-13.89255**	**15.45150**	**25.50947**
H	**-14.21321**	**17.08465**	**26.08495**
H	**-16.84969**	**14.31245**	**25.03450**
H	**-16.78492**	**14.92211**	**23.37342**
H	**-15.34052**	**14.23978**	**24.11371**
H	**-19.60450**	**18.65865**	**22.68411**
H	**-19.59634**	**19.02175**	**24.41408**
H	**-18.28181**	**19.59716**	**23.37294**
H	**-18.81227**	**15.31531**	**23.92654**
H	**-20.04975**	**16.45794**	**24.44267**
H	**-19.67907**	**16.27261**	**22.71665**
H	**-14.92840**	**20.25285**	**24.10731**
H	**-14.69452**	**18.54680**	**23.75872**
H	**-16.14078**	**19.38255**	**23.16908**
H	**-17.71527**	**20.55439**	**25.13231**
H	**-17.33966**	**20.12813**	**26.80178**
H	**-16.19479**	**21.07717**	**25.86224**
H	**-21.46722**	**16.16809**	**27.80472**
H	**-22.19159**	**15.25694**	**29.13369**
H	**-22.92738**	**16.77214**	**28.62050**
H	**-21.45029**	**17.75376**	**31.85533**
H	**-22.90907**	**17.24688**	**31.00783**
H	**-21.78664**	**16.02856**	**31.61336**
H	**-20.94820**	**13.98939**	**30.13874**
H	**-19.52371**	**13.60117**	**29.15360**
H	**-19.67306**	**12.96457**	**30.79614**
H	**-17.10317**	**15.52842**	**31.46923**
H	**-17.58232**	**13.83793**	**31.65272**
H	**-17.14423**	**14.48058**	**30.05734**
H	**-18.16665**	**18.32720**	**33.09078**
H	**-19.74454**	**17.57531**	**32.87232**
H	**-18.27672**	**16.59198**	**32.82390**
H	**-18.91235**	**19.58416**	**29.72367**

H	**-20.05366**	**19.45430**	**31.06708**
H	**-18.39561**	**19.98602**	**31.36361**
H	**-18.49448**	**12.45320**	**26.63932**
H	**-15.29000**	**13.25331**	**27.14769**
H	**-15.85451**	**13.06314**	**28.80494**
H	**-16.45522**	**11.96589**	**27.53375**
H	**-21.01004**	**14.10963**	**24.96009**
H	**-20.59520**	**12.55657**	**25.73232**
H	**-21.61585**	**13.74634**	**26.57599**

Table S20 I Atomic coordinates of **PyrDPE-Ru$_{acac}^{2+}$ (T)** from its DFT structure.

C	**-33.01327**	**28.81839**	**22.53218**
C	**-25.24740**	**23.36632**	**25.27662**
C	**-31.89877**	**28.03222**	**22.91986**
C	**-31.88566**	**26.64985**	**22.67121**
C	**-30.80366**	**28.64004**	**23.55641**
C	**-30.79534**	**25.86652**	**23.05081**
H	**-32.73563**	**26.18801**	**22.17760**
C	**-29.69716**	**27.88649**	**23.94835**
H	**-30.82338**	**29.70953**	**23.74424**
C	**-29.68512**	**26.48364**	**23.69722**
C	**-30.75652**	**24.45108**	**22.81060**
C	**-28.56486**	**28.48245**	**24.60054**
C	**-28.56828**	**25.70147**	**24.09155**
C	**-29.68808**	**23.70292**	**23.18759**
H	**-31.60699**	**23.98753**	**22.31764**
C	**-27.49678**	**27.73419**	**24.97819**
H	**-28.58105**	**29.55298**	**24.78709**
C	**-28.55625**	**24.29851**	**23.84096**
C	**-27.45884**	**26.31851**	**24.73933**
H	**-29.67176**	**22.63249**	**23.00046**
H	**-26.64628**	**28.19761**	**25.47120**
C	**-27.45126**	**23.54433**	**24.23640**
C	**-26.37076**	**25.53446**	**25.12345**
C	**-26.35841**	**24.15160**	**24.87718**
H	**-27.43221**	**22.47459**	**24.04992**
H	**-25.52218**	**25.99588**	**25.61985**
C	**-33.96395**	**29.50833**	**22.20611**
C	**-35.06534**	**30.29782**	**21.82767**
C	**-35.05436**	**31.70671**	**22.08983**
C	**-36.17128**	**29.71802**	**21.19252**
C	**-36.13828**	**32.46977**	**21.71539**
O	**-33.93751**	**32.15887**	**22.68184**
C	**-37.26228**	**30.49016**	**20.81306**
H	**-36.14601**	**28.65189**	**21.00562**
H	**-36.14222**	**33.53362**	**21.91506**
C	**-37.26368**	**31.90605**	**21.06622**
C	**-33.81408**	**33.54633**	**23.00164**
O	**-38.36267**	**30.00632**	**20.22153**

C	-38.38930	32.67157	20.64220
C	-34.53316	33.90681	24.28640
H	-34.14971	34.15455	22.15287
H	-32.73768	33.69784	23.11007
C	-38.45204	28.62118	19.86791
C	-38.56779	34.03877	20.81766
H	-39.15666	32.09841	20.13440
H	-35.61456	33.75719	24.21022
H	-34.15881	33.29714	25.11425
H	-34.35117	34.95997	24.52446
C	-37.71146	28.31237	18.58293
H	-38.11172	28.00309	20.70615
H	-39.52387	28.45204	19.74579
H	-37.75527	34.54605	21.35273
Ru	-39.93145	35.36030	20.39686
H	-36.63489	28.48470	18.67534
H	-37.86669	27.26165	18.31743
H	-38.09260	28.93337	17.76655
C	-41.03160	34.27264	19.43647
P	-38.73951	35.86719	18.24617
P	-41.19887	34.70240	22.47846
O	-41.19702	37.10136	20.13199
O	-38.69109	36.66333	21.53074
O	-41.77725	33.64069	18.80959
C	-39.27560	37.39320	17.28703
C	-36.87337	36.09531	18.30108
C	-39.07187	34.56822	16.91439
C	-40.05341	33.93511	23.75253
C	-42.28758	35.91884	23.39311
C	-42.45258	33.34615	22.07508
C	-40.99152	38.28136	20.55763
C	-38.85152	37.89748	21.79062
H	-38.72380	37.29471	16.34437
C	-40.77028	37.36536	16.96018
C	-38.84262	38.72977	17.88859
H	-36.65765	36.63877	17.36977
C	-36.06896	34.79518	18.28793
C	-36.40801	36.95370	19.47876
H	-40.15760	34.65658	16.77847

C	**-38.41301**	**34.87189**	**15.56280**
C	**-38.81044**	**33.11284**	**17.30382**
H	**-39.63898**	**33.08764**	**23.18934**
C	**-38.87414**	**34.82576**	**24.15577**
C	**-40.73657**	**33.38940**	**25.00737**
H	**-42.75495**	**35.29207**	**24.16399**
C	**-41.55972**	**37.05323**	**24.10941**
C	**-43.39765**	**36.47082**	**22.49522**
H	**-42.89607**	**33.69460**	**21.13432**
C	**-43.61232**	**33.13401**	**23.05552**
C	**-41.77285**	**32.00519**	**21.79611**
C	**-39.90969**	**38.70461**	**21.34777**
C	**-42.01100**	**39.30758**	**20.13420**
C	**-37.79220**	**38.50408**	**22.67187**
H	**-41.37956**	**37.34238**	**17.86723**
H	**-41.03000**	**38.26638**	**16.39163**
H	**-41.04574**	**36.50639**	**16.34018**
H	**-39.17259**	**38.86684**	**18.92118**
H	**-37.75639**	**38.85413**	**17.85881**
H	**-39.27370**	**39.53994**	**17.28806**
H	**-35.00634**	**35.03987**	**18.40538**
H	**-36.34685**	**34.13345**	**19.11471**
H	**-36.17179**	**34.23941**	**17.35385**
H	**-36.96275**	**37.88799**	**19.58295**
H	**-36.50581**	**36.40732**	**20.42016**
H	**-35.35014**	**37.20407**	**19.33392**
H	**-38.62978**	**34.04613**	**14.87539**
H	**-38.79373**	**35.78240**	**15.09374**
H	**-37.32359**	**34.95430**	**15.63491**
H	**-37.74940**	**32.89028**	**17.43403**
H	**-39.32811**	**32.82642**	**18.21709**
H	**-39.18704**	**32.46905**	**16.50004**
H	**-38.42838**	**35.35292**	**23.31081**
H	**-39.17162**	**35.57276**	**24.89784**
H	**-38.10579**	**34.19824**	**24.62358**
H	**-41.43132**	**32.57403**	**24.79625**
H	**-39.96737**	**32.99362**	**25.68183**
H	**-41.27522**	**34.17000**	**25.55593**
H	**-40.87546**	**36.68997**	**24.87954**

H	-41.00072	37.68525	23.41402
H	-42.30394	37.68682	24.60770
H	-43.93738	35.69477	21.94475
H	-44.12689	37.00590	23.11493
H	-42.99704	37.16916	21.76057
H	-44.25999	32.34977	22.64532
H	-43.28092	32.79586	24.04015
H	-44.23379	34.02122	23.19320
H	-40.94817	32.08803	21.08702
H	-41.38396	31.55149	22.71417
H	-42.50602	31.30998	21.37170
H	-39.89356	39.74706	21.64493
H	-41.86903	39.53187	19.06963
H	-43.02234	38.90443	20.24425
H	-41.92464	40.23934	20.69751
H	-36.80161	38.30870	22.24759
H	-37.92286	39.58007	22.80357
H	-37.82397	38.02055	23.65551
C	-24.29872	22.68216	25.62021
C	-23.20007	21.90400	26.02910
C	-23.18058	20.49761	25.75471
C	-22.12455	22.49566	26.70418
C	-22.10352	19.74544	26.16974
O	-24.25028	20.04324	25.08262
C	-21.03750	21.73610	27.11837
H	-22.16955	23.56121	26.89100
H	-22.08527	18.67970	25.98117
C	-21.00356	20.32340	26.84962
C	-24.35207	18.65471	24.76059
O	-19.98292	22.22450	27.78487
C	-19.86360	19.58035	27.27515
C	-24.85615	17.83009	25.92812
H	-23.39100	18.28991	24.37820
H	-25.06690	18.62636	23.93499
C	-19.87233	23.62754	28.05034
C	-19.64508	18.22100	27.08586
H	-19.11035	20.16940	27.78520
H	-24.16354	17.84955	26.77511
H	-25.82583	18.20649	26.26757

H	-24.98130	16.78865	25.61405
C	-19.37777	24.39683	26.84268
H	-20.82730	24.00953	28.42798
H	-19.14842	23.68220	28.86605
H	-20.44439	17.69119	26.55218
Ru	-18.26940	16.92671	27.55056
H	-20.08181	24.34783	26.00648
H	-19.24122	25.44910	27.11216
H	-18.41458	23.99938	26.50829
C	-17.08529	18.09117	28.29535
P	-17.13723	17.36958	25.35023
P	-19.31610	16.64735	29.83011
O	-17.00209	15.19488	27.87521
O	-19.63472	15.52622	26.71020
O	-16.28313	18.77690	28.78007
C	-15.74755	16.21034	24.83689
C	-18.20489	17.39980	23.80240
C	-16.16245	18.99075	25.33543
C	-21.14931	17.04965	29.79526
C	-19.11636	15.05354	30.78825
C	-18.57289	17.88419	31.05228
C	-17.22607	13.99062	27.53405
C	-19.50862	14.27046	26.55869
H	-15.32042	16.71288	23.96120
C	-14.65397	16.12337	25.90404
C	-16.18858	14.82982	24.35187
H	-17.47696	17.26536	22.98916
C	-18.94660	18.71547	23.56436
C	-19.21337	16.25095	23.74573
H	-15.38832	18.79978	26.09000
C	-15.44746	19.27868	24.00882
C	-16.91156	20.23953	25.80180
H	-21.13719	18.08867	29.43778
C	-21.95409	16.23436	28.77914
C	-21.85402	17.01633	31.15235
H	-19.58704	15.28251	31.75344
C	-19.83742	13.84078	30.20613
C	-17.63893	14.74219	31.04146
H	-17.50004	17.83165	30.83118

C	**-18.72758**	**17.58760**	**32.54904**
C	**-19.03227**	**19.31463**	**30.76999**
C	**-18.38855**	**13.50439**	**26.91376**
C	**-16.11091**	**13.02005**	**27.82640**
C	**-20.70042**	**13.57993**	**25.95094**
H	**-15.04192**	**15.72695**	**26.84557**
H	**-13.85936**	**15.45654**	**25.54843**
H	**-14.18952**	**17.09361**	**26.10659**
H	**-16.80175**	**14.29102**	**25.07817**
H	**-16.74619**	**14.89040**	**23.41286**
H	**-15.29409**	**14.22665**	**24.15474**
H	**-19.58778**	**18.60077**	**22.68198**
H	**-19.59334**	**18.97604**	**24.40857**
H	**-18.27785**	**19.55637**	**23.37109**
H	**-18.77522**	**15.27400**	**23.95824**
H	**-20.02215**	**16.41204**	**24.46297**
H	**-19.64795**	**16.21399**	**22.73950**
H	**-14.92544**	**20.23851**	**24.09602**
H	**-14.69249**	**18.53150**	**23.75303**
H	**-16.14209**	**19.36414**	**23.16730**
H	**-17.73471**	**20.51867**	**25.14100**
H	**-17.30878**	**20.13134**	**26.80885**
H	**-16.20464**	**21.07756**	**25.82195**
H	**-21.44943**	**16.13440**	**27.81703**
H	**-22.17006**	**15.22848**	**29.15172**
H	**-22.91921**	**16.73050**	**28.62023**
H	**-21.46944**	**17.76093**	**31.85189**
H	**-22.91850**	**17.23300**	**31.00077**
H	**-21.78987**	**16.03039**	**31.62576**
H	**-20.92061**	**13.97875**	**30.16994**
H	**-19.48389**	**13.59396**	**29.20144**
H	**-19.64127**	**12.97397**	**30.84931**
H	**-17.09959**	**15.56939**	**31.51186**
H	**-17.56366**	**13.87646**	**31.71009**
H	**-17.12184**	**14.50612**	**30.11102**
H	**-18.19267**	**18.36873**	**33.10266**
H	**-19.76750**	**17.61122**	**32.88277**
H	**-18.29693**	**16.63093**	**32.85171**
H	**-18.92151**	**19.59518**	**29.72193**

H	**-20.08062**	**19.46420**	**31.05009**
H	**-18.43107**	**20.01108**	**31.36540**
H	**-18.42951**	**12.44165**	**26.70432**
H	**-15.24004**	**13.27691**	**27.21160**
H	**-15.80038**	**13.10945**	**28.87261**
H	**-16.39227**	**11.98514**	**27.62062**
H	**-20.95817**	**14.05718**	**24.99936**
H	**-20.52723**	**12.51482**	**25.78438**
H	**-21.56339**	**13.69914**	**26.61657**

Table S31 I Atomic coordinates of **PyrDPE-Ru$_{acac}^{2+}$ (OSS)** from its DFT structure.

C	**-33.01724**	**28.80384**	**22.57849**
C	**-25.28789**	**23.36961**	**25.34255**
C	**-31.91658**	**28.02518**	**22.96985**
C	**-31.89087**	**26.64093**	**22.69894**
C	**-30.83029**	**28.62980**	**23.63738**
C	**-30.80669**	**25.86133**	**23.08239**
H	**-32.73087**	**26.18507**	**22.18363**
C	**-29.73154**	**27.87796**	**24.03379**
H	**-30.86094**	**29.69601**	**23.84081**
C	**-29.70630**	**26.47464**	**23.75936**
C	**-30.75656**	**24.44897**	**22.81847**
C	**-28.61283**	**28.47036**	**24.71530**
C	**-28.59809**	**25.69691**	**24.15582**
C	**-29.69090**	**23.70154**	**23.19881**
H	**-31.59700**	**23.99050**	**22.30449**
C	**-27.54821**	**27.72255**	**25.09765**
H	**-28.63934**	**29.53743**	**24.91860**
C	**-28.57207**	**24.29382**	**23.88026**
C	**-27.49863**	**26.31005**	**24.83442**
H	**-29.66402**	**22.63466**	**22.99453**
H	**-26.70812**	**28.18075**	**25.61244**
C	**-27.47293**	**23.54207**	**24.27616**
C	**-26.41576**	**25.53004**	**25.22033**
C	**-26.38873**	**24.14615**	**24.94748**
H	**-27.44153**	**22.47619**	**24.07118**
H	**-25.57705**	**25.98543**	**25.73815**
C	**-33.96976**	**29.49633**	**22.24296**
C	**-35.05855**	**30.27685**	**21.85798**
C	**-35.05885**	**31.68763**	**22.13177**
C	**-36.15950**	**29.69891**	**21.19807**
C	**-36.13905**	**32.45065**	**21.74630**
O	**-33.95616**	**32.13767**	**22.74415**
C	**-37.24042**	**30.46899**	**20.81184**
H	**-36.12766**	**28.63446**	**21.00254**
H	**-36.14881**	**33.51283**	**21.95423**
C	**-37.25247**	**31.89073**	**21.07544**
C	**-33.83727**	**33.52415**	**23.07643**
O	**-38.33323**	**29.99389**	**20.20008**

C	-38.37383	32.65096	20.63867
C	-34.57263	33.87190	24.35510
H	-34.16355	34.13742	22.22814
H	-32.76230	33.67403	23.19879
C	-38.42167	28.61125	19.83893
C	-38.55654	34.01445	20.81871
H	-39.12992	32.07739	20.11538
H	-35.65281	33.72264	24.26344
H	-34.20817	33.25551	25.18231
H	-34.39399	34.92305	24.60405
C	-37.66533	28.30665	18.56184
H	-38.09289	27.98859	20.67861
H	-39.49216	28.44488	19.70208
H	-37.75027	34.51748	21.36809
Ru	-39.90754	35.35875	20.39451
H	-36.58994	28.47808	18.66795
H	-37.81817	27.25704	18.29068
H	-38.03623	28.93096	17.74331
C	-41.00519	34.29426	19.41279
P	-38.69745	35.87312	18.26268
P	-41.20041	34.68080	22.44426
O	-41.14258	37.13235	20.14608
O	-38.65725	36.63553	21.55680
O	-41.74900	33.67233	18.77109
C	-39.21325	37.40882	17.30681
C	-36.82959	36.08723	18.32575
C	-39.03073	34.58790	16.91691
C	-40.07873	33.91622	23.74166
C	-42.31229	35.89706	23.33008
C	-42.44334	33.31991	22.02151
C	-40.91667	38.30512	20.57845
C	-38.79167	37.87161	21.81995
H	-38.66095	37.30830	16.36472
C	-40.70760	37.39802	16.97758
C	-38.76750	38.73895	17.91313
H	-36.60372	36.63629	17.40012
C	-36.03562	34.78077	18.30810
C	-36.36518	36.93219	19.51334
H	-40.11547	34.68369	16.77853

C	**-38.36621**	**34.89652**	**15.56932**
C	**-38.77948**	**33.12802**	**17.29549**
H	**-39.64850**	**33.07274**	**23.18411**
C	**-38.91177**	**34.81071**	**24.17044**
C	**-40.78389**	**33.36424**	**24.98139**
H	**-42.79437**	**35.28244**	**24.10178**
C	**-41.59654**	**37.04214**	**24.04150**
C	**-43.40258**	**36.43100**	**22.39743**
H	**-42.87909**	**33.67261**	**21.07874**
C	**-43.61185**	**33.09396**	**22.98862**
C	**-41.75518**	**31.98420**	**21.73943**
C	**-39.82690**	**38.70466**	**21.37109**
C	**-41.92547**	**39.34907**	**20.17166**
C	**-37.72700**	**38.45143**	**22.71350**
H	**-41.31755**	**37.37773**	**17.88427**
H	**-40.95783**	**38.30349**	**16.41166**
H	**-40.99115**	**36.54364**	**16.35476**
H	**-39.09883**	**38.87643**	**18.94518**
H	**-37.67972**	**38.85109**	**17.88691**
H	**-39.18774**	**39.55575**	**17.31379**
H	**-34.97193**	**35.01464**	**18.43820**
H	**-36.32881**	**34.11381**	**19.12542**
H	**-36.13461**	**34.23504**	**17.36763**
H	**-36.91374**	**37.86979**	**19.62159**
H	**-36.47490**	**36.37833**	**20.44909**
H	**-35.30425**	**37.17561**	**19.37857**
H	**-38.58037**	**34.07365**	**14.87747**
H	**-38.74433**	**35.80916**	**15.10220**
H	**-37.27697**	**34.97815**	**15.64650**
H	**-37.71860**	**32.89493**	**17.40804**
H	**-39.28410**	**32.84364**	**18.21655**
H	**-39.17449**	**32.49163**	**16.49451**
H	**-38.44472**	**35.33184**	**23.33328**
H	**-39.22931**	**35.56265**	**24.89928**
H	**-38.15564**	**34.18709**	**24.66309**
H	**-41.46232**	**32.53928**	**24.75536**
H	**-40.02623**	**32.97998**	**25.67543**
H	**-41.34634**	**34.13851**	**25.51495**
H	**-40.92960**	**36.68840**	**24.83124**

H	-41.01908	37.66004	23.34852
H	-42.34781	37.68695	24.51423
H	-43.97506	35.63873	21.90643
H	-44.10824	37.03689	22.97829
H	-42.97592	37.05555	21.61218
H	-44.25751	32.31782	22.56005
H	-43.28923	32.73864	23.96999
H	-44.23336	33.97933	23.13719
H	-40.92835	32.07612	21.03427
H	-41.36669	31.52896	22.65704
H	-42.48277	31.28619	21.30967
H	-39.79021	39.74523	21.67306
H	-41.86559	39.50322	19.08757
H	-42.93911	38.99652	20.38850
H	-41.76174	40.30672	20.67047
H	-36.73734	38.24198	22.29361
H	-37.83862	39.52852	22.85390
H	-37.77338	37.96013	23.69267
C	-24.33246	22.68446	25.68484
C	-23.23922	21.91716	26.08348
C	-23.20169	20.51249	25.78249
C	-22.16589	22.50610	26.77827
C	-22.11728	19.76403	26.18461
O	-24.26177	20.05953	25.10095
C	-21.07915	21.75147	27.17810
H	-22.22250	23.56721	26.98601
H	-22.08713	18.70318	25.97265
C	-21.02527	20.33766	26.87896
C	-24.34022	18.67931	24.73279
O	-20.02994	22.22989	27.85960
C	-19.87882	19.60250	27.29253
C	-24.83337	17.80883	25.87104
H	-23.37180	18.34511	24.34197
H	-25.05272	18.66806	23.90500
C	-19.93441	23.62568	28.16370
C	-19.65464	18.24897	27.08544
H	-19.12953	20.19129	27.80875
H	-24.14050	17.80511	26.71795
H	-25.80755	18.16058	26.22364

H	-24.94626	16.77825	25.51887
C	-19.44446	24.43348	26.97913
H	-20.89488	23.98692	28.54829
H	-19.21333	23.66575	28.98273
H	-20.45720	17.72473	26.55074
Ru	-18.27631	16.93629	27.52020
H	-20.14490	24.40021	26.13925
H	-19.32032	25.47918	27.27845
H	-18.47584	24.05593	26.63758
C	-17.07797	18.08921	28.25234
P	-17.17993	17.38531	25.31170
P	-19.28756	16.65072	29.80640
O	-17.01879	15.18544	27.80922
O	-19.66753	15.55164	26.68793
O	-16.26691	18.77301	28.72820
C	-15.82266	16.21066	24.74929
C	-18.26615	17.45660	23.77689
C	-16.17319	18.98594	25.31268
C	-21.11676	17.07446	29.80869
C	-19.09619	15.04816	30.75254
C	-18.51300	17.86772	31.02991
C	-17.26159	13.98646	27.46746
C	-19.55697	14.29550	26.52984
H	-15.41325	16.71332	23.86487
C	-14.70175	16.09898	25.78503
C	-16.29975	14.84065	24.26858
H	-17.55446	17.30365	22.95264
C	-18.97007	18.79508	23.55250
C	-19.30779	16.33724	23.72896
H	-15.41552	18.77556	26.07870
C	-15.43358	19.26550	23.99825
C	-16.90339	20.24747	25.77396
H	-21.09709	18.11725	29.46289
C	-21.94807	16.28240	28.79543
C	-21.80073	17.03304	31.17598
H	-19.54606	15.27732	31.72750
C	-19.84680	13.85112	30.17526
C	-17.62000	14.71113	30.97814
H	-17.44478	17.80917	30.78892

C	**-18.64322**	**17.55714**	**32.52606**
C	**-18.96493**	**19.30494**	**30.77071**
C	**-18.44117**	**13.51510**	**26.86612**
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C	**-20.76404**	**13.62035**	**25.93375**
H	**-15.07204**	**15.70767**	**26.73593**
H	**-13.92970**	**15.41798**	**25.40703**
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H	**-16.90383**	**14.30950**	**25.00797**
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H	**-15.42193**	**14.22224**	**24.04502**
H	**-19.63563**	**18.70032**	**22.68584**
H	**-19.58604**	**19.08055**	**24.41159**
H	**-18.27651**	**19.61112**	**23.34015**
H	**-18.89277**	**15.34733**	**23.92766**
H	**-20.10021**	**16.51383**	**24.46084**
H	**-19.75975**	**16.31966**	**22.72974**
H	**-14.92328**	**20.23200**	**24.08248**
H	**-14.66642**	**18.52174**	**23.76942**
H	**-16.11166**	**19.33177**	**23.14117**
H	**-17.66296**	**20.58273**	**25.06478**
H	**-17.38192**	**20.12031**	**26.74256**
H	**-16.16727**	**21.05392**	**25.87576**
H	**-21.45688**	**16.18343**	**27.82621**
H	**-22.17546**	**15.27629**	**29.16086**
H	**-22.90706**	**16.79574**	**28.65366**
H	**-21.39517**	**17.76315**	**31.87907**
H	**-22.86466**	**17.26551**	**31.04465**
H	**-21.74208**	**16.04021**	**31.63569**
H	**-20.92821**	**14.00671**	**30.16117**
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H	**-19.65219**	**12.97580**	**30.80744**
H	**-17.05902**	**15.52716**	**31.44286**
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H	**-18.09828**	**18.33204**	**33.07883**
H	**-19.67754**	**17.57835**	**32.87713**
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H	**-18.88145**	**19.59128**	**29.72169**

H	**-20.00360**	**19.46267**	**31.08120**
H	**-18.34045**	**19.99115**	**31.35412**
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H	**-20.60694**	**12.55288**	**25.76569**
H	**-21.61931**	**13.75148**	**26.60703**