Synthesis, Electrochemistry and Density Functional Theory of Osmium(II) Containing Different 2,2′:6′,2″-Terpyridines

Supplementary Materials

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1 ^{1}H NMR spectra

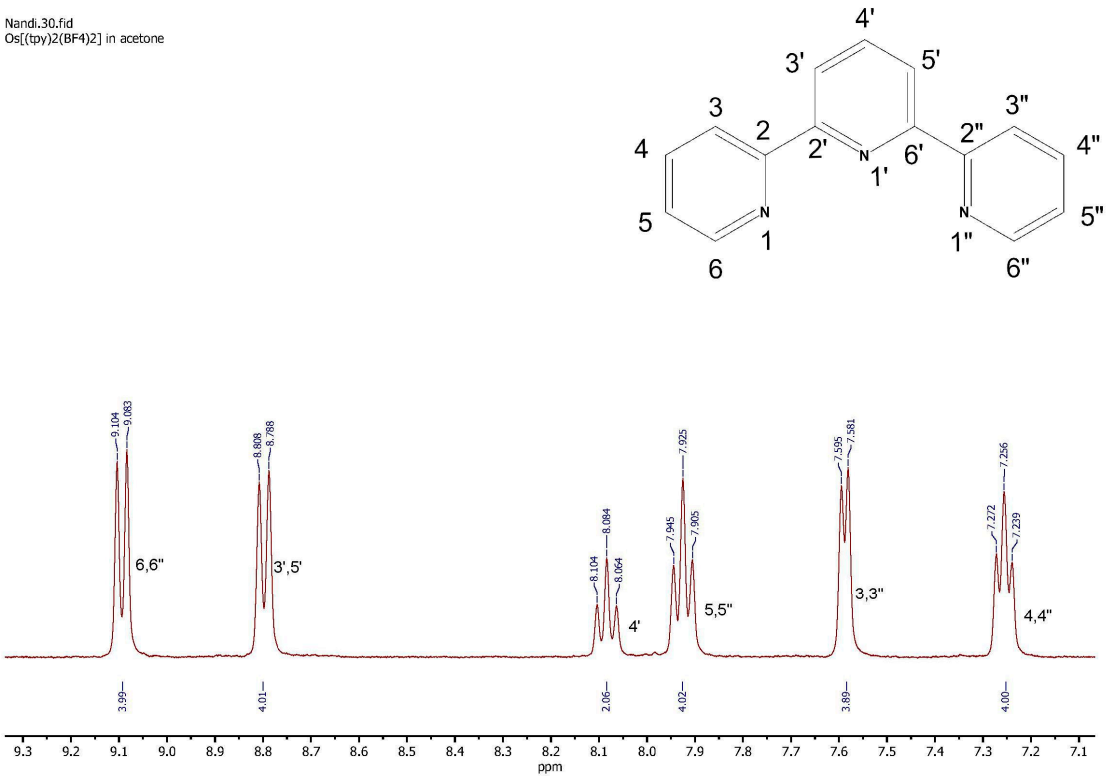


Figure S 1. ^{1}H NMR of [Os (2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (1).

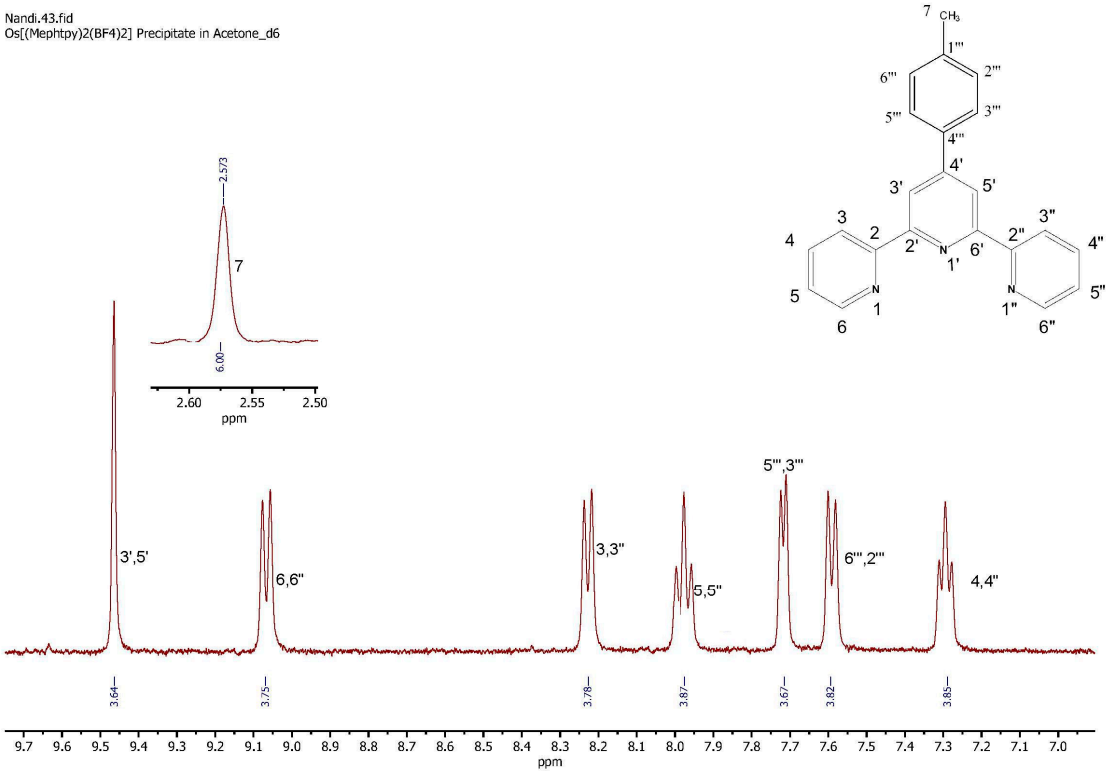


Figure S 2. ^{1}H NMR of [Os (4'-(4-methylphenyl)-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (2).

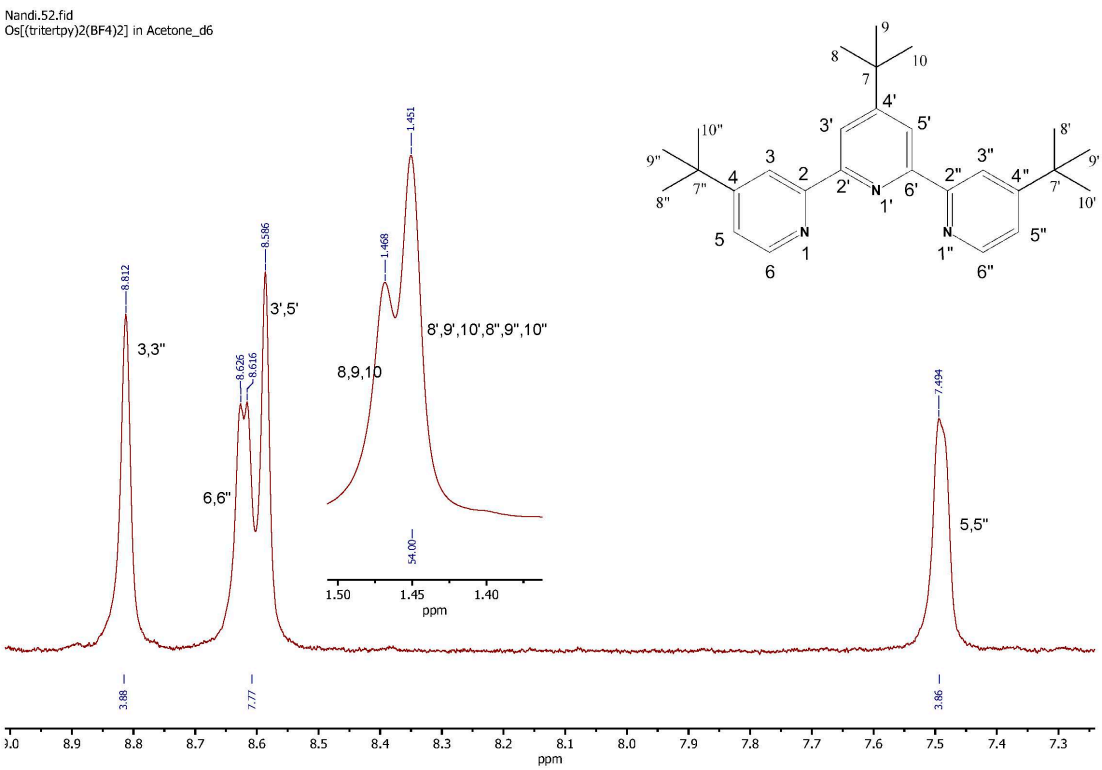


Figure S 3. ^{1}H NMR of [Os (4,4',4"-tri-tert-Butyl-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (3).

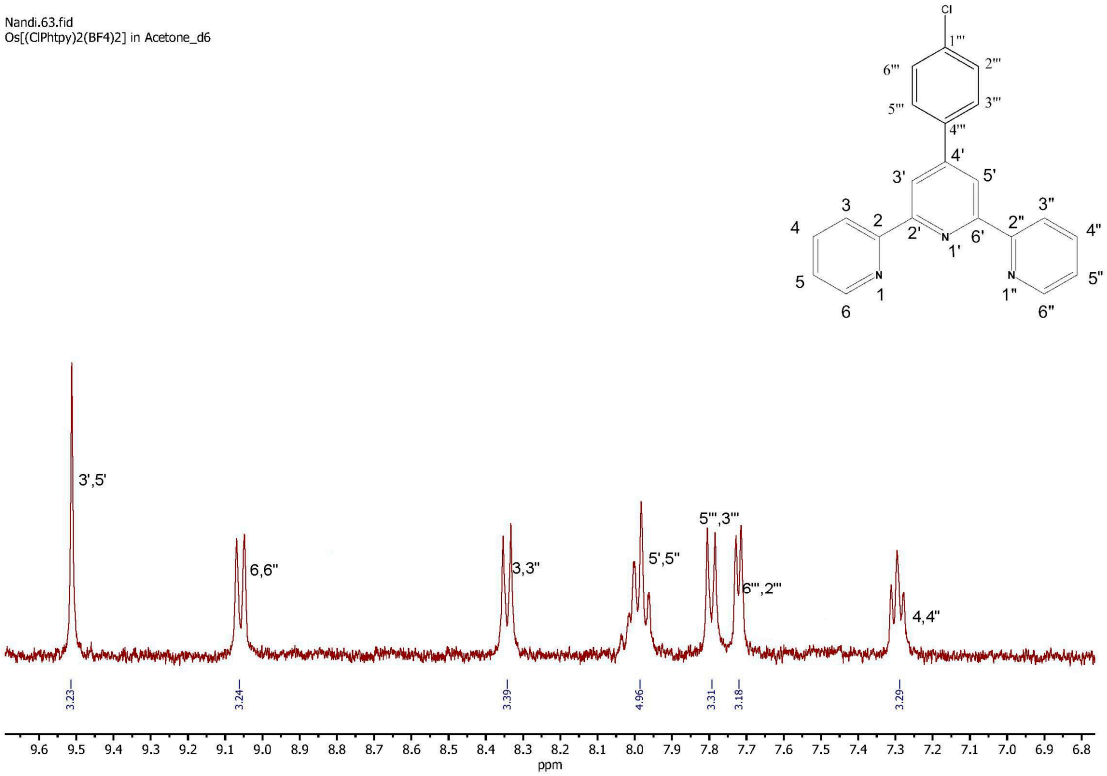


Figure S 4. ^{1}H NMR of [Os (4'-(4-chlorophenyl)-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (4).

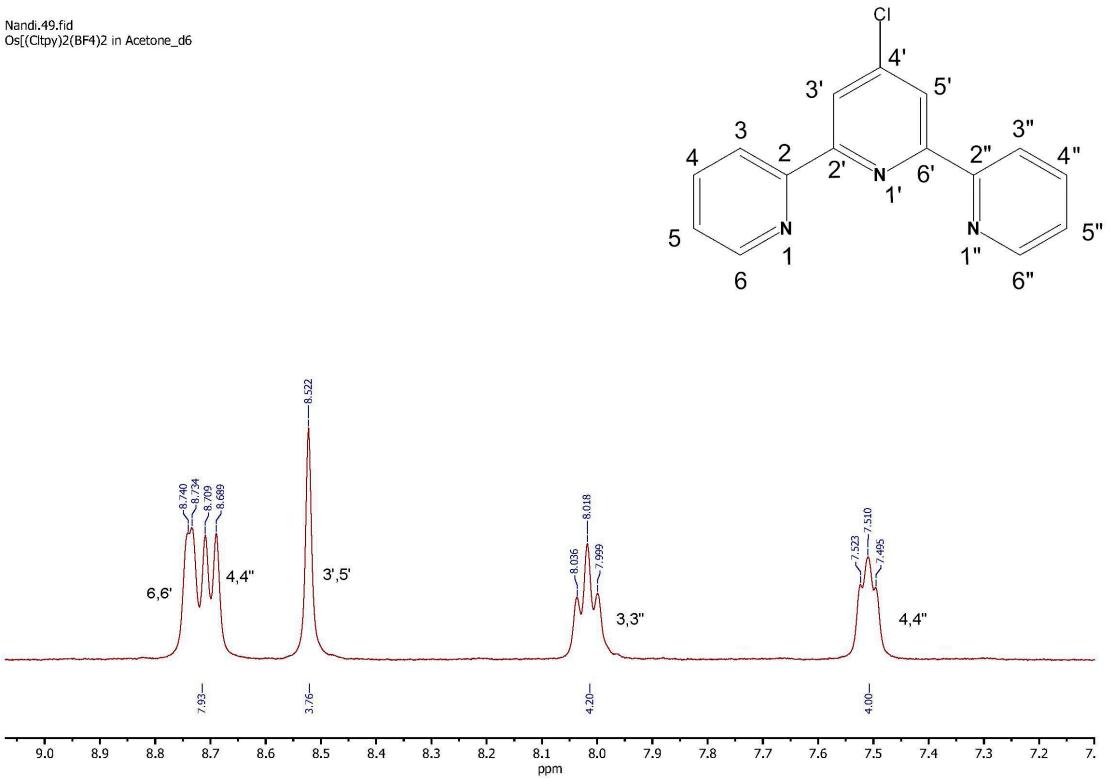


Figure S 5. ^{1}H NMR of [Os (4'-chloro-2,2′:6′,2′′-terpyridine)$_2$](BF$_4$)$_2$ (5).

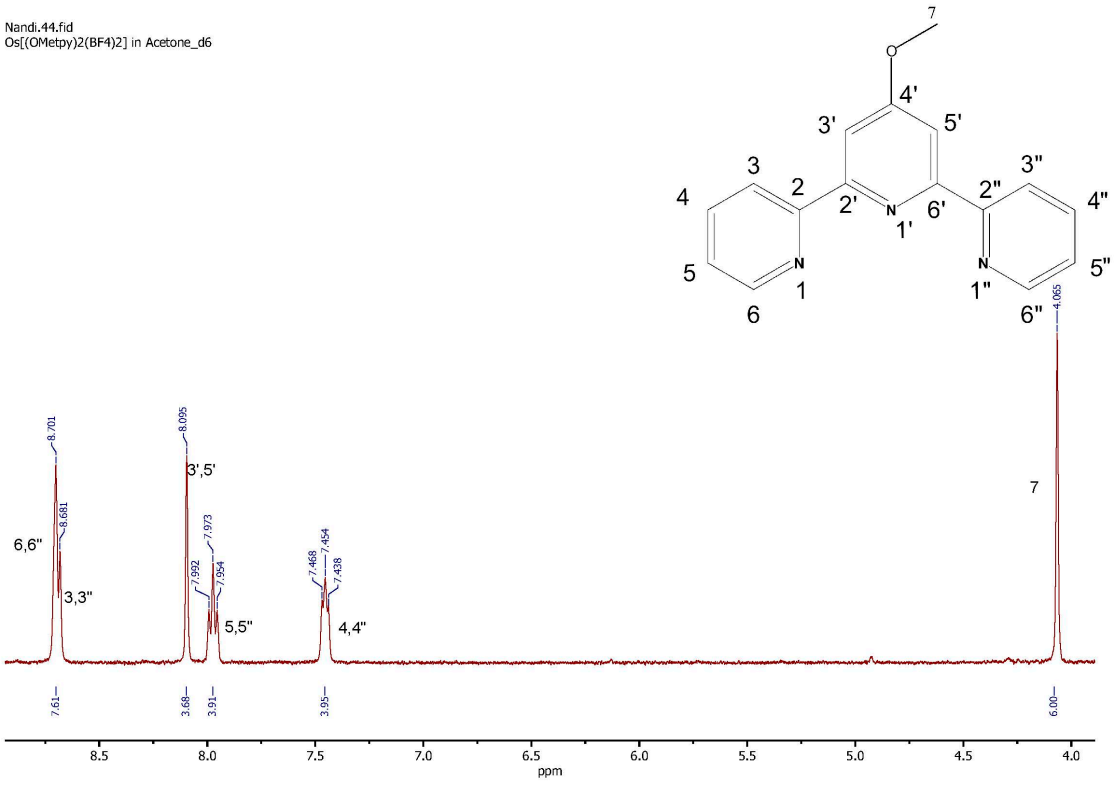


Figure S 6. ^{1}H NMR of [Os (4'-methoxy)-2,2′:6′,2′′-terpyridine)$_2$](BF$_4$)$_2$ (6).

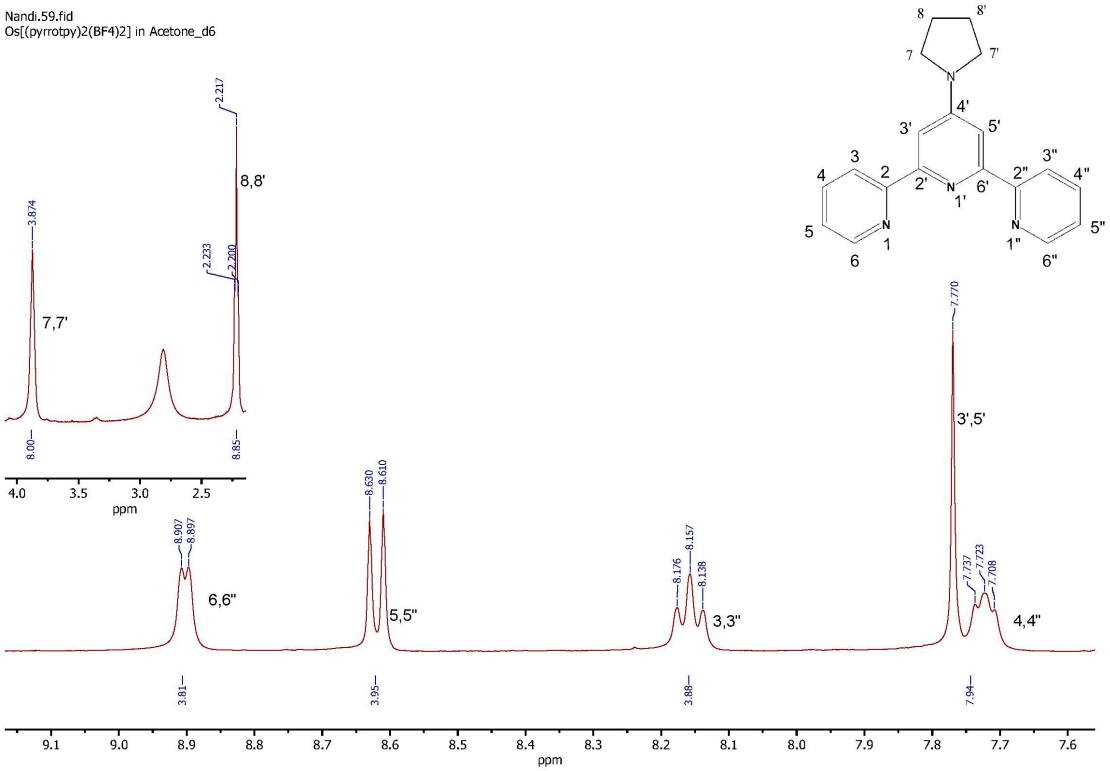


Figure S 7. ^{1}H NMR of [Os 4'-(N-Pyrrolidinyl)-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (7).

2 ^{13}C NMR spectra

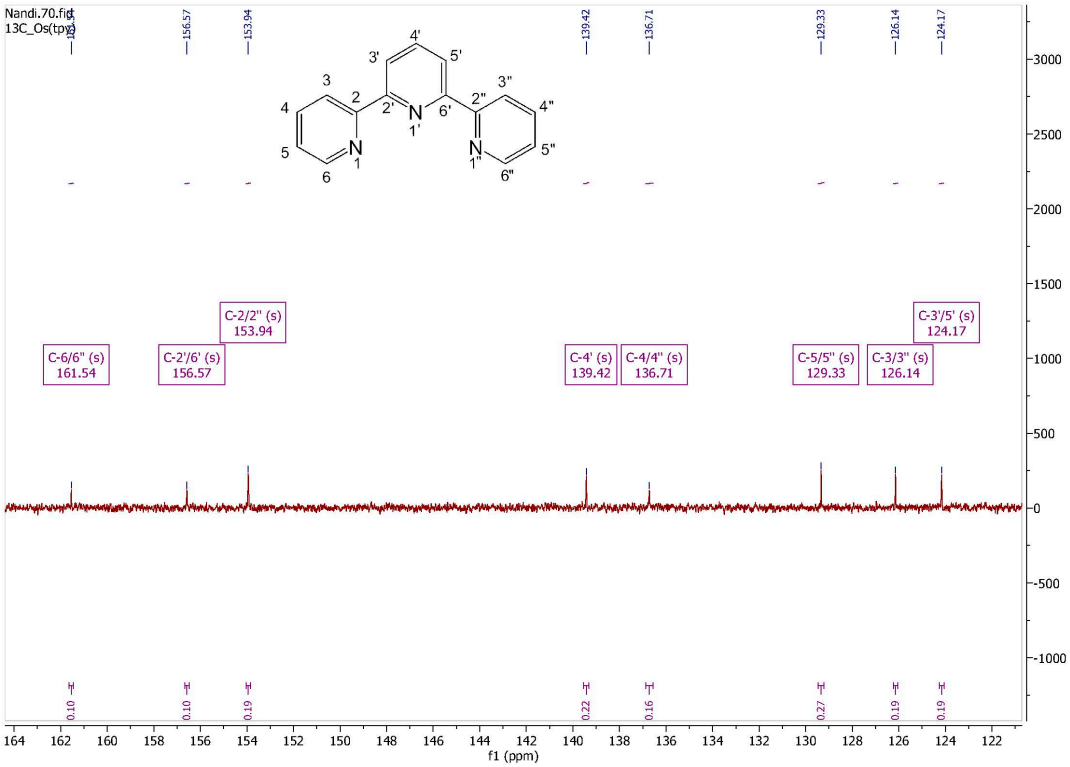


Figure S 8. ^{13}C NMR of [Os (2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (1).

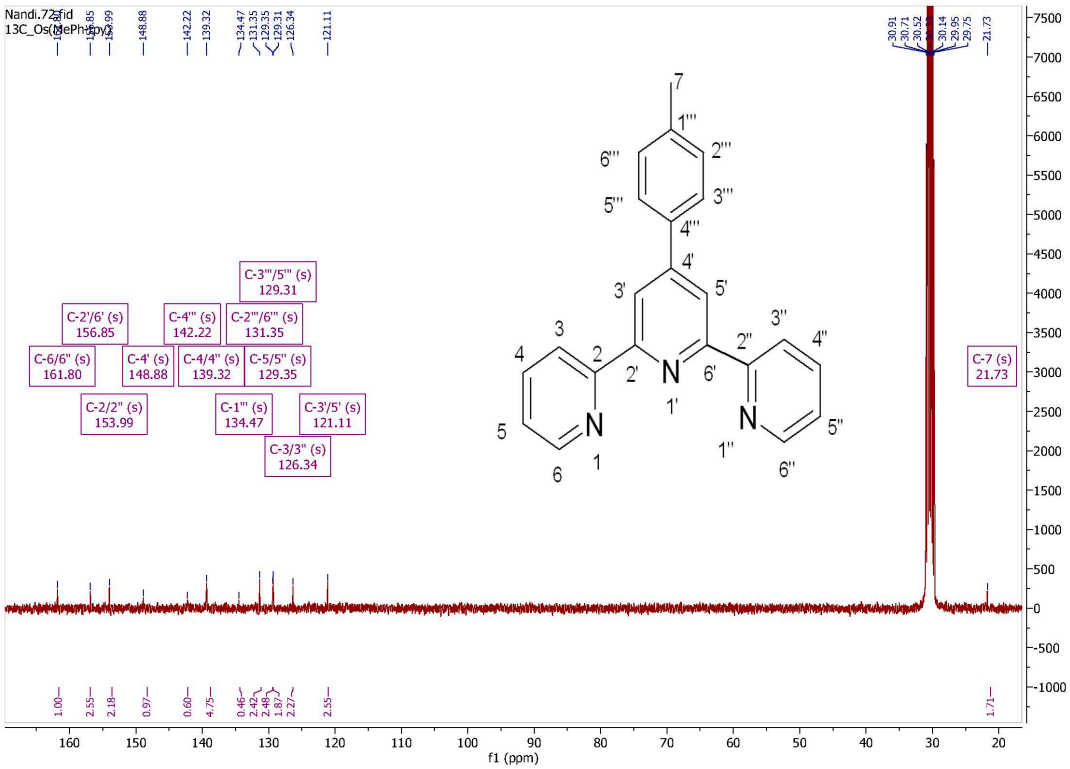


Figure S 9. ^{13}C NMR of [Os (4'-(4-methylphenyl)-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (2).

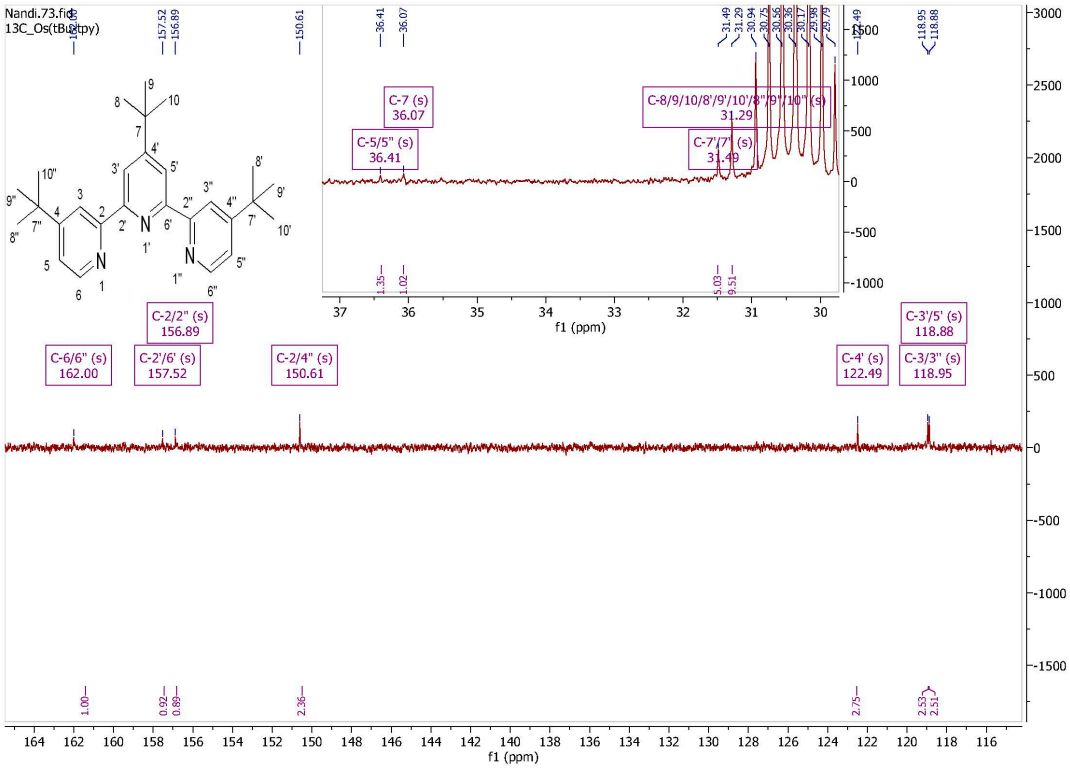


Figure S 10. ^{13}C NMR of [Os (4,4',4"-tri-tert-Butyl-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (3).

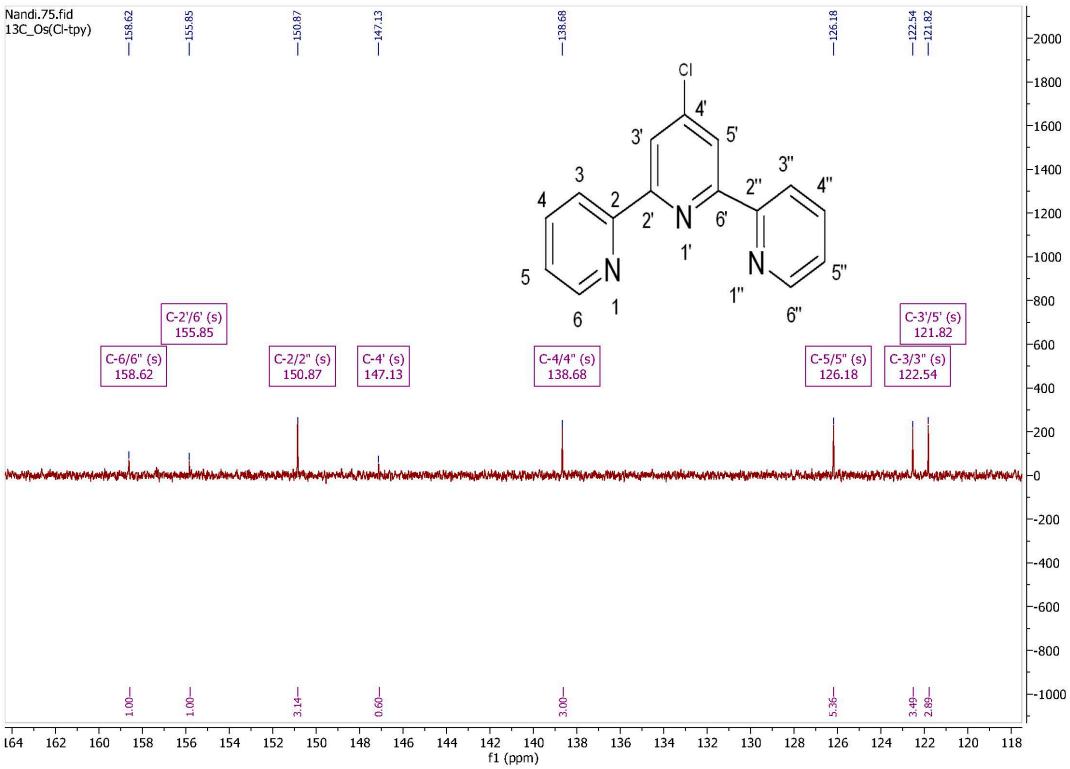


Figure S 11. ^{13}C NMR of [Os (4'-chloro-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (5).

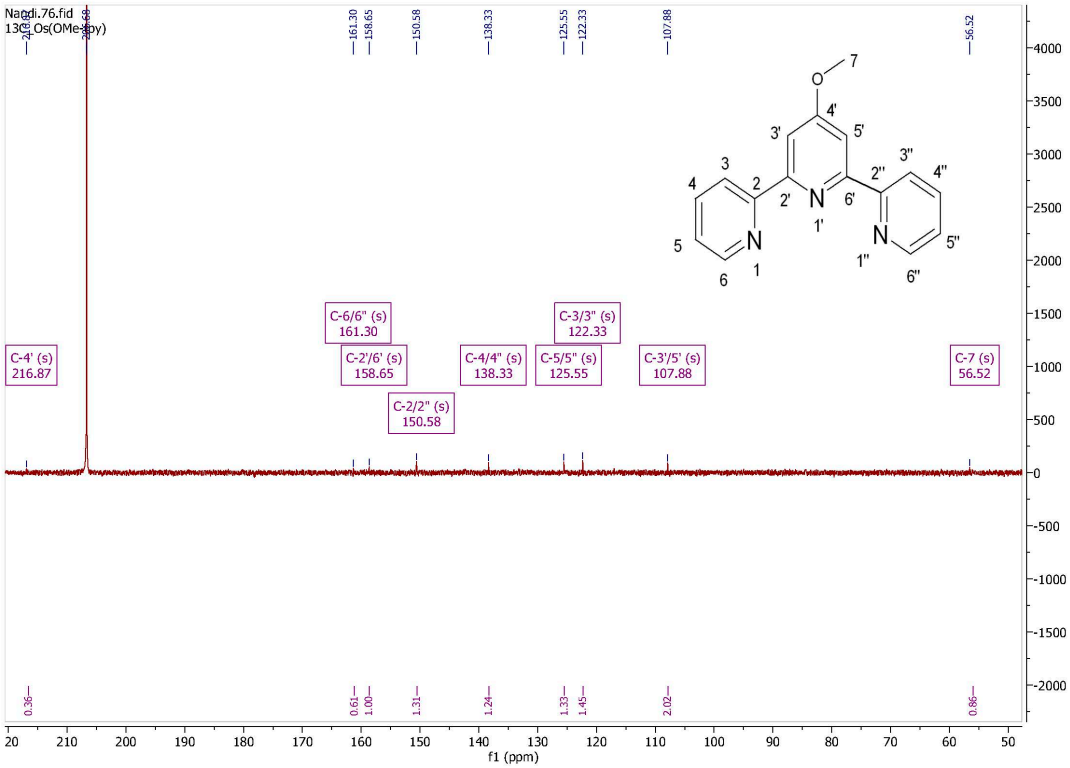


Figure S 12. ^{13}C NMR of [Os (4'-methoxy)-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (6).

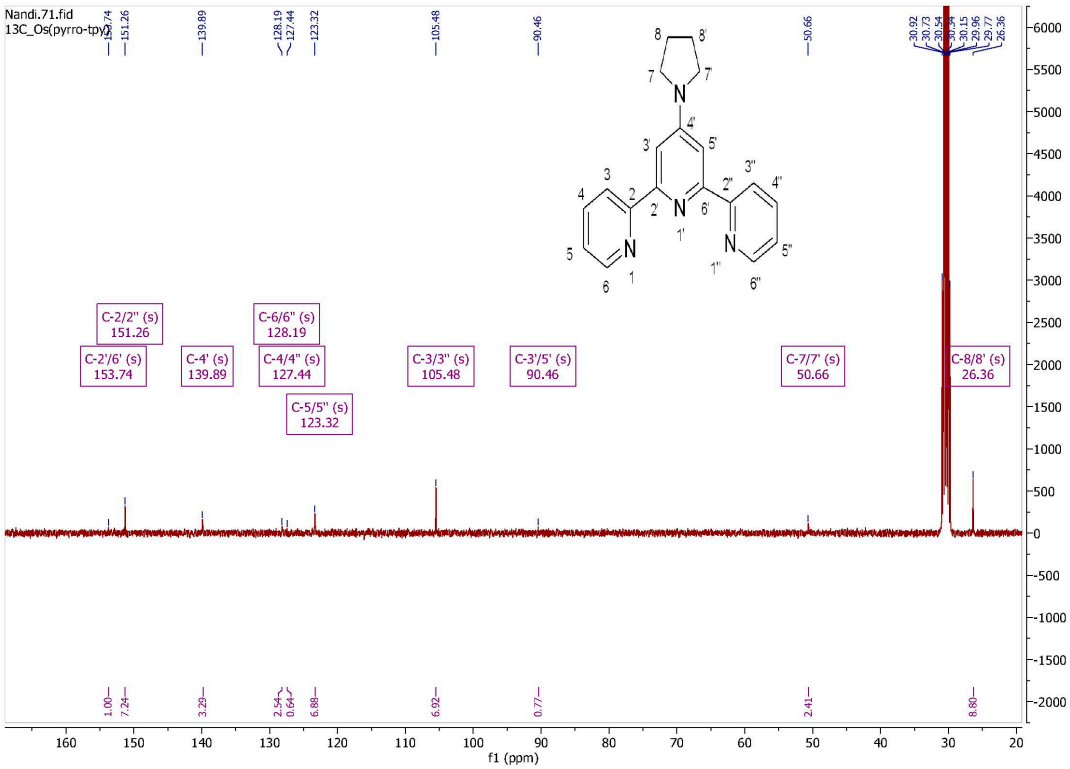


Figure S 13. ^{13}C NMR of [Os 4'-(N-Pyrrolidinyl)-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (7).

3 UV/Visible spectra

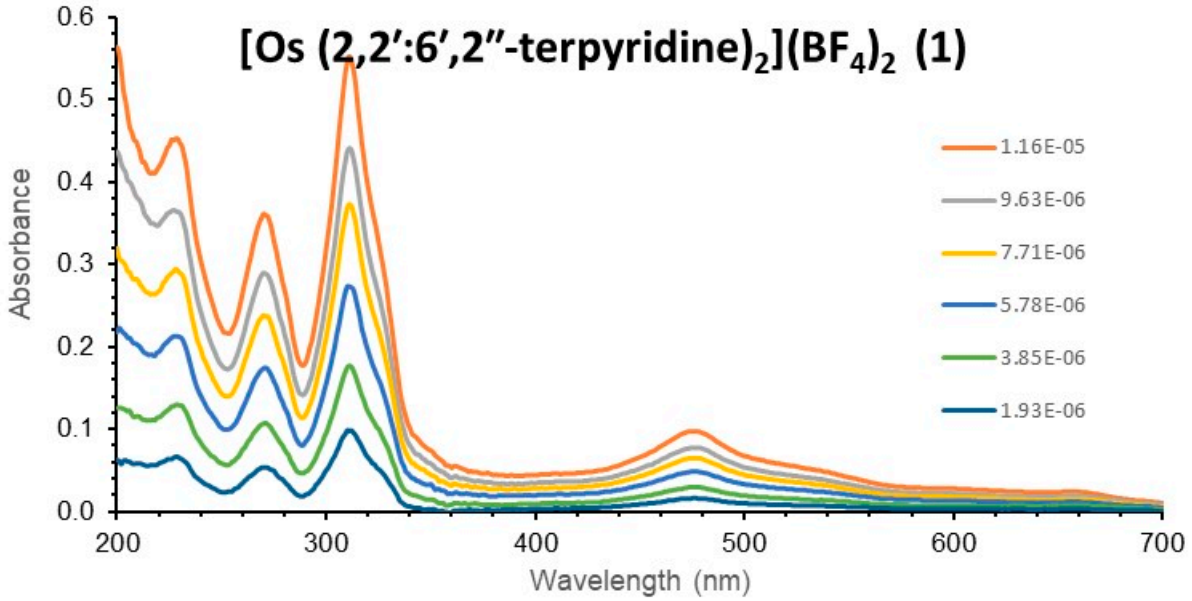


Figure S 14. UV/Visible spectra of [Os (2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (1). Concentration is indicated in mol dm^{-3}.

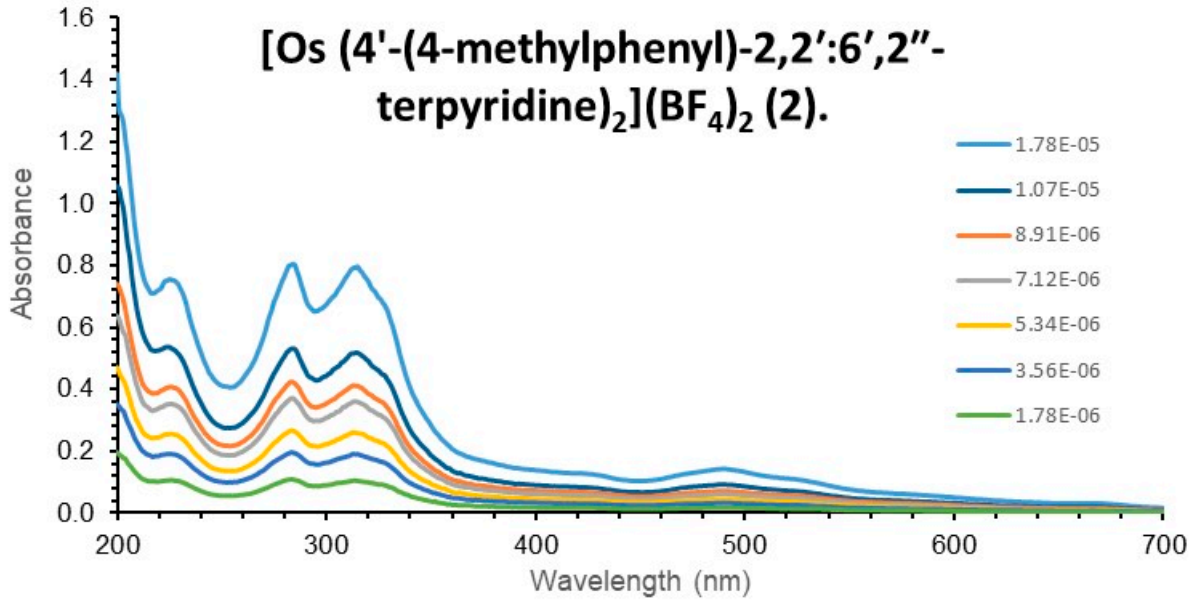


Figure S 15. UV/Visible spectra of [Os (4'-(4-methylphenyl)-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (2). Concentration is indicated in mol dm^{-3}.

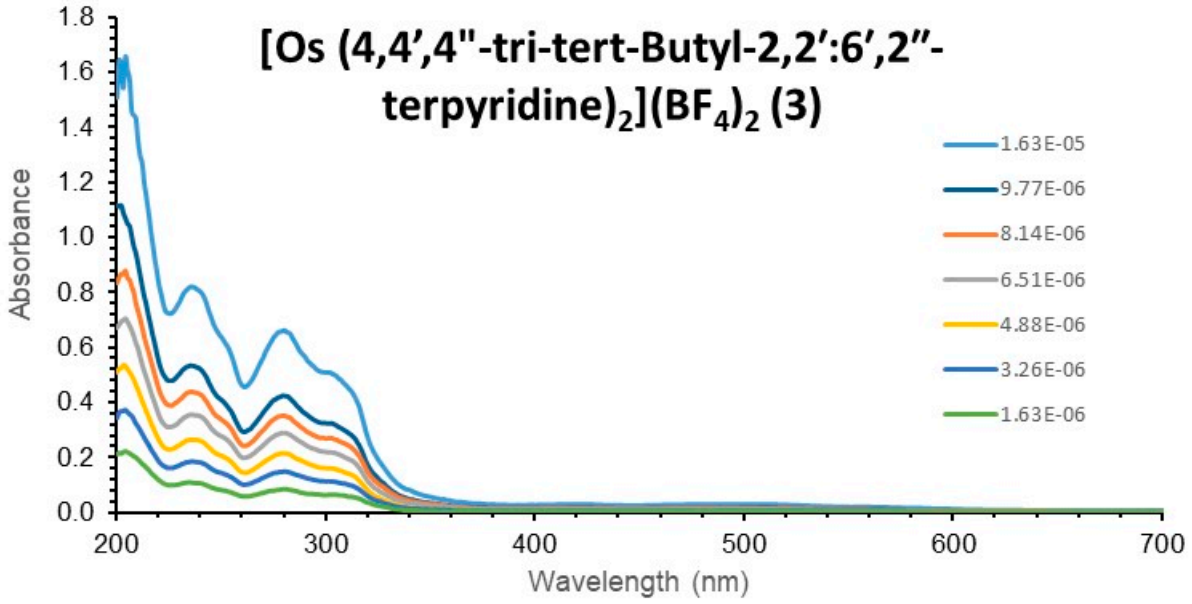


Figure S 16. UV/Visible spectra of [Os (4,4',4"-tri-tert-Butyl-2,2′:6′,2″-terpyridine)$_2$]$(BF_4)_2$ (3). Concentration is indicated in mol dm^{-3}.

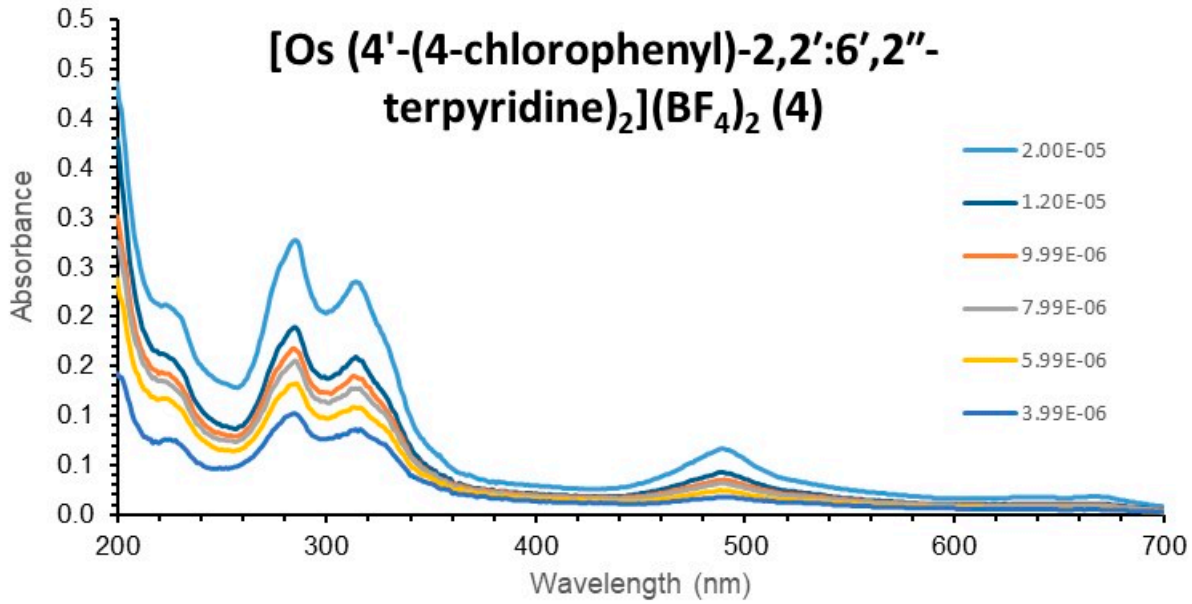


Figure S 17. UV/Visible spectra of [Os (4'-(4-chlorophenyl)-2,2′:6′,2″-terpyridine)$_2$]$(BF_4)_2$ (4). Concentration is indicated in mol dm^{-3}.

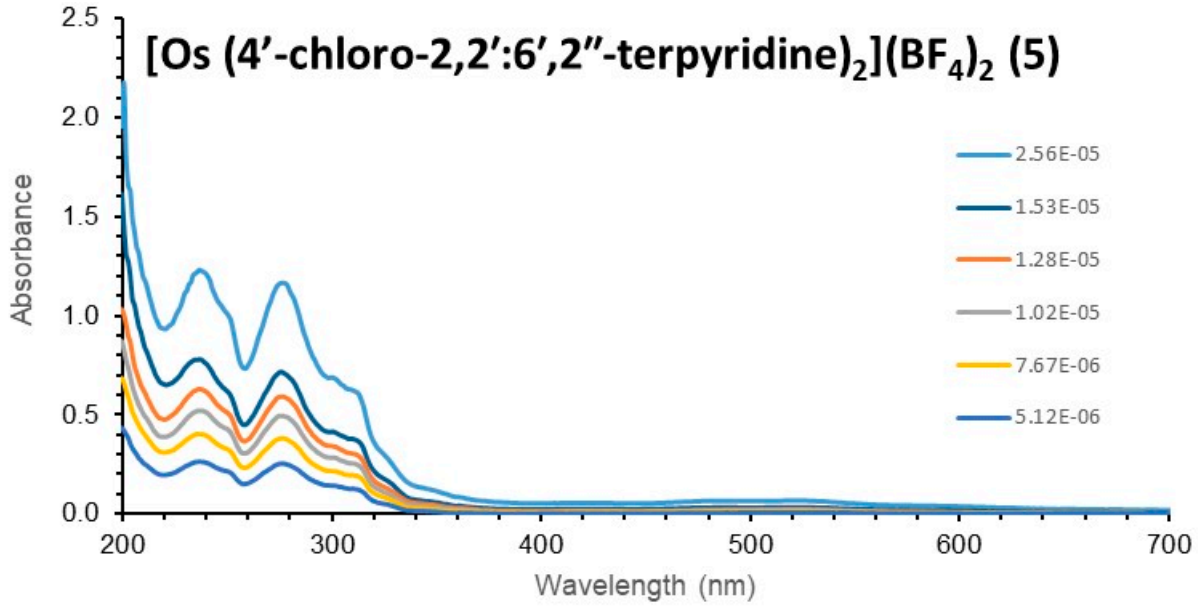


Figure S 18. UV/Visible spectra of [Os (4'-chloro-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (5). Concentration is indicated in mol dm^{-3}.

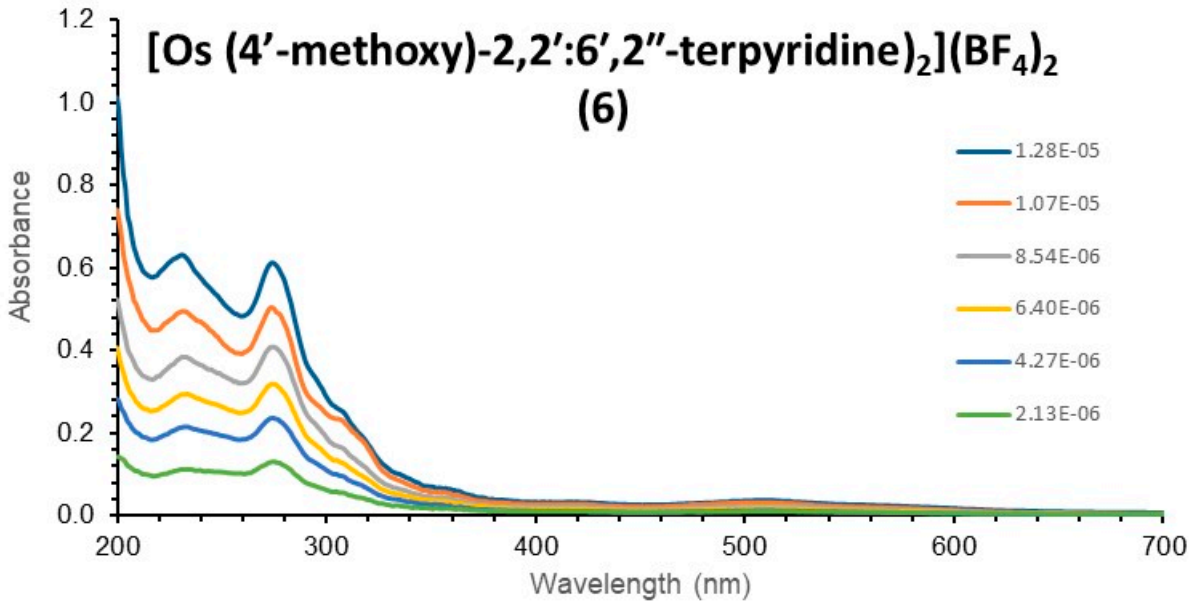


Figure S 19. UV/Visible spectra of [Os (4'-methoxy)-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (6). Concentration is indicated in mol dm^{-3}.

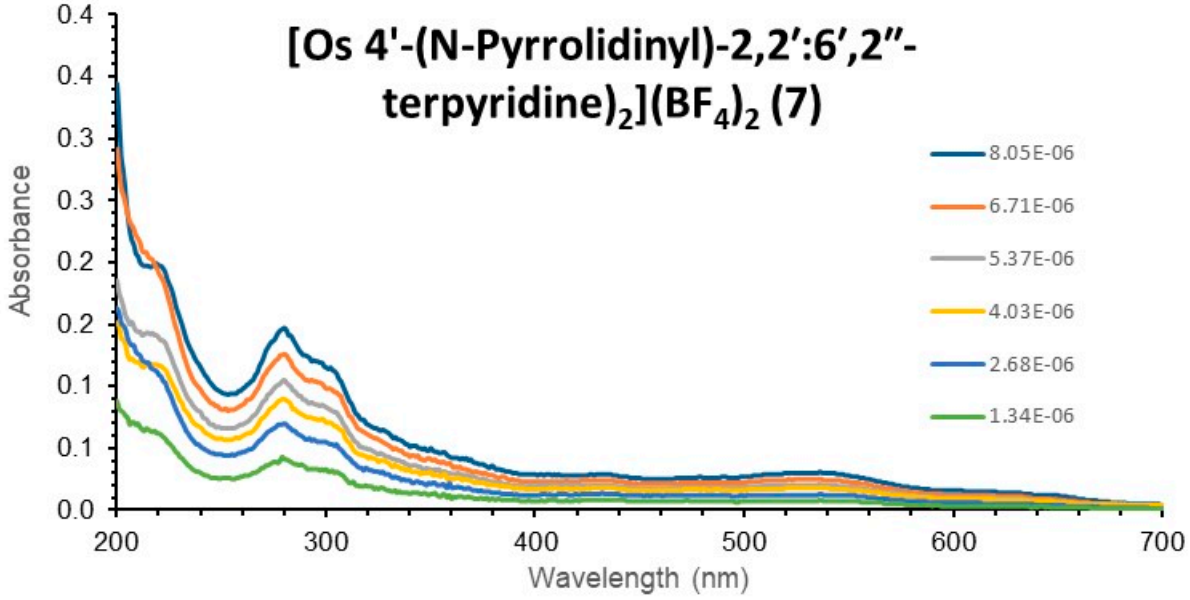


Figure S 20. UV/Visible spectra of [Os 4'-(N-Pyrrolidinyl)-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (7). Concentration is indicated in mol dm^{-3}.

4 FTIR spectra

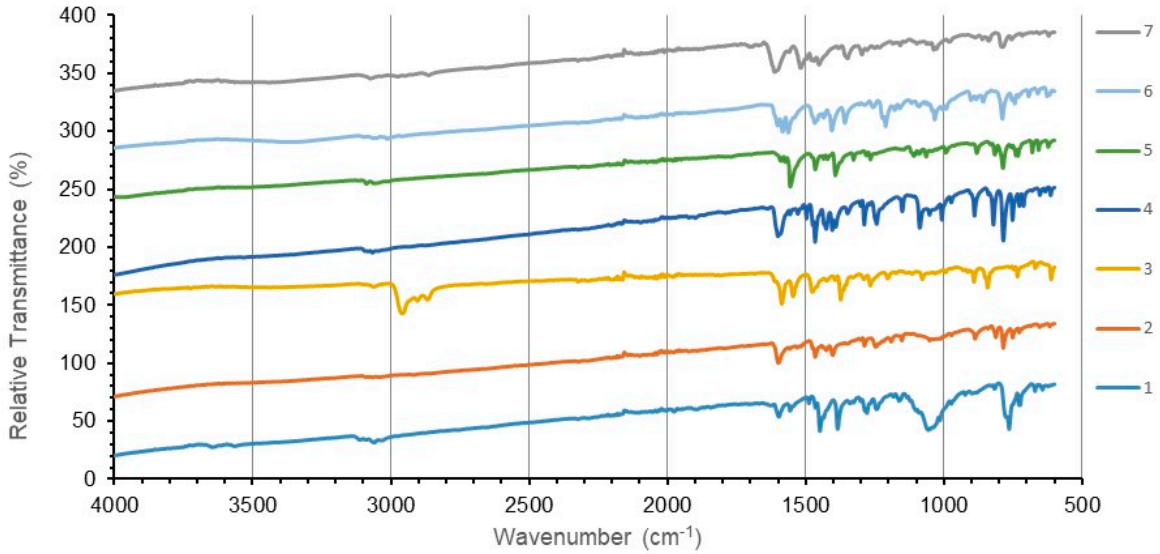


Figure S 21. Experimental IR spectra of (1) – (7).

5 PXRD

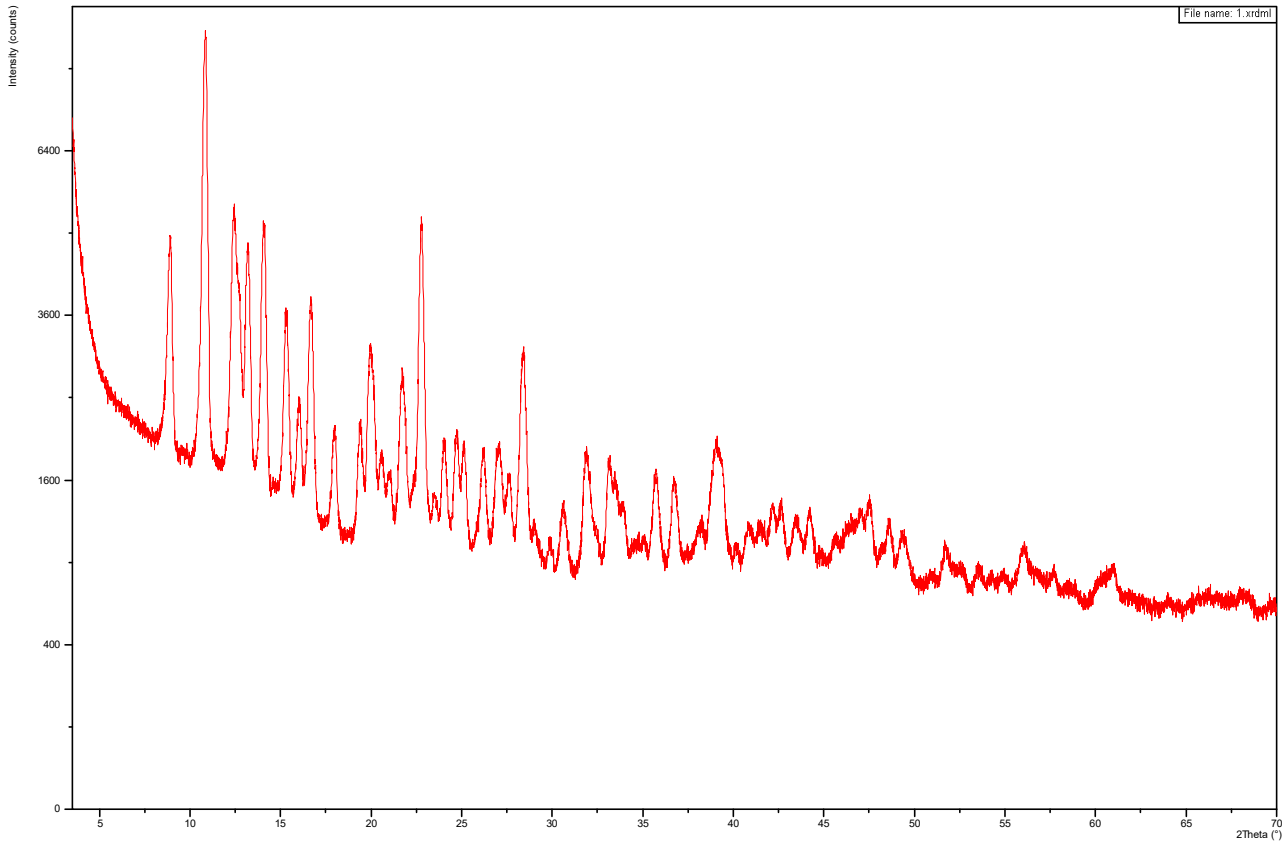


Figure S 22. XRD of [Os (2,2′:6′,2′′-terpyridine)$_2$](BF$_4$)$_2$ (1).

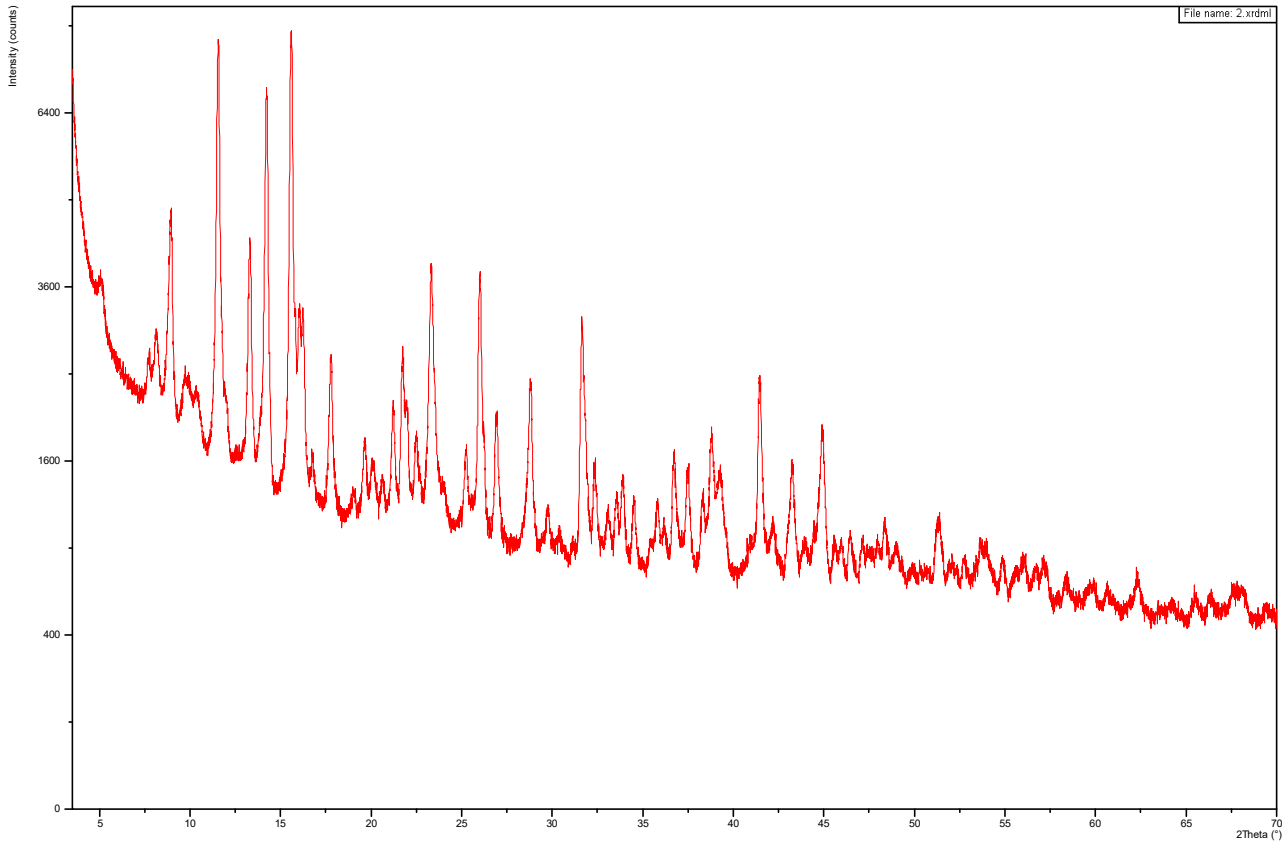


Figure S 23. XRD of [Os (4'-(4-methylphenyl)-2,2′:6′,2′′-terpyridine)$_2$](BF$_4$)$_2$ (2).

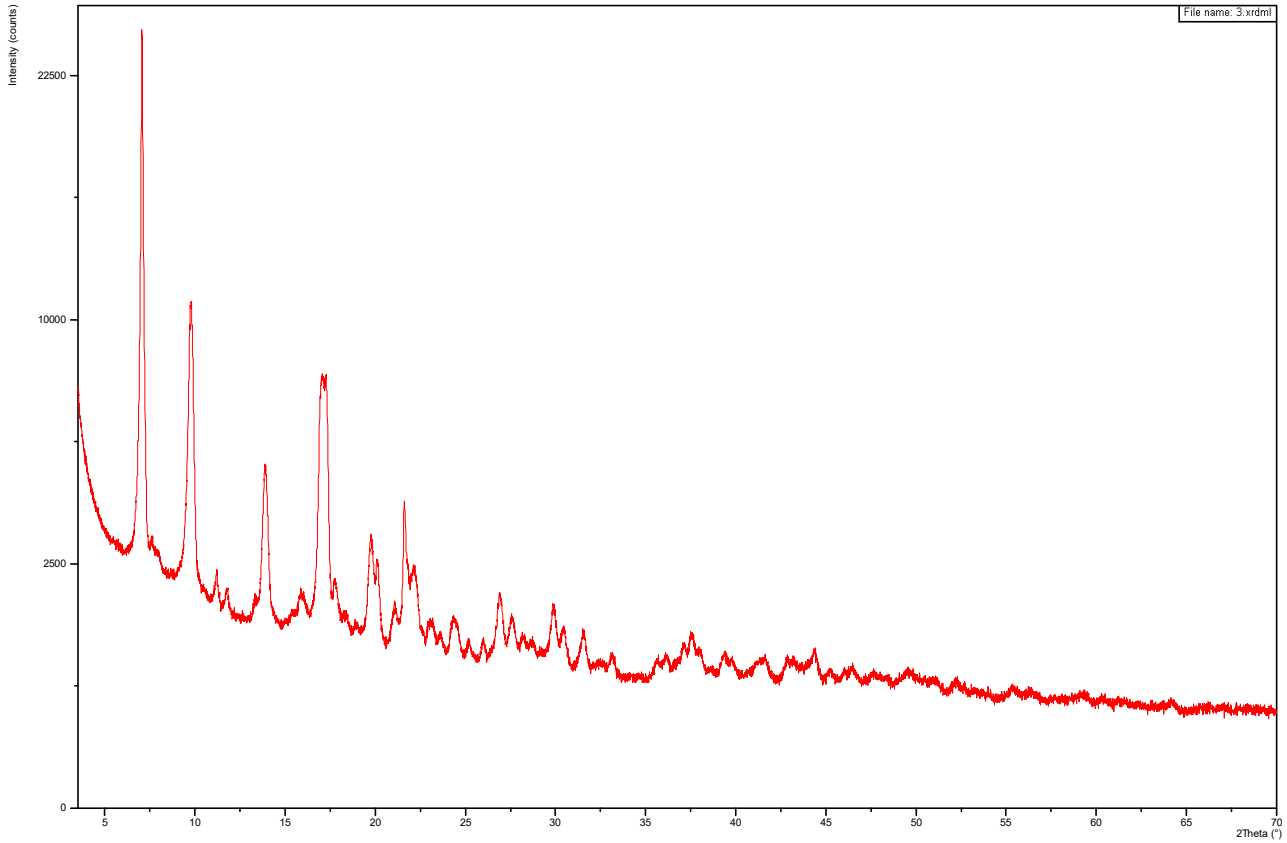


Figure S 24. XRD of [Os (4,4',4"-tri-tert-Butyl-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (3).

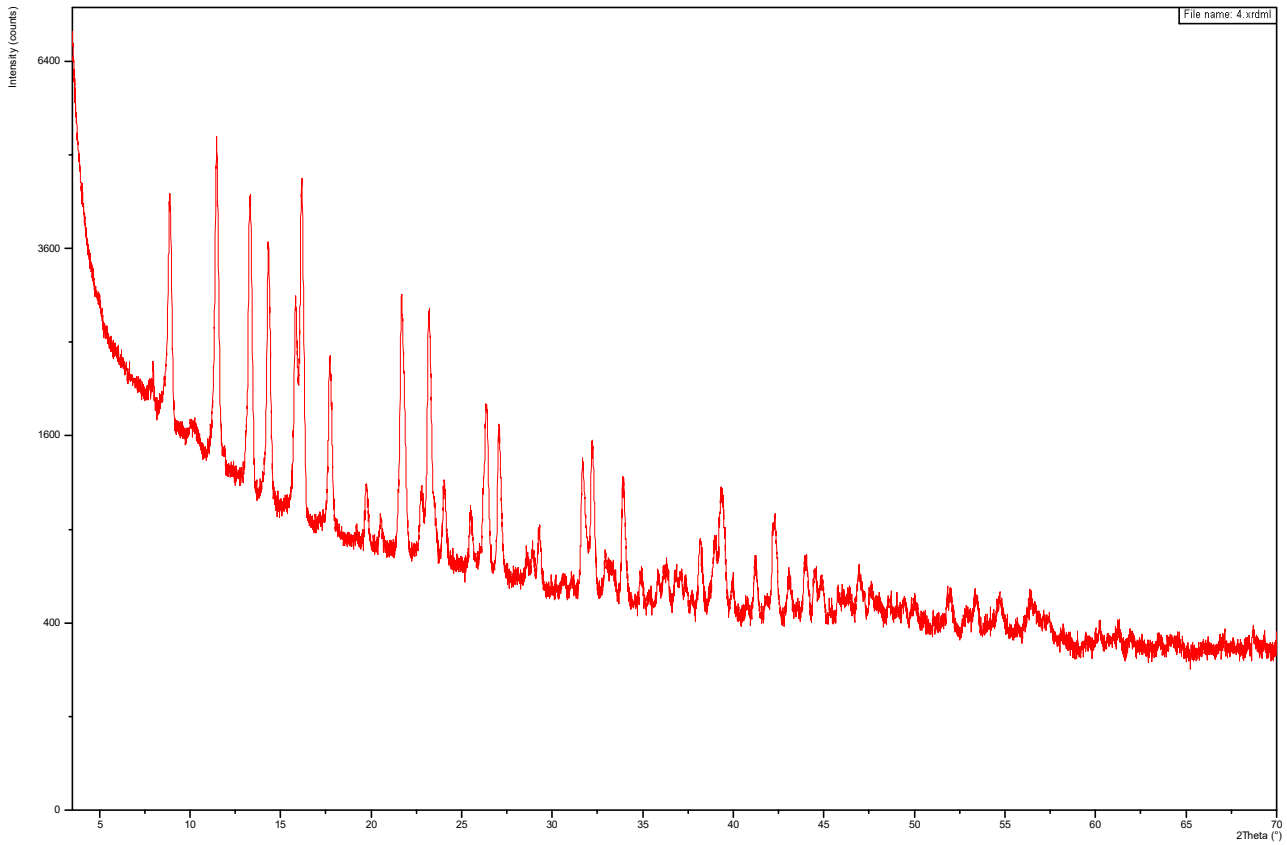


Figure S 25. XRD of [Os (4'-(4-chlorophenyl)-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (4).

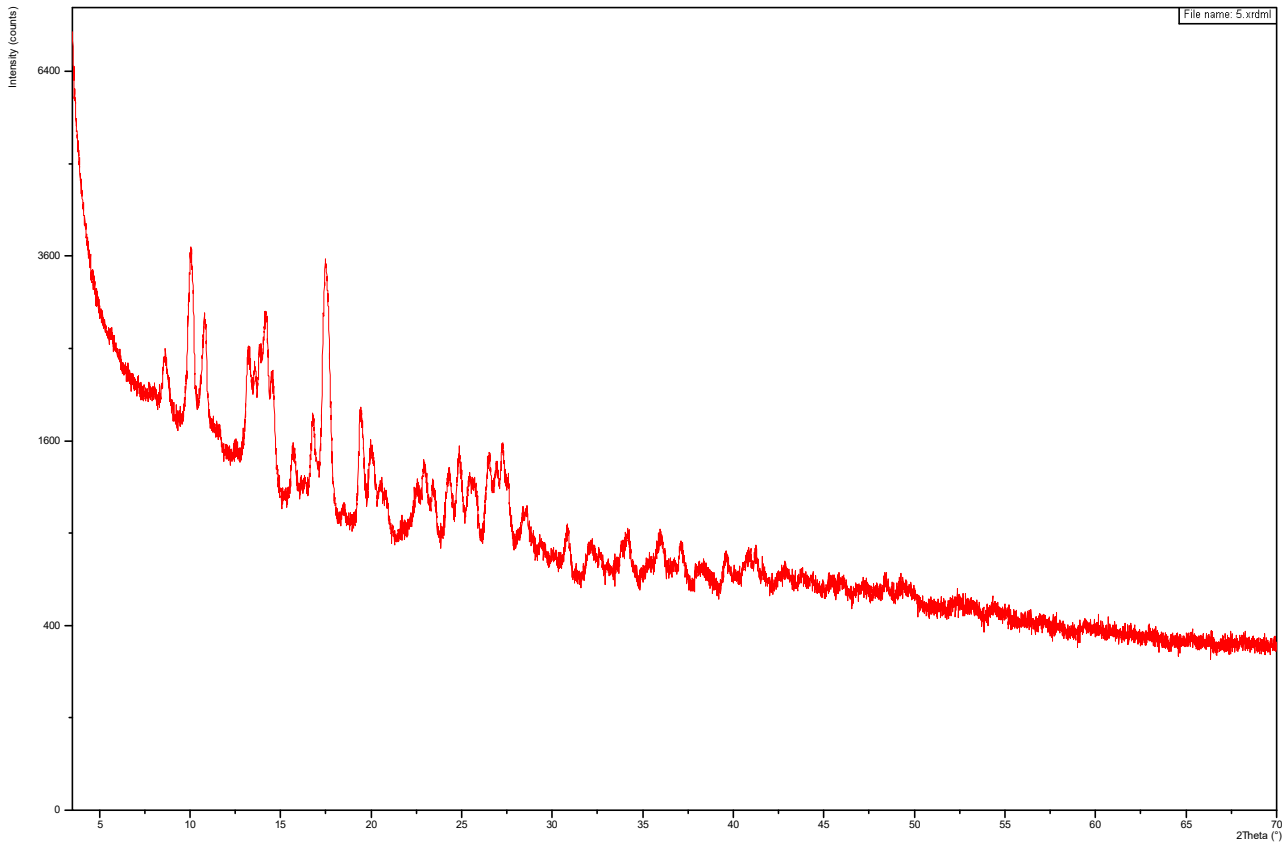


Figure S 26. XRD of [Os (4'-chloro-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (5).

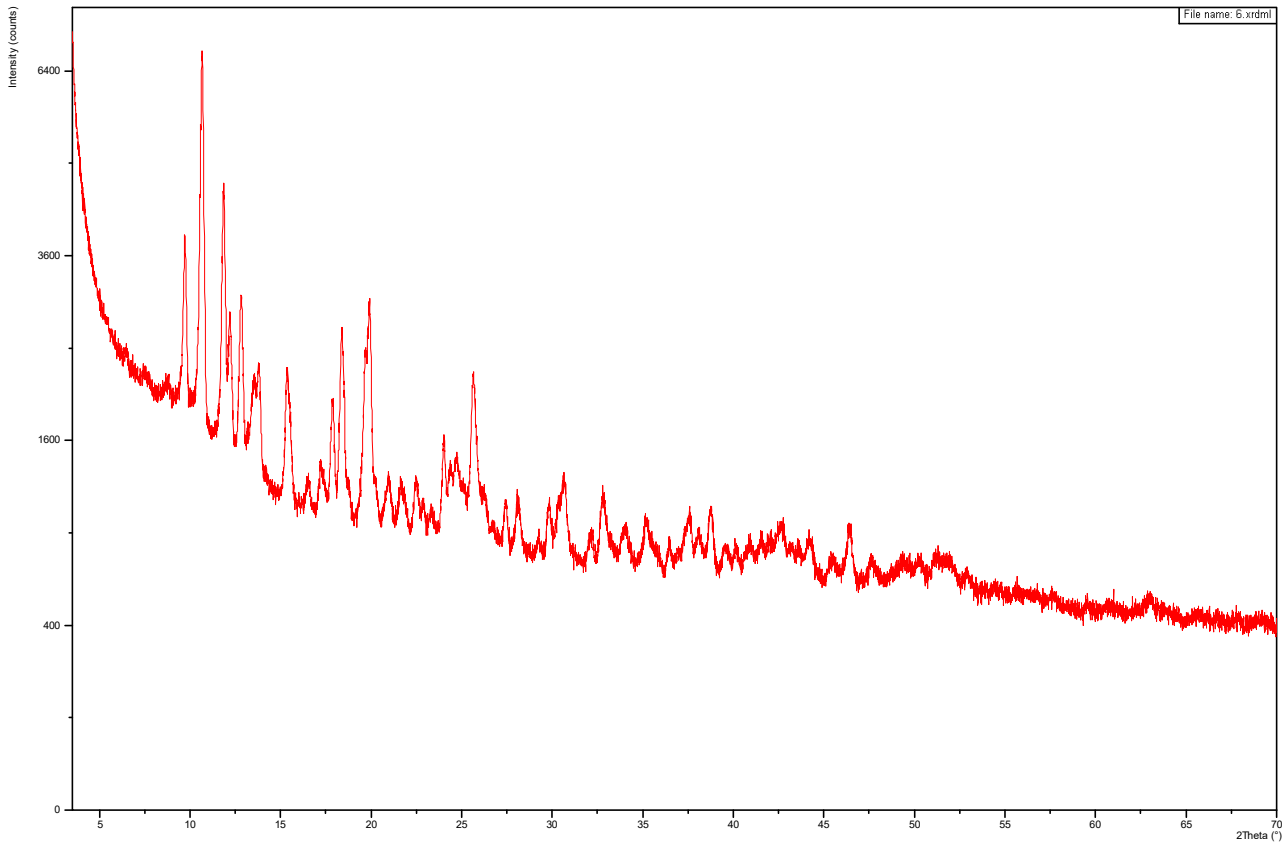


Figure S 27. XRD of [Os (4'-methoxy)-2,2′:6′,2″-terpyridine)$_2$](BF$_4$)$_2$ (6).

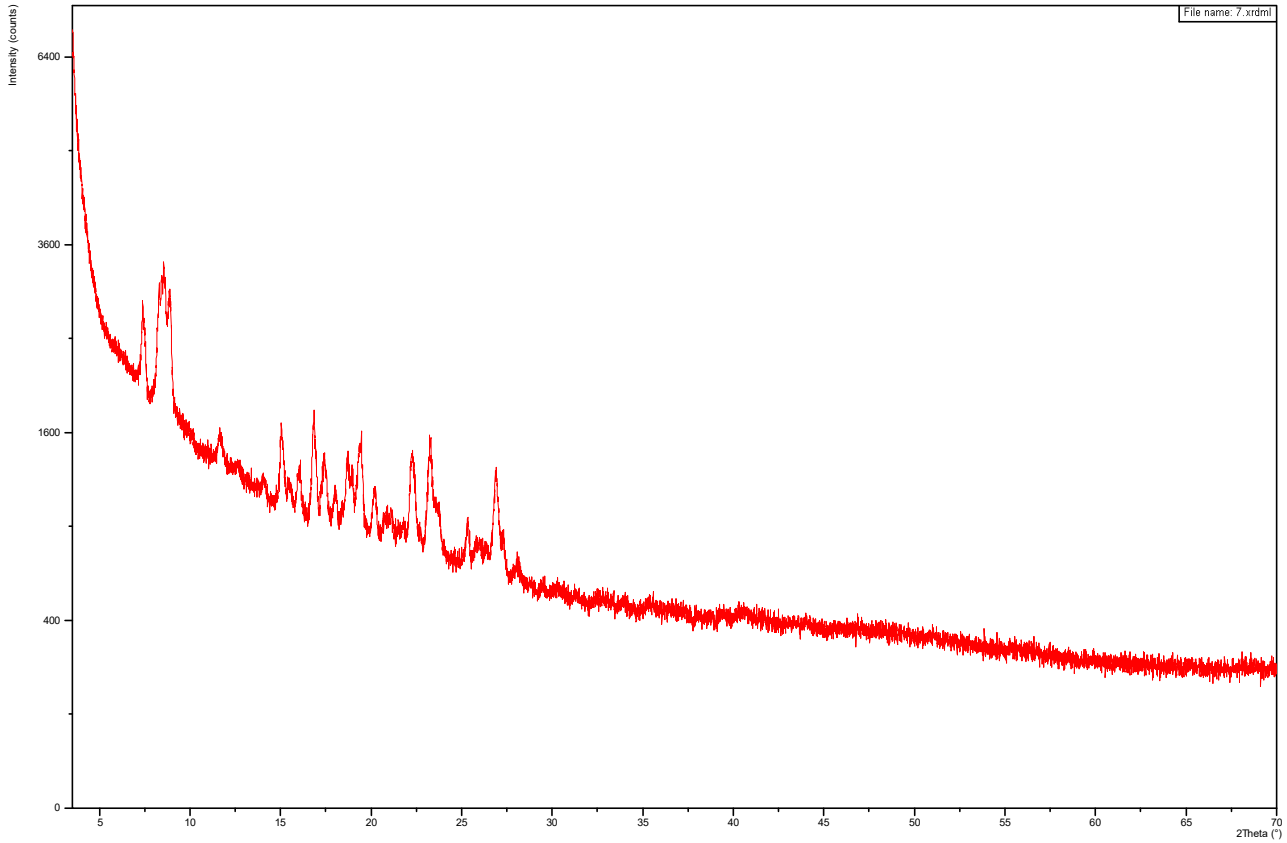


Figure S 28. XRD of [Os 4'-(N-Pyrrolidinyl)-2,2′:6′,2″-terpyridine)$_2$]$(BF_4)_2$ (7).

6 Optimized coordinates

Density functional theory (DFT) calculations were performed using the B3LYP functional which is composed of the Becke 88 exchange functional [1] in combination with the LYP correlation functional [2], as implemented in the Gaussian 16 package [3]. The triple-ζ basis set 6-311G(d,p) was used for lighter atoms (C, H, F, O) and the def2-TZVPP basis set for both the core and valence electrons of Os. Optimizations were performed in CH_3CN as solvent, using the implicit solvent Polarizable Continuum Model (PCM) [4] that uses the integral equation formalism variant (IEFPCM) [5].

6.1 [Os (2,2′:6′,2″-terpyridine)$_2$]$^{2+}$

Os	0.000000000	0.000000000	0.000000000
N	2.058234000	0.000000000	0.426799000
N	0.000000000	2.058234000	-0.426799000
N	0.000000000	0.000000000	2.008594000
N	0.000000000	0.000000000	-2.008594000
N	-2.058234000	0.000000000	0.426799000
N	0.000000000	-2.058234000	-0.426799000
C	4.710669000	0.000000000	1.295888000
C	3.669992000	0.000000000	2.214926000
C	4.407073000	0.000000000	-0.062079000
C	0.000000000	4.407073000	0.062079000
C	0.000000000	4.710669000	-1.295888000
C	2.350347000	0.000000000	1.769797000
C	1.207023000	0.000000000	4.062426000
C	3.077807000	0.000000000	-0.454232000
C	0.000000000	3.077807000	0.454232000
C	0.000000000	3.669992000	-2.214926000
C	1.187818000	0.000000000	2.670056000
C	0.000000000	0.000000000	4.756563000
C	0.000000000	2.350347000	-1.769797000
C	-1.207023000	0.000000000	4.062426000
C	0.000000000	1.187818000	-2.670056000
C	0.000000000	1.207023000	-4.062426000
C	-1.187818000	0.000000000	2.670056000
C	0.000000000	0.000000000	-4.756563000
C	-2.350347000	0.000000000	1.769797000
C	0.000000000	-1.187818000	-2.670056000
C	0.000000000	-1.207023000	-4.062426000
C	-3.669992000	0.000000000	2.214926000
C	0.000000000	-3.077807000	0.454232000
C	0.000000000	-2.350347000	-1.769797000
C	-3.077807000	0.000000000	-0.454232000
C	-4.710669000	0.000000000	1.295888000
C	0.000000000	-4.407073000	0.062079000
C	0.000000000	-3.669992000	-2.214926000

C	-4.407073000	0.000000000	-0.062079000
C	0.000000000	-4.710669000	-1.295888000
H	5.738526000	0.000000000	1.634997000
H	3.879909000	0.000000000	3.275344000
H	5.182841000	0.000000000	-0.816007000
H	0.000000000	5.182841000	0.816007000
H	0.000000000	5.738526000	-1.634997000
H	2.144247000	0.000000000	4.601106000
H	0.000000000	2.805292000	1.500365000
H	0.000000000	3.879909000	-3.275344000
H	0.000000000	0.000000000	5.838597000
H	2.805292000	0.000000000	-1.500365000
H	0.000000000	2.144247000	-4.601106000
H	-2.144247000	0.000000000	4.601106000
H	0.000000000	0.000000000	-5.838597000
H	0.000000000	-2.805292000	1.500365000
H	-3.879909000	0.000000000	3.275344000
H	0.000000000	-2.144247000	-4.601106000
H	-2.805292000	0.000000000	-1.500365000
H	0.000000000	-5.182841000	0.816007000
H	0.000000000	-3.879909000	-3.275344000
H	-5.738526000	0.000000000	1.634997000
H	-5.182841000	0.000000000	-0.816007000
H	0.000000000	-5.738526000	-1.634997000

6.2 [Os (4'-(4-methylphenyl)-2,2′:6′,2″-terpyridine)$_2$]$^{2+}$

Os	-0.000002000	0.003688000	-0.001165000
N	-0.430841000	-1.620269000	-1.266036000
N	0.429456000	-1.260909000	1.623398000
N	-2.006713000	0.003455000	-0.001484000
N	2.006709000	0.002246000	-0.000121000
N	-0.431733000	1.628282000	1.262759000
N	0.433105000	1.267865000	-1.625164000
C	-1.300789000	-3.710177000	-2.898300000
C	-2.219604000	-2.891889000	-2.255077000
C	0.057367000	-3.469522000	-2.714606000
C	-0.060245000	-2.707542000	3.473781000
C	1.297719000	-2.892383000	3.714649000
C	-1.774333000	-1.851850000	-1.442712000
C	-4.062044000	-0.950887000	-0.733490000
C	0.449920000	-2.422131000	-1.896474000
C	-0.451946000	-1.889846000	2.425733000
C	2.217193000	-2.250720000	2.895881000
C	-2.673244000	-0.934692000	-0.722930000
C	-4.786685000	0.000376000	0.001519000
C	1.772756000	-1.438761000	1.855165000
C	-4.062599000	0.953536000	0.734563000
C	2.672421000	-0.720607000	0.937490000
C	4.061220000	-0.734627000	0.952270000
C	-2.673765000	0.940356000	0.721035000
C	4.786677000	-0.001831000	-0.000035000

C	-1.775363000	1.859026000	1.439517000
C	2.674575000	0.723300000	-0.937604000
C	4.063411000	0.733331000	-0.952228000
C	-2.221283000	2.899777000	2.250620000
C	-0.446514000	1.898543000	-2.428101000
C	1.776925000	1.443404000	-1.855758000
C	0.448524000	2.431709000	1.891921000
C	-1.302973000	3.719636000	2.892552000
C	-0.052471000	2.715841000	-3.475588000
C	2.223674000	2.254891000	-2.895850000
C	0.055328000	3.479831000	2.708811000
C	1.306020000	2.898395000	-3.715217000
H	-1.640290000	-4.519937000	-3.531176000
H	-3.279895000	-3.059229000	-2.383677000
H	0.810512000	-4.079728000	-3.194834000
H	-0.813890000	-3.186541000	4.084334000
H	1.636564000	-3.524910000	4.524955000
H	-4.587285000	-1.685563000	-1.326908000
H	-1.498047000	-1.724114000	2.208758000
H	3.277357000	-2.380117000	3.063442000
H	1.496187000	-2.205348000	-1.731545000
H	4.585551000	-1.329715000	1.686219000
H	-4.587984000	1.686826000	1.329538000
H	-1.493079000	1.734495000	-2.212099000
H	-3.281688000	3.066544000	2.379079000
H	4.589717000	1.326553000	-1.686303000
H	1.494924000	2.215549000	1.727034000
H	-0.804749000	3.196314000	-4.086670000
H	3.284206000	2.382534000	-3.062415000
H	-1.642959000	4.529981000	3.524417000
H	0.808106000	4.091273000	3.188041000
H	1.646659000	3.530589000	-4.525031000
C	-6.266902000	-0.002237000	0.003572000
C	-6.991920000	1.197677000	0.061904000
C	-6.987144000	-1.204879000	-0.047974000
H	-6.469017000	2.146835000	0.081031000
H	-6.460563000	-2.152082000	-0.063009000
C	-8.381806000	1.191054000	0.064376000
C	-8.377481000	-1.203964000	-0.039549000
H	-8.915967000	2.134541000	0.102493000
H	-8.907920000	-2.149898000	-0.064596000
C	-9.102629000	-0.008048000	0.012772000
C	6.266898000	-0.004290000	-0.000635000
C	6.988850000	0.046804000	-1.202173000
C	6.990205000	-0.062550000	1.200412000
H	6.463663000	0.061916000	-2.150146000
H	6.465900000	-0.081174000	2.148807000
C	8.379273000	0.037926000	-1.199228000
C	8.380008000	-0.065461000	1.195814000
H	8.911081000	0.062706000	-2.144389000
H	8.912787000	-0.103417000	2.140099000
C	9.102627000	-0.014414000	-0.002331000
C	10.610433000	0.007971000	-0.000063000
H	11.015504000	-0.383980000	-0.935024000

H	10.982837000	1.031626000	0.115827000
H	11.015622000	-0.580572000	0.825937000
C	-10.610418000	-0.008522000	-0.010563000
H	-11.017362000	0.827702000	0.561976000
H	-10.982286000	0.086960000	-1.036537000
H	-11.014236000	-0.936698000	0.398588000

6.3 [Os (4,4',4"-tri-tert-Butyl-2,2′:6′,2′′-terpyridine)$_2$]$^{2+}$

Os	-0.004223000	-0.001959000	0.002156000
N	-0.387192000	-2.068889000	0.017713000
N	0.422188000	0.025140000	2.059694000
N	-2.010615000	-0.052509000	-0.000298000
N	2.003120000	0.053772000	0.009867000
N	-0.489693000	2.042417000	-0.016929000
N	0.436296000	-0.006344000	-2.053278000
C	-1.218039000	-4.775020000	0.042743000
C	-2.135852000	-3.725138000	0.033577000
C	0.136512000	-4.410035000	0.037680000
C	-0.046419000	0.024281000	4.415163000
C	1.310852000	0.061829000	4.747562000
C	-1.718523000	-2.395642000	0.021458000
C	-4.036173000	-1.302408000	0.015751000
C	0.506058000	-3.078928000	0.025427000
C	-0.444258000	0.007164000	3.087361000
C	2.206788000	0.081804000	3.672774000
C	-2.648355000	-1.252812000	0.012143000
C	-4.796948000	-0.122692000	0.006512000
C	1.764528000	0.064340000	2.356279000
C	-4.101250000	1.090282000	-0.006574000
C	2.665977000	0.084583000	1.191442000
C	4.058326000	0.132383000	1.212918000
C	-2.708262000	1.109417000	-0.009929000
C	4.788622000	0.149158000	0.020680000
C	-1.840641000	2.299984000	-0.021319000
C	2.675290000	0.066257000	-1.171044000
C	4.062785000	0.113636000	-1.180513000
C	-2.321028000	3.603151000	-0.035402000
C	-0.423609000	-0.039001000	-3.085987000
C	1.780166000	0.028486000	-2.341687000
C	0.347024000	3.094414000	-0.025824000
C	-1.455880000	4.703142000	-0.044751000
C	-0.017334000	-0.041111000	-4.411376000
C	2.231028000	0.026836000	-3.655110000
C	-0.089036000	4.410153000	-0.039387000
C	1.341925000	-0.008582000	-4.735399000
H	-3.195556000	-3.929293000	0.036167000
H	0.921107000	-5.154900000	0.043633000
H	-0.815400000	0.007075000	5.173548000
H	-4.529561000	-2.264009000	0.026434000
H	-1.493636000	-0.021604000	2.827105000
H	3.271235000	0.110591000	3.857273000

H	1.549202000	-2.793622000	0.022029000
H	4.567952000	0.157882000	2.163705000
H	-4.638872000	2.025781000	-0.013105000
H	-1.474595000	-0.064034000	-2.831909000
H	-3.390840000	3.757343000	-0.039305000
H	4.583623000	0.124888000	-2.127417000
H	1.403757000	2.863919000	-0.021771000
H	-0.781405000	-0.068953000	-5.174401000
H	3.296662000	0.052910000	-3.833436000
H	0.657994000	5.190445000	-0.045565000
C	6.323071000	0.206289000	-0.012829000
C	-6.330873000	-0.199701000	0.013887000
C	1.827363000	0.079157000	6.190969000
C	1.867712000	-0.012560000	-6.175499000
C	-2.013751000	6.131064000	-0.059699000
C	-1.630593000	-6.251035000	0.058483000
C	6.860857000	-1.043759000	-0.748729000
H	7.953190000	-1.012271000	-0.780112000
H	6.561366000	-1.960151000	-0.233336000
H	6.500463000	-1.099912000	-1.778297000
C	6.765453000	1.482287000	-0.767723000
H	7.857054000	1.532248000	-0.799671000
H	6.401777000	1.496396000	-1.797599000
H	6.398221000	2.381037000	-0.265247000
C	6.933241000	0.240371000	1.399638000
H	6.678588000	-0.652991000	1.976167000
H	8.021867000	0.281133000	1.320561000
H	6.611141000	1.120699000	1.962351000
C	-6.793651000	-0.935660000	1.293638000
H	-6.399495000	-1.952958000	1.346148000
H	-6.472217000	-0.399962000	2.190757000
H	-7.884884000	-1.000074000	1.308264000
C	-6.805911000	-0.981372000	-1.233742000
H	-6.491190000	-0.479933000	-2.152746000
H	-6.415018000	-2.001090000	-1.252264000
H	-7.897352000	-1.043643000	-1.236627000
C	-6.981850000	1.194668000	-0.008482000
H	-6.707760000	1.787508000	0.868308000
H	-6.711765000	1.756904000	-0.906468000
H	-8.068530000	1.084582000	-0.003795000
C	-2.884445000	6.346168000	1.201071000
H	-3.727871000	5.653125000	1.239157000
H	-2.294061000	6.214485000	2.111657000
H	-3.287759000	7.362235000	1.200818000
C	-1.053683000	-6.919577000	1.329008000
H	-1.335164000	-7.975688000	1.348747000
H	0.036576000	-6.863977000	1.361144000
H	-1.445557000	-6.445790000	2.232909000
C	-3.159041000	-6.428784000	0.062216000
H	-3.622448000	-5.997555000	-0.829225000
H	-3.397461000	-7.494664000	0.073717000
H	-3.620277000	-5.978892000	0.945539000
C	-1.056614000	-6.946616000	-1.198716000
H	0.033562000	-6.891806000	-1.234558000

H	-1.338075000	-8.002926000	-1.195165000
H	-1.450594000	-6.492336000	-2.111659000
C	-0.894012000	7.186514000	-0.068623000
H	-0.261855000	7.116816000	0.820518000
H	-0.258091000	7.097776000	-0.953349000
H	-1.338556000	8.184200000	-0.080233000
C	-2.881077000	6.321045000	-1.326779000
H	-2.288128000	6.172047000	-2.233007000
H	-3.724068000	5.626924000	-1.353694000
H	-3.284947000	7.336664000	-1.347387000
C	2.665826000	1.360284000	6.413367000
H	3.037267000	1.382795000	7.441246000
H	3.529782000	1.405437000	5.746515000
H	2.061996000	2.256752000	6.249901000
C	2.714642000	-1.166976000	6.423572000
H	2.145304000	-2.087384000	6.269319000
H	3.578198000	-1.184766000	5.754830000
H	3.088591000	-1.166034000	7.450819000
C	0.677858000	0.061572000	7.213914000
H	0.064793000	-0.838848000	7.122283000
H	1.093460000	0.076391000	8.223955000
H	0.028119000	0.934707000	7.111016000
C	0.724701000	-0.042869000	-7.205388000
H	1.146684000	-0.043706000	-8.212888000
H	0.109190000	-0.940591000	-7.104400000
H	0.076132000	0.832962000	-7.119380000
C	2.754212000	-1.263454000	-6.384308000
H	3.612647000	-1.273718000	-5.708830000
H	2.181853000	-2.180539000	-6.221707000
H	3.135860000	-1.277386000	-7.408612000
C	2.709765000	1.263863000	-6.410871000
H	3.569992000	1.316797000	-5.739800000
H	3.087075000	1.271429000	-7.436835000
H	2.106641000	2.163568000	-6.263333000

6.4 [Os (4'-(4-chlorophenyl)-2,2′:6′,2′′-terpyridine)$_2$]$^{2+}$

Os	0.000000000	0.000000000	-0.000001000
N	-2.047130000	0.214368000	0.430135000
N	-0.214372000	-2.047129000	-0.430136000
N	0.000000000	0.000000000	2.006021000
N	0.000000000	0.000000000	-2.006023000
N	2.047130000	-0.214368000	0.430135000
N	0.214372000	2.047129000	-0.430136000
C	-4.684543000	0.489676000	1.299602000
C	-3.649838000	0.378938000	2.218721000
C	-4.382884000	0.461142000	-0.058475000
C	-0.461150000	-4.382882000	0.058475000
C	-0.489680000	-4.684542000	-1.299602000
C	-2.337311000	0.242260000	1.773474000
C	-1.196908000	0.121269000	4.061021000
C	-3.060991000	0.322914000	-0.451011000

C	-0.322922000	-3.060989000	0.451010000
C	-0.378937000	-3.649838000	-2.218721000
C	-1.178121000	0.118403000	2.672062000
C	0.000000000	0.000000000	4.782279000
C	-0.242257000	-2.337311000	-1.773475000
C	1.196908000	-0.121269000	4.061021000
C	-0.118397000	-1.178122000	-2.672064000
C	-0.121260000	-1.196910000	-4.061023000
C	1.178121000	-0.118403000	2.672062000
C	0.000000000	0.000000000	-4.782279000
C	2.337311000	-0.242260000	1.773474000
C	0.118397000	1.178122000	-2.672064000
C	0.121260000	1.196910000	-4.061023000
C	3.649838000	-0.378938000	2.218721000
C	0.322922000	3.060989000	0.451010000
C	0.242257000	2.337311000	-1.773475000
C	3.060991000	-0.322914000	-0.451011000
C	4.684543000	-0.489676000	1.299602000
C	0.461150000	4.382882000	0.058475000
C	0.378937000	3.649838000	-2.218721000
C	4.382884000	-0.461142000	-0.058475000
C	0.489680000	4.684542000	-1.299602000
H	-5.706767000	0.596209000	1.638929000
H	-3.860658000	0.398697000	3.278876000
H	-5.154827000	0.543868000	-0.811732000
H	-0.543881000	-5.154824000	0.811732000
H	-0.596216000	-5.706766000	-1.638928000
H	-2.133275000	0.239886000	4.587335000
H	-0.296500000	-2.790222000	1.497407000
H	-0.398695000	-3.860658000	-3.278876000
H	-2.790226000	0.296490000	-1.497408000
H	-0.239883000	-2.133277000	-4.587338000
H	2.133275000	-0.239886000	4.587335000
H	0.296500000	2.790222000	1.497407000
H	3.860658000	-0.398697000	3.278876000
H	0.239883000	2.133277000	-4.587338000
H	2.790226000	-0.296490000	-1.497408000
H	0.543881000	5.154824000	0.811732000
H	0.398695000	3.860658000	-3.278876000
H	5.706767000	-0.596209000	1.638929000
H	5.154827000	-0.543868000	-0.811732000
H	0.596216000	5.706766000	-1.638928000
C	0.000000000	0.000000000	6.263729000
C	1.030402000	0.624286000	6.981743000
C	-1.030402000	-0.624286000	6.981743000
H	1.827350000	1.136737000	6.456832000
H	-1.827350000	-1.136737000	6.456832000
C	1.035517000	0.630083000	8.372116000
C	-1.035517000	-0.630083000	8.372116000
H	1.829464000	1.124593000	8.915998000
H	-1.829464000	-1.124593000	8.915998000
C	0.000000000	0.000000000	9.053895000
C	0.000000000	0.000000000	-6.263728000
C	-0.624325000	1.030378000	-6.981740000

C	0.624325000	-1.030378000	-6.981740000
H	-1.136808000	1.827304000	-6.456828000
H	1.136808000	-1.827304000	-6.456828000
C	-0.630122000	1.035493000	-8.372114000
C	0.630122000	-1.035493000	-8.372114000
H	-1.124666000	1.829418000	-8.915995000
H	1.124666000	-1.829418000	-8.915995000
C	0.000000000	0.000000000	-9.053892000
Cl	0.000000000	0.000000000	10.815313000
Cl	0.000000000	0.000000000	-10.815310000

6.5 [Os (4'-chloro-2,2′:6′,2″-terpyridine)$_2$]$^{2+}$

Os	0.000000000	0.000000000	0.000000000
N	2.059438000	0.000000000	0.429112000
N	0.000000000	2.059438000	-0.429112000
N	0.000000000	0.000000000	2.008442000
N	0.000000000	0.000000000	-2.008442000
N	-2.059438000	0.000000000	0.429112000
N	0.000000000	-2.059438000	-0.429112000
C	4.711487000	0.000000000	1.302941000
C	3.669235000	0.000000000	2.220673000
C	4.409385000	0.000000000	-0.054720000
C	0.000000000	4.409385000	0.054720000
C	0.000000000	4.711487000	-1.302941000
C	2.351462000	0.000000000	1.772372000
C	1.212865000	0.000000000	4.060982000
C	3.080366000	0.000000000	-0.449531000
C	0.000000000	3.080366000	0.449531000
C	0.000000000	3.669235000	-2.220673000
C	1.186614000	0.000000000	2.670211000
C	0.000000000	0.000000000	4.743115000
C	0.000000000	2.351462000	-1.772372000
C	-1.212865000	0.000000000	4.060982000
C	0.000000000	1.186614000	-2.670211000
C	0.000000000	1.212865000	-4.060982000
C	-1.186614000	0.000000000	2.670211000
C	0.000000000	0.000000000	-4.743115000
C	-2.351462000	0.000000000	1.772372000
C	0.000000000	-1.186614000	-2.670211000
C	0.000000000	-1.212865000	-4.060982000
C	-3.669235000	0.000000000	2.220673000
C	0.000000000	-3.080366000	0.449531000
C	0.000000000	-2.351462000	-1.772372000
C	-3.080366000	0.000000000	-0.449531000
C	-4.711487000	0.000000000	1.302941000
C	0.000000000	-4.409385000	0.054720000
C	0.000000000	-3.669235000	-2.220673000
C	-4.409385000	0.000000000	-0.054720000
C	0.000000000	-4.711487000	-1.302941000
H	5.738763000	0.000000000	1.643564000
H	3.878944000	0.000000000	3.281060000

H	5.186107000	0.000000000	-0.807587000
H	0.000000000	5.186107000	0.807587000
H	0.000000000	5.738763000	-1.643564000
H	2.145696000	0.000000000	4.605099000
H	0.000000000	2.811024000	1.496298000
H	0.000000000	3.878944000	-3.281060000
H	2.811024000	0.000000000	-1.496298000
H	0.000000000	2.145696000	-4.605099000
H	-2.145696000	0.000000000	4.605099000
H	0.000000000	-2.811024000	1.496298000
H	-3.878944000	0.000000000	3.281060000
H	0.000000000	-2.145696000	-4.605099000
H	-2.811024000	0.000000000	-1.496298000
H	0.000000000	-5.186107000	0.807587000
H	0.000000000	-3.878944000	-3.281060000
H	-5.738763000	0.000000000	1.643564000
H	-5.186107000	0.000000000	-0.807587000
H	0.000000000	-5.738763000	-1.643564000
Cl	0.000000000	0.000000000	-6.488830000
Cl	0.000000000	0.000000000	6.488830000

6.6 [Os (4'-methoxy)-2,2′:6′,2″-terpyridine$_2$]$^{2+}$

Os	0.000000000	0.000000000	0.036790000
N	1.402467000	0.590992000	-1.413443000
N	-1.402467000	-0.590992000	-1.413443000
N	-0.216793000	2.001182000	0.036218000
N	0.216793000	-2.001182000	0.036218000
N	-1.493111000	0.269761000	1.491978000
N	1.493111000	-0.269761000	1.491978000
C	3.186062000	1.666180000	-3.274653000
C	2.350332000	2.496885000	-2.540336000
C	3.117346000	0.292011000	-3.066606000
C	-3.117346000	-0.292011000	-3.066606000
C	-3.186062000	-1.666180000	-3.274653000
C	1.464009000	1.950789000	-1.615082000
C	0.409734000	4.140686000	-0.818164000
C	2.219503000	-0.202768000	-2.134115000
C	-2.219503000	0.202768000	-2.134115000
C	-2.350332000	-2.496885000	-2.540336000
C	0.541910000	2.754379000	-0.794474000
C	-0.522213000	4.742974000	0.035413000
C	-1.464009000	-1.950789000	-1.615082000
C	-1.296572000	3.942315000	0.891080000
C	-0.541910000	-2.754379000	-0.794474000
C	-0.409734000	-4.140686000	-0.818164000
C	-1.126033000	2.569755000	0.873735000
C	0.522213000	-4.742974000	0.035413000
C	-1.846474000	1.582668000	1.697090000
C	1.126033000	-2.569755000	0.873735000
C	1.296572000	-3.942315000	0.891080000
C	-2.823441000	1.924307000	2.628362000

C	2.114643000	0.682954000	2.214743000
C	1.846474000	-1.582668000	1.697090000
C	-2.114643000	-0.682954000	2.214743000
C	-3.455242000	0.931671000	3.365785000
C	3.092665000	0.394778000	3.153604000
C	2.823441000	-1.924307000	2.628362000
C	-3.092665000	-0.394778000	3.153604000
C	3.455242000	-0.931671000	3.365785000
H	3.876930000	2.085134000	-3.994843000
H	2.387191000	3.567608000	-2.684770000
H	3.747518000	-0.396035000	-3.614132000
H	-3.747518000	0.396035000	-3.614132000
H	-3.876930000	-2.085134000	-3.994843000
H	1.016675000	4.732843000	-1.484916000
H	-2.139845000	1.264473000	-1.945883000
H	-2.387191000	-3.567608000	-2.684770000
H	2.139845000	-1.264473000	-1.945883000
H	-1.016675000	-4.732843000	-1.484916000
H	-2.010775000	4.422451000	1.544721000
H	1.808491000	1.702062000	2.023940000
H	-3.087151000	2.962601000	2.774516000
H	2.010775000	-4.422451000	1.544721000
H	-1.808491000	-1.702062000	2.023940000
H	3.555852000	1.203189000	3.703354000
H	3.087151000	-2.962601000	2.774516000
H	-4.215507000	1.190542000	4.091379000
H	-3.555852000	-1.203189000	3.703354000
H	4.215507000	-1.190542000	4.091379000
O	0.748870000	-6.064984000	0.110903000
O	-0.748870000	6.064984000	0.110903000
C	0.000000000	-6.953211000	-0.733409000
H	0.187232000	-6.737795000	-1.788132000
H	0.360193000	-7.950261000	-0.494064000
H	-1.069009000	-6.886726000	-0.517530000
C	0.000000000	6.953211000	-0.733409000
H	-0.360193000	7.950261000	-0.494064000
H	1.069009000	6.886726000	-0.517530000
H	-0.187232000	6.737795000	-1.788132000

6.7 [Os 4'-(N-Pyrrolidinyl)-2,2′:6′,2″-terpyridine)$_2$]$^{2+}$

Os	0.000000000	0.000000000	0.000000000
N	1.454163000	1.452826000	0.436843000
C	1.661523000	1.656973000	1.782512000
C	2.597835000	2.588092000	2.225375000
C	3.335060000	3.325090000	1.308018000
C	3.119230000	3.113699000	-0.050353000
C	2.177497000	2.175778000	-0.441963000
N	0.000000000	0.000000000	2.016854000
C	0.836061000	0.832540000	2.687248000
C	0.857958000	0.856957000	4.070777000
C	0.000000000	0.000000000	4.809324000

C	-0.857958000	-0.856957000	4.070777000
C	-0.836061000	-0.832540000	2.687248000
N	-1.454163000	-1.452826000	0.436843000
C	-1.661523000	-1.656973000	1.782512000
C	-2.597835000	-2.588092000	2.225375000
C	-3.335060000	-3.325090000	1.308018000
C	-3.119230000	-3.113699000	-0.050353000
C	-2.177497000	-2.175778000	-0.441963000
N	1.454163000	-1.452826000	-0.436843000
C	1.661523000	-1.656973000	-1.782512000
C	2.597835000	-2.588092000	-2.225375000
C	3.335060000	-3.325090000	-1.308018000
C	3.119229000	-3.113699000	0.050353000
C	2.177496000	-2.175778000	0.441963000
N	0.000000000	0.000000000	-2.016854000
C	0.836060000	-0.832540000	-2.687248000
C	0.857957000	-0.856957000	-4.070777000
C	0.000000000	0.000000000	-4.809324000
C	-0.857957000	0.856957000	-4.070777000
C	-0.836060000	0.832540000	-2.687248000
N	-1.454163000	1.452826000	-0.436843000
C	-1.661523000	1.656973000	-1.782512000
C	-2.597835000	2.588092000	-2.225375000
C	-3.335060000	3.325090000	-1.308018000
C	-3.119229000	3.113699000	0.050353000
C	-2.177496000	2.175778000	0.441963000
H	2.749914000	2.735485000	3.285442000
H	4.063480000	4.049654000	1.648822000
H	3.668488000	3.662930000	-0.803499000
H	1.982624000	1.983573000	-1.488018000
H	1.519538000	1.533835000	4.588468000
H	-1.519538000	-1.533835000	4.588468000
H	-2.749914000	-2.735485000	3.285442000
H	-4.063480000	-4.049654000	1.648822000
H	-3.668488000	-3.662930000	-0.803499000
H	-1.982624000	-1.983573000	-1.488018000
H	2.749914000	-2.735485000	-3.285442000
H	4.063480000	-4.049654000	-1.648822000
H	3.668488000	-3.662930000	0.803499000
H	1.982624000	-1.983574000	1.488018000
H	1.519537000	-1.533836000	-4.588468000
H	-1.519537000	1.533836000	-4.588468000
H	-2.749914000	2.735485000	-3.285442000
H	-4.063480000	4.049654000	-1.648822000
H	-3.668488000	3.662930000	0.803499000
H	-1.982624000	1.983574000	1.488018000
N	0.000000000	0.000000000	-6.162177000
C	-0.924948000	0.797701000	-6.983167000
H	-0.661032000	1.861504000	-6.935798000
H	-1.953139000	0.686884000	-6.629610000
H	-0.946301000	0.974078000	-9.165351000
C	-0.731395000	0.232924000	-8.394995000
H	-1.398907000	-0.619475000	-8.548170000
C	0.731395000	-0.232924000	-8.394995000

H	1.398907000	0.619475000	-8.548170000
H	0.946301000	-0.974078000	-9.165351000
C	0.924948000	-0.797701000	-6.983167000
H	1.953139000	-0.686884000	-6.629610000
H	0.661032000	-1.861504000	-6.935798000
N	0.000000000	0.000000000	6.162177000
C	0.924948000	0.797701000	6.983166000
H	0.661032000	1.861504000	6.935798000
H	1.953140000	0.686884000	6.629610000
H	0.946301000	0.974078000	9.165351000
C	0.731395000	0.232924000	8.394995000
H	1.398907000	-0.619475000	8.548170000
C	-0.731395000	-0.232924000	8.394995000
H	-1.398907000	0.619475000	8.548170000
H	-0.946301000	-0.974078000	9.165351000
C	-0.924948000	-0.797701000	6.983166000
H	-1.953140000	-0.686884000	6.629610000
H	-0.661032000	-1.861504000	6.935798000

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