

New Donor-Acceptor Conjugates based on a Trifluorenylporphyrin linked to a Redox-Switchable Ruthenium Unit.

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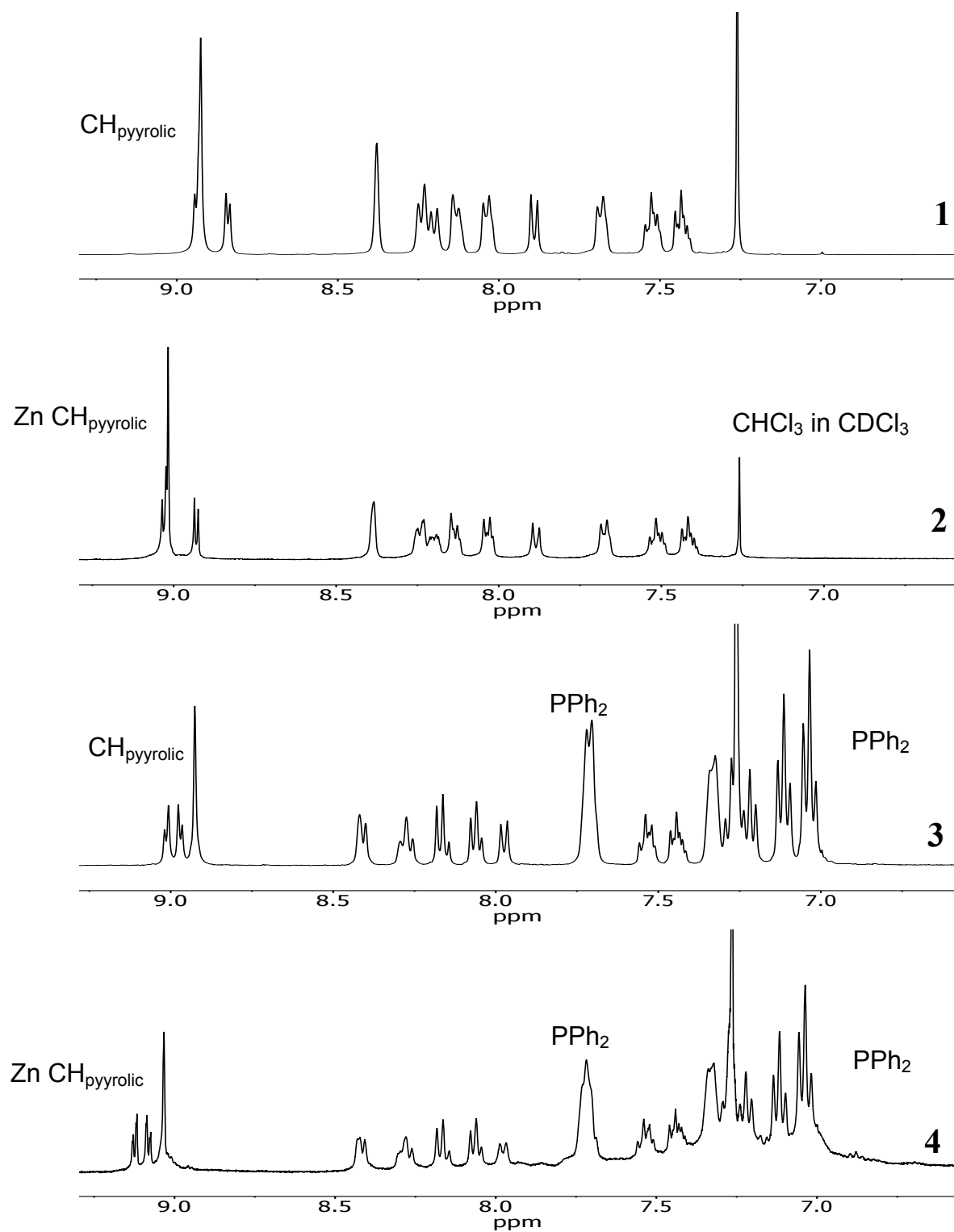


Figure S1. ^1H NMR spectra for 1-4 in CHCl_3 shown between 9.3 and 6.5 ppm for comparison.

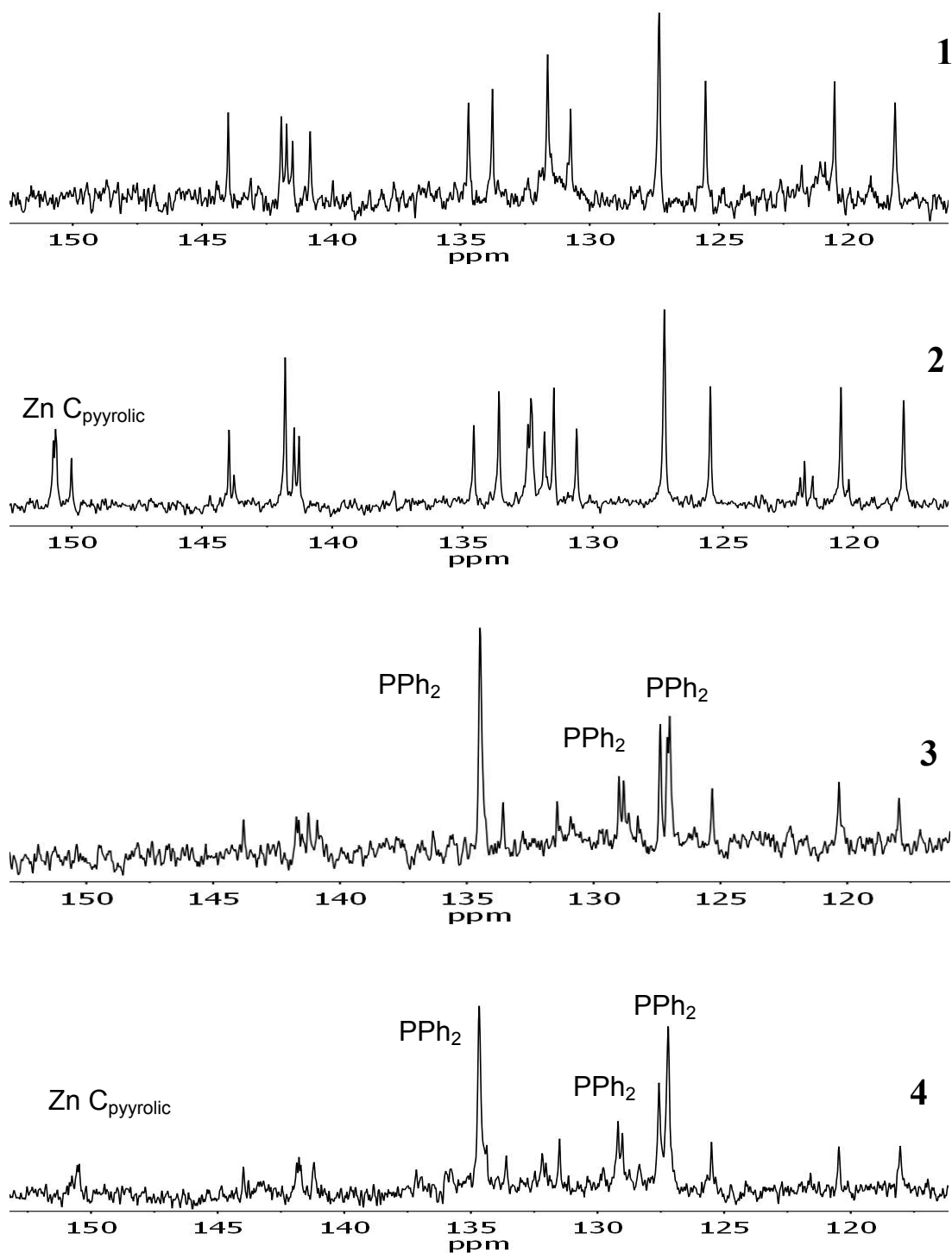


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectra for **1-4** in CHCl_3 shown between 152 and 116 ppm for comparison.

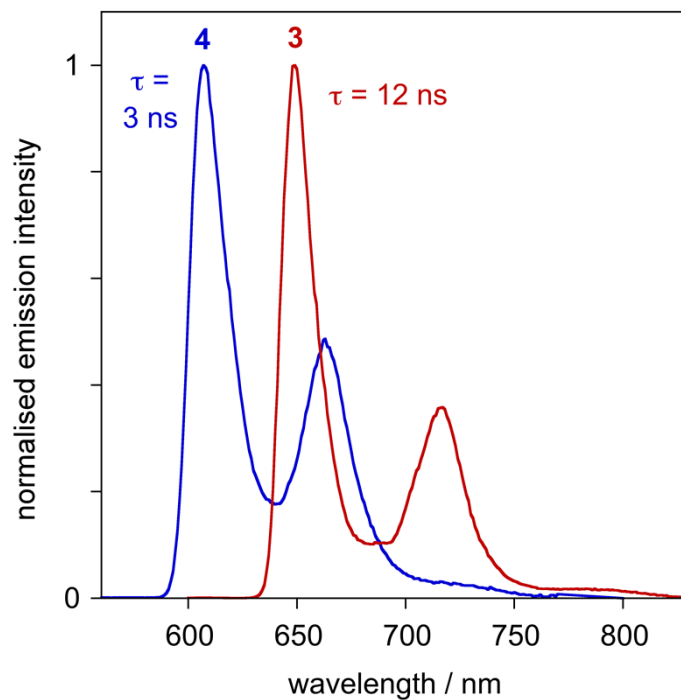


Figure S3. Emission spectra for **3** and **4** in a mixed solvent system of diethyl ether / isopentane / ethanol (2:2:1 v/v) at 77 K.

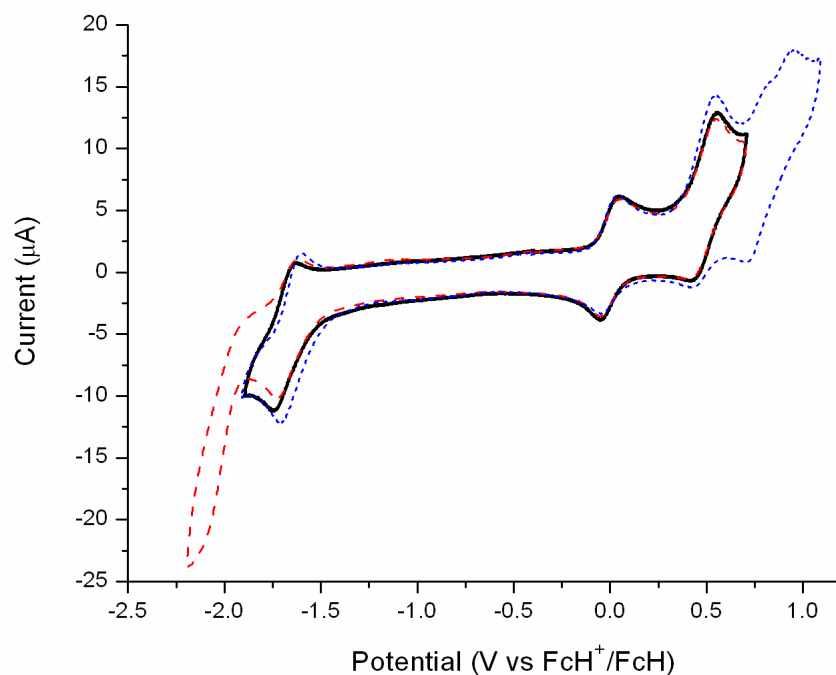


Figure S4. Cyclic voltammograms showing the irreversible waves on third oxidation and on second reduction for **3** in 0.1 M $[\text{Bu}_4\text{N}][\text{PF}_6]/\text{DCM}$.

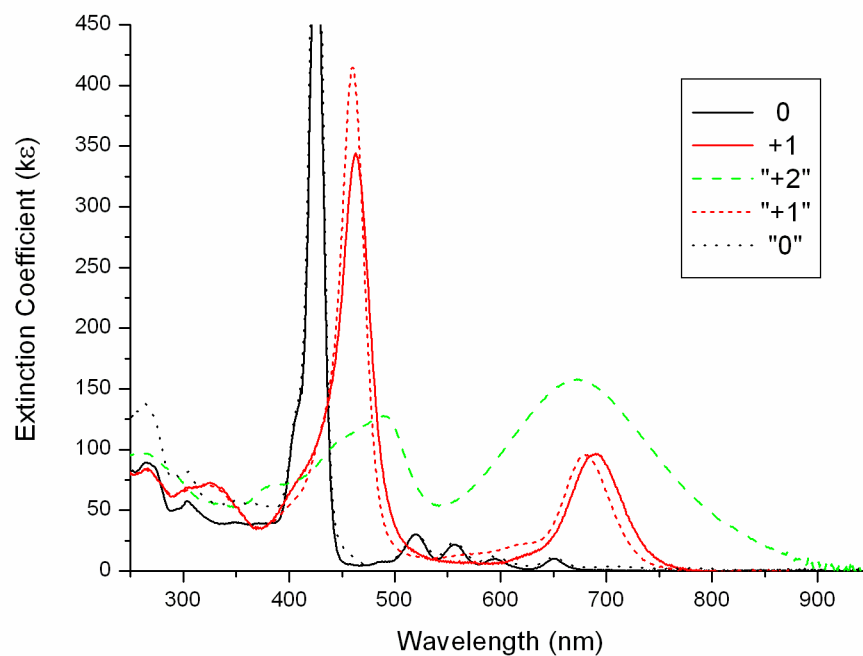


Figure S5. UV-visible absorption spectra for **1** on oxidation to the dication in 0.1 M $[\text{Bu}_4\text{N}][\text{PF}_6]/\text{DCM}$ from a SEC cell. Back reduction of the dication to its monocation and neutral species shows that their spectra are not identical to the spectra from the initial monocation and neutral species.

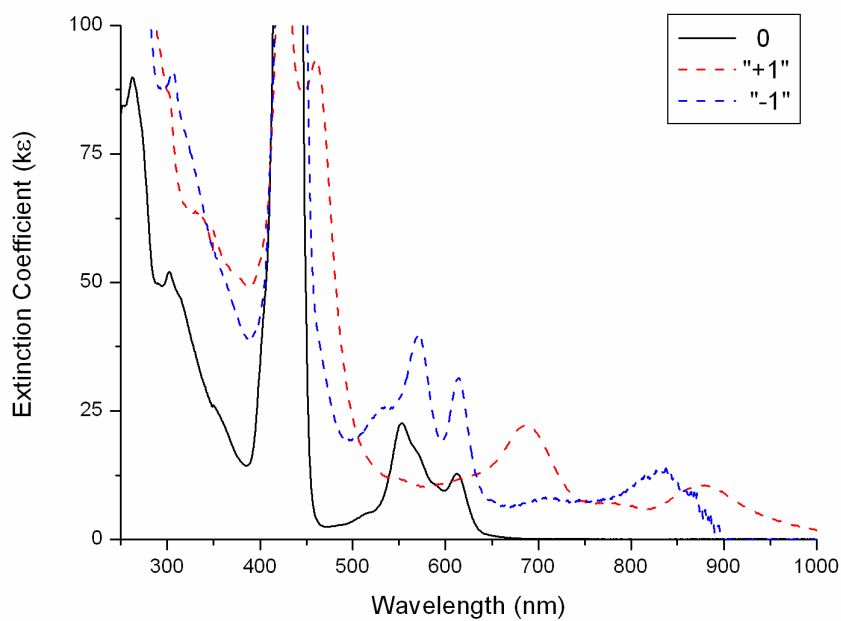


Figure S6. UV-visible absorption spectra for **2** and its unstable oxidised and reduced species in 0.1 M $[\text{Bu}_4\text{N}][\text{PF}_6]/\text{DCM}$ obtained by SEC.

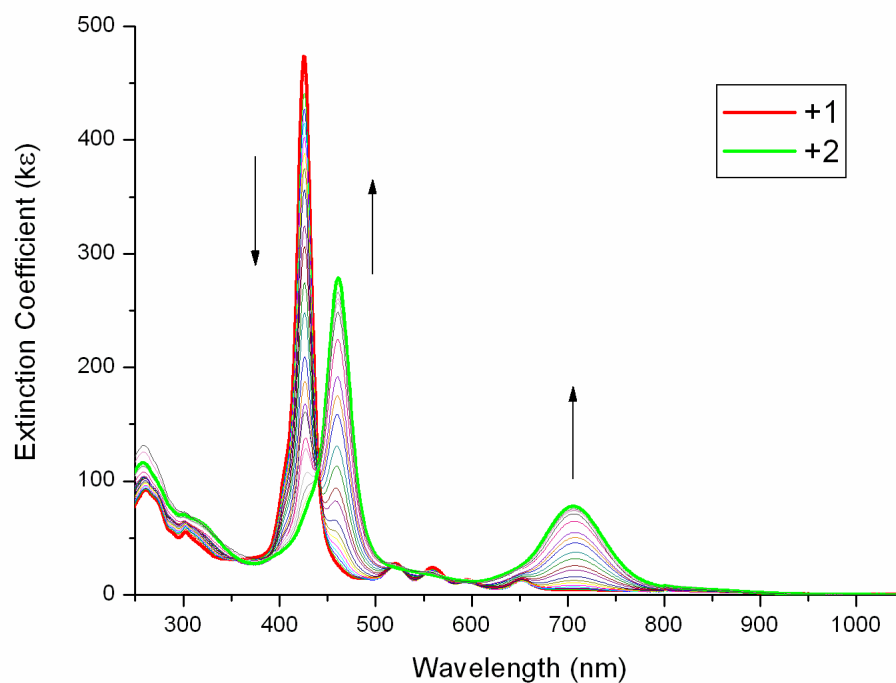


Figure S7. Progression in the UV-visible absorption spectra for **3** from its monocation to its dication in 0.1 M $[\text{Bu}_4\text{N}][\text{PF}_6]/\text{DCM}$ with a SEC cell.

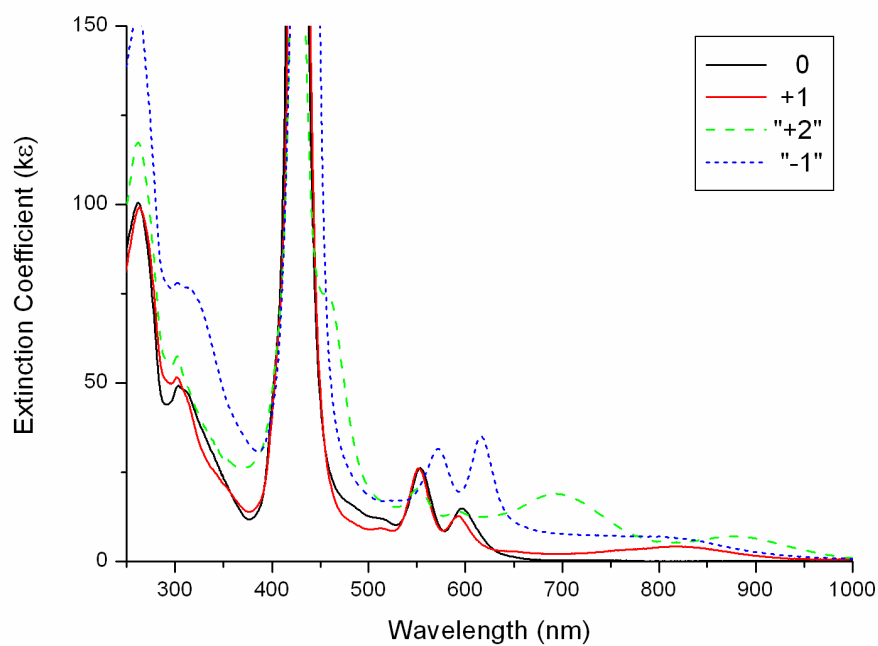


Figure S8. UV-visible absorption spectra for **4**, its stable monocation, unstable dication and unstable reduced species in 0.1 M $[\text{Bu}_4\text{N}][\text{PF}_6]/\text{DCM}$ obtained by SEC means.

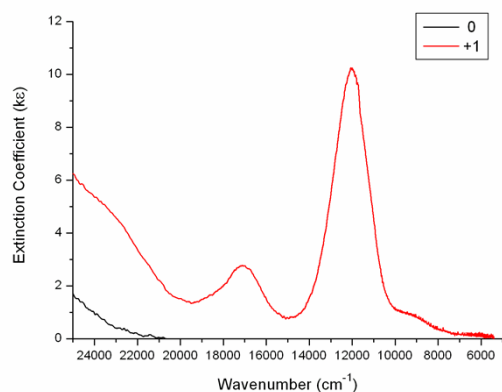


Figure S9. Near-IR (NIR) absorption spectra for the known ruthenium complex $\text{Ru}(\text{dppe})_2(\text{C}\equiv\text{CPh})\text{Cl}$ and its monocation in 0.1 M $[\text{Bu}_4\text{N}][\text{PF}_6]/\text{DCM}$. A Perkin-Elmer Lambda 900 spectrometer was used to record these SEC spectra.

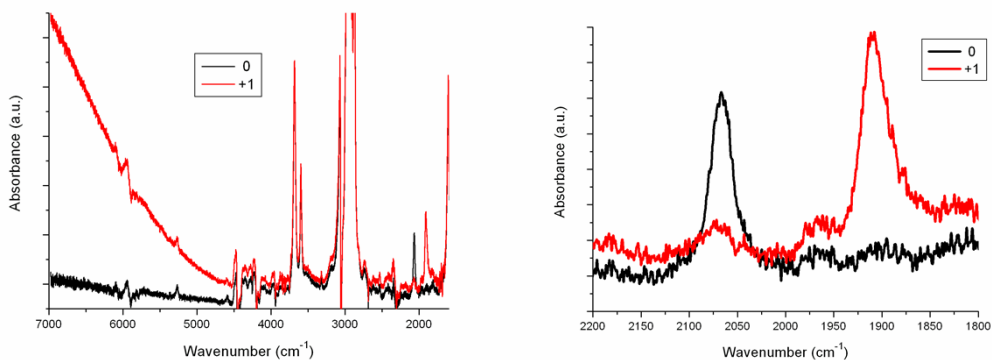


Figure S10. Near-Infrared – Infrared (NIR-IR) absorption spectra for **3** and its oxidised species in 0.1 M $\text{TBAPF}_6/\text{DCM}$ obtained by SEC.

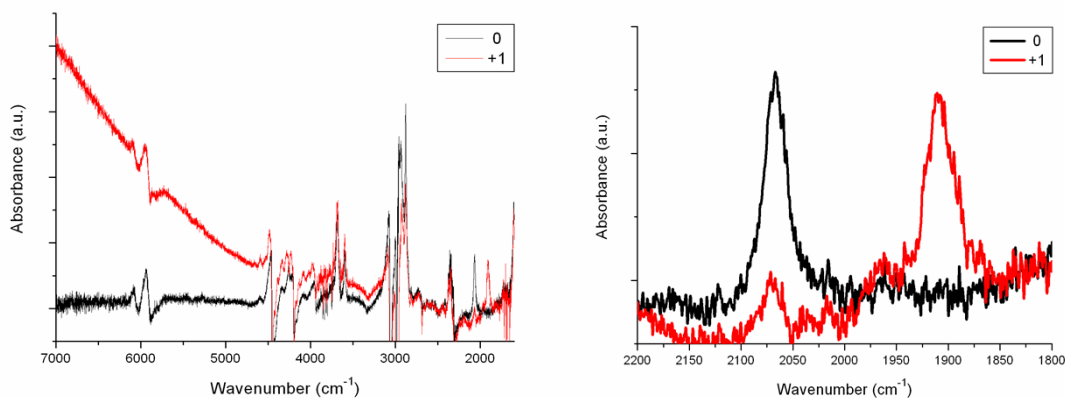


Figure S11. NIR-IR absorption spectra for **4** and its oxidised species in 0.1 M $[\text{Bu}_4\text{N}][\text{PF}_6]/\text{DCM}$.

Table S1. Orbital energies and % atom contributions for **1**, porp = porphyrin unit, F11 is the fluorene unit with H attached to N by the ethynylphenylene (HC≡C-C₆H₄) unit, F12 = fluorene unit opposite ethynylphenylene (HC≡C-C₆H₄) unit.

MO		eV	C≡CH	C ₆ H ₄	porp	F11	F12	F13
243	L+6	-0.48	2	6	76	6	5	5
242	L+5	-0.85	2	7	5	37	13	36
241	L+4	-0.86	7	22	6	12	43	10
240	L+3	-0.88	5	18	4	27	17	29
239	L+2	-0.99	6	20	23	15	19	17
238	L+1	-2.26	0	1	93	3	0	3
237	LUMO	-2.27	0	3	93	1	3	1
236	HOMO	-4.97	0	2	86	4	4	4
235	H-1	-5.37	0	0	98	1	1	1
234	H-2	-5.98	0	0	4	56	39	1
233	H-3	-5.99	0	0	4	7	22	66
232	H-4	-6.06	0	1	13	29	32	25
231	H-5	-6.26	0	0	98	0	0	0
230	H-6	-6.38	8	16	72	1	1	1

Table S2. Orbital energies and % atom contributions for **2**. F11 and F13 are ‘identical’ fluorene groups, F12 = unique fluorene unit.

MO		eV	C≡CH	C ₆ H ₄	porp	F11	F12	F13	Zn
257	L+6	-0.42	1	4	82	5	4	4	0
256	L+5	-0.83	3	10	5	31	20	30	0
255	L+4	-0.85	5	17	5	20	39	14	0
254	L+3	-0.88	5	18	3	27	12	33	0
253	L+2	-0.94	7	24	16	14	22	16	0
252	L+1	-2.15	0	1	93	3	1	3	0
251	LUMO	-2.17	0	3	93	1	3	1	0
250	HOMO	-5.05	0	2	77	3	3	3	12
249	H-1	-5.27	0	0	98	0	0	0	0
248	H-2	-5.28	0	1	62	1	1	1	33
247	H-3	-5.97	0	0	4	15	61	21	0
246	H-4	-5.97	0	0	5	53	0	42	0
245	H-5	-6.07	1	2	9	26	32	30	0
244	H-6	-6.43	12	20	62	1	2	0	4

Table S3. Orbital energies and % atom contributions for **3**. C α and C β represent the C attached to Ru and the second ethynyl carbon respectively.

MO	eV	Ru	Cl	C α	C β	C ₆ H ₄	dppe	porp	FI1	FI2	FI3
485 L+8	-0.52	1	0	0	0	0	98	0	0	0	0
484 L+7	-0.56	4	1	0	0	0	94	0	0	0	0
483 L+6	-0.61	1	0	0	0	1	98	0	0	0	0
482 L+5	-0.80	0	0	0	0	0	0	5	55	2	39
481 L+4	-0.80	0	0	0	0	0	0	4	5	72	19
480 L+3	-0.82	24	0	0	0	0	76	0	0	0	0
479 L+2	-0.88	0	0	0	0	1	0	16	32	17	34
478 L+1	-2.11	0	0	0	0	3	0	93	1	3	1
477 LUMO	-2.12	0	0	0	0	0	0	93	3	0	3
476 HOMO	-4.61	26	4	7	14	17	3	26	1	1	1
475 H-1	-4.86	40	12	4	17	2	4	19	1	1	1
474 H-2	-4.91	23	6	4	11	5	3	42	2	2	2
473 H-3	-5.22	0	0	0	0	1	0	98	0	0	0
472 H-4	-5.72	8	36	8	3	10	31	2	0	0	1
471 H-5	-5.82	2	35	8	9	2	44	0	0	0	0
470 H-6	-5.91	0	0	0	0	0	0	4	31	63	2
469 H-7	-5.93	0	0	0	0	0	0	5	29	6	60

Table S4. Orbital energies and % atom contributions for **4**.

MO	eV	Ru	Cl	C α	C β	C ₆ H ₄	dppe	porp	FI1	FI2	FI3	Zn
499 L+8	-0.51	1	0	0	0	0	98	0	0	0	0	0
498 L+7	-0.55	5	1	0	0	0	94	0	0	0	0	0
497 L+6	-0.60	1	0	0	0	0	98	0	0	0	0	0
496 L+5	-0.78	0	0	0	0	0	0	5	33	10	52	0
495 L+4	-0.80	0	0	0	0	0	0	4	25	71	0	0
494 L+3	-0.81	24	0	0	0	0	76	0	0	0	0	0
493 L+2	-0.85	0	0	0	0	0	0	10	36	11	42	0
492 L+1	-2.01	0	0	0	0	2	0	93	1	3	1	0
491 LUMO	-2.02	0	0	0	0	0	0	93	3	1	3	0
490 HOMO	-4.63	32	5	9	17	19	4	13	0	0	0	1
489 H-1	-4.87	47	14	6	21	3	5	4	0	0	0	0
488 H-2	-4.95	8	2	1	4	2	1	61	2	2	2	14
487 H-3	-5.13	0	0	0	0	0	0	98	0	0	0	0
486 H-4	-5.14	2	1	0	0	1	0	62	1	1	1	30
485 H-5	-5.71	8	36	8	3	10	31	2	1	1	1	0
484 H-6	-5.82	2	36	8	9	2	43	0	0	0	0	0
483 H-7	-5.90	0	0	0	0	0	0	4	11	67	18	0
482 H-8	-5.92	0	0	0	0	0	0	6	51	0	43	0

Cartesian coordinates

1

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2

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C	2.750800	0.843614	-0.330577	C	-0.971465	4.900562	0.672872
C	3.271253	2.195618	-0.322612	H	-1.228188	4.342131	1.565940
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C	-0.285581	2.728724	-0.401309	H	-1.092972	11.666381	-1.321572
C	-1.427358	1.930210	-0.362234	C	-1.725742	10.960345	0.610871
C	-2.778252	2.448976	-0.430739	H	-1.986607	11.950620	0.965785
H	-3.028220	3.491748	-0.514782	C	-1.898114	9.853139	1.452520
C	-3.621415	1.381906	-0.394687	H	-2.290656	9.984913	2.454895
H	-4.695999	1.380922	-0.442357	C	-1.558990	8.591237	0.981625
C	-2.801824	0.191092	-0.303959	C	-4.802758	-1.279334	-0.265528
C	-3.314890	-1.104604	-0.274995	C	-5.551121	-0.905117	0.866550
C	-2.516576	-2.246417	-0.247288	H	-5.039359	-0.495481	1.730054
C	-3.037900	-3.594508	-0.147602	C	-6.928125	-1.075778	0.859734
H	-4.083123	-3.842546	-0.093612	C	-7.581447	-1.620788	-0.269850
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H	-1.973321	-5.509249	-0.023248	H	-7.335123	-2.406661	-2.268406
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C	1.189707	-6.229630	1.079022	C	-9.027587	-1.689723	0.006496
H	1.436801	-5.615664	1.936742	C	-9.264355	-1.189052	1.307707
C	1.355382	-7.610491	1.137454	C	-10.554380	-1.143791	1.820631
H	1.732943	-8.079543	2.037433	H	-10.742611	-0.761465	2.817942
C	1.026862	-8.415364	0.029391	C	-11.616077	-1.601888	1.028644
C	0.529484	-7.798620	-1.134967	H	-12.627440	-1.572121	1.417170
H	0.280397	-8.411736	-1.992044	C	-11.382619	-2.097556	-0.259127
C	0.367329	-6.417052	-1.186245	H	-12.215609	-2.447487	-0.857803
H	-0.008146	-5.946978	-2.087215	C	-10.086312	-2.145232	-0.780267
C	5.036865	-0.121233	-0.250653	H	-9.910369	-2.529986	-1.778472
C	5.772042	-0.409474	0.914755	C	8.156240	-0.474929	2.034342
H	5.250354	-0.752652	1.800965	H	7.944911	0.164699	2.900778
C	7.149224	-0.240721	0.910532	H	8.152592	-1.521169	2.365640
C	7.815976	0.217305	-0.249478	C	-1.648218	7.237844	1.683159
C	7.091824	0.505545	-1.406861	H	-2.680890	7.000040	1.968663
H	7.592742	0.852909	-2.303318	C	-1.023319	7.210219	2.584938
C	5.705490	0.333863	-1.399979	C	-7.947862	-0.760665	1.951982
H	5.126930	0.545972	-2.291119	H	-7.951280	0.307928	2.202136
C	9.259554	0.302192	0.036133	H	-7.743543	-1.331069	2.867052
C	9.480963	-0.101090	1.373393	C	1.337808	-11.031595	0.132811
C	10.765680	-0.114508	1.901191	C	1.195375	-9.832470	0.085469
H	10.942174	-0.422629	2.925926	H	1.462937	-12.084942	0.174211
C	11.837526	0.277697	1.087891	Zn	0.117764	-0.702298	-0.319782

3

N	4.453388	1.626212	0.225739	C	10.923298	0.129070	0.231647
N	7.381078	1.546077	0.270269	C	11.619540	0.592927	1.361545
N	7.432097	-1.355088	0.147406	H	11.052501	0.941078	2.216345
N	4.504240	-1.276660	0.171309	C	13.015694	0.600726	1.395389
C	2.455748	0.143535	0.190991	H	13.536554	0.957615	2.276650
C	3.090865	1.389213	0.265084	C	13.723227	0.137415	0.285321
C	2.457077	2.674436	0.407644	C	13.029693	-0.330289	-0.854768
H	1.394263	2.815924	0.486348	C	11.642525	-0.336101	-0.885997
C	3.436066	3.634999	0.438480	H	11.101309	-0.682160	-1.759220
H	3.310143	4.697229	0.547738	C	15.171820	0.030799	0.035806
C	4.713958	2.980684	0.320424	C	16.263309	0.356470	0.842055
C	5.969888	3.597666	0.317568	H	16.116885	0.762488	1.836563
C	7.195880	2.917353	0.270042	C	17.553679	0.150391	0.345191
C	8.489893	3.610114	0.199485	H	18.411772	0.398314	0.959220
H	8.617055	4.677878	0.161092	C	17.749256	-0.372794	-0.938040
C	9.446299	2.650446	0.172884	H	18.756630	-0.525742	-1.307553
H	10.513120	2.775172	0.108275	C	16.654687	-0.700647	-1.749682
C	8.750552	1.357595	0.226785	H	16.813466	-1.105684	-2.743152
C	9.425278	0.126424	0.218695	C	15.370465	-0.498230	-1.260792
C	8.793935	-1.121018	0.201891	C	5.899342	-4.825230	0.045841
C	9.429635	-2.413117	0.248120	C	6.379601	-5.508132	-1.087795
H	10.492744	-2.560748	0.313347	H	6.749185	-4.939424	-1.933468
C	8.451392	-3.373796	0.212856	C	6.359067	-6.895495	-1.107231
H	8.578393	-4.441104	0.243906	C	5.862329	-7.624690	-0.002240
C	7.172223	-2.713626	0.143449	C	5.383645	-6.952778	1.123366
C	5.917529	-3.327122	0.089142	H	5.004189	-7.501368	1.978001
C	4.690902	-2.643730	0.074940	C	5.405412	-5.556414	1.140101
C	3.400213	-3.329821	-0.068634	H	5.044681	-5.016561	2.007204
H	3.276122	-4.391822	-0.189329	C	5.960695	-9.064502	-0.301576
C	2.443139	-2.370426	-0.044694	C	6.513506	-9.221696	-1.593970
H	1.378239	-2.487314	-0.142862	C	6.714610	-10.489401	-2.124696
C	3.134586	-1.084902	0.118888	H	7.138011	-10.616219	-3.115088
C	0.961099	0.139577	0.198209	C	6.361572	-11.609217	-1.359432
C	0.233260	0.761860	-0.830972	H	6.513382	-12.604132	-1.761712
H	0.770960	1.234220	-1.645197	C	5.814908	-11.454762	-0.080382
C	-1.157841	0.761160	-0.823489	H	5.548065	-12.331946	0.497708
H	-1.710052	1.244782	-1.620652	C	5.610016	-10.181112	0.458464
C	-1.879650	0.130789	0.217108	H	5.186280	-10.066617	1.449784
C	-1.141763	-0.491864	1.251530	C	5.075570	8.265235	-1.675797
H	-1.680067	-0.965897	2.062149	H	5.646621	8.169626	-2.608110
C	0.249505	-0.483285	1.238366	H	4.008346	8.161814	-1.909821
H	0.801775	-0.953852	2.043779	C	14.023790	-0.766300	-1.929078
C	5.985831	5.095164	0.374901	H	13.903899	-1.827539	-2.181747
C	5.504562	5.850514	-0.711498	H	13.906061	-0.175207	-2.846256
H	5.134486	5.338003	-1.592156	C	6.807039	-7.854700	-2.207944
C	5.524480	7.236136	-0.640313	H	7.874124	-7.736302	-2.435413
C	6.022010	7.891868	0.509492	H	6.235387	-7.698171	-3.131640
C	6.500602	7.148305	1.589039	Ru	-6.531013	-0.101805	0.061116
H	6.880445	7.640052	2.477417	P	-6.425935	0.735938	-2.189390
C	6.478765	5.753773	1.514883	P	-5.933565	-2.185198	-1.002535
H	6.839126	5.158943	2.345384	P	-6.610894	-0.905673	2.324621
C	5.924190	9.347958	0.304475	P	-7.104305	1.987256	1.124063
C	5.369850	9.589366	-0.974110	Cl	-9.092354	-0.293472	-0.084765
C	5.169401	10.889286	-1.420592	C	-4.532872	0.063850	0.187434
H	4.745196	11.080955	-2.400178	C	-3.302049	0.107667	0.212088
C	5.525069	11.956520	-0.584524	C	-4.923119	-1.640127	-2.468610
H	5.374156	12.975671	-0.921109	H	-4.025258	-1.138432	-2.097748
C	6.073792	11.718499	0.680708	H	-4.634105	-2.498446	-3.084011
H	6.343360	12.555848	1.313954	C	-5.779475	-0.646367	-3.286662
C	6.277767	10.412218	1.135004	H	-6.633117	-1.173638	-3.724044
H	6.703655	10.232927	2.115747	H	-5.190562	-0.220983	-4.104967

C	-7.378238	0.435563	3.401789	C	-3.457883	-3.253414	-0.126708
H	-8.036028	-0.037105	4.137907	H	-2.996358	-2.374850	-0.554208
H	-6.581836	0.953010	3.943704	C	-7.630061	-2.366209	2.789879
C	-8.172365	1.458340	2.554763	C	-8.419147	-3.026008	1.839469
H	-8.463544	2.320027	3.164697	H	-8.439634	-2.659264	0.824079
H	-9.063426	0.982029	2.139399	C	-9.212034	-4.117206	2.208596
C	-5.272781	2.101078	-2.638493	H	-9.820072	-4.611546	1.459504
C	-4.549151	2.791711	-1.658818	C	-9.226781	-4.558329	3.531531
H	-4.665234	2.516639	-0.622110	H	-9.842501	-5.403395	3.818021
C	-3.658863	3.810757	-2.013551	C	-8.446816	-3.903474	4.490417
H	-3.105335	4.328622	-1.238526	H	-8.454203	-4.241517	5.520518
C	-3.482480	4.151881	-3.354309	C	-7.655046	-2.816273	4.124133
H	-2.791066	4.939741	-3.630639	H	-7.039237	-2.327238	4.870407
C	-4.204209	3.474537	-4.342607	C	-5.041632	-1.262186	3.222631
H	-4.077535	3.739503	-5.386164	C	-4.276682	-0.235034	3.800793
C	-5.091920	2.459814	-3.988730	H	-4.596001	0.796088	3.729710
H	-5.661875	1.957630	-4.762362	C	-3.076856	-0.519264	4.454264
C	-7.951117	1.228737	-3.087950	H	-2.506011	0.288749	4.897773
C	-8.252701	2.580232	-3.317610	C	-2.609057	-1.833148	4.528038
H	-7.576565	3.351008	-2.972615	H	-1.677961	-2.053309	5.038071
C	-9.427111	2.943147	-3.979311	C	-3.345974	-2.857888	3.931783
H	-9.643179	3.992372	-4.142649	H	-2.985721	-3.879253	3.959928
C	-10.318731	1.964603	-4.419171	C	-4.550716	-2.576986	3.285473
H	-11.227792	2.247173	-4.937876	H	-5.101359	-3.383952	2.821352
C	-10.038828	0.618098	-4.176499	C	-8.113043	3.262073	0.270418
H	-10.733117	-0.149413	-4.499211	C	-7.506729	4.435815	-0.215766
C	-8.870913	0.252462	-3.508780	H	-6.442370	4.587606	-0.087548
H	-8.687890	-0.794829	-3.306783	C	-8.268653	5.419969	-0.846990
C	-7.107660	-3.317176	-1.876845	H	-7.786675	6.321904	-1.207390
C	-8.487580	-3.066450	-1.917333	C	-9.646472	5.248637	-1.002625
H	-8.892778	-2.209811	-1.389373	H	-10.240320	6.019200	-1.481309
C	-9.340567	-3.914267	-2.635222	C	-10.252585	4.077712	-0.544415
H	-10.404801	-3.707052	-2.651473	H	-11.317253	3.927045	-0.680253
C	-8.828632	-5.014306	-3.320830	C	-9.494594	3.086092	0.080747
H	-9.490384	-5.669379	-3.876094	H	-9.965332	2.162186	0.387452
C	-7.453824	-5.272392	-3.287787	C	-5.906527	3.061427	2.036821
H	-7.048638	-6.127850	-3.816528	C	-4.533408	2.778061	2.075675
C	-6.601279	-4.434449	-2.572305	H	-4.145734	1.923782	1.534459
H	-5.540864	-4.656554	-2.538241	C	-3.660485	3.586544	2.815158
C	-4.852371	-3.415863	-0.173645	H	-2.602240	3.350812	2.828159
C	-5.422815	-4.549392	0.436297	C	-4.147651	4.680526	3.527742
H	-6.496502	-4.690355	0.418201	H	-3.471640	5.305622	4.100019
C	-4.615504	-5.502437	1.058791	C	-5.516452	4.970321	3.500725
H	-5.070970	-6.373274	1.516790	H	-5.902719	5.820239	4.052013
C	-3.227293	-5.340236	1.083137	C	-6.386848	4.171341	2.762797
H	-2.599784	-6.087376	1.555925	H	-7.441650	4.418909	2.734015
C	-2.654138	-4.211556	0.494896	H	5.163624	0.895383	0.178222
H	-1.580146	-4.067344	0.519566	H	6.721290	-0.623201	0.150077

N	4.350431	1.538147	0.256944	C	5.987714	10.400289	1.130762
N	7.178395	1.533746	0.319662	H	6.373100	10.232693	2.130149
N	7.174847	-1.286850	0.164146	C	10.718252	0.119635	0.231626
N	4.347023	-1.286395	0.225059	C	11.430921	0.518070	1.375649
C	2.300941	0.128366	0.236069	H	10.876988	0.816830	2.257540
C	2.966723	1.353980	0.281764	C	12.827700	0.524215	1.389669
C	2.296279	2.632813	0.394602	H	13.361699	0.829875	2.282257
H	1.229931	2.758109	0.456879	C	13.518402	0.125956	0.244455
C	3.260212	3.592678	0.424168	C	12.807673	-0.276197	-0.910115
H	3.135795	4.657221	0.515977	C	11.420188	-0.280587	-0.921127
C	4.538544	2.918645	0.334549	H	10.865559	-0.579548	-1.803349
C	5.767350	3.577211	0.357936	C	14.963189	0.034796	-0.032608
C	6.994100	2.917216	0.336602	C	16.066992	0.314567	0.774073
C	8.275220	3.592138	0.296842	H	15.935973	0.662591	1.792444
H	8.403156	4.660110	0.280727	C	17.349622	0.138722	0.246460
C	9.236378	2.629898	0.264017	H	18.216958	0.351990	0.860528
H	10.303404	2.757656	0.216054	C	17.525541	-0.309580	-1.067590
C	8.560976	1.348478	0.282878	H	18.527107	-0.439949	-1.460790
C	9.220013	0.121254	0.238190	C	16.418587	-0.591609	-1.879574
C	8.557972	-1.104521	0.194631	H	16.562019	-0.938972	-2.896935
C	9.230922	-2.387307	0.205474	C	15.142032	-0.419155	-1.360115
H	10.297910	-2.517069	0.248735	C	5.757796	-4.824908	0.063536
C	8.267667	-3.347576	0.173441	C	6.186967	-5.489837	-1.100574
H	8.393191	-4.415911	0.185369	H	6.511010	-4.907590	-1.955726
C	6.987845	-2.669966	0.142258	C	6.178706	-6.877014	-1.135347
C	5.759950	-3.327620	0.120360	C	5.744644	-7.623727	-0.015626
C	4.532536	-2.666933	0.142335	C	5.317217	-6.969600	1.140493
C	3.253381	-3.337799	0.042117	H	4.986917	-7.531630	2.006737
H	3.127337	-4.401659	-0.055518	C	5.326510	-5.573132	1.172316
C	2.291640	-2.375690	0.069427	H	5.004897	-5.047182	2.063252
H	1.225505	-2.497629	-0.002297	C	5.841318	-9.059034	-0.336613
C	2.964176	-1.098808	0.192160	C	6.330485	-9.195985	-1.656610
C	0.805855	0.129047	0.234605	C	6.516396	-10.455423	-2.211971
C	0.086694	0.702070	-0.828128	H	6.891131	-10.566462	-3.223642
H	0.631142	1.138825	-1.657614	C	6.212426	-11.587496	-1.443730
C	-1.304534	0.702916	-0.830780	H	6.353140	-12.576150	-1.865024
H	-1.850115	1.151674	-1.652532	C	5.729158	-11.453099	-0.137193
C	-2.034851	0.121792	0.232282	H	5.499603	-12.339404	0.443007
C	-1.305466	-0.452360	1.299901	C	5.539700	-10.187818	0.426447
H	-1.849919	-0.889878	2.126762	H	5.165220	-10.089204	1.439090
C	0.086107	-0.443801	1.297074	C	4.919626	8.220050	-1.708406
H	0.631378	-0.876481	2.128330	H	5.528145	8.120834	-2.616324
C	5.767824	5.074689	0.404980	H	3.863406	8.106350	-1.983953
C	5.327269	5.817107	-0.706983	C	13.785417	-0.651171	-2.021708
H	4.995756	5.294152	-1.596864	H	13.661870	-1.697220	-2.329895
C	5.333592	7.203313	-0.646664	H	13.653525	-0.011220	-2.903490
C	5.777408	7.872512	0.517398	C	6.581382	-7.819216	-2.267768
C	6.215378	7.141643	1.622435	H	7.635226	-7.687877	-2.544521
H	6.553275	7.643617	2.521983	H	5.964704	-7.657602	-3.161121
C	6.207348	5.746213	1.558819	Ru	-6.686135	-0.105578	0.049402
H	6.536561	5.161308	2.409305	P	-6.566154	0.711683	-2.208381
C	5.677335	9.326164	0.295696	P	-6.087614	-2.199859	-0.991121
C	5.175363	9.552268	-1.007101	P	-6.782224	-0.888493	2.319284
C	4.984776	10.846681	-1.473410	P	-7.258934	1.994673	1.089651
H	4.600725	11.026593	-2.471617	Cl	-9.247075	-0.292825	-0.110415
C	5.297324	11.923822	-0.632889	C	-4.688076	0.056830	0.185946
H	5.153523	12.938829	-0.984785	C	-3.457461	0.099648	0.217765
C	5.793705	11.701016	0.656507	C	-5.069765	-1.670363	-2.458053
H	6.030304	12.545858	1.292976	H	-4.173145	-1.165596	-2.088261

H	-4.778806	-2.535050	-3.063494	C	-7.846533	-2.777531	4.130307
C	-5.922556	-0.684384	-3.289060	H	-7.236222	-2.282137	4.876901
H	-6.776993	-1.214929	-3.720954	C	-5.220153	-1.241738	3.231148
H	-5.331785	-0.270389	-4.111836	C	-4.455341	-0.211113	3.803205
C	-7.551721	0.464719	3.379643	H	-4.769289	0.820476	3.716702
H	-8.215472	0.000791	4.115987	C	-3.262623	-0.492877	4.470730
H	-6.756992	0.984543	3.921772	H	-2.692207	0.317869	4.909868
C	-8.337482	1.482188	2.518626	C	-2.801636	-1.807929	4.564547
H	-8.629416	2.350341	3.118908	H	-1.876303	-2.026213	5.085770
H	-9.227758	1.005197	2.102334	C	-3.537709	-2.836320	3.973652
C	-5.402898	2.065536	-2.665275	H	-3.182310	-3.858860	4.017025
C	-4.681553	2.762945	-1.688698	C	-4.735528	-2.557793	3.313651
H	-4.805424	2.499693	-0.649870	H	-5.285701	-3.367810	2.854334
C	-3.783445	3.773094	-2.048918	C	-8.258954	3.264502	0.218361
H	-3.231177	4.295776	-1.276270	C	-7.646664	4.432428	-0.274303
C	-3.597166	4.098810	-3.392129	H	-6.582755	4.582856	-0.140639
H	-2.899506	4.879652	-3.672626	C	-8.402240	5.412829	-0.918859
C	-4.316661	3.414840	-4.377505	H	-7.915826	6.310438	-1.284072
H	-4.182232	3.667879	-5.423060	C	-9.779461	5.243432	-1.081636
C	-5.211917	2.408688	-4.018214	H	-10.368396	6.011156	-1.570841
H	-5.779727	1.901226	-4.789990	C	-10.391324	4.078057	-0.616974
C	-8.084207	1.203732	-3.119222	H	-11.455498	3.928809	-0.758175
C	-8.375686	2.554016	-3.368076	C	-9.639751	3.090213	0.021716
H	-7.695764	3.324677	-3.030357	H	-10.114729	2.170306	0.333877
C	-9.544820	2.915930	-4.039632	C	-6.063767	3.073880	1.999821
H	-9.753259	3.964313	-4.217674	C	-4.691272	2.788813	2.047450
C	-10.440912	1.937538	-4.470659	H	-4.302524	1.929504	1.515121
H	-11.345798	2.219218	-4.997100	C	-3.820469	3.602107	2.784154
C	-10.170989	0.592494	-4.209174	H	-2.762583	3.365217	2.803478
H	-10.868918	-0.174588	-4.524982	C	-4.309289	4.702593	3.485489
C	-9.008583	0.228031	-3.531322	H	-3.634925	5.331510	4.055513
H	-8.833225	-0.817593	-3.314529	C	-5.677522	4.994179	3.449742
C	-7.258937	-3.338547	-1.860750	H	-6.065010	5.849274	3.992107
C	-8.638452	-3.086941	-1.909619	C	-6.545742	4.190579	2.714275
H	-9.045133	-2.225182	-1.391197	H	-7.599946	4.439853	2.678289
C	-9.489073	-3.940133	-2.623905	Zn	5.762221	0.123983	0.271967
H	-10.553006	-3.731999	-2.646801				
C	-8.975183	-5.046537	-3.297720				
H	-9.635101	-5.705703	-3.850317				
C	-7.600816	-5.305670	-3.256206				
H	-7.194107	-6.166086	-3.775656				
C	-6.750634	-4.462396	-2.544142				
H	-5.690636	-4.685430	-2.503367				
C	-5.012371	-3.423947	-0.144904				
C	-5.586840	-4.552489	0.470484				
H	-6.660329	-4.693990	0.445774				
C	-4.783750	-5.500042	1.106687				
H	-5.242202	-6.367285	1.568523				
C	-3.395858	-5.336908	1.140023				
H	-2.771594	-6.079645	1.623926				
C	-2.818929	-4.212878	0.546588				
H	-1.745251	-4.067750	0.578481				
C	-3.618281	-3.260550	-0.089297				
H	-3.154165	-2.385335	-0.520783				
C	-7.808801	-2.341637	2.791644				
C	-8.591101	-3.009750	1.841498				
H	-8.601935	-2.653638	0.822263				
C	-9.389710	-4.095230	2.215059				
H	-9.992257	-4.596086	1.465858				
C	-9.417195	-4.522196	3.542410				
H	-10.037437	-5.362736	3.832437				
C	-8.644097	-3.858959	4.501104				
H	-8.661330	-4.186012	5.534634				

