Electronic Supplementary Material (ESI) for New Journal of Chemistry.

SUPPORTING INFORMATION

DOI:

Title: Carbon-Rich Cyclopentadienyl Ruthenium Allenylidene Complexes

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Experimental Section

Determination of Stoichiometry

The determination of the stoichiometric coefficients was performed by recording Job plots, a method of *Continuous Variations*. Therefore, a series of measurements of ten samples was prepared in which the concentrations of pyrene and the complexes **1-5** were modified whereas the total concentration was kept constant. For each sample, an UV/Vis spectrum was recorded at ambient temperature. The change of absorption ΔA multiplied by the mole fraction χ_R was plotted against the mole fraction $\chi_R = \frac{[S]}{[S]+[R]}$. The maximum of the acquired curve shows the stoichiometric ratio of substrate and receptor.[1]

Table S1: Pipetting scheme of the sample preparation for a Job plot via UV/Vis titration.[a]

Sample	**V_R [µL]**	**V_S [µL]**	**V_{Solv} [µL]**	**V_{Total} [µL]**
1	100	0	3000	3100
2	90	10	3000	3100
3	80	20	3000	3100
4	70	30	3000	3100
5	60	40	3000	3100
6	50	50	3000	3100
7	40	60	3000	3100
8	30	70	3000	3100
9	20	80	3000	3100
10	10	90	3000	3100

[a] Measurement with *Varian Cary 5000*.

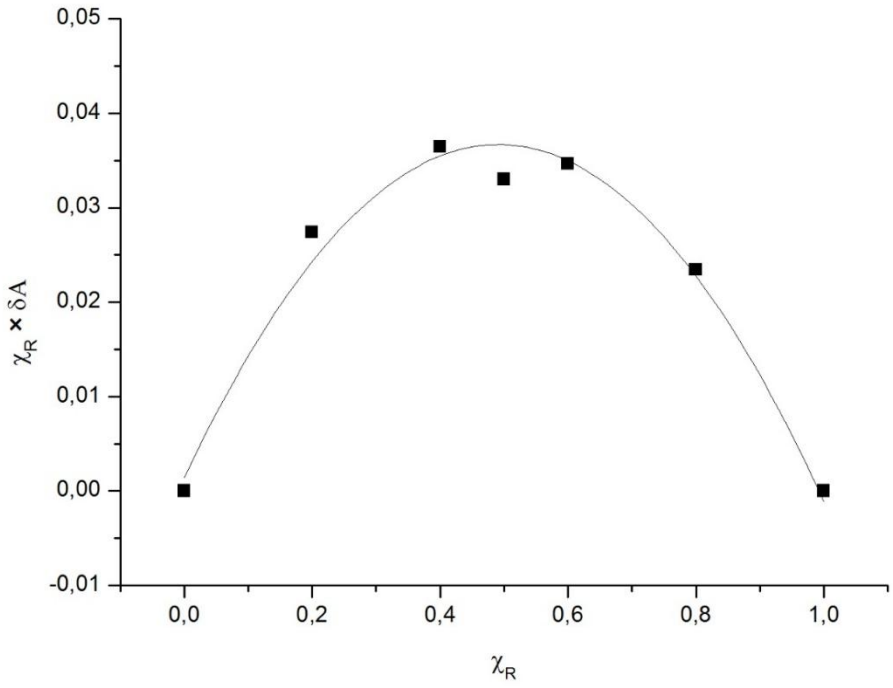

Figure S1: Job plot of the aggregation of **1** with pyrene by UV/Vis titration experiments in CH_2Cl_2.

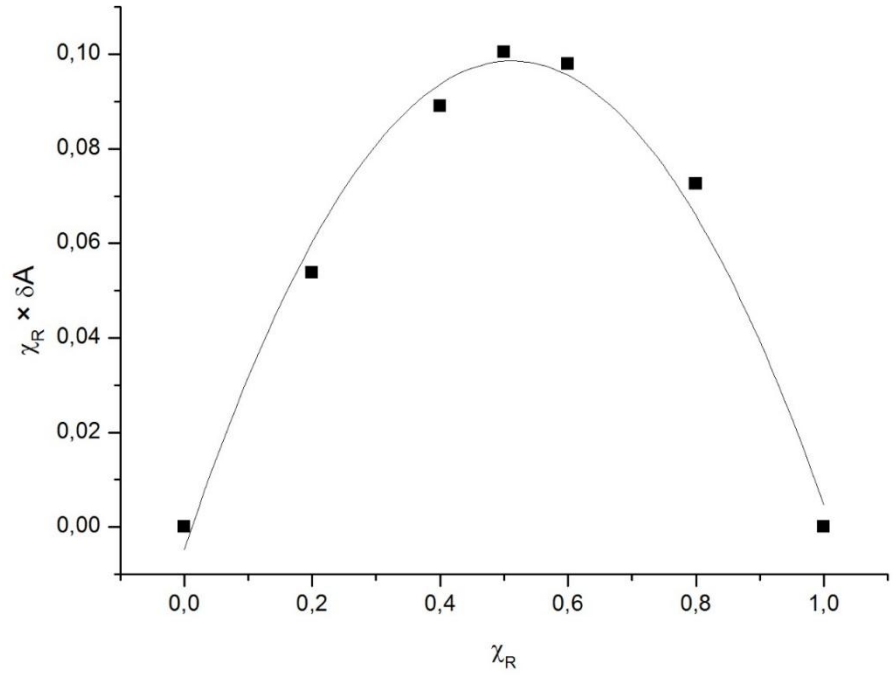

Figure S2: Job plot of the aggregation of **4** with pyrene by UV/Vis titration experiments in CH_2Cl_2.

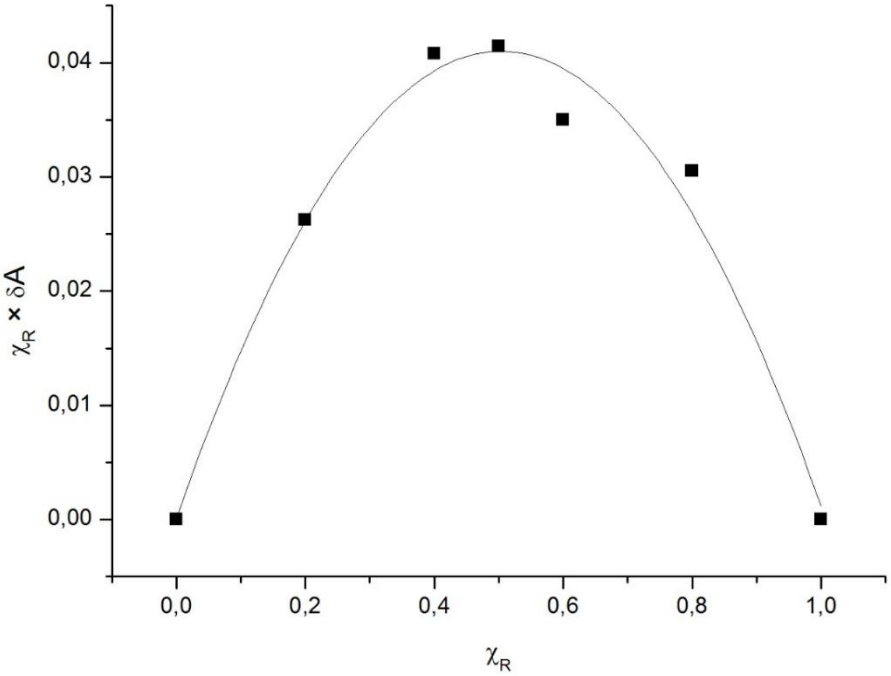

Figure S3: Job plot of the aggregation of **5** with pyrene by UV/Vis titration experiments in CH_2Cl_2.

CSI-MS Measurements

The samples were prepared by the following procedure. The appropriate complex and pyrene, in a concentration of about 10^{-6} mol × L^{-1} , were dissolved in acetonitrile and placed in an ultrasonic bath for 5 h. After that, the samples were measured immediately.

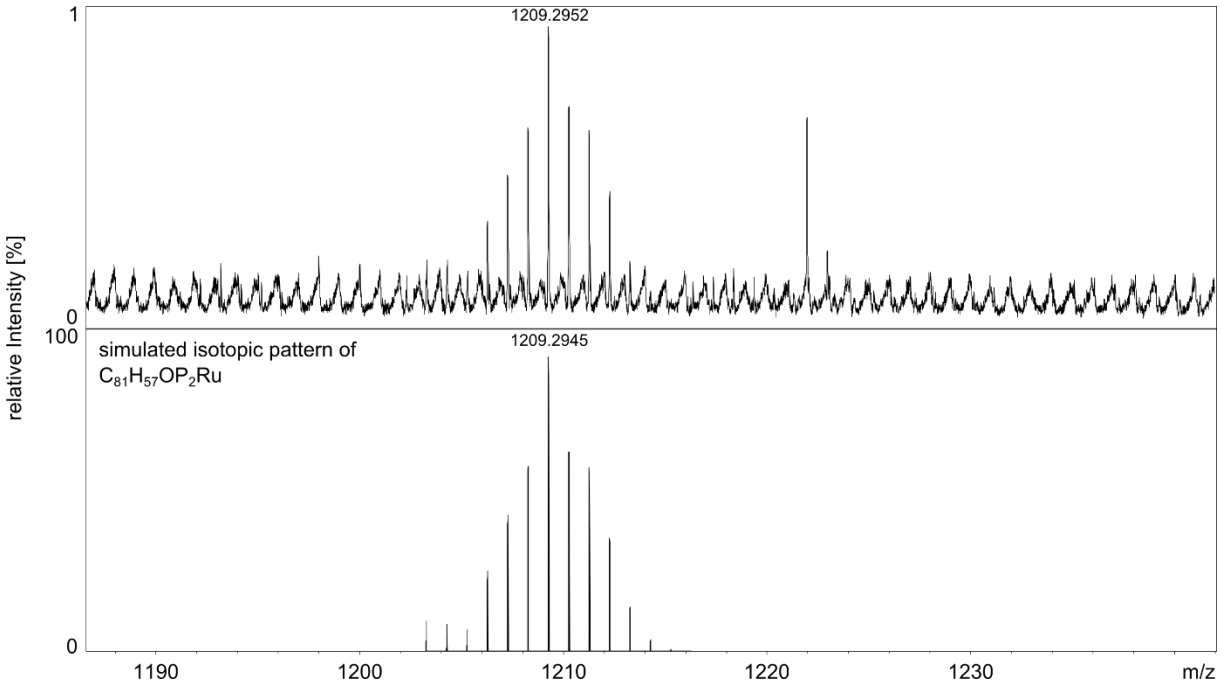

Figure S4: CSI-MS of **2** with pyrene (1:1 adduct) with a spray gas temperature of –40 °C and a dry gas temperature of –35 °C above and the corresponding simulated isotopic pattern below.

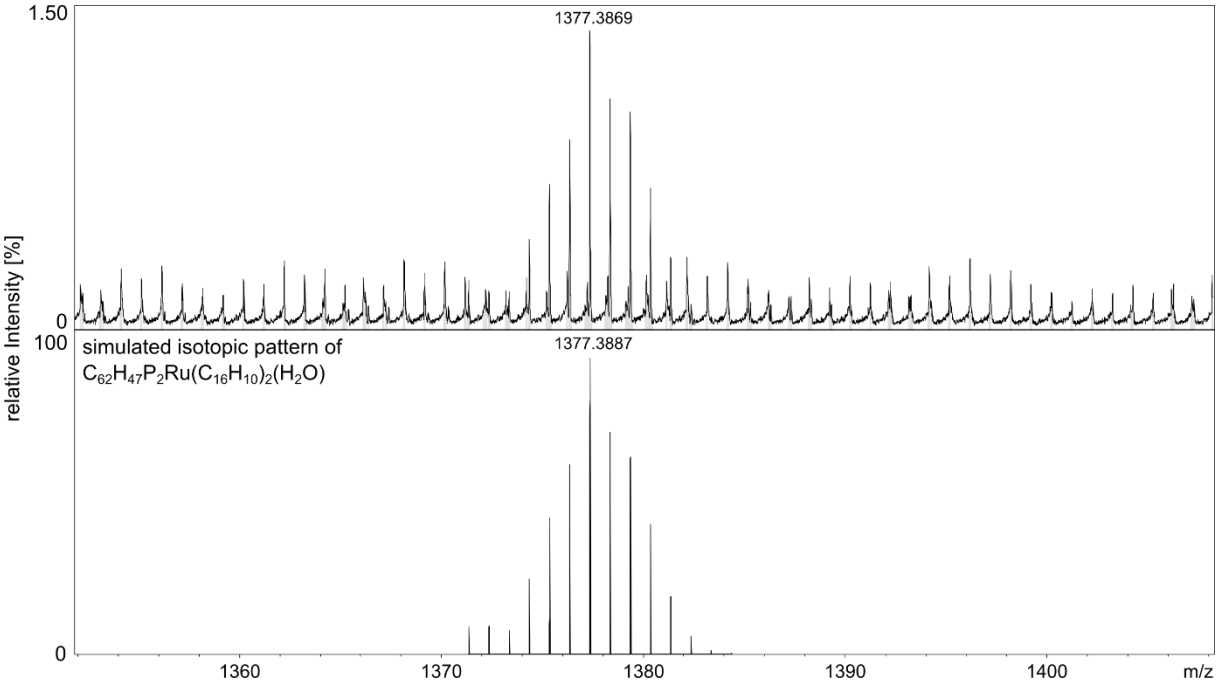

Figure S5: CSI-MS of **5** with pyrene (1:2 adduct) with a spray gas temperature of –40 °C and a dry gas temperature of –35 °C above and the corresponding simulated isotopic pattern below.

Cyclic voltammetry

Cyclic voltammetry experiments were measured with an *AUTOLAB PGSTAT 100*. A three-electrode cell was used: a gold disk working electrode, a platinum wire counter electrode and a silver wire as a pseudo-reference electrode. Cyclic voltammetry was performed in CH_2Cl_2 solution (1.00 mM complex) containing 0.1 M *n*-Bu_4NPF_6 as supporting electrolyte. All solutions were deoxygenated with N_2 before each experiment and a blanket of N_2 was used over the solution during the experiment. The potential values (E) were calculated using the following equation: $E = (E_{pc} + E_{pa})/2$, in which E_{pc} and E_{pa} correspond to the cathodic and anodic peak potentials, respectively. Potentials are referenced to the ferrocenium/ferrocene ($FeCp_2^+$/ $FeCp_2^0$) couple used as an internal standard.[2]

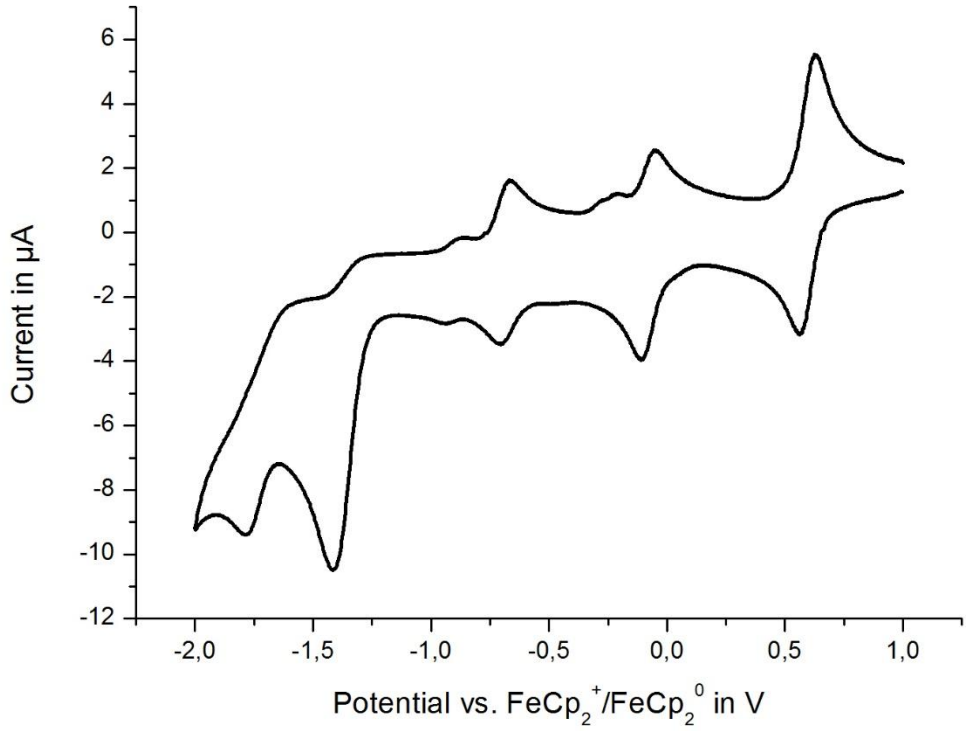

Figure S6: Cyclic voltammogram of **1** (1.00 mM) in *n*-Bu_4NPF_6 (0.1 M) solution of CH_2Cl_2 at a scan rate of 100 mV/s with potentials plotted against $FeCp_2^+$/$FeCp_2^0$.

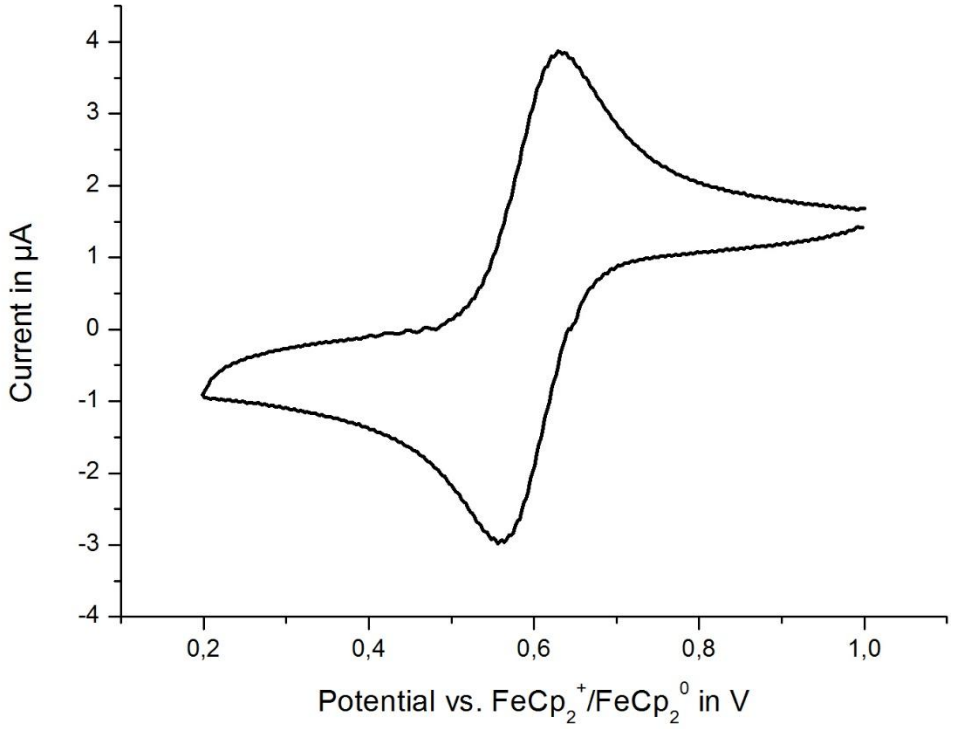

Figure S6.1: Positive part of the cyclic voltammogram of **1**.

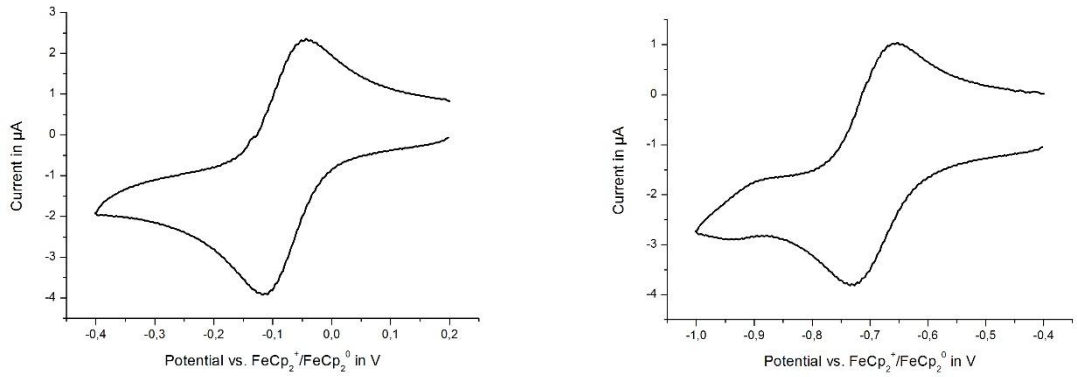

Figure S6.2: Isolated reduction processes of **1**.

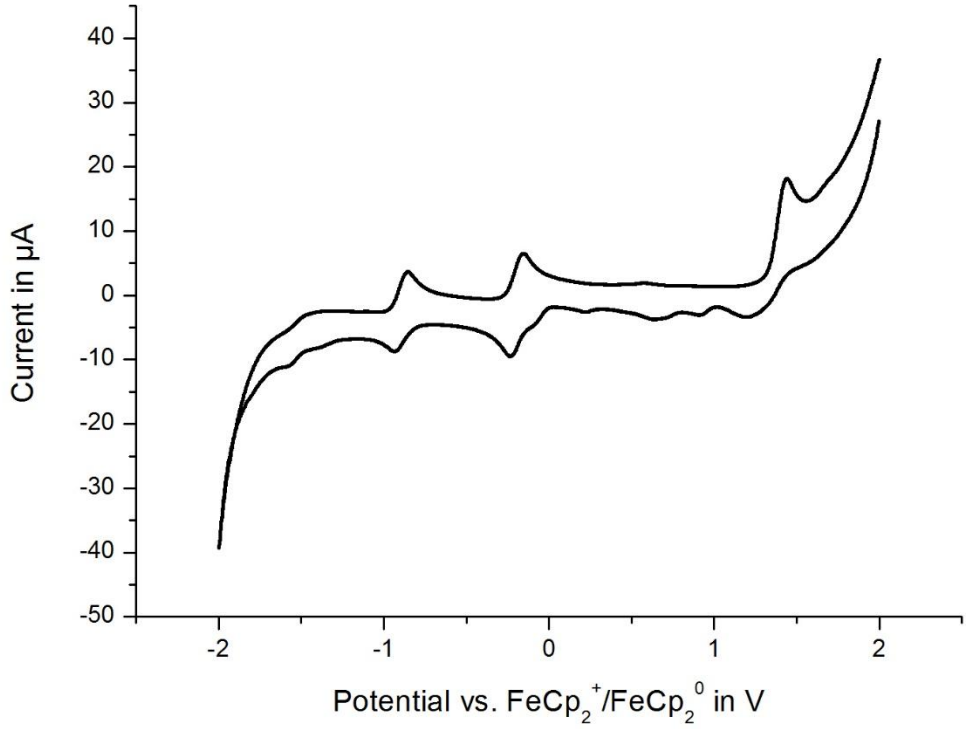

Figure S7: Cyclic voltammogram of **2** (1.00 mM) in *n*-Bu_4NPF_6 (0.1 M) solution of CH_2Cl_2 at a scan rate of 100 mV/s with potentials plotted against $FeCp_2^+/FeCp_2^0$.

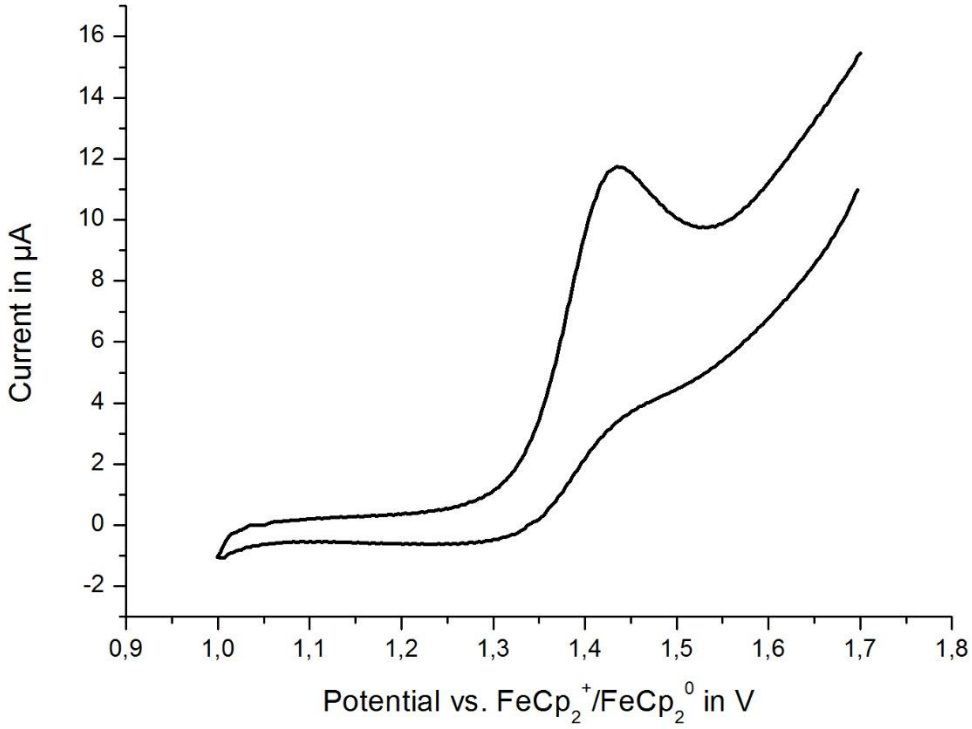

Figure S7.1: Positive part of the cyclic voltammogram of **2**.

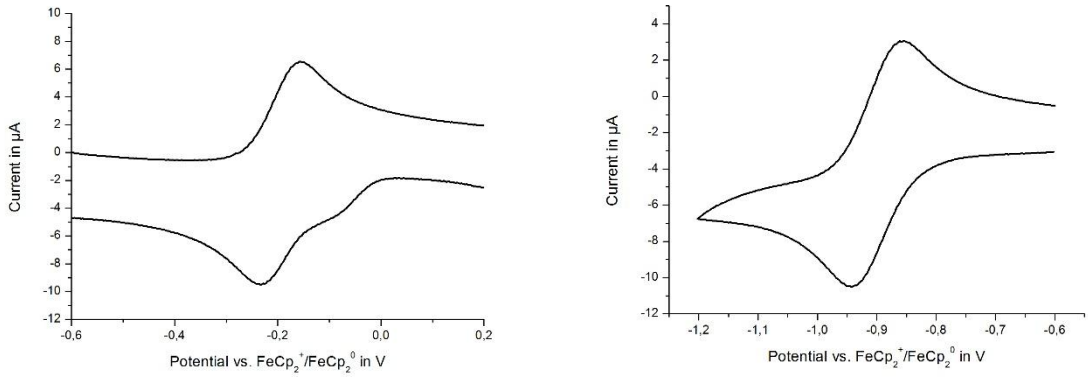

Figure S7.2: Isolated reduction processes of **2**.

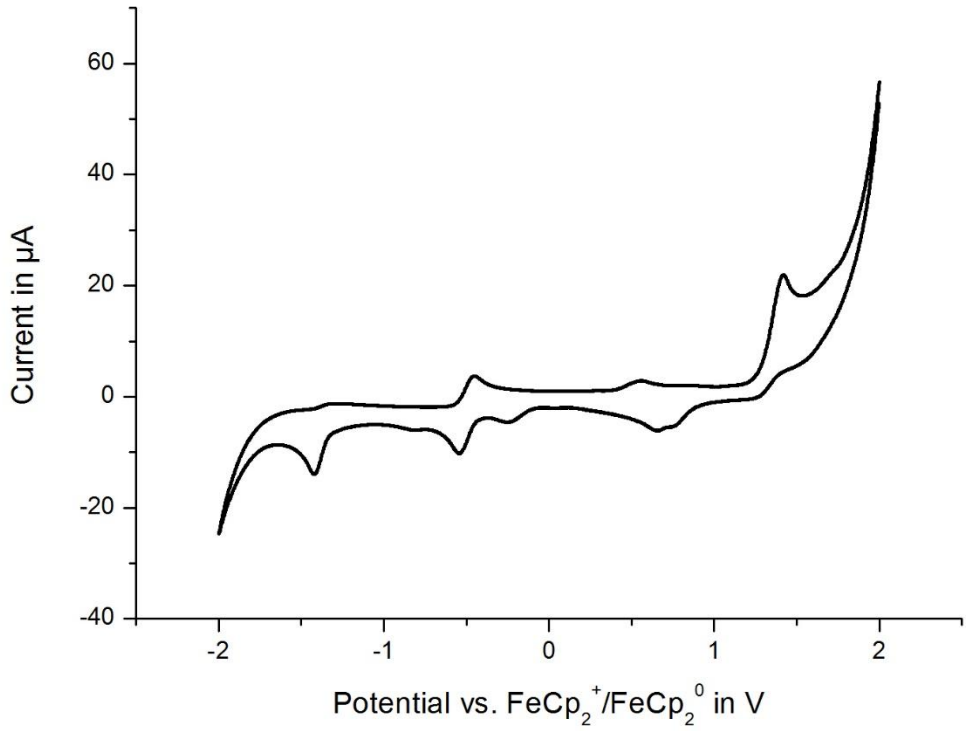

Figure S8: Cyclic voltammogram of **3** (1.00 mM) in *n*-Bu_4NPF_6 (0.1 M) solution of CH_2Cl_2 at a scan rate of 100 mV/s with potentials plotted against $FeCp_2^{+}/FeCp_2^{0}$.

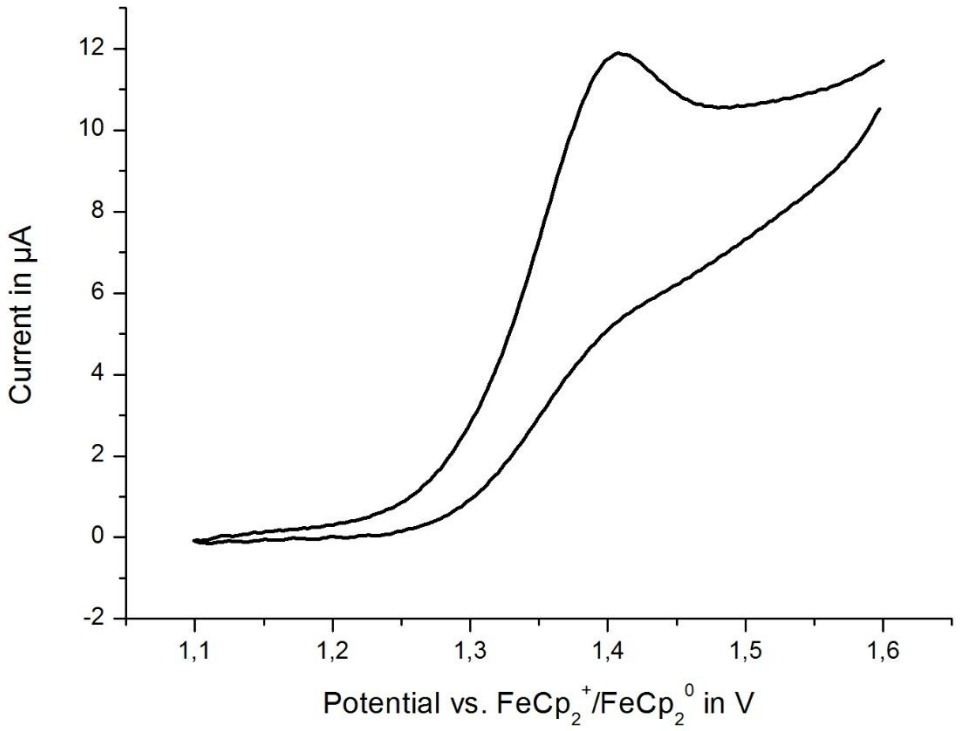

Figure S8.1: Positive part of the cyclic voltammogram of **3**.

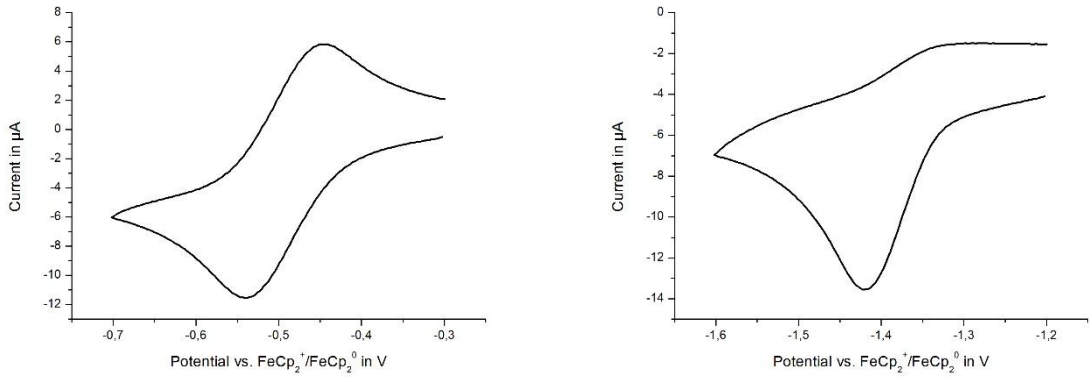

Figure S8.2: Isolated reduction processes of **3**.

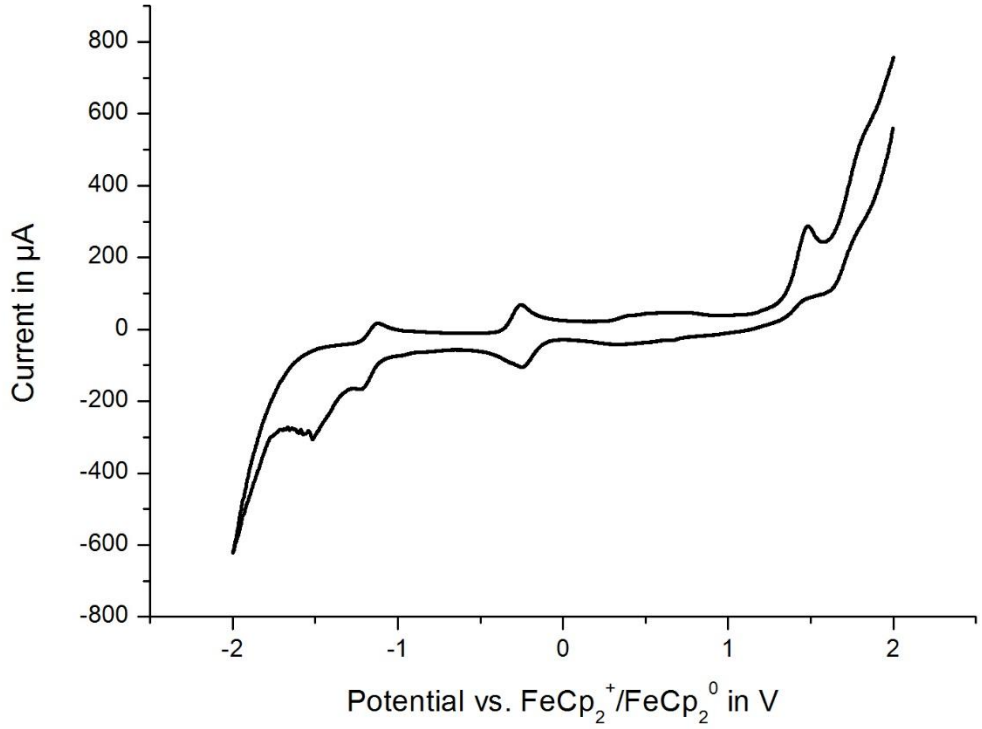

Figure S9: Cyclic voltammogram of **4** (1.00 mM) in *n*-Bu_4NPF_6 (0.1 M) solution of CH_2Cl_2 at a scan rate of 100 mV/s with potentials plotted against $FeCp_2^+/FeCp_2^0$.

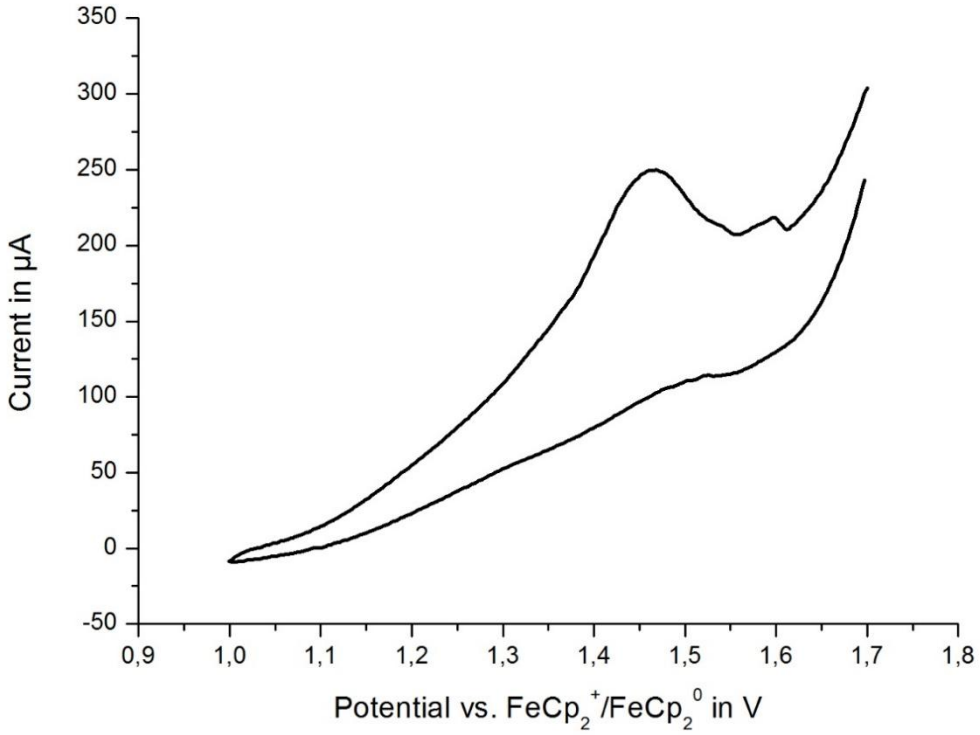

Figure S9.1: Positive part of the cyclic voltammogram of **4**.

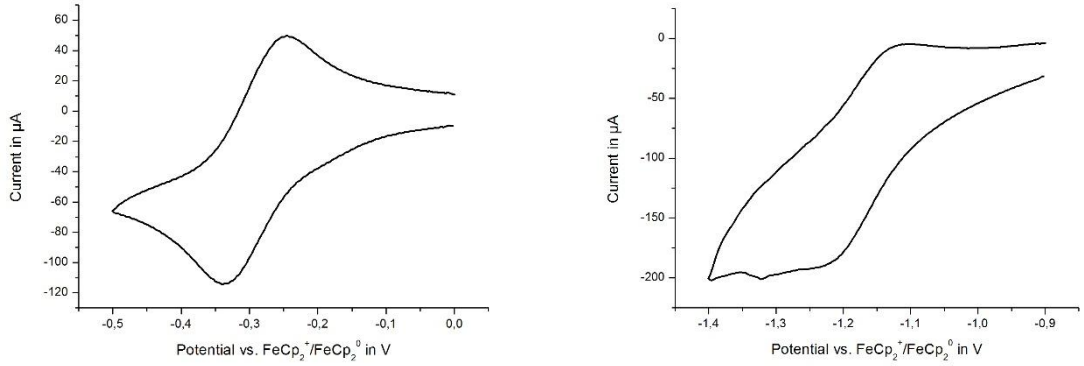

Figure S9.2: Isolated reduction processes of **4**.

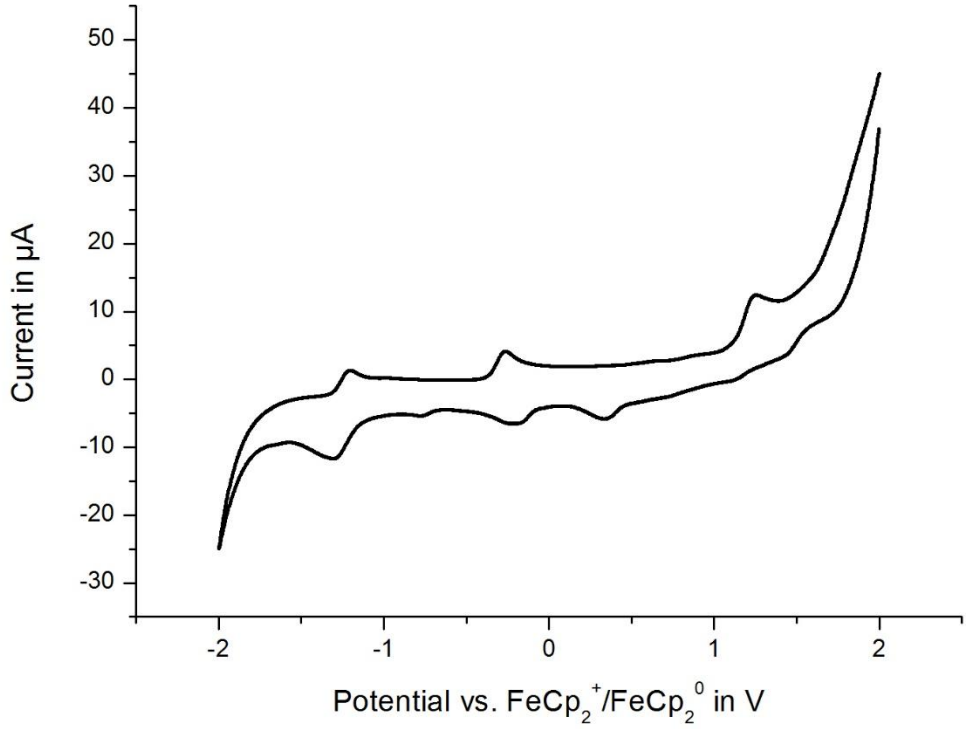

Figure S10: Cyclic voltammogram spectrum of **5** (1.00 mM) in *n*-Bu_4NPF_6 (0.1 M) solution of CH_2Cl_2 at a scan rate of 100 mV/s with potentials plotted against $FeCp_2^+/FeCp_2^0$.

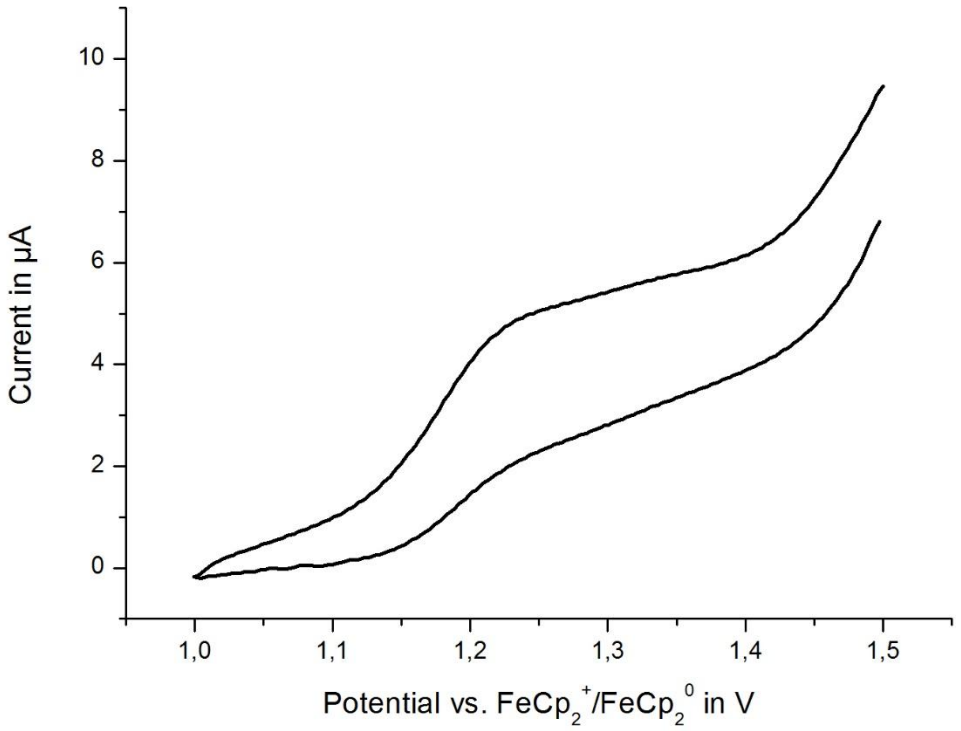

Figure S10.1: Positive part of the cyclic voltammogram of **5**.

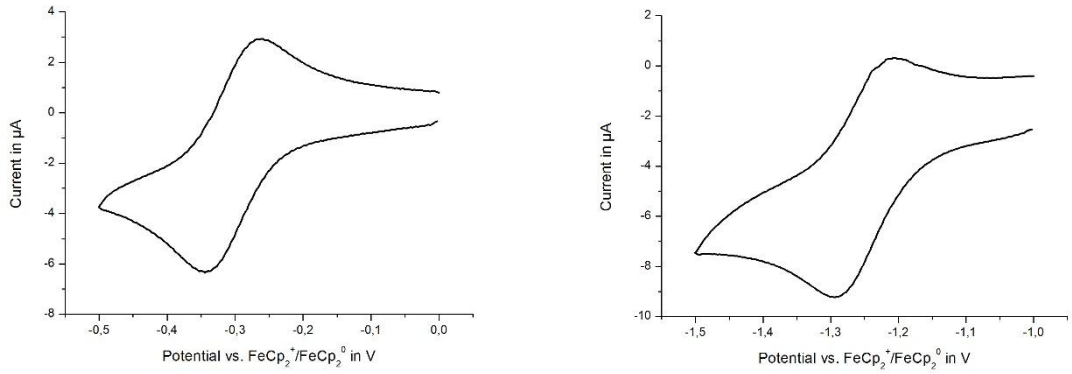

Figure S10.2: Isolated reduction processes of **5**.

UV/Vis Spectroscopy

UV/Vis spectroscopy was performed with a *Varian Cary 5000* spectrometer. The spectra were recorded in CH_2Cl_2 and the measuring range is from 2000 nm up to 200 nm.

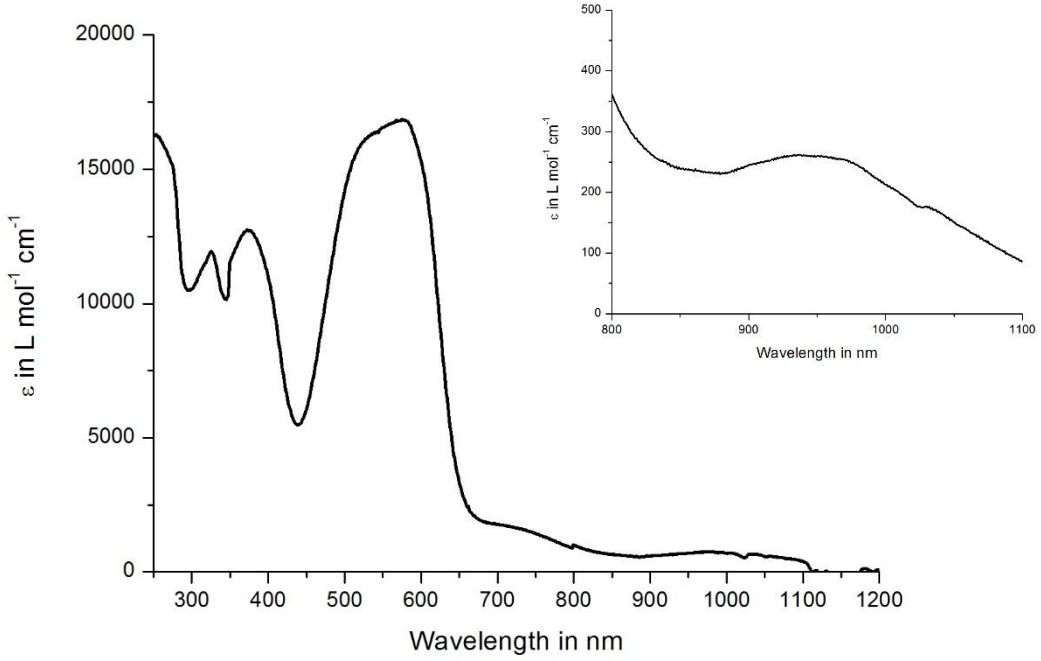

Figure S11: Absorption spectrum of **1** and part of the absorption spectrum (800 – 1100 nm) in CH_2Cl_2.

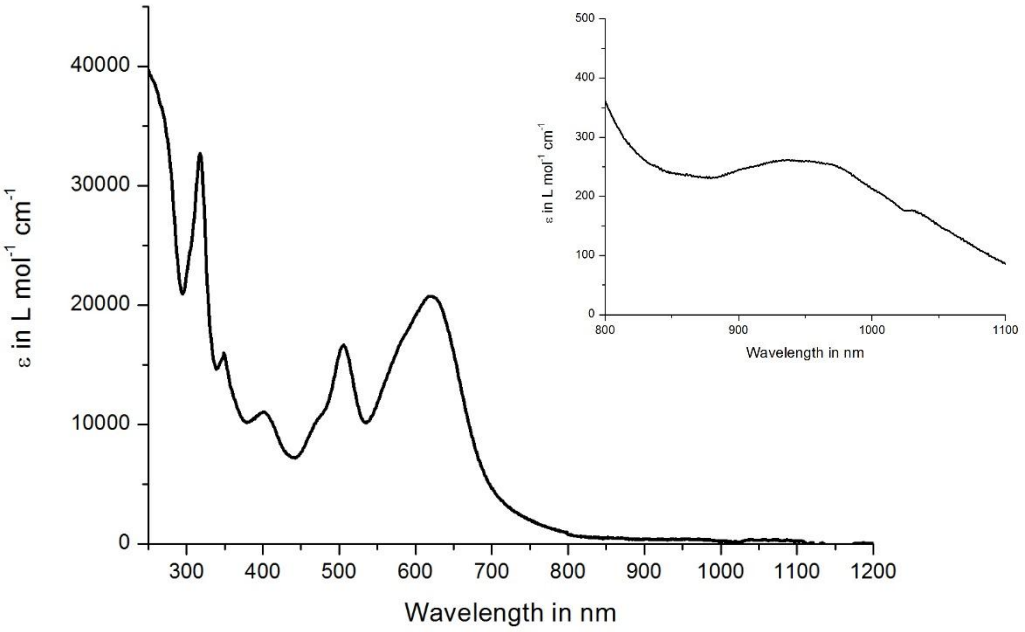

Figure S12: Absorption spectrum of **2** and part of the absorption spectrum (800 – 1100 nm) in CH_2Cl_2.

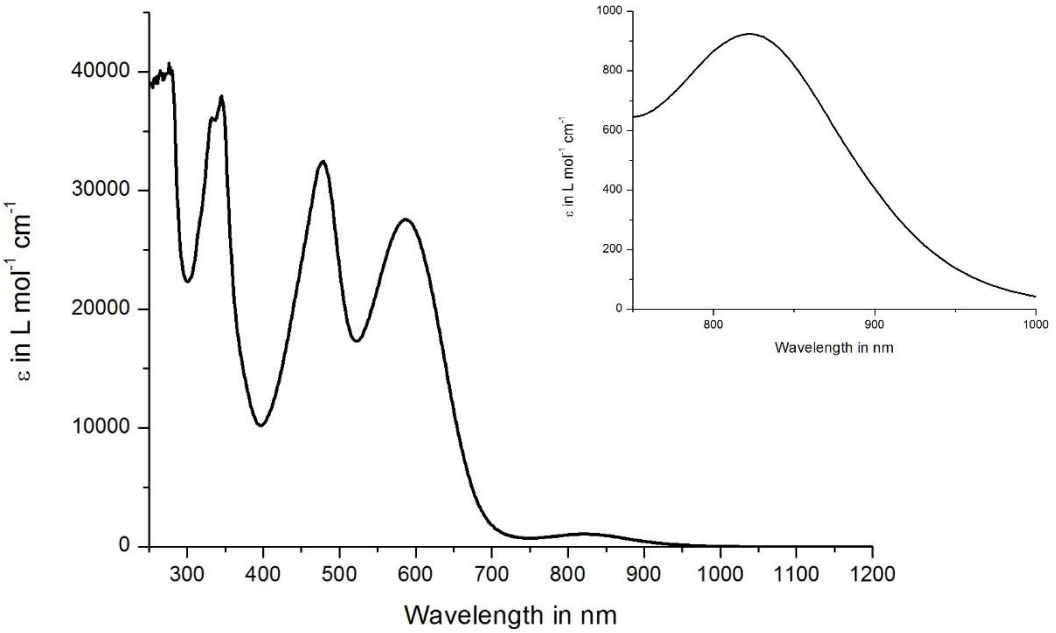

Figure S13: Absorption spectrum of **3** and part of the absorption spectrum (800 – 1100 nm) in CH_2Cl_2.

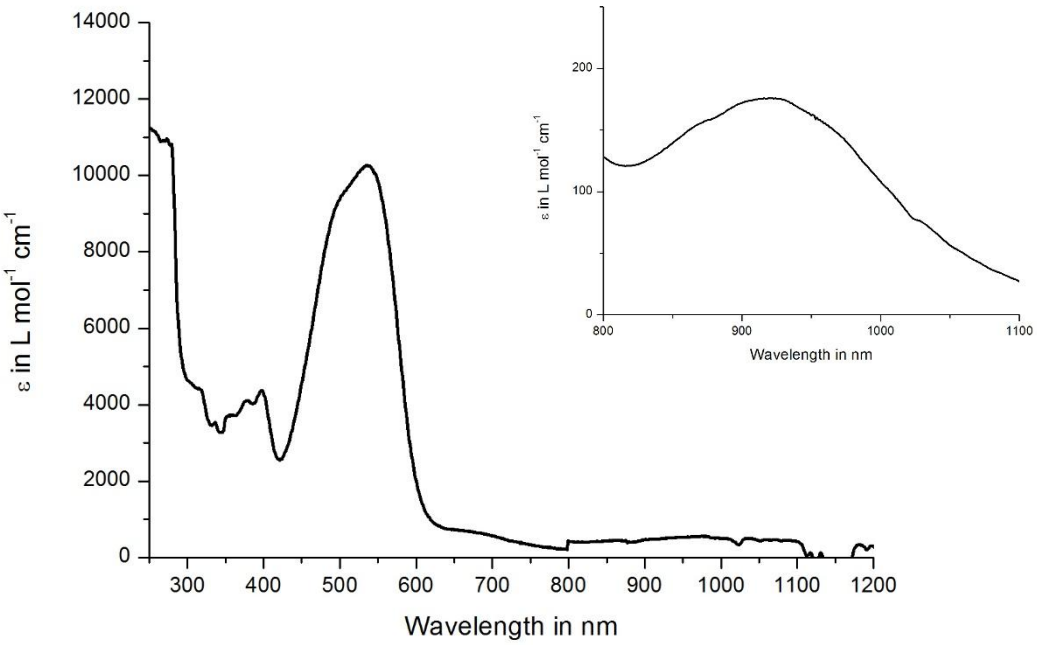

Figure S14: Absorption spectrum of **4** and part of the absorption spectrum (800 – 1100 nm) in CH_2Cl_2.

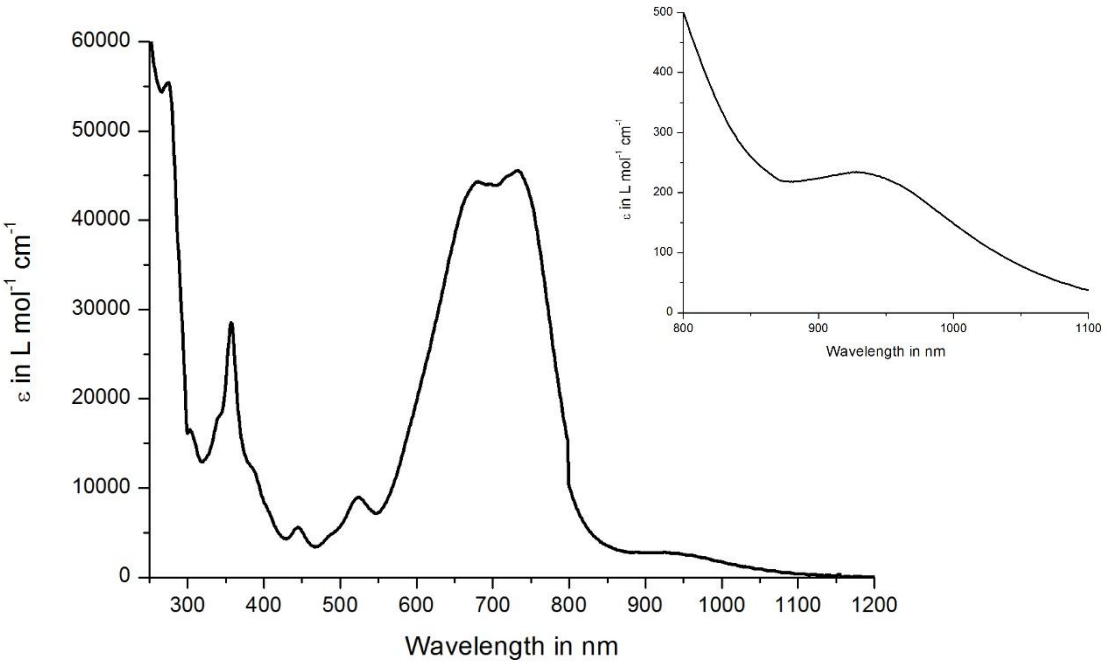

Figure S15: Absorption spectrum of **5** and part of the absorption spectrum (800 – 1100 nm) in CH_2Cl_2.

X-ray structure determination

The structure determination for **1** and **2** were carried out on a *Bruker-Nonius Kappa-CCD* diffractometer. For the structure of **5** X-ray intensity data was collected on an *Agilent Supernova Dual Source* diffractometer equipped with an Atlas S2 CCD detector. In all cases Mo-K_α radiation (λ = 0.71073 Å) was used. Single crystals of **1**, **2** and **5** were coated with perfluoropolyether, picked with a glass fiber or loop, and immediately mounted in the nitrogen cold gas stream of the diffractometer. The structures were solved by using direct methods and refined with full-matrix least squares against F^2 (SHELX-97).[3] A weighting scheme was applied in the last steps of the refinement with $w = 1/[\sigma^2(F_o^2) + (aP)^2 + bP]$ and $P = [2F_c^2 + \max(F_o^2,0)]/3$. The hydrogen atoms were included in their calculated positions and refined in a riding model. The asymmetric unit of **1** contains one disordered diethyl ether molecule that was refined in a 1:1 ratio on two positions. The asymmetric unit of **2** contains one acetone and one diethyl ether molecule and in case of complex **5** one dichloromethane and half a molecule of disordered *n*-hexane were found. Since it was not possible to resolve the disorder of this *n*-hexane SQUEEZE was applied in case of **5**.[4,5] The structure pictures were prepared with the program Mercury.[6]

Crystal data

Table S2. Selected distances and angles for complex **1**, **2** and **5** determined from the X-ray crystal structure and theoretical calculations (LACVP*/B3LYP) for complex **2**.

	1 Experimental	**2** Experimental	**2** Theroretical	**5** Experimental
Distances in Å				
Ru-C_α	1.895(4)	1.907 (6)	1.918	1.925(3)
C_α-C_β	1.251(6)	1.256 (8)	1.260	1.250(5)
C_β-C_γ	1.356(6)	1.360(8)	1.368	1.378(4)
Angles in °				
Ru-C_α-C_β	172.1(4)	168.7(5)	173.64	176.2(4)
C_α-C_β-C_γ	167.4(4)	169.7(6)	174.90	175.4(4)

Table S3: Details for the structure determination of **1**,**2** and **5**.

	1	**2**	**5**
empirical formula	$C_{57}H_{43}F_6OP_3Ru \times Et_2O$	$C_{65}H_{47}F_6OP_3Ru \times Et_2O \times H_3CCOCH_3$	$C_{62}H_{47}F_6P_3Ru \times CH_2Cl_2$
CCDC-No.	CCDC 1406943	CCDC 1406944	CCDC 1417389
formula mass	1126.01	1284.2	1182.88
crystal colour/habit	purple block	purple needle	green block
crystal system	orthorhombic	triclinic	monoclinic
space group, *Z*	*P*nma, 62	*P-1*, 2	*I*2/a, 8
a [Å]	26.143 (3)	10.0465 (8)	20.6123 (6)
b [Å]	25.5375 (12)	15.3950 (12)	22.6218 (6)
c [Å]	16.4850 (16)	20.6856 (18)	25.5409 (7)
α [°]	90	73.300 (6)	90
β [°]	90	84.013 (6)	105.389 (3)
γ [°]	90	75.746 (7)	90
V [Å^3]	11005.8 (17)	2968.1 (4)	11482.4 (6)
Θ [°]	2.71 to 27.5	2.74 to 25.03	2.889 to 25.35
h	–33 to 33	–11 to 11	–28 to 27
k	–31 to 33	–18 to 18	–30 to 30
l	–21 to 21	–24 to 24	–35 to 34
F(000), *Z*	4624, 8	1324	4816, 8
μ (Mo-K$_\alpha$) [mm^{-1}]	0.71073	0.71073	0.71073
crystal size [mm]	0.76 × 0.20 × 0.11	0.40 × 0.10 × 0.08	0.3058 × 0.2526 × 0.1162
$D_{calcd.}$ [g cm^{-3}], *T* [K]	1.359, 150	1.437, 150	1.369, 100
reflections collected	100441	53667	38940
independent reflections	12797	10308	10493
obs. Reflections, $I > 2\sigma I$	9846	8050	9065
parameter	682	768	703
weight parameter *a*	0.0988	0.1695	0.0680
weight parameter *b*	43.0095	7.3888	47.9990
R_1 (observed)	0.0599	0.0731	0.0437

R_1 (overall)	0.0830	0.0984	0.0513
wR_2 (observed)	0.1745	0.2016	0.1249
wR_2 (overall)	0.1953	0.241	0.1298
diff. peak/hole [e/Å]	-1.776 / 2.510	-1.803 / 1.027	-1.157 / 1.553
goodness-of-fit on F^2	1.099	1.044	1.057

Computational Data

All density-functional theory (DFT)-calculations were carried out by using the Jaguar 7.7.107 software running on Linux 2.6.18-238.el5 SMP (x86_64) on two AMD Phenom II X6 1090T processor workstations (Beowulf-cluster) parallelized with OpenMPI.[7] The X-ray crystal structure of **2** was used as starting geometry. Complete geometry optimization was carried out on the implemented LACVP* (Hay-Wadt effective core potential (ECP) basis on heavy atoms, N31G6* for all other atoms) basis set and with the B3LYP density functional. The calculated structure was proven to be a true minima by the absence of large imaginary frequencies. Orbital Plots were obtained using Maestro 9.1.207, the graphical interface of Jaguar. UV/VIS transistions were obtained by time dependent (TD) DFT-cacluclations on the geometry of the minimized structure.

Details for the calculation of **2**

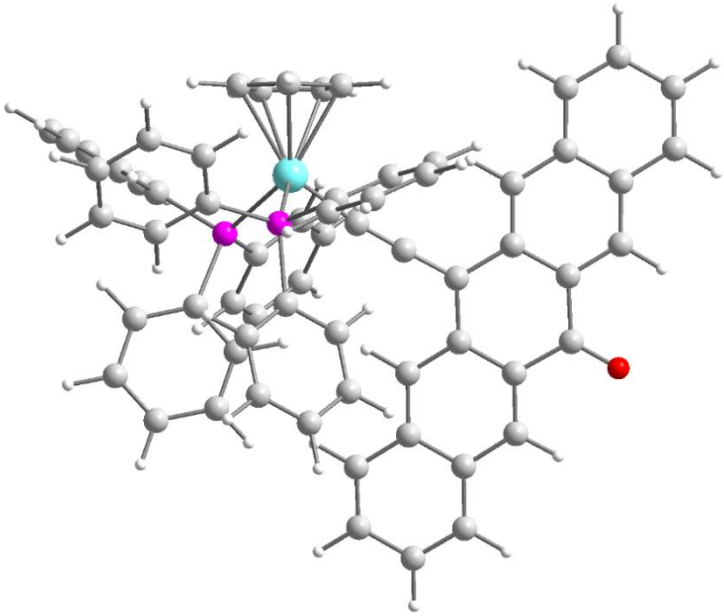

Figure S16: Calculated geometry of **2**.

Time-dependent DFT calculations of the excited states of **2**

Excited State 1: 1.5784 eV, 785.48 nm
orbitals in excitation / CI coeff.

242 => 246 / 0.22406
243 => 246 / 0.22458
244 => 246 / –0.82204
245 => 246 / –0.44797
Transition dipole moment (debye):
X = –0.4176, Y = 0.1145, Z = –0.7823, Tot = 0.8941
Oscillator strength, f = 0.0048

Excited State 2: 1.9371 eV, 640.05 nm
orbitals in excitation / CI coeff.

242 => 246 / –0.24501
243 => 246 / –0.84930
244 => 246 / –0.39639
245 => 246 / 0.16575
Transition dipole moment (debye):
X = 0.2136, Y = 0.0387, Z = 0.8747, Tot = 0.9012
Oscillator strength, f = 0.0060

Excited State 3: 2.3285 eV, 532.47 nm
orbitals in excitation / CI coeff.

238 => 246 / 0.11558

240 => 246 / –0.14614
241 => 246 / –0.14914
242 => 246 / 0.11713
243 => 246 / 0.30278
244 => 246 / –0.34352
245 => 246 / 0.81560
Transition dipole moment (debye):
X = –0.4657, Y = –1.1859, Z = 6.3725, Tot = 6.4986
Oscillator strength, f = 0.3729

Excited State 4: 2.4241 eV, 511.47 nm
orbitals in excitation / CI coeff.
237 => 246 / –0.14311
239 => 246 / 0.11554
242 => 246 / –0.89800
243 => 246 / 0.31053
244 => 246 / –0.13126
237 => 247 / 0.11125
Transition dipole moment (debye):
X = –4.2126, Y = 1.9985, Z = –0.1471, Tot = 4.6649
Oscillator strength, f = 0.2000

Excited State 5: 2.6371 eV, 470.16 nm
orbitals in excitation / CI coeff.
237 => 246 / 0.24197
239 => 246 / 0.92467
239 => 247 / 0.23439
Transition dipole moment (debye):
X = 0.5759, Y = –0.2726, Z = 0.2035, Tot = 0.6689
Oscillator strength, f = 0.0045

Excited State 6: 2.6996 eV, 459.27 nm
orbitals in excitation / CI coeff.
240 => 246 / 0.44865
241 => 246 / –0.85742
Transition dipole moment (debye):
X = –0.1951, Y = 0.4201, Z = –2.9310, Tot = 2.9674
Oscillator strength, f = 0.0901

Excited State 7: 2.8246 eV, 438.94 nm
orbitals in excitation / CI coeff.
236 => 246 / 0.12551
237 => 246 / –0.12427
238 => 246 / 0.23210
240 => 246 / 0.85075
241 => 246 / 0.35313
245 => 246 / 0.15311
Transition dipole moment (debye):
X = –0.2192, Y = –0.4192, Z = 4.0269, Tot = 4.0546
Oscillator strength, f = 0.1761

Excited State 8: 2.9336 eV, 422.63 nm
orbitals in excitation / CI coeff.

237 => 246 / –0.41590
238 => 246 / –0.36454
239 => 246 / 0.13975
242 => 247 / –0.10890
243 => 248 / –0.37340
244 => 248 / –0.62893
Transition dipole moment (debye):
X = 1.6700, Y = –1.4751, Z = 0.2675, Tot = 2.2442
Oscillator strength, f = 0.0560

Excited State 9: 2.9394 eV, 421.80 nm
orbitals in excitation / CI coeff.

237 => 246 / –0.58642
238 => 246 / –0.43252
239 => 246 / 0.18364
242 => 246 / 0.13590
242 => 247 / –0.15020
243 => 248 / 0.28637
244 => 248 / 0.46640
Transition dipole moment (debye):
X = 2.9526, Y = –0.9684, Z = 0.7816, Tot = 3.2042
Oscillator strength, f = 0.1144

Excited State 10: 2.9842 eV, 415.47 nm
orbitals in excitation / CI coeff.

231 => 246 / –0.11325
225 => 248 / 0.13707
241 => 248 / 0.10422
242 => 248 / 0.31760
243 => 248 / 0.64651
244 => 248 / –0.31728
245 => 248 / –0.44957
Transition dipole moment (debye):
X = 0.7971, Y = 0.2920, Z = –0.6301, Tot = 1.0571
Oscillator strength, f = 0.0126

Excited State 11: 2.9936 eV, 414.16 nm
orbitals in excitation / CI coeff.

232 => 246 / 0.17035
233 => 246 / –0.10461
234 => 246 / 0.13160
235 => 246 / 0.19321
237 => 246 / 0.54714
238 => 246 / –0.69560
240 => 246 / 0.15054
241 => 246 / 0.16135
245 => 246 / 0.11734

245 => 247 / –0.10768
Transition dipole moment (debye):
X = –0.6033, Y = –0.2025, Z = 3.2907, Tot = 3.3517
Oscillator strength, f = 0.1275

Excited State 12: 3.0284 eV, 409.41 nm
orbitals in excitation / CI coeff.

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235 => 246 / 0.27545
236 => 246 / –0.93796
240 => 246 / 0.10344
Transition dipole moment (debye):
X = –0.1106, Y = 0.3079, Z = 0.8001, Tot = 0.8644
Oscillator strength, f = 0.0086

Cartesian coordinates for the computed species 2

atom	x	y	z
C1	3.9745777586	2.9179795237	5.5026465769
C2	3.8072111703	2.8379418743	6.7484903481
C3	3.7166955063	2.8307241958	8.1133911994
C4	4.8092827934	2.2950793759	8.9282241966
C5	5.8440159050	1.5737345574	8.3412177349
H6	5.8270643141	1.4106616015	7.2676342992
C7	6.8983490225	1.0279248313	9.1043443405
C8	7.9401434938	0.2610467439	8.5167078614
H9	7.9261837526	0.0883427655	7.4434560060
C10	8.9474747798	–0.2621248682	9.2947975756
H11	9.7375617933	–0.8512412039	8.8376781294
C12	8.9619866705	–0.0420324978	10.6941721009
H13	9.7633973534	–0.4640461625	11.2938684980
C14	7.9676007122	–0.6978701779	11.2958673352
H15	7.9749161506	0.8653033905	12.3692932990
C16	6.9137491367	1.2480517252	10.5241083005
C17	5.8650621812	1.9999283791	11.1058964007
H18	5.8543095522	2.1854713178	12.1759285167
C19	4.8299257800	2.5042135776	10.3480124332
C20	3.7482432158	3.2557105641	11.0379412934
C21	2.5718986530	3.6310993476	10.2104092959
C22	1.4809246348	4.1969440841	10.8354244396
H23	1.5424949676	4.3845502217	11.9033833021
C24	0.2970729105	4.5110773826	10.1248079007
C25	–0.8349576369	5.0861555646	10.7555396193
H26	–0.7869931137	5.3122964236	11.8171187509
C27	–1.9788174489	5.3496495049	10.0338574829
H28	–2.8417110210	5.7903851399	10.5255165334
C29	–2.0428104166	5.0433354926	8.6523469736
H30	–2.9564338592	5.2497582448	8.1013368527
C31	–0.9609317360	4.4852803684	8.0088964742
H32	–1.0109840538	4.2471675061	6.9499312110
C33	0.2388239484	4.2125129512	8.7208696675
C34	1.3776675784	3.6600763706	8.0936767816

H35	1.3324970320	3.4229004266	7.0360045155
C36	2.5442999536	3.3815915041	8.7973954369
C37	5.5455565739	0.8902282251	3.6267630684
H38	5.3254867775	0.1121900662	4.3451092601
C39	6.5173525192	1.9224190130	3.7778259830
H40	7.1778068678	2.0624390245	4.6216538465
C41	6.4930936835	2.7148304146	2.5909354031
H42	7.1282352805	3.5677645490	2.3957749652
C43	5.5208381092	2.1786733626	1.7008855083
H44	5.2944786238	2.5322905952	0.7059484446
C45	4.9230039882	1.0572112311	2.3549656004
H46	4.1511858879	0.4238883601	1.9395258233
C47	6.2421650046	5.8800550051	4.3764225246
C48	6.9113071373	5.0764969770	5.3078888549
H49	6.5305282104	4.0864149945	5.5305150480
C50	8.0420294093	5.5520956729	5.9780515672
H51	8.5440289864	4.9151683658	6.7017985546
C52	8.5191516306	6.8380486218	5.7280674411
H53	9.3985169909	7.2076959338	6.2478463149
C54	7.8464782814	7.6555766622	4.8154722862
H55	8.1983538816	8.6660027068	4.6250750842
C56	6.7137811154	7.1866013133	4.1534620545
H57	6.1913603466	7.8463791948	3.4669749375
C58	3.5376768596	6.5208660024	4.4542340485
C59	3.2961192566	6.3197694435	5.8230169511
H60	3.6453342378	5.4147381881	6.3072543610
C61	2.6173727222	7.2762566988	6.5754115144
H62	2.4442247922	7.1016497694	7.6340862486
C63	2.1653708147	8.4522367114	5.9729857174
H64	1.6397478045	9.2011757236	6.5597157469
C65	2.4010837686	8.6624142825	4.6155658296
H66	2.0600481298	9.5769158696	4.1371190089
C67	3.0879063485	7.7090904754	3.8605541500
H68	3.2768630843	7.9106923516	2.8124929669
C69	4.7509770001	5.9283724241	1.8568910374
C70	5.9787423487	6.1348569481	1.2088773847
H71	6.9111424137	6.0055263420	1.7491893059
C72	6.0191850972	6.5309484445	–0.1294357740
H73	6.9797863959	6.6915983158	–0.6115426460
C74	4.8365602901	6.7326741320	–0.8405465018
H75	4.8699774468	7.0520836998	–1.8785804410
C76	3.6090655942	6.5250396579	–0.2084892521
H77	2.6807324829	6.6824352862	–0.7517413912
C78	3.5649559155	6.1174940387	1.1249840454
H79	2.5996578737	5.9590336854	1.5967966961
C80	1.1573237322	1.5030336351	4.0660026386
C81	1.8294852882	0.4724757836	4.7379687426
H82	2.9119456774	0.4221706920	4.6980645805
C83	1.1214303601	–0.4798390103	5.4729318115
H84	1.6596193611	–1.2693212412	5.9910407435
C85	–0.2697947268	–0.4155052145	5.5492085702

H86	–0.8207318376	–1.1534339001	6.1262110424
C87	–0.9510517676	0.6043940776	4.8827541846
H88	–2.0352642192	0.6621576461	4.9351594872
C89	–0.2457231382	1.5550017112	4.1453110683
H90	–0.7933743048	2.3375851686	3.6300106032
C91	0.9208342667	4.1521258469	3.0505668585
C92	0.7056640633	4.8154799351	4.2690826012
H93	1.2764682829	4.5305260490	5.1457691989
C94	–0.2288936326	5.8449050604	4.3655730523
H95	–0.3729667162	6.3513157291	5.3158439163
C96	–0.9630193276	6.2321912229	3.2424088442
H97	–1.6919116498	7.0351006652	3.3159141723
C98	–0.7557113642	5.5833407162	2.0257827600
H99	–1.3278277484	5.8731356981	1.1480486738
C100	0.1762843677	4.5465217977	1.9281511471
H101	0.3062116871	4.0400600746	0.9778134448
C102	1.8879936230	2.0498895535	1.3142142164
C103	2.4580722903	2.7441215750	0.2325424032
H104	3.0214078476	3.6555341443	0.4084996522
C105	2.2965569729	2.2841652210	–1.0741476129
H106	2.7356568368	2.8425160497	–1.8970639327
C107	1.5753873432	1.1137495518	–1.3256031142
H108	1.4522136597	0.7535397136	–2.3431142555
C109	1.0145471117	0.4131205165	–0.2584874695
H110	0.4509179830	–0.4982460469	–0.4402150272
C111	1.1639985451	0.8769628226	1.0518365525
H112	0.7076341051	0.3212529138	1.8639873984
P113	4.6571847895	5.3179018169	3.5937596554
P114	2.0938417164	2.7211439145	3.0300189928
Ru116	4.4060860429	2.9245664589	3.6338690819
O123	3.8048660805	3.5167775614	12.2357083828
X	5.7999689748	1.7526724493	2.8102751126

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