Supplementary Material (ESI) for Chemical Communications

π-FACE DONOR PROPERTIES OF N-HETEROCYCLIC CARBENES

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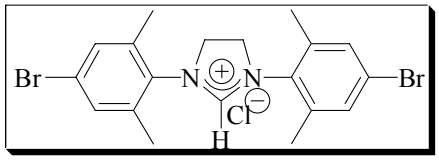
Cyclic Voltammetry (EG&G Princeton Applied Research Model 263A potentiostat)
CV measurements were done with a three electrode arrangement. The working electrode was soft glas coated platinum wire (diameter 1 mm). The platinum wire counter electrode was coiled around the glass tube of the working electrode. The pseudoreference electrode was a silver wire. All potential were referenced against the formal potentials of octamethylferrocene (CH_2Cl_2, -10 mV vs. Ag/AgCl) or ferrocen (CH_2Cl_2, 460 mV vs. Ag/AgCl). All CV measurements were done in dry CH_2Cl_2 under an Ar-atmosphere NBu_4PF_6 als supporting electrolyte.

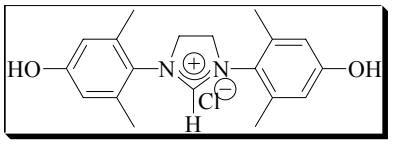
Gas chromatography (Firma Perkin Elmer, Modell Auto System with a CP-SIL_8 AB column, l = 15 m, d_i = 0.25 mm, d_p = 10m)) using nitrogen as the carrier gas and FID detection. Quantification of the GC signals was made by referencing with authentic samples.

^{1}H-NMR und **^{13}C-NMR**-Spectra: Bruker WM 300 and AC-300 at 300 MHz or 75.5 MHz and a Bruker Avance at 500 MHz or 125.75 MHz, **^{31}P-NMR**-Spectra (Bruker AC 200, 80.96 MHz). All measurements were done at 295 K, referenced to added TMS (0.00 ppm) or internal ^{1}H impurities in deuterated solvents .

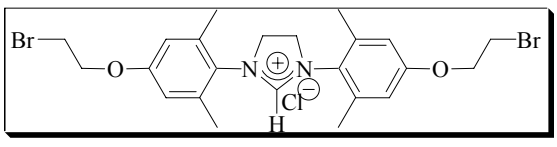
^{1}H- ^{13}C-NMR data of the imidazolinium and imidazolium chlorides



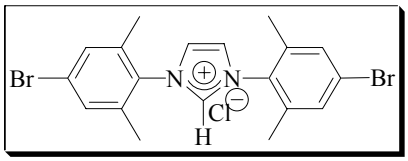
^{1}H-NMR (300 MHz, [D_6]-DMSO): δ 2.41 (s, 12H, *ortho*-CH_3), 4.50 (s, 4H, NCH_2CH_2N), 7.56 (s, 4H, CH_{meta}), 9.25 (s, 1H, im-H^2). ^{13}C-NMR (75.5 MHz, [D_6]-DMSO): δ 17.1, 50.7, 122.8, 131.3, 132.7, 138.5, 160.3.



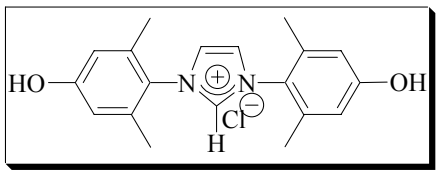
^{1}H-NMR (300 MHz, [D_6]-DMSO): δ 2.29 (s, 12H, *ortho*-CH_3), 4.39 (s, 4H, NCH_2CH_2N), 6.67 (s, 4H, CH_{meta}), 8.94 (s, 1H, im-H^2), 10.1 (bs, 1H, O*H*). ^{13}C-NMR (75.5 MHz, [D_6]-DMSO): δ 17.3, 51.0, 115.2, 124.6, 136.8, 137.4 158.3.



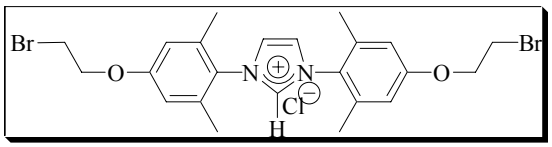
^{1}H-NMR (500 MHz, CD_3CN): δ 2.30 (s, 12H, *ortho*-CH_3), 3.64 (t, *J* = 5.3 Hz, 4H, CH_2Br), 4.25 (t, *J* = 5.3 Hz, 4H, CH_2O), 4.32 (s, 4H, NCH_2CH_2N), 6.72 (s, 4H, CH_{meta}), 8.56 (s, 1H, im-H^2). ^{13}C-NMR (125 MHz, CD_3CN): δ 17.0, 29.8, 51.1, 67.8, 114.3, 126.0, 137.4, 158.6, 160.0.



^{1}H-NMR (300 MHz, [D$_6$]-DMSO): δ 2.16 (s, 12H, *ortho*-C*H*$_3$), 7.69 (s, 4H, C*H*$_{meta}$), 8.34 (s, 2H, im-*H*^{4,5}), 9.79 (s, 1H, im-*H*^{2}). ^{13}C-NMR (75.5 MHz, [D$_6$]-DMSO): δ 16.7, 123.8, 124.6, 131.4, 132.7, 137.3, 138.6.

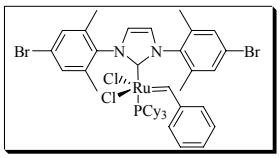


^{1}H-NMR (300 MHz, [D$_6$]-DMSO): δ 2.03 (s, 12H, *ortho*-C*H*$_3$), 6.75 (s, 4H, C*H*$_{meta}$), 8.19 (s, 2H, im-*H*^{4,5}), 9.58 (s, 1H, im-*H*^{2}), 10.21 (bs, 1H, O*H*). ^{13}C-NMR (75.5 MHz, [D$_6$]-DMSO): δ 18.3, 114.2, 128.6, 137.9, 141.8, 154.2 162.8.

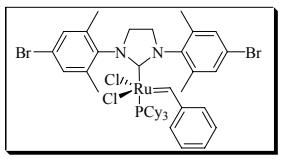


^{1}H-NMR (300 MHz, CDCl$_3$): δ 2.09 (s, 12H, *ortho*-C*H*$_3$), 3.58 (t, *J* = 6.0 Hz, 4H, C*H*$_2$Br), 4.23 (t, *J* = 6.0 Hz, 4H, C*H*$_2$O), 6.66 (s, 4H, C*H*$_{meta}$), 7.58 (s, 2H, C*H*=N), 10.95 (s, 1H, im-*H*^{2}). ^{13}C-NMR (75 MHz, CDCl$_3$): δ 18.2, 29.0, 68.1, 115.1, 124.7, 126.6, 136.3, 140.5, 159.4.

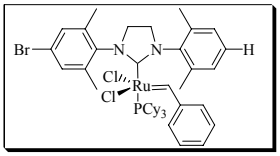
Spectroscopic data of the Grubbs-II-complexes



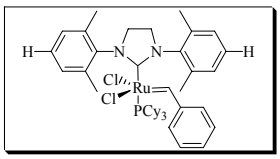
^{1}H-NMR (200 MHz, C$_6$D$_6$): δ 1.12-2.44 (m, 45H), 5.95 (s, 2H, NC*H*C*H*N), 7.01-7.36 (m, 9H), 19.83 (s, 1H, RuC*H*Ar). ^{31}P-NMR (81.0 MHz, C$_6$D$_6$): δ 32.0.



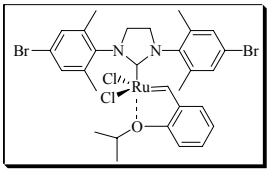
^{1}H-NMR (200 MHz, C$_6$D$_6$): δ 1.11-3.09 (m, 49H) 7.05-7.36 (s, 9H), 19.54 (s, 1H, RuC*H*Ar). ^{31}P-NMR (81.0 MHz, C$_6$D$_6$): δ 30.2.



^{1}H-NMR (200 MHz, C$_6$D$_6$): δ 1.08-3.30 (m, 49H) 7.00-7.15 (m, 10H), 19.68 (s, 1H, RuC*H*Ar). ^{31}P-NMR (81.0 MHz, C$_6$D$_6$): δ 29.2.

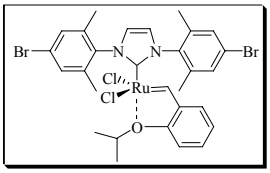


^{1}H-NMR (200 MHz, C_6D_6): δ 1.08-3.30 (m, 49H) 7.00-7.15 (m, 11H), 19.66 (s, 1H, RuC*H*Ar). ^{31}P-NMR (81.0 MHz, C_6D_6): δ 29.1.



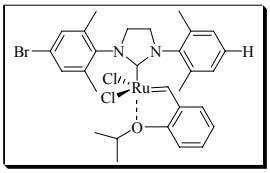
^{1}H-NMR (500 MHz, C_6D_6): δ 1.27 (d, 6H, *J* = 6.1 Hz, (C*H*$_3$)$_2$CHOAr), 2.32 (bs, 12H, *ortho*-C*H*$_3$), 3.21 (s, 4H, NC*H*$_2$C*H*$_2$N), 4.42 (sept., 1H, *J* = 6.1 Hz, (CH$_3$)$_2$C*H*OAr), 6.23 (d, 1H, *J* = 8.3 Hz, aromat.-C*H*), 6.58 (t,1H, *J* = 7.4 Hz, aromat.-C*H*), 7.02 (m, 1H, aromat-C*H*), 7.19 (d, 1H, *J* = 7.6 Hz, aromat.-C*H*), 7.25 (s, 4H, C*H*$_{meta}$), 16.47 (s, 1H, RuC*H*Ar).

^{13}C-NMR (125.75 MHz, C_6D_6): δ 18.1, 19.9, 49.5, 74.1, 111.9, 121.0, 121.2, 128.2, 130.5, 140.8, 144.3, 151.4, 212.7, 295.0.



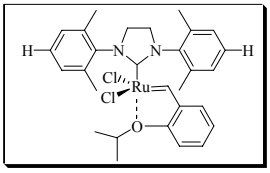
^{1}H-NMR (500 MHz, C_6D_6): δ 1.34 (d, 6H, *J* = 6.1 Hz, (C*H*$_3$)$_2$CHOAr), 2.15 (s, 12H, *ortho*-C*H*$_3$), 4.43 (sept., 1H, *J* = 6.2 Hz, (CH$_3$)$_2$C*H*OAr), 6.05 (s, 2H, NC*H*C*H*N) 6.25 (d, 1H, *J* = 8.3 Hz, aromat.-C*H*), 6.63 (d,1H, *J* = 7.5 Hz, aromat.-C*H*), 7.05 (m, 1H, aromat-C*H*), 7.24 (s, 4H, C*H*$_{meta}$), 7.28 (d, 1H, *J* = 7.6 Hz, aromat.-C*H*), 16.60 (s, 1H, RuC*H*Ar).

^{13}C-NMR (125.75 MHz, C_6D_6): δ 19.2, 21.4, 75.6, 113.3, 122.1, 122.5, 123.7, 124.2, 130.3, 131.6, 137.8, 141.1, 145.9, 152.9, 179.2, 287.5.



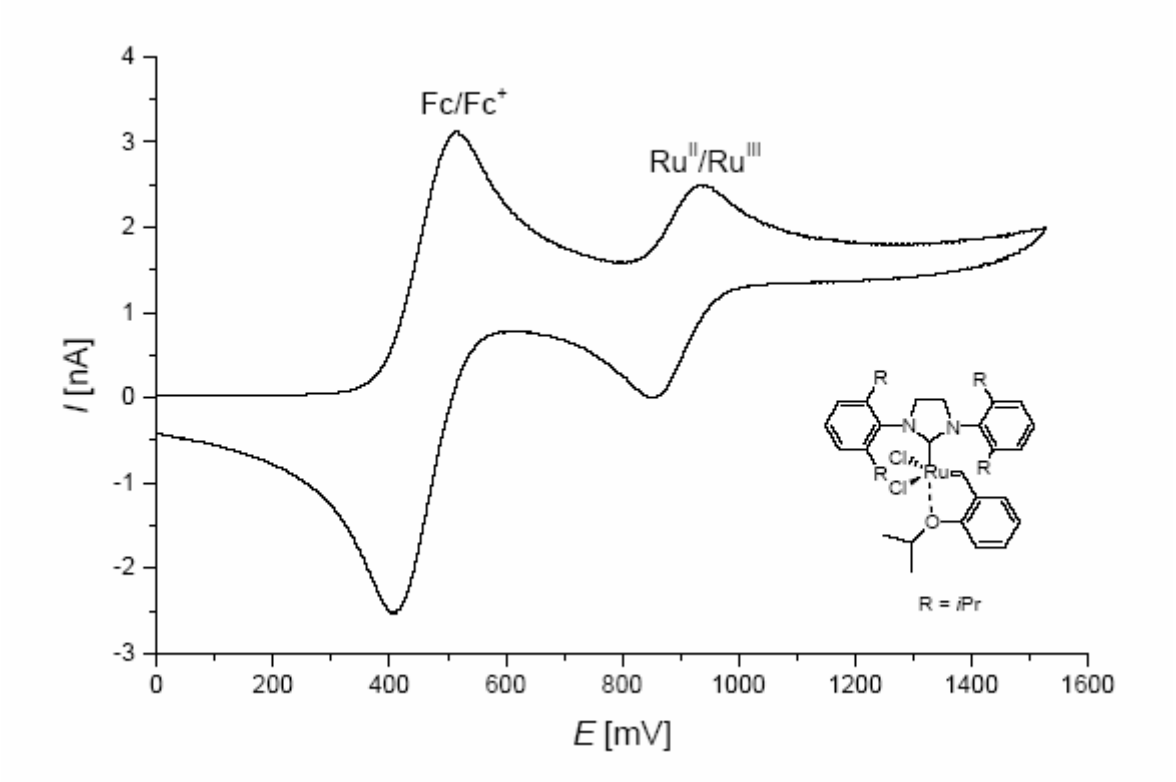
^{1}H-NMR (500 MHz, C_6D_6): δ 1.28 (d, 6H, *J* = 6.1 Hz, (C*H*$_3$)$_2$CHOAr), 2.41 (bs, 6H, *ortho*-C*H*$_3$), 2.45 (bs, 6H, *ortho*-C*H*$_3$), 3.26 (m, 2H, NC*H*$_2$), 3.33 (m, 2H, C*H*$_2$N), 4.43 (sept., 1H, *J* = 6.1 Hz, (CH$_3$)$_2$C*H*OAr), 6.26 (d, 1H, *J* = 8.5 Hz, aromat.-C*H*), 6.58 (t,1H, *J* = 7.6 Hz, aromat.-C*H*), 7.04-7.15 (m, 6H, C*H*$_{meta}$, C*H*$_{para}$, aromat-C*H*), 7.19 (m, 1H, aromat.-C*H*), 16.48 (s, 1H, RuC*H*Ar).

^{13}C-NMR (125.75 MHz, C_6D_6): δ 19.3, 20.0, 21.3, 50.7, 51.35, 72.3, 113.2, 122.2, 122.5, 123.0, 129.24, 131.77, 139.4, 142.6, 145.7, 152.7, 213.5, 291.7.



^{1}H-NMR (500 MHz, C_6D_6): δ 1.30 (d, 6H, *J* = 6.0 Hz, $(CH_3)_2$CHOAr), 2.56 (bs, 12H, *ortho*-CH_3), 3.39 (s, 4H, NCH_2CH_2N), 4.52 (sept., 1H, *J* = 6.2 Hz, $(CH_3)_2CH$OAr), 6.31 (d, 1H, *J* = 7.9 Hz, aromat.-C*H*), 6.60 (t, 1H, *J* = 7.4 Hz, aromat.-C*H*), 7.06-7.10 (m, 7H, CH_{meta}, CH_{para}, aromat-C*H*), 7.17 (d, 1H, *J* = 8.0 Hz, aromat.-C*H*), 16.50 (s, 1H, RuC*H*Ar). ^{13}C-NMR (125.75 MHz, C_6D_6): δ 19.7, 21.4, 51.2, 73.1, 113.2, 122.1, 122.5, 129.0, 139.5, 145.7, 152.7, 213.0, 291.8.

Cyclic Voltammograms of several Olefin Metathesis Catalysts



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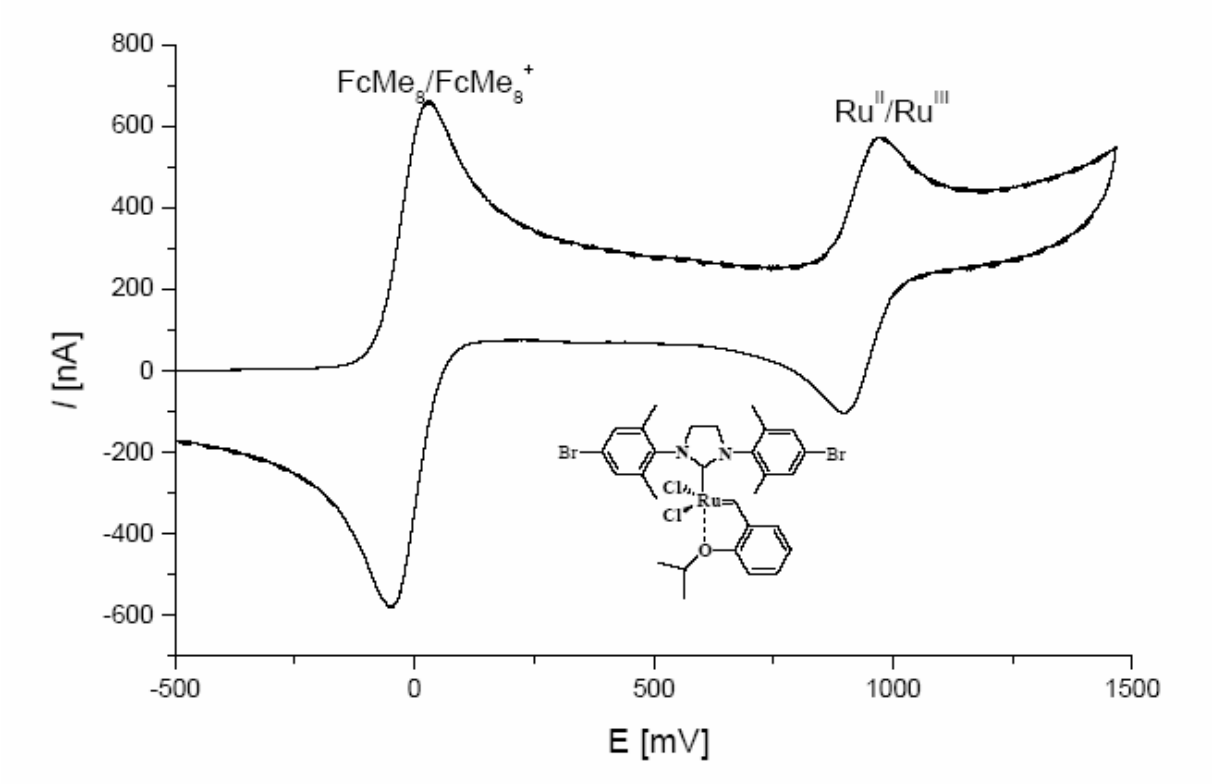

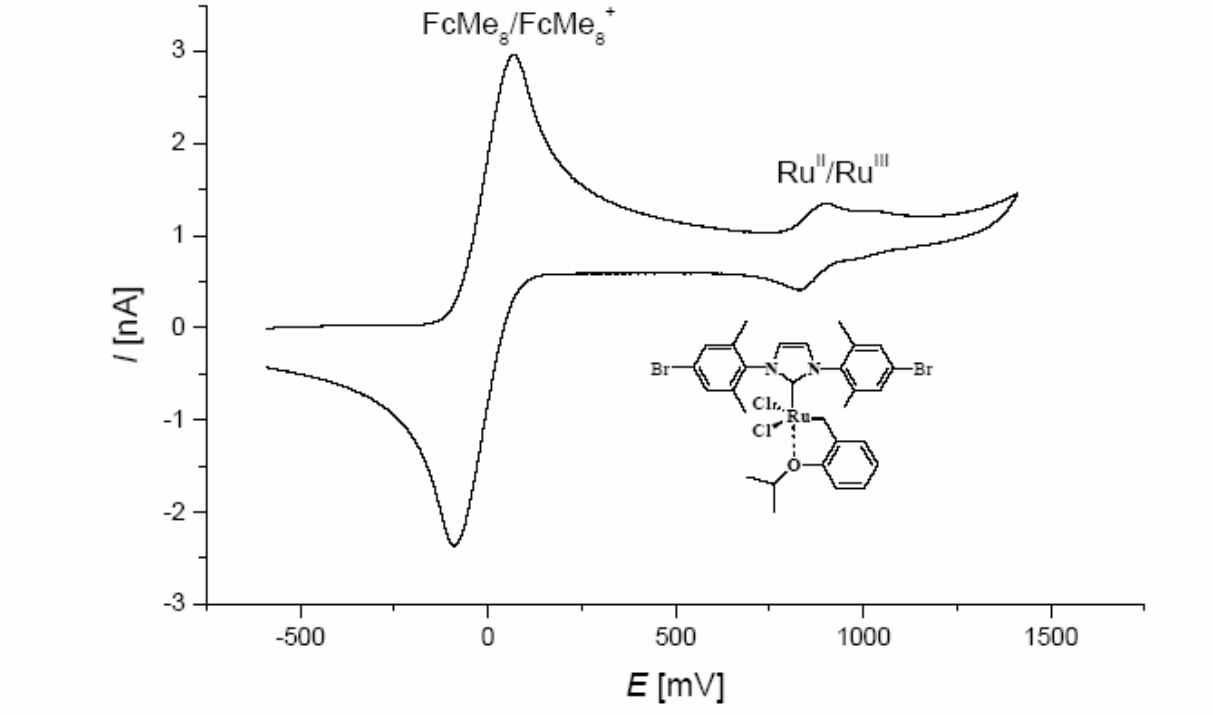

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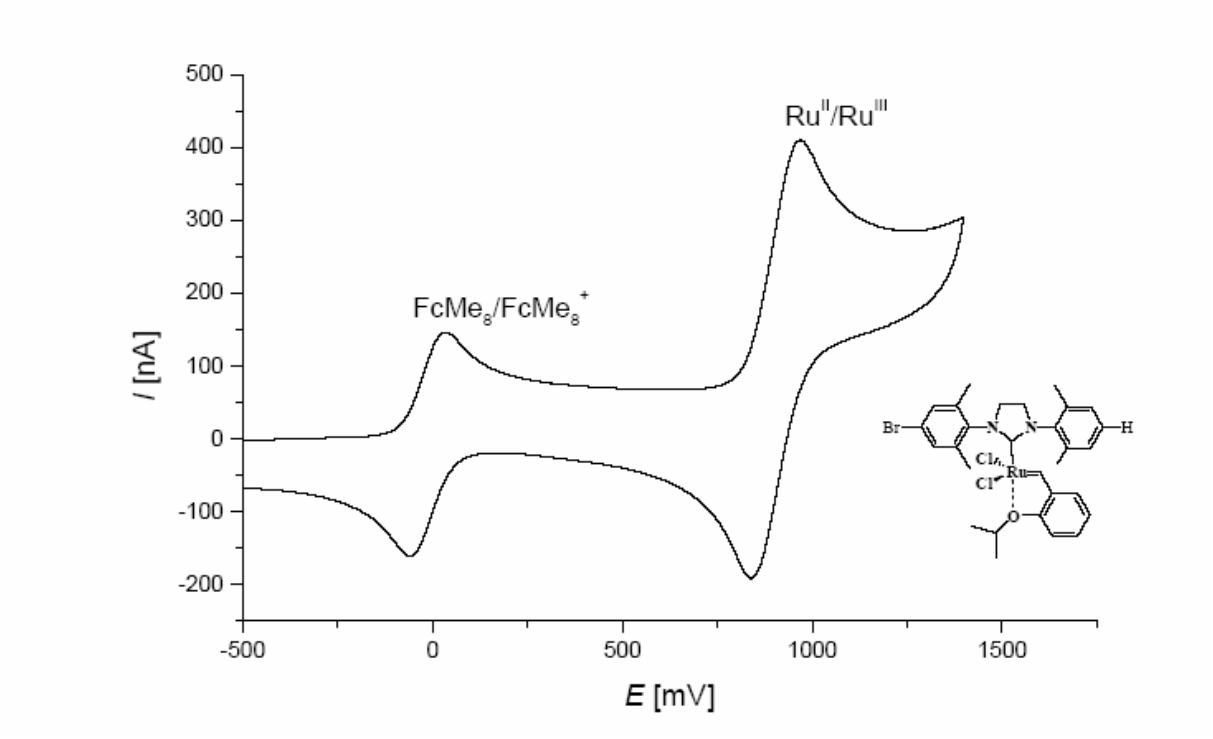

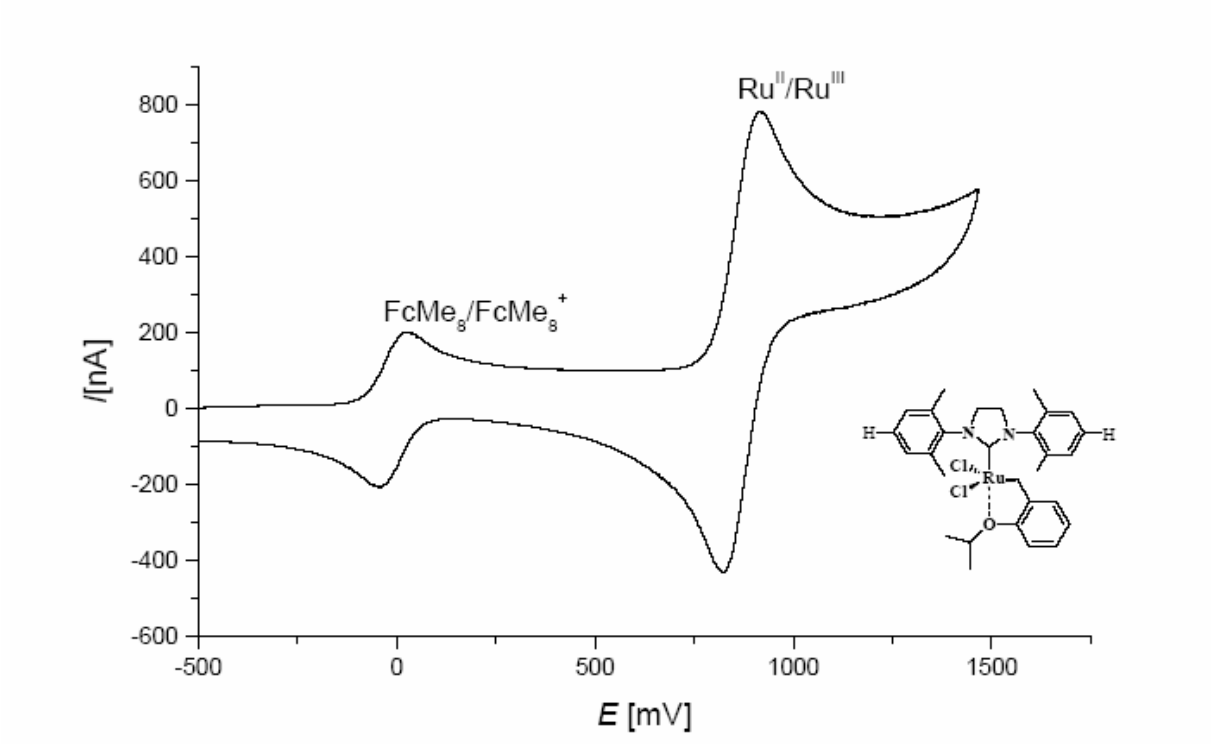

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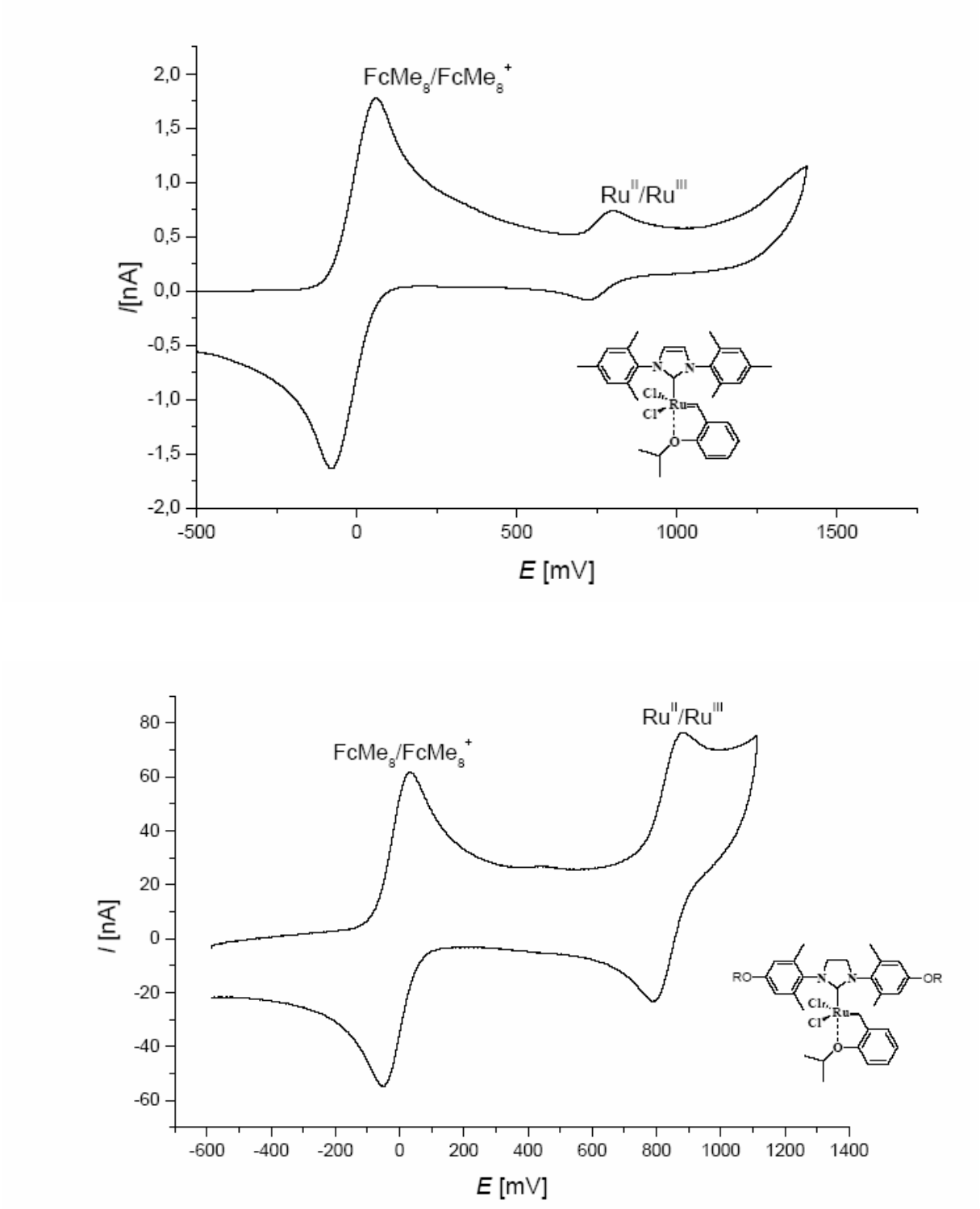

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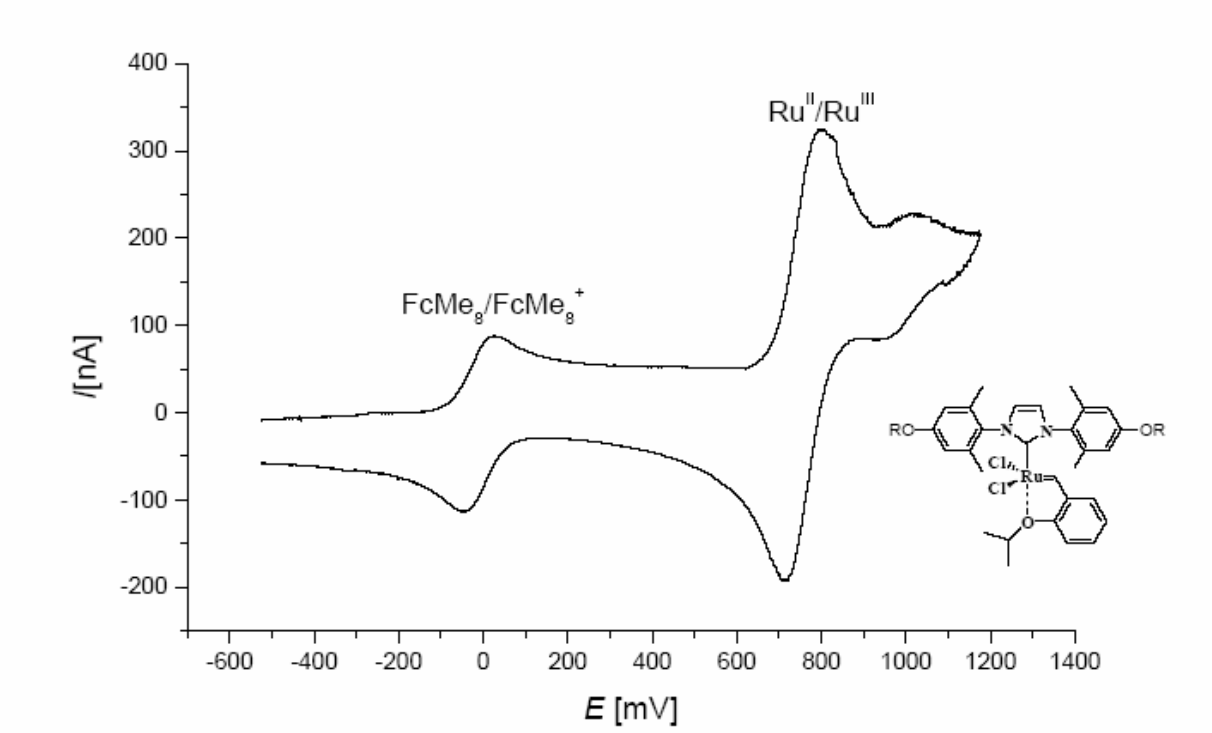

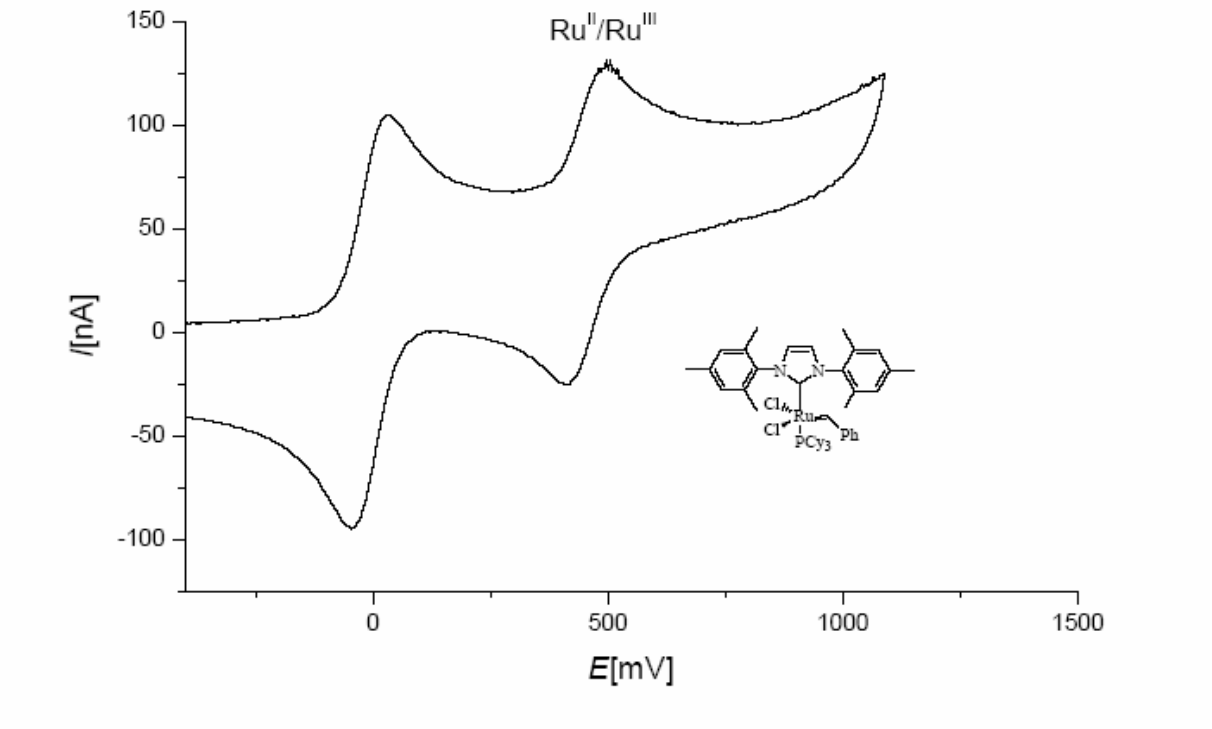

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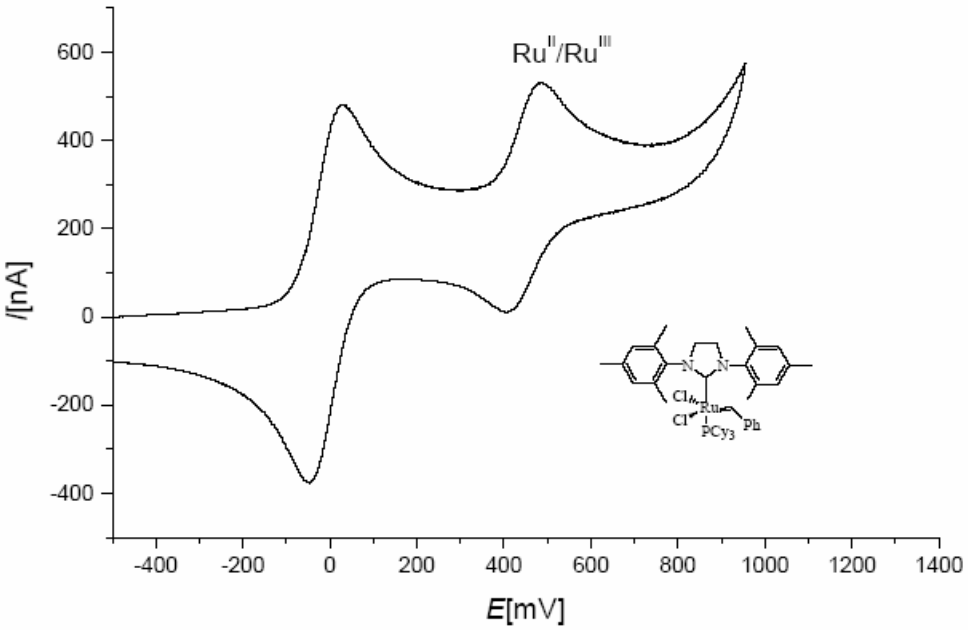

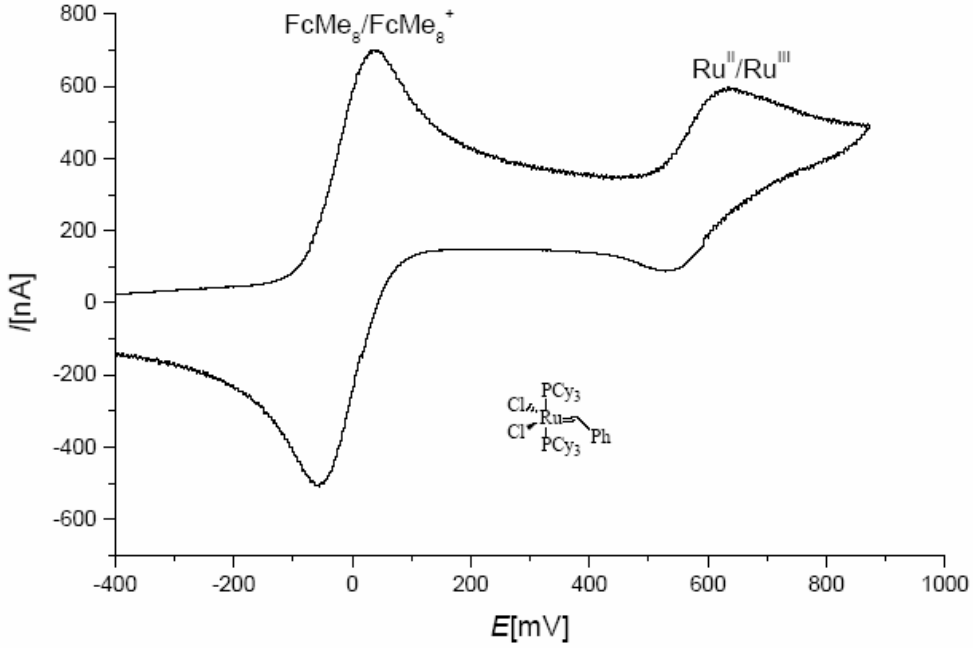

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