

Supporting Information

Effect of iodide based organic salts and ionic liquid additives in dye-sensitized solar cell performance

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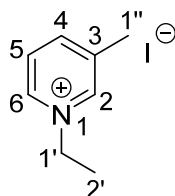
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Synthesis

General method for the synthesis of N-ethyl-methylpyridinium iodides:

A mixture of methylpyridine, iodoethane (1.2 eq) and 10 mL of acetonitrile was heated to 60°C in the microwave equipment with stirring until completion. After evaporating the solvent, the product was washed 5 times with diethyl ether and dried.

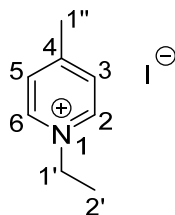
N-ethyl-3-methylpyridinium iodide (**5**):



Starting from 10 g (107.4 mmol) of 3-methylpyridine and 20.1 g of iodoethane, 24.8 g (92.7%) of N-ethyl-3-methylpyridinium iodide were obtained.

¹H NMR (400 MHz, Methanol-*d*₄) δ (ppm) 8.94 (s, 1H), 8.86 (d, *J* = 6.1 Hz, 1H), 8.44 (d, *J* = 8.0 Hz, 1H), 8.01 (t, *J* = 7.2 Hz, 1H), 4.67 (q, *J* = 7.4 Hz, 2H), 2.61 (s, 3H), 1.67 (t, *J* = 7.4 Hz, 3H).

N-ethyl-4-methylpyridinium iodide (**7**):



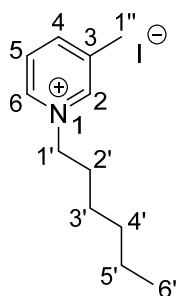
Starting from 8.5 g (91.3 mmol) of 4-methylpyridine and 17.1 g of iodoethane, 21.8 g (95.9%) of N-ethyl-4-methylpyridinium iodide were obtained.

¹H NMR (400 MHz, Methanol-*d*₄) δ (ppm) 8.89 (d, *J* = 6.3 Hz, 2H), 7.98 (d, *J* = 6.1 Hz, 2H), 4.67 (q, *J* = 7.4 Hz, 2H), 2.72 (s, 3H), 1.67 (t, *J* = 7.4 Hz, 3H).

General method for the synthesis of N-hexyl-methylpyridinium iodides:

A mixture of methylpyridine and iodoethane (1.2 eq) was heated to 80°C in the microwave equipment with stirring until completion. The product was washed 5 times with diethyl ether and dried.

N-hexyl-3-methylpyridinium iodide (**6**):

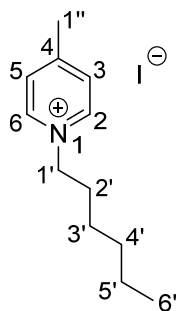


Starting from 10 g (91.3 mmol) of 3-methylpyridine and 27.2 g of iodohexane, 31.6 g (96.4%) of N-hexyl-3-methylpyridinium iodide were obtained.

^1H NMR (400 MHz, Methanol- d_4) δ (ppm) 8.97 (s, 1H), 8.87 (d, J = 6.1 Hz, 1H), 8.45 (d, J = 8.1 Hz, 1H), 8.02 (t, J = 7.1 Hz, 1H), 4.63 (t, J = 7.7 Hz, 2H), 2.61 (s, 3H), 2.05 (p, J = 7.3 Hz, 2H), 1.41 (d, J = 10.4 Hz, 6H), 1.00 – 0.90 (m, 3H).

^{13}C NMR (101 MHz, Methanol- d_4) δ (ppm) 147.28, 145.54, 143.06, 141.29, 128.74, 62.93, 32.42, 32.26, 26.85, 23.44, 18.49, 14.24

N-hexyl-4-methylpyridinium iodide (**8**):

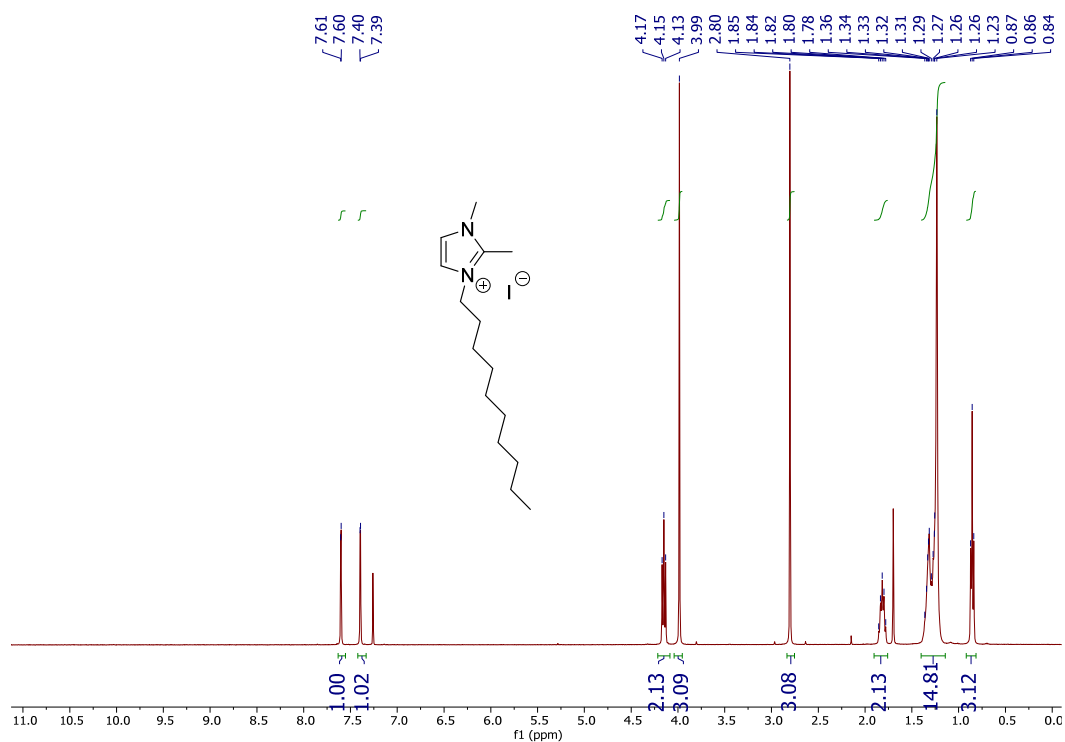


Starting from 9 g (96.6 mmol) of 4-methylpyridine and 24.6 g of iodohexane, 27.9 g (94.6%) of N-hexyl-4-methylpyridinium iodide were obtained.

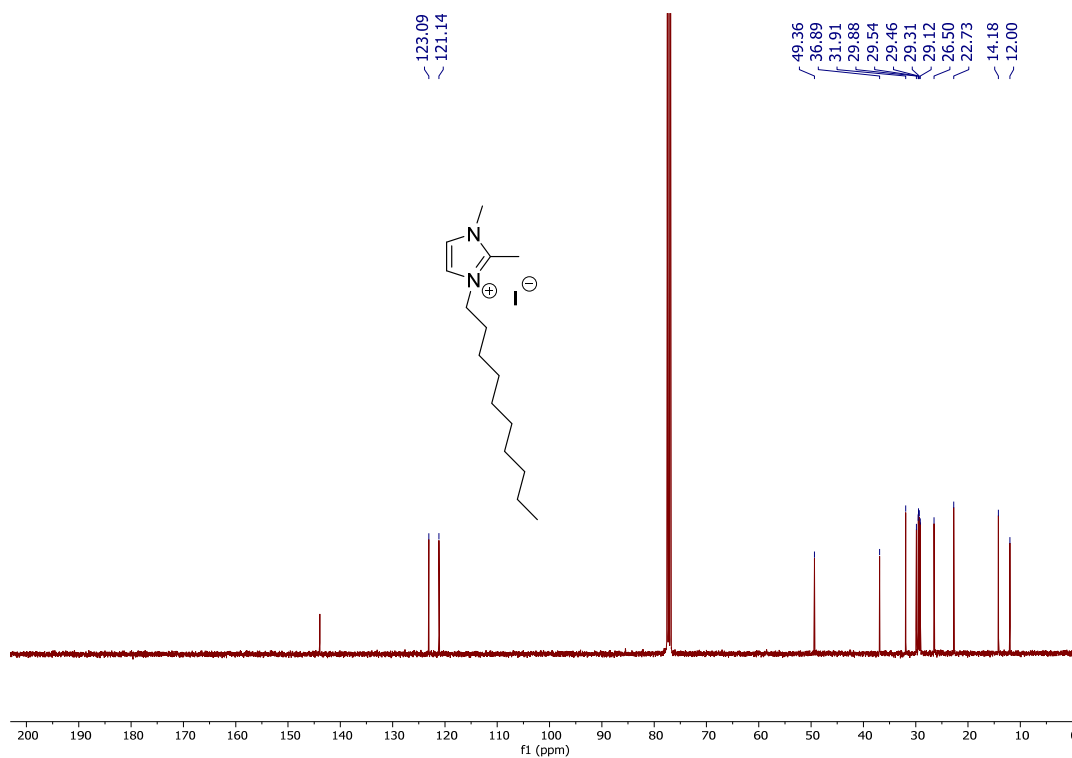
^1H NMR (400 MHz, Methanol- d_4) δ (ppm) 8.90 – 8.81 (m, 2H), 7.96 (d, J = 6.2 Hz, 2H), 4.59 (t, J = 7.6 Hz, 2H), 2.71 (s, 3H), 2.02 (t, J = 7.3 Hz, 2H), 1.38 (dq, J = 10.5, 6.4, 6.0 Hz, 6H), 0.96 – 0.91 (m, 3H).

Spectra

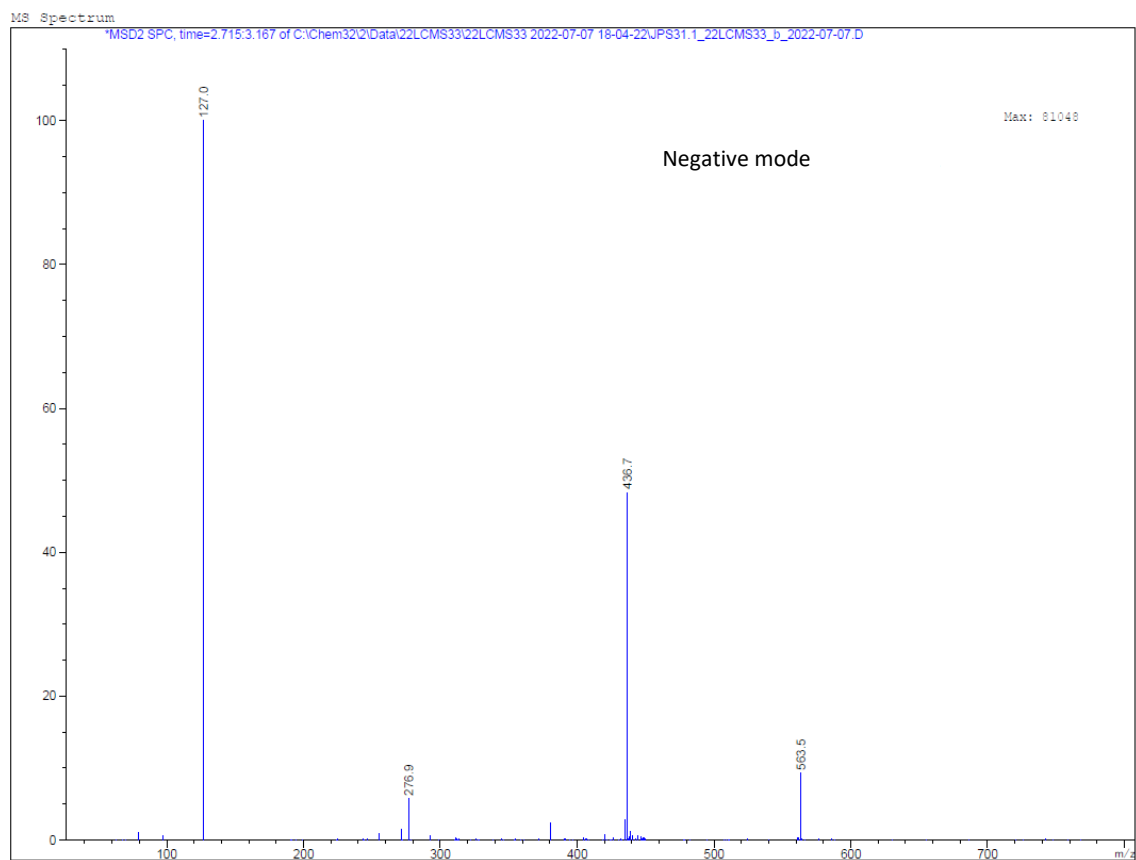
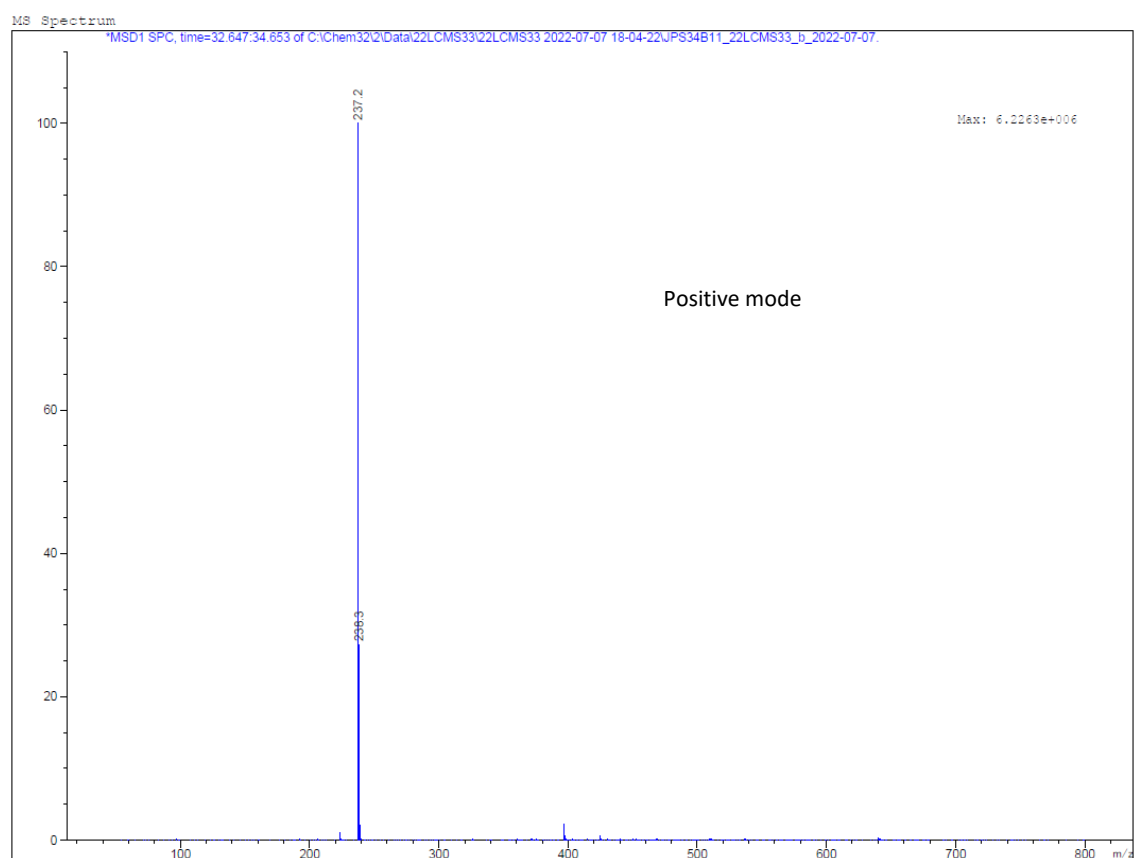
^1H -NMR (400 MHz, CDCl_3) spectrum of 3-decyl-1,2-dimethylimidazolium iodide (**4**):



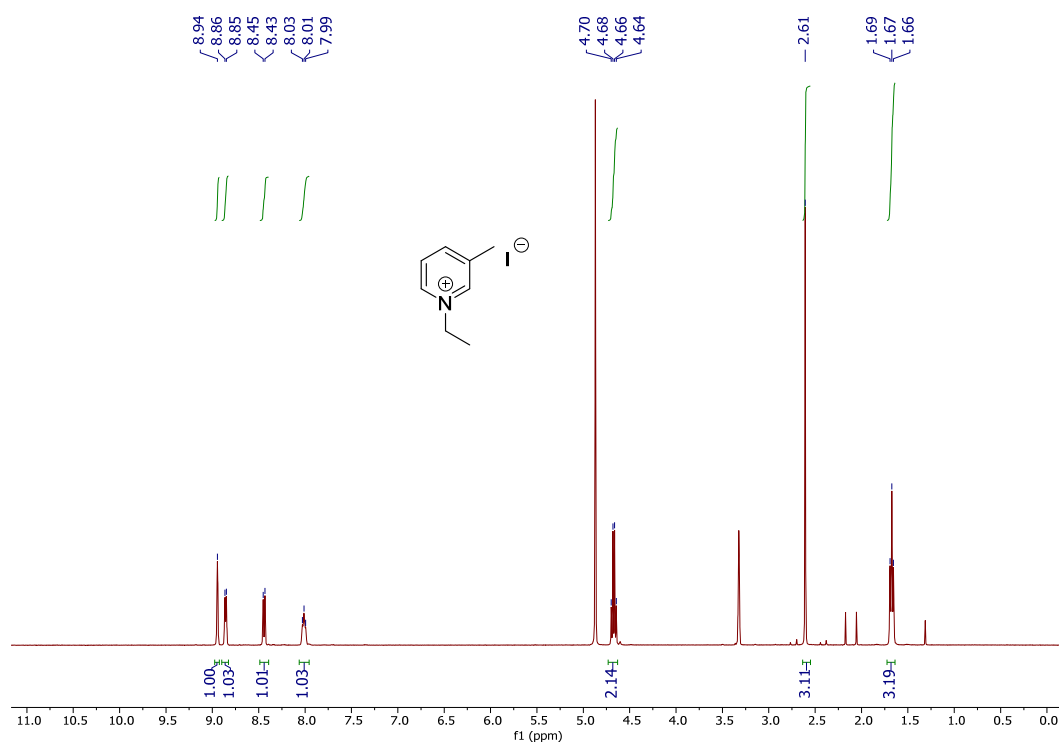
^{13}C -NMR (101 MHz, CDCl_3) spectrum of 3-decyl-1,2-dimethylimidazolium iodide (**4**)



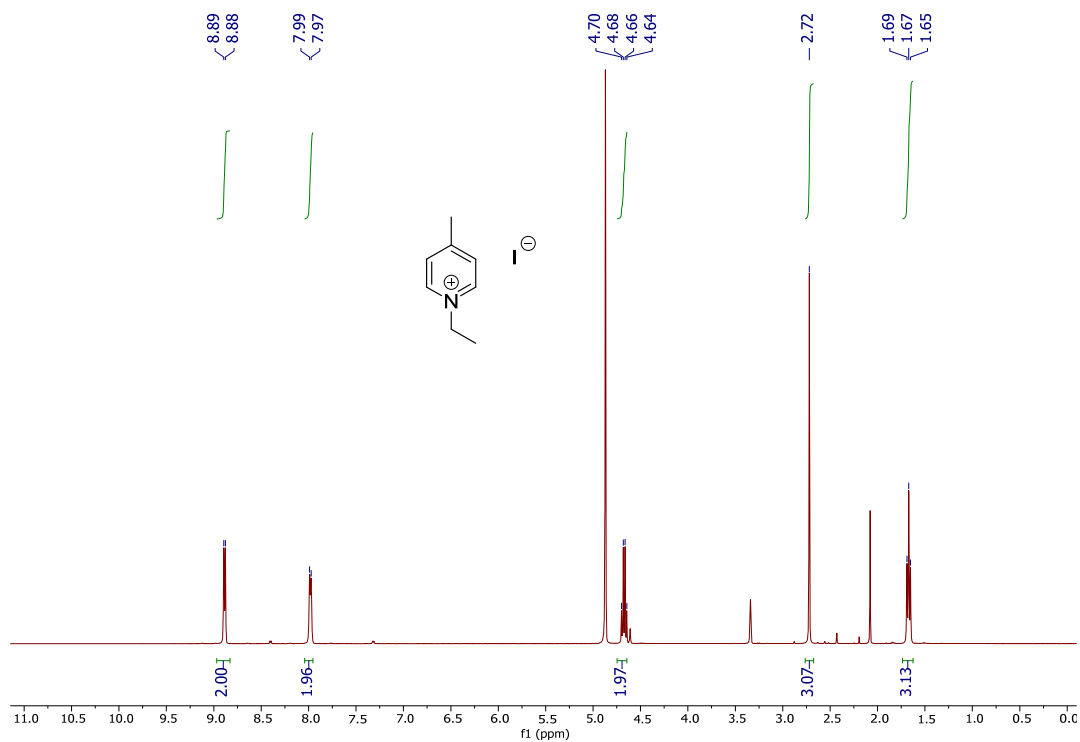
MS spectra of 3-decyl-1,2-dimethylimidazolium iodide (**4**):



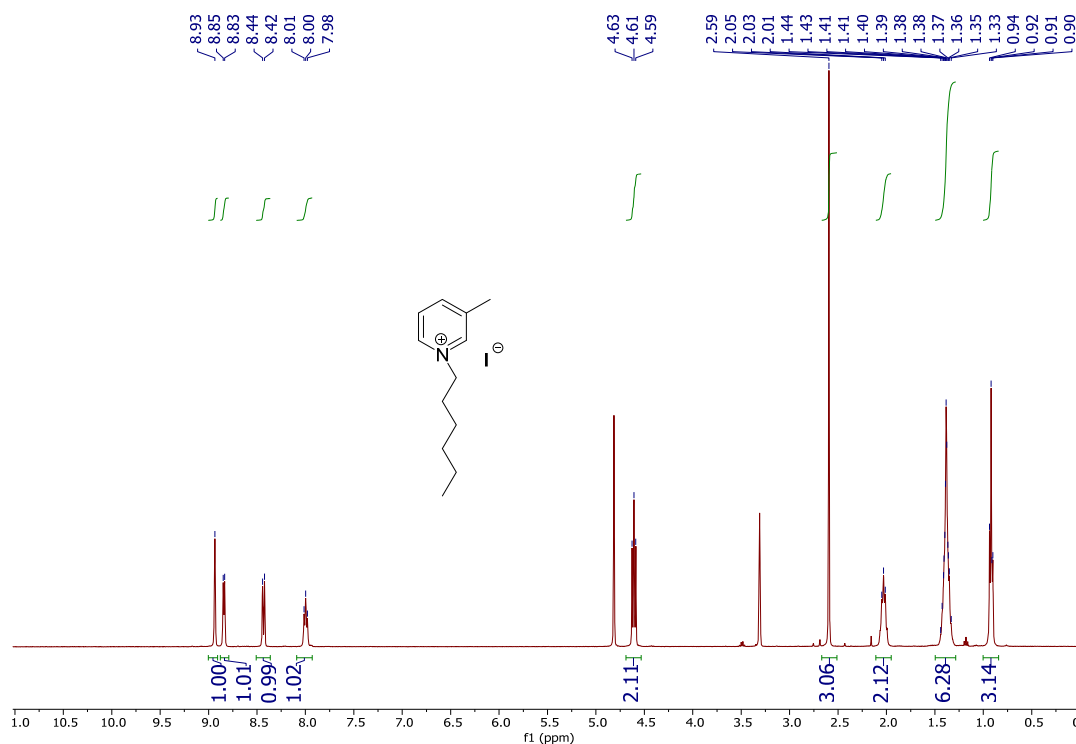
^1H -NMR (400 MHz, Methanol- d_4) spectrum of N-ethyl-3-methylpyridinium iodide (**5**):



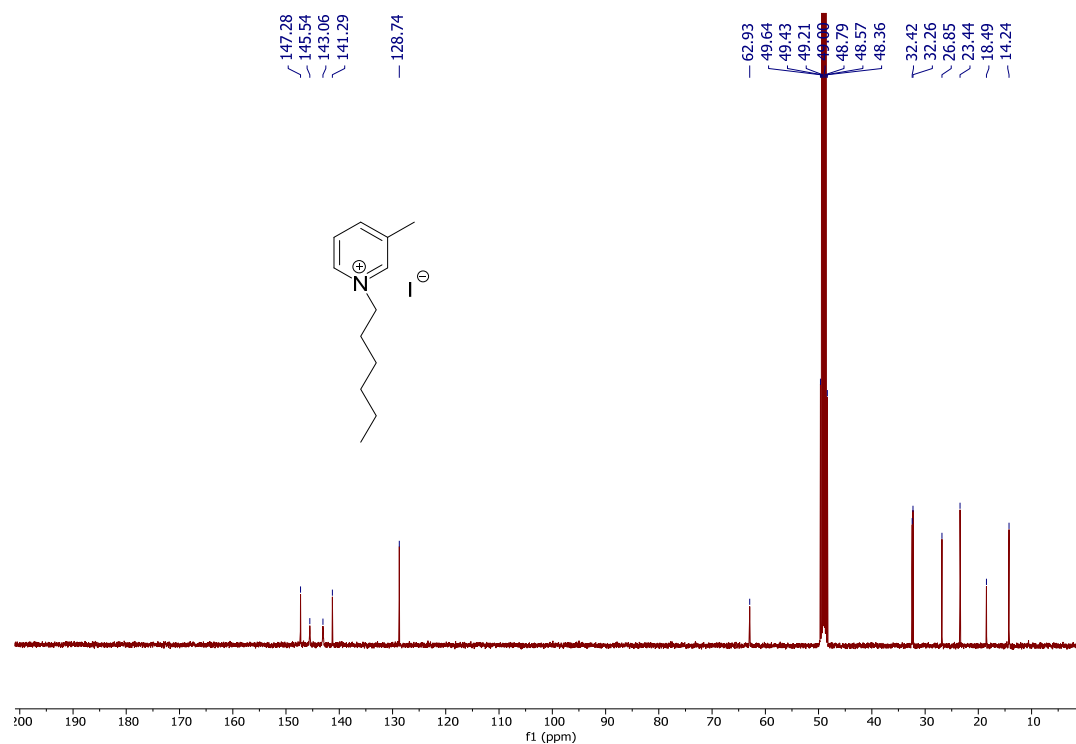
^1H -NMR (400 MHz, Methanol- d_4) spectrum of N-ethyl-4-methylpyridinium iodide (**7**):



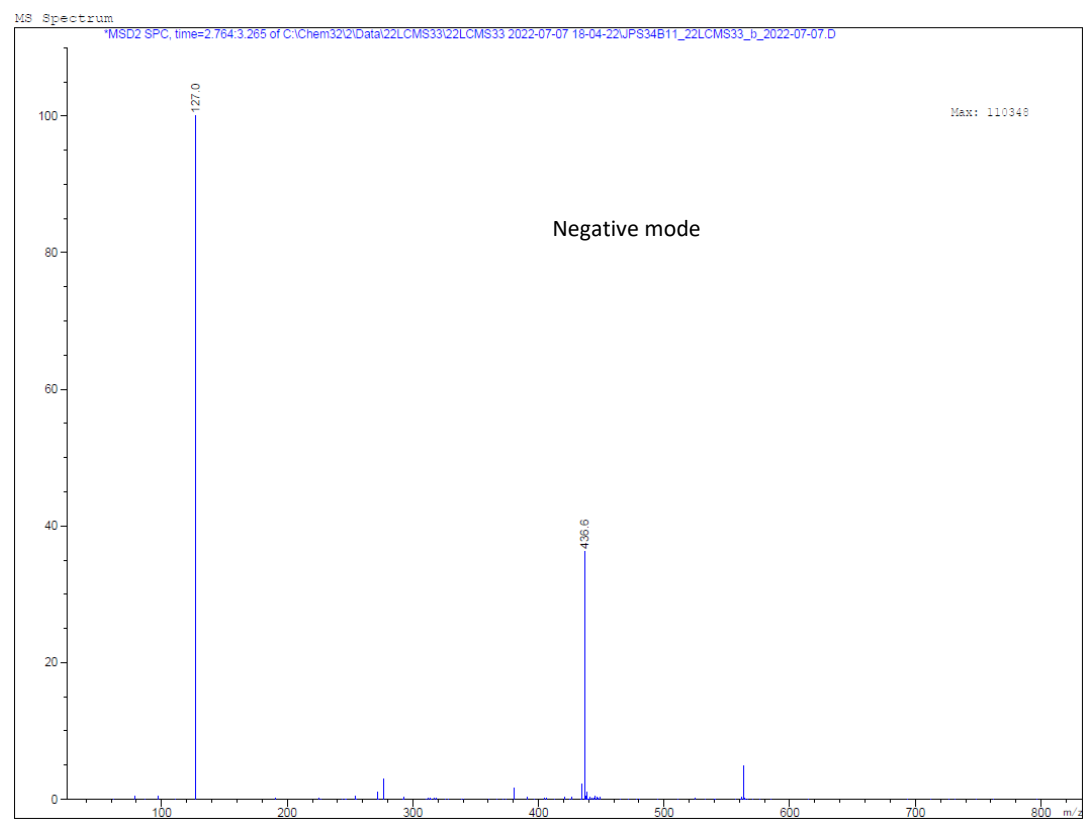
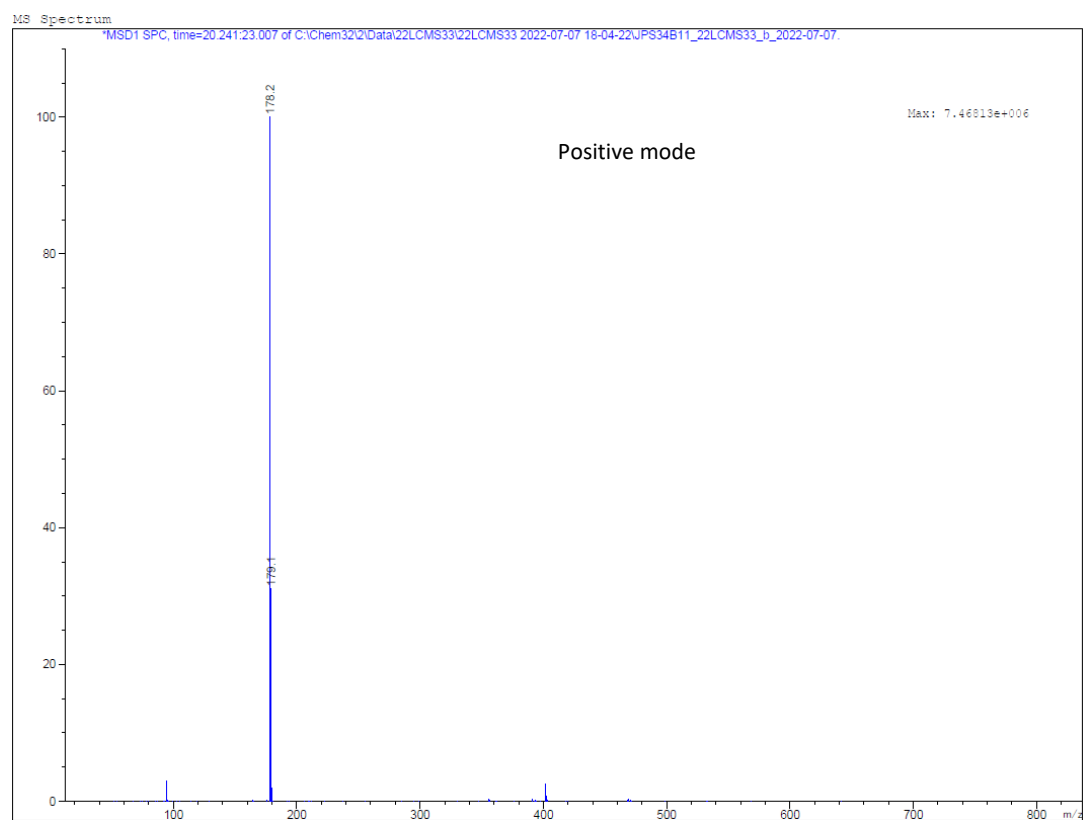
^1H -NMR (400 MHz, Methanol- d_4) spectrum of N-hexyl-3-methylpyridinium iodide (**6**):



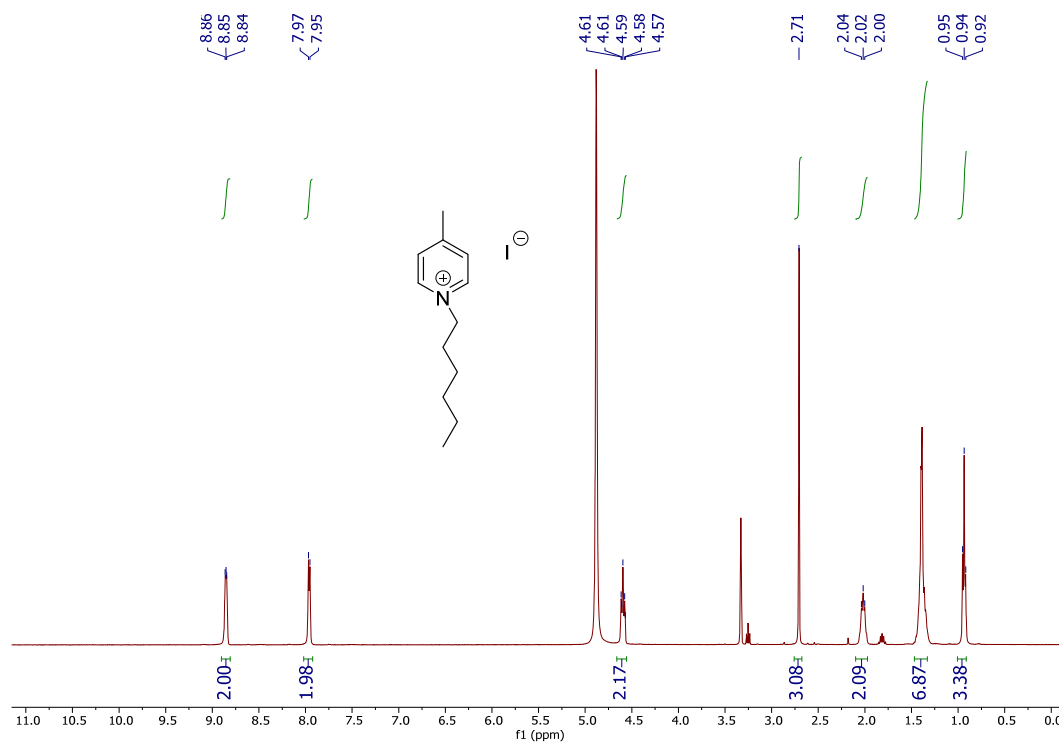
^{13}C -NMR (101 MHz, Methanol- d_4) spectrum of N-hexyl-3-methylpyridinium iodide (**6**):



MS spectra of N-hexyl-3-methylpyridinium iodide (6):



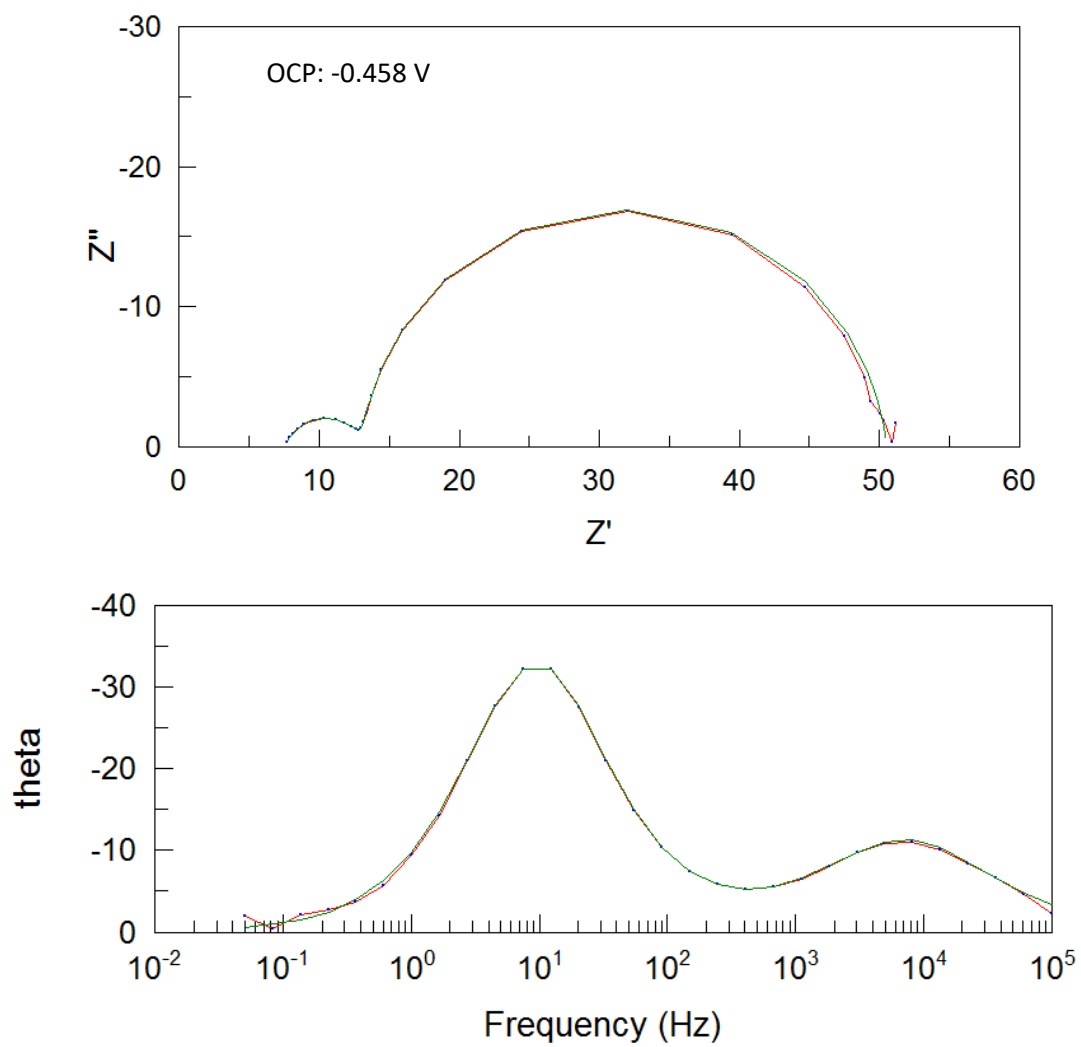
^1H -NMR (400 MHz, Methanol- d_4) spectrum of N-hexyl-4-methylpyridinium iodide (**8**):



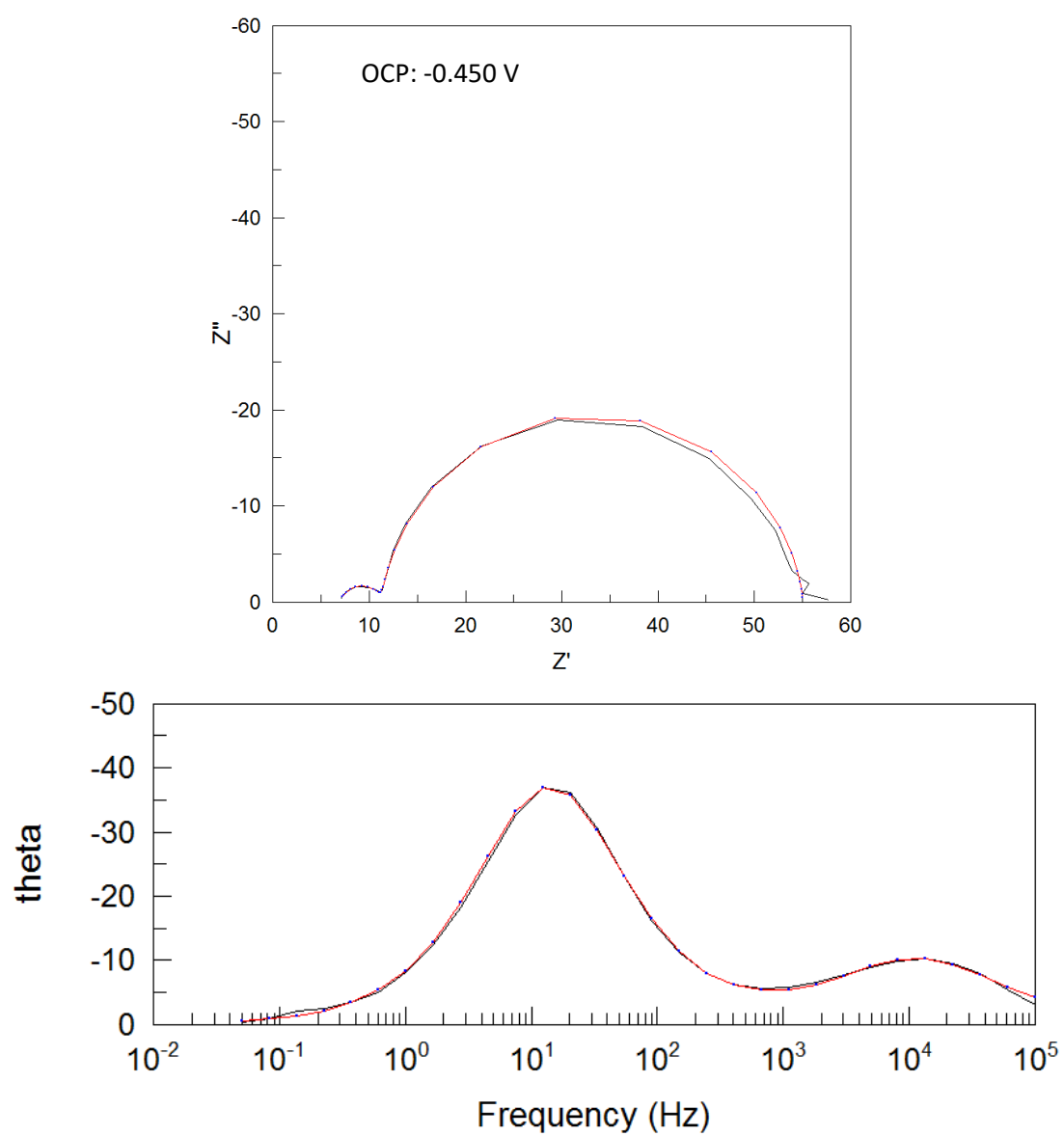
Electrochemical Impedance Spectroscopy

Without 4-TBP:

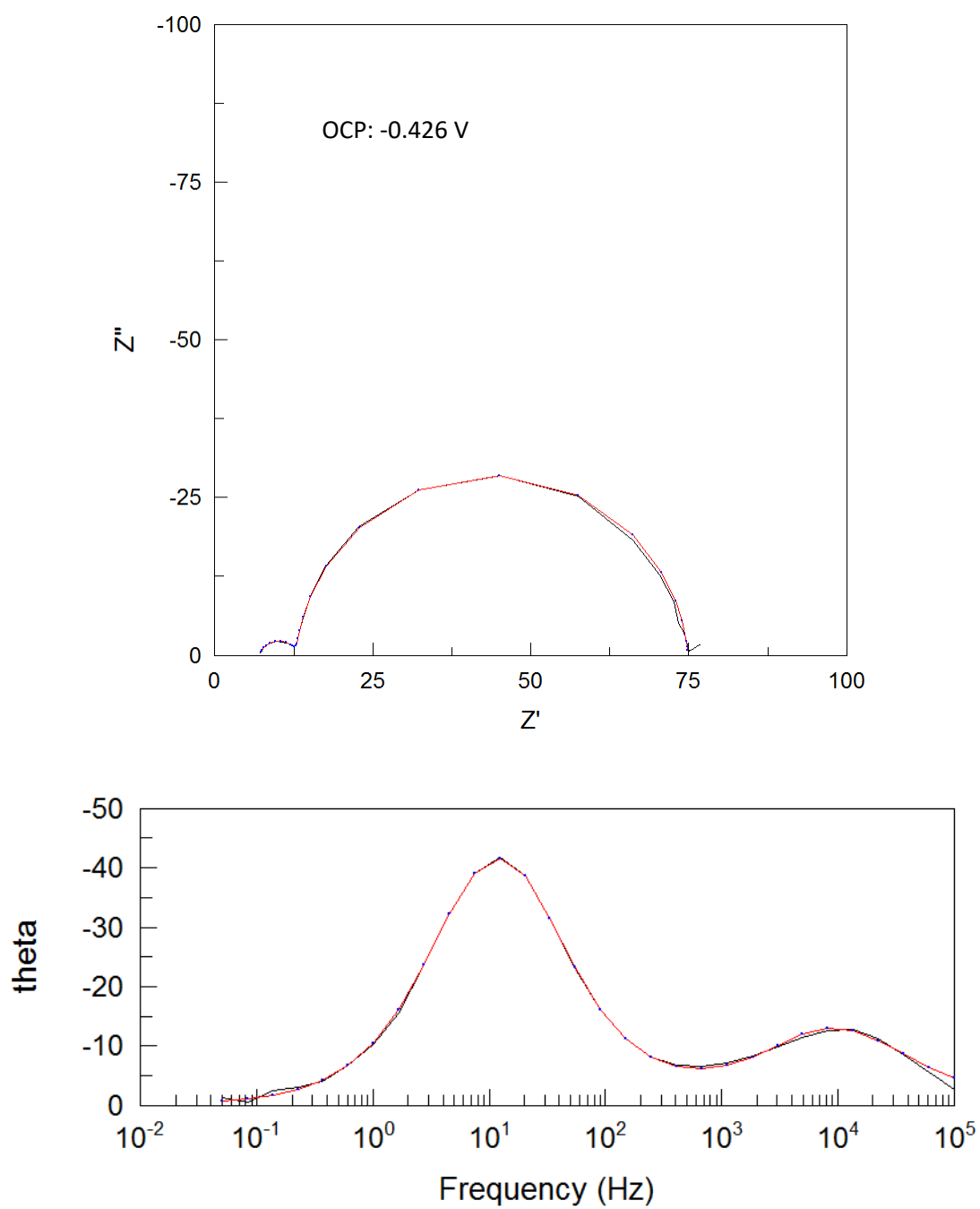
Nyquist (top) and Bode (bottom) plots of reference:



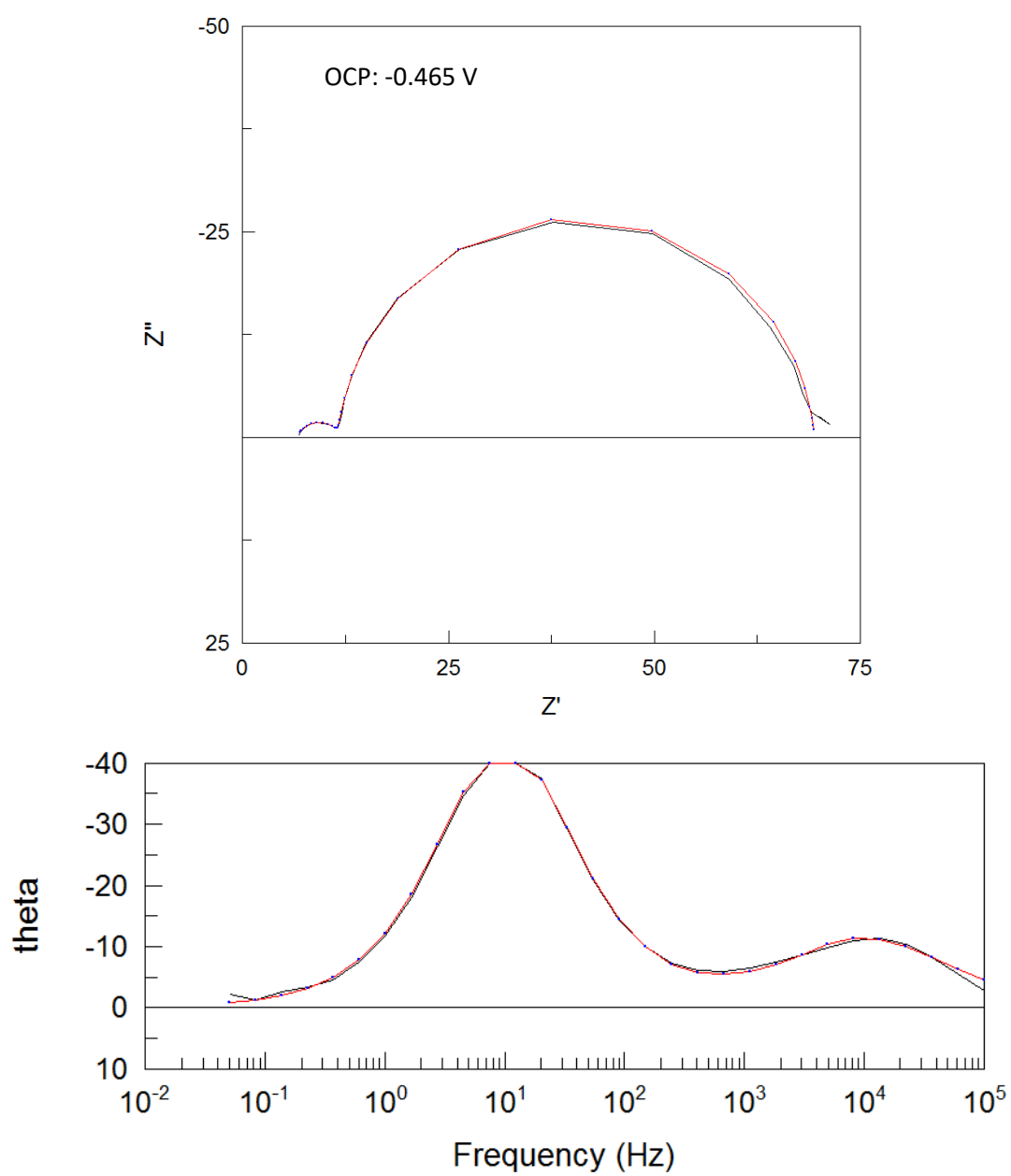
Nyquist (top) and Bode (bottom) plots of **E1**:



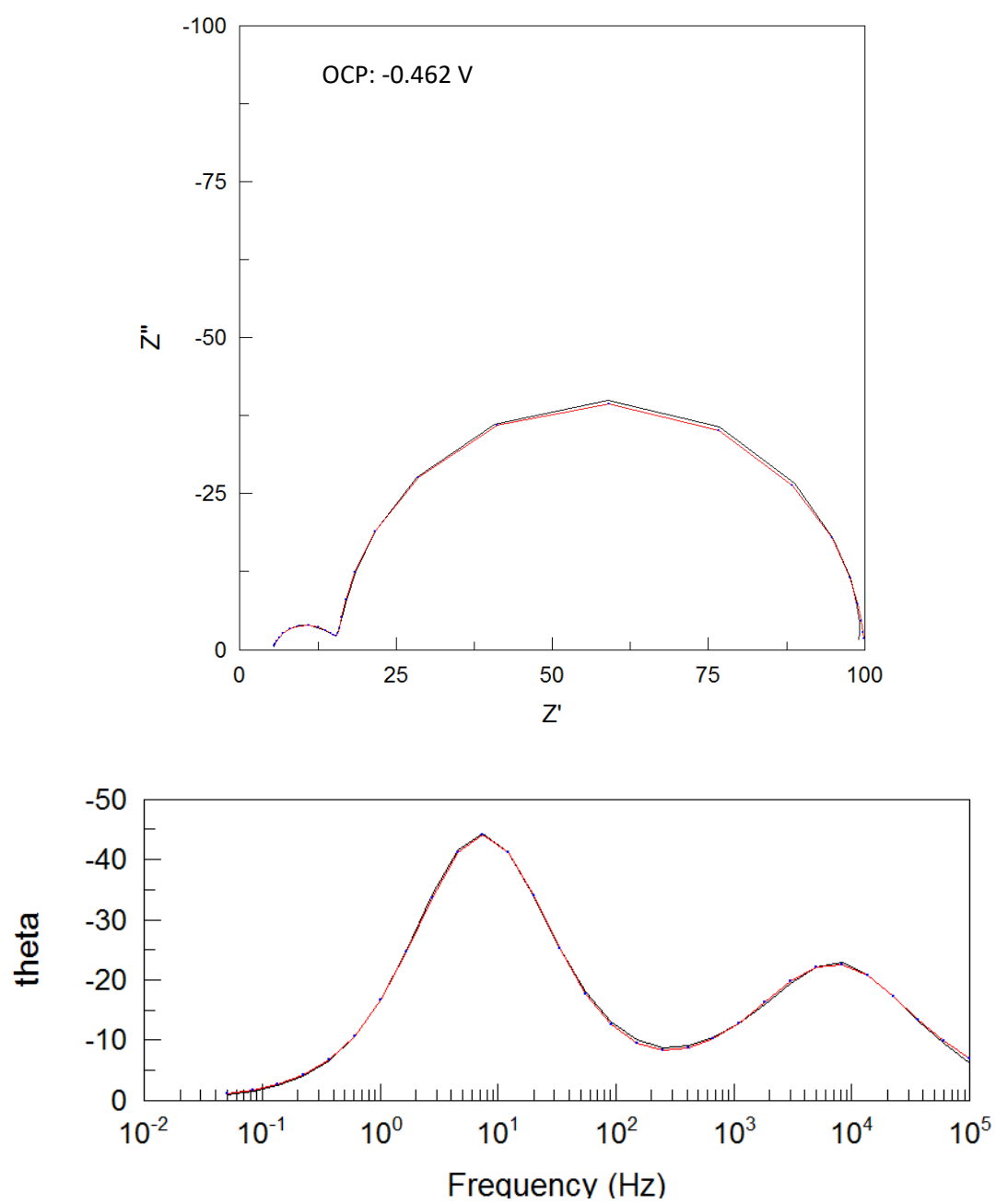
Nyquist (top) and Bode (bottom) plots of E2:



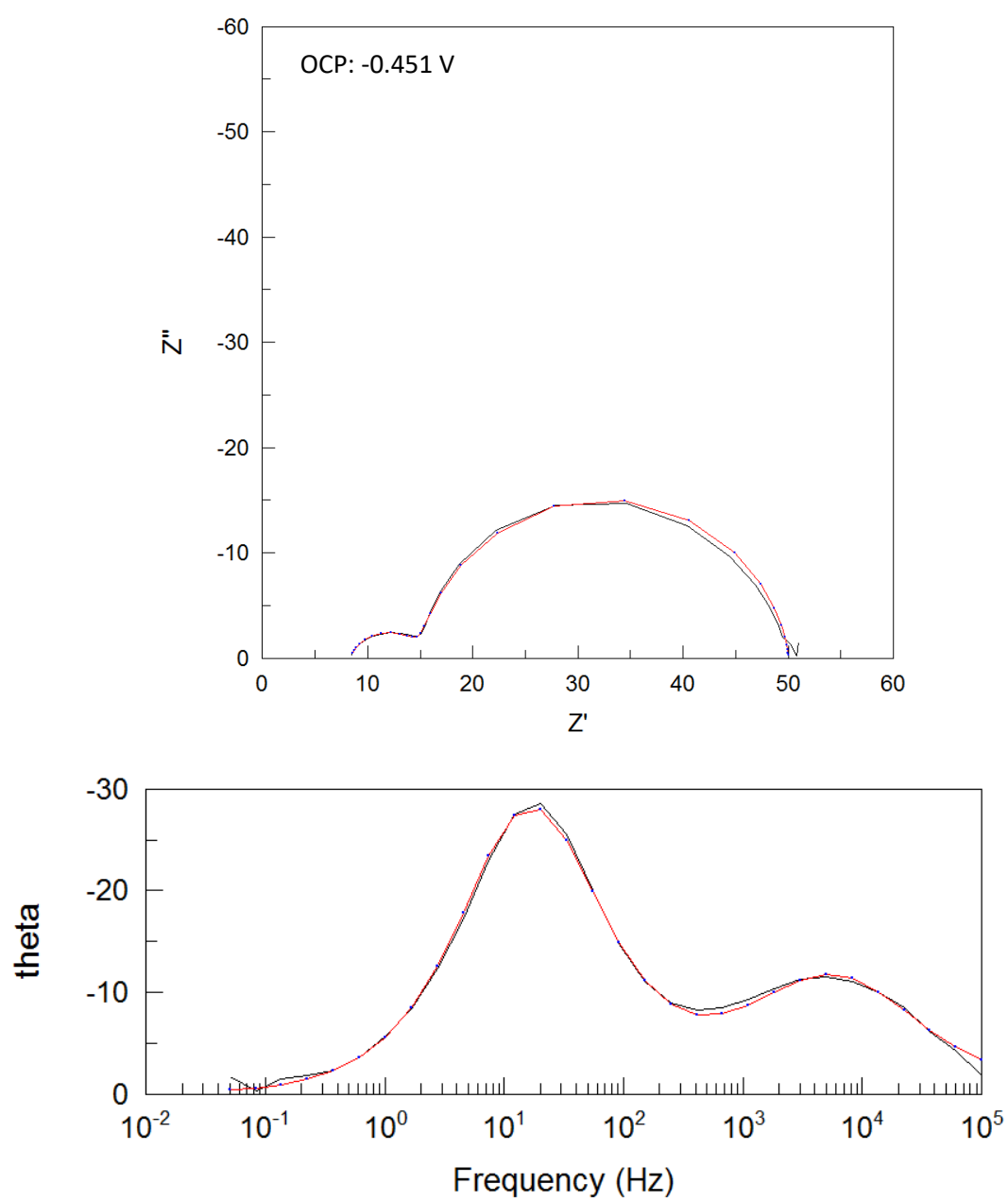
Nyquist (top) and Bode (bottom) plots of **E3**:



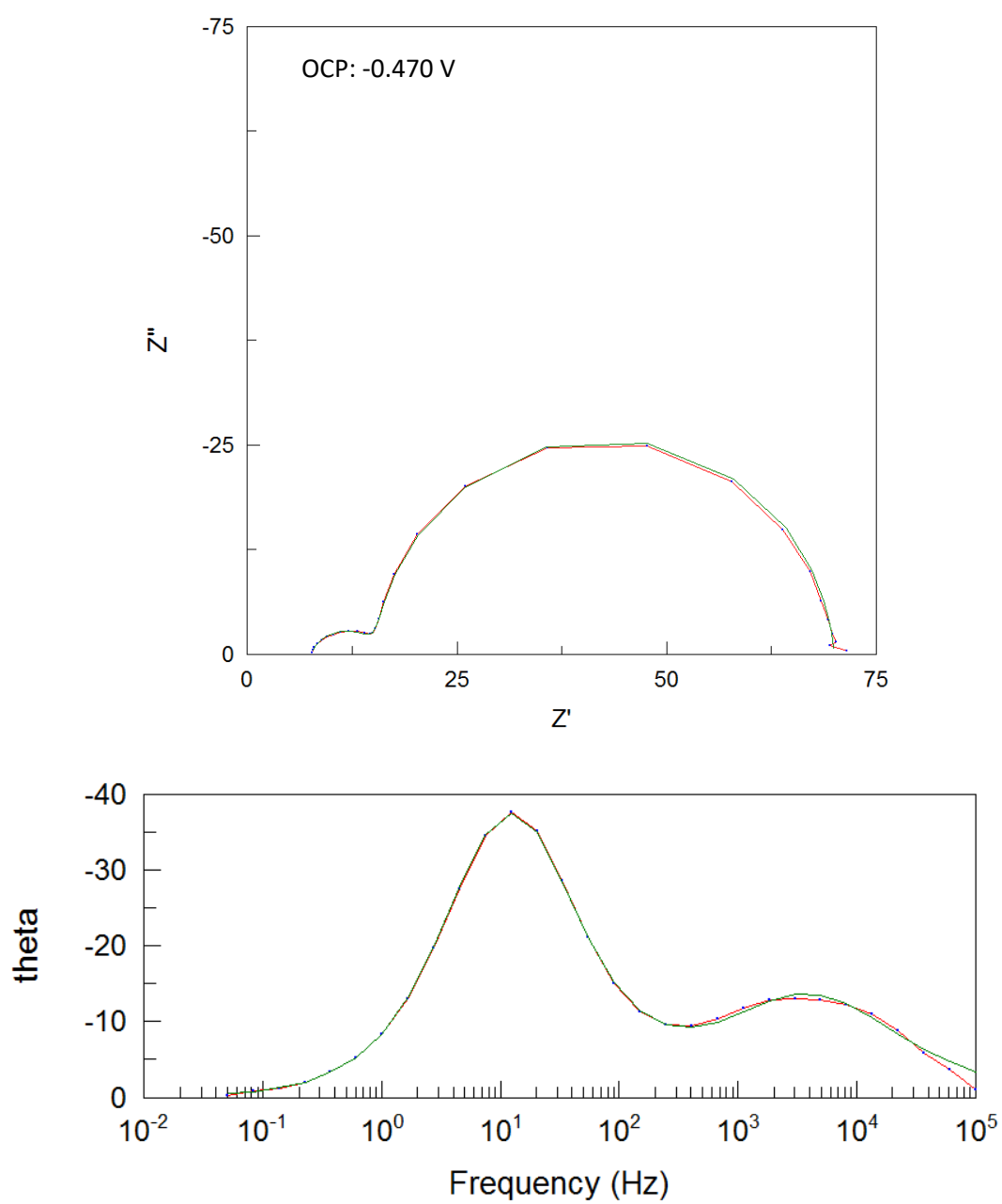
Nyquist (top) and Bode (bottom) plots of **E4**:



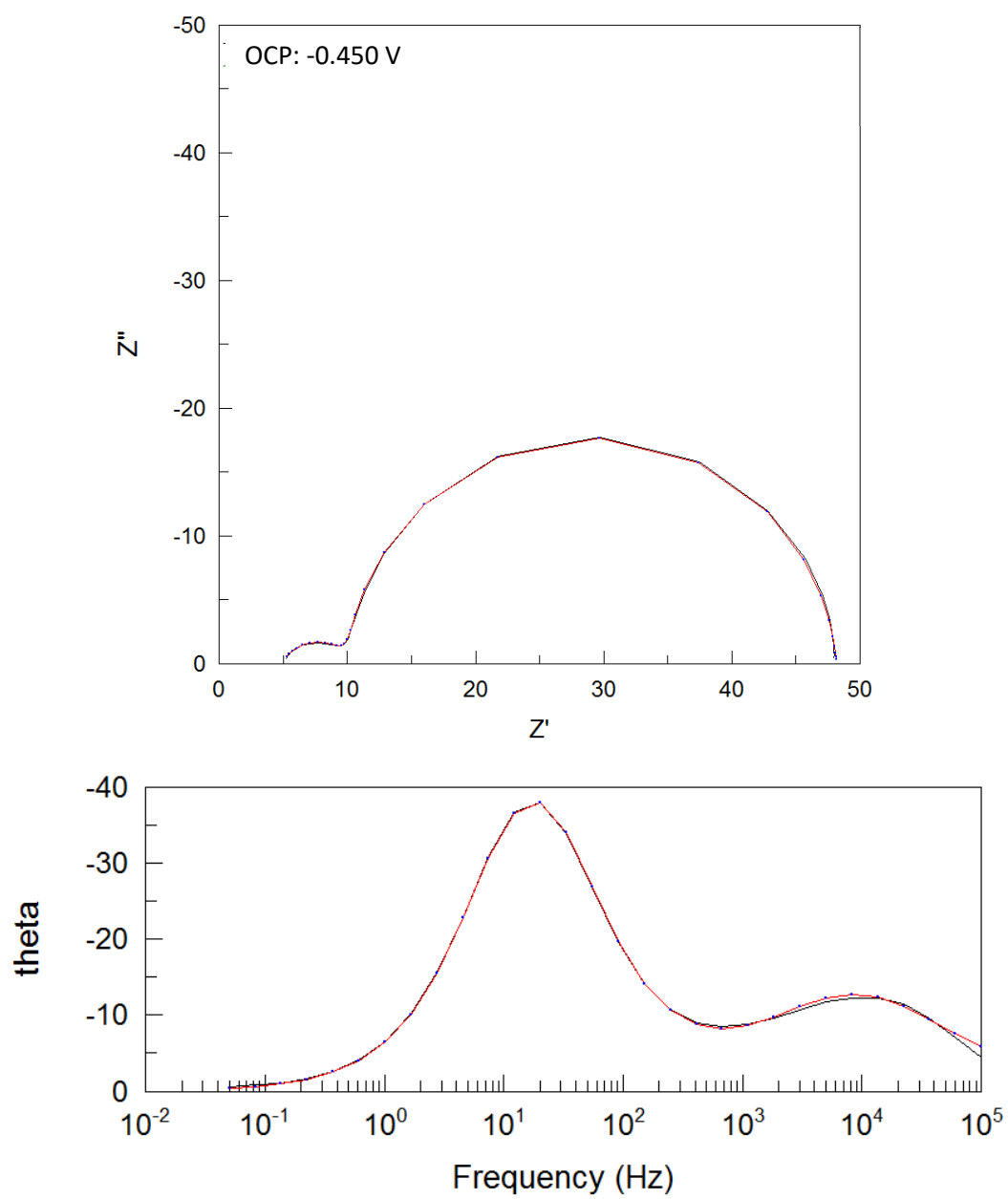
Nyquist (top) and Bode (bottom) plots of **E5**:



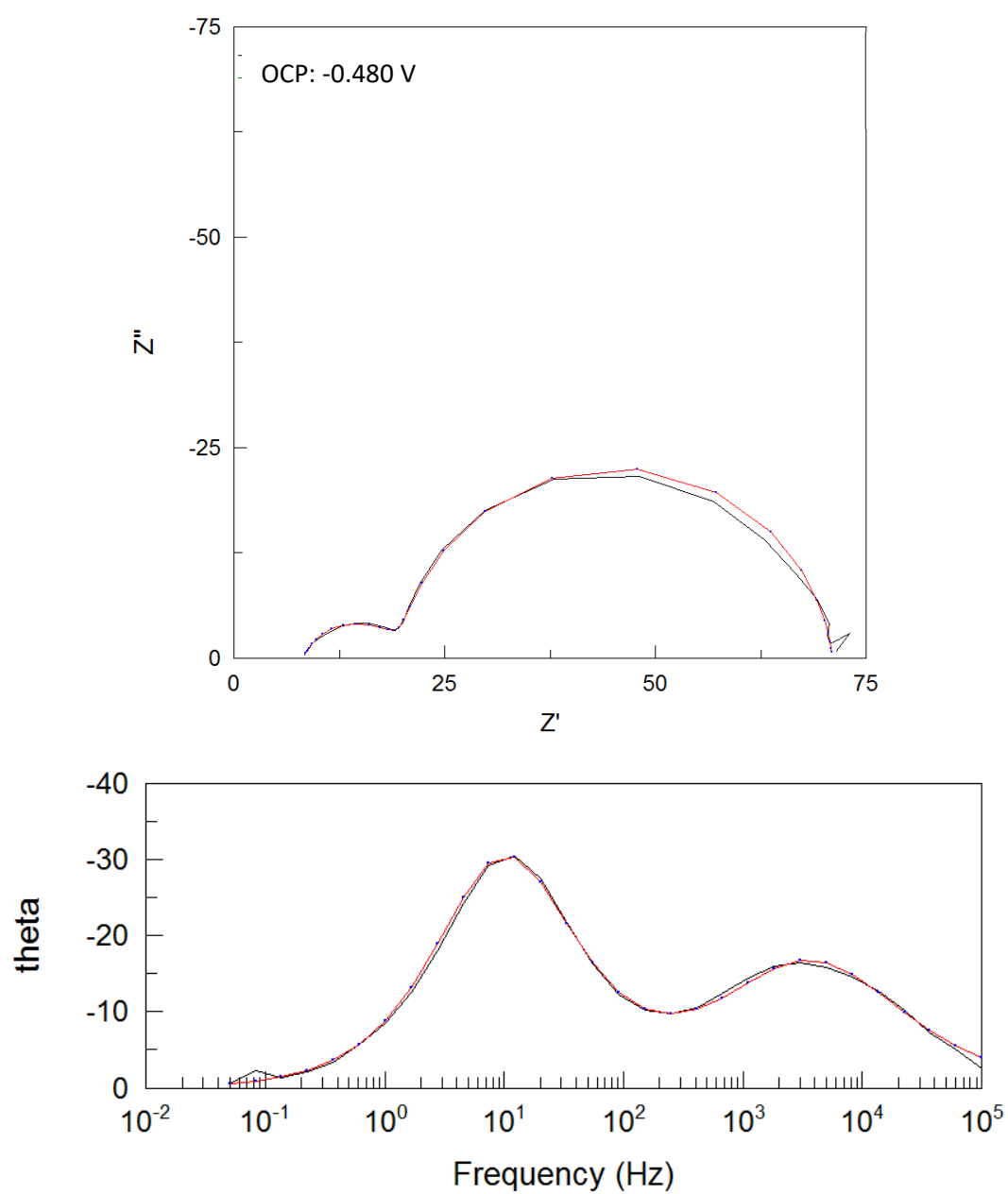
Nyquist (top) and Bode (bottom) plots of E6:



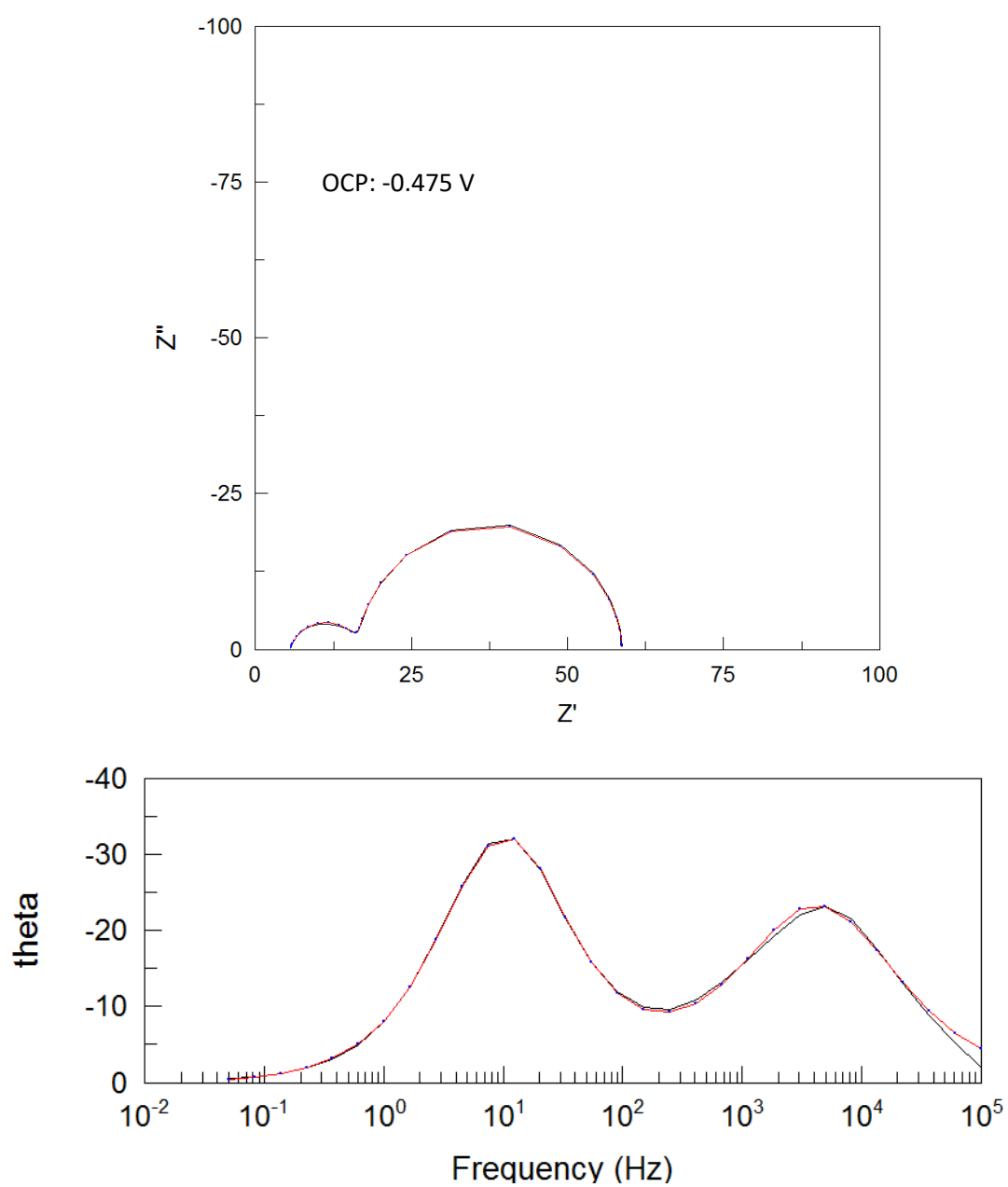
Nyquist (top) and Bode (bottom) plots of **E7**:



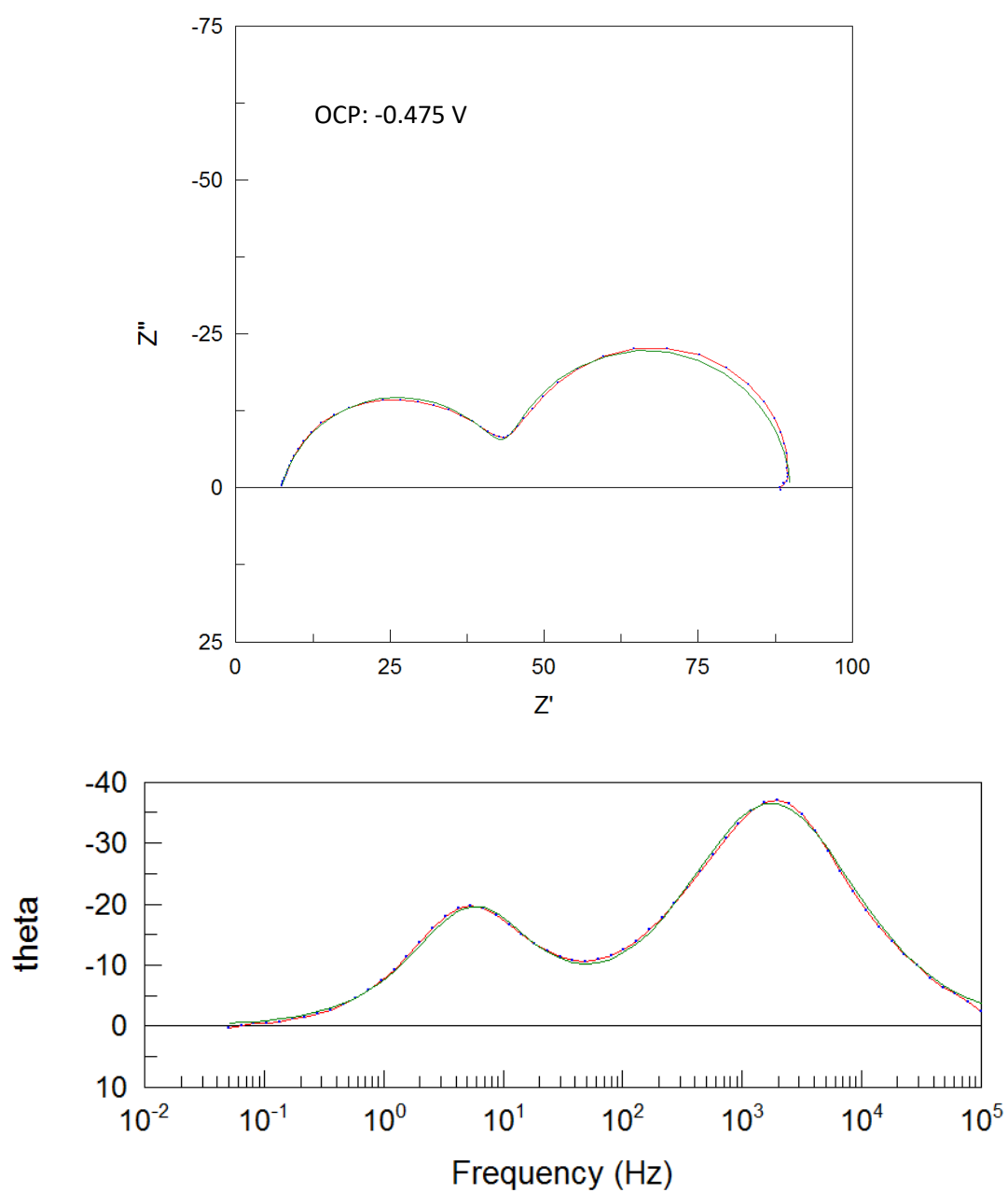
Nyquist (top) and Bode (bottom) plots of **E8**:



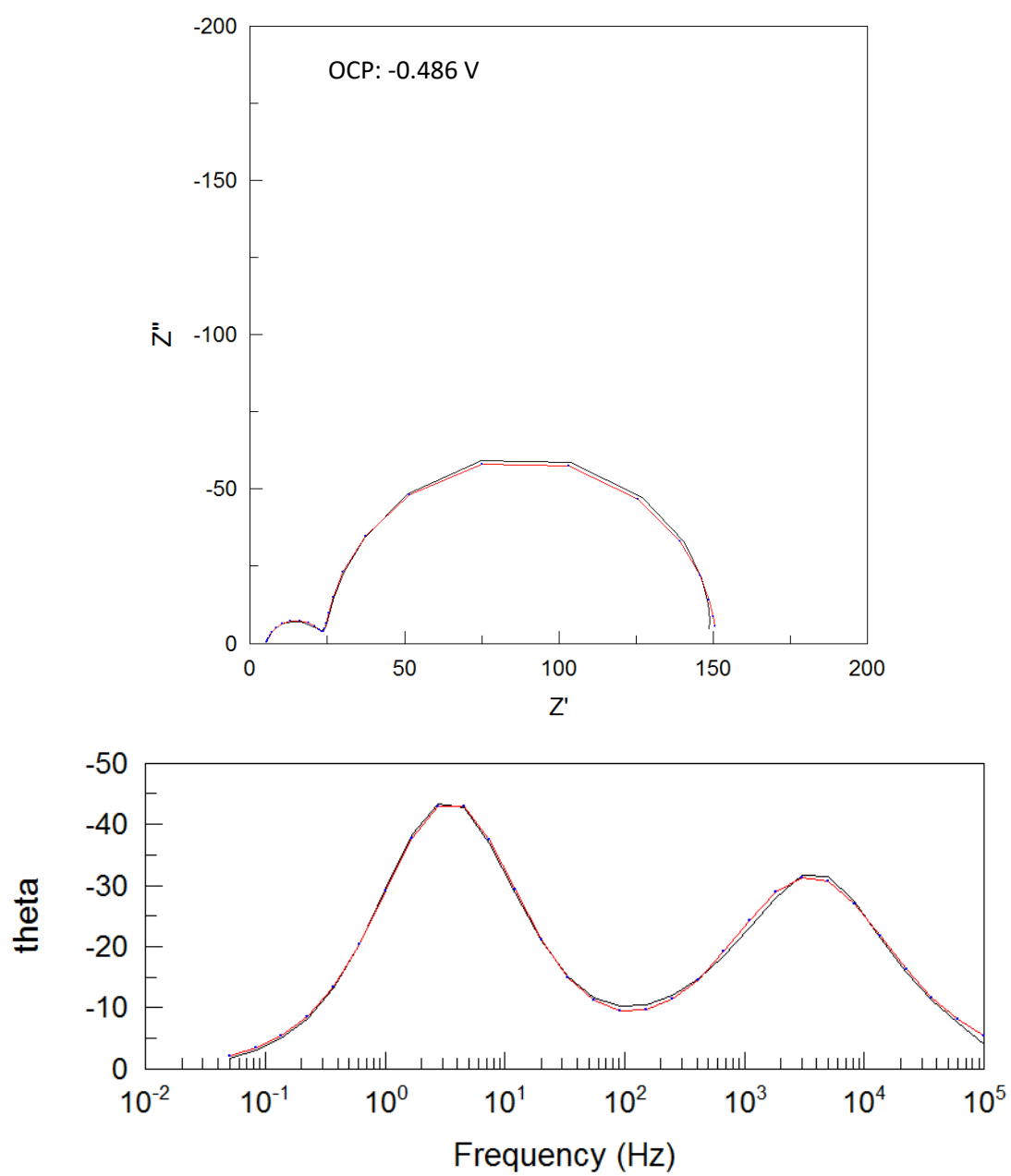
Nyquist (top) and Bode (bottom) plots of **E9**:



Nyquist (top) and Bode (bottom) plots of **E10**:

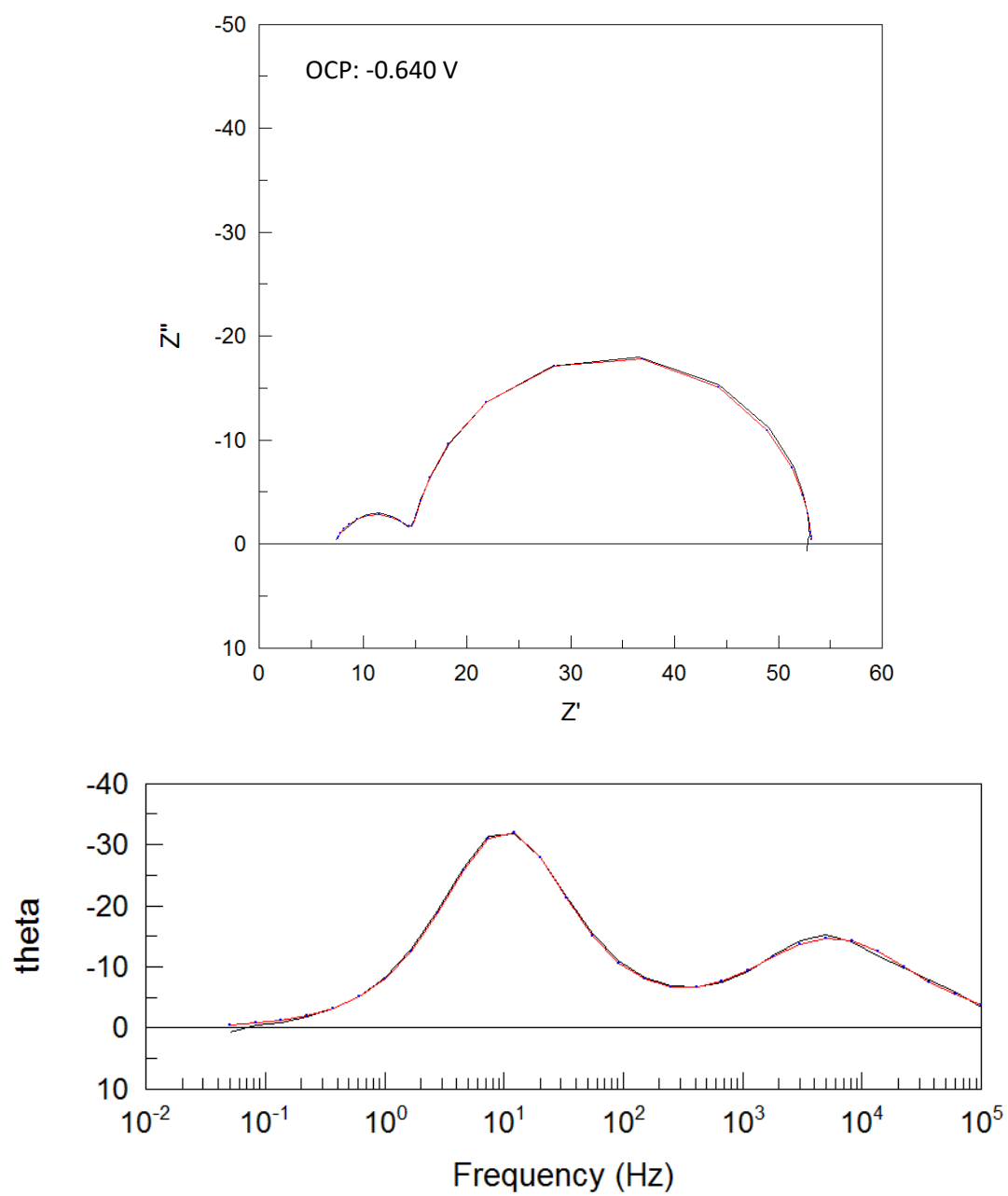


Nyquist (top) and Bode (bottom) plots of **E11**:

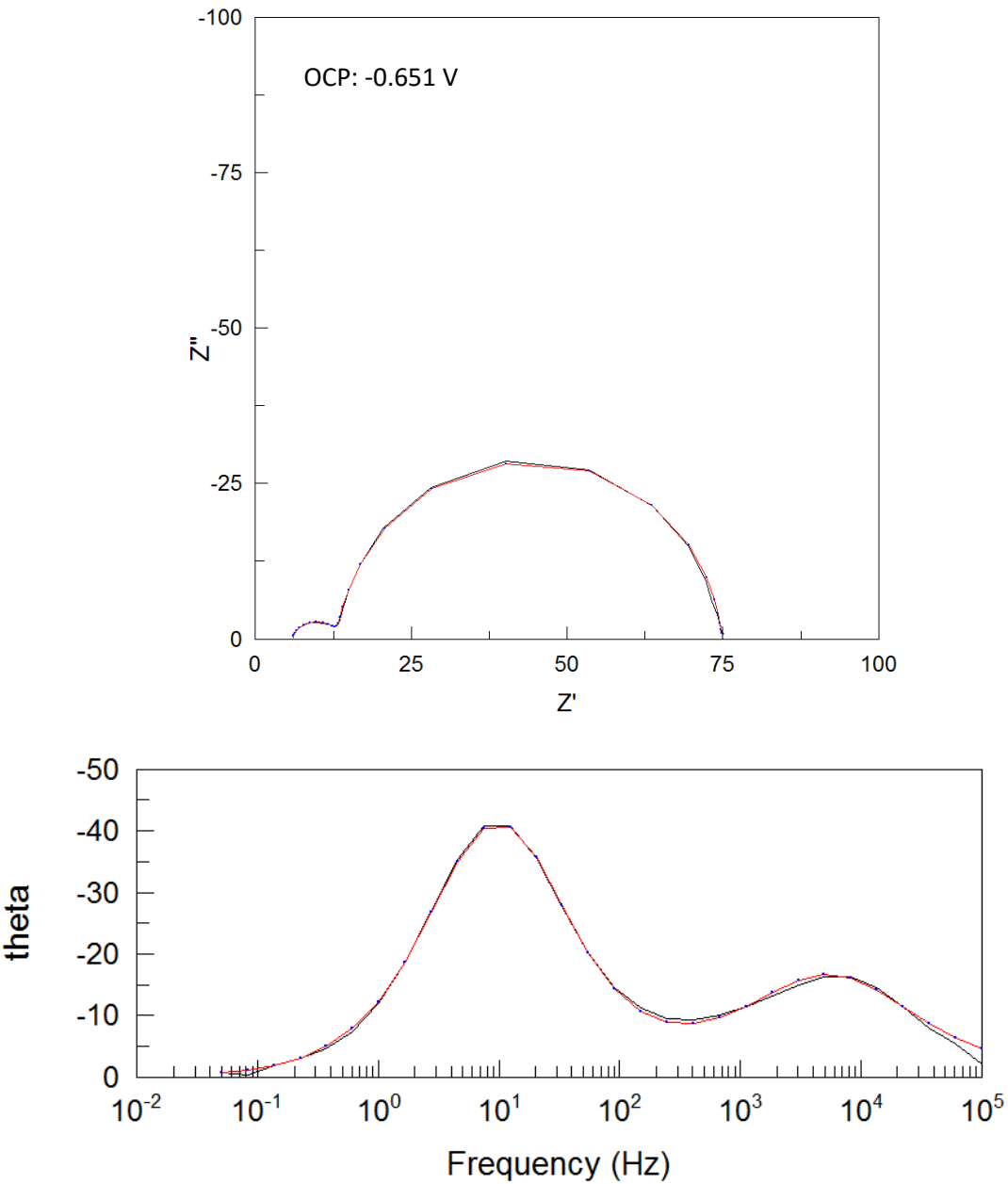


With 4-TBP:

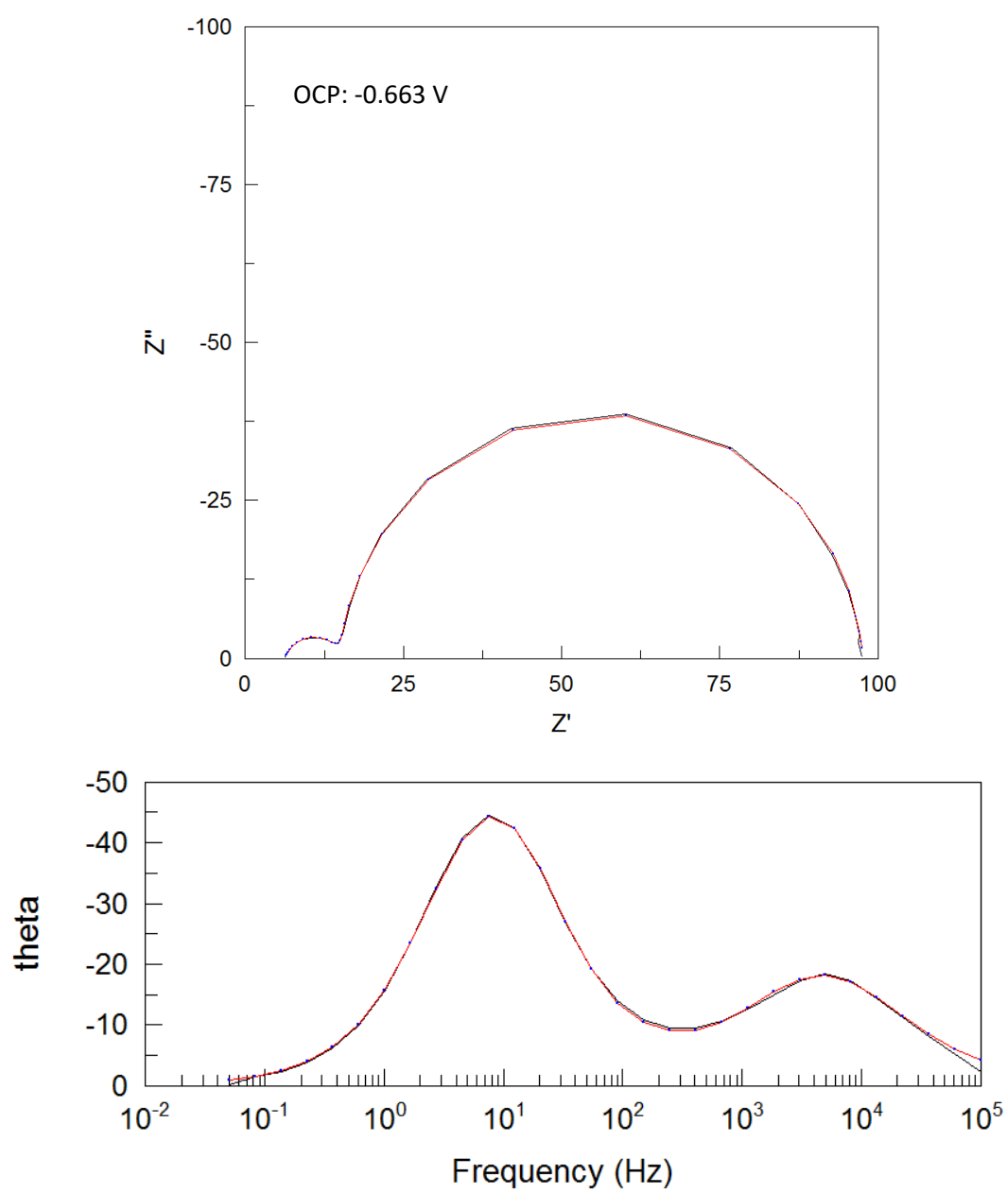
Nyquist (top) and Bode (bottom) plots of reference:



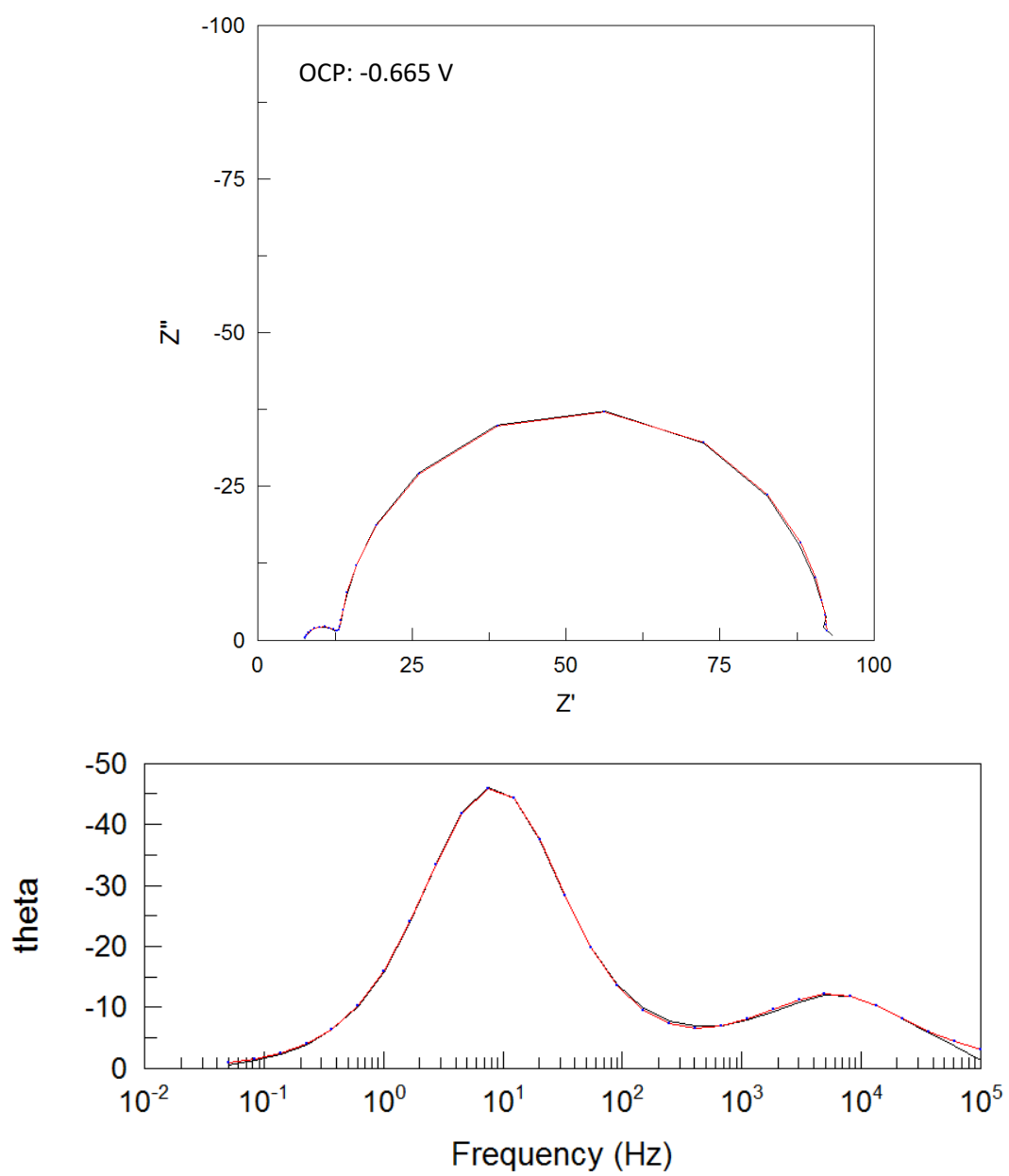
Nyquist (top) and Bode (bottom) plots of **E1**:



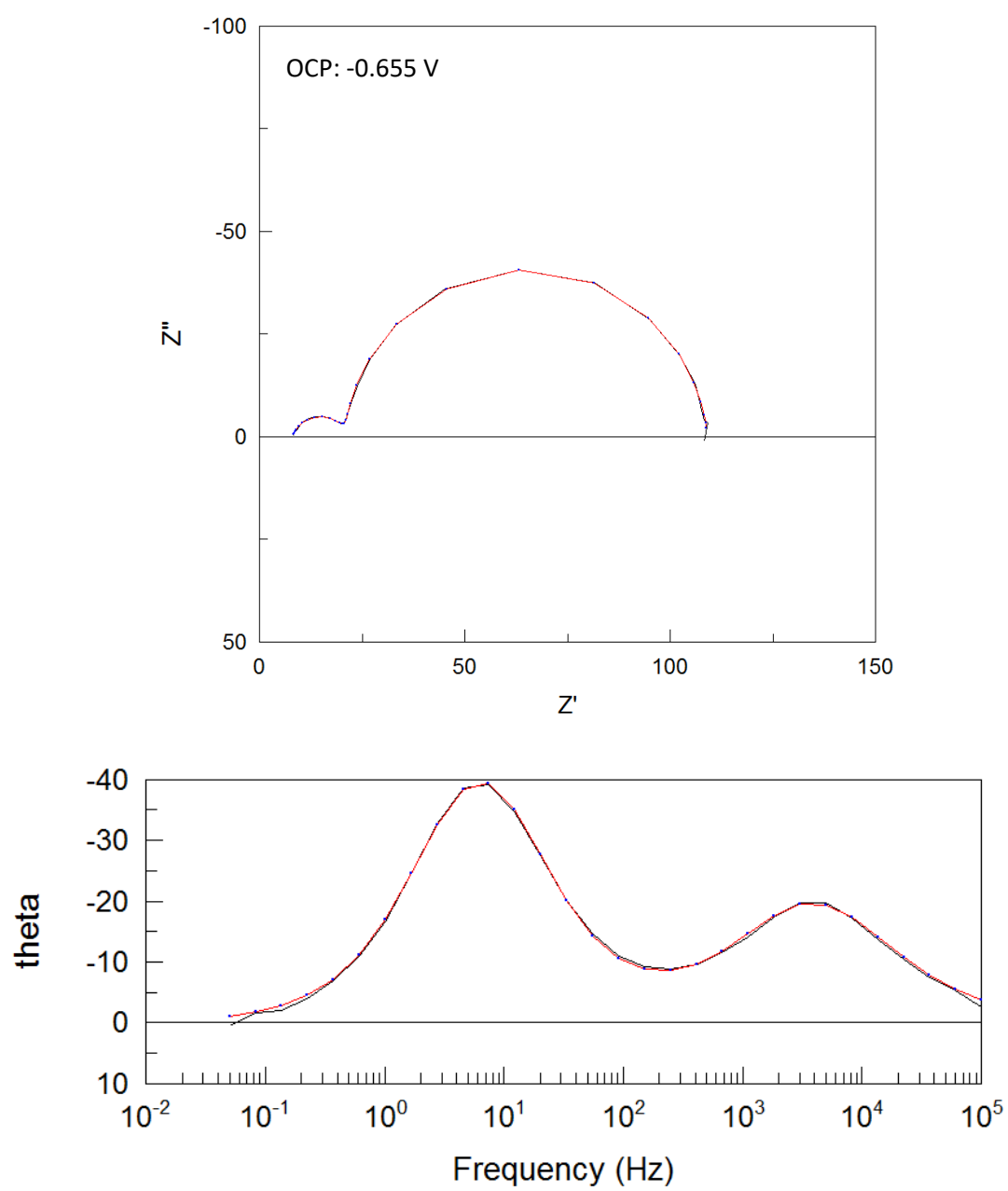
Nyquist (top) and Bode (bottom) plots of E2:



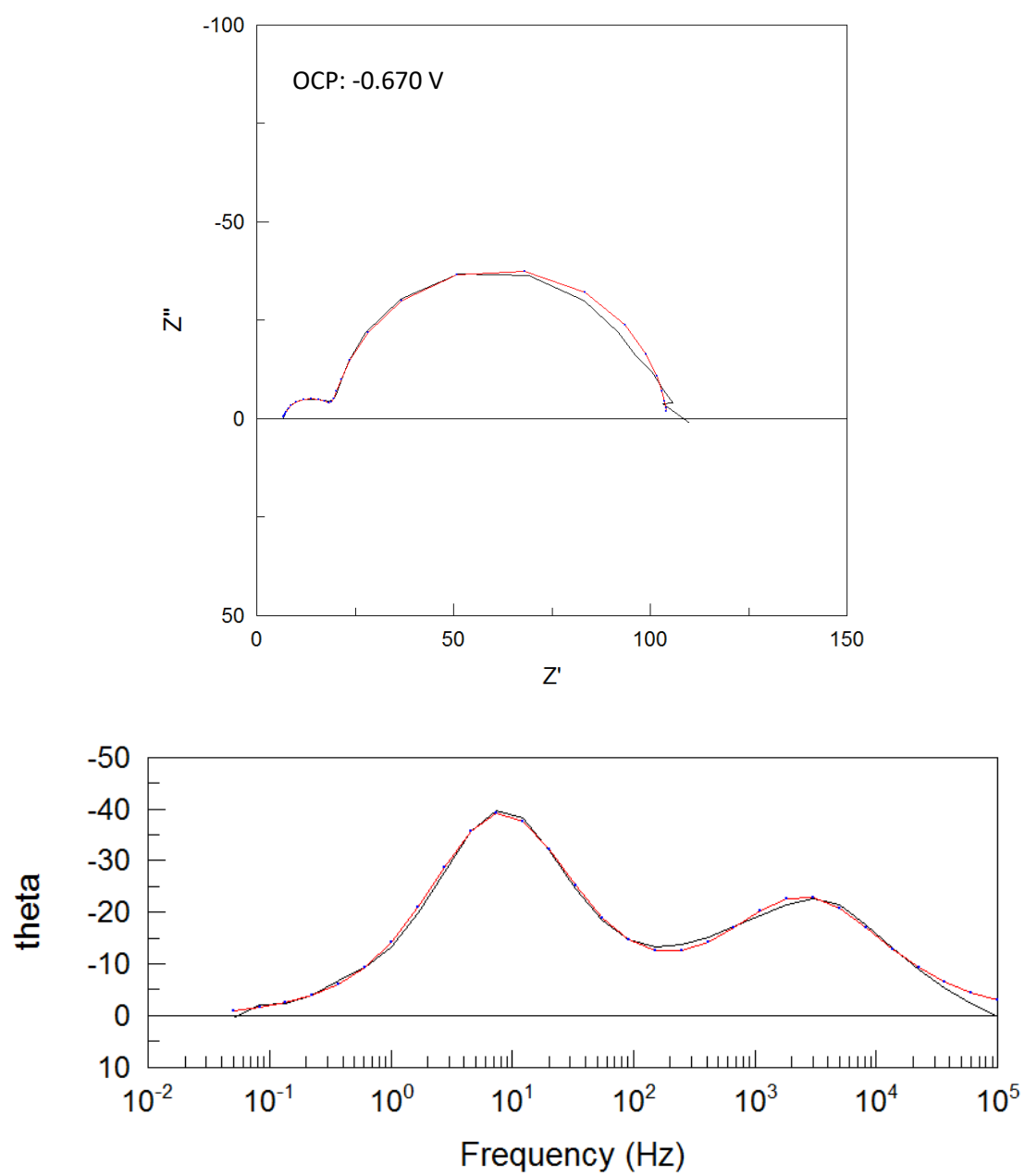
Nyquist (top) and Bode (bottom) plots of **E3**:



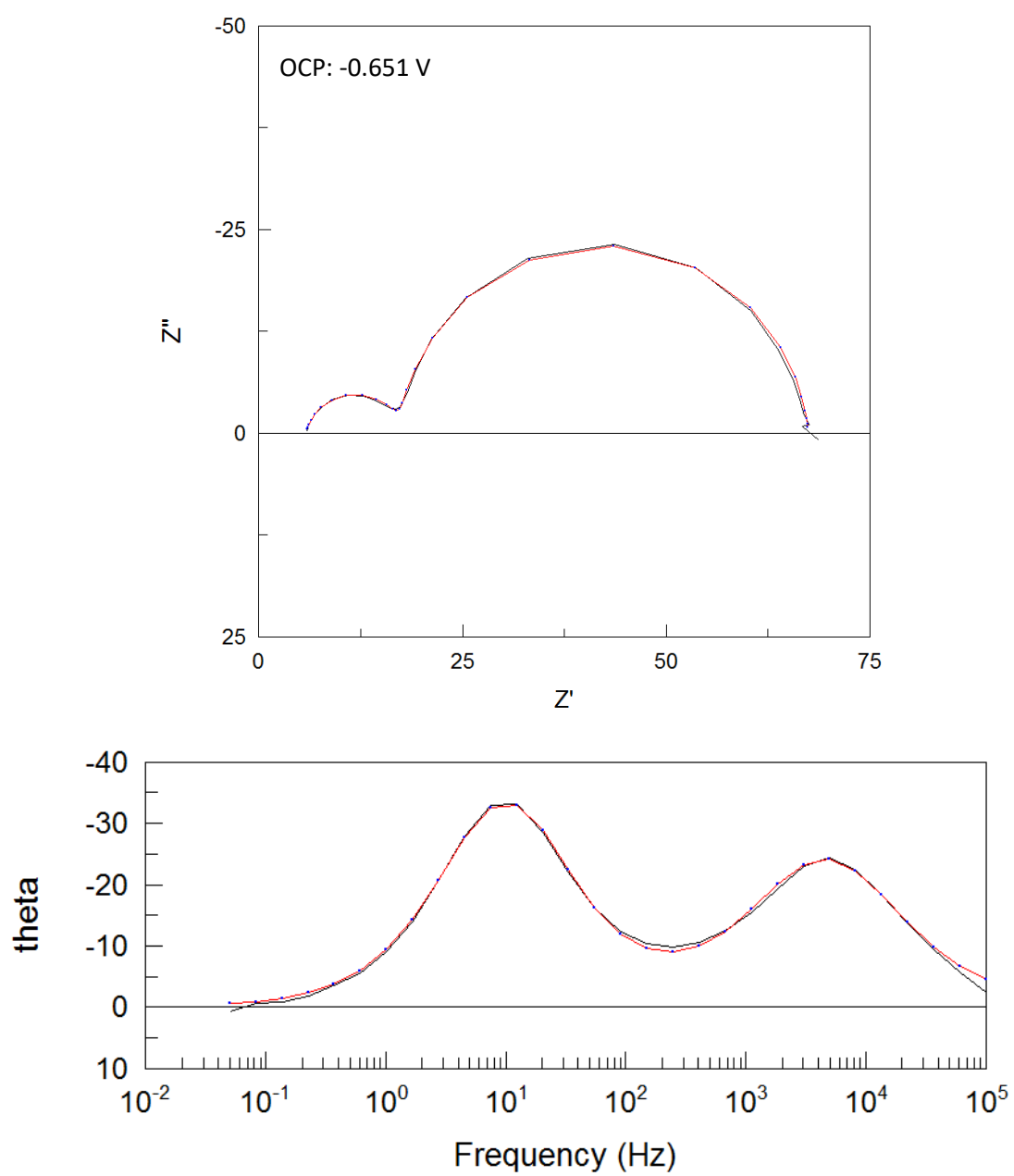
Nyquist (top) and Bode (bottom) plots of **E4**:



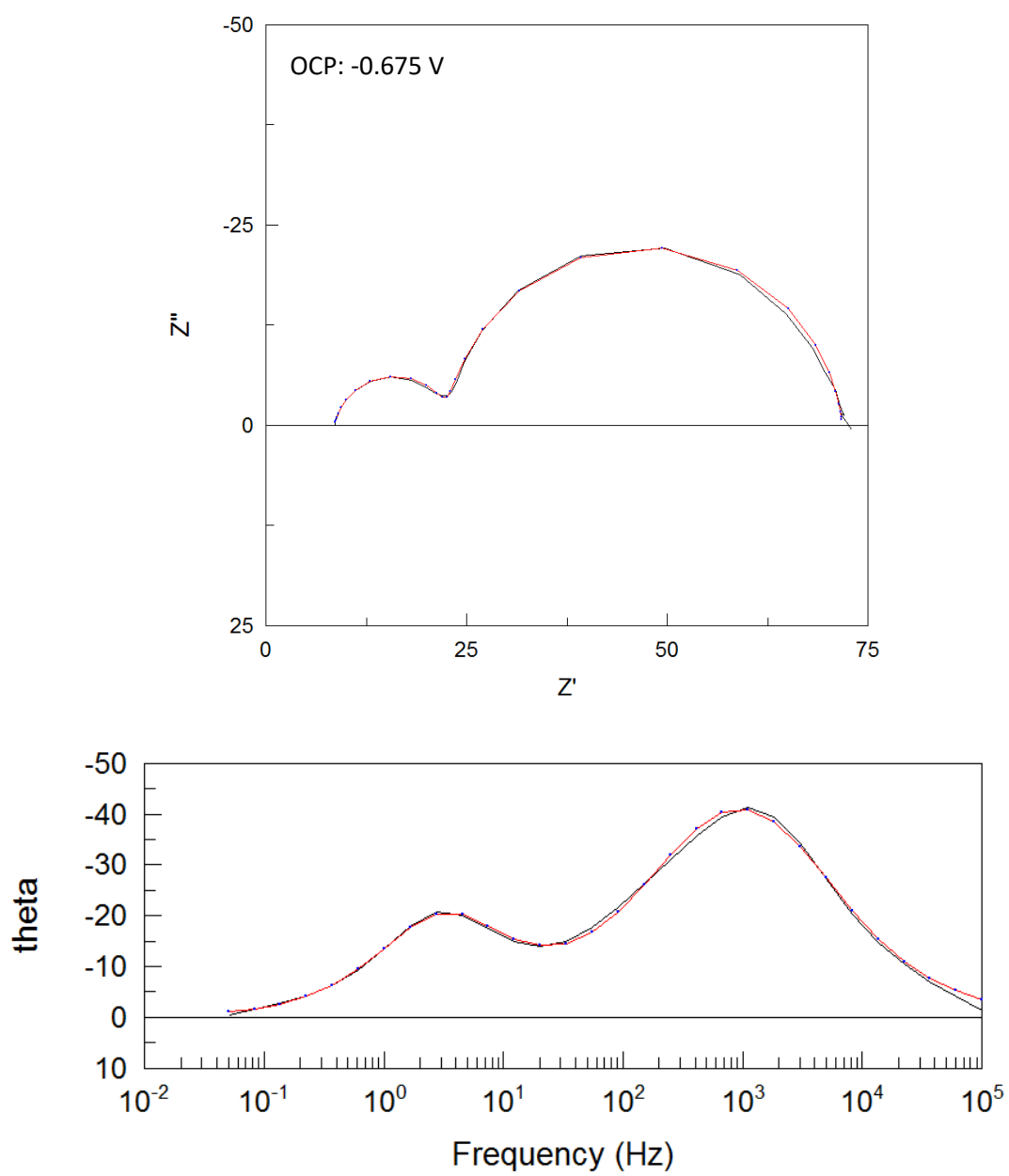
Nyquist (top) and Bode (bottom) plots of **E5**:



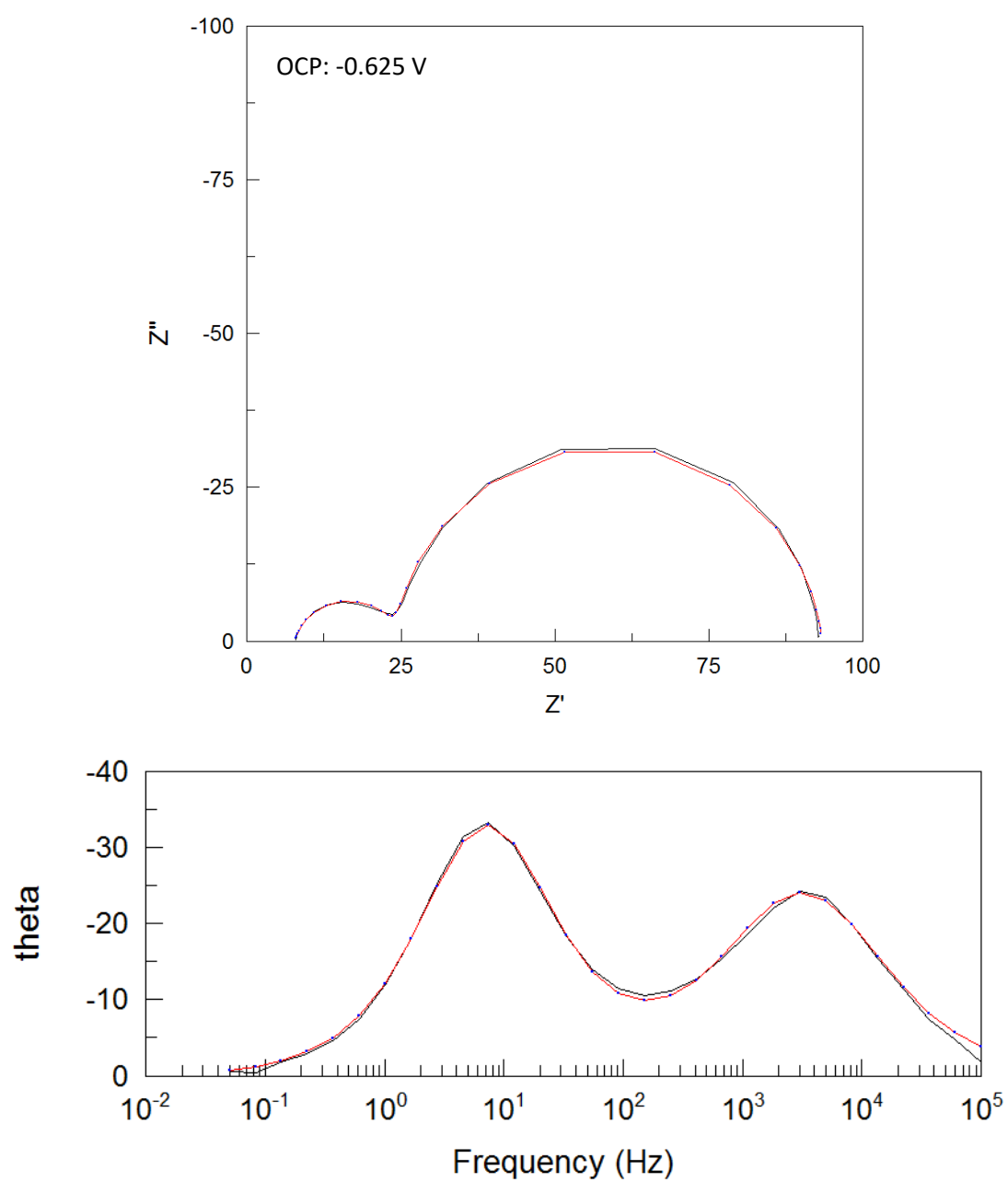
Nyquist (top) and Bode (bottom) plots of E6:



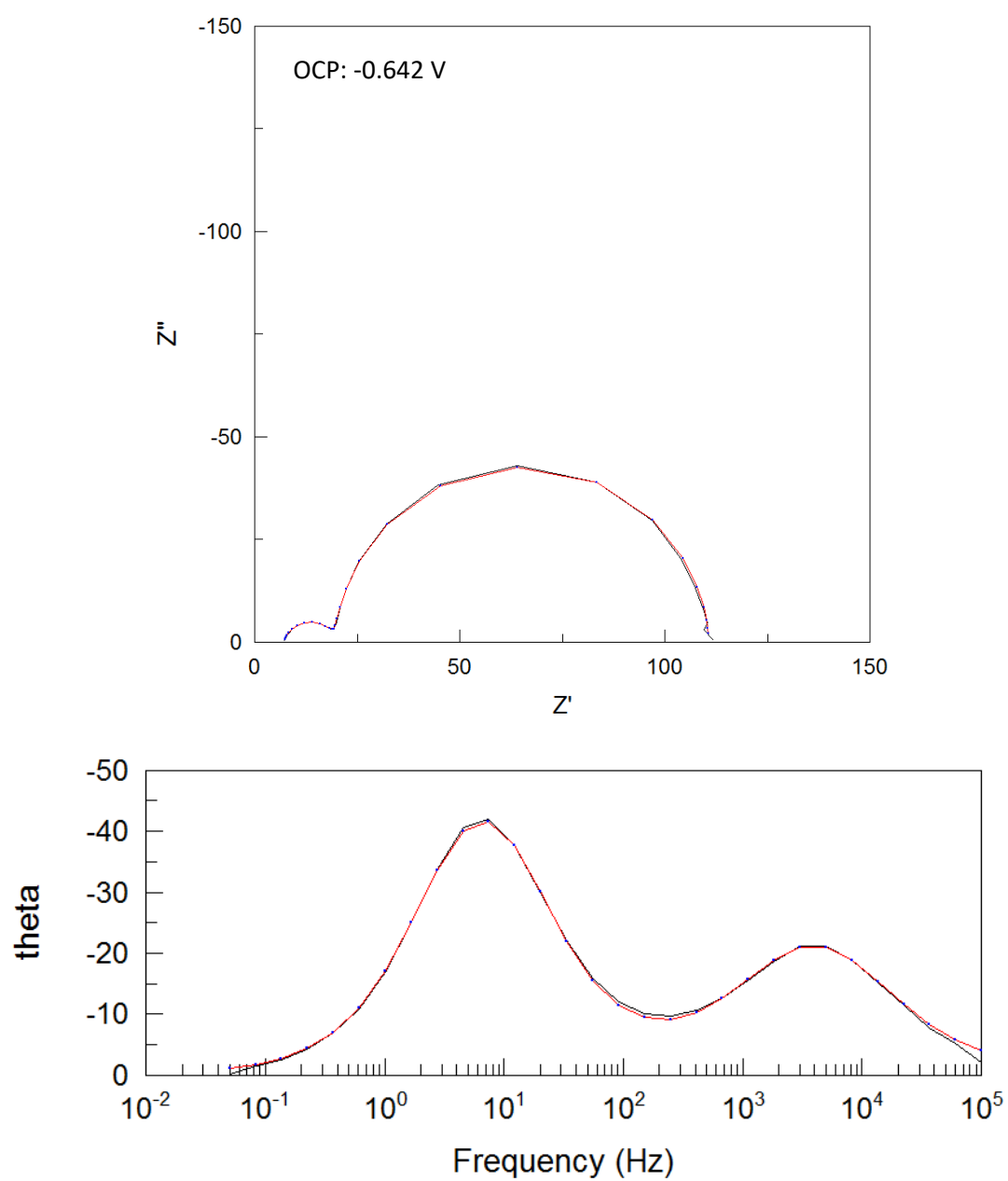
Nyquist (top) and Bode (bottom) plots of **E7**:



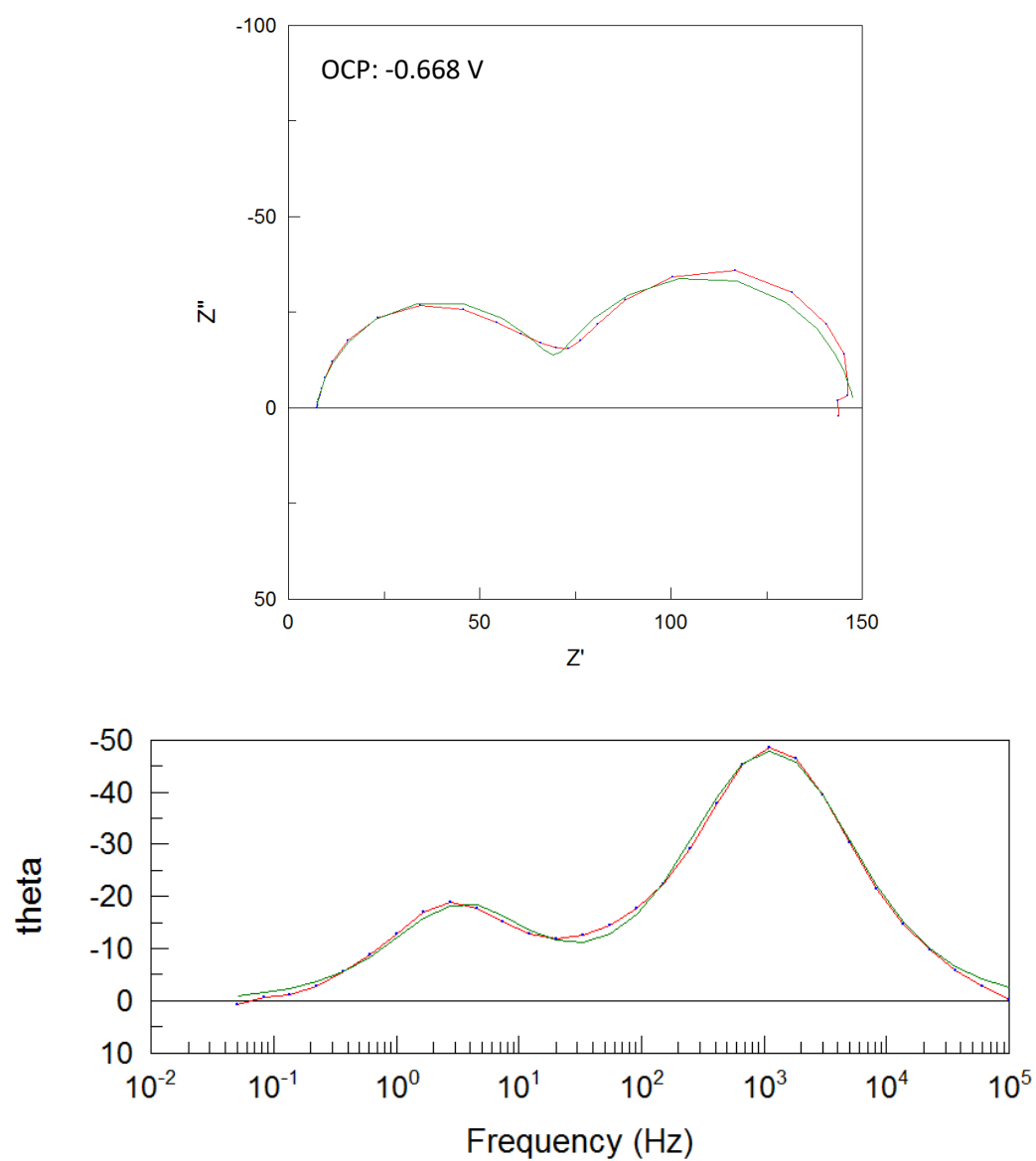
Nyquist (top) and Bode (bottom) plots of **E8**:



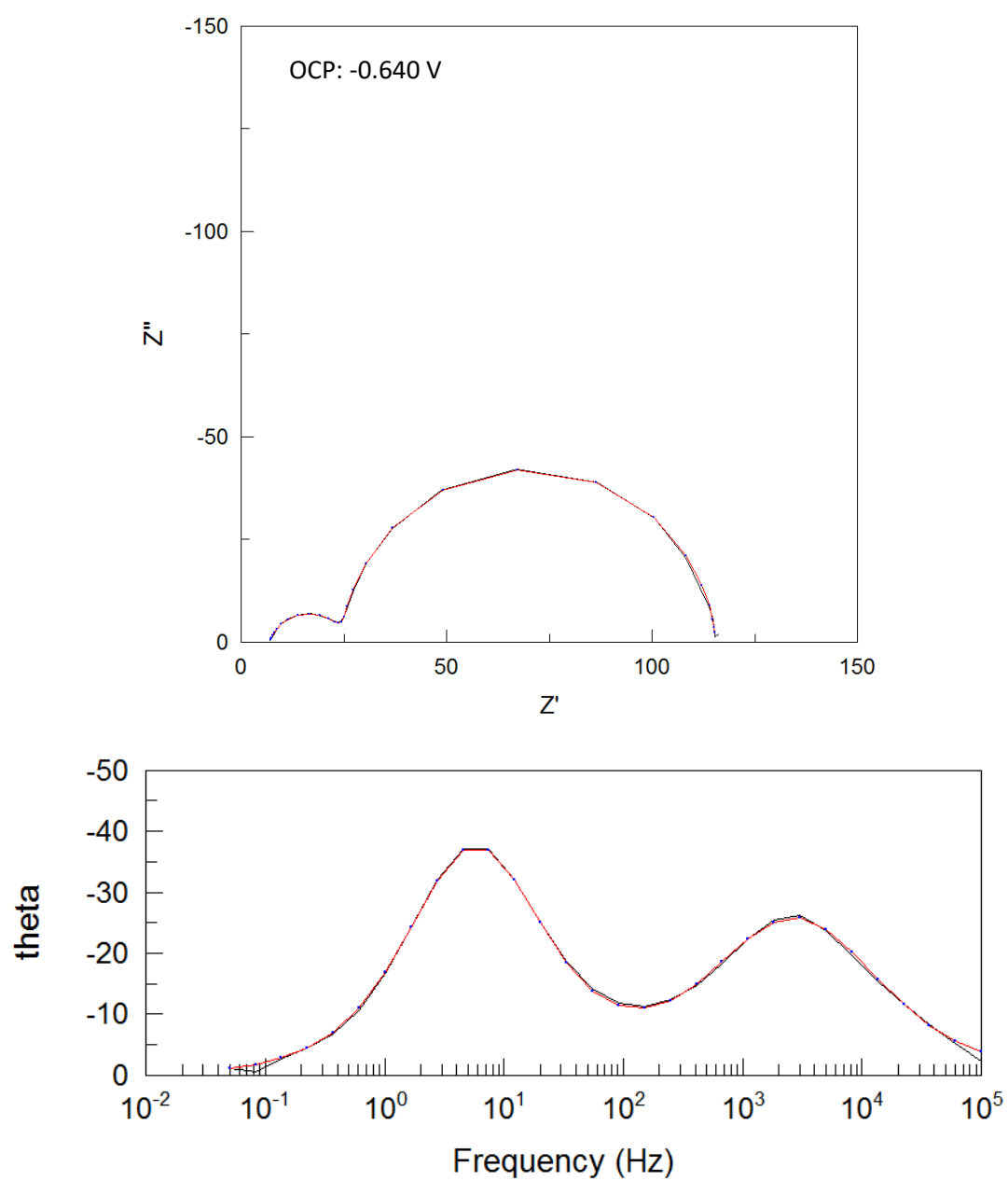
Nyquist (top) and Bode (bottom) plots of **E9**:



Nyquist (top) and Bode (bottom) plots of **E10**:



Nyquist (top) and Bode (bottom) plots of **E11**:



1. Huang, J.; Riisager, A.; Wasserscheid, P.; Fehrmann, R., Reversible physical absorption of SO₂ by ionic liquids. *Chem. Commun.* **2006**, (38), 4027-4029, doi: 10.1039/b609714f.