Supporting Information for

π-Conjugated Poly(aryleneethynylene)s Consisting of Salophen and Ni-Salophen Units in the π-Conjugated Main Chain: Preparation and Chemical Properties

Hiroki Fukumoto*, Kazuto Yamane, Yumiko Kase, and Takakazu Yamamoto*

Chemical Resources Laboratory, Tokyo Institute of Technology,

4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan.

X-ray Crystallography. The cyrstal of **Br_2-Salophen-Ni** was mounted in a glass capillary. Measurements were made on a Rigaku Saturn CCD area detector with graphite monochromated Mo-Kα radiation (λ = 0.71075 Å). The data were collected to a maximum 2θ value of 55.0 ° at 293 K. A total of 720 oscillation images were collected. The distance between the crystal and camera was 44.99 nm, and readout was performed in the 0.070 mm pixel mode.

The structure of **Br_2-Salophen-Ni** was solved by direct method (SIR92), and refined by full-matrix least-squares method. Non-hydrogen atoms and hydrogen atoms were refined anisotropically and isotropocally, respectively. All calculations were performed using Rigaku CrystalClear software package. Crystal data and data collection parameters, and selected bond distance and angles of **Br_2-Salophen-Ni** were summarized in Table S1 and Table S2, respectively. ORTEP drawing of the structure was shown in Figure S1. The crystal structure data of **Br_2-Salophen-Ni** (CCDC number 785112) was deposited at the Cambridge Crystallographic Data Centre. The data can be obtained free of charge via www.ccdc.cam.au.uk/data_request/cif.

Table S1. Crystal Data and Data Collection Parameters of **Br_2-Salophen-Ni**

Empirical formula	$C_{20}H_{12}Br_2N_2NiO_2$
Formula weight	530.83
Crystal system	orthorhombic
Space group	*P*bca (No.14)
a, Å	10.084(2)
b, Å	14.552(4)
c, Å	24.360(6)
V, Å^3	3574.5(15)
Z	8
D_{calcd}, g/cm^3	1.973
F(000)	2080
μ(MoKα), cm^{-1}	55.89
Crystal size, mm	0.22 x 0.22 x 0.15
No. of reflections measured	25041
No. of observation ($I > 3.00(\sigma)$)	2624
No. of variables	244
R^a ($I > 3.00(\sigma)$)	0.0518
$R_w{}^b$ ($I > 3.00(\sigma)$)	0.0681
GOF	0.838
$\Delta\rho$, e Å^{-3}	1.22, -1.31

a) $R = (\Sigma||Fo| - |Fc||) / (\Sigma|Fo|)$ b) $R_w = [\Sigma\, w\, (|Fo| - |Fc|)^2 / \Sigma\, wFo^2]^{1/2}$

Table S2. Selected Bond Distances and Angles of **Br_2-Salophen-Ni**

Distances (Å)			
Ni ─ N(1)	1.863(4)	Ni ─ N(2)	1.857(4)
Ni ─ O(1)	1.840(4)	Ni ─ O(2)	1.847(3)
N(1) ─ C(1)	1.307(5)	N(2) ─ C(3)	1.316 (6)
O(1) ─ C(2)	1.295(6)	O(2) ─ C(4)	1.303(6)
Angles (°)			
N(1) ─ Ni ─ O(1)	96.07(18)	N(1) ─ Ni ─ N(2)	85.01(19)
O(1) ─ Ni ─ O(2)	83.57(17)	O(2) ─ Ni ─ N(2)	95.39(18)

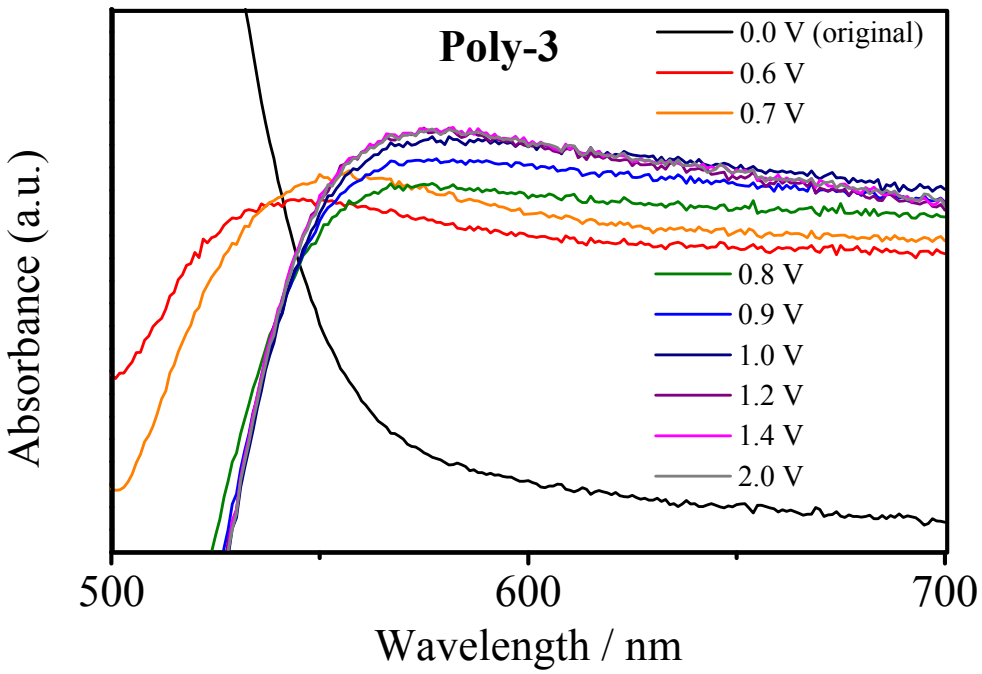

Figure S1. Differential UV-vis spectra of **Poly-3** film cast on an ITO glass electrode. Obtained at various applied potentials (vs. Ag^{+}/Ag). The UV-vis spectrum of the original **Poly-3** film is also shown.