Electronic Supplementary Information

Importance of Alkyl Chain-Length on the Self-Assembly of New Ni(qdt)$_2$ Complexes and Charge Transport Properties

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Experimental

General information

All the chemical reagents used in the experiments were purchased without further purification. All reactions were carried out under an inert atmosphere of dry N_2. NMR spectra were recorded on the Bruker-400 MHz spectrometer, and referenced to the residual proton solvent signals. Elemental analyses were performed at Elementary VARIOEL Micro Cube. Mass spectra were recorder with a mass spectrometer API-150EX. Single crystal X-ray diffraction data was collected by a Bruker X8 Proteum diffractometer using Cu-kα radiation (λ = 1.54178 Å) at 133 k. Lattice determination and data collection was performed using built-in SADSBS program of the program suite. The structure was solved by direct method (SHELXS) and refined by full-matrix least squares on F^2 (SHELXL) using the SHELX-97 program suite.

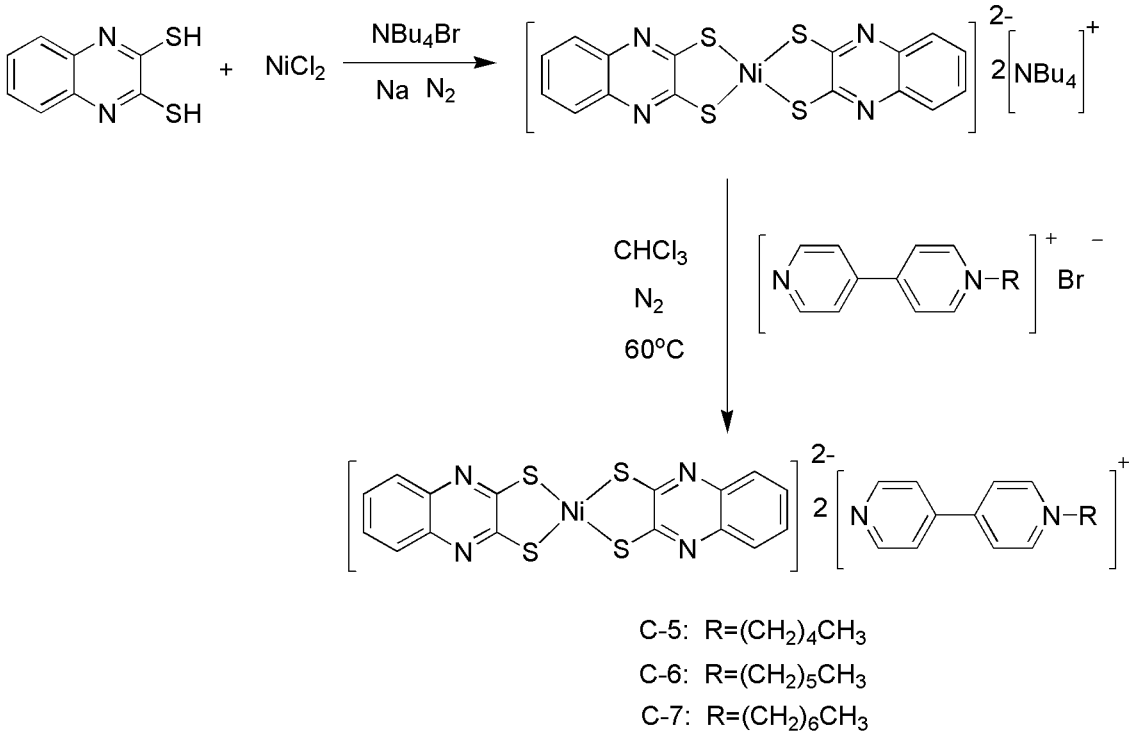
SEM was performed on a FEI/Philips XL30 environmental scanning electron microscope. TEM images and SAED patterns were obtained using a FEI / Philips Tecnai 12 BioTWIN transmission electron microscope. GIXRD data were collected using a Bruker D8 Advance (θ/θ) diffractometer with a Göbel mirror attachment.

The bottom gate bottom contact FET devices were fabricated by drop-casting the complex in dimethyl sulfoxide (DMSO) on the Si substrate with 100 nm SiO_2 as dielectric layer. The source and drain contacts were prefabricated using a standard photolithography lift-off process followed by E-beam evaporation of 100 nm Au contacts. The FET devices were characterized by Keithley 4200 semiconducting parameter analyzer. Field-effect mobility (μ) was calculated in the saturation regime of drain current using the following equation:

$$I_{DS} = \frac{W}{2L} C_i \mu (V_{GS} - V_T)^2$$

Where, W is the channel width, L is the channel length, C_i is the capacitance per unit area of the SiO_2 dielectric, I_{DS} is the drain current, V_{GS} and V_T are the gate and threshold voltages, respectively.

Synthesis of nickel complexes



C-5: R=$(CH_2)_4CH_3$
C-6: R=$(CH_2)_5CH_3$
C-7: R=$(CH_2)_6CH_3$

Scheme S1. Synthetic procedure for complexes **C-5, C-6, and C-7 .**

Single Crystal Structure Analysis:

Table S1. Crystal data for X-ray structures of complexes **C-5, C-6** and **C-7**

Compound name	C-5.2H_2O	C-6	C-7.2H_2O
Crystal system /Space group	Triclinic P-1	Monoclinic P 21/c	Monoclinic P 21/c
Lattice parameters	$a = 8.1895(2)$Å $b = 8.5987(3)$Å $c = 16.7988(2)$Å $\alpha = 92.215(2)^o$ $\beta = 102.812(1)^o$ $\gamma = 105.961(2)^o$ $V = 1102.75(6)$Å^3	$a = 14.8356(2)$Å $b = 10.8116(2)$Å $c = 13.3564(2)$Å $\alpha = 90^o$ $\beta = 93.711(1)^o$ $\gamma = 90^o$ $V = 2137.83(6)$Å^3	$a = 15.2630(3)$Å $b = 9.2809(2)$Å $c = 16.8903(3)$Å $\alpha = 90^o$ $\beta = 93.097(2)^o$ $\gamma = 90^o$ $V = 2389.09(8)$Å^3
Molecular Formula	$C_{46}H_{50}N_8NiO_2S_4$	$C_{48}H_{50}N_8NiS_4$	$C_{50}H_{58}N_8NiO_2S_4$
Molecular Weight	933.90	925.93	989.99
Z	2	2	2
D_x(gcm^{-3})	1.406	1.438	1.376
μ, mm^{-1} (Cukα)	2.793	2.841	2.609
F(000)	490.0	972.0	1044.0
Max θ, °	67.390	66.990	66.990
Observed data [I>2σ]	3018	8371	9078
Parameters/restrain	273/2	278/0	302/2
R_1 [a]/wR_2 [b]	0.0662/0.1888	0.026, 0.071	0.0307, 0.0859
Goodness of fit S	1.041	1.062	1.033
Residual electron density	0.204	0.247	0.464

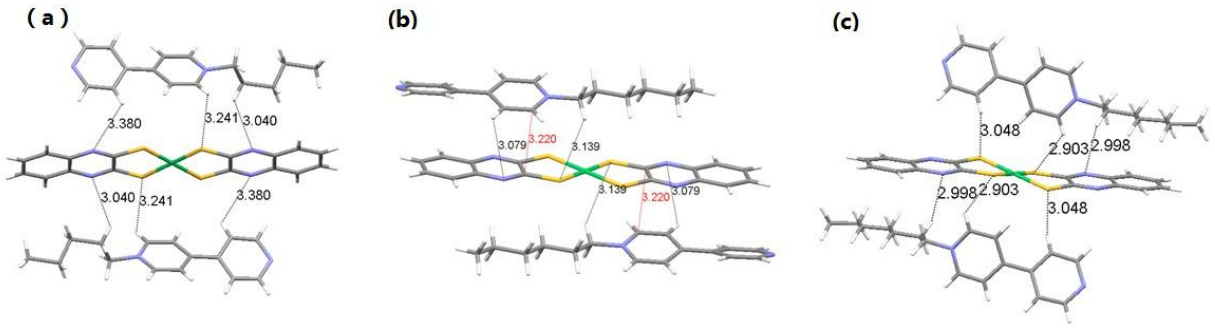


Fig.S1 Crystal structures (a, b, and c) with bond distances of C-5, C-6, and C-7, respectively.

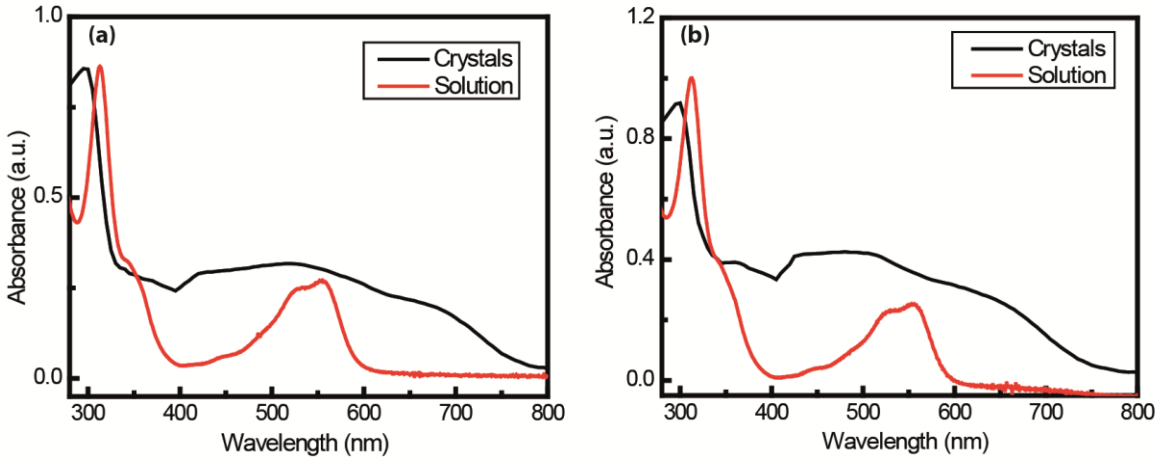


Fig.S2 UV-vis absorption spectra of solution and crystal of C-5 (a) and C-7 (b).

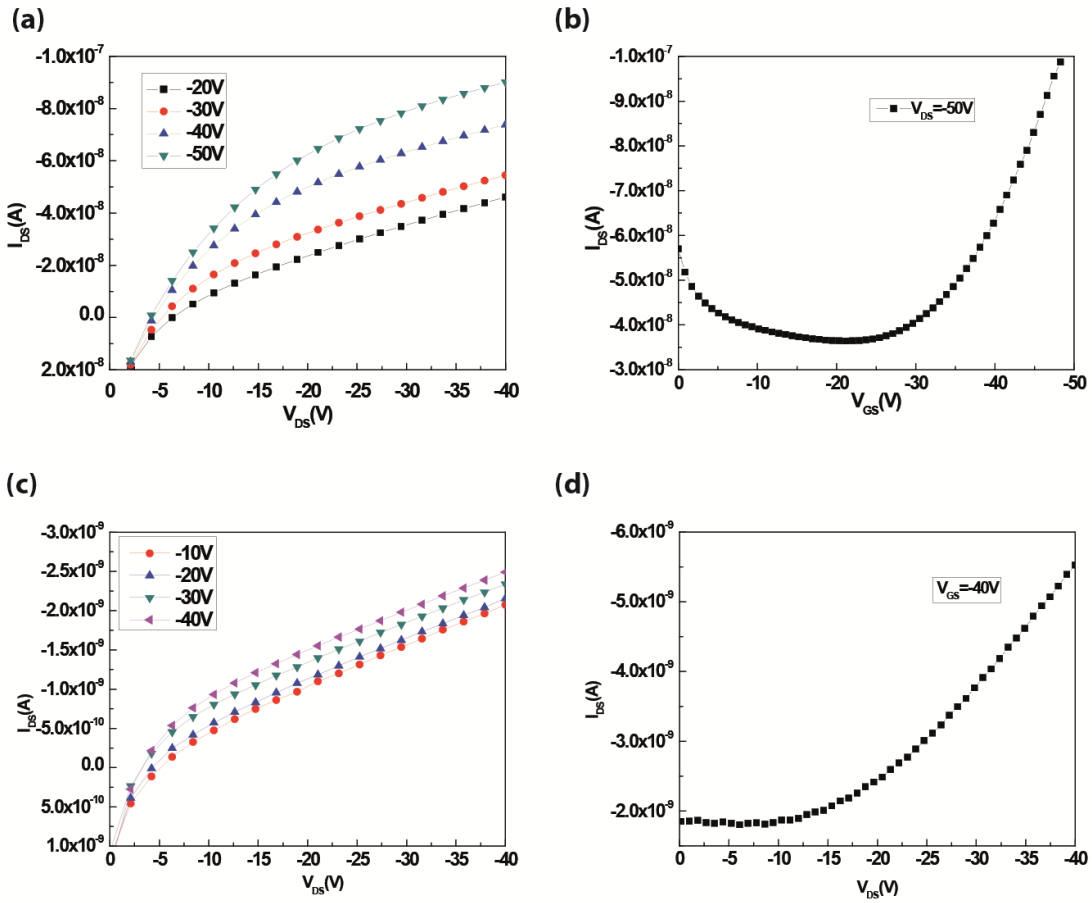


Fig.S3 (a) Output characteristics and (b) transfer characteristics of the FET device of C-5 (c) Output characteristics and (d) transfer characteristics of the FET device of C-7.