Electronic Supplementary Information

for

Conjugated Coordination Polymers Based on 8-Hydroxyquinoline Ligands: Impact of Polyhedral Oligomeric Silsesquioxanes on Solubility and Luminescence

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Material Synthesis:

5-Formyl-8-hydroxyquinoline (FHQ) was synthesized and characterized following a reported procedure.[33] ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of FHQ was shown in Figures S1.

Two methods can be used to synthesize the benzamides according to the literature.[34] N-Propylheptakis(isobutyl) POSS-3,5-dinitrobenzamide was prepared from the condensation reaction of 3,5-dinitrobenzoic acid with POSS-NH_2 in the presence of DCC. Excess 3,5-dinitrobenzoic acid was used to allow a full conversion of POSS-NH_2 and N,N'-dicyclohexylurea (DCU) was completed removed by the precipitation cycle. However, we found that DCU could not removed completely from the product formed by the reaction of dodecylamine with 3,5-dinitrobenzoic acid catalyzed with DCC, even purified by silica gel column chromatography. Then N-Dodecyl-3,5-dinitrobenzamide was synthesized via the reaction of 3,5-dinitrobenzoyl chloride with dodecylamine.

Fluorometric Analysis:

The quantum yields of the polymers in solution were determined according to the

following equation:

$$\Phi_u = \Phi_s \frac{F_u A_s n_u^2}{F_s A_u n_s^2}$$

Where Φ is quantum yield; F is integrated area under the corrected emission spectra; A is absorbance at the excitation wavelength; n is the refractive index of the solution; the subscripts u and s refer to the unknown and the standard, respectively. Quinine bisulfate in 0.05 M H_2SO_4 solution was used as the standard.

^{1}H NMR characterization of the products:

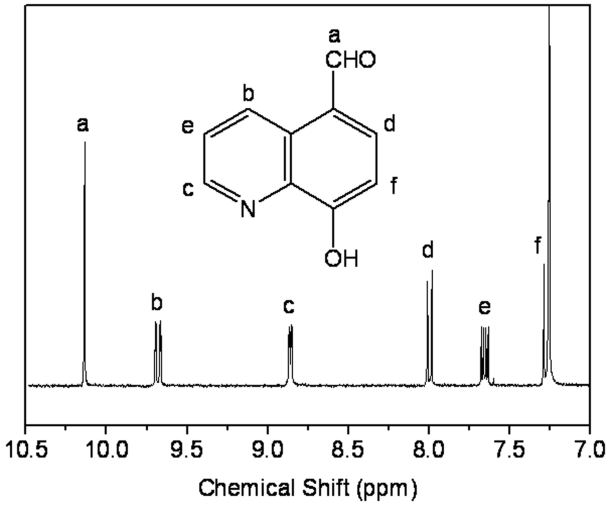

Figure S1. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of FHQ.

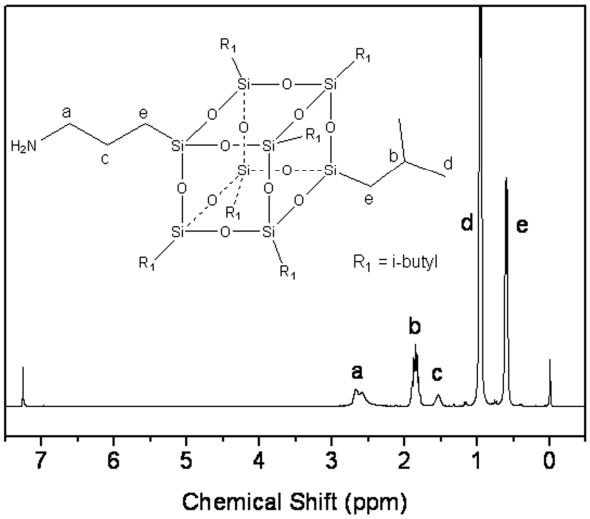

Figure S2. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of POSS-NH_2.

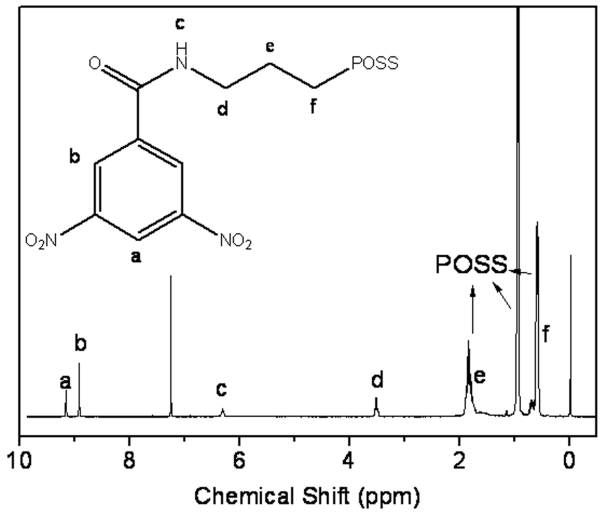

Figure S3. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of N-propyl POSS 3,5-dinitrobenzamide.

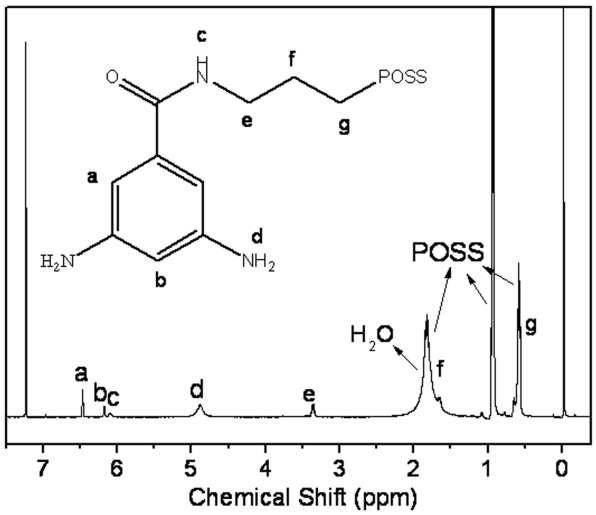

Figure S4. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of N-propyl POSS 3,5-diaminobenzamide.

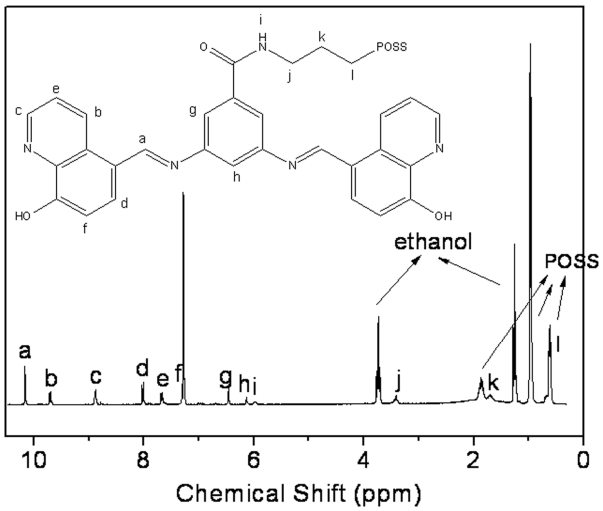

Figure S5. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1a**.

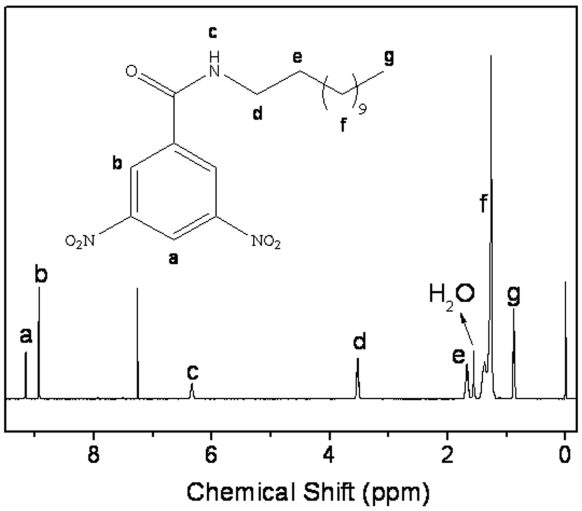

Figure S6. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of N-dodecyl 3,5-dinitrobenzamide.

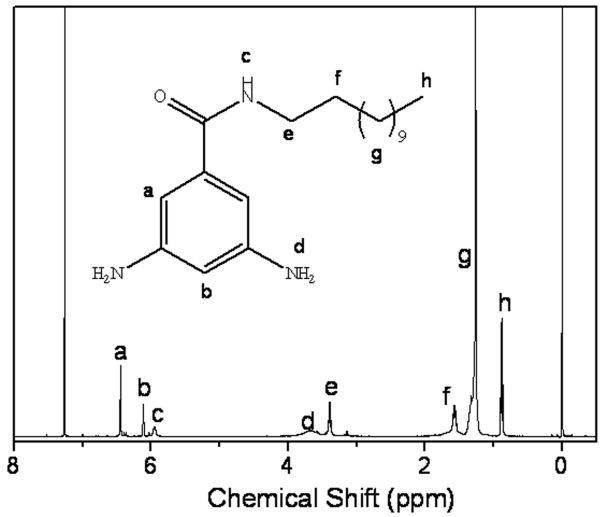

Figure S7. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of N-dodecyl 3,5-diaminobenzamide.

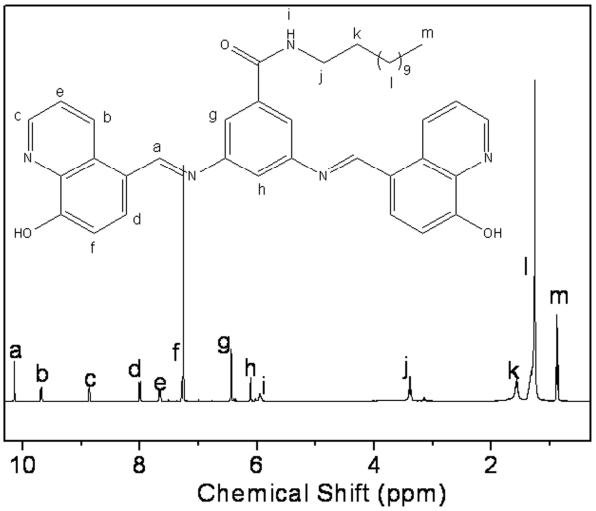

Figure S8. ^{1}H NMR spectrum ($CDCl_3$, 400 MHz) of **1b**.

^{13}C NMR characterization of the products:

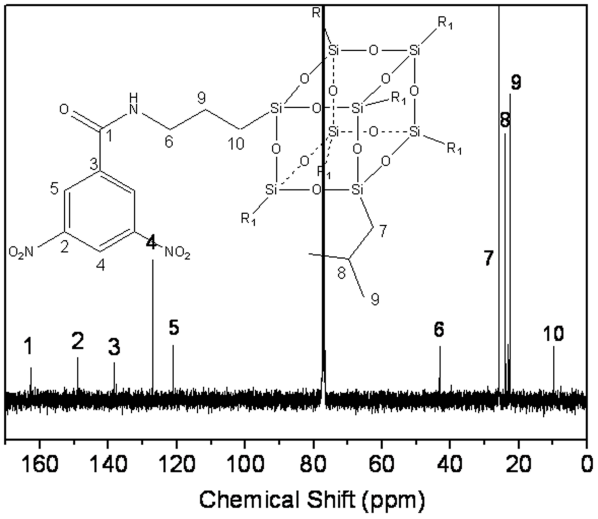

Figure S9. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of N-propyl POSS 3,5-dinitrobenzamide.

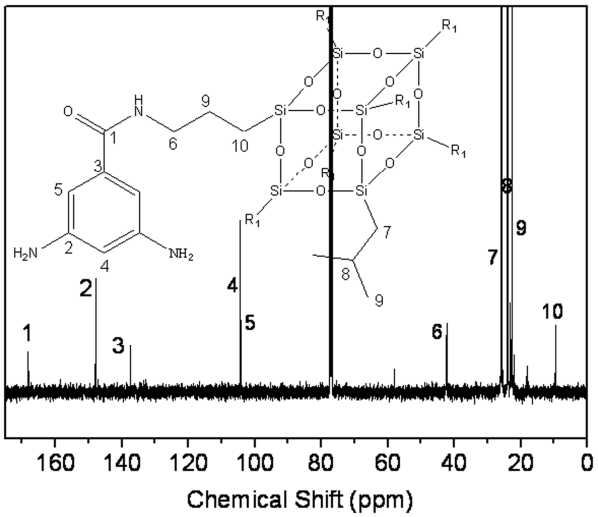

Figure S10. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of N-propyl POSS 3,5-diamonobenzamide (ethanol: 58.1 and 18.2 ppm).

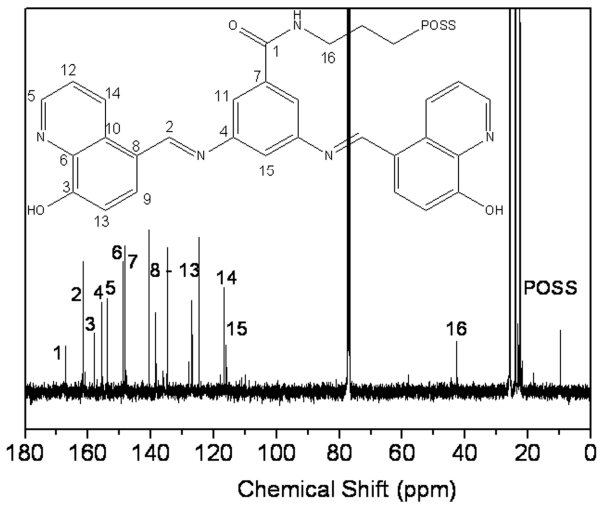

Figure S11. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of **1a**.

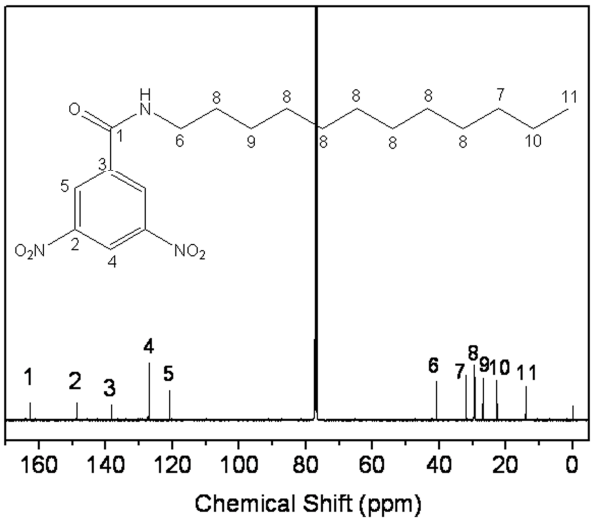

Figure S12. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of N-dodecyl 3,5-dinitrobenzamide.

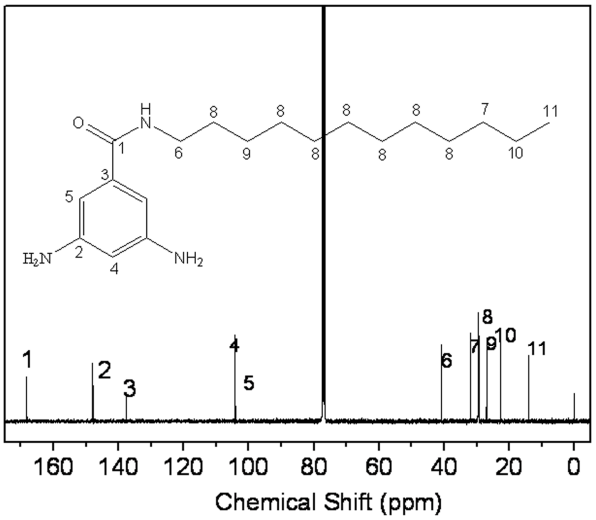

Figure S13. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of N-dodecyl 3,5-diaminobenzamide.

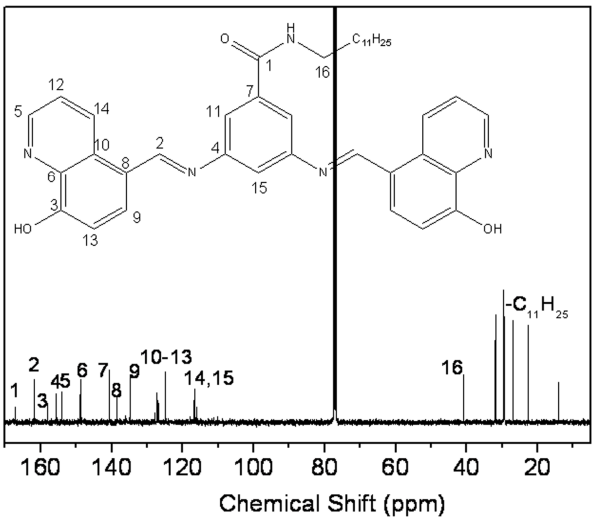

Figure S14. ^{13}C NMR spectrum ($CDCl_3$, 100 MHz) of **1b**.

UV-Vis absorption spectra:

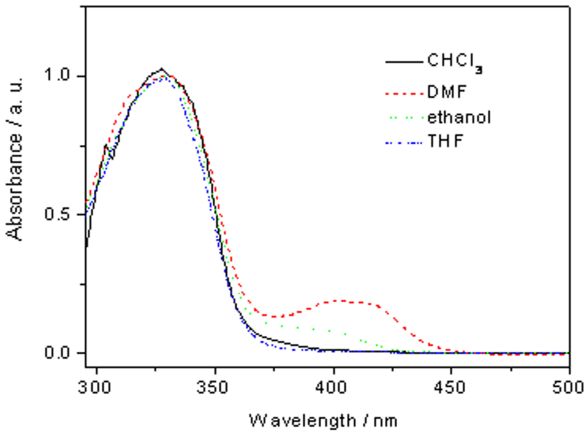

Figure S15. UV-Vis absorption spectra of FHQ in different solvents.

FHQ shows similar absorption spectra in $CHCl_3$ and THF with absorption maxima around 325 nm. In ethanol and DMF solution, the absorption at 400 nm is caused by the hydrogen bonds between FHQ and solvents. The emission of FHQ is very weak and the emission intensity was at the limit of instrument sensitivity, preventing reliable characterisation.

Thermogravimetric Analysis:

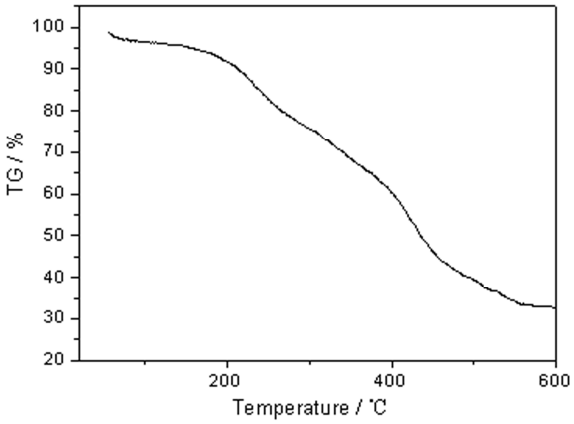

Figure S16. The TGA curve of **2b** measured in air.

PL spectra:

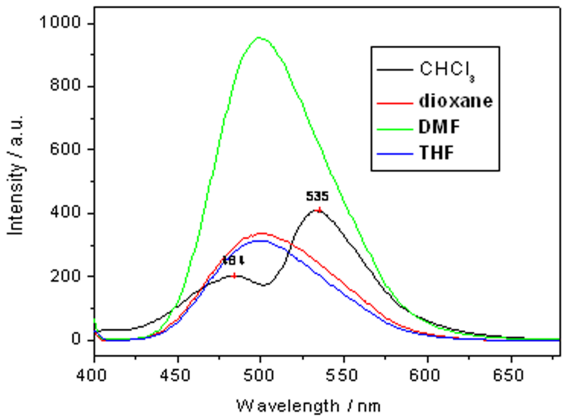

Figure S17. Fluorescence spectra of **2a** in different solutions excited at 385 nm: concentration of repeat units = 25 μM.

TEM image:

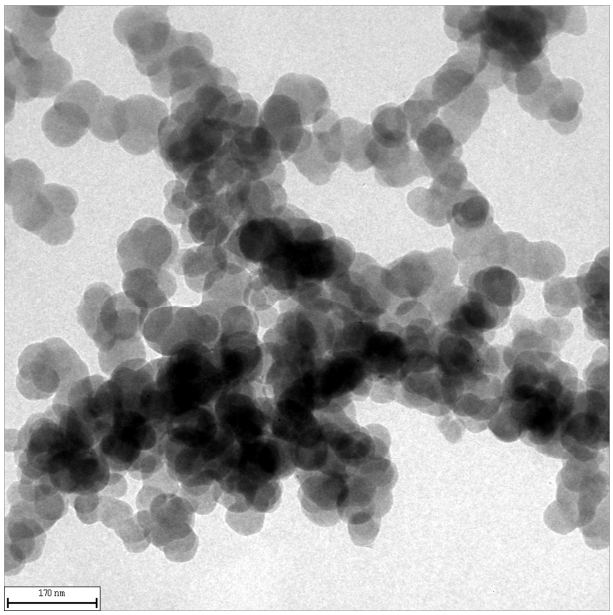

Figure S18. Typical TEM image obtained in 10^{-4} M (repeat units) $CHCl_3$ solution of **2a**.