Supplementary Information for:

INVESTIGATING THE POTENTIAL OF FLEXIBLE AND PRE-ORGANIZED TETRAAMIDE LIGANDS TO ENCAPSULATE ANIONS IN ONE DIMENSIONAL COORDINATION POLYMERS: SYNTHESIS, SPECTROSCOPIC STUDIES AND CRYSTAL STRUCTURES

Nur Shuhaila Haryani Abd Haris, ¹ Nafisah Mansor, ¹ Mohd Sukeri Mohd Yusof, ^{1,2} Christopher J. Sumby ³ and Maisara Abdul Kadir*^{1,2}

¹ Faculty of Science and Marine Environment, Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, Malaysia

² Advanced Nano Materials Research Group, Faculty of Science and Marine Environment, Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, Malaysia

³ School of Physical Sciences, Centre for Advanced Nanomaterials, The University of Adelaide, Adelaide, South Australia 5005, Australia

Correspondence: Email: maisara@umt.edu.my; Tel: +6096683294

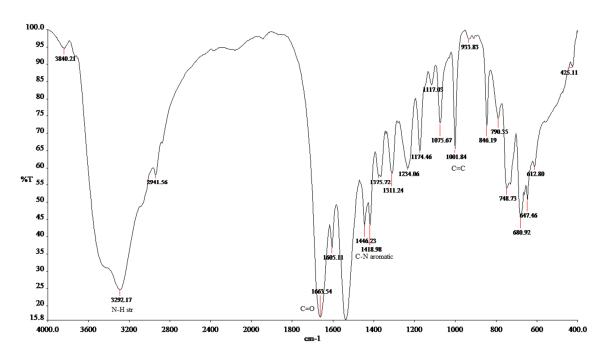


Figure S1. FTIR spectrum of L2

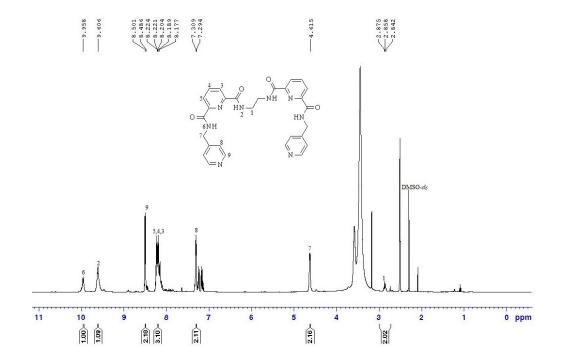


Figure S2. ¹H NMR spectrum of L2

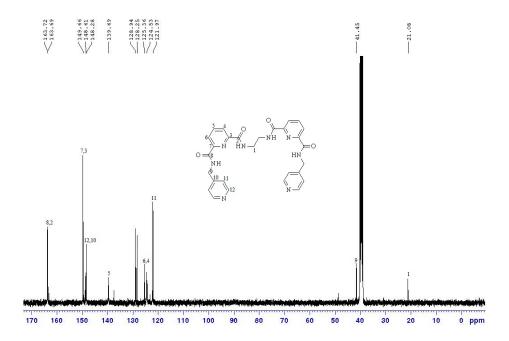


Figure S3. ¹³ C NMR spectrum of L2

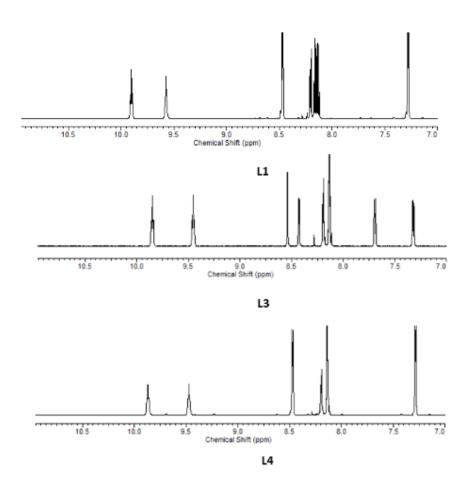


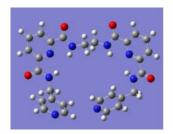
Figure S4. Enlargement of NH and proton pyridine peaks for L1, L3 and L4 in the ¹H NMR spectra

Table S1. The comparison of optimization energy between L2 with different shapes

Ligand Shape Optimization Energy (kJ/mol)

-4782816.68

S-shaped like structure



U-shaped like structure

-4782810.91