

Solvent Dependent Formation of Metallogels and Single-Crystal MOFs by La(III) and Ce(III) Connectors and 3,5-Pyridinedicarboxylate

Goutam Nandi*, Hatem M. Titi, Ranjit Thakuria and Israel Goldberg*

School of Chemistry, Sackler Faculty of Exact Sciences, Tel-Aviv University, Ramat-Aviv, 69978 Tel-Aviv, Israel. E-mail addresses: gtm.nnd@gmail.com goldberg@post.tau.ac.il

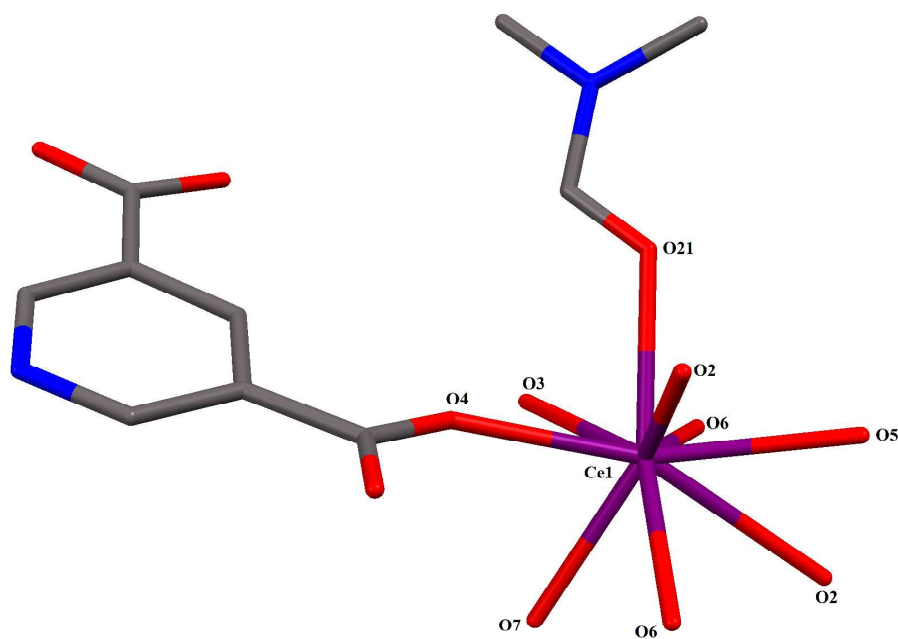


Figure S1 Coordination environment of Ce(III) ion (Hydrogen atoms are omitted for clarity). All the metal-coordinated O-sites (except for O21) are of the six surrounding 3,5-PDC linkers.

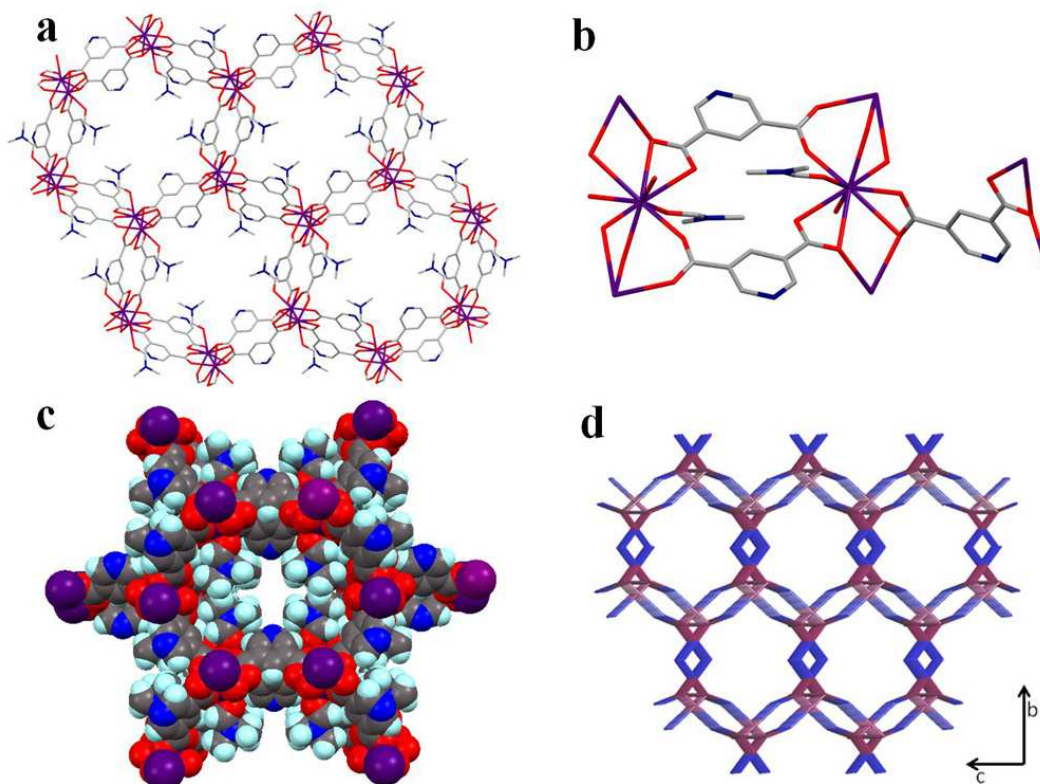


Figure S2 (a) Packing of **2** showing the hexagonal channel (down the *a*-axis). (b) The bridging between the two metal centers with their coordination environments. (c) View of the hexagonal channel formed by **2** in space-fill model, which is lined by the metal-coordinated DMF ligand and the pyridyl-N sites. (d) Simplified (node and linker) framework structure of metal complex **2** (purple = metal cluster, blue = ligand).

Table S1 Crystallographic and refinement data.

	[La(III)(3,5-PDC)_{1.5}(DMF)]_xDMF 1	[Ce(III)(3,5-PDC)_{1.5}(DMF)]_xDMF 2
Chemical formula	C ₂₇ H ₂₃ La ₂ N ₅ O ₁₄	C ₂₇ H ₂₃ Ce ₂ N ₅ O ₁₄
Formula weight	919.32	921.74
Crystal system	Orthorhombic	Orthorhombic
Space group	<i>Pnma</i>	<i>Pnma</i>
T/K	110(2)	110(2)

a/Å	8.1241(3)	8.1162(4)
b/ Å	30.3843(10)	30.2842(14)
c/ Å	15.6616(5)	15.6709(7)
α /°	90	90
β /°	90	90
γ /°	90	90
Z	4	4
V/ Å ³	3866.0(2)	3851.8(3)
D _{calc} /g cm ⁻³	1.579	1.589
μ /mm ⁻¹	2.243	2.397
Reflns collected	24239	15168
Unique reflns	3262	2869
R1[I > 2(I)]	0.0434	0.0401
wR2 (all)	0.1085	0.1004
Goodness-of-fit	1.080	1.087
CCDC No.	979166	979167

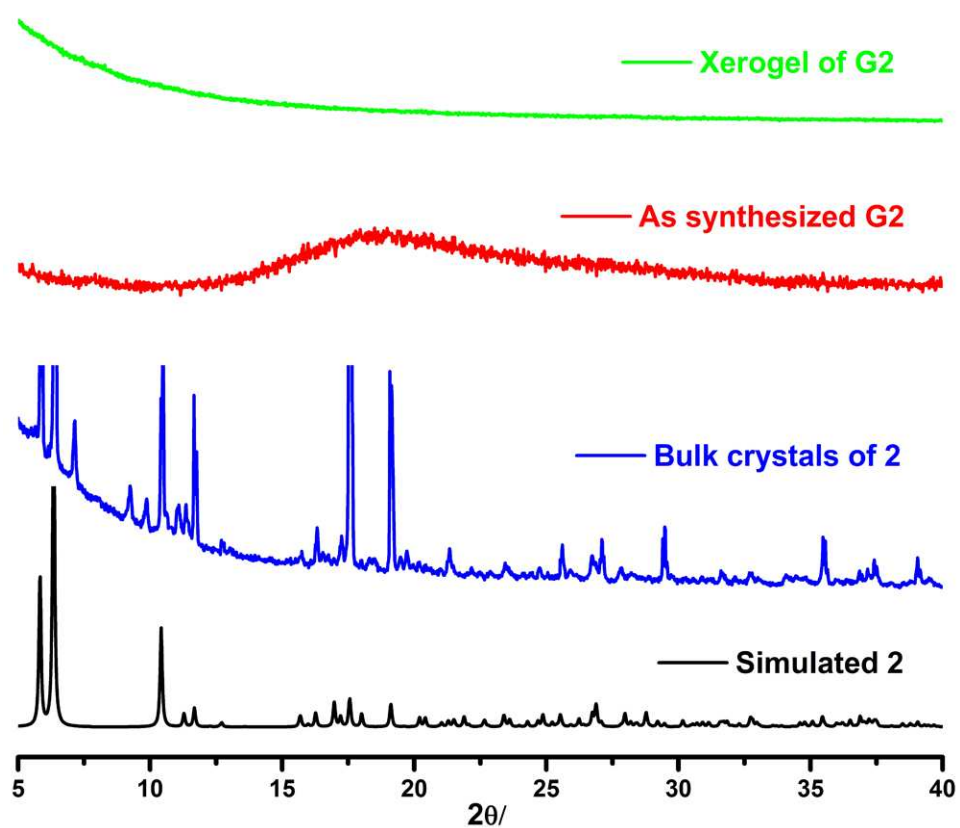


Figure S3 PXRD of as synthesized **G2** and xerogel of **G2** along with the simulated and experimental powder pattern of **2**.

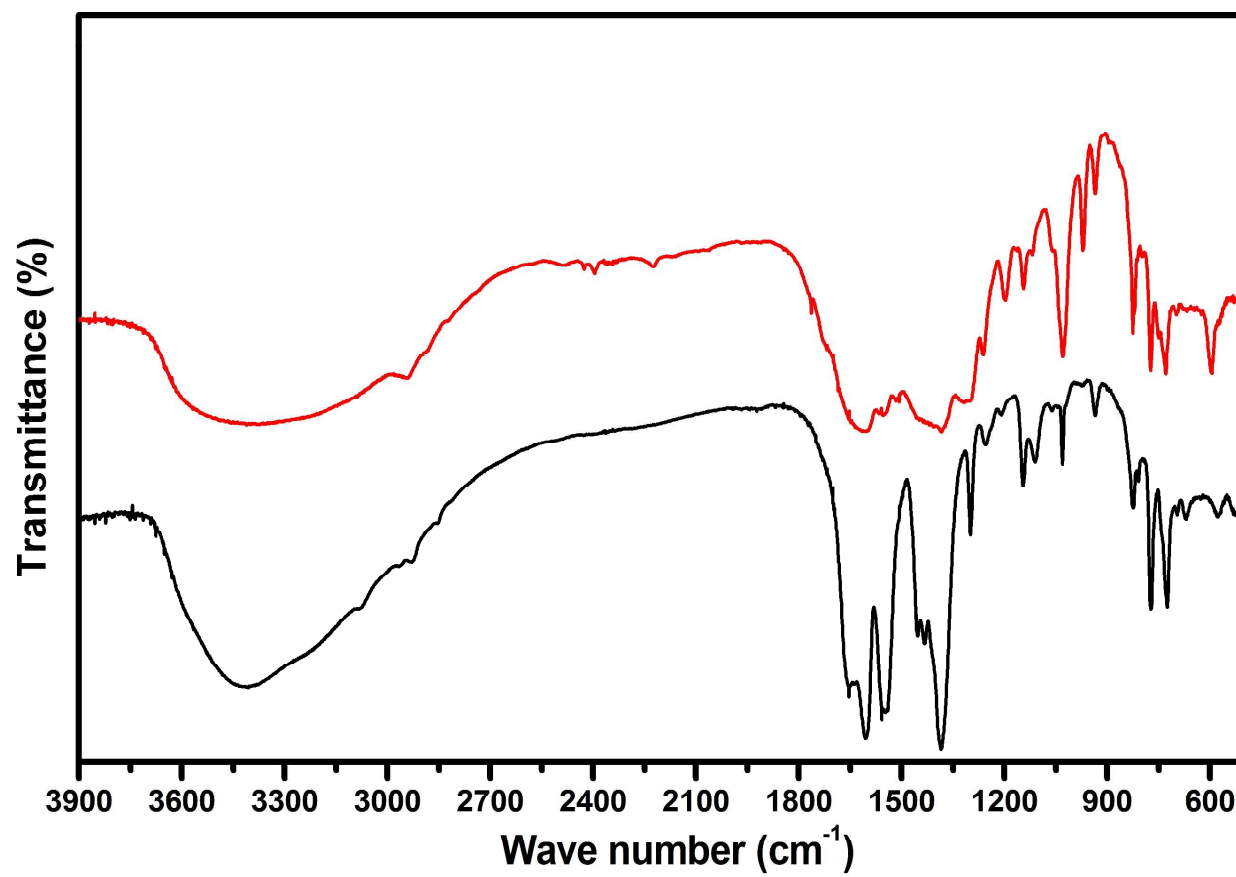


Figure S4 Comparison of FT-IR spectra of xerogel of **G1** (red) and bulk crystals of **1** (black).

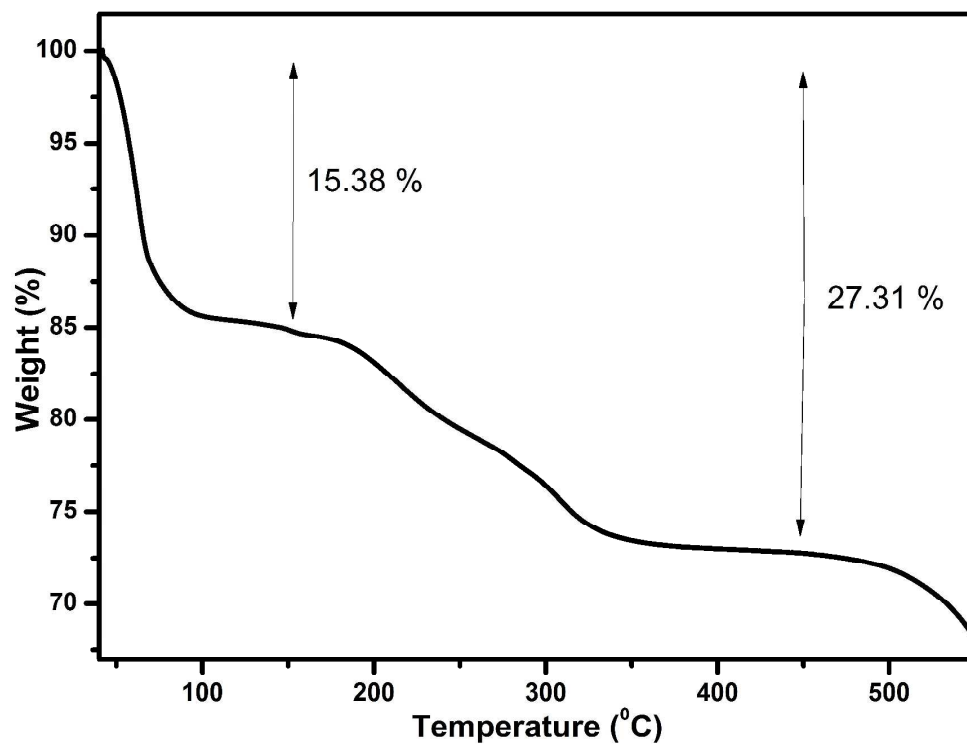


Figure S5 TGA of 1

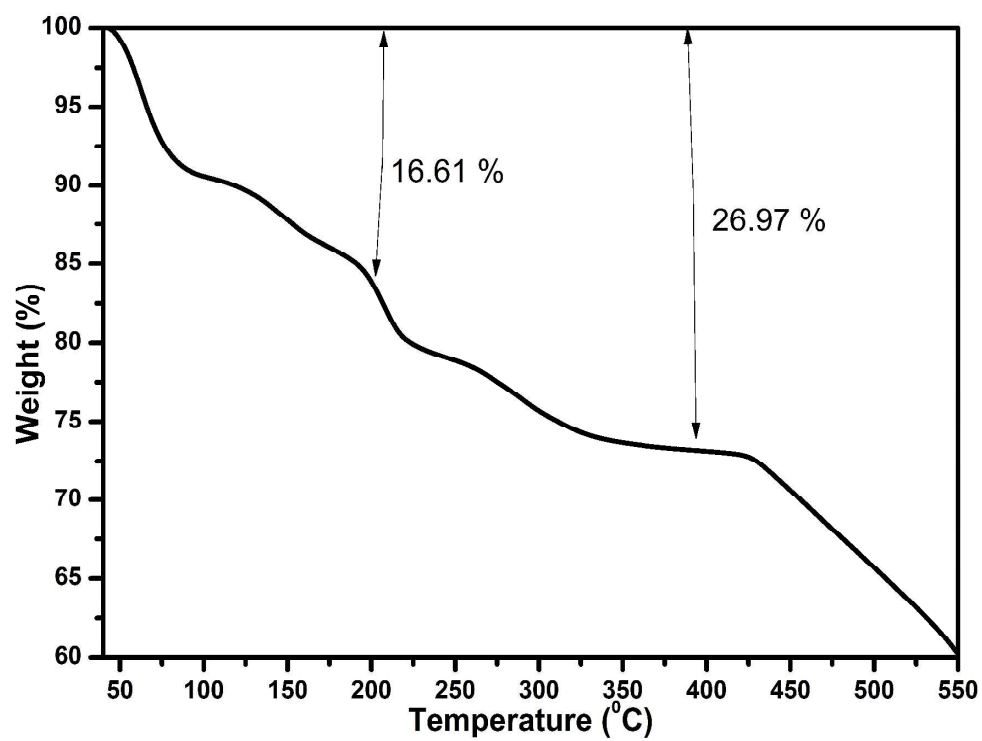


Figure S6 TGA of 2