ESI

EFFECT OF π- π STACKING INTERACTIONS ON THE EMISSION PROPERTIES OF NOVEL CADMIUM METAL-ORGANIC FRAMEWORKS BASED ON 1,4-BIS(4-PYRIDYL)-2,3-DIAZA-1,3-BUTADIENE.

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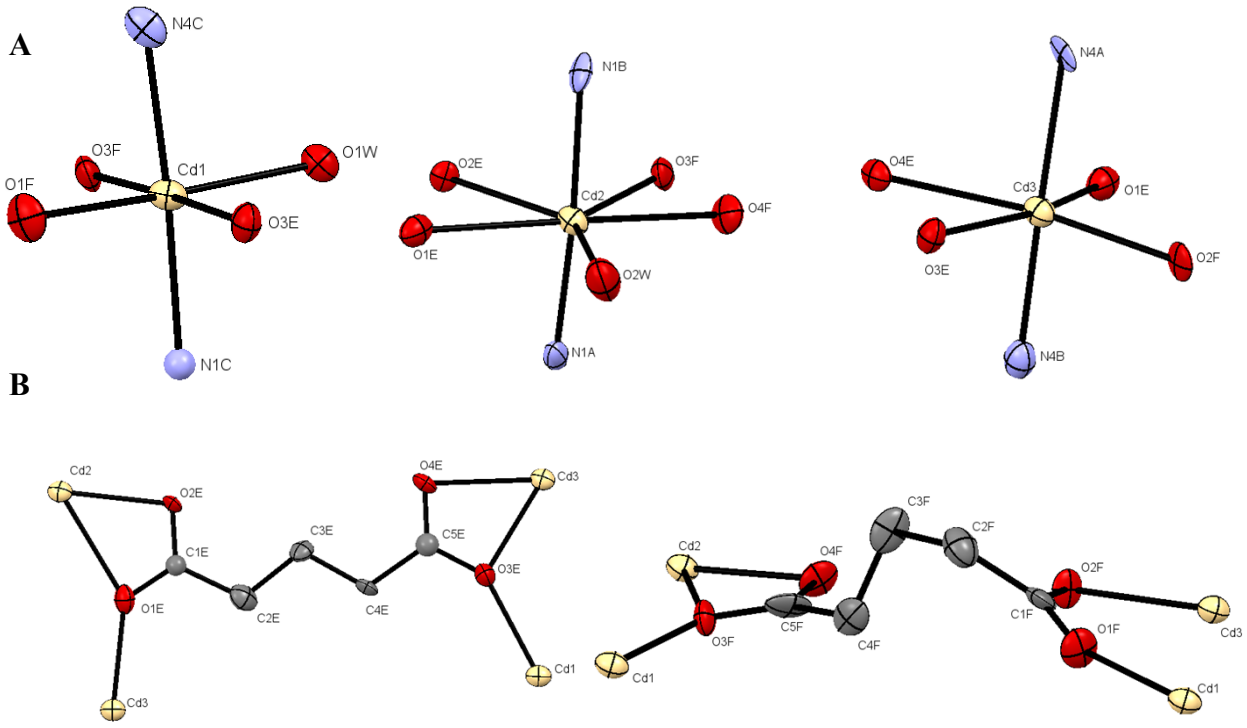
Figures and table for compound 1

Figure S1 (A) ORTEP representation of the three different cadmium environments in compound 1. (B) ORTEP representation of the two types of glutarate ligands. (C) ORTEP of the three types of 4-bpdb ligands. (D) Partial ORTEP view of a cadmium-glutarate sheet; (E) view of the topology[1] of compound1.



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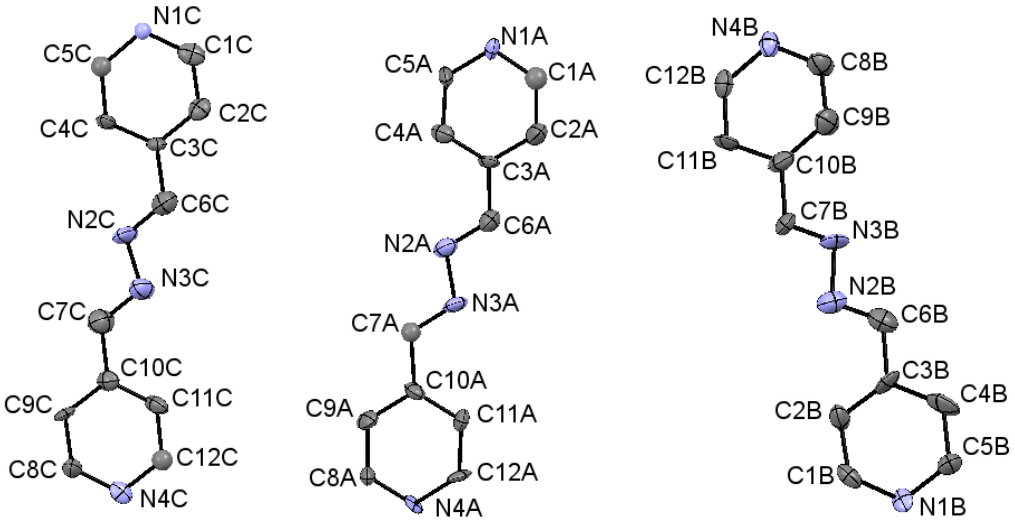
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C1C
C4C
C2C
C3C
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C7C
C10C
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C8C
C12C
N4C
N1A
C5A
C1A
C4A
C2A
C3A
N2A
C6A
N3A
C7A
C10A
C9A
C11A
C8A
C12A
N4A
N4B
C12B
C8B
C9B
C11B
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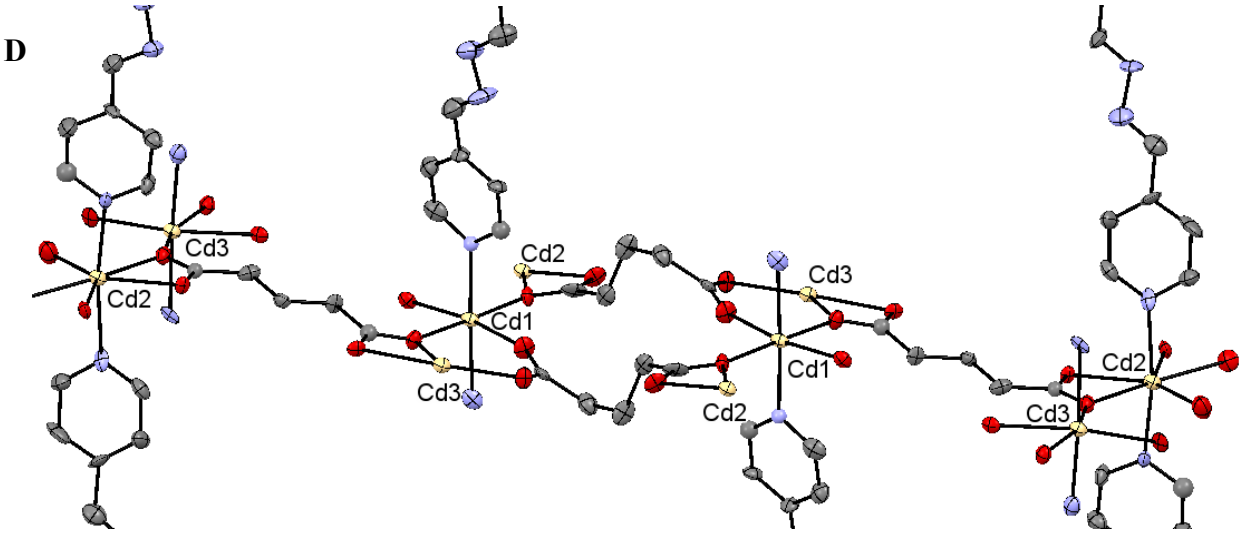
C6B
C3B
C4B
C2B
C5B
C1B
N1B

D


Cd3
Cd2
Cd2
Cd1
Cd3
Cd3
Cd1
Cd2
Cd2
Cd3

E

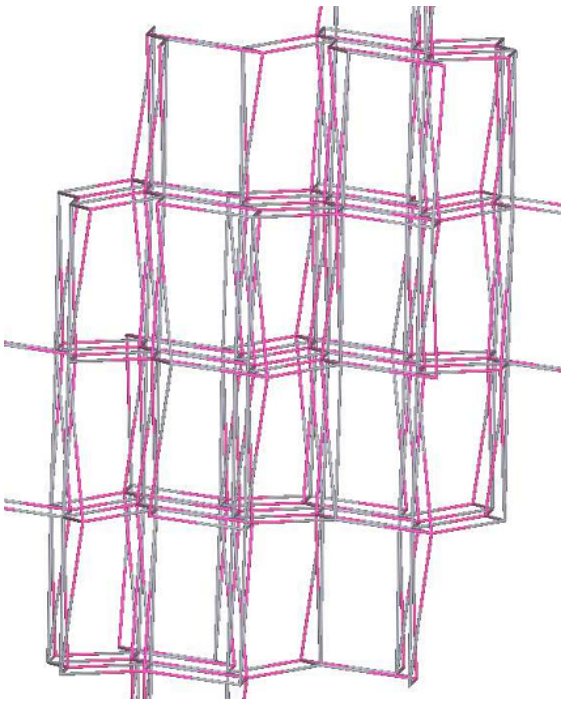


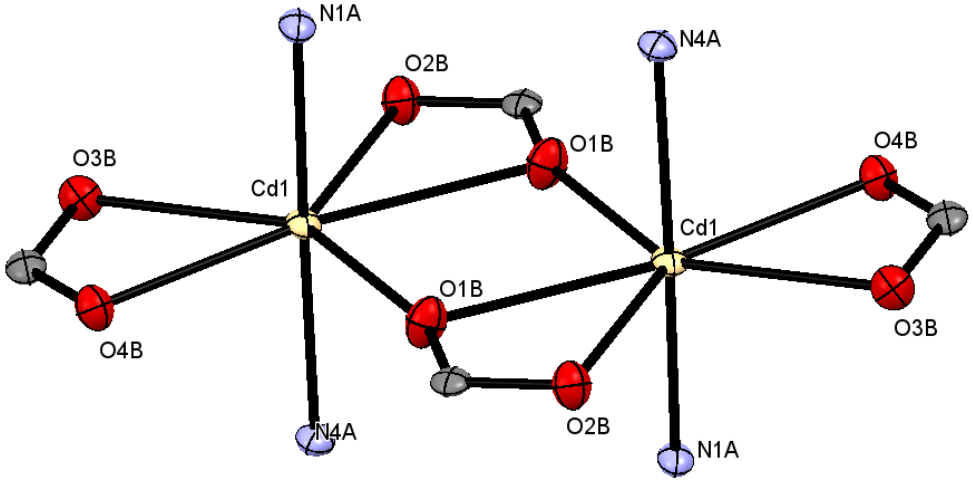
Table S1 – Selected bond distances (Å) and angles (°) in compound 1.

Cd1-N1C	2.272(7)	O1F-Cd1-O3E	79.9(3)
Cd1-O1F	2.310(7)	O1F-Cd1-O3F	99.1(2)
Cd1-O1W	2.283(7)	N4C-Cd1-N1C	174.1(3)
Cd1-O3E	2.315(7)		
Cd1-O3F	2.286(7)		
Cd1-N4C	2.303(11)		
Cd2-N1A	2.36(2)	O2E-Cd2-O1E	53.4(2)
Cd2-N1B	2.37(2)	O2W-Cd2-O4F	81.9(3)
Cd2-O1E	2.549(9)	O1E-Cd2-O2W	81.4(2)
Cd2-O2E	2.345(8)	O4F-Cd2-O3F	54.2(2)
Cd2-O2W	2.256(9)	O3F-Cd2-O2E	89.5(2)
Cd2-O3F	2.492(9)	N1B-Cd2-N1A	167.7(3)
Cd2-O4F	2.351(9)		
Cd3-O1E	2.307(6)	O4E-Cd3-O3E	55.3(2)
Cd3-N4A	2.330(7)	O3E-Cd3-O2F	109.9(2)
Cd3-N4B	2.360(10)	O2F-Cd3-O1E	88.5(2)
Cd3-O2F	2.262(7)	O1E-Cd3-O4E	106.2(2)
Cd3-OE3	2.333(7)	N4A-Cd3-N4B	166.3(3)
Cd3-O4E	2.420(7)		

Figures and table for compound 2

Figure S2 (A) ORTEP view of the dimeric compound and its coordination sphere; (B) ORTEP view of the 4-bpdb ligand in compound 2 (C) ORTEP view of the pimelate dianion (D) view of the topology[1] of compound 2.

A



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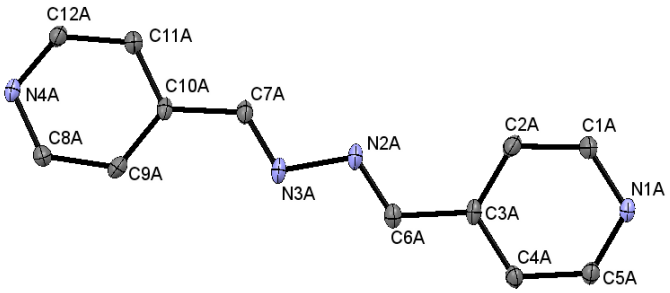

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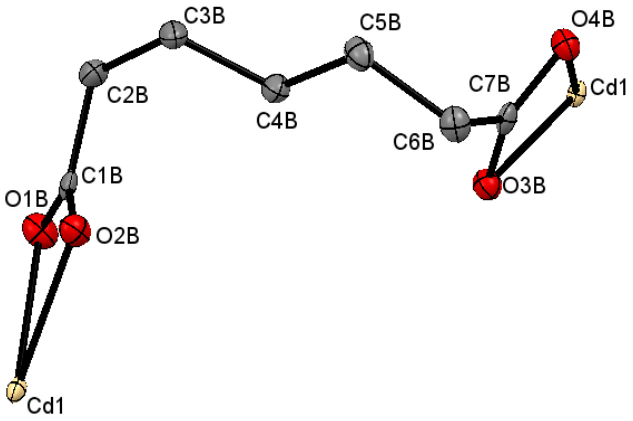

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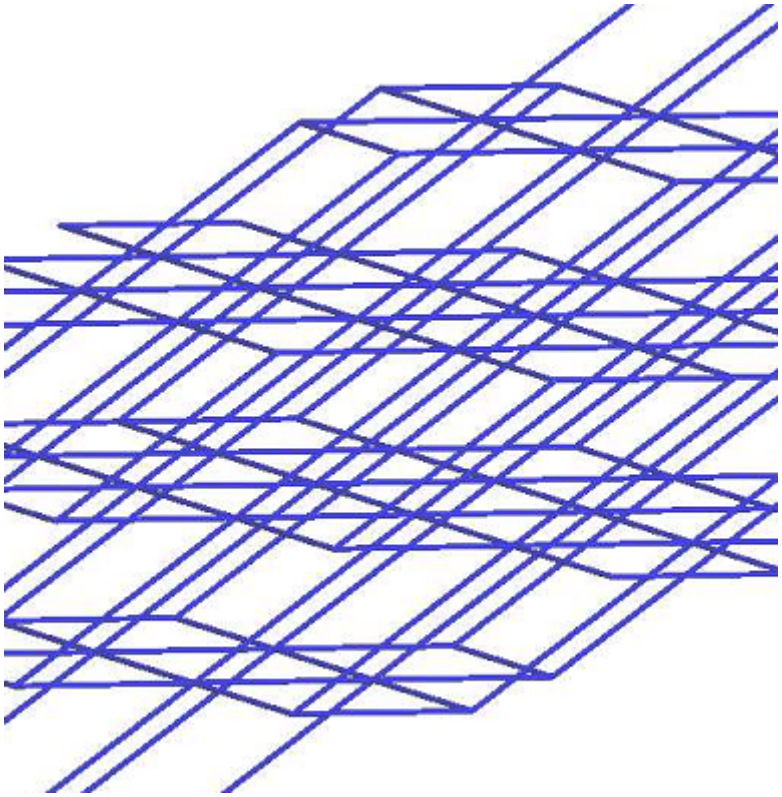


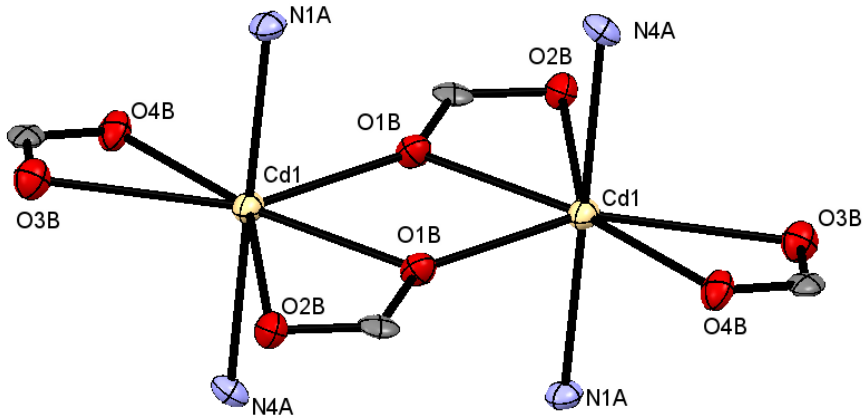
<u>Table S2</u> – Selected bond distances (Å) and angles (°) in compound 2

Cd1-N1A	2.322(1)	N1A-Cd1-N4A	172.85(5)
Cd1-O1B	2.344(1)	O1B-Cd1-O2B	53.49(5)
Cd1-O1B	2.447(1)	O2B-Cd1-O3B	89.05(5)
Cd1-O2B	2.407(1)	O3B-Cd1-O4B	55.30(4)
Cd1-N4A	2.352(1)	O4B-Cd1-O1B	89.38(5)
Cd1-O3B	2.385(1)	O1B-Cd1-O1B	72.88(5)
Cd1-O4B	2.375(1)		

Figures and table for compound 3

Figure S3 – (A) ORTEP view of the dimeric compound and its coordination sphere; (B) ORTEP view of the succinate dianion (C) ORTEP view of the 4-bpdb ligand (D) view of the topology[1] of compound 3.

A



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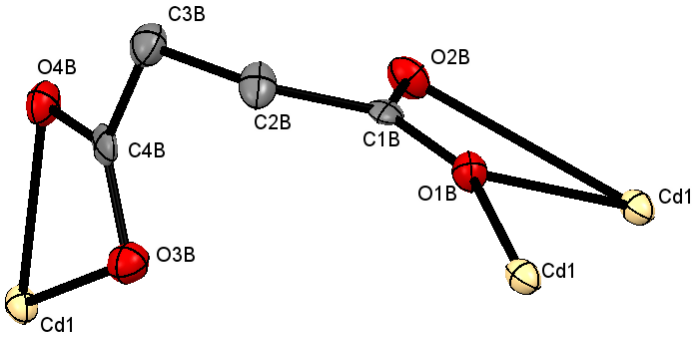

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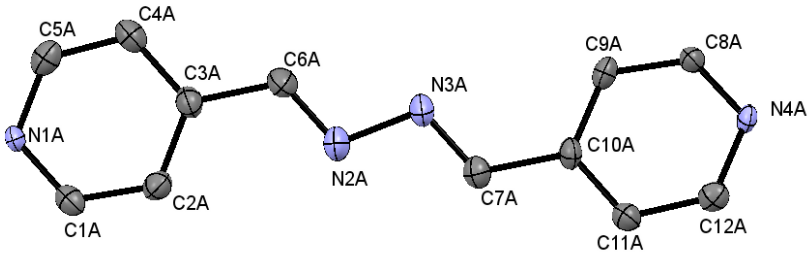

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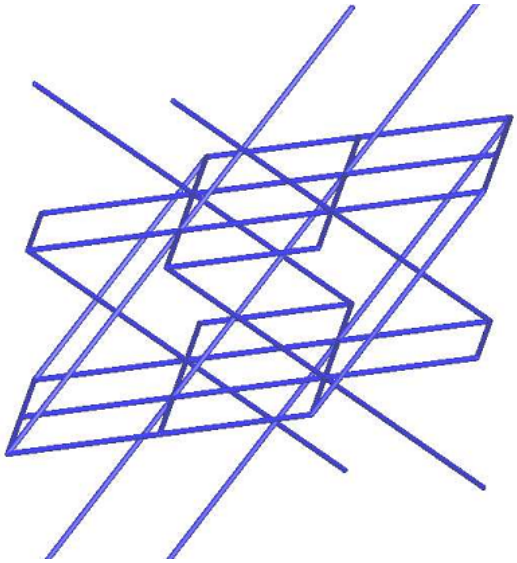


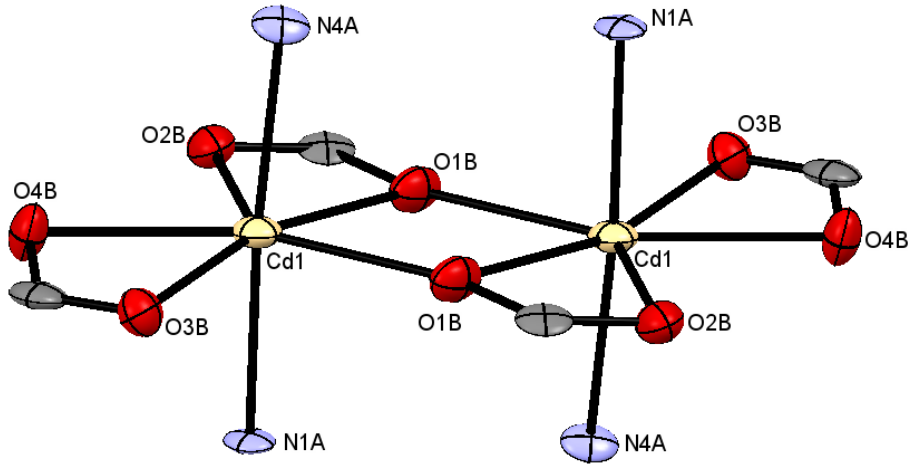
Table S3 – Selected bond distances (Å) and angles (°) in compound 3.

Cd1-N1A	2.314(4)	N1A-Cd1-N4A	178.9(1)
Cd1-O1B	2.313(3)	O3B-Cd1-O4B	54.5(1)
Cd1-O2B	2.751(3)	O4B-Cd1-O1B	92.3(1)
Cd1-O1B	2.384(3)	O1B-Cd1-O1B	72.26(9)
Cd1-N4A	2.329(4)	O1B-Cd1-O2B	50.77(9)
Cd1-O3B	2.492(3)	O2B-Cd1-O3B	91.02(9)
Cd1-O4B	2.319(3)		

Figures and table for compound 4

Figure S4 – (A) ORTEP view of the dimeric compound and its coordination sphere in compound 4; (B) ORTEP view of the glutarate dianion (C) ORTEP view of the 4-bpdb ligand

A



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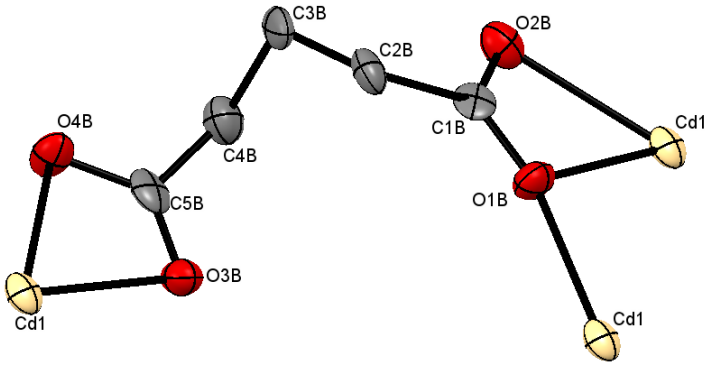

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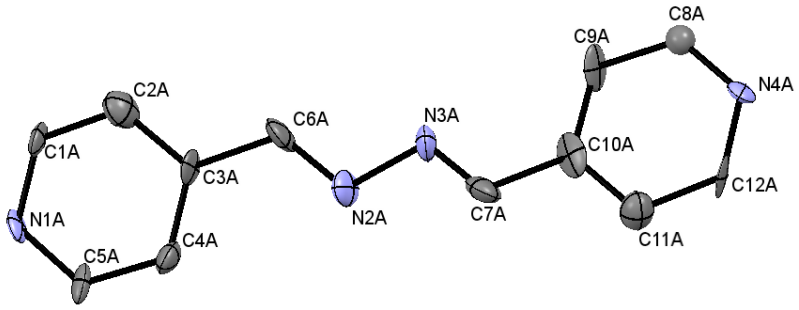


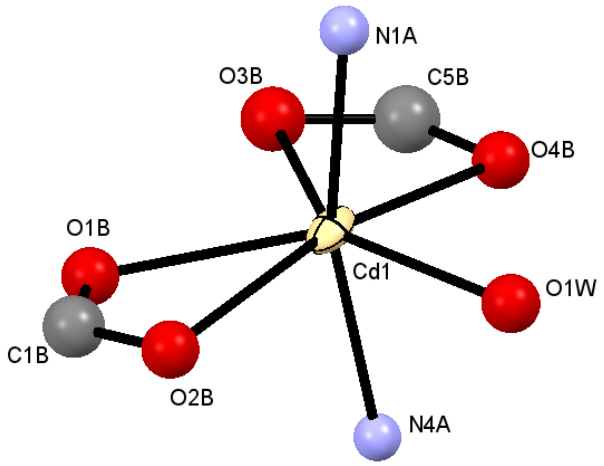
Table S4 – Selected bond distances (Å) and angles (°) in compound 4.

Cd1-N1A	2.309(3)	N4A-Cd-N1A	175.09(13)
Cd1-O1B	2.391(3)	O1B-Cd1-O2B	55.16(10)
Cd1-O3B	2.481(3)	O2B-Cd1-O4B	84.24(10)
Cd1-O4B	2.394(3)	O4B-Cd1-O3B	53.55(10)
Cd1-N4A	2.317(3)	O3B-Cd1-O1B	92.16(11)
Cd1-O1B	2.391(3)		
Cd1-O2B	2.381(3)		

Figures and table for compound 5

Figure S5 – (A) ORTEP view of the coordination sphere in compound 5; (B) ORTEP view of the glutarate dianion (C) ORTEP view of the 4-bpdb ligand

A



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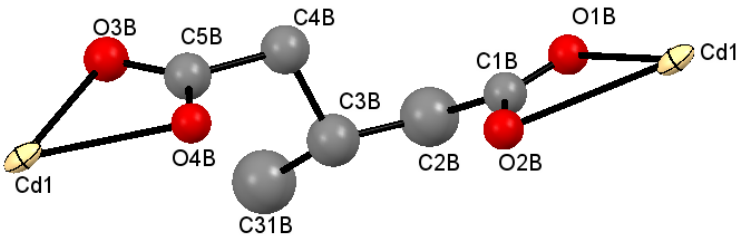

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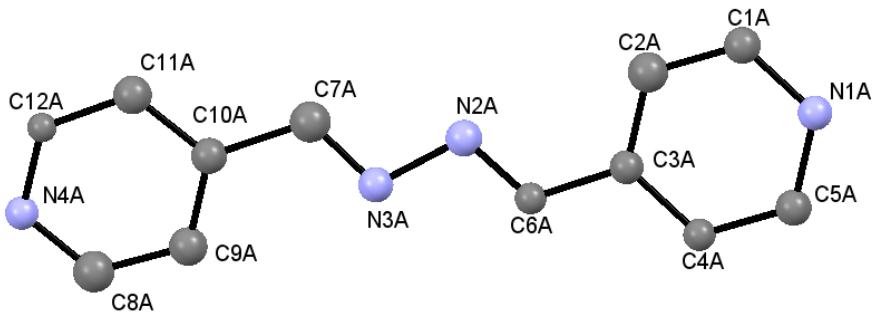


Table S5 – Selected bond distances (Å) and angles (°) in compound 5.

Cd1-N1A	2.330(4)	N4A-Cd1-N1A	165.46(14)
Cd1-O1B	2.338(8)	O4B-Cd1-O3B	54.6(4)
Cd1-O1W	2.302(3)	O1B-Cd1-O2B	53.1(3)
Cd1-O2B	2.514(13)	O3B-Cd1-O1B	79.41(17)
Cd1-N4A	2.370(7)	O2B-Cd1-O1W	86.4(4)
Cd1-O3B	2.306(8)	O1W-Cd1-O4B	87.4(4)
Cd1-O4B	2.486(12)		

Figure of compound 6

Figure S6 - Stick representation of the H-bond networks formed by 4-bpdb and glutaric acid in compound 6 from c axis(top) and from b axis (bottom); different 1D polymers have different color.

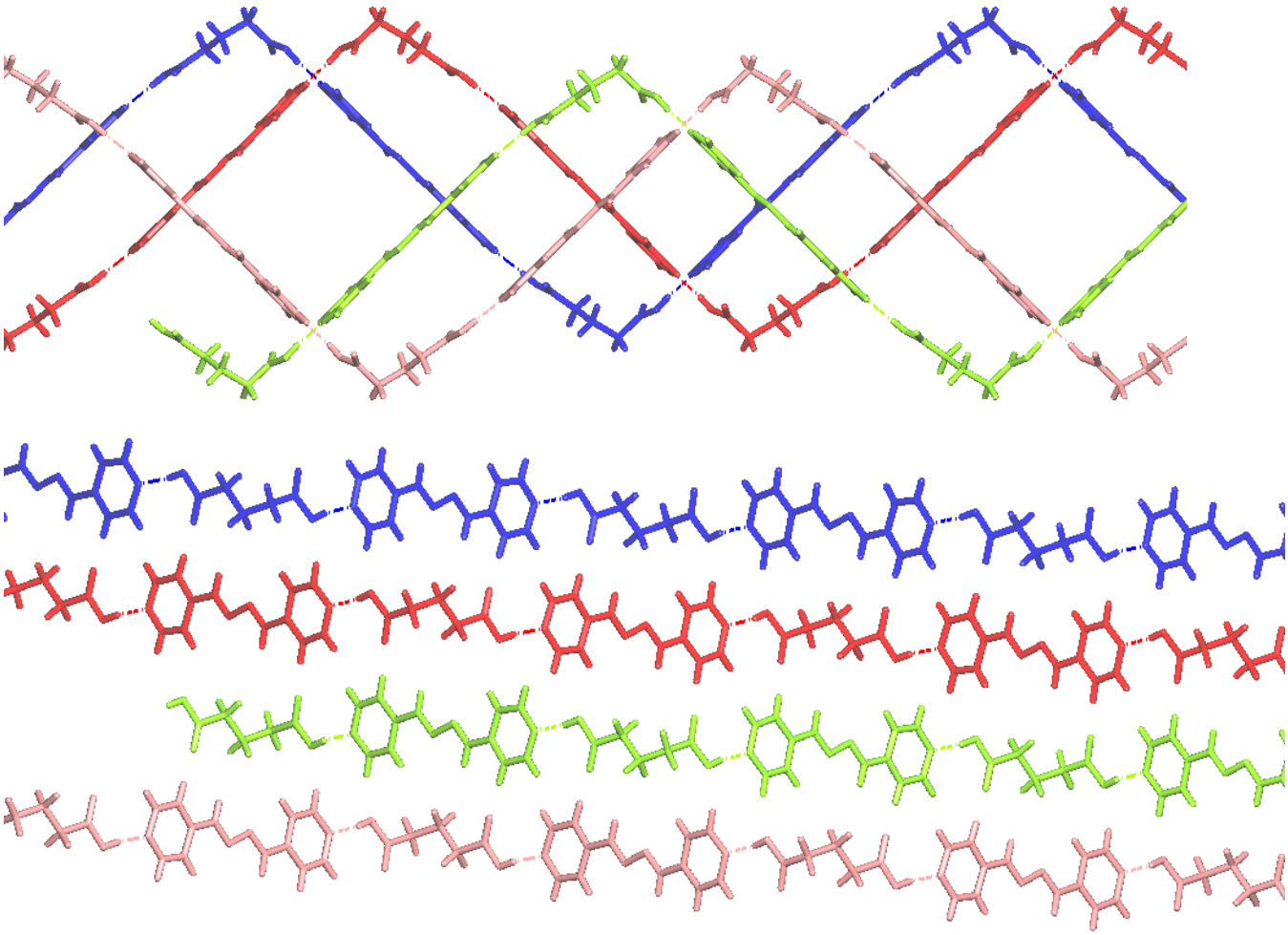


Figure of compound 7

Figure S7 - Stick representation of the H-bond networks formed by 4-bpdb and adipic acid in compound 7, viewed from a axis(top) and from b axis (bottom); different 1D polymers have different color.

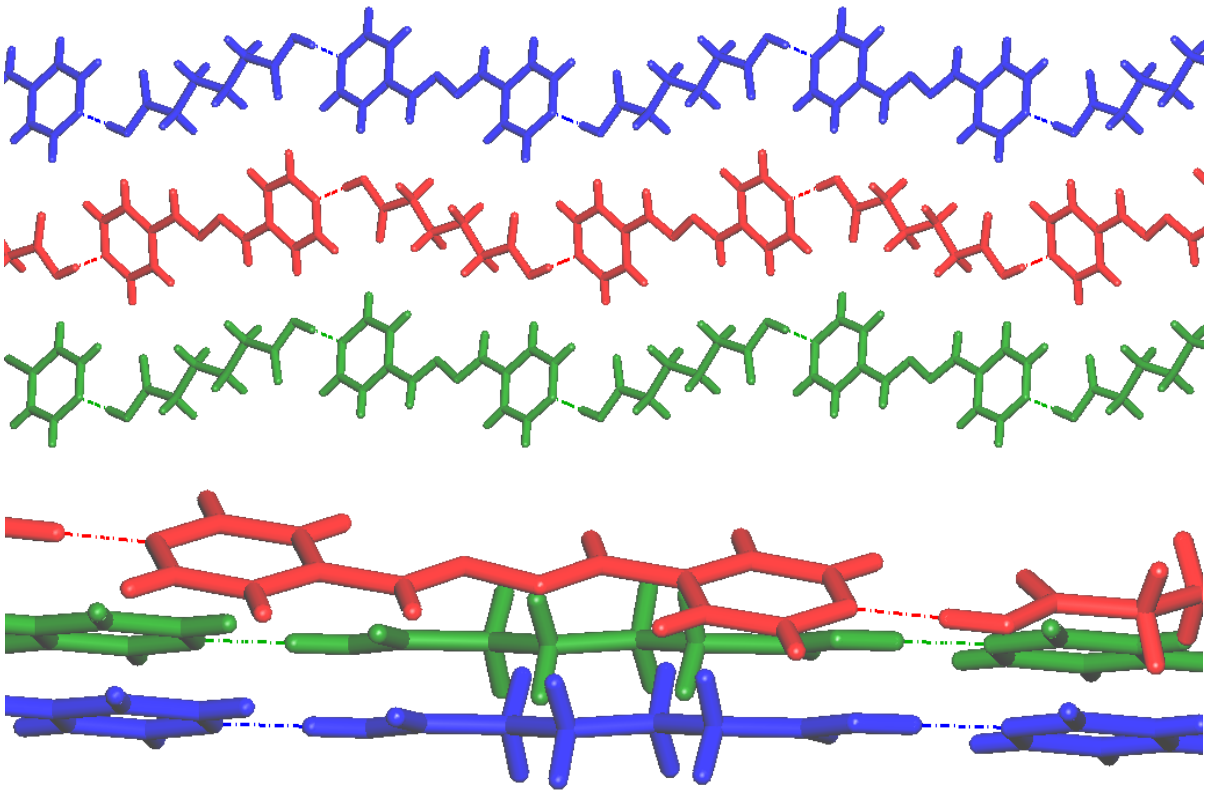
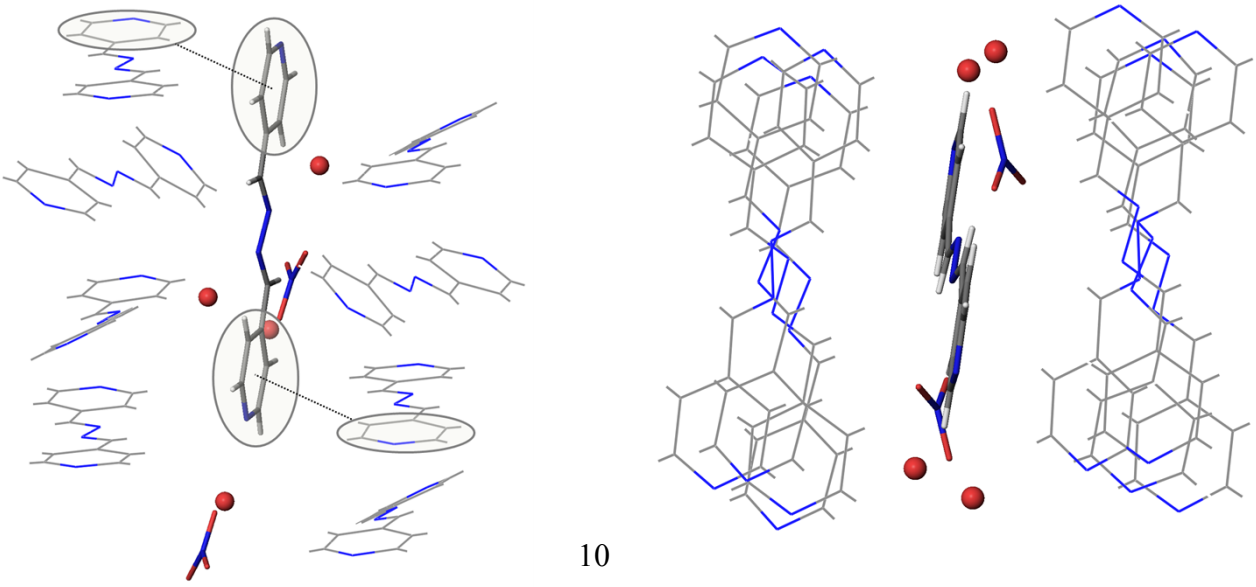


Figure S8 – Alternative views of the relative and non-interfering disposition of embedded guest molecules, water molecules (red spheres), nitrate ions and 4-bpdb ligands, with the stacked 4-bpdb ligands. The large distances (c.a. 4A) between the centroids of the embedded 4-bpdb pyridine moieties and the closest H atom of the closet staked pyridine moieties (inside circles) suggest a lack of an effect of the guest molecules with the stacking dependent emission.



LEBAIL REFINEMENTS FOR COMPUNDS 1-7

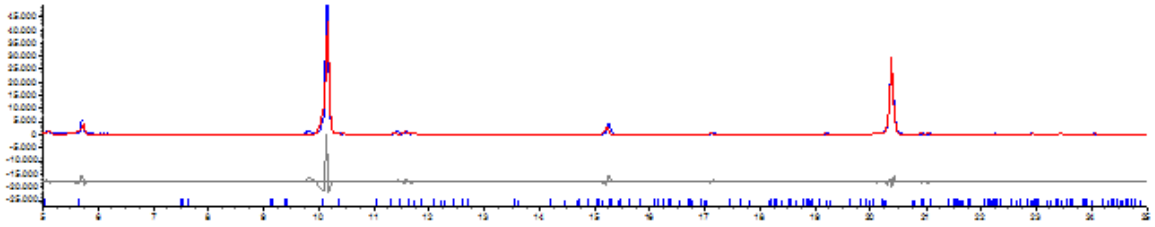


Figure S9. Lebail Refinement for **1**: a = 46.67, b =12.46, c =31.32, β =131.20, V =13697.47, *sample displacement* = -0.189mm.

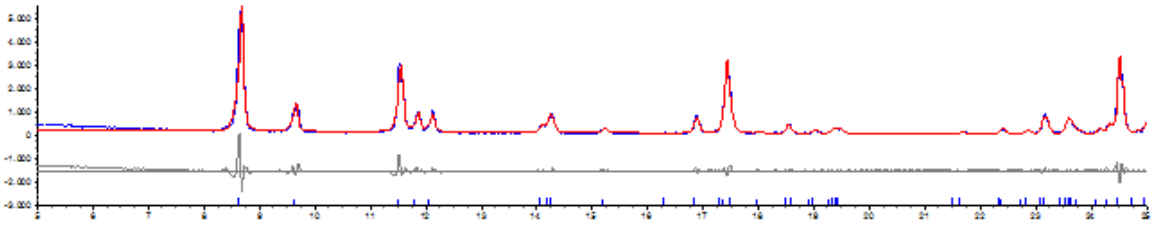


Figure S10. Lebail Refinement for **2**: a = 10.88, b =11.67, c =15.90, β =109.59, V =1902.60, *sample displacement* = -0.131mm.

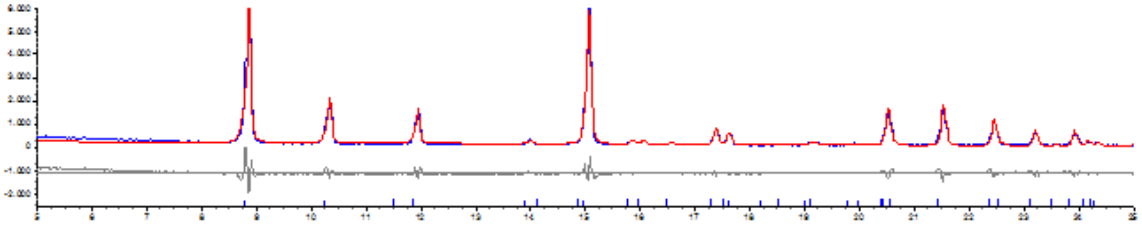


Figure S11. Lebail Refinement for **3**: a = 10.70, b =11.91, c =13.31, β =109.62, V =1597.16, *sample displacement* = -0.201mm.

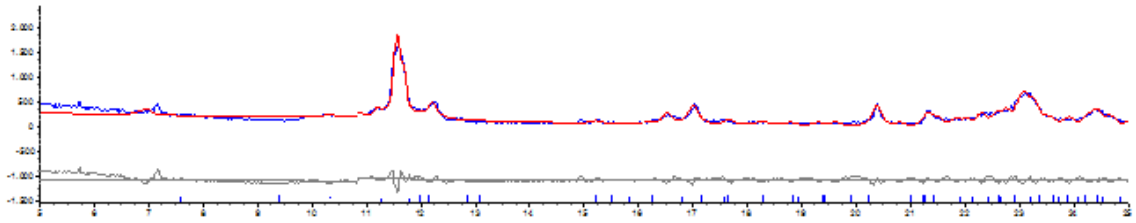


Figure S12. Lebail Refinement for **4**: a = 8.35, b =10.09, c = 12.19, α = 91.58, β =105.69, γ =109.82, V =922.04, *sample displacement* = 1.180mm

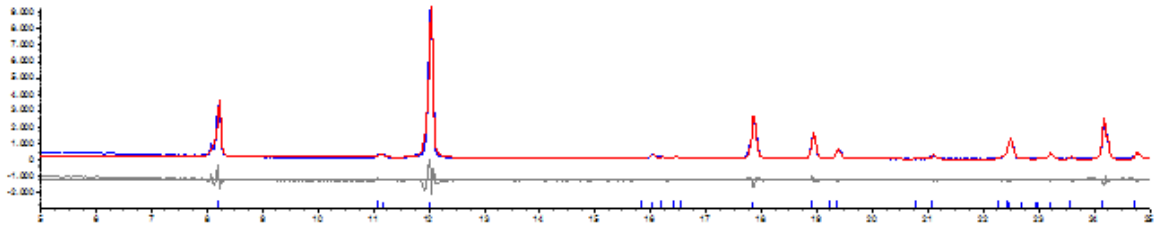


Figure S13. Lebail Refinement for **5**: a = 17.19, b =15.85, c =9.23, β =121.02, V =2154.67, *sample displacement* = - 0.079mm

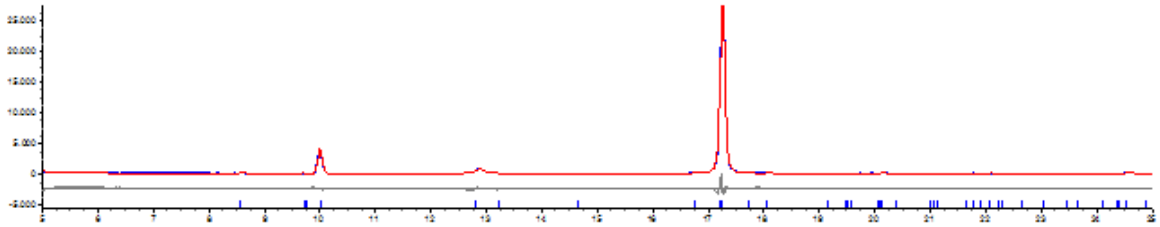


Figure S15. Lebail Refinement for **6**: a = 41.14, b =4.67, c =20.61, β =118.15, V =3488.39, *sample displacement* = -0.097

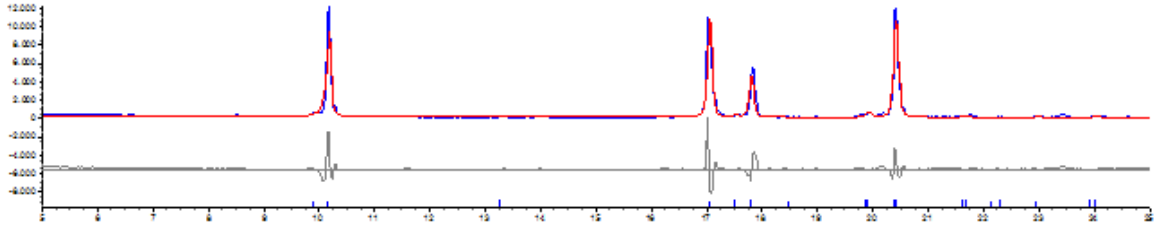


Figure S16. Lebail Refinement for **7**: a = 4.84, b = 10.40, c =17.55, β =97.62, V =875.19, -0.049mm

IR SPECTRA FOR COMPOUND 1-7

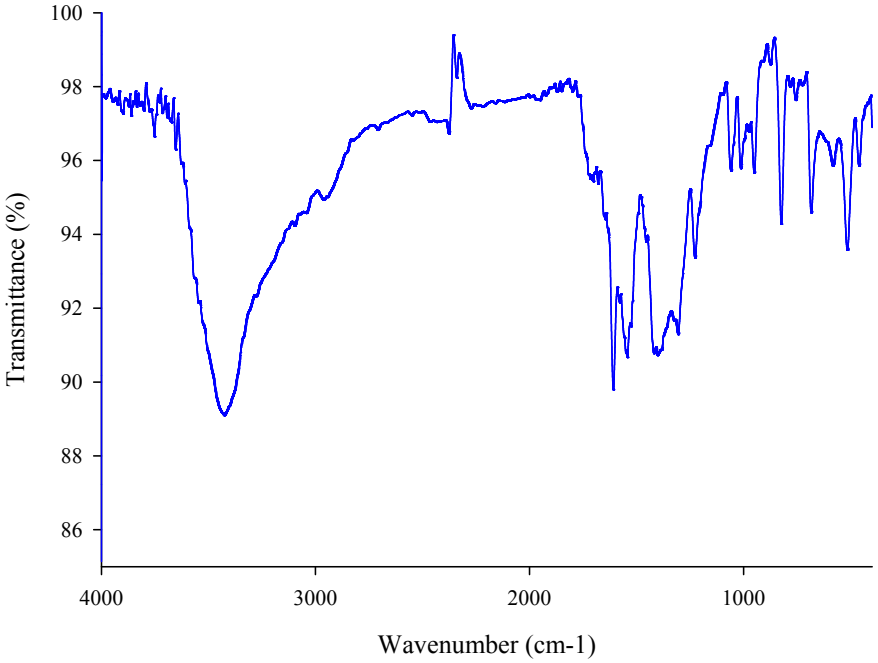


Figure S17. IR spectrum for compound **1**.

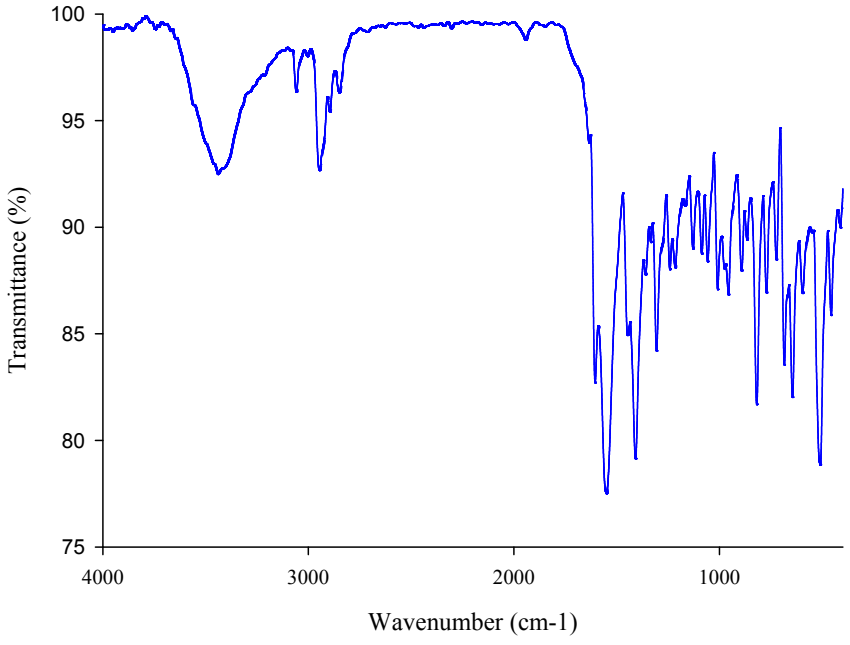


Figure S18. IR spectrum for compound **2**.

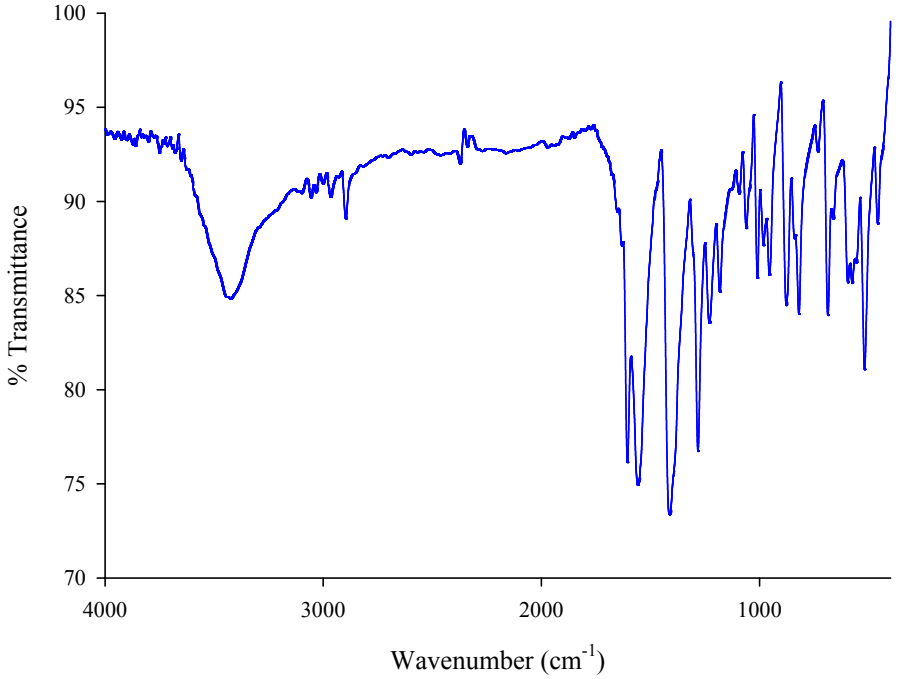


Figure S19. IR spectrum for compound **3**.

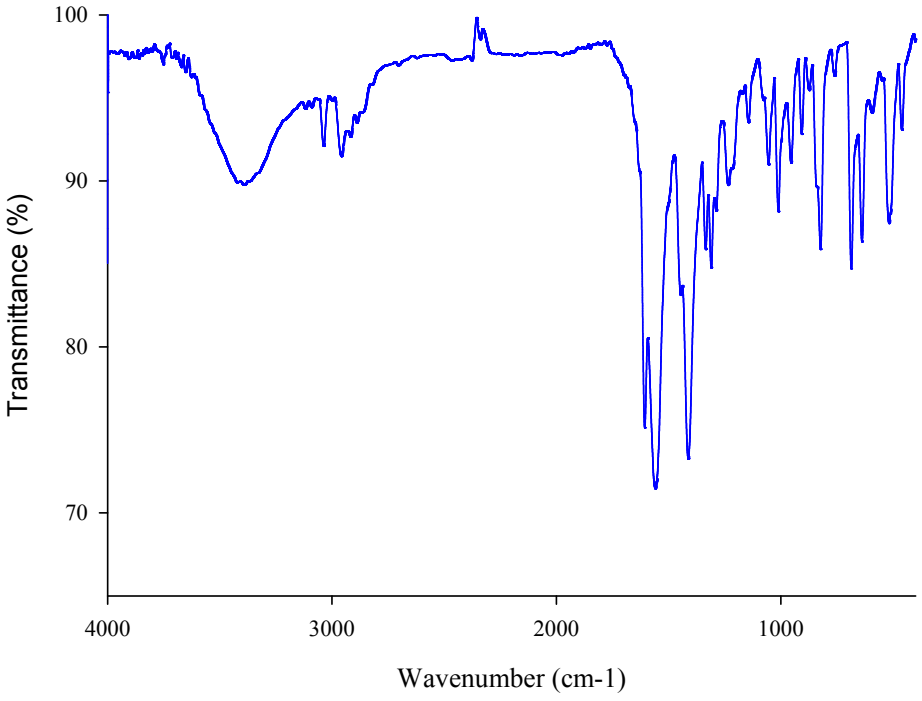


Figure S20. IR spectrum for compound **4**.

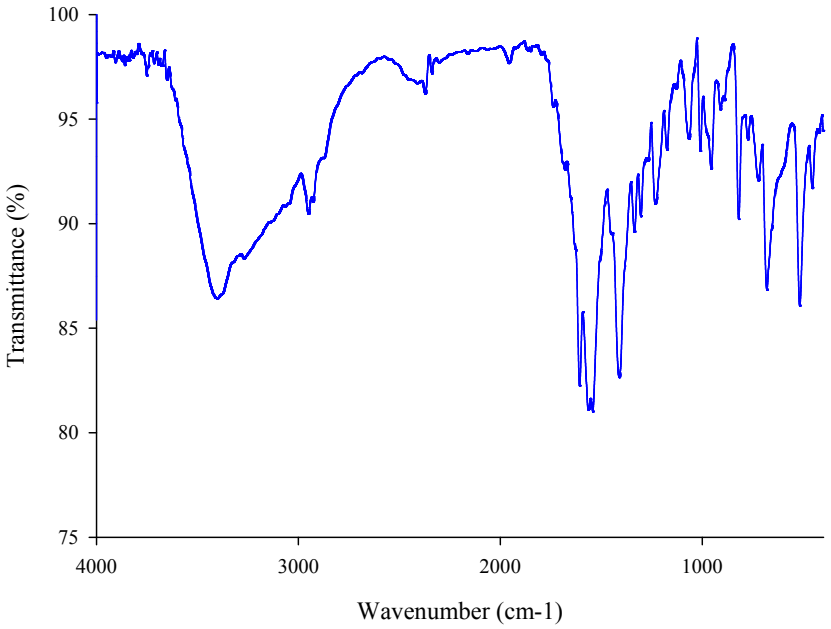


Figure S21. IR spectrum for compound **5**.

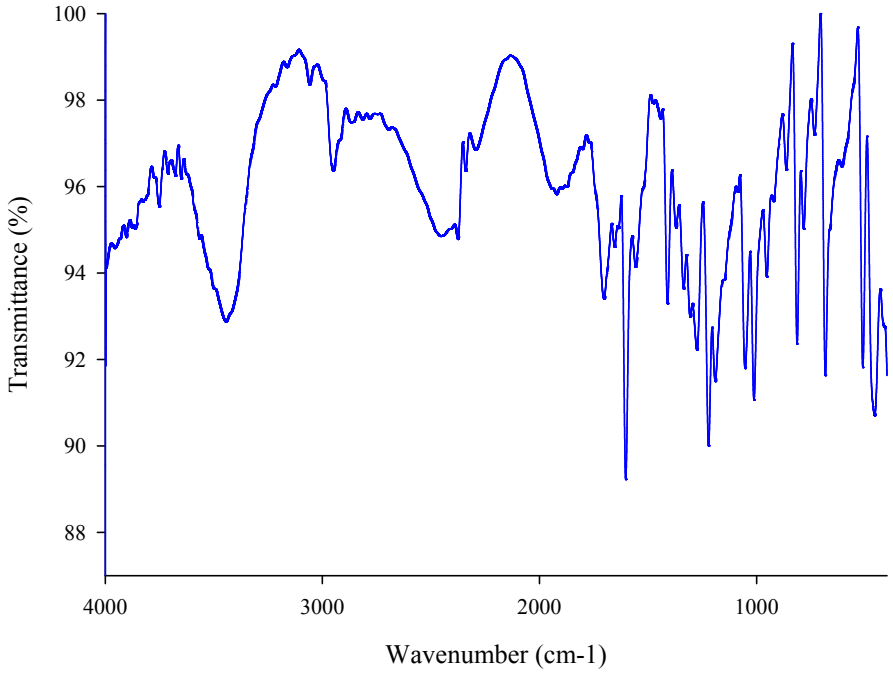


Figure S22. IR spectrum for compound **6**.

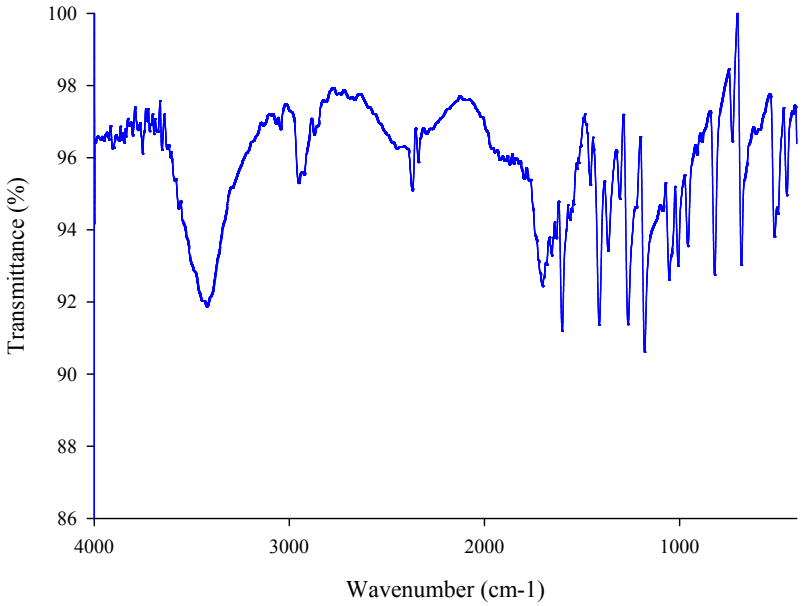


Figure S23. IR spectrum for compound **7**.

TG SPECTRUM FOR COMPOUND 1

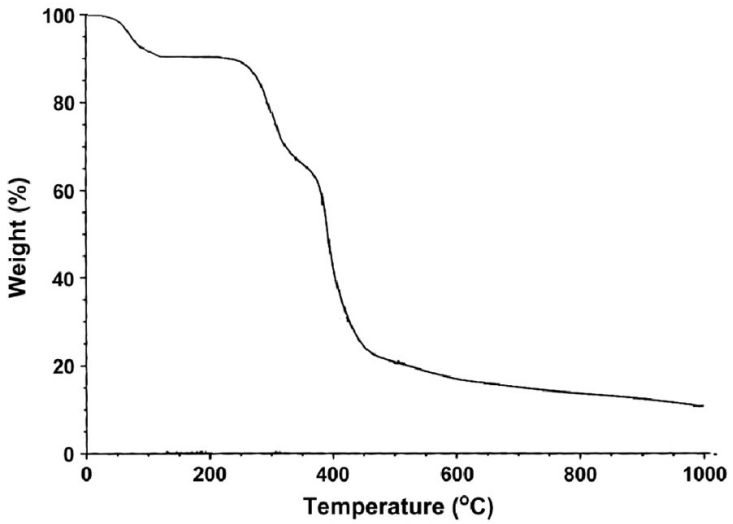


Figure S24. IR spectrum for compound **1**.

LUMINESCENCE VARIATION FOR 1

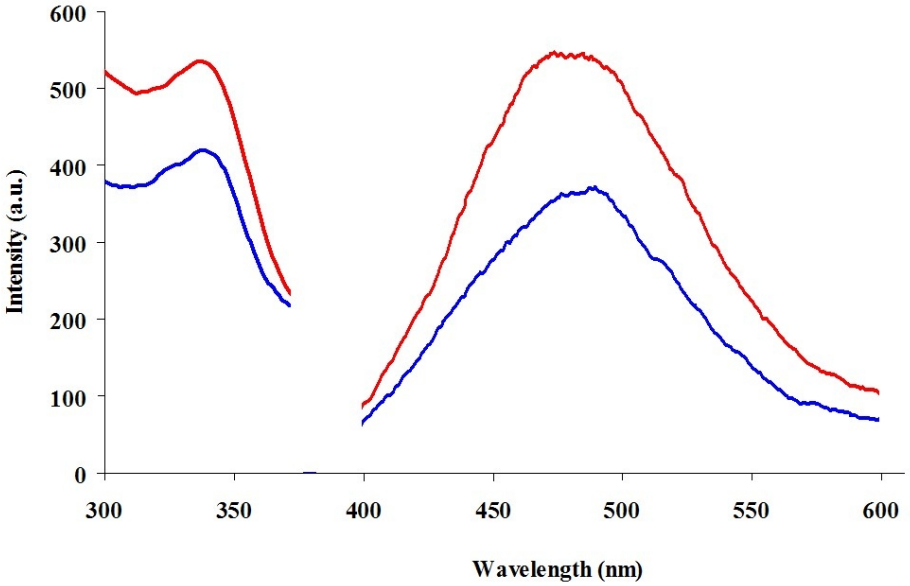


Figure S25. Luminescence variation intensities upon excitation and emission in photoluminescence studies using pristine and activated compounds IR spectrum for compound **1**.

REFERENCES

(1) Blatov, V.A.; Shevchenko, A.P. ; Proserpio, D.M. *Cryst. Growth Des.,* **2014**, 14, 3576.