

# **Synthesis, Structure and Magnetic Properties of Cobalt(II) Coordination Polymers from a New Tripodal Carboxylate Ligand: Weak Ferromagnetism and Metamagnetism**

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## **Supporting Information**

**Table S1.** Selected Bond Distances (Å) and Bond Angles (°) in **1-4**.

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| 1                    |                      |                      |
|----------------------|----------------------|----------------------|
| Co1 O2 2.151(4)      | Co1 O8 2.092(4)      | Co2 O6 1.963(4)      |
| Co1 O3 2.134(5)      | Co1 O8 2.115(4)      | Co2 O8 1.942(4)      |
| Co1 O4 2.077(4)      | Co2 O5 1.961(5)      | Co2 N1 2.031(5)      |
| Co1 O7 2.064(5)      |                      |                      |
| O3 Co1 O2 61.51(18)  | O7 Co1 O8 176.50(17) | O5 Co2 N1 103.2(2)   |
| O4 Co1 O2 101.57(17) | O7 Co1 O8 94.64(17)  | O6 Co2 N1 98.7(2)    |
| O4 Co1 O3 163.04(18) | O8 Co1 O2 96.31(17)  | O8 Co2 O5 106.57(18) |
| O4 Co1 O8 85.20(17)  | O8 Co1 O2 163.47(17) | O8 Co2 O6 109.72(19) |
| O4 Co1 O8 94.87(16)  | O8 Co1 O3 97.26(18)  | O8 Co2 N1 124.32(19) |
| O7 Co1 O2 86.50(19)  | O8 Co1 O3 102.08(17) | Co2 O8 Co1 99.35(17) |
| O7 Co1 O3 85.9(2)    | O5 Co2 O6 114.5(2)   | Co2 O8 Co1 128.5(2)  |
| O7 Co1 O4 92.2(2)    |                      |                      |
| 2                    |                      |                      |
| Co1 O1 2.029(5)      | Co1 OW1 2.205(5)     | Co2 O4 2.169(5)      |
| Co1 O3 2.046(5)      | Co1 OW2 2.145(6)     | Co2 O6 2.211(5)      |
| Co1 O8 2.073(5)      | Co2 O2 2.045(5)      | Co2 O7 2.099(5)      |
| Co1 O8 2.090(5)      | Co2 O4 2.129(5)      | Co2 O8 2.009(5)      |
| O1 Co1 O3 91.2(2)    | O8 Co1 OW1 89.8(2)   | O7 Co2 O4 99.91(18)  |
| O1 Co1 O8 92.6(2)    | O8 Co1 OW2 89.0(2)   | O7 Co2 O6 61.21(18)  |
| O1 Co1 O8 173.9(2)   | O8 Co1 OW2 103.1(2)  | O8 Co2 O2 96.2(2)    |
| O1 Co1 OW1 90.2(2)   | O2 Co2 O4 95.18(19)  | O8 Co2 O4 90.07(18)  |
| O1 Co1 OW2 91.8(2)   | O2 Co2 O4 172.69(18) | O8 Co2 O4 91.47(19)  |
| O3 Co1 O8 94.97(19)  | O2 Co2 O6 95.8(2)    | O8 Co2 O6 105.63(19) |
| O3 Co1 O8 167.7(2)   | O2 Co2 O7 92.5(2)    | O8 Co2 O7 165.00(19) |
| O3 Co1 OW1 84.8(2)   | O4 Co2 O6 86.16(18)  | OW2 Co1 OW1 173.0(2) |
| O3 Co1 OW2 88.4(2)   | O4 Co2 O6 158.53(18) | Co2 O8 Co1 119.9(2)  |
| O8 Co1 OW1 83.6(2)   | O7 Co2 O4 82.21(19)  | Co2 O8 Co1 124.7(2)  |
| 3                    |                      |                      |
| Co1 O2 2.161(4)      | Co2 O1 2.353(4)      | Co2 O6 2.025(5)      |
| Co1 O3 2.004(4)      | Co2 O2 2.121(4)      | Co2 N1 2.101(5)      |
| Co1 O7 2.078(4)      | Co2 O4 2.074(4)      | Co2 N2 2.153(5)      |
| O3 Co1 O2 85.85(16)  | O2 Co2 N2 89.53(18)  | O6 Co2 O4 105.11(19) |
| O3 Co1 O2 94.15(16)  | O4 Co2 O1 164.54(16) | O6 Co2 N1 84.78(19)  |
| O3 Co1 O7 83.56(18)  | O4 Co2 O2 108.66(16) | O6 Co2 N2 169.6(2)   |
| O3 Co1 O7 96.44(17)  | O4 Co2 N1 92.88(18)  | N1 Co2 O1 100.06(18) |

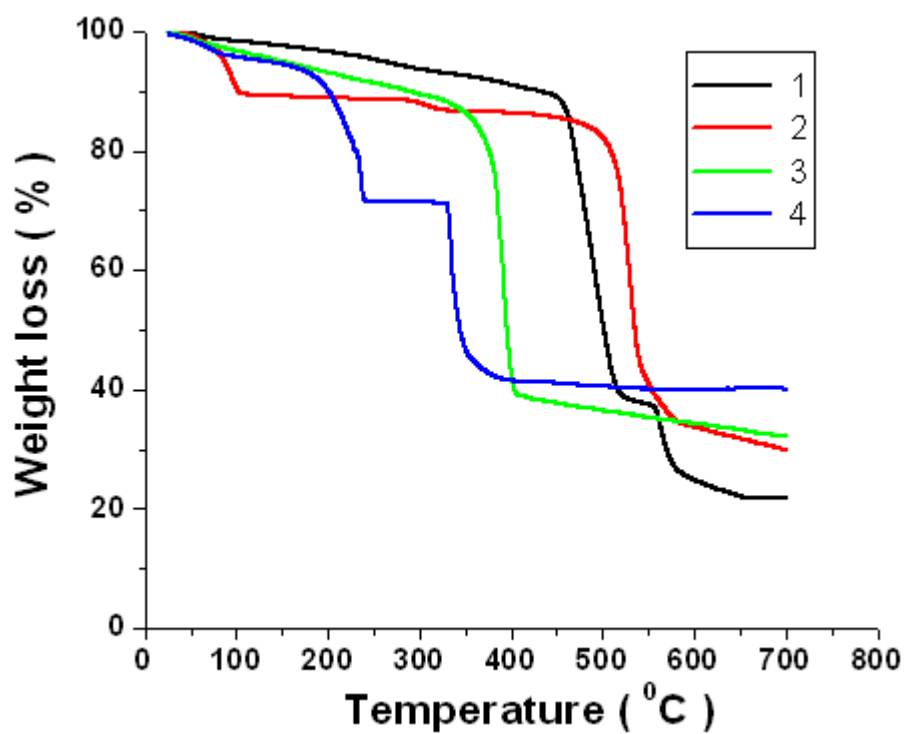
|                     |                     |                      |
|---------------------|---------------------|----------------------|
| O7 Co1 O2 84.63(16) | O4 Co2 N2 85.22(19) | N1 Co2 O2 158.42(18) |
| O7 Co1 O2 95.37(16) | O6 Co2 O1 84.62(18) | N1 Co2 N2 93.7(2)    |
| O2 Co2 O1 58.89(15) | O6 Co2 O2 88.20(17) | N2 Co2 O1 85.53(18)  |

**4**

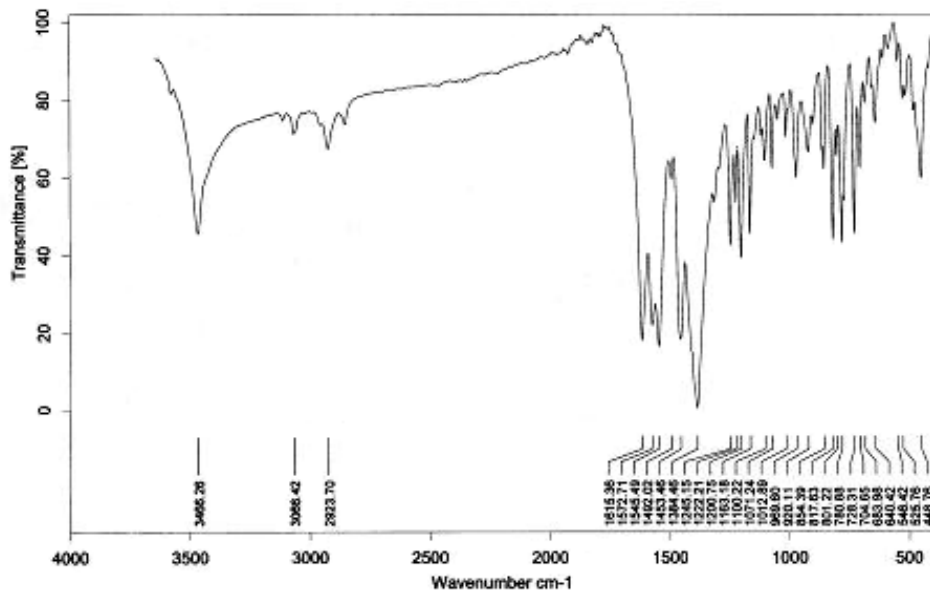
|                     |                      |                       |
|---------------------|----------------------|-----------------------|
| Co1 O1 2.114(4)     | Co2 O1 2.090(4)      | Co2 N1 2.178(6)       |
| Co1 O4 2.033(4)     | Co2 O3 2.036(4)      | Co2 N2 2.085(5)       |
| Co1 O6 2.091(4)     | Co2 O7 2.039(5)      |                       |
| <hr/>               |                      |                       |
| O4 Co1 O1 88.13(17) | O1 Co2 N1 83.29(18)  | O7 Co2 N1 165.16(19)  |
| O4 Co1 O1 91.87(17) | O3 Co2 O1 102.60(18) | O7 Co2 N2 89.57(19)   |
| O4 Co1 O6 84.98(16) | O3 Co2 O7 102.72(19) | N2 Co2 O1 159.9(2)    |
| O4 Co1 O6 95.02(16) | O3 Co2 N1 92.12(19)  | N2 Co2 N1 88.9(2)     |
| O6 Co1 O1 87.37(16) | O3 Co2 N2 96.2(2)    | Co2 O1 Co1 111.14(18) |
| O6 Co1 O1 92.63(16) | O7 Co2 O1 93.27(17)  |                       |

**Table S2.** Selected non-bonding distances (Å) in **1-4**.

|                     |                    |                     |
|---------------------|--------------------|---------------------|
| <b>1</b>            |                    |                     |
| Co1.....Co1' 3.144  | Co2.....Co2' 5.975 | Co1'.....Co2 3.635  |
| Co1'.....Co2' 3.095 | Co1.....Co2 3.095  | Co1.....Co2' 3.635  |
| O8.....Co2' 4.241   | O8'..... Co2 4.241 |                     |
| <b>2</b>            |                    |                     |
| Co1.....Co1' 3.160  | Co2.....Co2' 6.431 | Co2.....Co1' 3.548  |
| Co1'.....Co2' 3.616 | Co2.....Co2' 3.273 | Co1.....Co2' 3.548  |
| Co1 .....Co2 3.616  | O8..... Co2' 4.507 | O8'..... Co2 4.507  |
| <b>3</b>            |                    |                     |
| Co1.....Co2 3.443   | Co1.....Co2' 3.443 | Co2 .....Co2' 6.887 |
| <b>4</b>            |                    |                     |
| Co1.....Co2 3.468   | Co1.....Co2' 3.468 | Co2 .....Co2' 6.937 |



**Figure S1.** TGA of compound 1-4. Color code: Compound 1, black; Compound 2, red; Compound 3, green; Compound 4, blue.



**Figure S2.** IR spectrum of compound 1

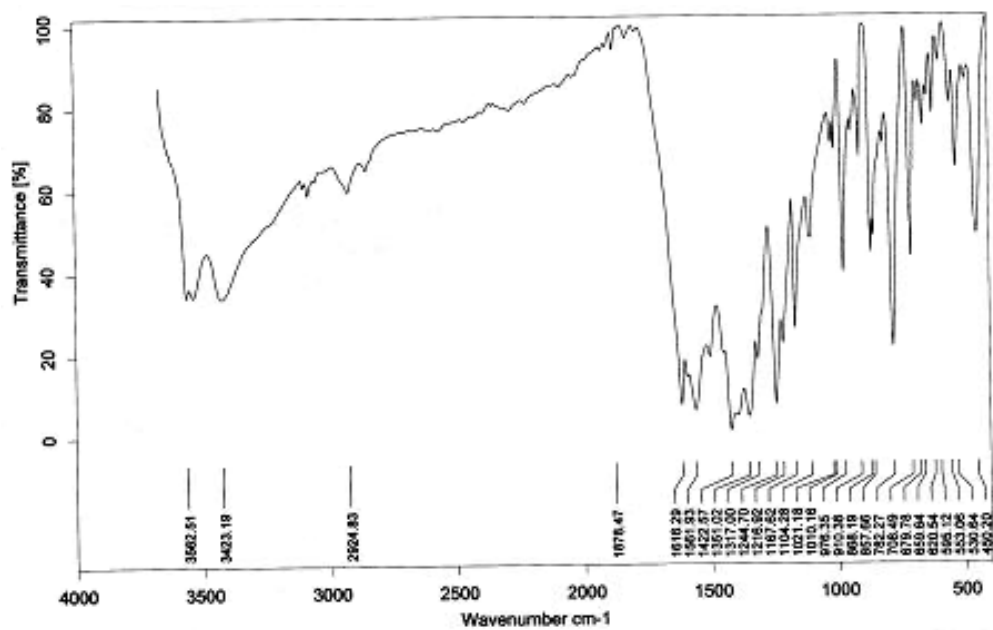


Figure S3. IR spectrum of compound 2

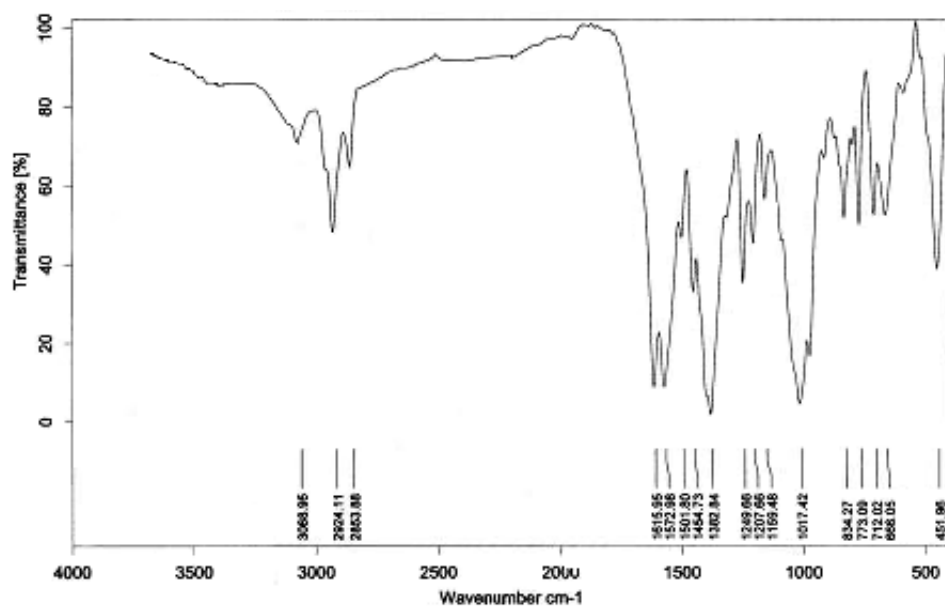


Figure S4. IR spectrum of compound 3

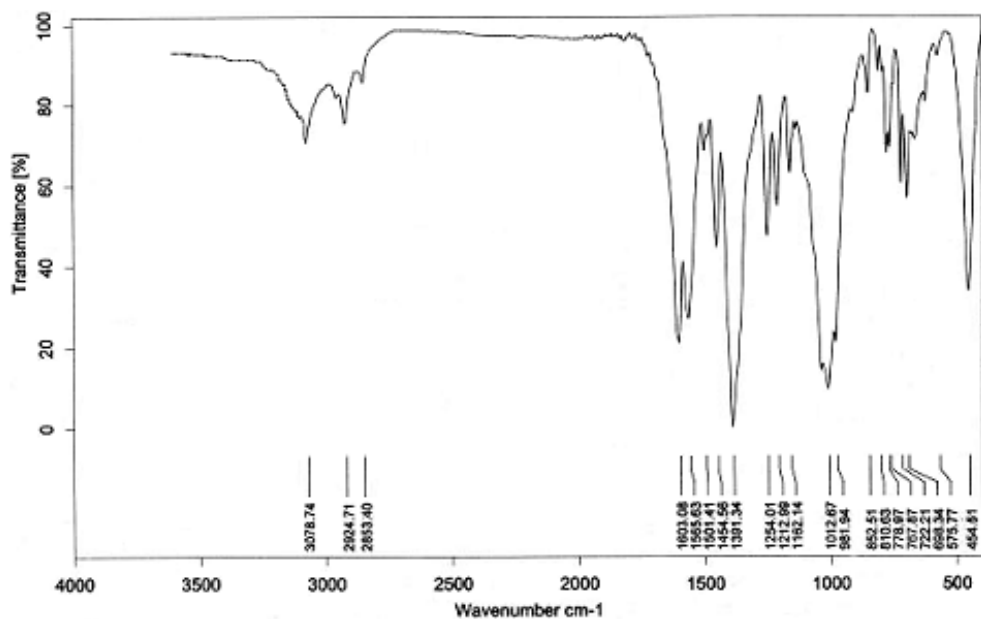


Figure S5. IR spectrum of compound 4

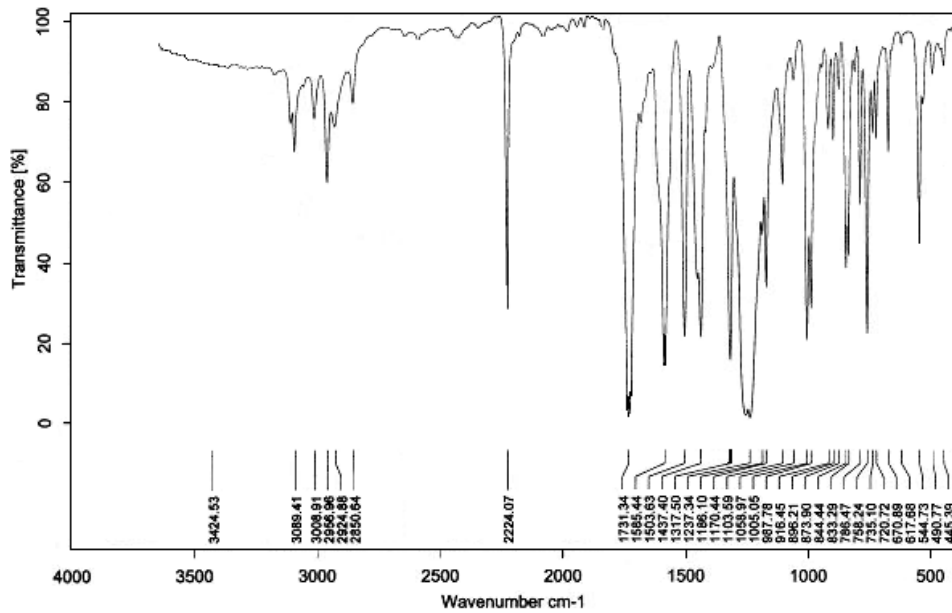


Figure S6. IR spectrum of dcpi.

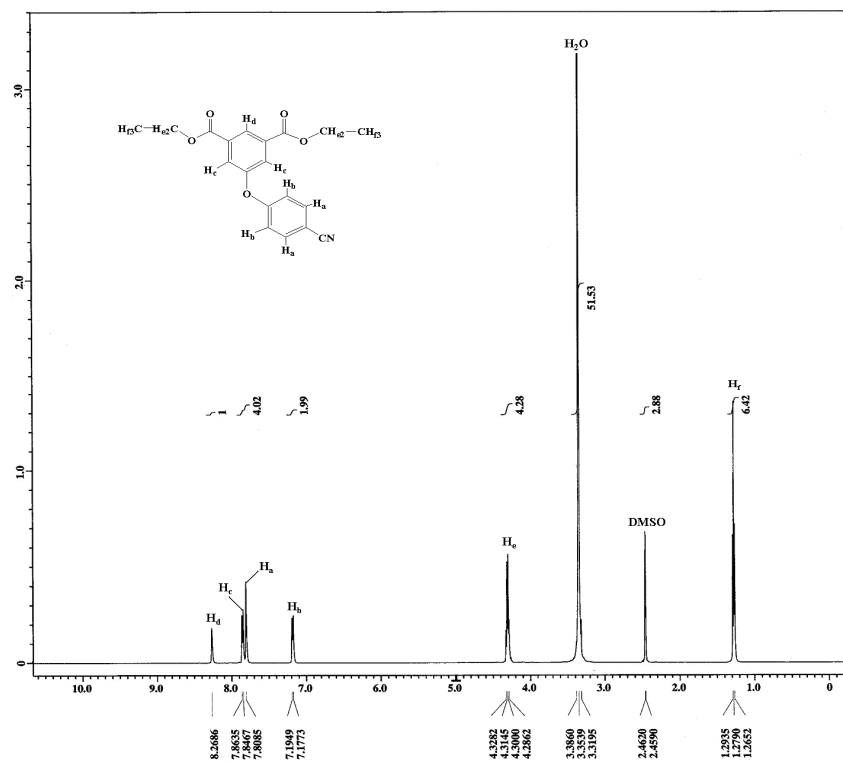


Figure S7. NMR spectrum of dpci

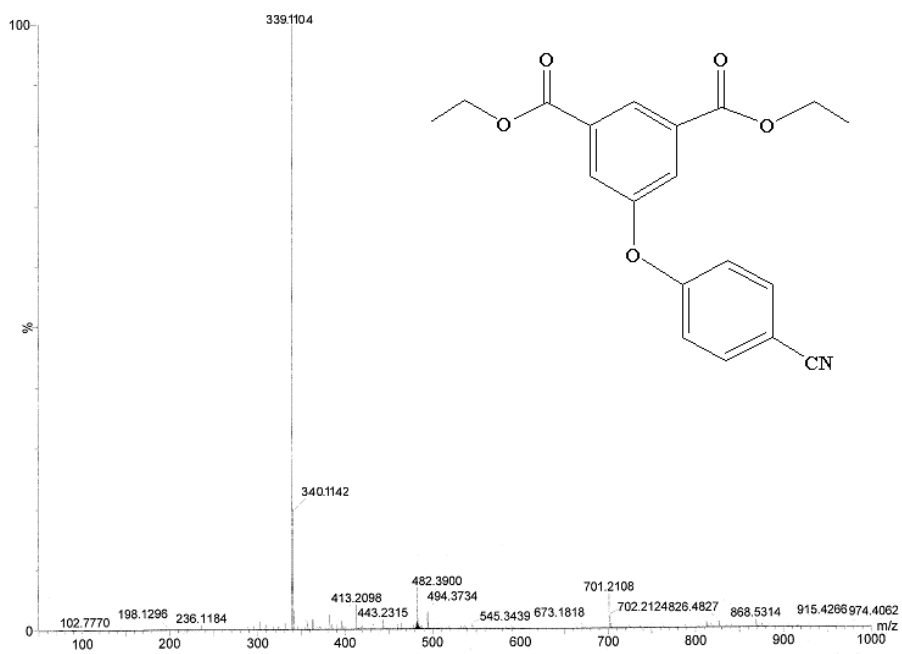


Figure S8. ESI-MS spectrum of dpci.

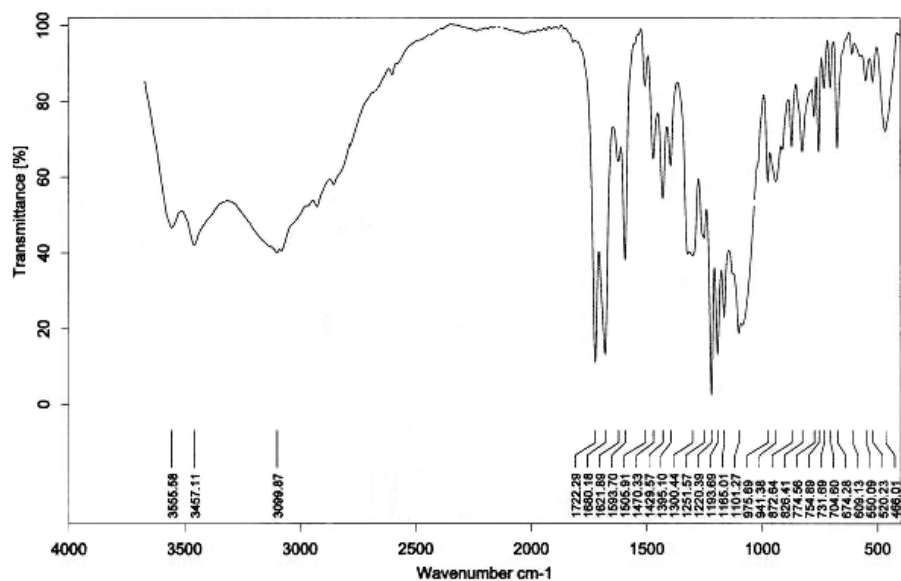


Figure S9. IR spectrum of cpiaH<sub>3</sub>

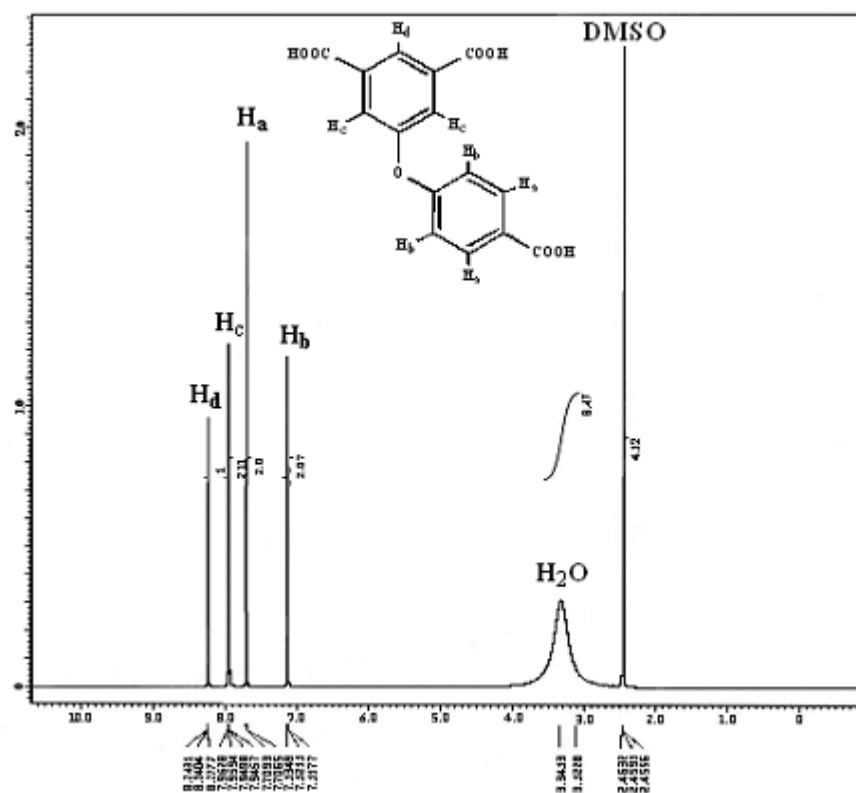


Figure S10. NMR spectrum of cpiaH<sub>3</sub>.



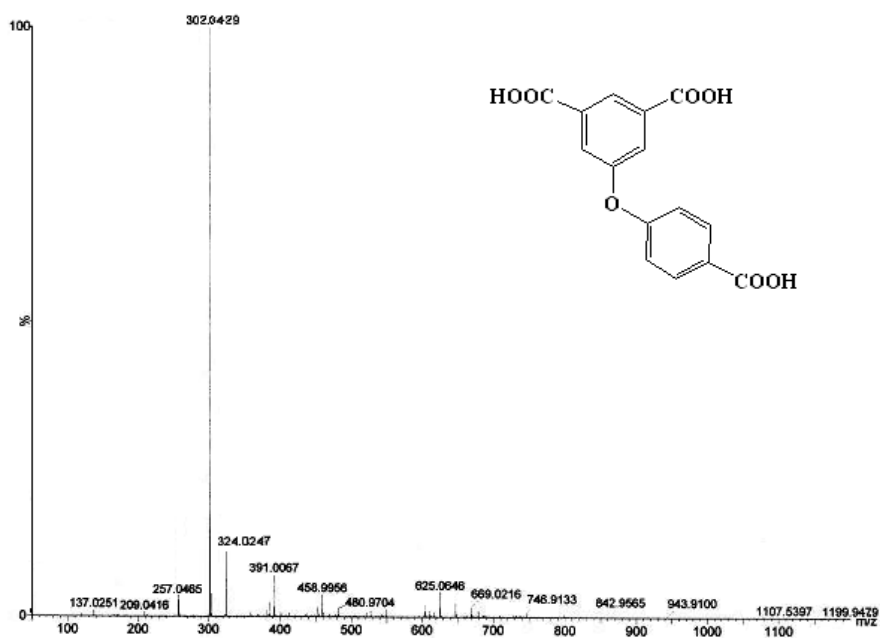


Figure S11. ESI-MS spectrum of cpiaH<sub>3</sub>.

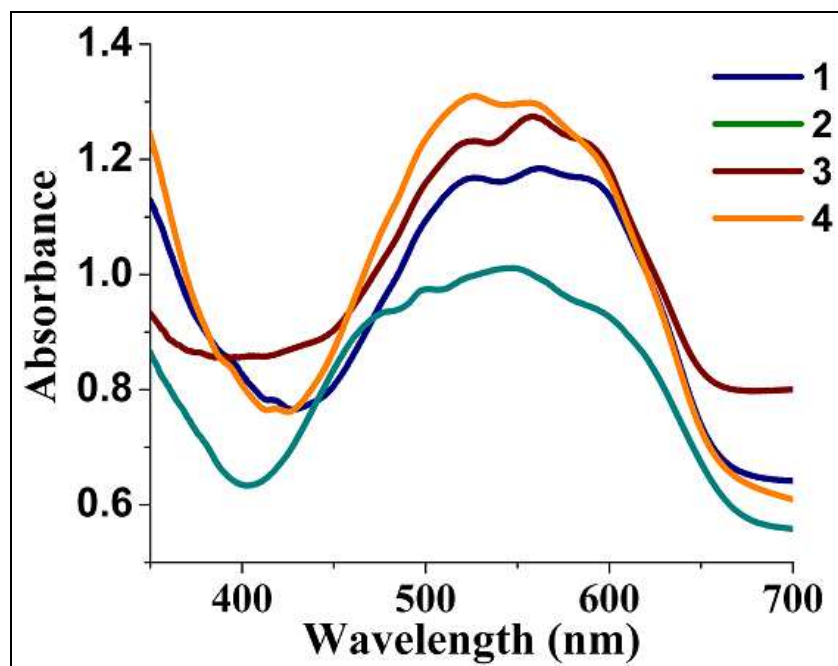
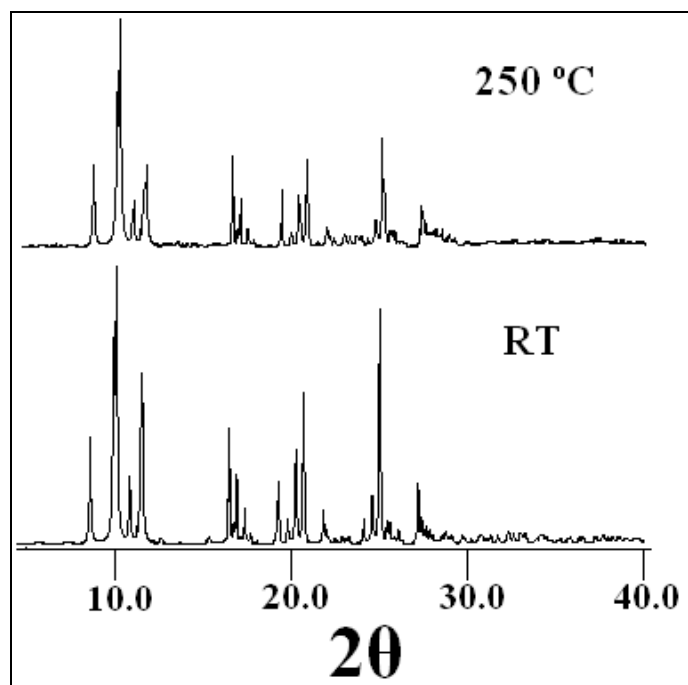
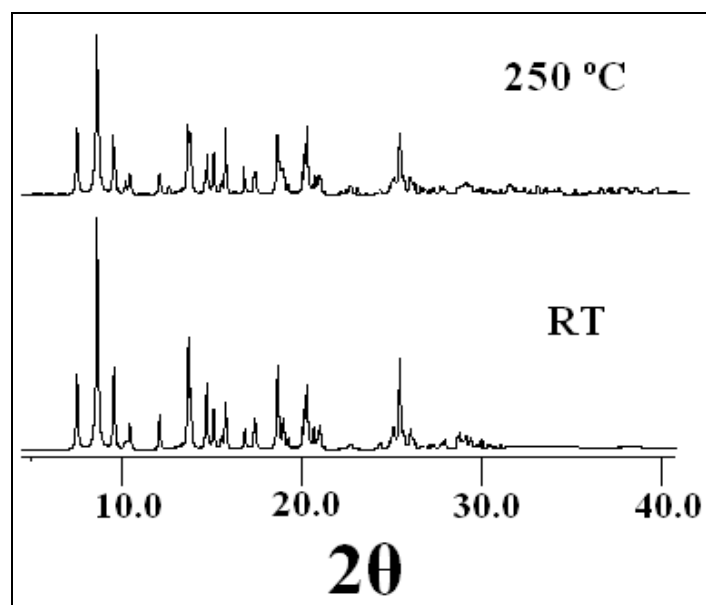


Figure S12. Solid state UV-vis spectra of compounds 1-4.



**Figure S13.** PXRD patterns of compound **1** as-synthesized (below) and after heating at 250 °C (above).



**Figure S14.** PXRD patterns of compound **3** as-synthesized (below) and after heating at 250 °C (above).