

Electronic Supplementary Information (ESI)

Crystal engineering of a series of complexes and coordination polymers based on pyrazole-carboxylic acid ligands†

Smaail Radi,^{*1} Mohamed El-Massadoudi,¹ Houria Benaissa,² N. N. Adarsh,² Marilena Ferbinteanu,³ Eamonn Devlin,⁴ Yiannis Sanakis,⁴ Yann Garcia^{*2}

*1*LCAE, Département de Chimie, Faculté des Sciences, Université Mohamed I, BP 524, 60 000 Oujda, Morocco.

*2*Institute of Condensed Matter and Nanosciences, Molecules, Solids and Reactivity (IMCN/MOST), Université catholique de Louvain, Place L. Pasteur 1, 1348 Louvain-la-Neuve, Belgium.

*3*University of Bucharest, Faculty of Chemistry, Inorganic Chemistry Department, Dumbrava Rosie 23, Bucharest 020462, Romania.

*4*Institute of Materials Science, NCSR Demokritos, Athens 15310, Greece.

E-mail: yann.garcia@uclouvain.be, radi_smaail@yahoo.fr

Fax: +32-10472330

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Table S1 - Hydrogen Bonding Parameters of 1-5

| D-H...A | D-H (Å) | H...A (Å) | D...A (Å) | D-H...A (°) | Symmetry operation for A |
|----------------------|----------|-----------|-----------|-------------|--------------------------|
| 1 | | | | | |
| O(5)-H(1)...O(2) | 1.23(15) | 1.70(16) | 2.868(8) | 158(12) | x, y, z |
| O(5)-H(2)...O(1) | 0.78(5) | 2.49(5) | 3.265(7) | 173(4) | 3/2-x, -1/2+y, z |
| O(5)-H(2)...O(2) | 0.78(5) | 2.44(5) | 3.032(8) | 134(5) | 3/2-x, -1/2+y, z |
| C(6)-H(6A)...O(5) | 0.97 | 2.60 | 3.513(9) | 157 | 2-x, 1-y, 1-z |
| 2 | | | | | |
| C(6)-H(6B)...O(4) | 0.97 | 2.58 | 3.489(6) | 157 | -1/2+x, 1/2-y, 1-z |
| 3 | | | | | |
| O(7)-H(3)...O(4) | 0.92(5) | 1.87(5) | 2.777(3) | 169(4) | -x, -y, -z |
| O(7)-H(4)...O(6) | 0.76(5) | 2.17(5) | 2.876(4) | 155(5) | -x, -y, 1-z |
| O(5)-H(6)...O(7) | 0.75(4) | 1.97(4) | 2.714(4) | 173(5) | x, y, z |
| O(5)-H(7)...O(6) | 0.86(4) | 1.93(4) | 2.780(3) | 171(4) | x, y, z |
| O(6)-H(8)...O(2) | 0.75(4) | 2.08(4) | 2.825(3) | 174(4) | x, -1+y, z |
| O(6)-H(9)...O(2) | 0.96(5) | 1.83(5) | 2.782(3) | 170(4) | -1-x, 1-y, 1-z |
| C(6)-H(6A)...O(7) | 0.97 | 2.50 | 3.456(4) | 168 | x, y, z |
| C(7)-H(7A)...O(3) | 0.97 | 2.48 | 3.415(3) | 162 | -x, 1-y, -z |
| C(7)-H(7B)...O(4) | 0.97 | 2.53 | 3.418(3) | 153 | 1+x, y, z |
| 4 | | | | | |
| O(7)-H(1)...O(14) | 0.64(5) | 2.14(5) | 2.770(5) | 167(7) | 3/2-x, -1/2+y, 3/2-z |
| O(7)-H(4)...O(12) | 0.91(9) | 1.83(9) | 2.742(5) | 177(9) | x, y, z |
| O(3)-H(6)...O(10) | 0.82(5) | 1.88(5) | 2.692(5) | 177(9) | x, y, z |
| O(3)-H(7)...O(9) | 0.82(5) | 1.99(5) | 2.719(5) | 150(5) | 3/2-x, 1/2+y, 5/2-z |
| C(3)-H(3C)...O(13) | 0.96 | 2.45 | 3.317(8) | 150 | x, y, z |
| C(14)-H(14C)...O(6) | 0.96 | 2.36 | 3.237(6) | 152 | 2-x, 1-y, 2-z |
| C(16)-H(16B)...O(14) | 0.97 | 2.56 | 3.419(5) | 147 | 3/2-x, -1/2+y, 3/2-z |
| C(17)-H(17C)...O(11) | 0.96 | 2.59 | 3.514(8) | 161 | 1/2+x, 1/2-y, -1/2+z |
| C(28)-H(28C)...O(2) | 0.96 | 2.59 | 3.238(6) | 125 | x, y, z |
| 5 | | | | | |
| C(10)-H(10A)...O(1) | 0.96 | 2.59 | 3.354(8) | 136 | x, 1+y, z |
| C(10)-H(10C)...Cl(1) | 0.96 | 2.82 | 3.752(7) | 163 | 3/2-x, 1/2+y, 3/2-z |
| C(14)-H(14A)...O(2) | 0.96 | 2.31 | 3.257(10) | 171 | 1/2+x, 1/2-y, -1/2+z |
| 6 | | | | | |
| C(6)-H(6B)...O(1) | 0.97 | 2.54 | 3.415(8) | 150 | 1-x, 1-y, 2-z |
| C(7)-H(7A)...N(2) | 0.97 | 2.61 | 2.961(9) | 101 | 2-x, 1-y, 2-z |
| C(9)-H(9B)...O(4) | 0.96 | 2.59 | 3.40(3) | 142 | 1-x, 1-y, 1-z |
| C(10)-H(10B)...O(4) | 0.96 | 2.59 | 3.34(3) | 136 | x, y, z |
| C(10)-H(10B)...O(5) | 0.96 | 2.57 | 3.451(14) | 152 | x, 1+y, z |

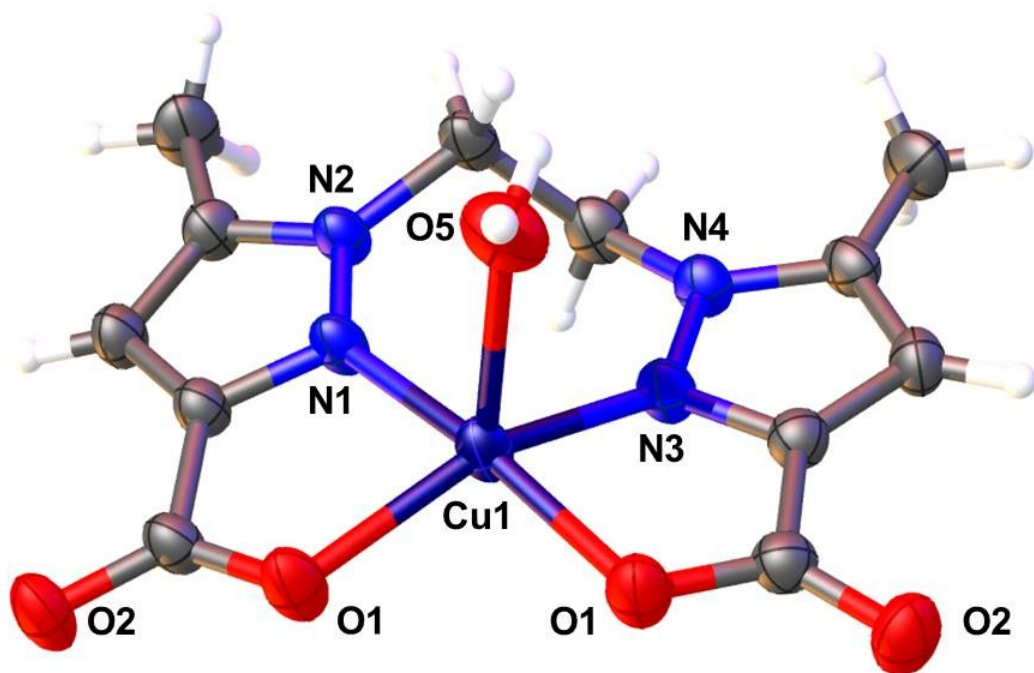


Figure S1: Crystal structure of **1**, displaying the coordination geometry of Cu(II)

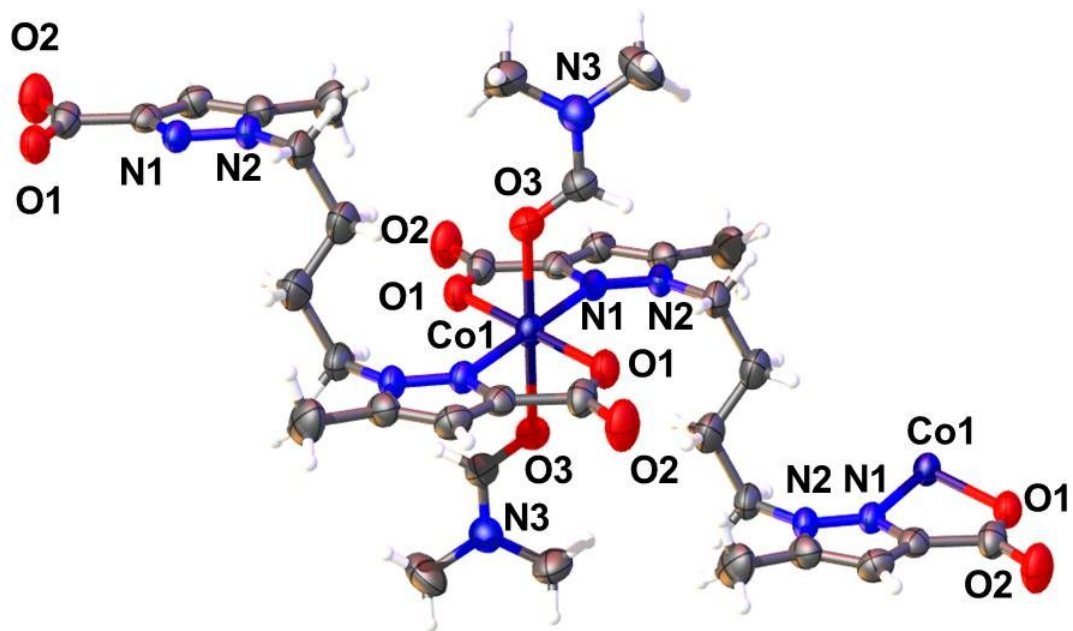


Figure S2: Crystal structure of **2**, displaying the coordination geometry of Co(II)

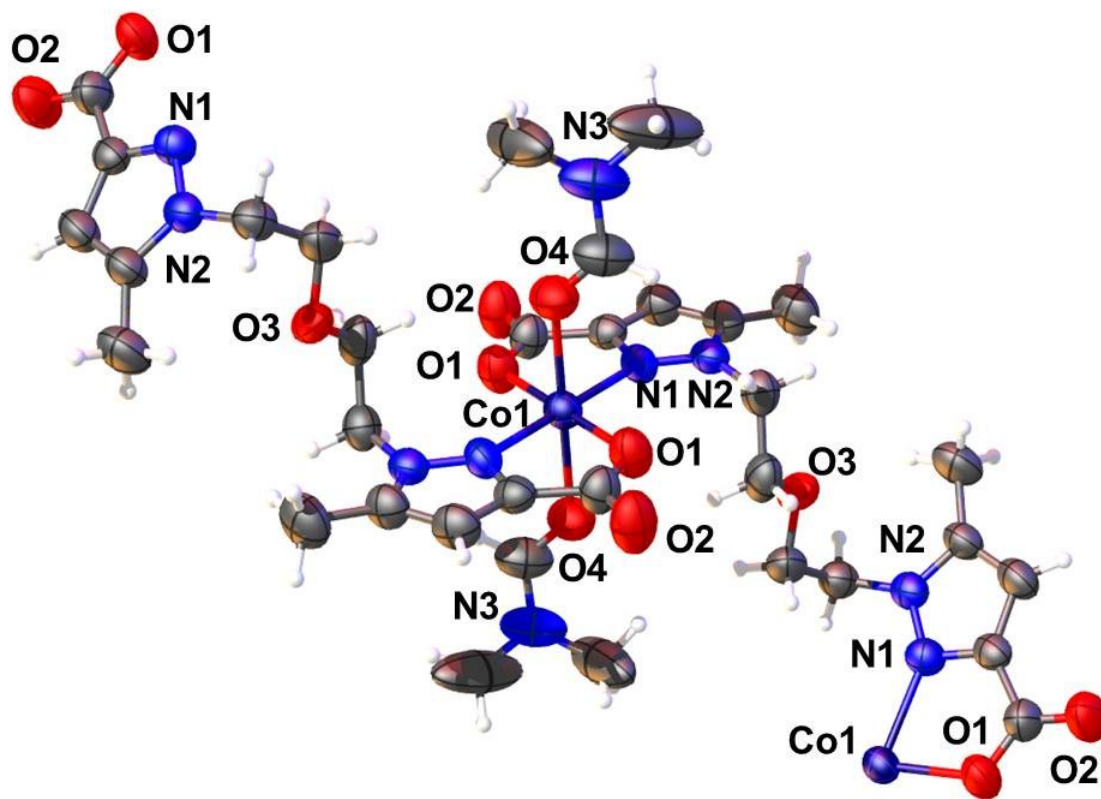


Figure S3: Crystal structure of 3, displaying the coordination geometry of Co(II)

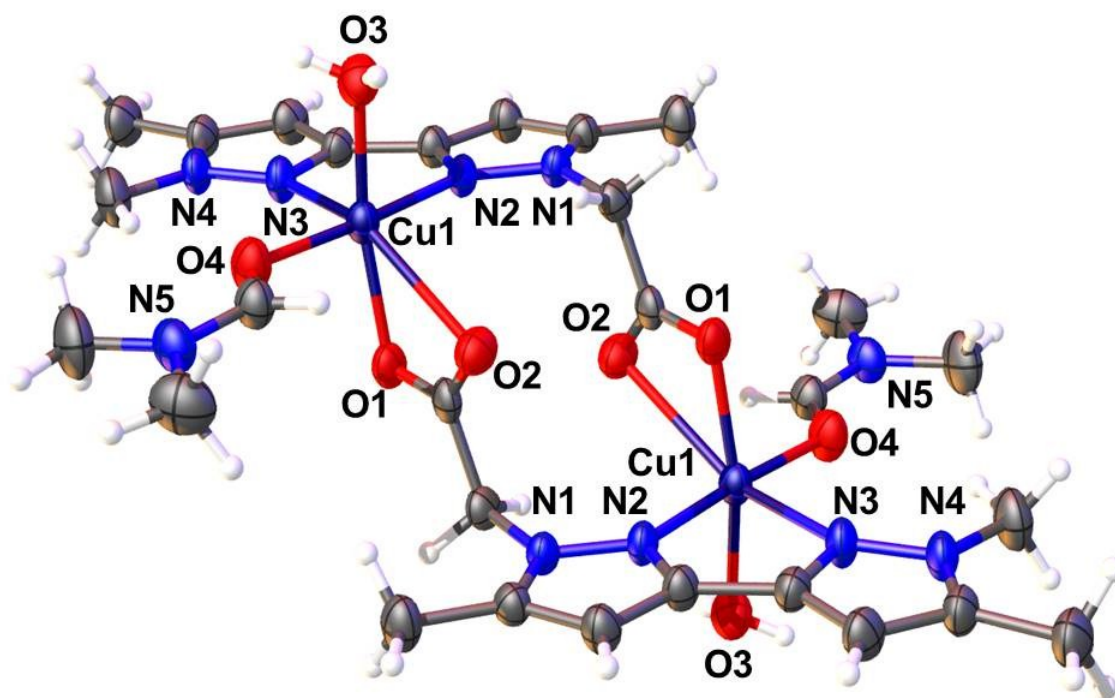


Figure S4: Crystal structure of 4, displaying the coordination geometry of Cu(II)

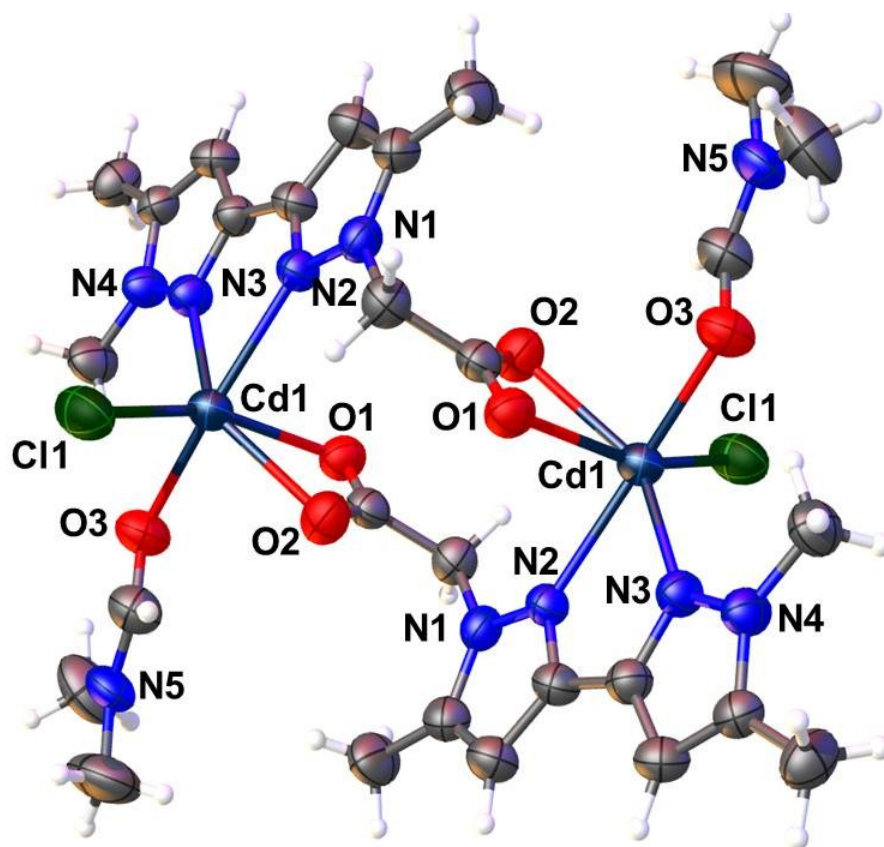


Figure S5: Crystal structure of **5**, displaying the coordination geometry of Cd(II)

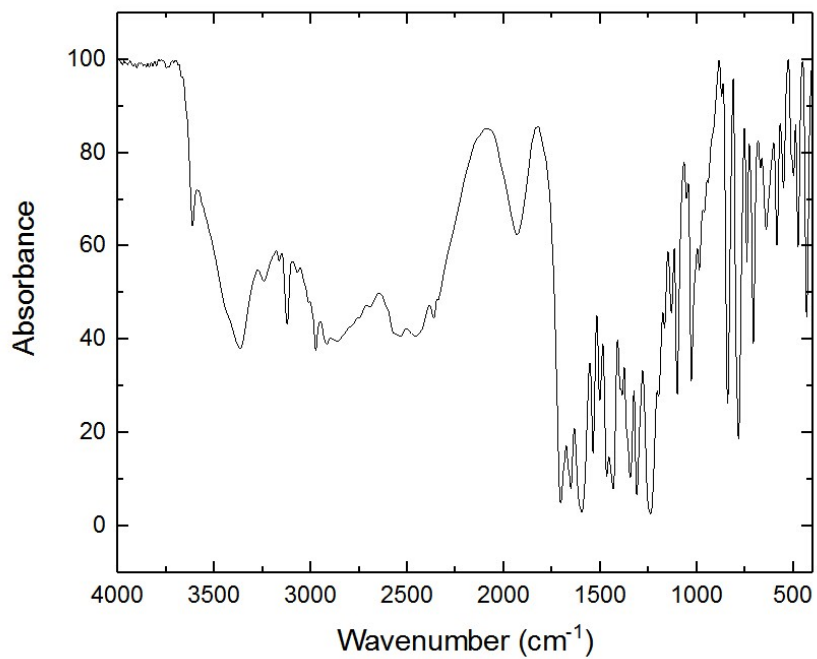


Figure S6: FT-IR data of complex 1.

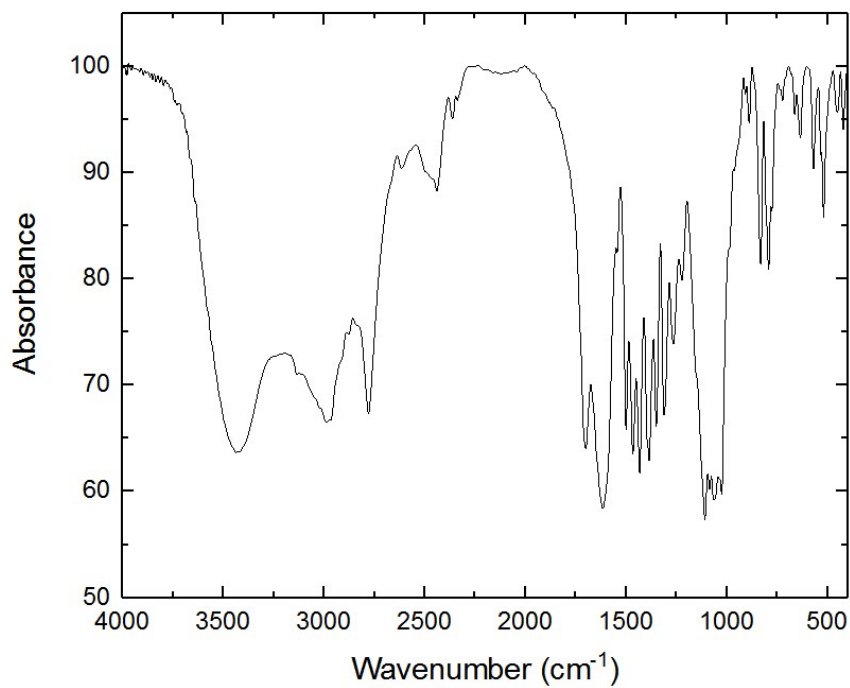


Figure S7: FT-IR data of complex 2.

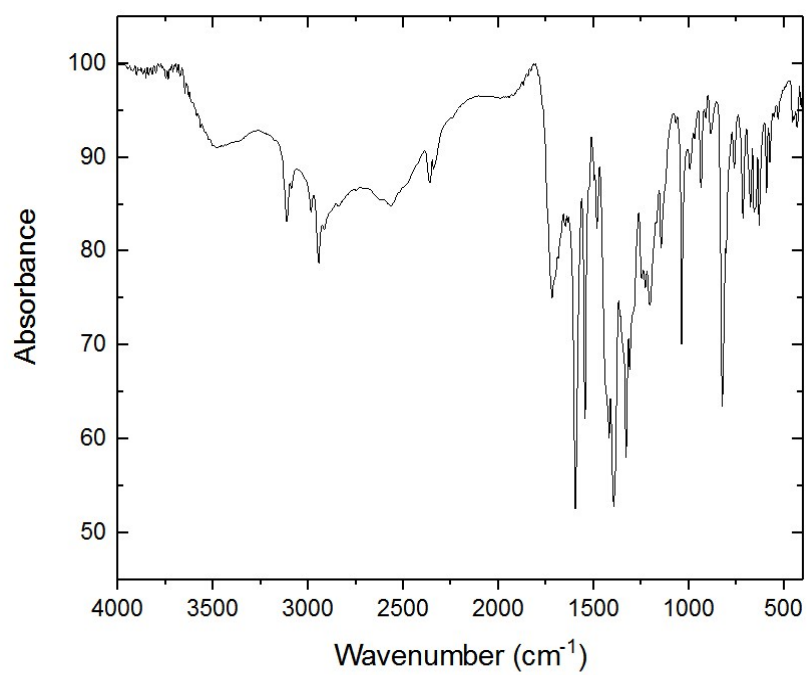


Figure S8: FT-IR data of complex 3.

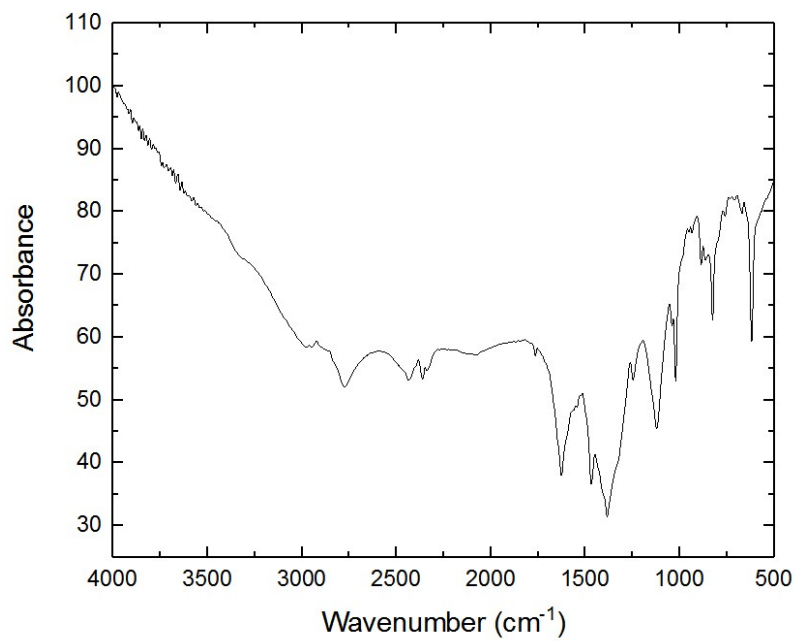


Figure S9: FT-IR data of complex 4.



Figure S10: FT-IR data of complex **5**.