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New iron tetrazolate frameworks: synthesis temperature effect, thermal behavior, Mössbauer and magnetic studies

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SUPPLEMENTARY INFORMATION

Table S1. Atomic coordinates and equivalent ADP of [Hdma]·(Fe₅F₈(H₂O)₂(amtetraz)₄) (1)

| Atom | Wyckoff position | τ | x | y | z | $B_{eq}(\text{\AA}^2)$ |
|------------|------------------|---------|-------------|------------|------------|------------------------|
| Fe(1) | 1d | 1 | ½ | 0 | 0 | 3,34(8) |
| Fe(2) | 1a | 1 | 0 | 0 | 0 | 3,24(8) |
| Fe(3) | 2l | 1 | ½ | 0.36593(9) | ½ | 1,83(3) |
| Fe(4) | 1f | 1 | 0 | ½ | ½ | 2,16(5) |
| F(1) | 2m | 1 | 0.190(2) | 0 | -0.1361(7) | 3,1(2) |
| F(2) | 4o | 1 | 0.2041(9) | 0.3842(4) | 0.5206(12) | 5,1(2) |
| F(3)/OW(3) | 2n | 0.5/0.5 | 0.587(2) | ½ | 0.6606(9) | 3,5(2) |
| F(4)/OW(4) | 2n | 0.5/0.5 | 0.044(2) | ½ | 0.7241(12) | 5,9(4) |
| N(1) | 4o | 1 | 0.209(2) | 0.1248(7) | 0.1406(12) | 4,3(4) |
| N(2) | 4o | 1 | 0.418(2) | 0.1234(7) | 0.1468(10) | 4,7(3) |
| N(3) | 4o | 1 | 0.522(2) | 0.1964(7) | 0.2489(11) | 4,3(3) |
| N(4) | 4o | 1 | 0.399(2) | 0.2479(4) | 0.3127(8) | 3,6(2) |
| N(5) | 4o | 1 | -0.0029(16) | 0.2336(8) | 0.2700(16) | 5,6(3) |
| C(1) | 4o | 1 | 0.204(2) | 0.2018(8) | 0.2425(12) | 3,9(3) |
| C(1)A | 2j | 0.5 | ½ | 0.401(3) | 0 | 3,5(6) |
| N(1)A | 2n | 0.25 | 0.457(8) | ½ | -0.107(6) | 2,8(9) |
| C(2)A | 2m | 0.50 | 0.185(3) | 0 | -0.503(4) | 2,1(3) |
| N(2)A | 4o | 0.125 | 0.003(11) | 0.044(4) | -0.446(6) | 2,4(9) |

Table S2. Atomic coordinates and equivalent ADP of [Hdma]_{11.5}·(Fe₅F₇(H₂O)(HCOO)(amtetraz)₄) (2)

| Atom | Wyckoff position | τ | x | y | z | $B_{eq}(\text{\AA}^2)$ |
|------------|------------------|-----------|-------------|-------------|------------|------------------------|
| Fe(1) | 1d | 1 | ½ | 0 | 0 | 1,24(2) |
| Fe(2) | 1a | 1 | 0 | 0 | 0 | 1,11(2) |
| Fe(3) | 2l | 1 | ½ | 0.36653(6) | ½ | 1,29(2) |
| Fe(4) | 1f | 1 | 0 | ½ | ½ | 1,46(2) |
| F(1) | 2m | 1 | 0.8042(5) | 0 | 0.1388(4) | 1,76(6) |
| F(2) | 4o | 1 | 0.2183(4) | 0.38055(18) | 0.5425(3) | 2,16(4) |
| F(3)/OW(3) | 2n | 0.25/0.75 | 0.6061(6) | ½ | 0.6660(5) | 2,03(6) |
| F(4)/OW(4) | 2n | 0.25/0.75 | -0.0035(8) | ½ | 0.2577(5) | 3,53(9) |
| N(1) | 4o | 1 | 0.7972(5) | 0.1250(3) | 0.8589(4) | 1,64(6) |
| N(2) | 4o | 1 | 0.5890(5) | 0.1212(3) | 0.8501(4) | 1,65(6) |
| N(3) | 4o | 1 | 0.4812(5) | 0.1927(3) | 0.7506(4) | 1,84(6) |
| N(4) | 4o | 1 | 0.6162(5) | 0.2471(3) | 0.6892(4) | 1,60(6) |
| C(1) | 4o | 1 | 0.8082(6) | 0.2050(3) | 0.7593(5) | 1,76(6) |
| N(5) | 4o | 1 | 0.9897(6) | 0.2360(4) | 0.7306(6) | 4,1(2) |
| C(4) | 2n | 0.50 | 0.176(2) | ½ | 0.2290(18) | 3,4(3) |
| C(1)A | 2j | 0.75 | ½ | 0.4010(7) | 0 | 3,9(3) |
| N(1)A | 2n | 0.375 | 0.437(2) | ½ | 0.9086(17) | 2,8(3) |
| C(2)A | 2m | 0.75 | -0.1875(16) | 0 | 0.5031(11) | 3,6(3) |
| N(2)A | 4o | 0.1875 | -0.050(4) | -0.0477(18) | 0.460(2) | 3,5(5) |

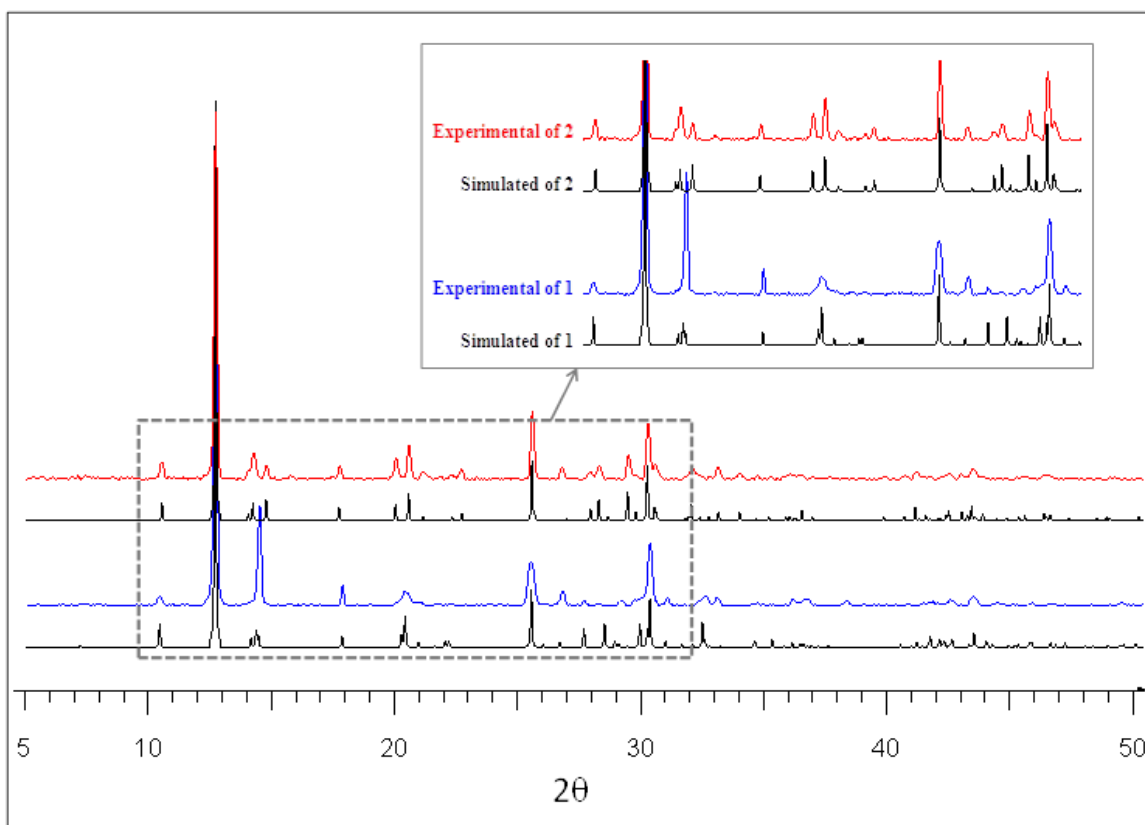


Figure S1. Experimental and simulated XRD patterns of $[\text{Hdma}] \cdot (\text{Fe}_5\text{F}_8(\text{H}_2\text{O})_2(\text{amtetraz})_4)$ (1) and $[\text{Hdma}]_{1.5} \cdot (\text{Fe}_5\text{F}_7(\text{H}_2\text{O})(\text{HCOO})(\text{amtetraz})_4)$ (2)

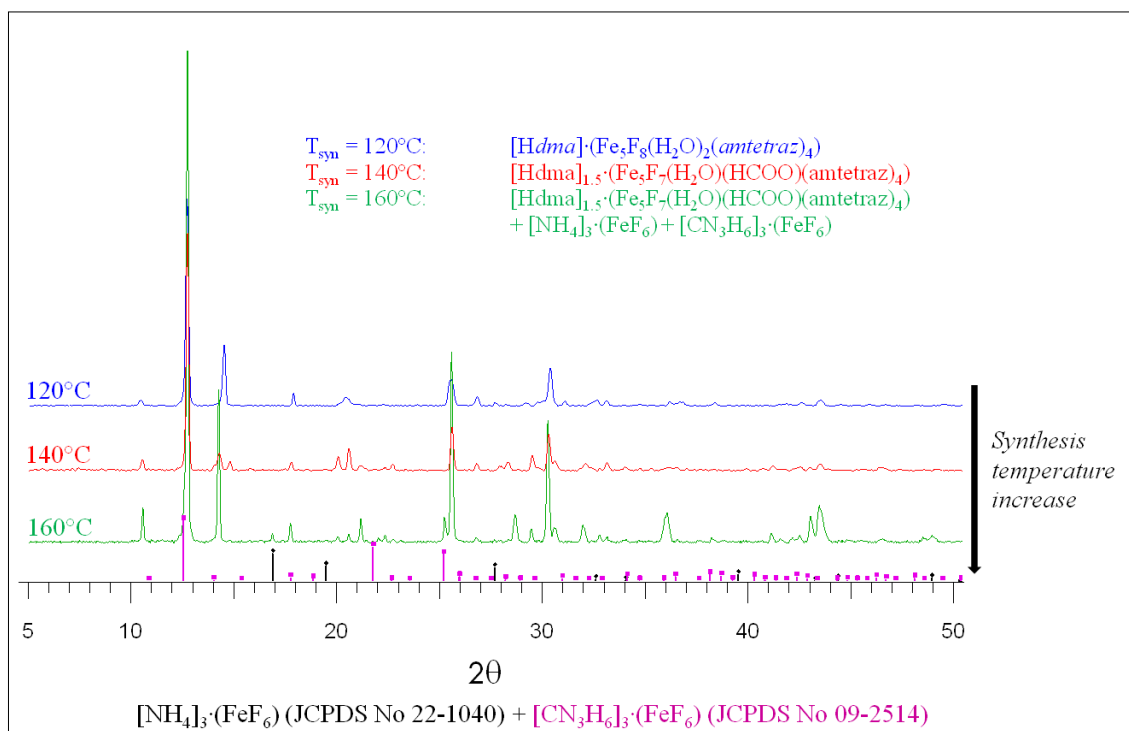


Figure S2. Evolution of XRD patterns and phase composition as a function of the synthesis temperature

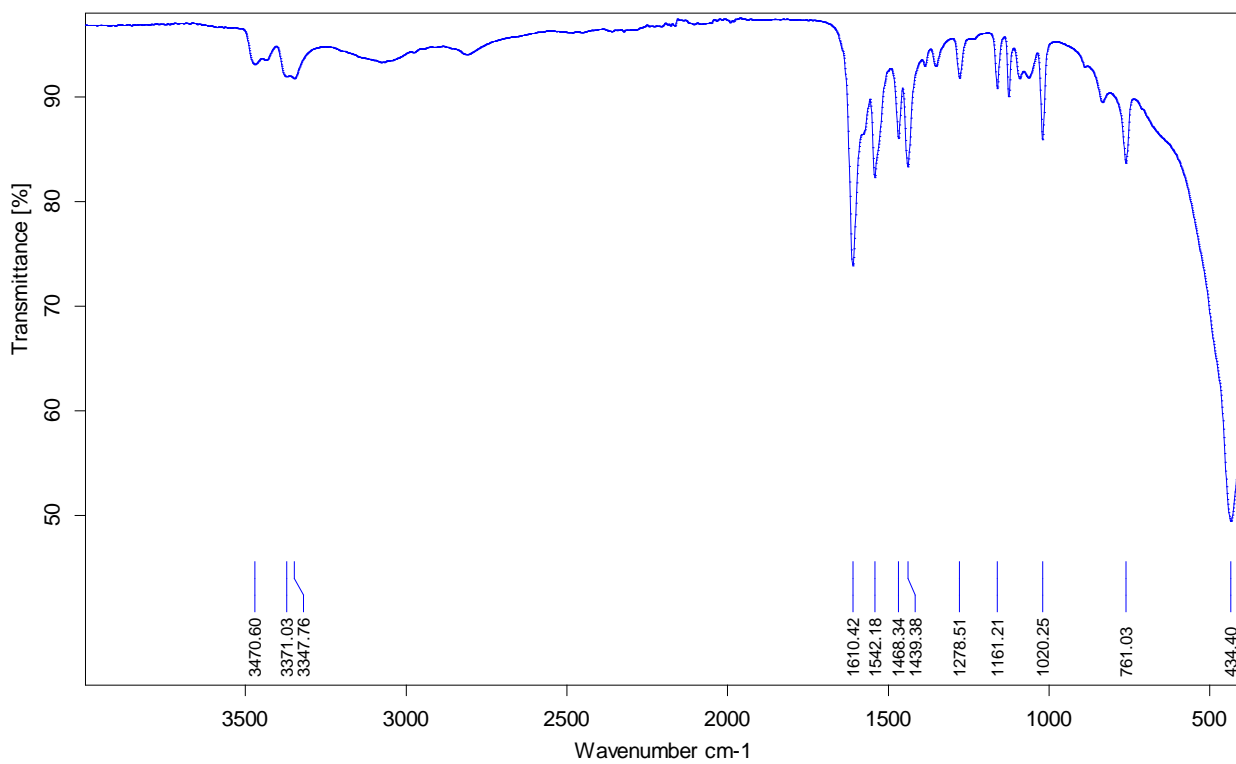


Figure S3. Infrared spectroscopy of $[Hdma] \cdot (Fe_5F_8(H_2O)_2(amtetraz)_4)$ (1)

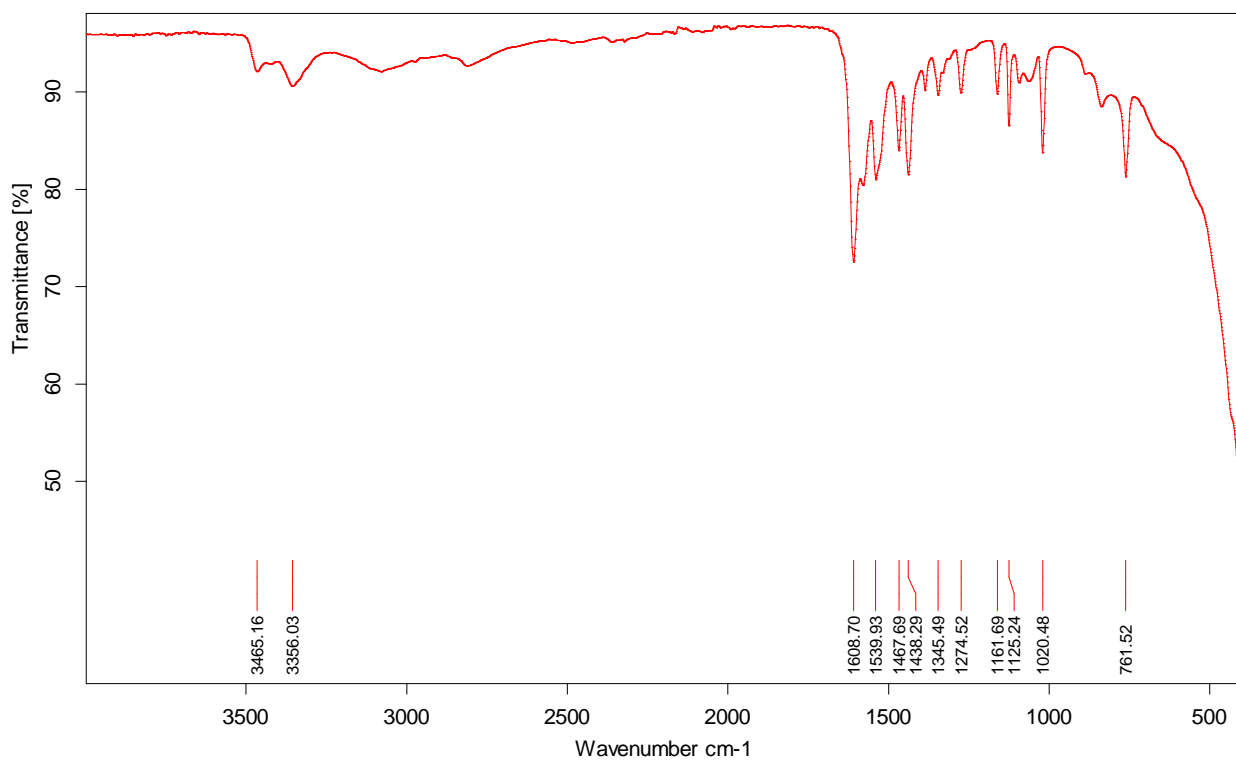


Figure S4. Infrared spectroscopy of $[Hdma]_{1.5} \cdot (Fe_5F_7(H_2O)(HCOO)(amtetraz)_4)$ (2)