



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

Vanessa Pimenta, Quang Hoang Hanh Le, Lucy Clark, Jérôme Lhoste, Annie Hémon-Ribaud, Marc Leblanc, Jean-Marc Greneche, Gilles Dujardin, Philip Lightfoot, Vincent Maisonneuve

► To cite this version:

Vanessa Pimenta, Quang Hoang Hanh Le, Lucy Clark, Jérôme Lhoste, Annie Hémon-Ribaud, et al.. New iron tetrazolate frameworks: synthesis, temperature effect, thermal behaviour, Mössbauer and magnetic studies. Dalton Transactions, 2015, 44 (17), pp.7951 - 7959. 10.1039/c5dt00281h . hal-01905643

HAL Id: hal-01905643

<https://univ-lemans.hal.science/hal-01905643>

Submitted on 30 Jan 2024

HAL is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

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

Vanessa Pimenta,^a Quang Hoang Hanh Le,^a Lucy Clark,^b Jérôme Lhoste,^{a,*} Annie Hémon-Ribaud,^a Marc Leblanc,^a Jean-Marc Grenèche,^a Gilles Dujardin,^a Philip Lightfoot^b and Vincent Maisonneuve.^a

^a*IMMM-UMR 6283 CNRS, LUNAM, Faculté des Sciences et Techniques, Université du Maine, Avenue Olivier Messiaen, 72085 Le Mans Cedex 9, France*

^b*School of Chemistry and EaStChem, University of St. Andrews, St. Andrews, Fife, KY16 9ST, United Kingdom*

* To whom correspondence should be addressed. E-mail: jerome.lhoste@univ-lemans.fr
Phone: (33).(0)2 43 83 33 59. Fax: (33).(0)2 43 83 35 06

SUPPLEMENTARY INFORMATION

Table S1. Atomic coordinates and equivalent ADP of [Hdma]·(Fe₃F₈(H₂O)₂(amtetraz)₄) (1)

Atom	Wyckoff position	τ	x	y	z	B _{eq} (Å ²)
Fe(1)	1d	1	$\frac{1}{2}$	0	0	3,34(8)
Fe(2)	1a	1	0	0	0	3,24(8)
Fe(3)	2l	1	$\frac{1}{2}$	0.36593(9)	$\frac{1}{2}$	1,83(3)
Fe(4)	1f	1	0	$\frac{1}{2}$	$\frac{1}{2}$	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)	$\frac{1}{2}$	0.6606(9)	3,5(2)
F(4)/OW(4)	2n	0.5/0.5	0.044(2)	$\frac{1}{2}$	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	$\frac{1}{2}$	0.401(3)	0	3,5(6)
N(1)A	2n	0.25	0.457(8)	$\frac{1}{2}$	-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]_{1.5}·(Fe₅F₇(H₂O)(HCOO)(amtetraz)₄) (2)

Atom	Wyckoff position	τ	x	y	z	B _{eq} (Å ²)
Fe(1)	1d	1	$\frac{1}{2}$	0	0	1,24(2)
Fe(2)	1a	1	0	0	0	1,11(2)
Fe(3)	2l	1	$\frac{1}{2}$	0.36653(6)	$\frac{1}{2}$	1,29(2)
Fe(4)	1f	1	0	$\frac{1}{2}$	$\frac{1}{2}$	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)	$\frac{1}{2}$	0.6660(5)	2,03(6)
F(4)/OW(4)	2n	0.25/0.75	-0.0035(8)	$\frac{1}{2}$	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)	$\frac{1}{2}$	0.2290(18)	3,4(3)
C(1)A	2j	0.75	$\frac{1}{2}$	0.4010(7)	0	3,9(3)
N(1)A	2n	0.375	0.437(2)	$\frac{1}{2}$	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)

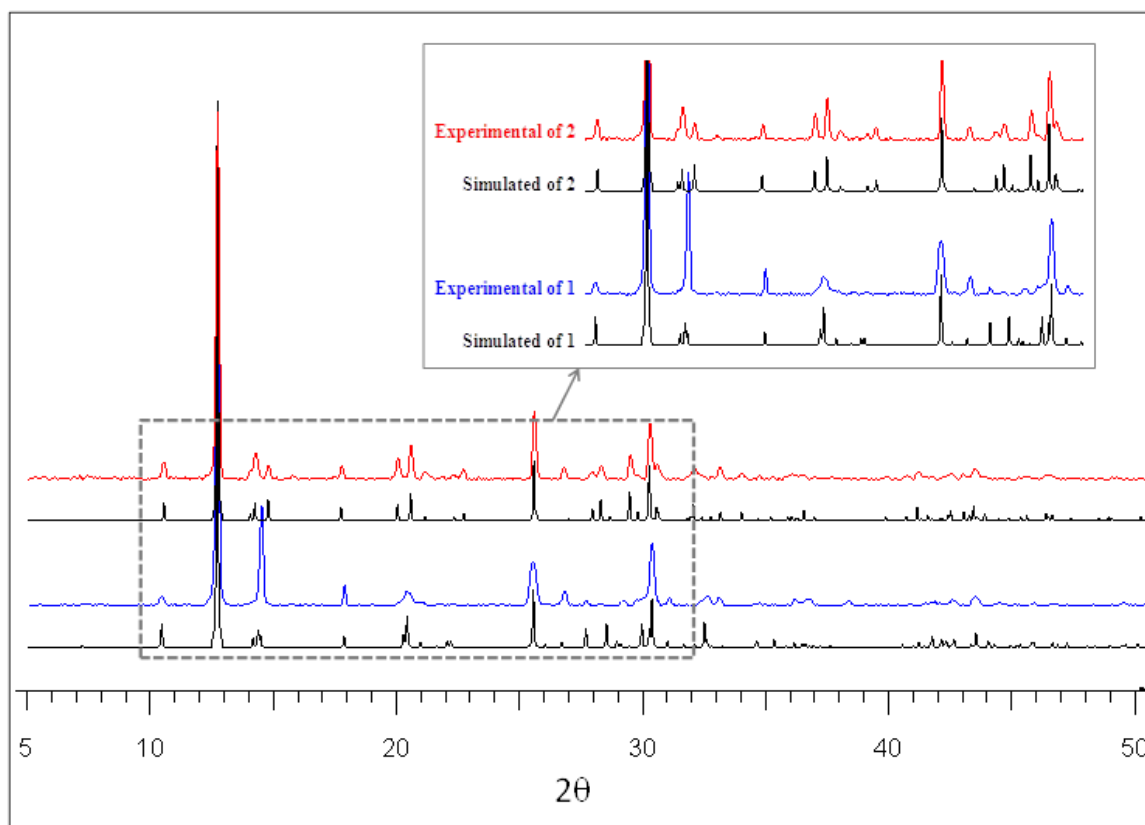


Figure S1. Experimental and simulated XRD patterns of $[\text{Hdma}] \cdot (\text{Fe}_5\text{F}_8(\text{H}_2\text{O})_2(\text{amtetraz})_4)$ (1) and $[\text{Hdma}]_{1.5} \cdot (\text{Fe}_5\text{F}_7(\text{H}_2\text{O})(\text{HCOO})(\text{amtetraz})_4)$ (2)

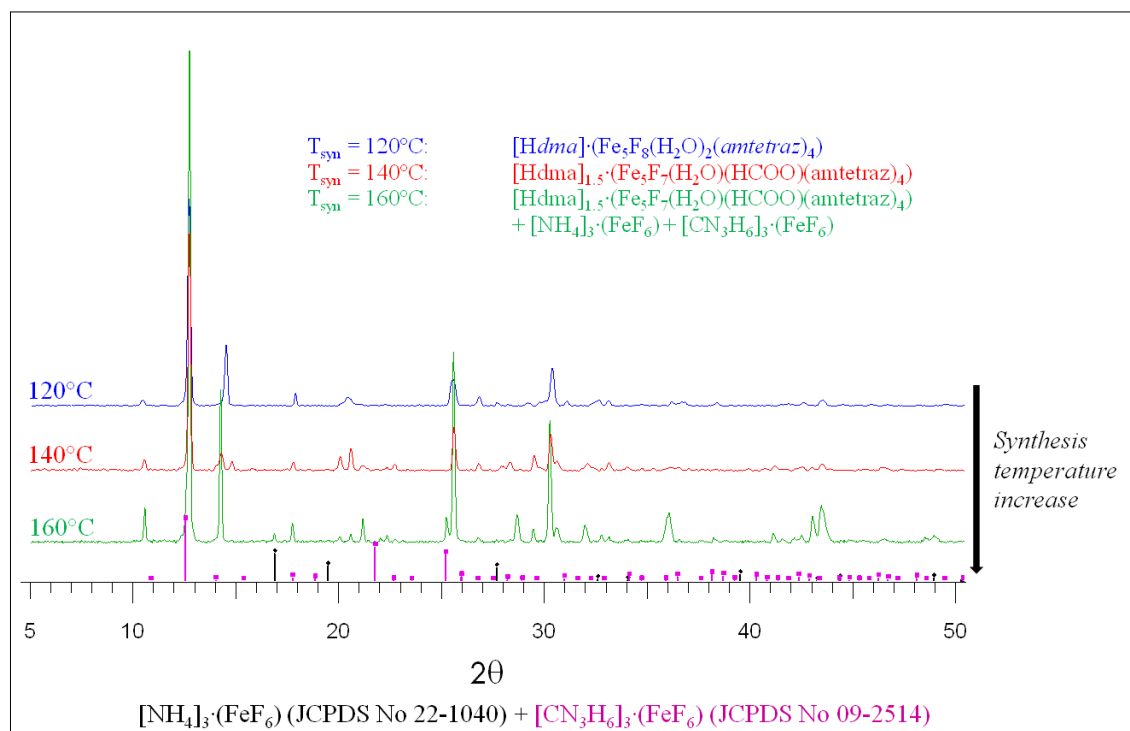


Figure S2. Evolution of XRD patterns and phase composition as a function of the synthesis temperature

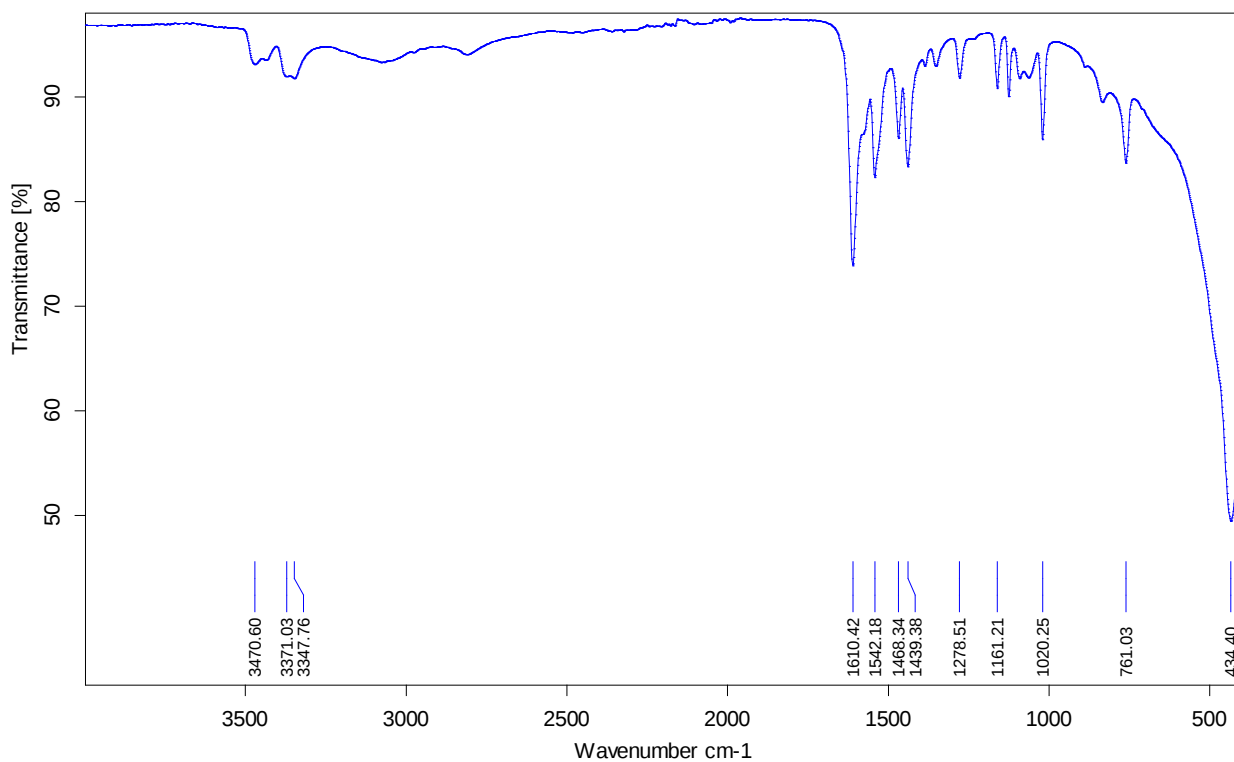


Figure S3. Infrared spectroscopy of [Hdma]·(Fe₅F₈(H₂O)₂(amtetraz)₄) (1)

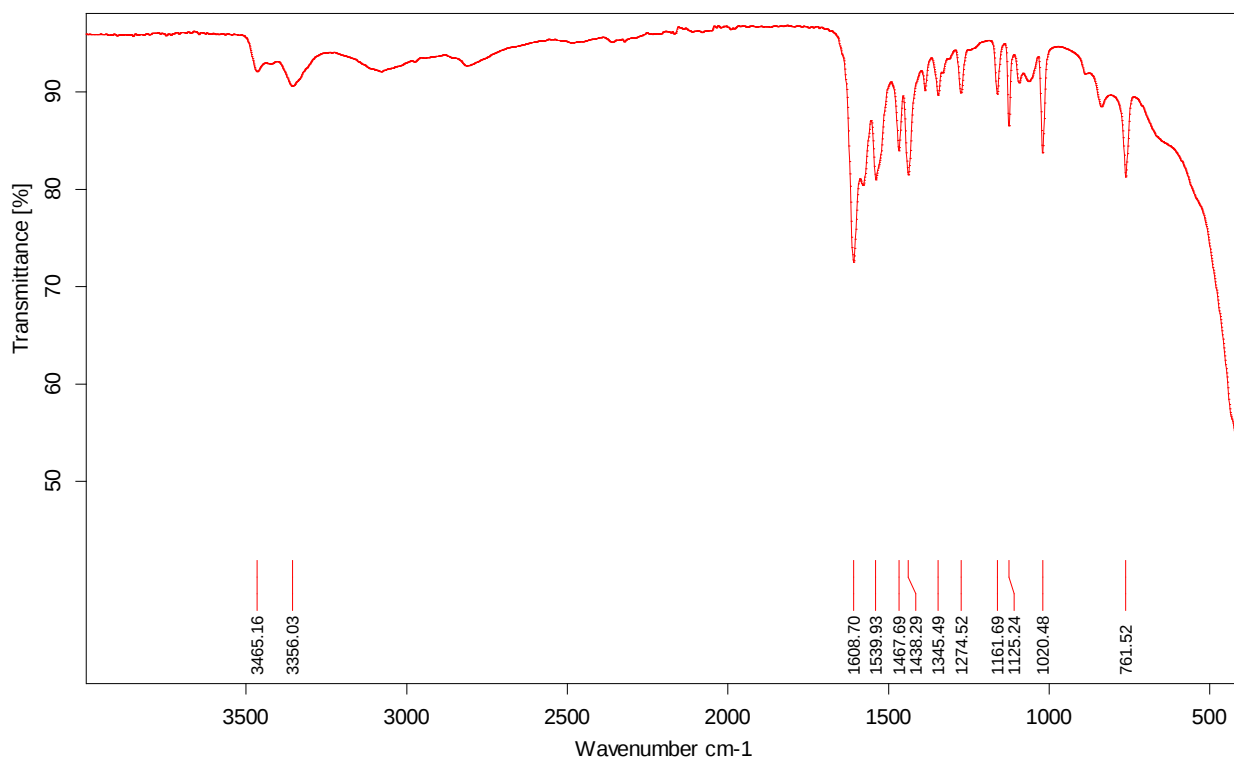


Figure S4. Infrared spectroscopy of [Hdma]_{1.5}·(Fe₅F₇(H₂O)(HCOO)(amtetraz)₄) (2)