

Supporting Information

Synthesis and characterization of CuFeO_2 delafossite type inorganic wires using Fe and Cu single source molecular precursors

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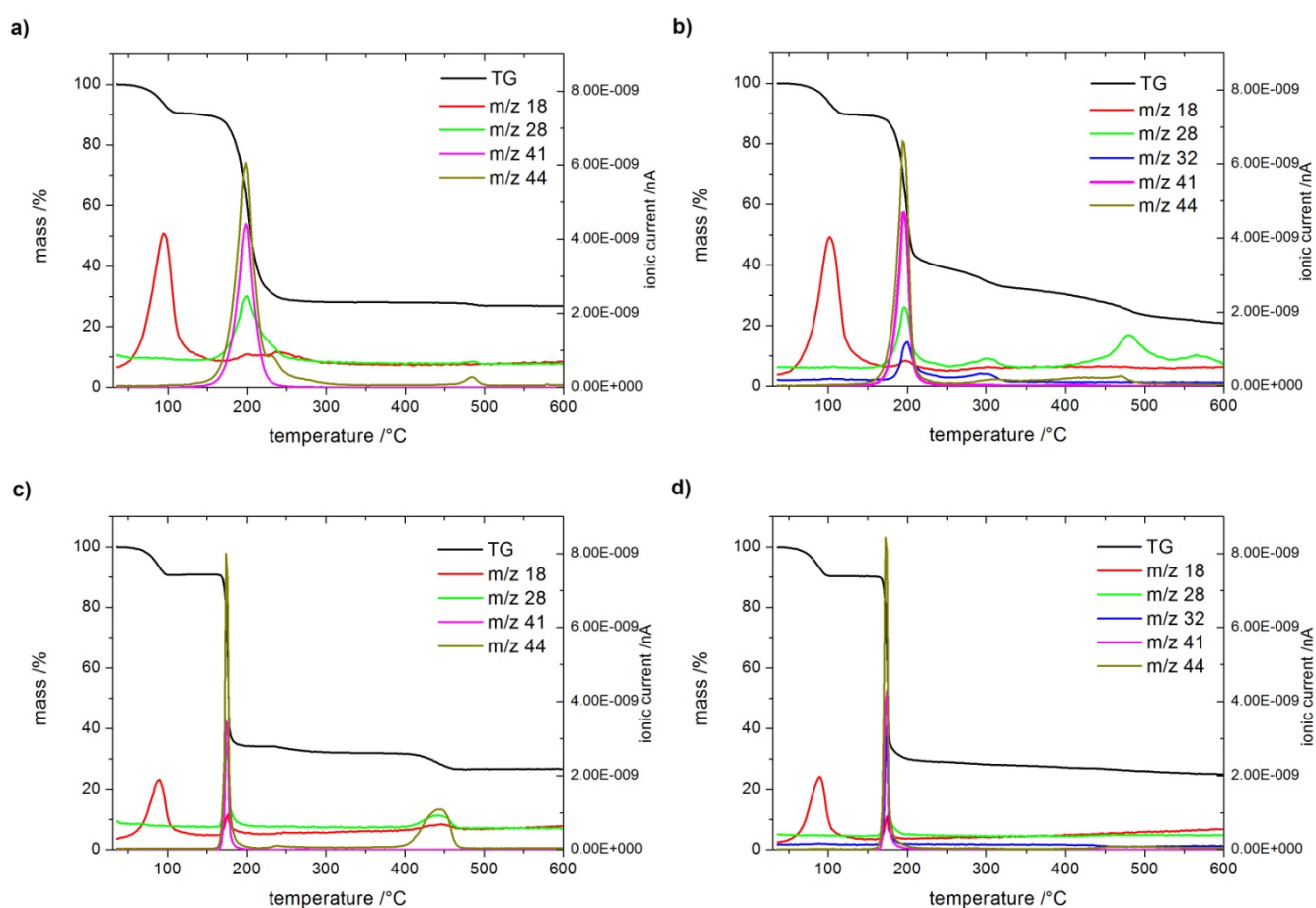


Figure S1. TG-coupled MS of di[2-(methoxyimino)propanoato]iron **1** in (a) oxygen and (b) helium and di[2-(methoxyimino)propanoato]copper **2** in (c) oxygen and (d) helium.

Table S1. Crystal data and structure refinement.

Compound	1	2
Empirical formula	C ₈ H ₁₆ Fe N ₂ O ₈	C ₈ H ₁₆ Cu N ₂ O ₈
Color	Yellow	light blue
Formula weight	324.08 g mol ⁻¹	331.77 g mol ⁻¹
Temperature	100 K	299 K
Wavelength	0.71073 Å	0.71073 Å
Crystal system	Monoclinic	Triclinic
Space group	P 2 ₁ /c, (no. 14)	P $\bar{1}$ (no. 2)
Unit cell dimensions		
a	10.0654(12) Å	6.109(1) Å
b	8.9084(10) Å	7.008(1) Å
c	7.2243(9) Å	9.152(2) Å
α		102.02(2)°
β	98.313(2)°	95.06(1)°
γ		112.48(2)°
Volume	640.97(13) Å ³	347.94(11) Å ³
Z	2	1
Density (calculated)	1.679 Mg m ⁻³	1.583 Mg m ⁻³
Absorption coefficient	1.214 mm ⁻¹	1.604 mm ⁻¹
F(000)	336 e	171 e
Crystal size	0.30 x 0.23 x 0.05 mm ³	0.30 x 0.20 x 0.06 mm ³
θ range for data collection	3.07 to 33.46°	3.26 to 26.36°
Index ranges	-15 ≤ h ≤ 15, -13 ≤ k ≤ 13, -11 ≤ l ≤ 11	-7 ≤ h ≤ 7, -7 ≤ k ≤ 8, -9 ≤ l ≤ 11
Reflections collected	20811	2162
Independent reflections	2508 [R _{int} = 0.013]	1422 [R _{int} = 0.012]
Reflections with I > 2σ(I)	2400	1371
Completeness to $\theta = 27.50^\circ$	99.9 %	99.7 %
Absorption correction	Gaussian	Multi-scan
Max. and min. transmission	0.94204, 0.71359	0.9099, 0.6447
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	2508 / 1 / 96	1422 / 2 / 94
Goodness-of-fit on F ²	1.093	1.078
Final R indices		
[I > 2σ(I)] R ₁ , wR ²	0.019, 0.053	0.03, 0.08
(all data) R ₁ , wR ²	0.02, 0.053	0.032, 0.082
Largest diff. peak and hole	0.5, -0.5 e Å ⁻³	0.4, -0.3 e Å ⁻³