SMARTER Crystallography of the fluorinated organic-inorganic compound $Zn_3Al_2F_{12}\cdot[HAmTAZ]_6$.

Charlotte Martineau, Amandine Cadiau, Boris Bouchevreau, Jürgen Senker, Francis Taulelle, Karim Adil

Electronic Supplementary Information

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Table 1. Conditions of single-crystal X-ray data collection and refinement parameters of $Zn_3Al_2F_{12}\cdot[HAmTAZ]_6$

Formula	C12 H24 Al2 F12 N24 Zn3
Formula weight	982.62
Crystal system, space group	Hexagonal, R -3
a	12.5761(5) 17.6463(9)
Volume, Z	2417.0(2), 3
Crystal size	0.24 x 0.14 x 0.08 mm
2Theta range (°)	5.94 to 55 deg.
Reflections collected / unique	4706 / 1037
Max. and min. transmission	0.7454, 0.6462
Data / restraints / parameters	1037 / 0 / 84
Goodness-of-fit	1.083
Final R indices [I>2sigma(I)]	R1 = 0.0216, wR2 = 0.0583
R indices (all data)	R1 = 0.0233, wR2 = 0.0593
Largest diff. peak and hole	0.331 and -0.373 $e.^{-3}$
CCDC number	863484

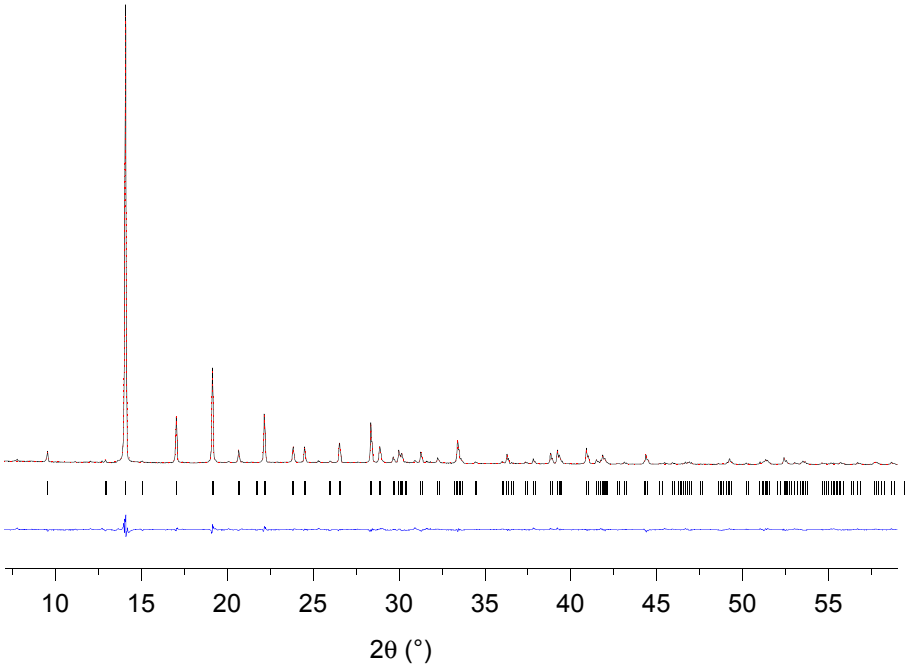

Fig. 1. Experimental (dark line) and calculated (red dots) XRPD diagram of $Zn_3Al_2F_{12}$·[HAmTAZ]$_6$ in the 9-40° 2θ region. The Bragg positions (black ticks) and the difference between experimental and calculated data (blue line) are shown below.

File 1. Instruction file for the space group determination of $Zn_3Al_2F_{12}$·[HAmTAZ]$_6$. The program used to run the calculation is available upon request to the corresponding author.

```
! Nuclei labels (on each line all data must be separated only by spaces)
Al F H C Zn
! Stoichiometric coefficients of precedent nuclei
2 12 24 12 3
! Crystal System Code ! Z Code ! Molar Mass (opt) ! Density (opt) ! Needed Cell Parameters (opt)
5 3
! Relative intensities of the different NMR lines (1 line per nucleus)
1
1 1
1 1 1 1
1 1
```

```
1 2
! Symetry Code of each precedent line (1 line per nucleus)
1
1 1
1 1 1 1
1 1
1 1


! Codes Information
!
! Crystal System Code (and optionally needed cell parameters if Z=0)
! 1 Triclinic ; a b c alpha beta gamma
! 2 Monoclinic (b or c unique) ;  a b c beta/gamma
! 3 Orthorhombic ; a b c
! 4 Tetragonal ; a c
! 5 Trigonal-h (hexagonal axes) ; a c
! 6 Trigonal-r (rhombohedral axes) ; a alpha
! 7 Hexagonal ; a c
! 8 Cubic ; a
!
! Z Code
! Z if known
! 0 if unknown but if Molar Mass, Density and Cell Parameters are known => the Z will be calculated.
! any negative number if unknown. Several Z values will be tried.
!
! Symetry Code
! 0 if eta=0
! 1 in all other cases
```

File 2. Output file for the space group determination of $Zn_3Al_2F_{12}$·[HAmTAZ]$_6$. The program used to run the calculation is available upon request to the corresponding author.

```
For Z=3,
(Partial) Chemical Formula : Al2F12H24C12Zn3
(Partial) Crystallochemical Formula : Al6F18F18H18H18H18H18C18C18Zn3Zn6
3 possible space groups :
R-3 (148)
R32 (155)
R-3m (166)
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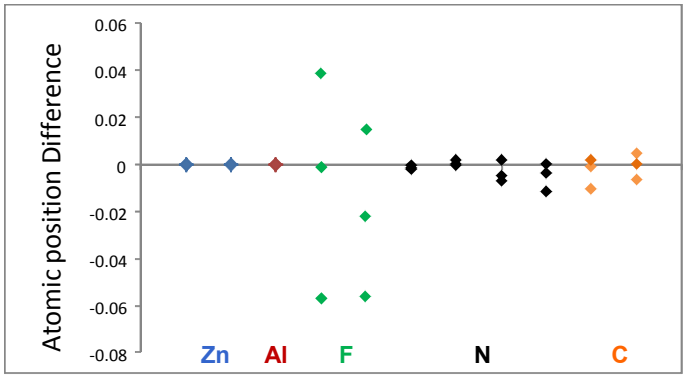

Fig. 2. Differences between the fractional atomic positions of the DFT-optimized structure and the model determined from single-crystal X-ray diffraction in $Zn_3Al_2F_{12}$·$[HAmTAZ]_6$.