CRYSTAL STRUCTURE OF NEW TERNARY COMPOUND $La_3Fe_{6.36}Zn_{29.64}$

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Introduction

Investigation of the La–Fe–Zn phase diagram in a region with high concentration of zinc has revealed a new compound with tetragonal symmetry and ~$LaFe_2Zn_{10}$ composition which may be interesting in terms of magnetic and hydrogen sorption properties.

Experimental

A sample for investigation was synthesized by direct reaction of metals in evacuated fused-silica ampoules heated to 900 °C and slowly cooled to 500 °C, than annealed at this temperature for 2 weeks and quenched in cold water. The crystal structure of the compound was investigated by single crystal X-ray diffraction (Bruker PLATFORM/SMART APEX II CCD diffractometer; Mo $K\alpha$-radiation, ω-scan, $2.46 < \theta < 26.33^{o}$). A structure solution by direct methods and refinement using full-matrix

least-squares refinements on F^2 were carried out using SHELXS-97 and SHELXL-97 [1, 2] program packages, respectively.

Results and Discussion

The title compound crystallizes in a derivate from the Ce_3Zn_{22}-type structure (Fig.) (space group $I4_1/amd$, Pearson code $tI144$) with lattice parameters $a = 8.9777(2)$ Å, $c = 21.4820(8)$ Å, $V = 1731.43(8)$ Å^3, ($R_1 = 0.0611$, $wR_2 = 0.124$) (Tab. 1, 2). Two split positions Zn1/Fe1 and Zn2/Fe2 are distinguishing feature of this structure. It should be noted that this compound is disordered derivate of the hexagonal $CaCu_5$-type (space group $P6/mmm$) as well as other Zn-rich ternary phases which often crystallize in different derivatives of this structure type such as Th_2Ni_{17}, Th_2Zn_{17}, $Ce_2Ge_3Zn_6$, $Gd_2Co_3Zn_{14}$ etc.

Table 1. Crystallographic data for $La_3Fe_{6.36}Zn_{29.64}$

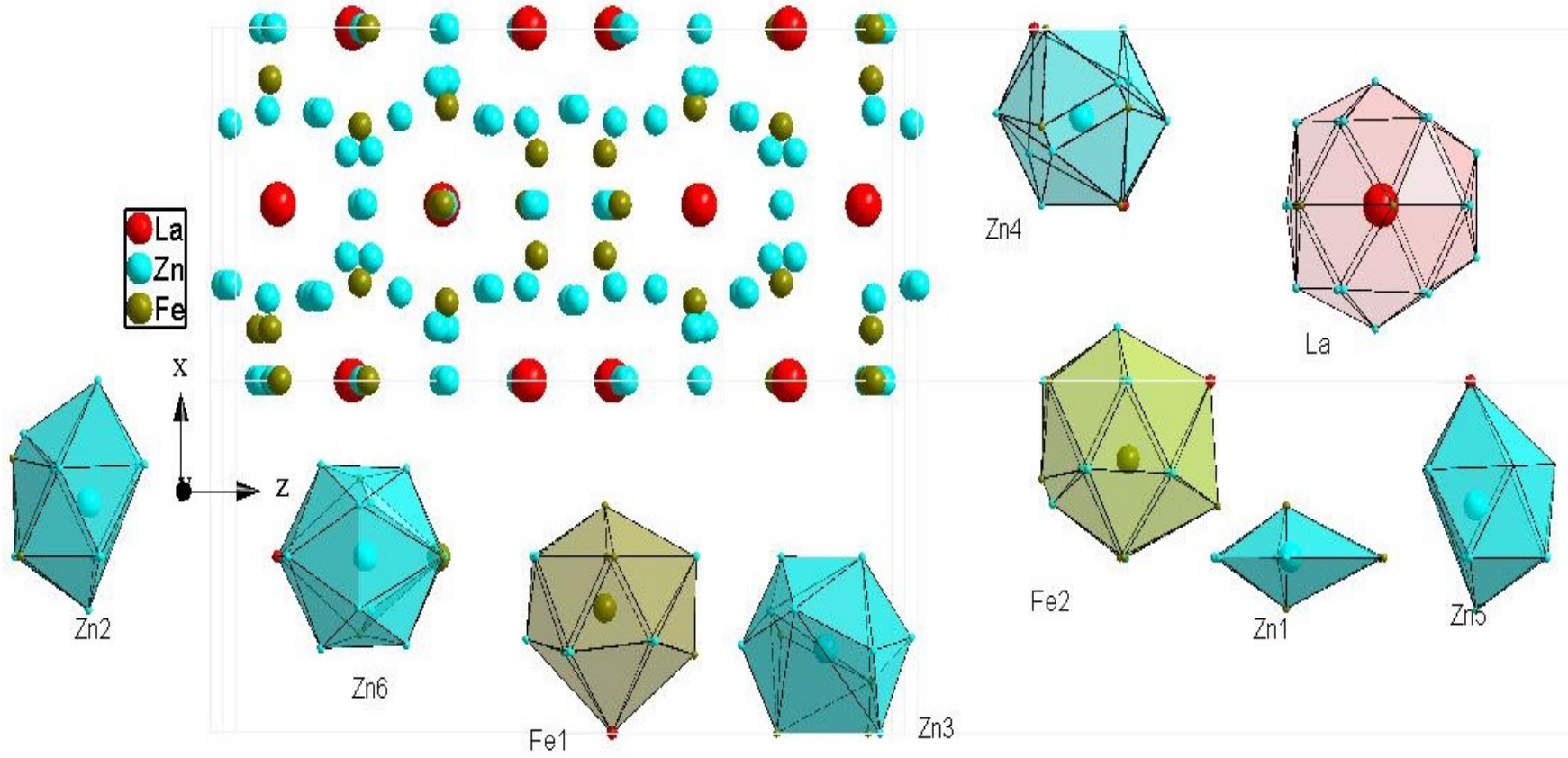
Formula	$La_3Fe_{6.36}Zn_{29.64}$
Temperature, K	296(2)
Space group	$I4_1/amd$
Pearson symbol	$tI144$
Lattice parameters	
a, Å	8.9777(2)
c, Å	21.4820(8)
V, Å^3	1731.43(8)
Calculated density, ρ (g/cm^3)	6.755
Absorption coefficient, μ (mm^{-1})	33.995
Radiation	Mo $K\alpha$, λ = 0, 71073 Å
Monochromator	graphite
Θ range for data collection (degrees)	2.46÷26.33
Total number of reflections	21235

Number of unique reflections	506
Number of reflections ($I_o > 2\sigma(I_o)$)	470
Number of parameters	40
Restrictions	$I_o > 2\sigma(I_o)$
Weighing scheme	$w = 1/[\sigma^2(F_o^2) + (0.0868P)^2 + 1531.20P]$, where $P = (\max F_o^2, 0) + 2 \cdot F_c^2)/3$
Extinction coefficient	0.0012(3)
R_P	0.0611
wR	0.1240
Goodness of fit, S	1.179
$\Delta\rho_{max}$(e·Å^{-3})	2.34
$\Delta\rho_{min}$(e·Å^{-3})	-2.32

Table 2. Atomic coordinates and isotropic displacement parameters for $La_3Fe_{6.36}Zn_{29.64}$

Atom	**Site**	**Occupation**	***x***	***y***	***z***	U_{eq}, Å^2
La1	8*e*	1.0	1/2	3/4	0.06585(15)	0.010(1)
Zn1	8*e*	0.50(1)	1/2	3/4	0.3109(4)	0.0149(18)
Fe1	16*h*	0.50(1)	1/2	0.6044(14)	0.3046(6)	0.010(2)
Zn2	16*h*	0.44(1)	0.6522(16)	3/4	0.2023(6)	0.016(3)
Fe2	16*h*	0.56(1)	0	0.4722(16)	0.0635(6)	0.015(3)
Zn3	16*g*	1.0	0.2393(4)	0.5107(4)	1/8	0.013(1)
Zn4	16*f*	1.0	0.2713(7)	1/2	0	0.024(1)
Zn5	16*h*	1.0	1/2	0.3985(5)	0.0739(2)	0.010(1)
Zn6	16*h*	1.0	1/2	0.5158(6)	0.1899(2)	0.014(1)

Figure. Crystal structure of $La_3Fe_{6.36}Zn_{29.64}$ compound



References

[1] Sheldrick, G. M. (2008). Acta Cryst. A64, 112–122.

[2] Sheldrick, G. M. (2015). Acta Cryst. C71, 3–8.