Crystal structure and hydrogenation properties of the MgNi2B6 ternary compound

N. Pavlyuk[1], A. Bondaruk[2], D.Kulawik[2], W.Ciesielski[2], V. Pavlyuk1,2

[1]Department of Inorganic Chemistry, Ivan Franko National University of Lviv, Kyryla & Mefodia str. 6, 79005 Lviv, Ukraine,

[2]Jan Długosz University in Częstochowa, Institute of Chemistry, al. Armii Krajowej 13/15, 42200 Częstochowa, Poland

Email of communicating v.pavlyuk@ujd.edu.pl

The intermetallic compounds based on magnesium are widely investigated now due to their excellent hydrogen storage and electrochemical properties [1]. During the systematic study of Mg–Ni-B alloys, the tetragonal phase $MgNi_2B_6$ was detected. The $MgNi_2B_6$ ternary compound was prepared in a tantalum crucible in a resistance furnace with a thermocouple controller. The single crystal of $MgNi_2B_6$ was investigated by means of an Oxford Diffraction Xcalibur3 diffractometer with a CCD detector. The crystal structure of the $MgNi_2B_6$ compound was successfully solved by direct methods and refined in the space group *Immm* (N°71). The refined lattice parameters are *a*=3.0985(8) Å, *b*=6.5572(13) Å, *c*=8.3176(17) Å, *V*=168.99(6) Å^3. The starting atomic parameters were taken from an automatic interpretation of direct methods followed by difference Fourier syntheses using the SHELX-97 package programs [2]. Finally, all parameters are refined to *R*1 = 0.047 and *wR*2 = 0.122 using 129 independent reflections with I > 2σ(I) and presented in Table 1. The ternary boride $MgNi_2B_6$ is isostructural to $CeCr_2B_6$ [3]. Boron nets are presented in Figure 1.

The prepared $MgNi_2B_6$ sample was hydrogenated by hydrogen gas at a pressure up to 20 bar and a temperature of 623 K. Under these conditions, $MgNi_2B_6$ absorbs up to 2.4 wt% H_2.

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2) for $MgNi_2B_6$

Atoms	Sites	*x*	*y*	*z*	U_{eq}
B1	4*h*	0	0.139(3)	1/2	0.041(3)
B2	8*l*	0	0.290(1)	0.332(1)	0.034(2)
Ni	4*j*	1/2	0	0.3484(3)	0.0492(7)
Mg	2*a*	0	0	0	0.035(1)

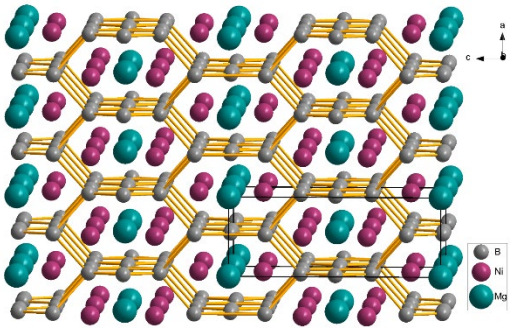

Figure 1. Boron nets in the $MgNi_2B_6$ structure

[1] Larpruenrudee, P., Bennett, N. S., Gu, Y., Fitch, R., & Islam, M. S. (2022). *Scientific Reports*, **12**(1), 13436.

[2] Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen,Germany.

[3] Kuz'ma Y.B., Svarichevskaya S.I., Fomenko V.N. *Inorg. Mater.* (1973) **9**, 1372-1374.