

Programme & The Book of Abstracts

*Twentieth Annual Conference*

# YUCOMAT 2018

Herceg Novi, Montenegro, September 3–7, 2018

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**TWENTIETH ANNUAL CONFERENCE**

# **YUCOMAT 2018**

Hunguest Hotel Sun Resort Herceg Novi, Montenegro,  
September 3-7, 2018  
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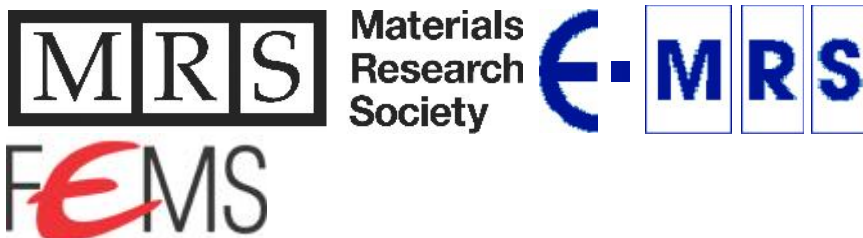
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### **Crystal structure and X-Ray spectroscopic properties of R.E.<sub>2</sub>Ni<sub>12</sub>P<sub>5</sub> compounds**

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We have studied experimentally and theoretically the electronic structure and x-ray absorption spectrum at the R.E.L3 - edge and x-ray emission spectra of Ni and P in the R.E.<sub>2</sub>Ni<sub>12</sub>P<sub>5</sub> compounds. Crystal structure of the ternary phosphate Ce<sub>2</sub>Ni<sub>12</sub>P<sub>5</sub> has been refined using X-ray powder diffraction pattern of the single phase sample with the same nominal composition, and the isotopic structure as for earlier known La<sub>2</sub>Ni<sub>12</sub>P<sub>5</sub>-type has been proved: space group P21/m, formula units Z = 2, lattice parameters are a = 1.07809(2) nm, b = 0.36869(1) nm, c = 1.31490(3) nm, b = 107.776(4), residual R-values are RI = 0.0681, RP = 0.0442, RwP = 0.0603. The theoretical calculations have been carried out by means of the ab initio fully-relativistic spin-polarized Dirac linear muffin-tin orbital method. The calculations show good agreement with the experimental measurements. R.E.LIII - absorption spectra in ternary R.E.<sub>2</sub>Ni<sub>12</sub>P<sub>5</sub> compounds were obtained at 78K and 300K using a tube spectrometer equipped with an RKD-01 co-ordinate detector. The mixed valence state of Ce and Eu was obtained in the Ce<sub>2</sub>Ni<sub>12</sub>P<sub>5</sub> and Eu<sub>2</sub>Ni<sub>12</sub>P<sub>5</sub> compounds.

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