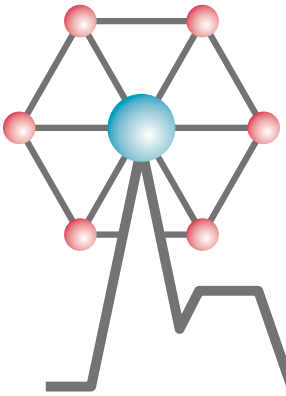
The 21st International Conference on Solid Compounds of Transition Elements



SCTE'18 VIENNA

March 25 - 29, 2018

Programme and Abstracts

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Mo-PO24

Calorimetric investigation of hydrogen interaction with $Ti_{0.9}Zr_{0.1}Mn_{1.3}V_{0.6}$

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We have investigated the hydrogen interaction with $Ti_{0.9}Zr_{0.1}Mn_{1.3}V_{0.6}$ applying the calorimeter of Tean-Calvet type connected with a Sieverts-type apparatus.

The sample $Ti_{0.9}Zr_{0.1}Mn_{1.3}V_{0.6}$ and its hydride $Ti_{0.9}Zr_{0.1}Mn_{1.3}V_{0.6}H_3$ were checked by X-ray diffraction which indicated that the starting sample was single-phase material with the hexagonal Laves phase structure C14 ($MgZn_2$) and hydride of $Ti_{0.9}Zr_{0.1}Mn_{1.3}V_{0.6}H_3$ was single phase material with the hexagonal Laves phase structure C14 ($MgZn_2$) too. The calorimetric study was carried out in the temperature range 60 - 130°C and a hydrogen pressure up to 50 atm. Absorption (desorption) partial molar enthalpy ΔHabs.(des.) was determined from the heat effect of the reaction:

$Ti_{0.9}Zr_{0.1}Mn_{1.3}V_{0.6}\ H_X + y/2\ H_2 \leftrightarrow Ti_{0.9}Zr_{0.1}Mn_{1.3}V_{0.6}\ H_{X+Y}$

$P=f(C)$, $\Delta H_{abs.(des)}=f(C)$ and $\Delta S_{abs.(des)}=f(C)$ dependences were obtained.

The calorimetric data obtained for the $Ti_{0.9}Zr_{0.1}Mn_{1.3}V_{0.6} - H_2$ system at 60ºC are presented in the Table:

H/IMC	$\Delta H_{abs.}$, kJ/molH_2	H/IMC	$\Delta H_{des.}$, kJ/molH_2
0.7-1.5	-30.3±-0.2	0.7-1.5	27.4±-0.5
1.5-2.3	-31.4±-0.2	1.8-2.2	31.2±-0.3
2.3-2.7	-33.4±-0.2	2.3-2.7	33.4±-0.8

As one can see from presented results the values of enthalpy of hydrogen reaction of absorption and desorption from the hydride phase increased with the rise of C. We assume that hydrogenation of IMC at definite conditions (increased temperature and pressure) may cause rearrangement of crystal structure of initial IMC and formation of some new different interstitial sites which are more energetic efficient for hydrogen.

It should be emphasized that $Ti_{0.9}Zr_{0.1}Mn_{1.3}V_{0.6}$ has very good hydrogen capacity (C~3) and very small hysteresis of pressure these properties are very important for the use of this compound in the technology purposes.

Mo-PO25

Thermodynamic properties of the two-dimensional quantum magnet $Cu(tn)Cl_2$ *

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Previous studies of polycrystalline $Cu(tn)Cl_2$, (tn = $C_3H_{10}N_2$) identified the compound as an excellent realization of a two-dimensional (2d) quantum magnet. While no phase transition to magnetic long-range order was observed down to 50 mK, the response of the material to the applied magnetic field mimics a field-induced Berezinskii-Kosterlitz-Thouless transition theoretically predicted for the Heisenberg antiferromagnet (HAF) on a square lattice†. While such behavior indicates extreme weakness of interlayer magnetic correlations, the character of the 2d magnetic lattice is not known†.

The present work is focused on the determination of intra-layer exchange interactions. For that purpose, specific heat, magnetic susceptibility and elastic properties of a single crystal were experimentally investigated nominally at temperatures from 0.3 to 300 K. Since the quantitative analysis of the magnetic specific heat is highly sensitive to the estimation of the phonon contribution, various approaches were applied for its determination as the use of the diamagnetic isomorph $Zn(tn)Cl_2$ and elastic constants. The resulting magnetic contribution was analyzed within a model of the spin ½ HAF on the spatially anisotropic square lattice with the nearest-neigbour coupling J and J'. The best agreement was obtained for $J'/J = 0.3$ and $J/k_B = 4.4$ K. However, susceptibility data suggest the co-existence of ferro and antiferromagnetic interactions within the magnetic layer, namely $J'/J = -0.5$ and $J/k_B = 4.4$ K. Additional steps including first-principles study are discussed.

* This work was supported by projects VEGA 1/0269/17, APVV-14-0073, DS-2016-0046 and VVGS-2017-252.

† A. Orendáčová et al, Phys. Rev. B 80, 144418 (2009).