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Phase stability, crystal structure and magnetism in $(U_{1-x}Nb_x)_2Ni_{21}B_6$ and $(U_yNb_{1-y})_3Ni_{20}B_6$. ALESSIA PROVINO, University of Genova, Italy, AMITAVA BHATTACHARYA, SUDESH K DHAR, Dept CMPMS, TIFR, Mumbai, India, MARCELLA PANI, FLAVIO GATTI, University of Genova, Italy, DURGA PAUDYAL, Ames Laboratory, Ames, IA, USA, PIETRO MANFRINETTI, University of Genova, Italy — Ternary phases with composition $T_2M_{21}X_6$ and $T_3M_{20}X_6$ (T = transition metal; M = $3d$ metal; X = B, C, P) are reported to crystallize with the $W_2Cr_{21}C_6$ -type and $Mg_3Ni_{20}B_6$ -type, respectively (ternary ordered derivatives of the cubic $Cr_{23}C_6$ -type, $cF116$). They attract interest due to their refractory, mechanical, and peculiar magnetic properties. Literature data on these compounds only concern apparently stoichiometric 2:21:6 and 3:20:6 phases. Often only nominal composition has been reported, with few structural refinements and no measurements of physical properties. Lack of detailed stoichiometry and crystallographic data does not allow sufficient understanding of the crystal chemistry and properties of these compounds. We studied stability, crystal structure and magnetism of $(U_{1-x}Nb_x)_2Ni_{21}B_6$ and $(U_yNb_{1-y})_3Ni_{20}B_6$; stable phases are $U_2Ni_{21}B_6$ and $Nb_3Ni_{20}B_6$, as also confirmed by theoretical calculations. The two pristine compounds solubilize Nb and U, respectively, up to a given extent. The substitution of U by Nb leads to a structural change from the $W_2Cr_{21}C_6$ - to the $Mg_3Ni_{20}B_6$ -type. While $U_2Ni_{21}B_6$ is a Pauli paramagnet (itinerant non-magnetic state of U- $5f$ electrons), in agreement with literature, magnetization data for $(U_yNb_{1-y})_3Ni_{20}B_6$ show itinerant ferromagnetism with $T_C > 300$ K.

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