Na_7RbTl_4: A New Ternary Alkali Metal Thallide including Tl_4^{8-} tetrahedra

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During our studies on alkali metal thallides with mixed alkali metals, we want to fill the gaps between the already known compounds, which still have remained, and investigate the influence of the different alkali metals on the structure [1]. One of these gaps remains at the A:Tl ratio of 2:1. For this composition, only the binary compounds Li_2Tl and Na_2Tl are known so far [2], but compounds including with the heavier alkali metals K, Rb or Cs still are missing. On our poster we present Na_7RbTl_4, the first ternary phase in the A:Tl ratio 2:1 (final R-values: R_1=0.0231, wR_2=0.0392). Single crystal x-ray structure analysis first suggested tetragonal symmetry of the unit cell, but no structure solution was possible within this crystal system. Structure solution and refinement succeeded when pseudo-merohedral twinning was taken into account, yielding a final model in space group *Pbam* (a=16.3584(4) Å, b=16.3581(4) Å, c=11.3345(3) Å, V=3033.04(14) $Å^3$). The structure motif is represented by Tl_4^{8-} tetrahedra embedded in a matrix of fully occupied alkali metal cations, which Hansen and Smith also described for Na_2Tl[2]. While the coordination sphere of the Tl_4 tetrahedra in Na_2Tl contains 23 Na (21: d(Na-Tl)<3.7 Å, +2: d(Na-Tl)<4.2 Å), the two different Tl_4 tetrahedra in Na_7RbTl_4 are surrounded by 16 Na (d(Na-Tl)<3.6 Å)and 5 Rb (d(Rb-Tl)<4.3 Å). The coordination number of sodium is very similar between those two compounds (Na_2Tl: 12 or 14, Na_7RbTl_4: 11, 12 or 14), while the coordination number of rubidium sums up to 18.

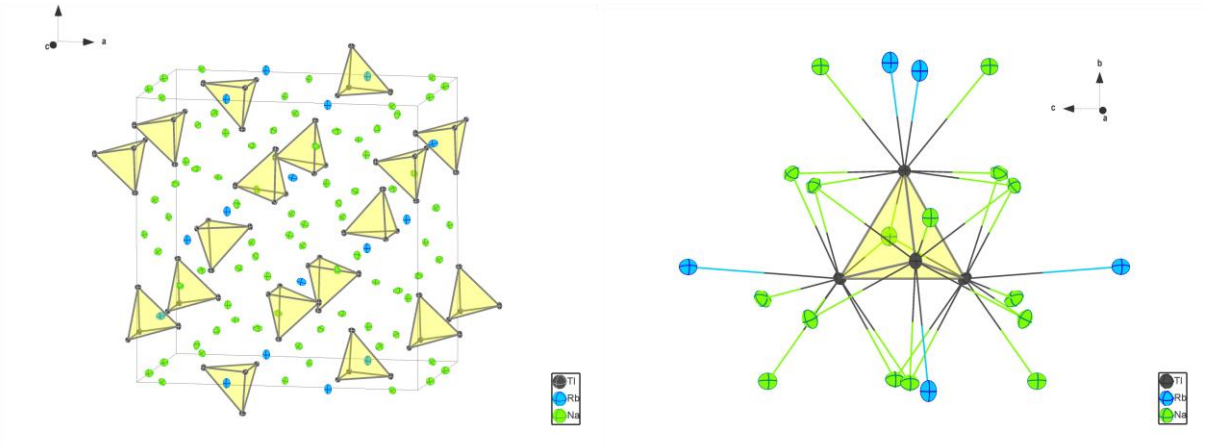

Fig. 1: Unit cell of Na_7RbTl_4 with isolated Tl_4^{8-} tetrahedra in a matrix of fully occupied alkali metal cations and coordination sphere of a Tl_4 tetrahedra

[1] Gärtner S., Spotlight on Alkali Metals: The Structural Chemistry of Alkali Metal Thallides. Crystals, 10, 1013 (2020)
[2] Stöhr J., Müller W., Schäfer H. Structural Principles of Lithium Group III Compounds. Acta Cryst. A, 37, C185 (1981); Hansen D.A., Smith J.F. Structure and Bonding Model for Na_2Tl. Acta Cryst., 22, 836-845 (1967)

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