Novel, crystalline, inorganic materials

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The chemistry of bi-anion system A-TM-Te-Cl (A = alkali-metal, TM = transition metal)

The chemical system A-TM-Te-Cl (A = alkali-metal, TM = transition metal) is to a large extent unknown but holds many possibilities. Both Te and Cl could appear as anions in a common crystalline lattice, which would most probably result in novel crystal structures, and possibly novel coordinations of transition metals (TMs), which is an excellent starting point for magnetic, optic, and electric properties. The ultimate goal is to get further understanding of the trinity: crystal structure – chemical composition – physical properties.

To synthesize the complex A-TM-Te-Cl compounds, we will use an exact method: the closed system reaction. All you place in the reaction should end up somewhere! And nothing unknown comes in. Naturally, there could be a reaction with the vessel itself, but that is all controllable and known influences. By this technique, we are able to force Nature to adapt to our suggests – if there is a possibility for a A-TM-Te-Cl compound, we will see the way, and then follow it. You will perform an almost holistic research, which can end up with anything from a novel compound, a new crystal structure, all the way to a (for example) new superconductor.

To the most important analyses, you will perform x-ray diffraction – on single crystals and powder – and evaluate those data with great accuracy (and several different software packages). From those data we can simulate the atomic arrangements that describe the whole crystals, including ordering of anions and rare TM-coordinations. From the crystal structure simulation, bond distances and angles are of revealed and of essence to get further understanding for the inorganic chemist. Electron microscopy investigations will reveal the true composition of samples, apart from showing the morphology of the crystallites. With each novel compound, we need to measure some “global” properties, like magnetism, to complete the trinity.

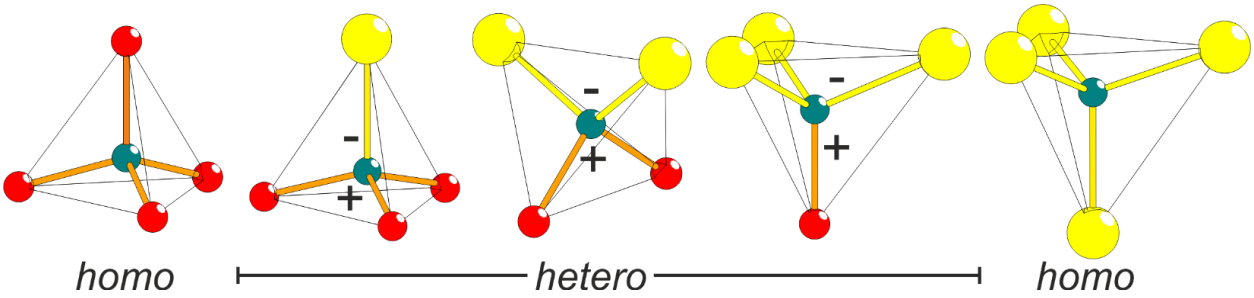

Figure: Two anions can cause strange (hetero-leptic) coordination, as compared to the homo-leptic coordination found in a single-anion lattice.