Components of Thermal Sensors: Synthesis and Properties of Thermochromic Crystals

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Thermochromic dyes find applications in fields like material processing and studying of thermal phenomena. I hypothesized that materials based on alkylammonium salts of transition metals, which are prone to phase transitions accompanied by change of various physical properties, could be used as thermal indicators or parts of electronic components. My project goal was to synthesize novel materials of these groups, to find ways to measure temperature, including the ability to visualize temperature fields on complex surfaces and ensure reversible or irreversible color change after a particular temperature is reached. I focused on: understanding why color change occurs; synthesizing suitable salts; establishing types and temperatures of color transitions. Various analysis techniques established the structure, qualitative and quantitative composition of the compounds. Twelve specimens were synthesized. Compounds with the general formula [NRxH4-x]y[MCl4] were synthesized (X=2,4; y=1,2; M=Cu,Co,Ni; R=Et,Bu,Ppz), and their phase transition temperatures and colour change in the range of 20–200°C were determined. The structure of these complex compounds was determined using IR and Raman spectroscopy, powder and single-crystal X-ray diffraction. Phase transition temperatures were found to depend on the structural hardness of the cationic moiety. Differential scanning calorimetry data demonstrated the presence of thermal transitions not accompanied by color change. Also, such transitions can be accompanied by change in the electrical properties of the crystals. An unknown phase, free from admixtures of starting reagents, was discovered by XRPD. This learning is a step to making indicators for industrial and consumer use that will augment safety and product knowledge.