

**Structural Insights into the Temperature-induced Color Changes of  $[(\text{CH}_3)_2\text{NH}_2]_2\text{NiCl}_4$** **T. Runčevski***Southern Methodist University, Dallas TX**truncevski@smu.edu*

The hybrid inorganic–organic material  $[(\text{CH}_3)_2\text{NH}_2]_2\text{NiCl}_4$  was reported to exhibit a remarkable thermochromism. [1] The color of this compound rapidly changes from deep red to deep blue upon heating at 383 K. Surprisingly, upon cooling to room temperature, the deep blue compound changes its color to dark, golden yellow. The so-produced yellow compound spontaneously transitions back to the starting deep red compound upon prolonged storage at ambient conditions. This color-change sequence can be cycled for a number of times without apparent degradation. Originally, it was believed that the color change originates from temperature-induced changes in the local geometry around the  $\text{Ni}^{+2}$  cations in the structure. To shine light at these processes, we performed detailed studies using synchrotron X-ray powder diffraction, with diffraction data collected as a function of temperature. We discover that rather than undergoing thermochemic transitions, this compound is in fact a reacting system and the different color originate from different crystalline phases. The crystal structure and composition of these phases was solved and refined using the diffraction data. These structures were used to rationalize the color changes. This contribution emphasized the importance of powder X-ray diffraction, and crystallography in general, in the mechanistic studies of the stimuli-responsive crystalline compounds.

[1] Bukleski, M., Petrusevski, M. V. (2009). *J. Chem. Ed.* **86**, 30.

**Keywords:** thermochromism; powder diffraction; Rietveld