Scientists describe the structure of a prospective luminesce substance

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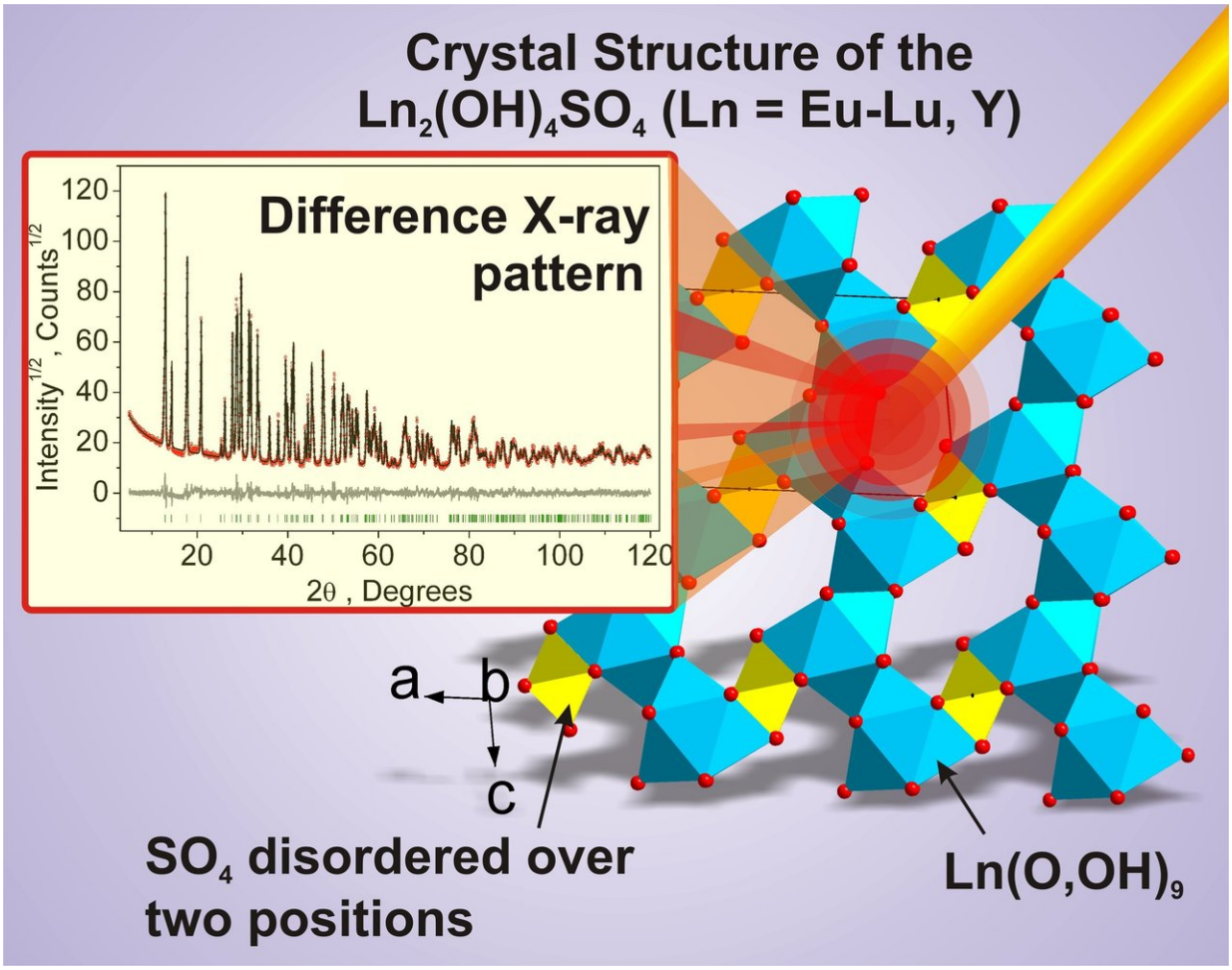

The structure of the new substance. Credit: Maksim Molokeev.

A physicist from Siberian Federal University (SFU) and Kirensky

Institute of Physics Federal Research Center KSC SB RAS (IF) has described the structure and properties of a new substance obtained by his Chinese colleagues. These are layered crystals of rare earth metal hydroxides $Ln_2(OH)_4SO_4$ (Ln=Eu-Lu, Y) that may be eco-friendly sources of phosphors (substances that transform different energies into light emission) for panels, screens and other electronic devices. The discovery was reported by *Chemistry: A European Journal*.

As usual, the discovery happened by chance. Chinese researchers synthesized a new powder substance mixing rare earth metal nitrates with ammonia sulfates and hydrates. The compound contained rare earth elements, and therefore had luminescent properties. However, its spectrum was unique and inconsistent with any expected result. Scientists were surprised to learn that its X-ray pattern was not comparable to any other from their database. Therefore, the substance not only had new composition, but belonged to a whole new class of compounds.

First of all, the researchers had to characterize the substance's crystal structure to determine the atoms it consists of and their location relative to each other.

"What was difficult about it is that we were unable to obtain the substance in the form of a monocrystal, so standard single-crystal X-ray methods could not be used. Determining structure from powder is a very complicated task that requires vast experience and knowledge," said Maksim Molokeev, a co-author of the work, candidate of physical and mathematical sciences, senior researcher of Kirensky Institute of Physics, and a senior tutor at SFU.

This was the task that Chinese scientists asked Maksim Molokeev to solve. He managed to successfully decode the X-ray pattern of the powder. It turned out that the new material consisted of SO_{42}- tetrahedra

and ions of rare earth elements surrounded by atoms of oxygen in the form of a three-caped trigonal prism. The SO_{42}- tetrahedra were disordered in several positions, i.e. these structural elements constantly changed their orientation in space and time (making the interpretation of the structure even more difficult).

After the structure of this layered compound was determined, it confirmed its unique nature. The substance was really a part of a new previously unknown class. Moreover, the researchers found out that the compound had very rare and valuable properties. When it is heated to 800º C, water is evaporated, leaving industrially useful phosphor appropriate for screens. Traditional production methods are "dirty," and cause emissions of toxic by-products. The new substance achieves the desired results in an eco-friendly way.

In the future, new iso-structural compounds (i.e. the compounds in which ions are replaced with different ones without material structural changes) are likely to be added to this class of substances. These new compounds may be used in the manufacturing of catalysts, microelectronics. UV protection, and other prospective scientific and technical areas.

Provided by Siberian Federal University