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## Molecular design and crystal engineering of a novel series of inorganicorganic hybrid architectures based Keggin-type polyoxometalates

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## ABSTRACT

The targeted synthesis of inorganic–organic hybrid supramolecular materials through crystal engineering is a principal challenge of modern chemistry research. Polyoxometalates (POMs), as metal–oxygen cluster species, are significant inorganic components for this goal because of their extreme versatility of compositions, high structural stability, and infinite variety of chemical, physical, and biological properties. Due to importance of this field, a novel series of inorganic-organic hybrid architectures based on Keggin-type POMs and lanthanoids coordination compounds have been synthesized under hydrothermal conditions. From the viewpoint of crystal engineering, the control of the dimensionality of the resulting hybrid compounds is still a great challenge, as the final structures are frequently modulated by various factors. The objective of the present research is to explore the effect of organic ligands, POMs charge density, size of the lanthanoide ions and synthetic conditions in final assemblies. The luminescent properties of some of these compounds have been investigated. Monte Carlo simulation has been employed for predicting the ability of these compounds to capture CH<sub>4</sub> and CO<sub>2</sub> and also to separate CH<sub>4</sub>/H<sub>2</sub> and CO<sub>2</sub>/N<sub>2</sub> mixtures.

Keywords: Inorganic-organic hybrid, Polyoxometalates, Lanthanoids, Luminescent property, Gas storage

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