DESIGN AND CRYSTALLIZATION OF CYCLODEXTRIN METAL-ORGANIC FRAMEWORKS USING TEMPLATE-DIRECTED SYNTHESIS

K. Krūkle-Bērziņa[1], S. Belyakov[1]

[1] *Latvian Institute of Organic Synthesis Aizkraukles iela 21, LV-1006, Riga, Latvia*

Email of communicating kkberzina@osi.lv

Cyclodextrin-based metal-organic frameworks (CD MOFs) are a unique class of supramolecular materials with promising applications in areas such as drug delivery, catalysis, and sensing, due to their biocompatibility, tunable porosity, and structural diversity [1]. However, precise control over their crystallization and phase outcomes remains a significant challenge.

This study investigates the application of **template-directed synthesis (TDS)** to influence and control the crystallization of γ-cyclodextrin MOFs (γCD MOFs) formed with sodium (Na^+) and potassium (K^+) ions. The TDS approach utilizes molecular templates to guide nucleation, favour specific packing arrangements, and enable the selective formation of particular phases under otherwise comparable experimental conditions.

A combination of single-crystal X-ray diffraction (SCXRD), powder X-ray diffraction (PXRD), and thermal analysis (TA) was used for characterization. Preliminary findings show that template mass has a pronounced impact on crystallization kinetics and product quality. For γCD-Na MOFs, increased template concentration led to significantly slower crystallization or complete suppression of crystal formation, although the resulting phase remained structurally consistent. In contrast, γCD-K MOF crystallization exhibited only a moderate response to the same template, but the final crystal phase differed from that obtained in template-free conditions.

These findings indicate a cation-specific response to the template, suggesting differences in nucleation and growth mechanisms between the Na^+ and K^+ systems. The results underscore the potential of template design as a tool for phase control in CD MOF synthesis and highlight the importance of continued exploration of additive effects, cation identity, and crystallization conditions. Ultimately, this approach could pave the way for reproducible synthesis of tailor-made CD MOFs with applications across pharmaceutical and materials science industries.

[1] Rajkumar, T.; Kukkar, D.; Kim, K. H.; Sohn, J. R.; Deep, A. (2019). *J. Ind. Eng. Chem*. **72**, 50.

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