

## MS20-P02 | SYNTHESIS AND STRUCTURE DETERMINATION OF SCM-15: A 3D LARGE PORE ZEOLITE WITH INTERCONNECTED STRAIGHT 12×12×10-RING CHANNELS

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SCM-15 (Sinopec Composite Material No. 15), the first zeolite containing a 3-dimensional channel system with interconnected 12-, 12-, and 10-ring channels, has been synthesized using 4-pyrrolidinopyridine as organic structure-directing agent (OSDA) [1]. Its structure has been determined by combining single-crystal electron diffraction (SCED) and synchrotron powder X-ray diffraction (SPXD) data. The complete framework structure of SCM-15 was determined directly using direct method (by *SHELXS*) based on SCED data, [2] as well as the rough locations of guest molecules such as OSDA and F<sup>-</sup> ions and framework atoms such as Ge. The more accurate framework structure and the locations of OSDA, F<sup>-</sup> ions, and Ge atoms were then obtained by refining the structure against the SPXD data. It was found that the results obtained from SCED data show good consistency with those from SPXD data, indicating the good reliability of the results from SCED data.

The determined structure demonstrates that the framework of SCM-15 is related to a class of frameworks (FOS-5, ITQ-7, PKU-16, ITQ-26, ITQ-21, Beta polymorph B, and SU-78B) that can be built from similar chains which are connected by shared 4-ring or d4r units. Six topologically reasonable 3D large or extra-large pore hypothetical zeolites are then predicted based on the relationship between those frameworks.

[1] Y. Luo, S. Smeets, Z. Wang, J. Sun, W. Yang, *Chem. -Eur. J.* 2019, 25, 2184-2188.

[2] G. M. Sheldrick, *Acta Crystallogr. A*, 2008, 64, 112-122.