Poster

Localization of Na^+ cations within nanozeolite ECR-1 using a 3D ED method

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Until now, the comprehensive structural analysis of single crystals of zeolite ECR-1, an aluminosilicate with the **EON** topology, has been hindered owing to the submicron dimensions of the obtained crystals. Additionally, this zeolite, which is characterized by a topology comprising alternating periodic building units of two other zeolites (**MAZ** and **MOR** layers), exhibits stacking faults that impede accurate refinement through the Rietveld method.

In this report, we present, for the first time, the structure of ECR-1 elucidated by studying a nanocrystal with a significantly reduced number of stacking faults [1]. The sample used was synthesized hydrothermally using trioxane as the organic structure-directing agent. The structure determination was conducted at 103 K by a 3 dimensional electron diffraction (3D ED) technique, namely precession electron diffraction (PED).

Results show that partial dehydration occurred in the structure owing to the high vacuum conditions in the TEM sample chamber. From the dynamical refinement (R_{obs} = 0.097), 8.16 Na^+ charge compensating cations were localized on six distinct crystallographic sites, along with approximately four water molecules per unit cell (Fig. 1). Furthermore, a canonical Monte Carlo computational study was conducted to compare the experimental cationic distribution and location of water molecules with the simulation.

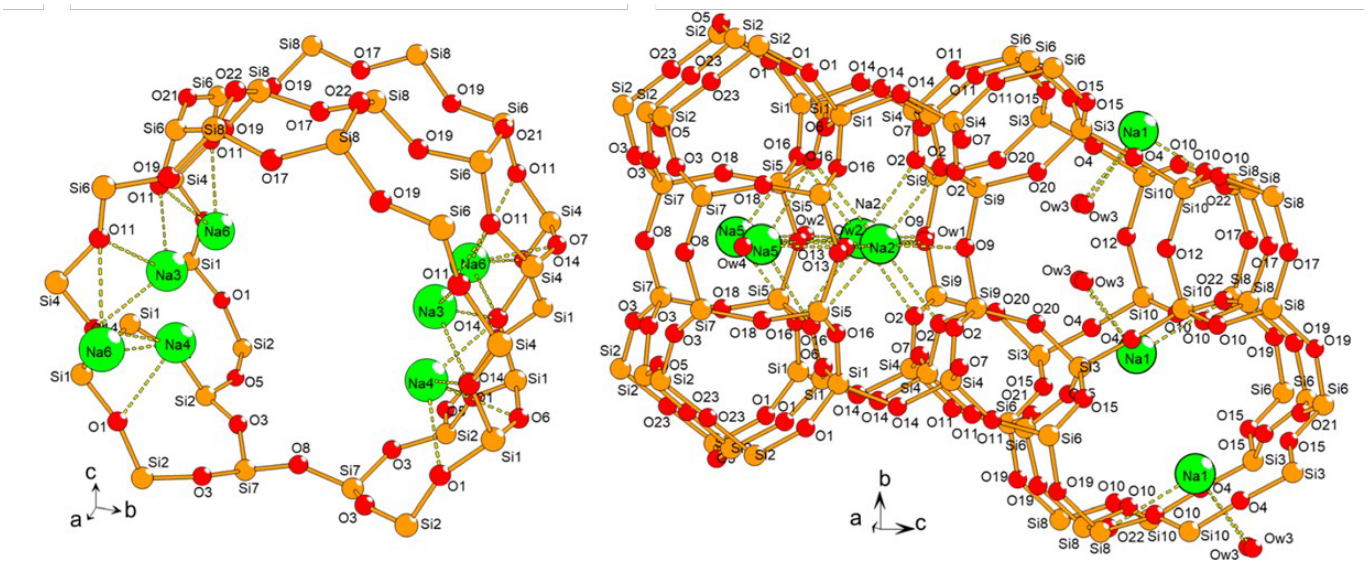

Figure 1. Overview of ECR-1 cationic sites from 3D ED.

[1] Örs, T., Deroche, I., Chatelard, C., Dodin, M., Martinez-Franco, R., Tuel, A. & Paillaud, J.-L. (2024). *Symmetry* **16**, 477.