Location of active species in zeolites, the case of Cu-omega

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Copper-exchanged zeolites are active materials for the partial oxidation of methane to methanol (MtM), which is a potential alternative to petroleum-derived building blocks for the petrochemical industry. Many copper-exchanged zeolites of varying structure type are active for this reaction ([1],[2],[3]). During the course of a study to test the performance of copper-exchanged zeolites with 8- and 10-rings, we found that the methanol yield obtained using Cu-omega (**MAZ** framework type) (4) was significantly higher than that obtained with Cu-MOR, which is the most-often used material for this reaction ([4]). The framework structure of zeolite omega ([5]) is composed of gmelinite (*gme*) cavities stacked in columns parallel to *c*. They are connected laterally via ellipsoidal 8-rings to form a hexagonal array of columns that define a round 12-ring channel parallel to *c*. The 8-ring channels between the *gme* columns are not unlike those found in mordenite, but they are not accessible from the 12-ring channel. However, they do connect the *gme* cavities via a convoluted 3-dimensional 8-ring channel system. To investigate the reason for the remarkable catalytic performance of this material, we are using different characterization techniques, such as FTIR, XAS and X-ray diffraction, combined with molecular simulation. In this work, we present the results from a structure analysis using synchrotron powder diffraction data collected *in situ* during the activation of Cu-omega under oxygen and during the reaction itself. In the activated material, copper species are found in the 6-rings in the *gme* columns. They are single copper species, as opposed to the dimers generally accepted as the active species in the partial oxidation of methane to methanol ([6]). This material contains a low Cu/Al ratio (0.07) and is not very active in MtM, indicative of low activity of copper ions.

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