Supporting Information for

Kinetic study and effect of water on methane oxidation to methanol over copper-exchanged mordenite

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Fig. S1. XRD patterns for the CuMOR material



Fig. S2. Nitrogen adsorption-desorption isotherms for CuMOR



Fig. S3. FTIR spectra of surface species formed over CuMOR after the activation at 673K in oxygen with subsequent reaction with methane at 473K for 30 min.



Fig. S4. FTIR spectra of gas phase acquired during the reaction of CuMOR with 100 torr of methane at 473K. Prior to the reaction, the sample was activated at 673K in oxygen for 1h.



Fig. S5. FTIR spectra of nitrogen monoxide adsorbed over CuMOR-673K after activation, reduction in hydrogen and reaction with methane with pre-adsorbed water. The figure duplicates the data presented in Figure 4 in the main text.

The band at 1805 cm⁻¹ corresponds to the Cu^I(NO) mononitrozyl species, while two bands at 1730 and 1825 cm⁻¹ are due to the Cu^I(NO)₂ dinitrozyl species, formed from the mononitrozyl upon the increase of the NO partial pressure. For the Cu^{II}(NO) monotrintozyls multiple bands due to the copper species of different structure appear in the region between 1900 and 2000 cm⁻¹. It is generally believed that the frequency of the bands is correlated with the nuclearity of the copper-oxo sites. Low frequency around 1900 cm⁻¹ indicates with presence of monomeric copper sites, while higher frequencies are typically associated with the copper dimers or trimers. With that, the spectra obtained for the copper-exchanged mordenite point to the existence of a mixture of multiple copper species in this material.



Fig. S6. TG data of CuMOR heating in a flow of dry mixture containing 20 vol% oxygen in nitrogen. The water content after the activation at 473K accounts for 88.65-8833 = 0.32 wt%.