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Crystal Structures of the No and No_2 Sorption Complexes of Dehydrated Fully Mn^{2+}-Exchanged Zeolite X. Yang Kim[a], Gyoung Hwa Jeong[a], Young Mi Lee[a], Karl Seff[b] [a]Dept. of Chemistry, Pusan National Univ., Pusan, Korea [b]Dept. of Chemistry, Univ. of Hawaii, Honolulu, Hawaii.

The crystal structures of the nitric oxide (crystal 1) and the nitrogen dioxide (crystal 2) complexes of fully dehydrated fully Mn^{2+}-exchanged zeolite X ($Mn_{46}Si_{100}Al_{92}O_{384}$ per unit cell) have been determined at 21(1)℃ by single-crystal X-ray diffraction techniques in the cubic space groups $Fd\bar{3}m$ and $Fd\bar{3}$, respectively. In crystal 1, Mn^{2+} ions are located at four crystallographic sites: 15 Mn^{2+} ions per unit cell at the octahedral site I (at the centers of hexagonal prisms), 2 at site Ij, and the remaining 29 at two different sites II. Sixteen nitrogen monoxide molecules lie in the supercage where they coordinate to site-II Mn^{2+} ions. The observed N-O bond length, 1.6(3) Å can be compared with that in NO gas, 1.15 Å. NO coordinates to Mn^{2+} in a lateral π -bonded manner with N somewhat favored. In crystal 2, Mn^{2+} ions are located at four crystallographic sites: 14 Mn^{2+} ions at site I, 4 at site Ij, 20 at site II and the remaining 8 at site IIIj. Twenty-eight nitrogen dioxide molecules per unit cell lie in the supercage; each of 20 coordinates via its N atom to a site-II Mn^{2+} ion and the remaining 8 coordinate similarly to site-IIIj Mn^{2+} ions. From bond lengths and color, Mn^{2+} does not appear to have been oxidized in either structure.