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In situ **neutron diffraction study of SII CO deuterohydrate clathrate** JINLONG ZHU, LANSCE-LC, Los Alamos National Laboratory, SHIYU DU, T-Division, Los Alamos National Laboratory, XIAOHUI YU, LANSCE-LC, Los Alamos National Laboratory, HONGWU XU, EES, Los Alamos National Laboratory, SVEN VOGEL, LANSCE-LC, Los Alamos National Laboratory, CHANGQING JIN, Institute of Physics, Chinese Academy of Sciences, YUSHENG ZHAO, HiPSEC, University of Nevada — SII CO clathrate has been successfully synthesized at $\sim$ 100 bar and 252 K. During the synthesis process, SI CO clathrate was formed first as an intermediate phase and then transformed to SII clathrate. Structural parameters of SII CO clathrate at temperatures from 25 K to 260 K have been determined from Rietveld analysis of neutron diffraction data. With decreasing temperature, the decrease of lattice parameter can be described by a two-order polynomial thermal expansion equation. The molecular lengths of CO in the small and large cages decrease linearly with decreasing temperature. There is one CO molecule in each small cage, whereas two CO molecules occupy in each large cage. CO molecules are not localized at the cage centers. Rather, they exhibit disordered distributions in both small and large cages, while the CO in small cage shows a donut shape nuclear distributions around the cage center, the CO in large cage delocalized from the cage center and more disordered with increasing temperature.

Jinlong Zhu
LANSCE-LC, Los Alamos National Laboratory

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