High-Pressure Studies of Abnormal Guest-Dependent Expansion in $\{[Cu(CO_3)_2](CH_6N_3)_2\}_n$

Qian Li,[†,§] Shourui Li,[†,§] Kai Wang,[,†] Jing Liu,[#] Ke Yang,[‡] Bingbing Liu,[†] Guangtian Zou,[†] and Bo Zou[*,†]*

[†]State Key Laboratory of Superhard Materials, Jilin University, Changchun 130012, P. R. China

[#]Beijing Synchrotron Radiation Laboratory, Institute of High Energy Physics, Chinese Academy of Sciences, Beijing 100039, China

[‡]Shanghai Synchrotron Radiation Facilities, Shanghai Institute of Applied Physics, Chinese Academy of Sciences, Shanghai 201204, China

Supporting Information

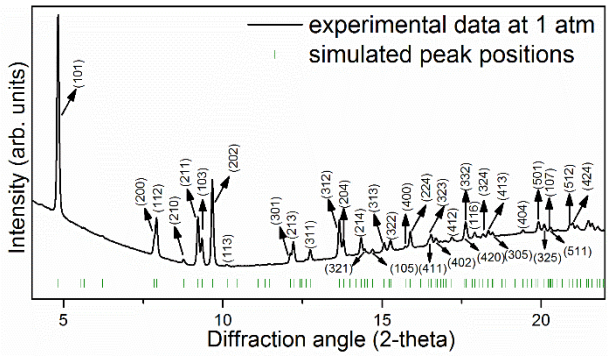

Figure S1. Comparison between the experimental and simulated data, together with the detailed identification of the diffraction peaks.

The softening at pressures above 2.5 GPa

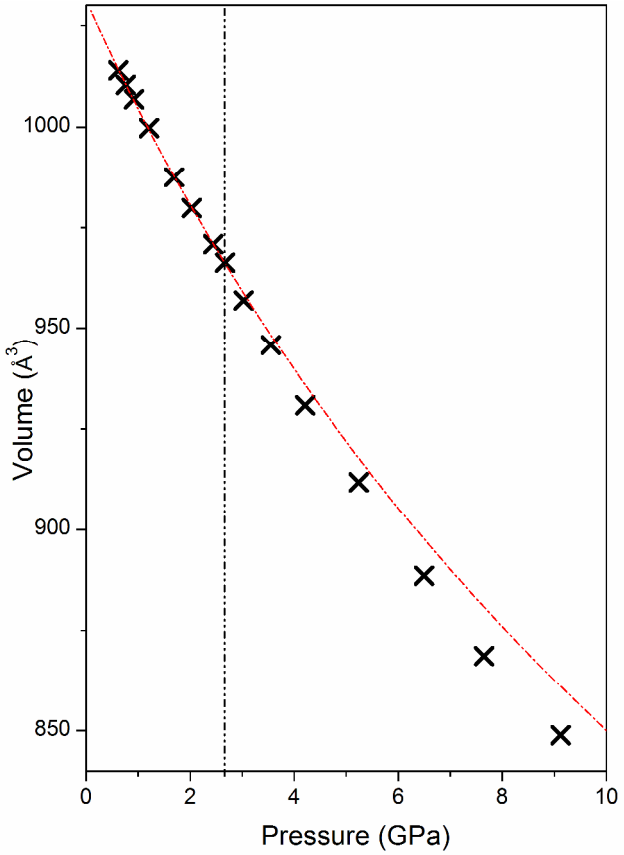

Figure S2. The curve of third order Birch-Murnaghan equation of state fit to the P–V data in the pressure range 0–9 GPa.

When methanol-ethanol is applied as PTM, the pressure condition and quality of the data is the best. So the fitting of the P-V data is performed based on the result in methanol-ethanol. As shown in Figure S5, the curve of third order Birch-Murnaghan equation of state fit to the P–V data in the pressure range 0–2.7 GPa also deviates the experimental data over 2.7 GPa. This result is coincident with the one obtained from the high-pressure single X-ray diffraction investigation. Meanwhile, the values of V_0 = 1031.38(4), K_0 = 36.6(7) GPa, K' = 3.4(6) we solved are very close to the ones shown in the previous study.[4]

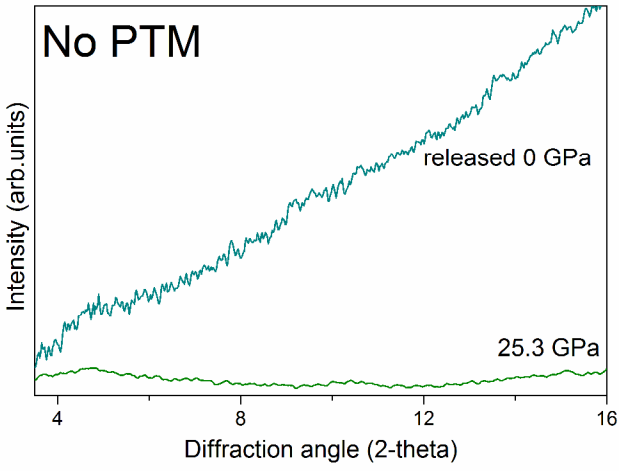

Figure S3. The ADXRD patterns without PTM at ~25 GPa and after releasing pressure.

After increasing highest pressure to ~25 GPa, the released ADXRD pattern shows that GCC becomes amorphous completely.

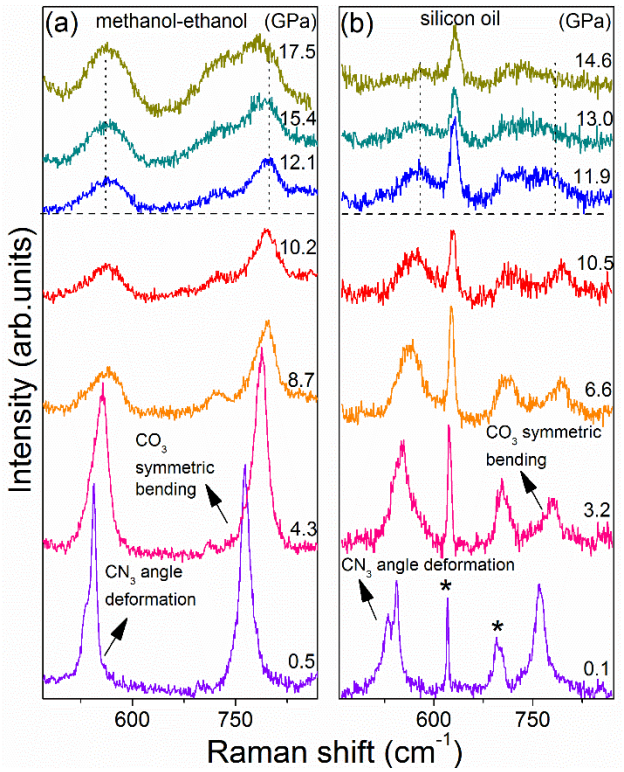

Figure S4. Selected Raman spectra of GCC at various pressures (a) with methanol-ethanol and (b) with silicon oil in the spectra region 460 – 870 cm^{-1}. The two peaks marked by the asterisks in (b) are the signal of silicon oil.

The Raman spectra of GCC are strongly influenced by the PTM molecules. When silicon oil is applied, the Raman signal of PTM can affect the observation of the peaks of GCC, and the Raman signal of GCC is too weak to be detected above 14.6 GPa. However, the results are the same in essence in these two sets of experiments. Furthermore, as can be seen in Figure S4b, evolution of the two peaks (marked by the stars) is continuous, indicating silicon oil and GCC have not affected each other at high pressure.