Supporting Information

High-Pressure Sorption of Hydrogen in Urea

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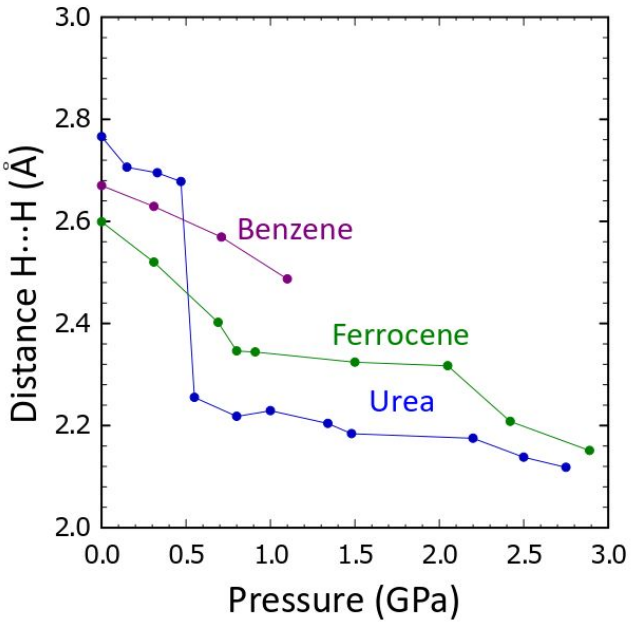

Figure S1 Shortest H···H bond in urea, ferrocene, and benzene up to 3.0 GPa.[1,2] The lines joining the points were drawn to guide the eye only.

Table 1. Phase transitions of urea in the literature.

References	*Transition*	*T (K)/P (GPa)*	*Space group*
*Bridgman, P. W. (Proc. Am. Acad. Arts Sci. **1916**)*	*I→II, III*	*0.48 GPa/296 K*	
*Olejniczak, A. et.al (J. Phys. Chem. C **2009**)*	*I→III*	*0.48 GPa/296 K*	$P\bar{4}2m \rightarrow P2_12_12_1$
	III→IV	*2.8 GPa/296 K*	$P2_12_12_1 \rightarrow P2_12_12$
*Weber, H. P. et.al (J. Appl. Crystallogr. **2002**)*	*IV →V*	*7.2 GPa/296 K*	$P2_12_12_1 \rightarrow Pmcn$

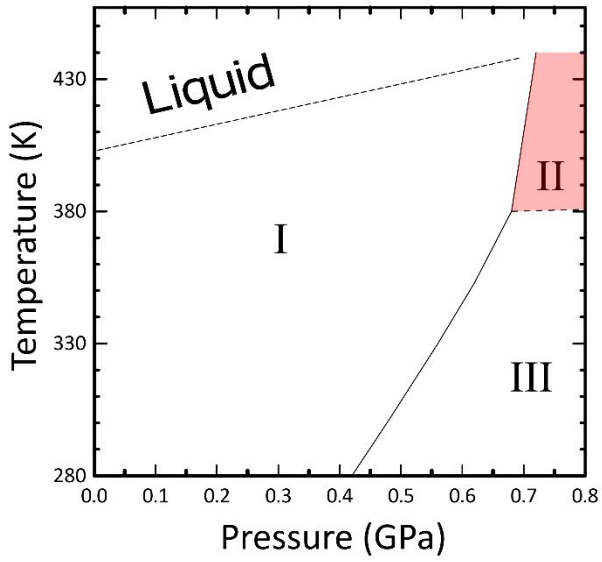

Figure S2 Phase diagram of urea obtained in Volumetric experiment with no pressure transmitting medium by P.W. Bridgman.[3] Postulated phase II (marked red) was not confirmed by other methods.[6,9]

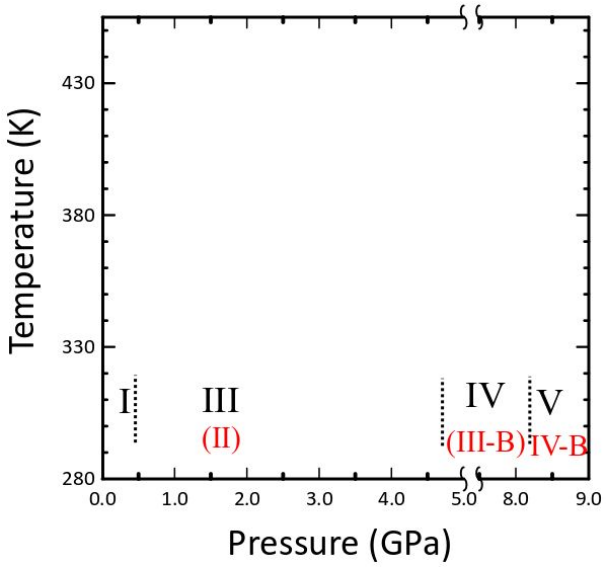

Figure S3 Phase diagram of urea from Lamelas *et.al* by Raman and derived from X-ray diffraction on the sample compressed in Ar.[4]

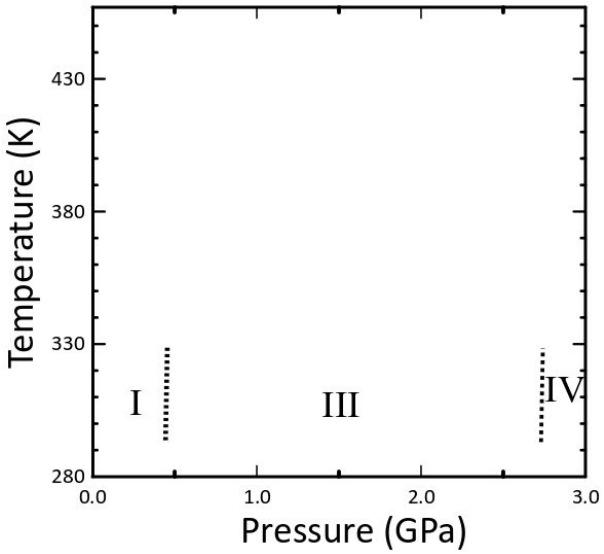

Figure S4 Phase boundaries of urea at 296 K based on the sample recrystallizations under pressure from the solutions in water (phases I and III) and in the methanol:ethanol:water mixture (phases III and V).[5,6]

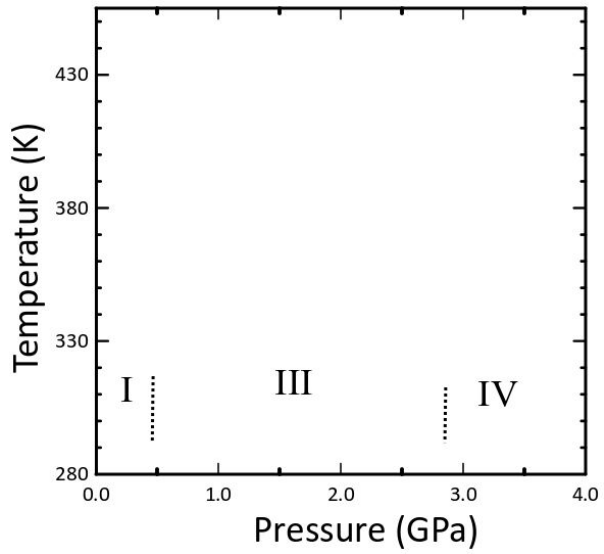

Figure S5 Measurements performed by neutron diffraction for deuterated urea compressed in deuterium at room temperature by Donnelly *et.al.*[7]

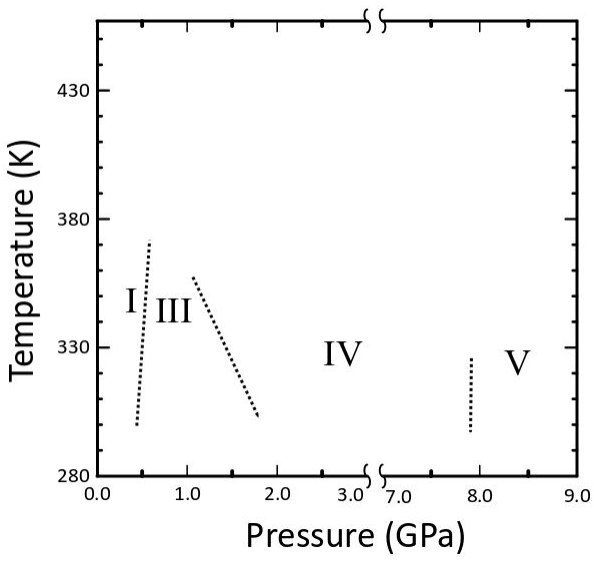

Figure S6 Phase diagram of pure urea by FTIR from Dziubek *et.al*.[8,9]

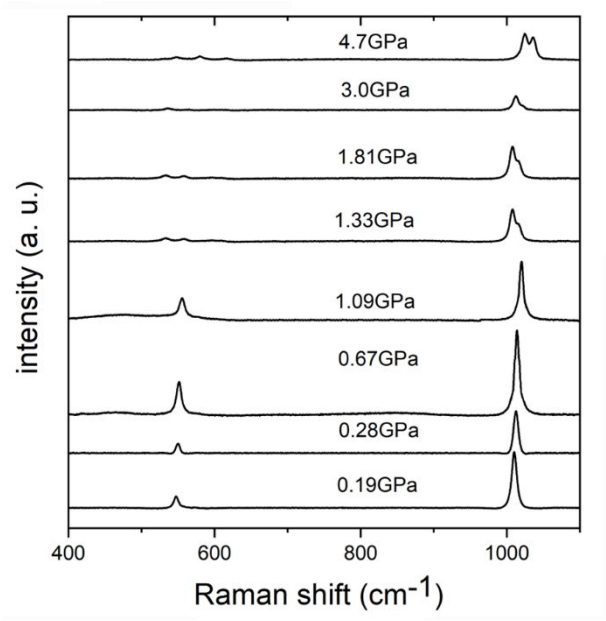

Figure S7 Raman spectra of urea in immersion oil up to 4.7 GPa, the intensities of spectra are normalized to allow comparison all mode.

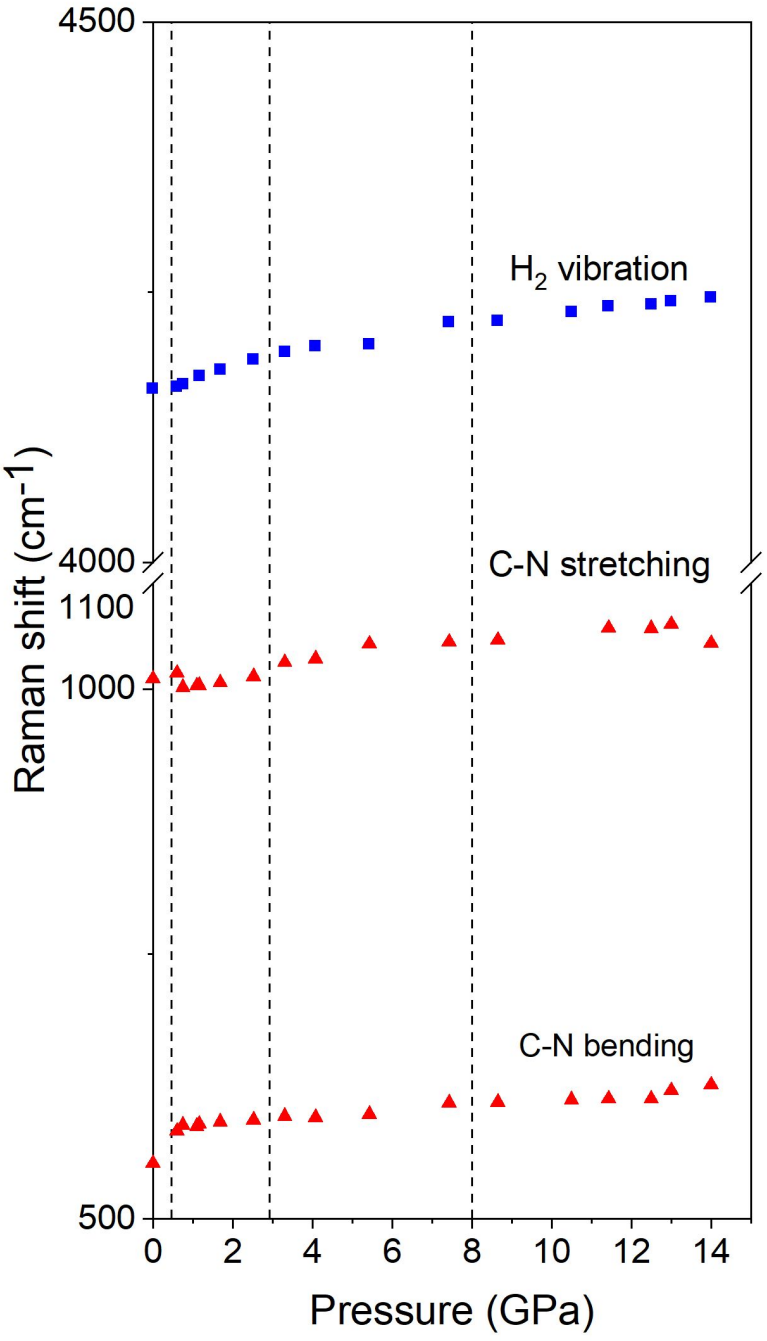

Figure S8 Hydrogen (Q_1-branch) and urea frequencies as a function of pressure up to 14.0 GPa. The hydrogen frequencies are indicated in blue and those of urea in red.

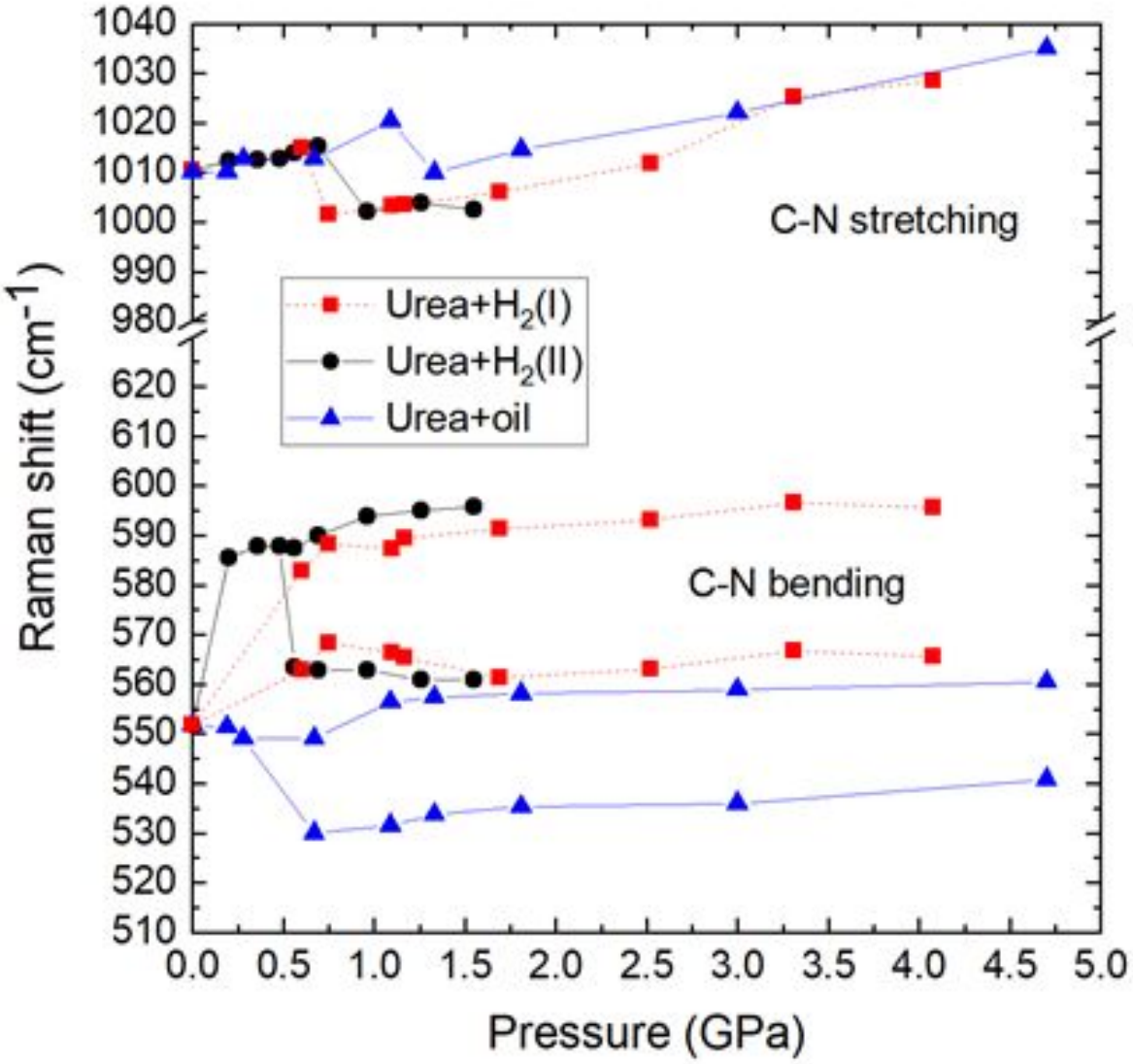

Figure S9. Raman shifts frequencies as a function of pressure measured for urea powder compressed in oil and in hydrogen (see the legend). The lines joining the points are for guiding the eye only.

References

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