Electronic Supplementary Material (ESI) for RSC Advances.

Supplemental material

Structural investigation of three distinct amorphous forms of Ar hydrate

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Figure S1. Ar hydrate density vs. pressure obtained from molecular dynamics (MD) calculations (black line) compared to experimental results, split in ^{Nat}Ar (black crosses) and ^{36}Ar clathrate hydrate (red squares) datasets. Simulated data extended to 3 GPa (broken line), past the pressure-induced amorphization.

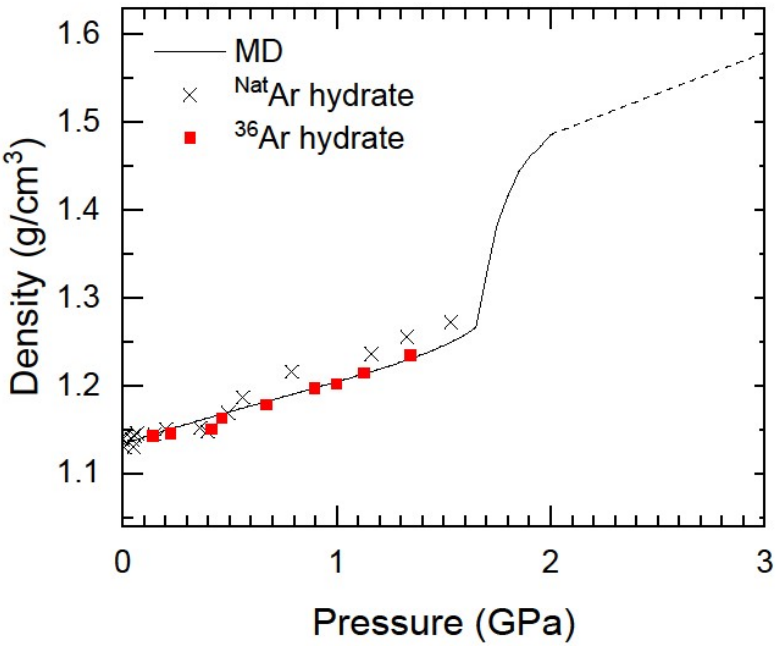

Figure S2. Mean square displacement of H_2O molecules in simulated heating of amorphous Ar hydrate at 2.0 GPa pressure. Curves represent temperature steps on heating from 95 K. Diffusion constants (D) shown in 10^{-8} cm^2 s^{-1} were extracted from MD trajectories with GROMACS.

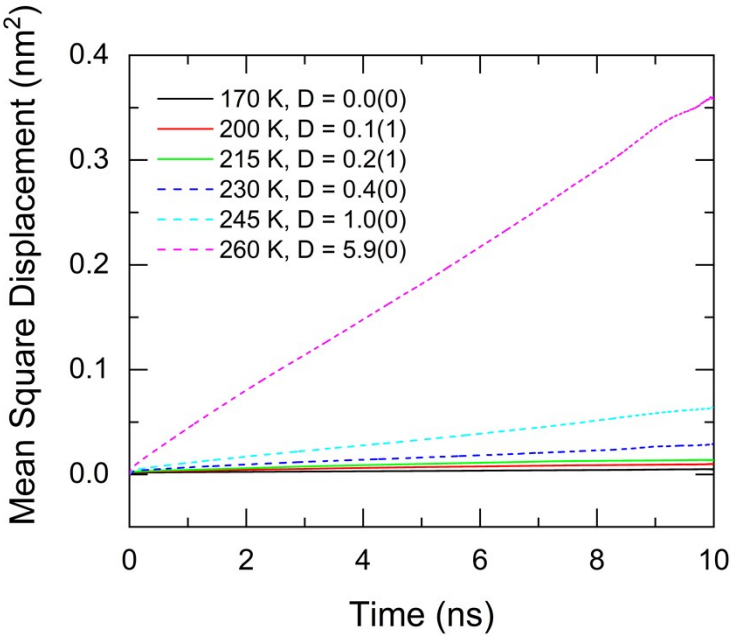

Figure S3. Experimental neutron structure factors, S(Q), for amorphous Ar clathrate hydrate samples with ^{2}H and ^{36}Ar as compared to ^{Nat}Ar isotope substitution at 95 K. **(a)** High-density amorphous (HDA) at 2 GPa; **(b)** Very-high-density amorphous (VHDA) at 2 GPa; and **(c)** Recovered amorphous (RA) at atmospheric pressure.

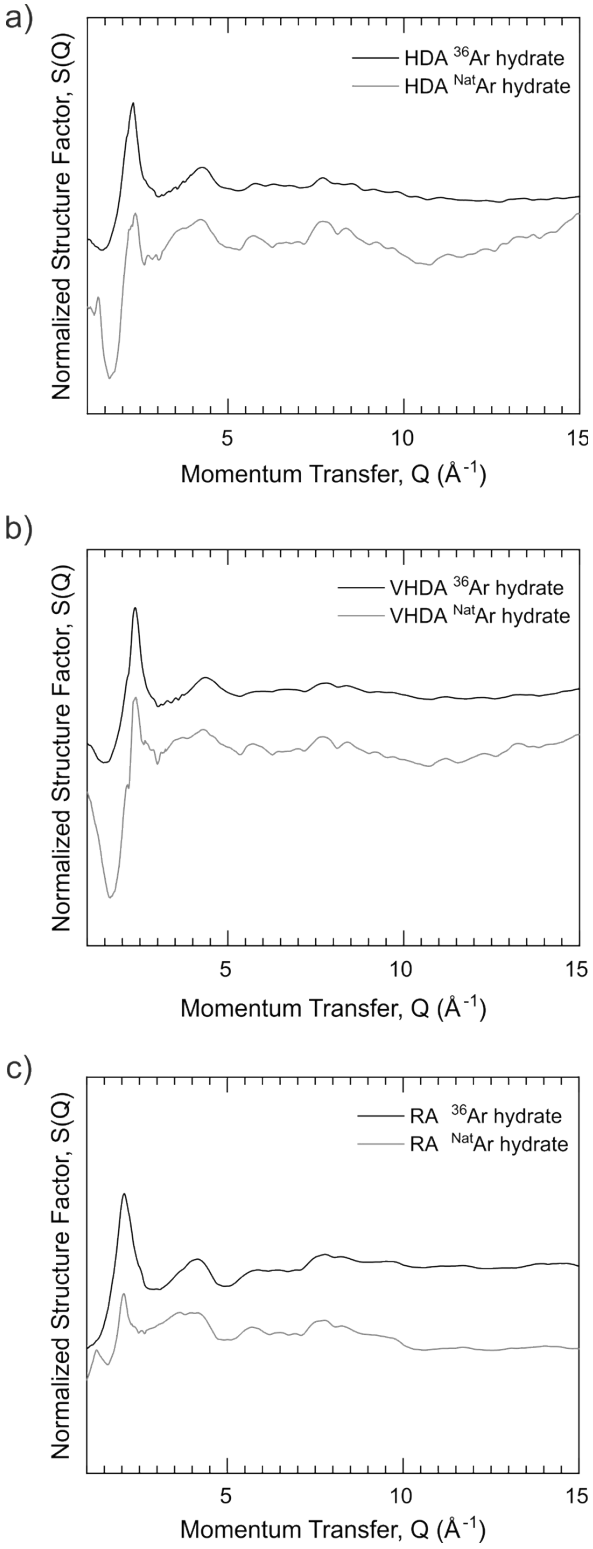

Figure S4. Partial correlation functions for **(a)** O−H and **(b)** H−H interactions for HDA at 2 GPa, 95 K (gray line); VHDA at 2 GPa, 95 K (red line); and RA at atmospheric pressure, 95 K (blue line).