nature chemistry

SUPPLEMENTARY INFORMATION

DOI: 10.1038/NCHEM.827

To circumvent usual scaling issues with simulations of shock compression[1], we use the Multi-Scale Shock Technique (MSST)[2–6]. MSST is a simulation methodology based on the Navier-Stokes equations for compressible flow. Instead of simulating a shock wave within a large computational cell with many atoms[1], the MSST computational cell follows a Lagrangian point through the shock wave as if the shock were passing over it. This is accomplished by time-evolving equations of motion for the atoms and volume of the computational of cell to constrain the stress in the propagation direction to the Rayleigh line and the energy of the system to the Hugoniot energy condition[2–4]. In the case of a shock, conservation of mass, momentum, and energy across the shock front leads to the Hugoniot relation $E-E_0 = \frac{1}{2}(P+P_0)(V_0-V)$, where E is the energy, P is the negative of the diagonal component of the stress tensor in the direction of the shock (uniaxial stress), and V is the volume. A subscript 0 refers to the pre-shocked state, while quantities without subscripts refer to the post-shocked state. The Rayleigh line $P - P_0 = U_S^2\rho_0\left(1-\frac{\rho_0}{\rho}\right)$ (where U_S is the shock velocity and ρ is the density) describes the thermodynamic path connecting the initial state of the system to its final (Hugoniot) state. For a given shock speed, these two relations describe a steady planar shock wave within continuum theory. By constraining the MD system to obey these relations, MSST enables simulation of the shock wave with significantly fewer atoms and consequently with significantly smaller computational cost. Linear scaling of computational work with simulation duration has enabled simulation lengths of up to 0.2 ns of tight-binding *ab initio* molecular dynamic simulations of shock compressed nitromethane[5].

An example of the time evolution of the thermodynamic properties of the shock compressed astrophysical ice is shown in Fig. S1. We used a planewave cutoff of 400 Ry and an optimized DZVP (double zeta valence polarized) basis set for all elements in the system, although we observed the system energy and stress to be converged with a planewave cutoff as low as 280 Ry. Calculations with an optimized TZVP (triple zeta valence polarized) basis set yielded virtually identical results to the DZVP basis set. For all of our shock compression simulations, we observe an average drift in the Hugoniot energy of 3% or less. Simulations with the PBE (Perdew-Burke-Ernzerhof) exchange correlation functional[7] at a shock velocity of 7 km/s yielded a pressure and density within 5% and a temperature within 9% of the

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results from BLYP, all within the standard deviation of these quantities. In order to test finite system size effects, we conducted a shock compression simulation at 7 km/s with a simulation cell doubled in the shock compressed direction, i. e., the a lattice vector. For this simulation cell we compute the Hugoniot pressure and density to deviate by less than 1%, and the temperature to deviate by less than 2% from the undoubled simulation.

The final Hugoniot states as well as the duration of each shock compression simulation are shown in Table SI. The computed shock Hugoniot for our astrophysical ice mixture is compared to that of water in Fig. S2. We show validation of our simulations over a wide range of pressures and temperatures. The deviation of our computed data from the water Hugoniot starting at 47 GPa is likely due to carbon condensation and the formation of novel compounds. The average lifetimes for the C–N bonded species, the lifetimes of the longest lived C–N bonded species, and the mole fraction of all C–N bonded species formed in our shock compression simulations are shown in Fig. S3.

The time over which a cometary ice would be held in its shock compressed state before arrival of a rarefaction wave and subsequent decompression can be approximated by the size of the comet divided by its sound speed c, where $c^2 = (\partial P/\partial \rho)$, and P and ρ are the pressure and density of the Hugoniot state, respectively. Based on our computed Hugoniot curve, for a comet experiencing a shock wave of 9 km/s we compute via finite differences a sound speed of ∼8.7 km/s. From this we compute that a comet with a radius of 1.61 km will remain in its compressed state for approximately 0.4 seconds. In order to get a sense of the degree of chemical equilibration on the time scales of our shock compression simulations, we have simulated a shock velocity of 9 km/s for ∼20 ps using a system half the size of that reported in our manuscript (105 atoms) and with the smaller SZV (single zeta valence) basis set (with GTH pseudopotentials and the BLYP functional). This simulation achieved a Hugoniot pressure of 49.6 GPa along the direction of the shock compression and a Hugoniot temperature of 3228 K, very similar to our results reported in the manuscript (47 GPa and 3141 K). The number density of C–C, C–N, and O–H bonds as a function of time are shown in Fig. S4. We observe that the C–N and O–H bonds all achieve a steady state within the first few picoseconds of shock compression. However, the C–C bonds are still increasing monotonically after 20 ps. These results are similar to previous simulations for water[8] and C-N-O-H containing energetic materials[9].

The computed isentrope for water is shown in Fig. S5, starting at 47 GPa and 3141 K.

All of our simulations were between 52-57% water by mole fraction upon expansion. As a result, we approximated the isentropic expansion curve of the cometary ice mixture using this equation of state. The equation of state used to compute the isentropic expansion thermodynamic path was based on a fit to experimental data, and has been shown to accurately reproduce a number of different types of experimental data at high pressure, including the shock Hugoniot curves and speeds of sound[10]. The astrophysical ice simulations at these conditions were expanded in discrete steps by performing constant pressure-temperature (NPT) simulations for 2-4 ps per step, using velocity scaling to control the temperature at each thermodynamic point. The system was expanded until the pressure of the initial configuration was reached. The simulation temperature was then quenched in discrete steps of approximately 400 K, also using velocity scaling to control the temperature. After equilibration at 300 K for several ps, the system temperature was controlled by using Nosé-Hoover thermostats[11] for all nuclear degrees of freedom for 10-20 ps. The total simulation time for all expansion steps plus cooling and thermal equilibration for our longest simulation was ∼50 ps.

We show simulated mass spectra results for the C–N bonded species from two isentropic expansions in addition to what we report in the manuscript: one that was begun after only 3 ps of shock compression but was expanded along the same seven points along the water isentrope (Fig. S6), and one rapid expansion conducted at the conclusion of the shock compression simulation (Fig. S7) that was expanded along only four points along the isentrope (35 GPa, 16.6 GPa, 9.7 GPa, 0.5 GPa). For the expansion after 3 ps of shock compression, we observe the formation of NH_2-$(CH_2)_2$-COOH as well as complexes with that combined with CO_2 and other moieties, found at higher mass peaks. For the rapid expansion, we observe a complex at 230 au of glycine, CO_2, formic acid and a C–N bonded alcohol. Thus, while the exact amino acid complex formed will depend on the point at which we expand our simulations, the formation of complexes with amino acids is consistent throughout. Both expansions shown here contain a mass peak at 61 amu corresponding to formamide, NH_2-COOH.

In order to calculate the Gibbs Free energy of reaction (ΔG_{rxn}) in solution for the formation of glycine, we used the quantum-chemical solvation model COSMO-RS[12]. COSMO-RS uses a statistical distribution of the surface charge density for each solute and solvent molecule in order to compute all necessary chemical potentials and subsequently the ΔG_{rxn}.

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COSMO-RS has been shown to accurately model the solubility of molecular crystals[13] and CO_2[14]. For our calculations, we modeled the solvent as 85% water and 15% formic acid. This composition is consistent with results from our quenched and expanded simulations. Increasing the fraction of formic acid to 40% caused a decrease in ΔG_{rxn} for both H_3O^+ and NH_4^+ reactions of $\sim$2 kcal/mol.

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Table SI: Table of final thermodynamic states and durations for our shock compression simulations. Error bars were determined by calculating the standard deviation over five time segments except for the 10 km/s trajectory, which was computed over three time segments. U_s and U_p refer to the shock and particle velocity, respectively.

U_s (km/s)	Temperature (K)	Pressure (GPa)	Density (g/cc)	Time (ps)	U_p (km/s)
5	706 ± 2	10.1 ± 0.1	1.66 ± 0.01	11.0	1.99
6	1020 ± 8	15.9 ± 0.3	1.82 ± 0.02	5.0	2.70
7	1589 ± 30	24.3 ± 0.7	2.00 ± 0.03	5.0	3.50
8	2348 ± 10	34.3 ± 0.2	2.17 ± 0.02	10.0	4.31
9	3141 ± 15	46.5 ± 0.5	2.35 ± 0.02	6.8	5.14
10	4083 ± 16	59.0 ± 0.4	2.50 ± 0.02	1.6	6.00

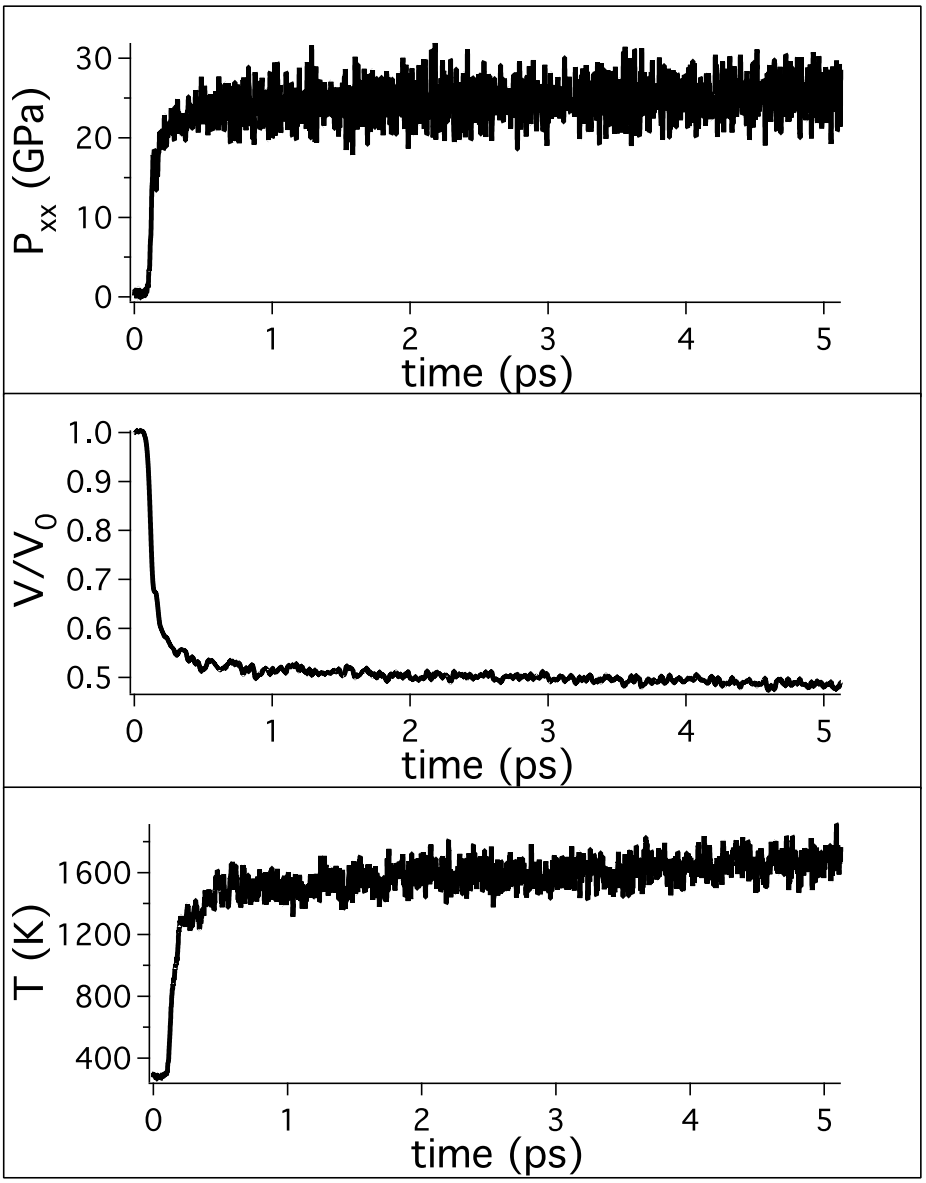

Figure S 1: Time evolution of the thermodynamic states induced by the 7 km/s shock velocity.

DOI: 10.1038/NCHEM.827

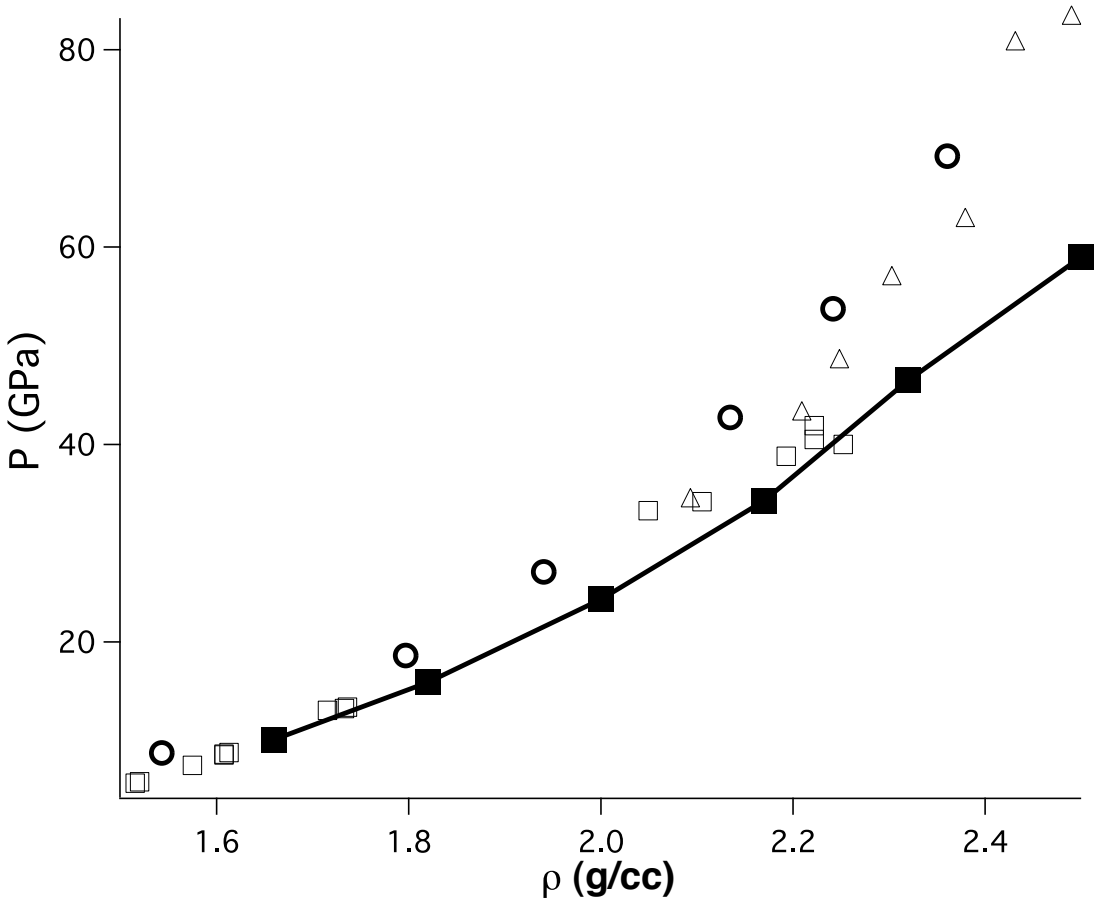

Figure S 2: Plot of the pressure vs. density Hugoniot results compared to published results for water. The thick line with filled squares corresponds to simulation results for the astrophysical ice mixture. The open squares correspond to the experimental results from Walsh et al.[15], the open triangles to experimental results from Mitchell and Nellis[16], and the bold open circles to simulation results from Goldman et al.[8], all for water.

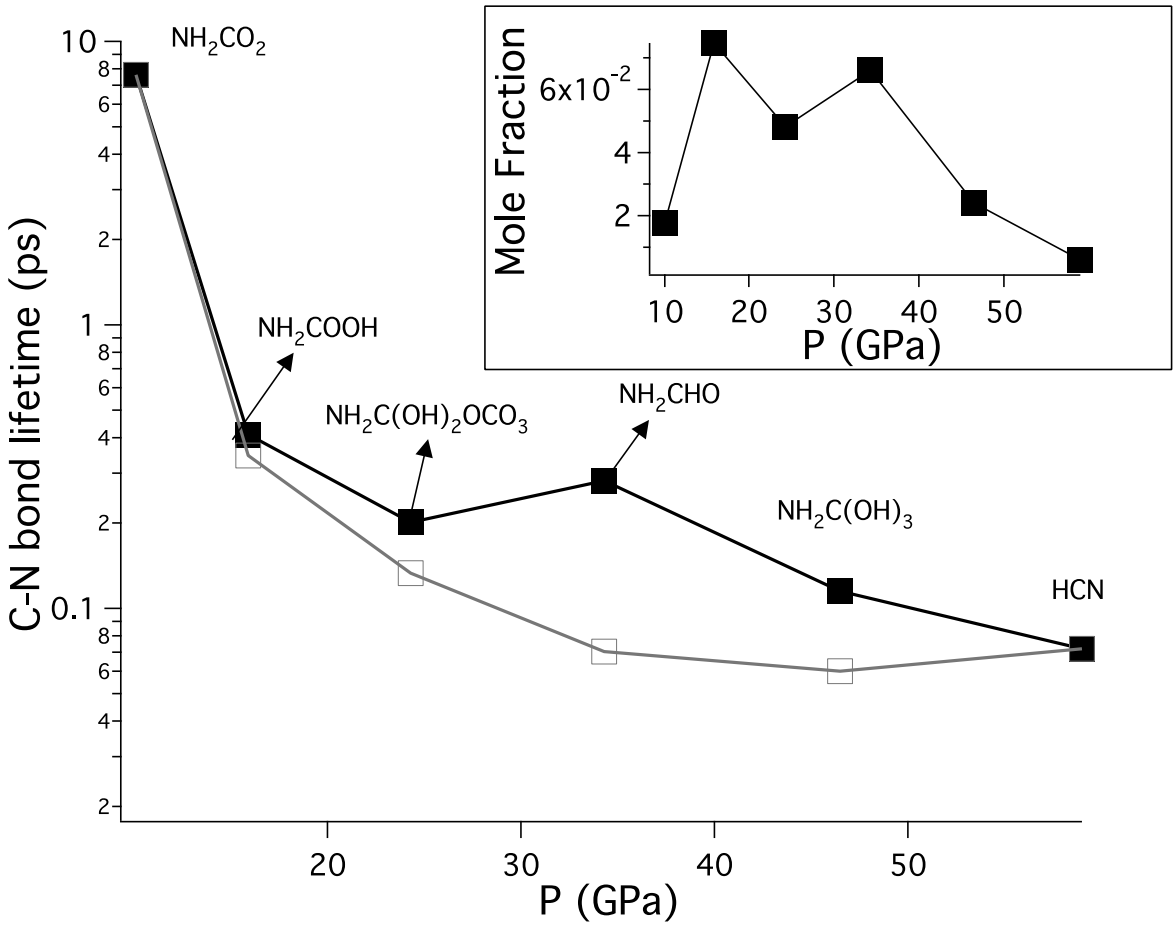

Figure S 3: Lifetimes of the C–N bonded species in our shock compression simulations. The black curve (filled squares) corresponds to the longest lived C–N bonded species in each simulation, the formulas for which are indicated above the curve. The gray curve (open squares) corresponds to the concentration weighted average C–N bond lifetime for each simulation. Inset: the total mole fraction of all C–N bonded species at each shock compression.

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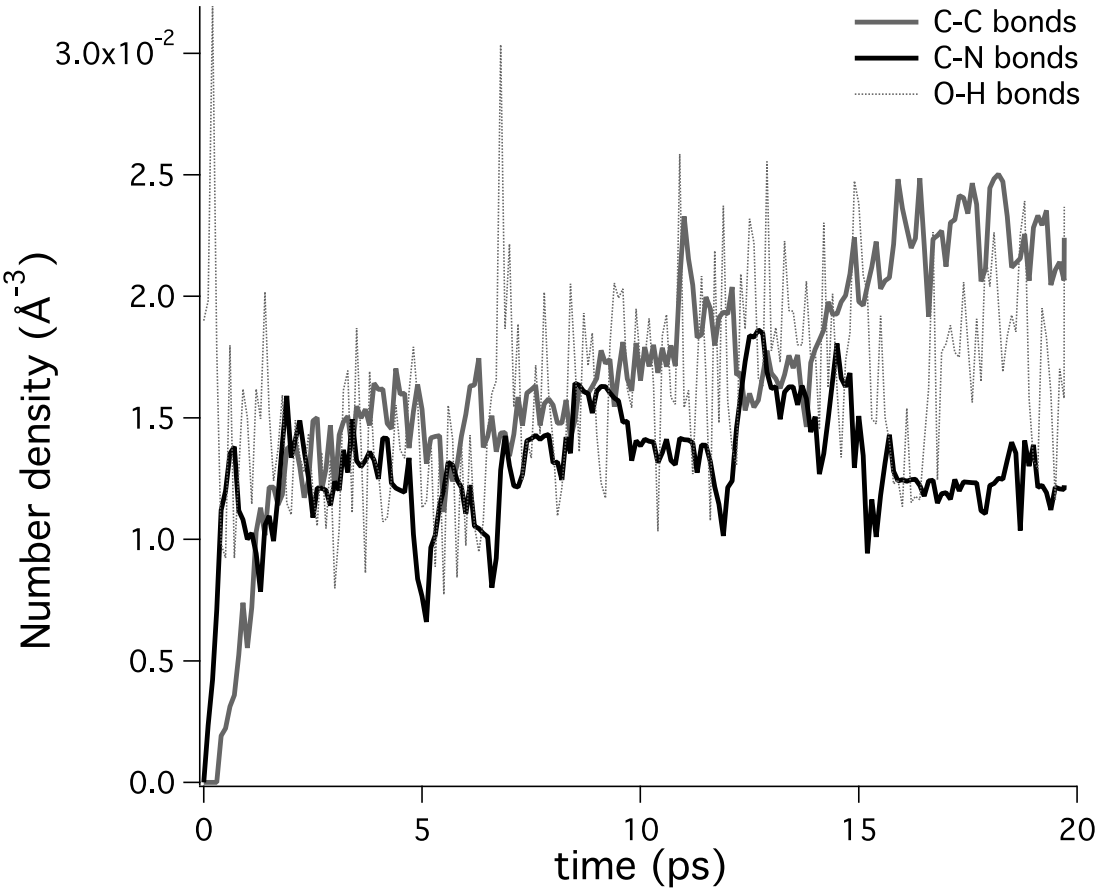

Figure S 4: Number density of different types of bonds as a function of time in our simulations of shock compression at 9 km/s with a system of 105 atoms.

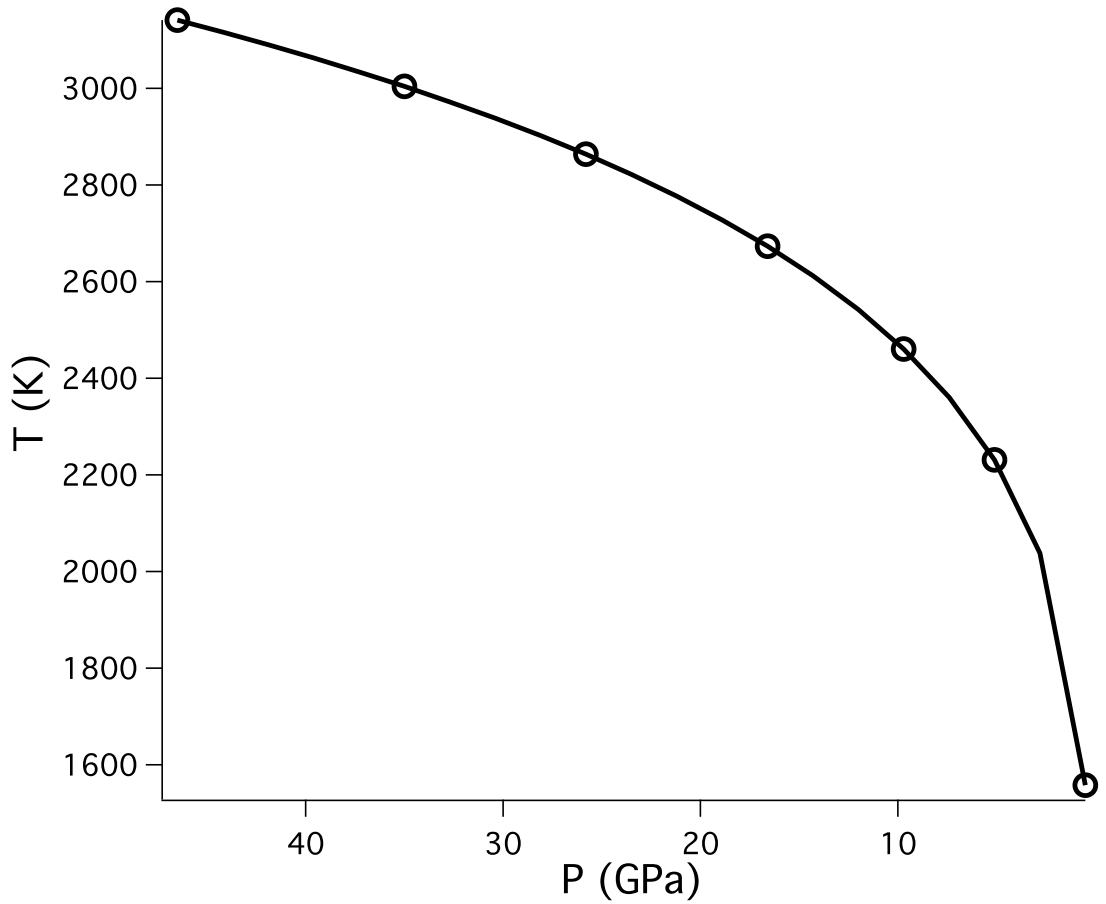

Figure S5: Plot of the isentropic expansion states. The solid line corresponds to the result computed from the equation of state model for water[10]. The circles correspond to the constant pressure-temperature points of the expansion discussed in the manuscript.

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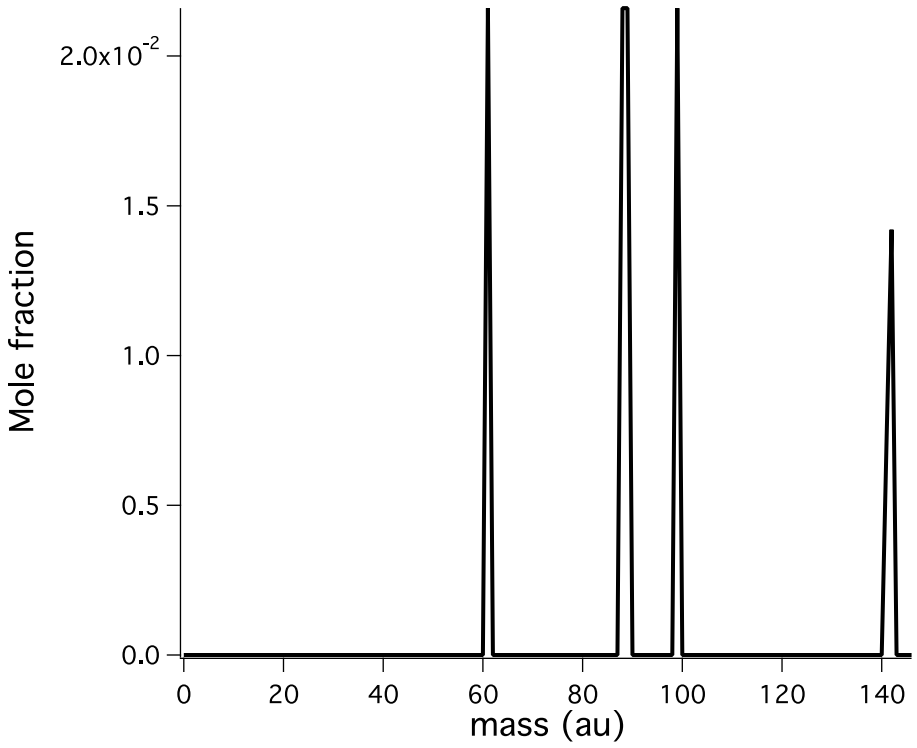
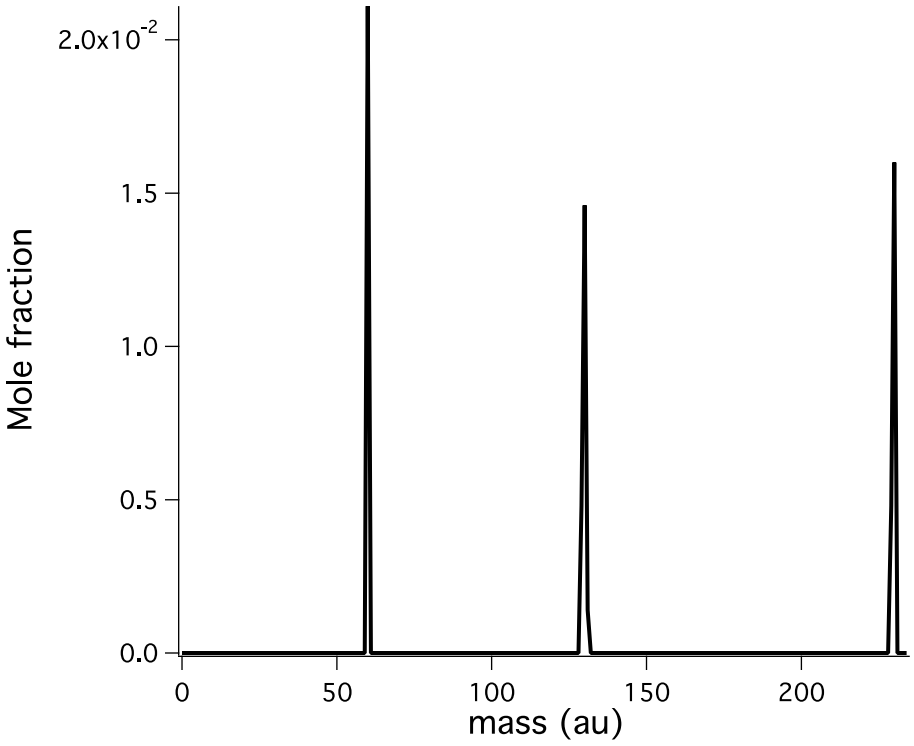
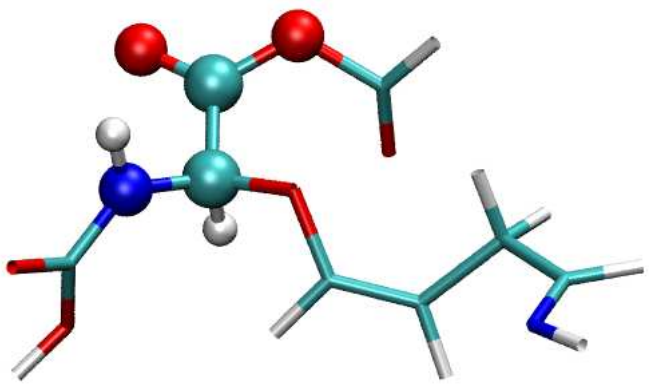


Figure S 6: Simulated mass spectrum C–N bonded species of the isentropic expansion after 3 ps of shock compression. The broad mass peak at 88-89 au corresponds to the deprotonated reactant and protonated product of the reaction NH_2-$(CH_2)_2$-COO^- + H^+ ↔ NH_2-$(CH_2)_2$-COOH. The mass peak at 60 au corresponds to NH_2-COO^-, the peak at 99 au to CH_2=N-CH=CH-COOH, and the peak at 142 au to CH_2=N-CH=CH-C(NH_2)-C(O)-CO_2^-.



(a)



(b)

Figure S 7: Simulated mass spectrum of C–N bonded species for the rapid isentropic expansion mentioned above. The graphic in (b) corresponds to the C–N oligomer at a mass peak of 230 au. The highlighted atoms (shown as colored spheres) correspond to a sequence very close to glycine. The mass peak at 60 au corresponds to NH_2-C(O)-NH_2, and the peak at 130 au to CHO-C(CHO)=NH-COOH.