# Structural Dynamics of 1,2-Diiodoethane in Cyclohexane Probed By Picosecond X-Ray Liquidography

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Supporting Information

Supplementary Figure S1. Kinetic scheme considering all the possible intermediate and product species involved in the reaction. The reaction pathways starting from $C_2H_4I_2$ parent molecule, C_2H_4I radical, C_2H_4I-I isomer, and I atom are indicated by black, red, green, and blue arrows, respectively.
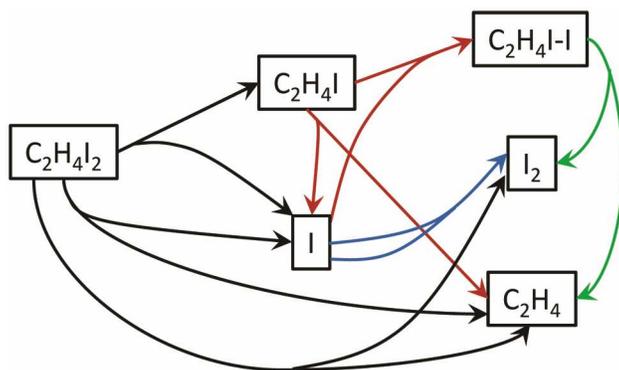
Supplementary Figure S2. The pair distribution functions, $g(r)$, calculated for each atom-atom pair in all of the chemical species involved in the photodissociation of $C_2H_4I_2$. Since a solute molecule has a relatively stable geometry formed by chemical bonds, $g(r)$ of an atomic pair in the solute molecule has a sharp distribution at the atom-atom distance calculated by DFT calculation. In contrast, due to dynamic solute-solvent interaction, $g(r)$ of an atomic pair between solute and solvent molecules (i.e. cage term) has a broad distribution obtained from molecular dynamics (MD) simulation. From these $g(r)$'s, scattering intensities of solute and cage terms are calculated. Also, by using the peak positions of $g(r)$'s as shown in Figure 4 in the main text, the oscillatory features in the difference scattering curves measured by TRXL can be assigned on the basis of atomic pairs.
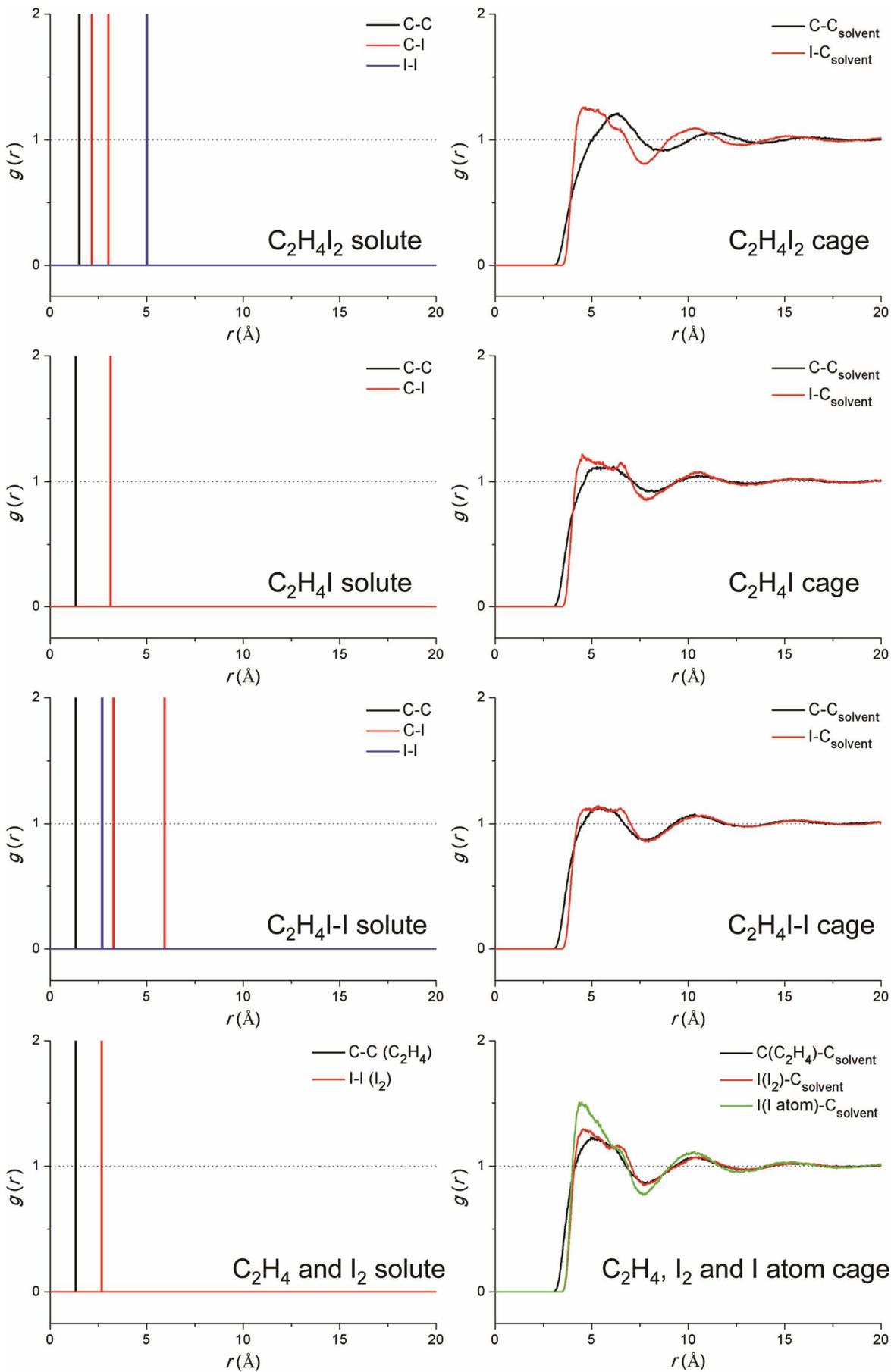
Supplementary Figure S3. Comparison of the bridged model and the anti model. The fitting qualities of the two models at each time point are compared by the ratio of reduced chi-square values obtained from the global fitting using the two models. At 100 ps, where the concentration of $C_2H_4I\cdot$ radical is high, the ratio is significantly below 1, indicating that the bridged model fits the experimental data much better than the anti model. As the concentration of C_2H_4I radical decreases at later time delays, the ratio expectedly approaches 1.