Variation and Decomposition of the Partial Molar Volume of Small Gas Molecules in Different Organic Solvents Derived from Molecular Dynamics Simulations

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Figure S1: Scheme of how XCav locates empty space in solutions. First, the simulation box is divided into cubic cells of predefined size. Centered on each atom (shown together with bonds in red) a sphere with corresponding van der Waals radius was placed (in orange). Atom specific van der Waals radii were derived from the used force field. For each cell, the distances between the cell center and all atoms were calculated. Whenever at least one of these distances was found to be smaller than the sum of atomic van der Waals radius and half of the cell side length, this cell was considered to be inside one of the spheres and thus deleted. The remaining cells (in green) indicate unoccupied space in the structure.
Figure S2: Orientation of cylindrical coordinate system to describe pair distributions of solute and empty space cells, $g_{sx}(r,z)$ as defined in eq 9. The origin of the coordinate system is the center-of-mass of the solute (shown in red). The z-axis is oriented in the direction of the solute velocity, $\vec{v}$, with z-values decreasing in that direction. The coordinate $r$ designates the radial distance of the cell from the z-axis, i.e. it is the component perpendicular to the solute movement. Shown is the center of one empty space cell at point $(r,z)$. Surrounding solvent molecules (blue) envelop the solvent cage (white). The solvent cage is represented by empty space cells as indicated by the grid that were previously found by XCav.
Figure S3: Changes of total energy (upper half) and volume (lower half) during the production run of the MD simulation of 10 CO₂ solvated in acetone.
Figure S4: Changes of total energy (upper half) and volume (lower half) during the production run of the MD simulation of 10 CO$_2$ solvated in methanol.
Figure S5: Changes of total energy (upper half) and volume (lower half) during the production run of the MD simulation of 10 CO₂ solvated in heptane.
**Figure S6:** Changes of total energy (upper half) and volume (lower half) during the production run of the MD simulation of 10 CO$_2$ solvated in diethylether.
Figure S7: Radial distribution function, $g^{\text{rdf}}$, as a function of the center-of-mass distance, $r$, between pairs of CO$_2$ and acetone. Shown are the RDFs that were derived from averaging over the entire production run of 5 ns (black), the first nanosecond of the production run (red) and the last nanosecond of the production run (blue), respectively.
Figure S8: Radial distribution function, $g^{\text{def}}$, as a function of the center-of-mass distance, $r$, between pairs of CO$_2$ and methanol. Shown are the RDFs that were derived from averaging over the entire production run of 5 ns (black), the first nanosecond of the production run (red) and the last nanosecond of the production run (blue), respectively.
Figure S9: Radial distribution function, $g^{\text{.rdf}}$, as a function of the center-of-mass distance, $r$, between pairs of CO$_2$ and heptane. Shown are the RDFs that were derived from averaging over the entire production run of 5 ns (black), the first nanosecond of the production run (red) and the last nanosecond of the production run (blue), respectively.
Figure S10: Radial distribution function, \( g_{df} \), as a function of the center-of-mass distance, \( r \), between pairs of CO\(_2\) and diethylether. Shown are the RDFs that were derived from averaging over the entire production run of 5 ns (black), the first nanosecond of the production run (red) and the last nanosecond of the production run (blue), respectively.