Supporting Information
Deep Eutectic Solvents Mixed with Fluorinated Refrigerants for Absorption Refrigeration:
A Molecular Simulation Study

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Table S1. Non-bonded parameters for levulinic acid

| Atom name	GAFF atom type	Partial charge (e)	vdW radius (A)	Well depth (kcal/mol)
CF	c	0.7715	1.9080	0.0860
CG	c3	-0.1103	1.9080	0.1094
CH	c3	-0.0358	1.9080	0.1094
CI	c	0.6301	1.9080	0.0860
CJ	c3	-0.4086	1.9080	0.1094
OF	o	-0.5962	1.6612	0.2100
OHF	oh	-0.6871	1.7210	0.2104
OI	o	-0.5632	1.6612	0.2100
HOF	ho	0.4583	0.1120	0.0010
HG1	hc	0.0652	1.4870	0.0157
HG2	hc	0.0652	1.4870	0.0157
HH1	hc	0.0277	1.4870	0.0157
HH2	hc	0.0277	1.4870	0.0157
HJ1	hc	0.1185	1.4870	0.0157
HJ2	hc	0.1185	1.4870	0.0157
HJ3	hc	0.1185	1.4870	0.0157

All bonded parameters are taken from the GAFF force field

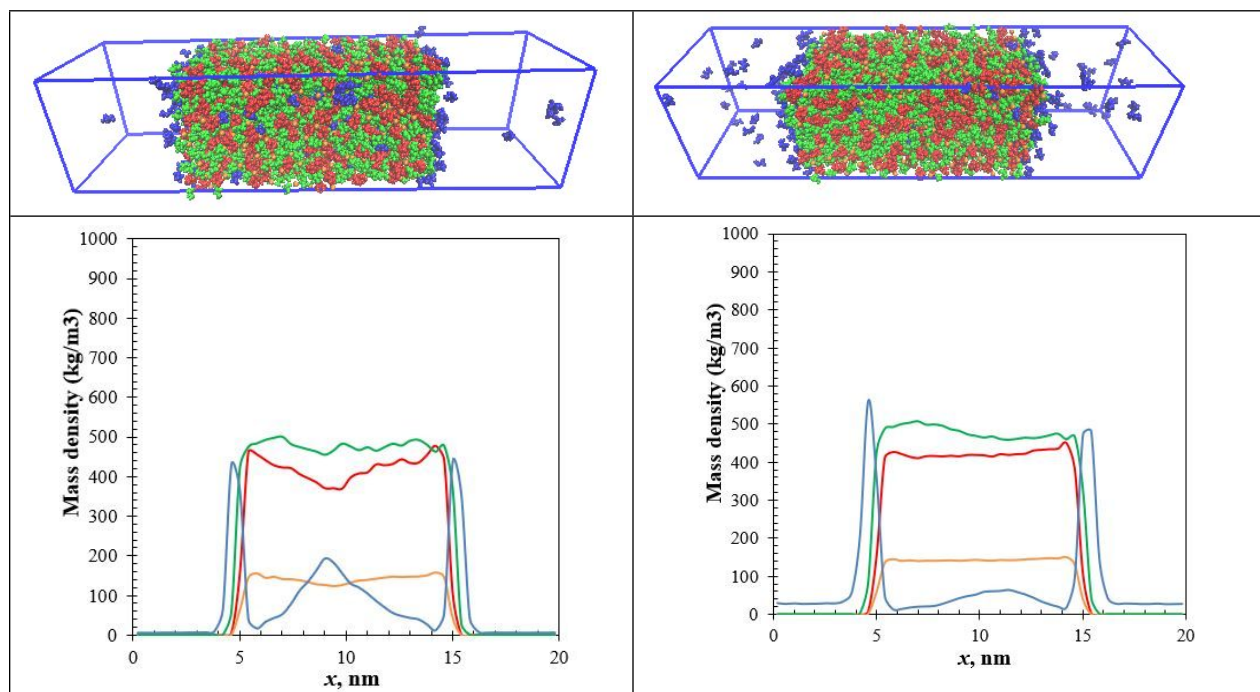* Corresponding author. E-mail: f.hung@northeastern.edu
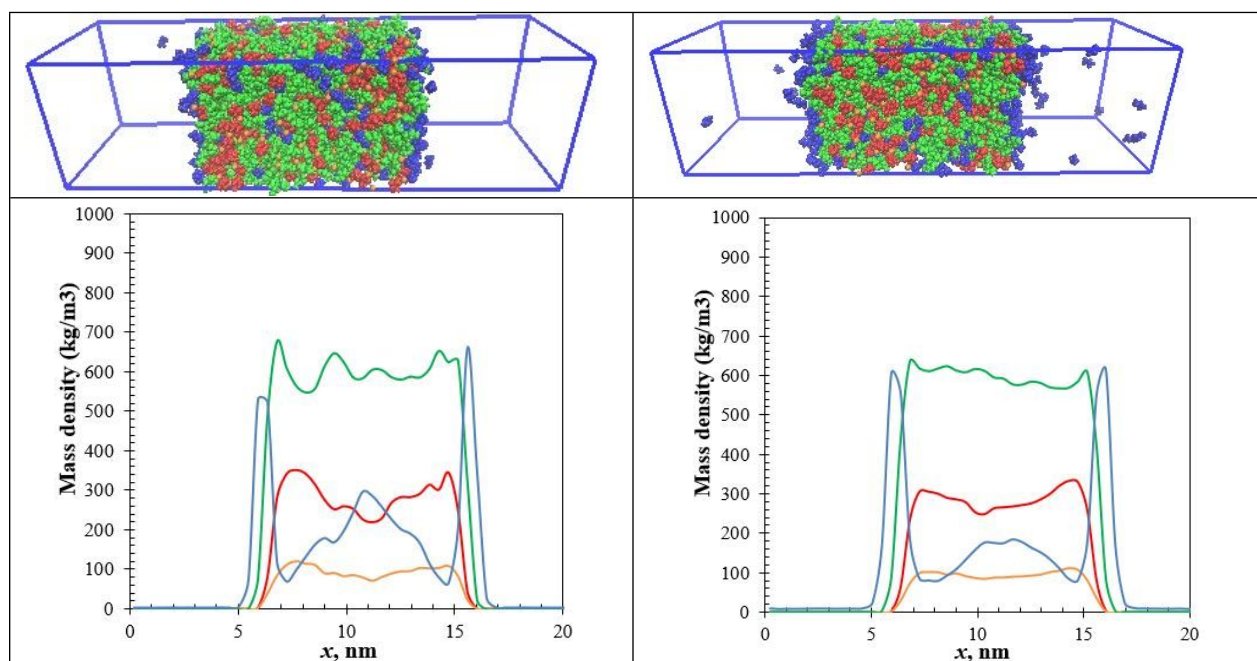
Figure S1. Representative simulation snapshots (top) and local density profiles (bottom) of systems of R245fa in levuline, from *NVT* simulations in elongated boxes with *T* = 298 K (left) and *T* = 343 K (right). Red = choline (cation), orange = chlorine (anion), green = levulinic acid (HBD), and blue = R245fa (refrigerant).
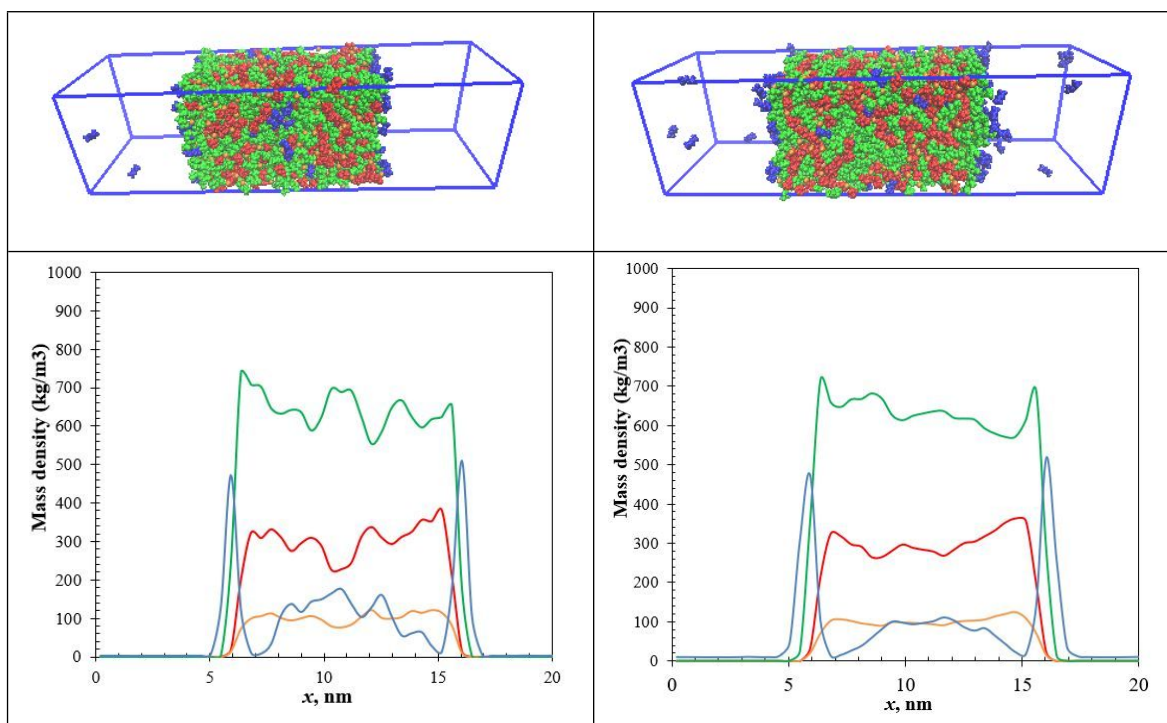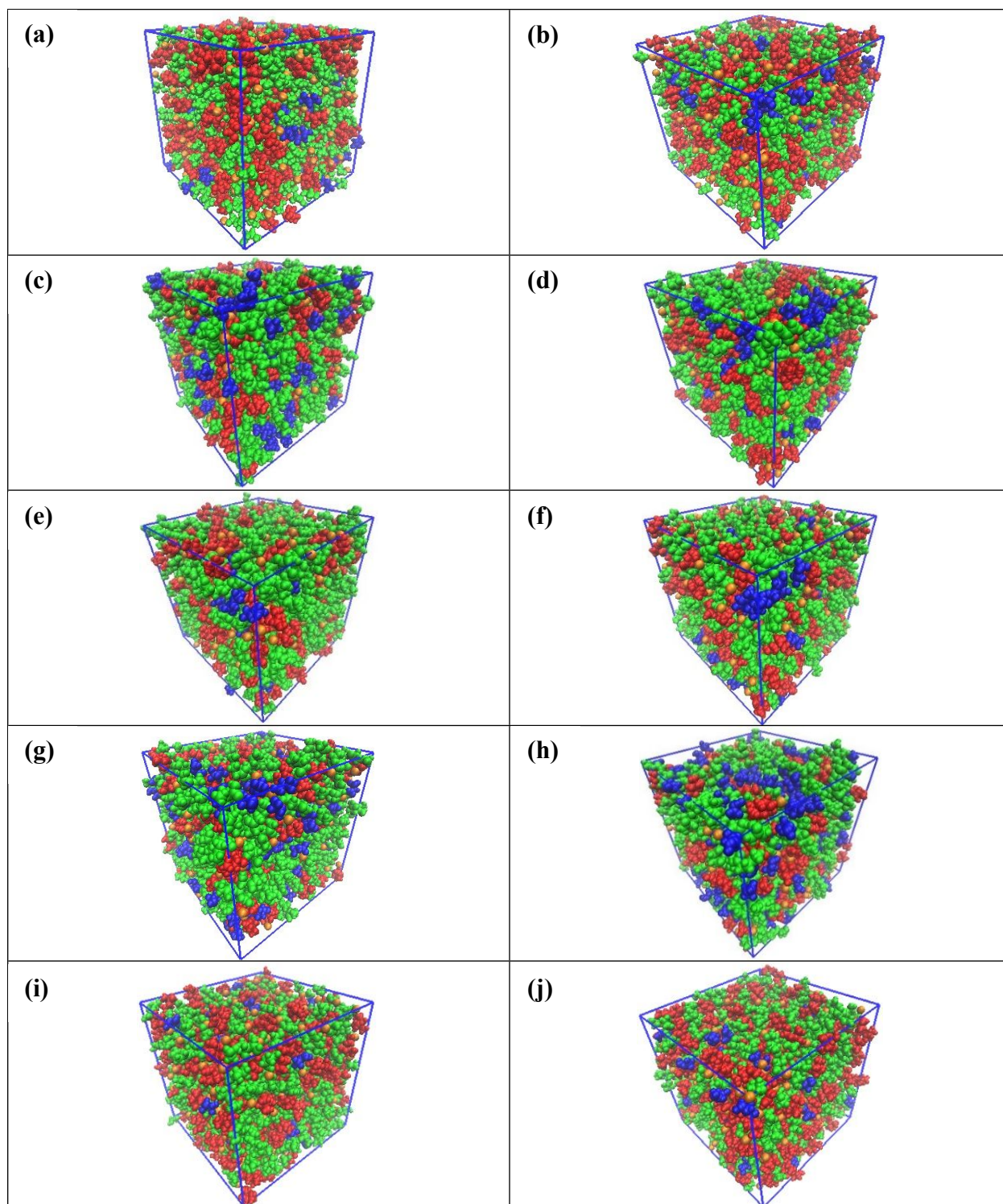
Figure S2. Representative simulation snapshots (top) and local density profiles (bottom) of systems of HFO1336mzzE in levuline, from NVT simulations in elongated boxes with $T = 298$ K (left) and $T = 343$ K (right). Red = choline (cation), orange = chlorine (anion), green = levulinic acid (HBD), and blue = HFO1336mzzE (refrigerant).
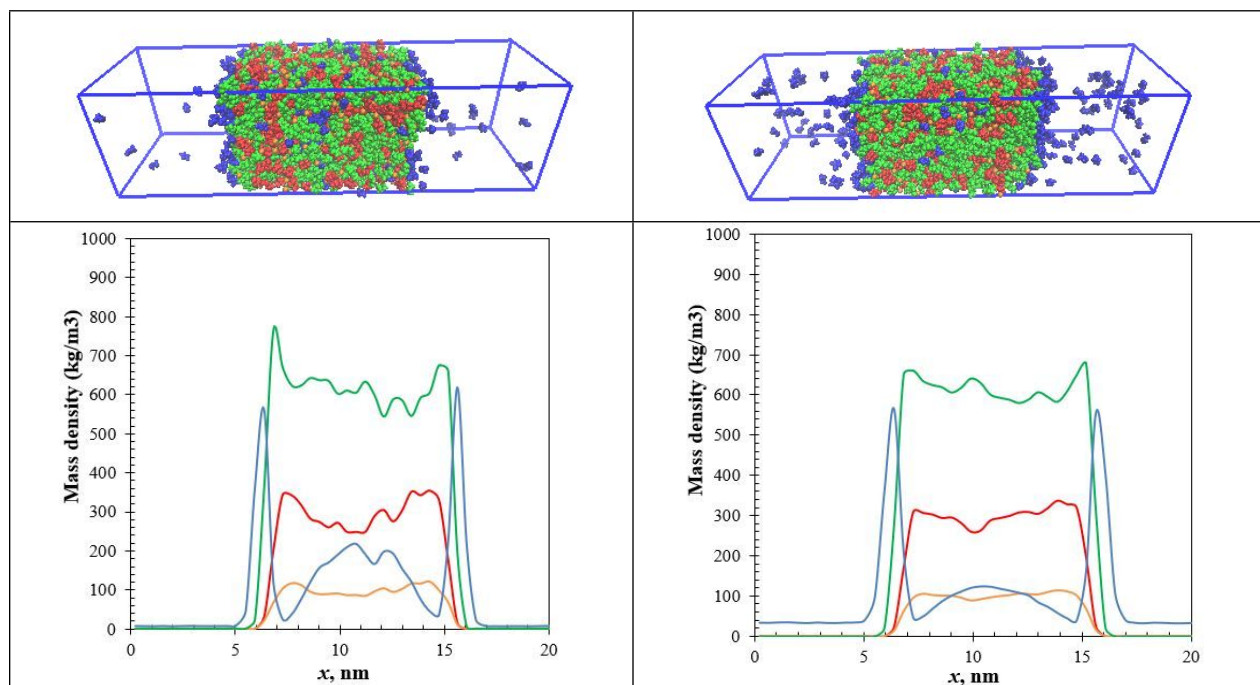
Figure S3. Representative simulation snapshots (top) and local density profiles (bottom) of systems of R1234zeE in levuline, from *NVT* simulations in elongated boxes with $T = 298$ K (left) and $T = 343$ K (right). Red = choline (cation), orange = chlorine (anion), green = levulinic acid (HBD), and blue = R1234zeE (refrigerant).

Figure S4. Representative simulation snapshots (top) and local density profiles (bottom) of systems of R1234zeE in ethaline, from *NVT* simulations in elongated boxes with *T* = 298 K (left) and *T* = 343 K (right). Red = choline (cation), orange = chlorine (anion), green = ethylene glycol (HBD), and blue = R1234zeE (refrigerant).

Figure S5. Representative simulation snapshots of refrigerant-DES mixtures at T_5 = 298 K (left column) and T_8 = 343 K (right column). (a,b) R245fa-ethaline, x_R = 5%, P_5 = 1.0 bar, P_8 = 2.5 bar; (c,d) R245fa-levuline, x_R = 15%, P_5 = 1.0 bar, P_8 = 2.5 bar; (e,f) HFO1336mzzE-levuline, x_R = 5%, P_5 = 1.4 bar, P_8 = 3.2 bar; (g,h) R1234zeE-levuline, x_R = 20%, P_5 = 3.7 bar, P_8 = 7.7 bar; (i,j) R1234zeE-ethaline, x_R = 5%, P_5 = 3.7 bar, P_8 = 7.7 bar. Red = choline (cation), orange = chlorine (anion), green = HBD, and blue = refrigerant.
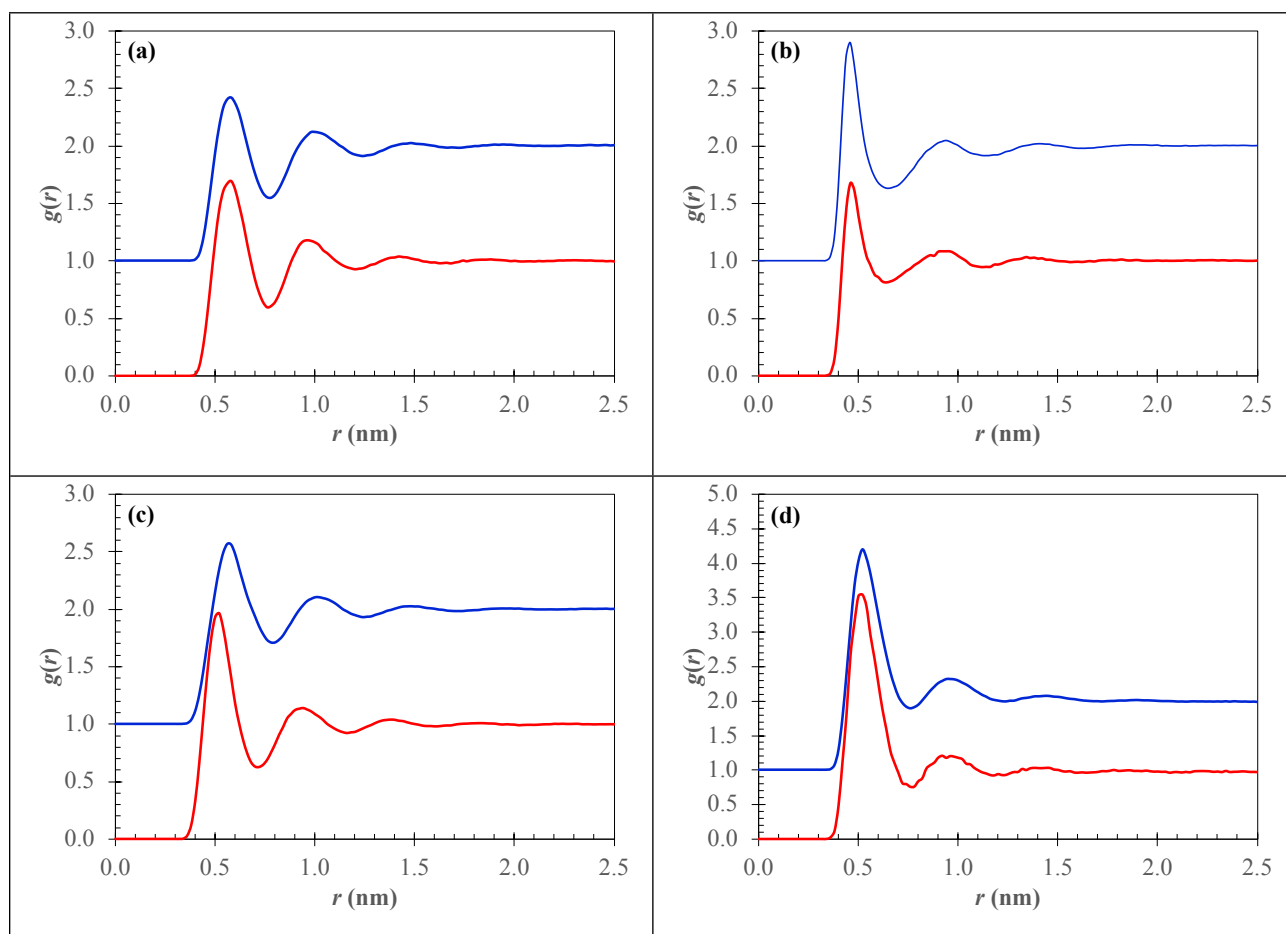
Figure S6. Center-of-mass radial distribution functions $g(r)$ at $T_5 = 298$ K for (a) cation-refrigerant, (b) anion-refrigerant, (c) HBD-refrigerant, and (d) refrigerant-refrigerant pairs. Blue = R1234zeE-levuline, $P_5 = 3.7$ bar, $x_R = 20\%$; red = R1234zeE-ethaline, $P_5 = 3.7$ bar, $x_R = 5\%$.
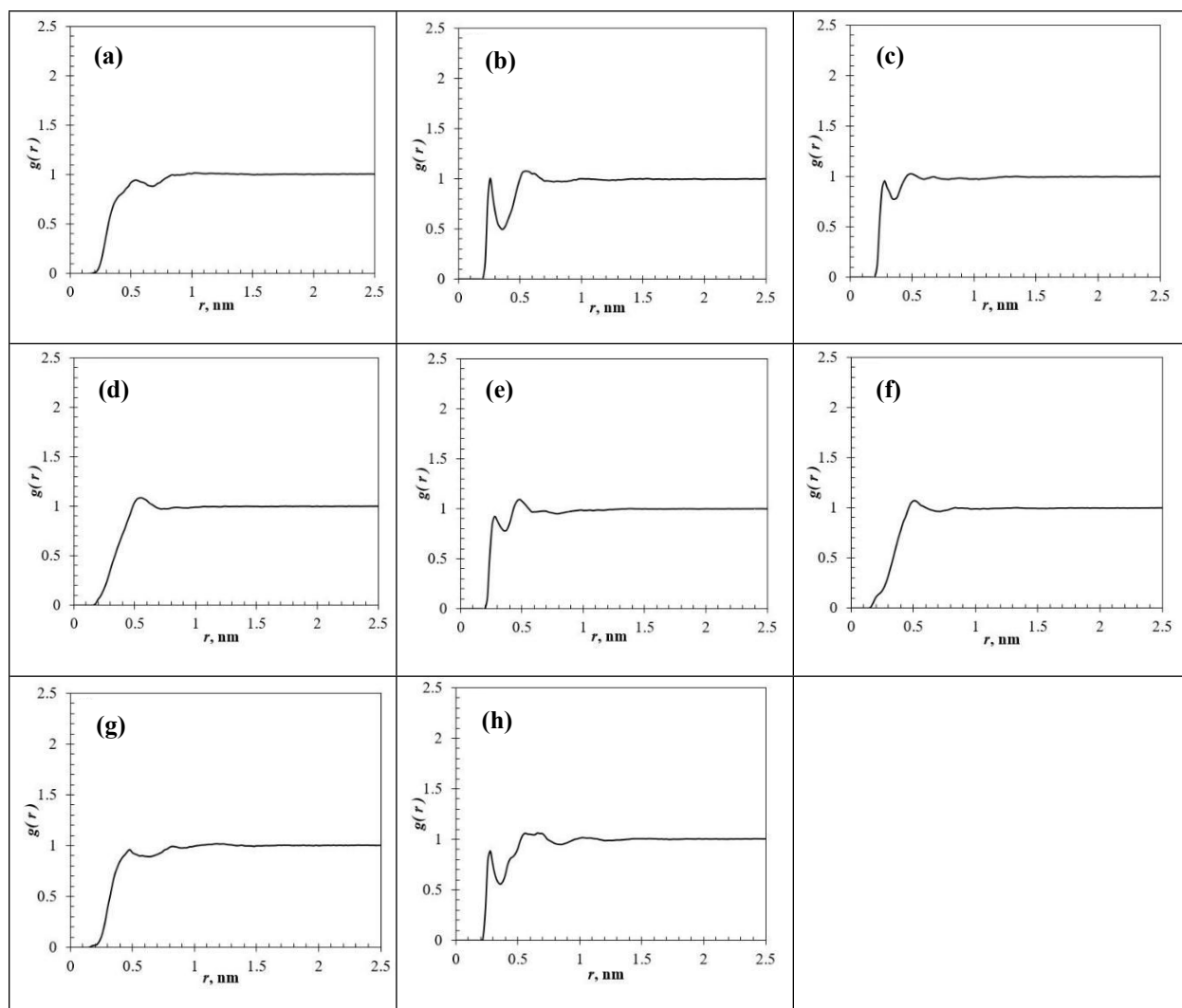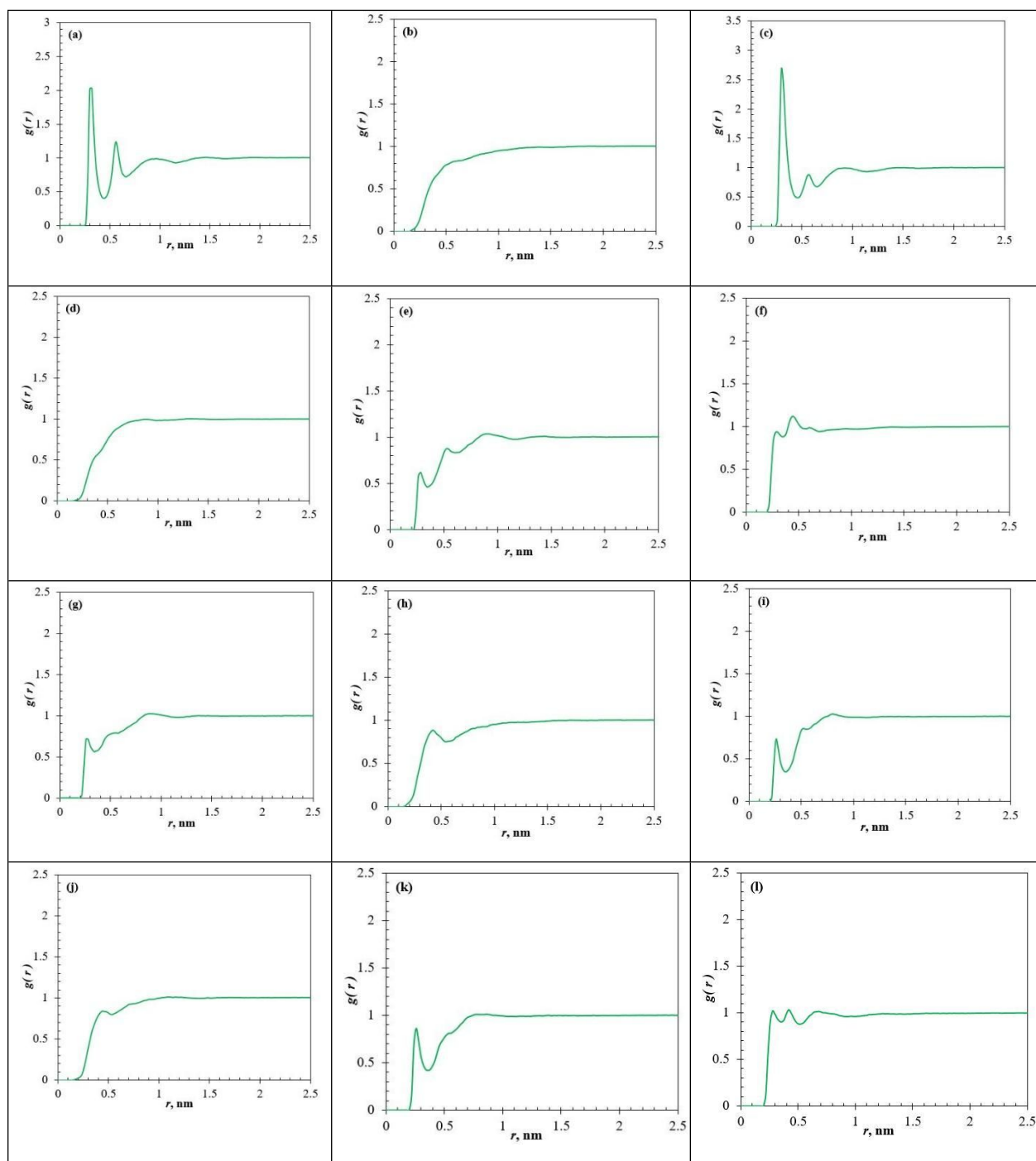
Figure S7. Atom-atom radial distribution functions *g*(*r*) in systems containing R245fa (5% molar) and ethaline at 298 K and 1 bar, for the following pairs: (a) FAA (R245fa) – HO1 (cation), (b) HAH (R245fa) – OAA (HBD), (c) FAC (R245fa) – HAC (HBD), (d) FAA (R245fa) – HAA (HBD), (e) FAA (R245fa) – HAC (HBD), (f) FAC (R245fa) – HAA (HBD), (g) FAC (R245fa) – HO1 (cation), (h) HAF (R245fa) – OAA (HBD).
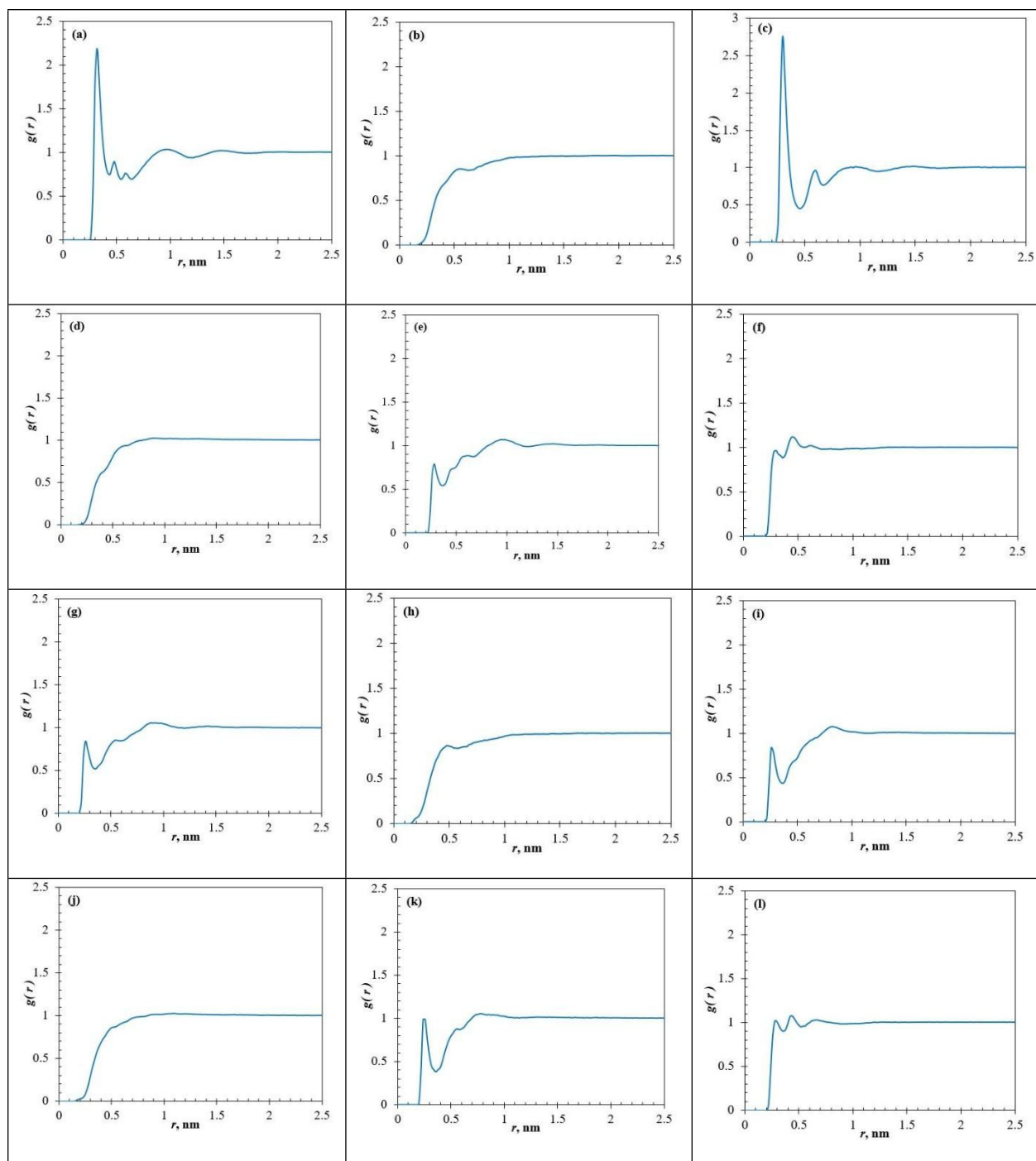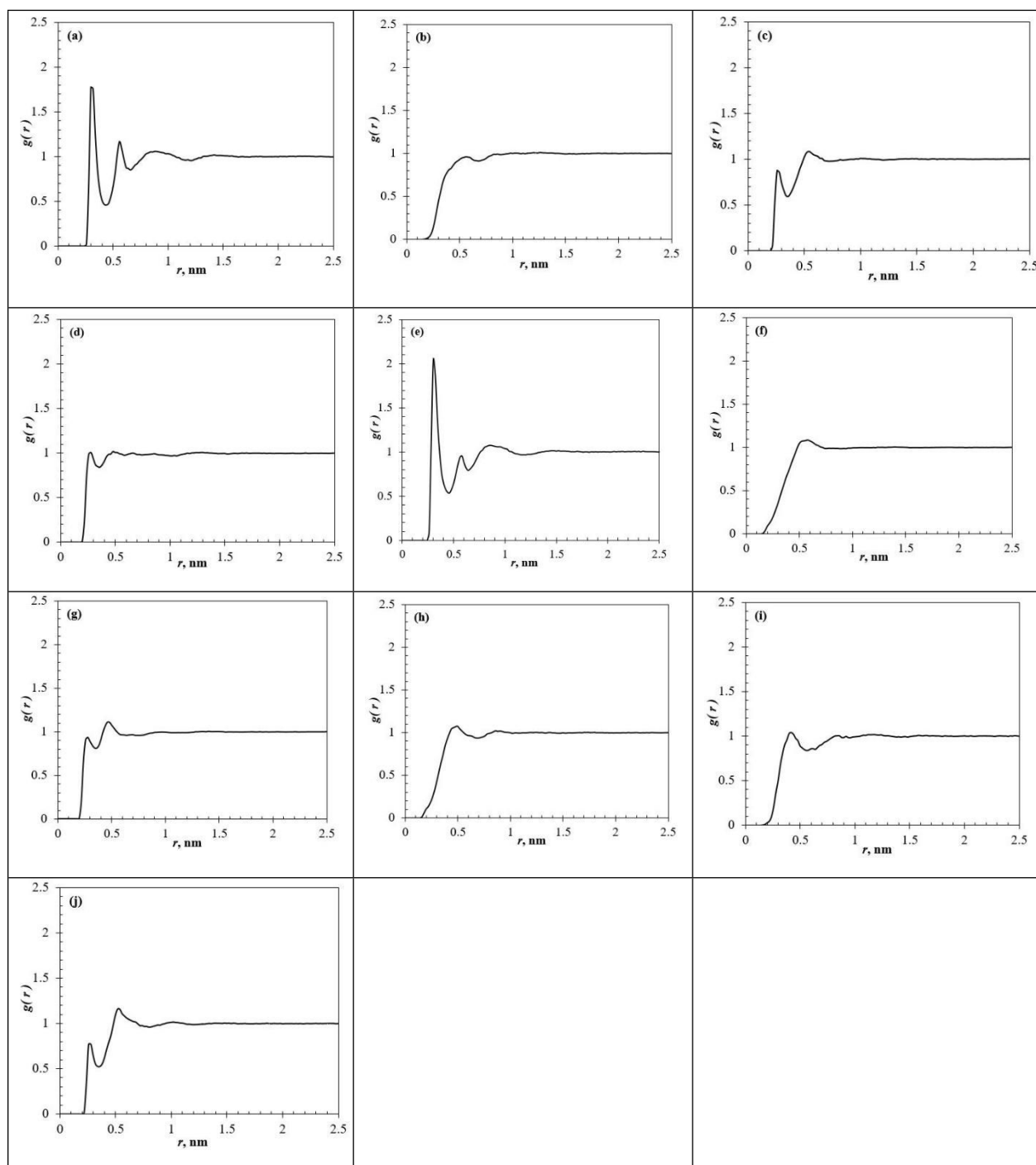
Figure S8. Atom-atom radial distribution functions g(r) in systems containing R245fa (15%) and levuline at 298 K and 1 bar, for the following pairs: (a) HAF (R245fa) – Cl (anion), (b) FAA (R245fa) – HO1 (cation), (c) HAH (R245fa) – Cl (anion), (d) FAA (R245fa) – HOF (HBD), (e) HAF (R245fa) – OHF (HBD), (f) FAA (R245fa) – HJ1 (HBD), (g) HAH (R245fa) – OHF (HBD), (h) FAC (R245fa) – HO1 (cation), (i) HAF (R245fa) – OF (HBD), (j) FAC (R245fa) – HOF (HBD), (k) HAH (R245fa) – OF (HBD), (l) FAC (R245fa) – HJ1 (HBD).
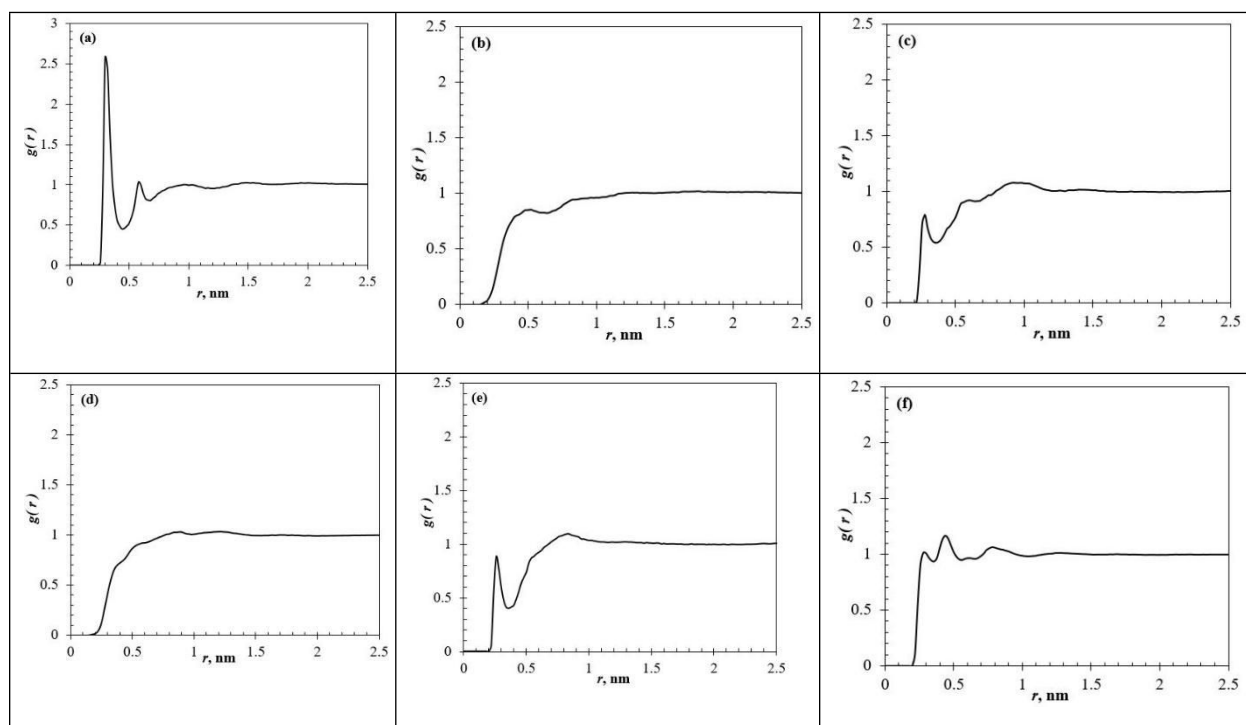
Figure S9. Atom-atom radial distribution functions g(r) in systems containing HFO1336mzzE (5%) and levuline at 298 K and 1.4 bar, for the following pairs: (a) HAF (HFO-1336mzzE) – Cl (anion), (b) FAA (HFO-1336mzzE) – HO1 (cation), (c) HAF (HFO-1336mzzE) – OHF (HBD), (d) FAA (HFO-1336mzzE) – HOF (HBD), (e) HAF (HFO-1336mzzE) – OF (HBD), (f) FAA (HFO-1336mzzE) – HJ1 (HBD).

Figure S10. Atom-atom radial distribution functions g(r) in systems containing R1234zeE (20%) and levuline at 298 K and 3.7 bar, for the following pairs: (a) HAE (R1234zeE) – Cl (anion), (b) FAA (R1234zeE) – HO1 (cation), (c) HAD (R1234zeE) – Cl (anion), (d) FAA (R1234zeE) – HOF (HBD), (e) HAE (R1234zeE) – OHF (HBD), (f) FAA (R1234zeE) – HJ1 (HBD), (g) HAD (R1234zeE) – OHF (HBD), (h) FAC (R1234zeE) – HO1 (cation), (i) HAE (R1234zeE) – OF (HBD), (j) FAC (R1234zeE) – HOF (HBD), (k) HAD (R1234zeE) – OF (HBD), (l) FAC (R1234zeE) – HJ1 (HBD).

Figure S11. Atom-atom radial distribution functions g(r) in systems containing R1234zeE (5%) and ethaline at 298 K and 3.7 bar, for the following pairs: (a) HAE (R1234zeE) – Cl (anion), (b) FAA (R1234zeE) – HO1 (cation), (c) HAD (R1234zeE) – OAA (HBD), (d) FAC (R1234zeE) – HAC (HBD), (e) HAD (R1234zeE) – Cl (anion), (f) FAA (R1234zeE) – HAA (HBD), (g) FAA (R1234zeE) – HAC (HBD), (h) FAC (R1234zeE) – HAA (HBD), (i) FAC (R1234zeE) – HO1 (cation), (j) HAE (R1234zeE) – OAA (HBD).
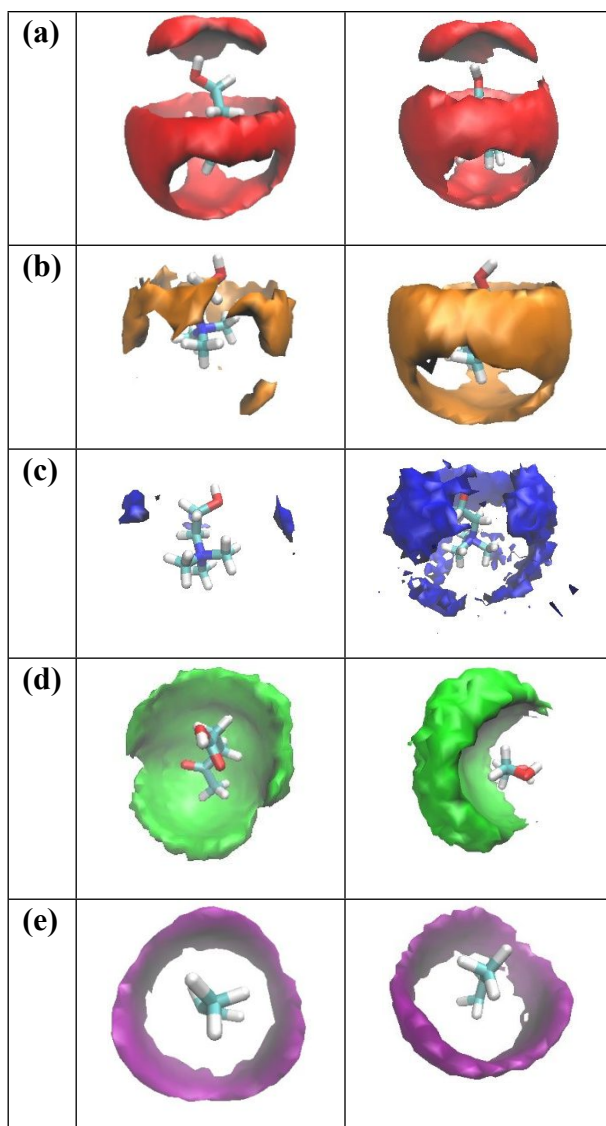
Figure S12. Spatial distribution functions (SDFs) at $T_5 = 298$ K of the following refrigerant-DES mixtures: (left column) R1234zeE-levuline, $x_R = 20\%$, $P_5 = 3.7$ bar and (right column) R1234zeE-ethaline, $x_R = 5\%$, $P_5 = 3.7$ bar. SDFs for the following pairs are presented: (a) cation-anion, (b) cation-HBD, (c) cation-refrigerant, (d) HBD-refrigerant, (e) refrigerant-anion.
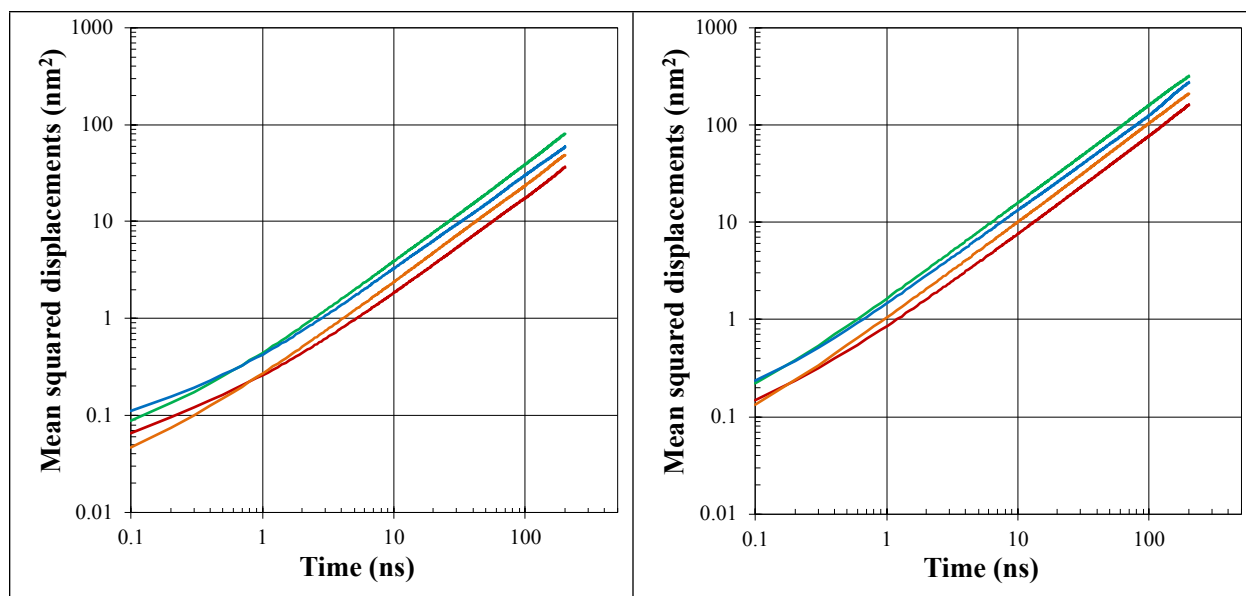
Figure S13. Mean squared displacements as a function of time in systems of R245fa in ethaline, at T_5 = 298 K and P_5 = 1.0 bar (left), and at T_8 = 343 K and P_8 = 2.5 bar (right). Red = choline (cation), orange = chlorine (anion), green = ethylene glycol (HBD), and blue = R245fa (refrigerant).