Electronic Supplementary Information to: From Cold to Hot, The Structure and Structural Dynamics of Dense Ionic Fluids

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1 Simulation Methods

Simulation methods for sections other than 2.1 in the main article have been previously described and are appropriately referenced. For section 2.1 a description is provided below.

1.1 PIM Simulation Methods

PIM molecular dynamics simulations at constant temperature (900 °C) and pressure (1 bar) of UCl_3, UCl_3-KCl (20-80 mol %), and KCl were run using the Metalwalls software (release 20.05)[1] using an identical protocol for equilibration and production as previously described for $LaCl_3$ and its mixtures in reference 2. The number of ions used in this study are listed in Table 1; other parameters for the PIM model are provided in Tables 2 and 3. As proposed in reference 3, the polarizabilities of K^+ and Cl^- are taken to be 4.7 $bohr^3$ and 20.0 $bohr^3$ respectively; U^{3+} is taken as non-polarizable.

Table 1 Number of Ions Used in PIM Simulations

Salt	Ion Type		
	# U	# K	# Cl
UCl_3	1000	0	3000
UCl_3-KCl (20-80)	300	1200	2100
KCl	0	2000	2000

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Table 2 Charge-Dipole Damping Parameters

Ion-Pair	b_4^{ij}=b_4^{ji}	c_4^{ij}	c_4^{ji}	Ref.
U^{3+}-Cl^-	1.258	1.000	N/A	[4]
K^+-Cl^-	1.632	3.000	0.917	[3]

Table 3 BMH Parameters

Ion-Pair	α_{ij}	B_{ij}	C_{ij}^6	C_{ij}^8	b_{ij}^6	b_{ij}^8	Ref.
U^{3+}-U^{3+}	3.000	15.0	47.70	100.0	1.50	1.00	[4]
U^{3+}-K^+	3.000	10.0	34.80	94.6	1.50	1.00	[4]
K^+-K^+	5.000	1.0	1.0	10.0	1.70	1.70	[3]
U^{3+}-Cl^-	1.800	400.0	97.22	600.0	1.50	1.00	[4]
K^+-Cl^-	1.833	208.6	29.40	128.3	1.70	1.70	[3]
Cl^--Cl^-	1.797	275.1	140.0	280.0	1.70	1.70	[3]

References

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