Molten Alkali Halides - Temperature Dependence of Structure, Dynamics and Thermodynamics - Supporting Information

Marie-Madeleine Walz and David Van der Spoel*

Department of Cell and Molecular Biology, Uppsala University, Husargatan 3, Box 596, SE-75124 Uppsala, Sweden

E-mail: david.vanderspoel@icm.uu.se

Evaluation methods

The interionic distances reported for X-ray diffraction can stem from a direct evaluation of the average total correlation function G(r),[1–3] radial distribution function D(r)[4,5] or D(r)/r,[2] or partial radial distribution functions.[6] The terms correlation function and radial distribution function are sometimes used interchangeably; the difference between G(r) and D(r) being a factor $\frac{1}{4\pi r^2}$. Ohno et al.[2,7] evaluate the first neighbour distance from D(r), D(r)/r and G(r) for molten LiBr and NaCl; the maximum differences were found to be 4 pm and 8 pm, respectively, this is within the usually stated experimental error of ± 10 pm. While it is common for X-ray diffraction experiments to evaluate the total radial or correlation distribution function, for Neutron diffraction data the partial radial distribution function is evaluated in certain cases.

There are also different methods to evaluate the coordination number. Biggin et al.[8] list four methods using either the partial g(r) or the total G(r) correlation functions: (i) symmetrical rg(r),

---

*To whom correspondence should be addressed

(ii) symmetrical $r^2g(r)$, integration to the first minimum in (iii) g(r) or (iv) $r^2g(r)$. The authors evaluate the different methods for NaCl using g(r) which results in values from 3.9 to 5.3 (ΔCN 1.4). For G(r) the difference is lower, and results in 4.0 to 4.5 (ΔCN 0.5). For X-ray diffraction experiments, usually G(r) (or D(r)) is evaluated.

Overall it can be concluded, that despite the fact that there are different methods to evaluate both the interionic distance and the CNs, it is not likely that the large observed discrepancies originate from the specific methods used, although they certainly contribute to fluctuations. In computational sciences, usually the partial radial distribution function is evaluated for reading out interionic distances and for determining the CN by integrating to the first minimum. This is a straightforward approach that should result in reproducible numbers.

In this paper we use the term radial distribution function (the equation is given in the main paper) that is nowadays often used for what was in older literature referred to as pair correlation function.

Radial distribution functions at the melting point T$_m$

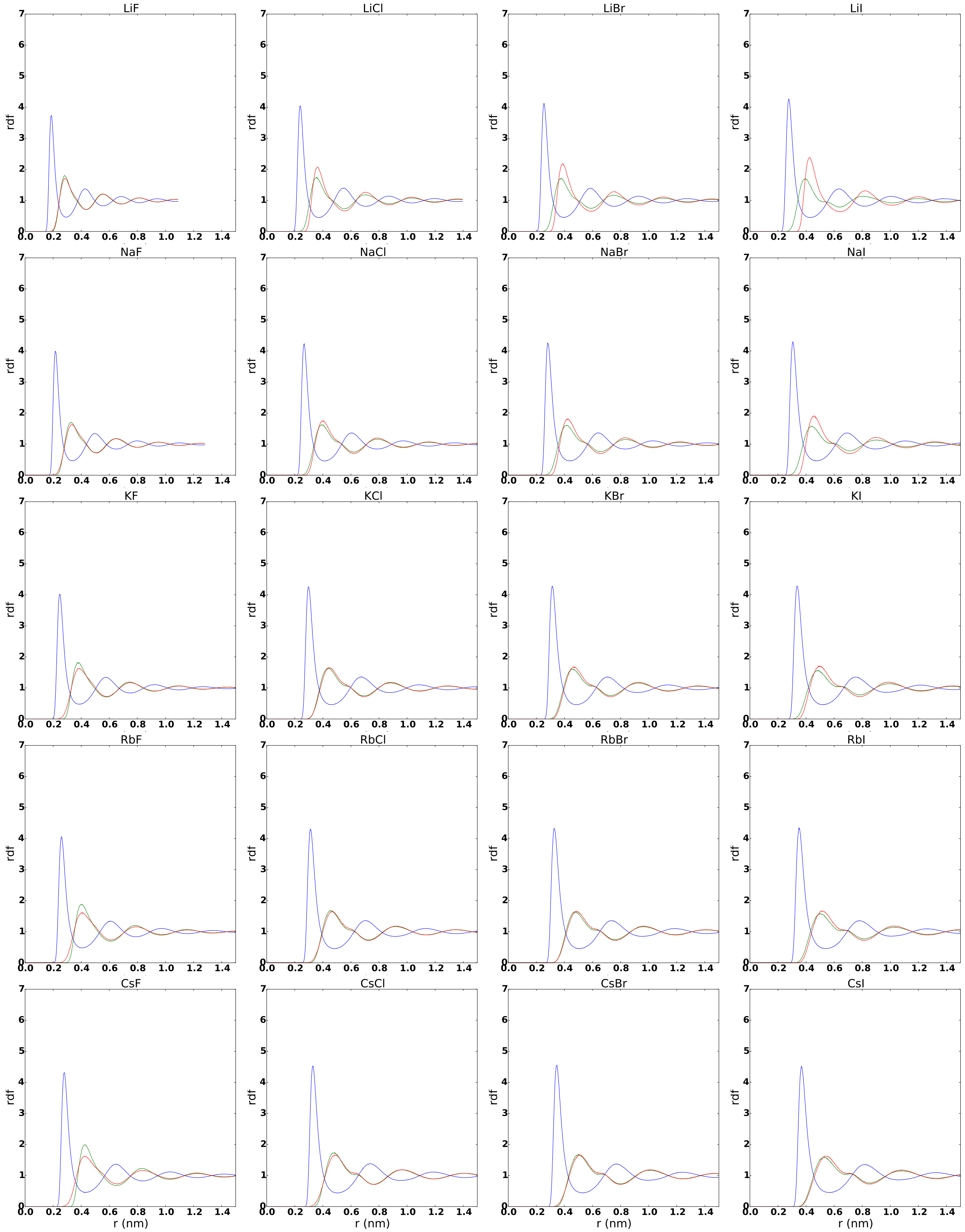

Figure S1: Radial distribution functions for all alkali halide melts at $T_{m,exp}$ simulated with our polarisable WBK force field. In dark blue $g(r)_{+-}$, in green $g(r)_{++}$ and in red $g(r)_{--}$.

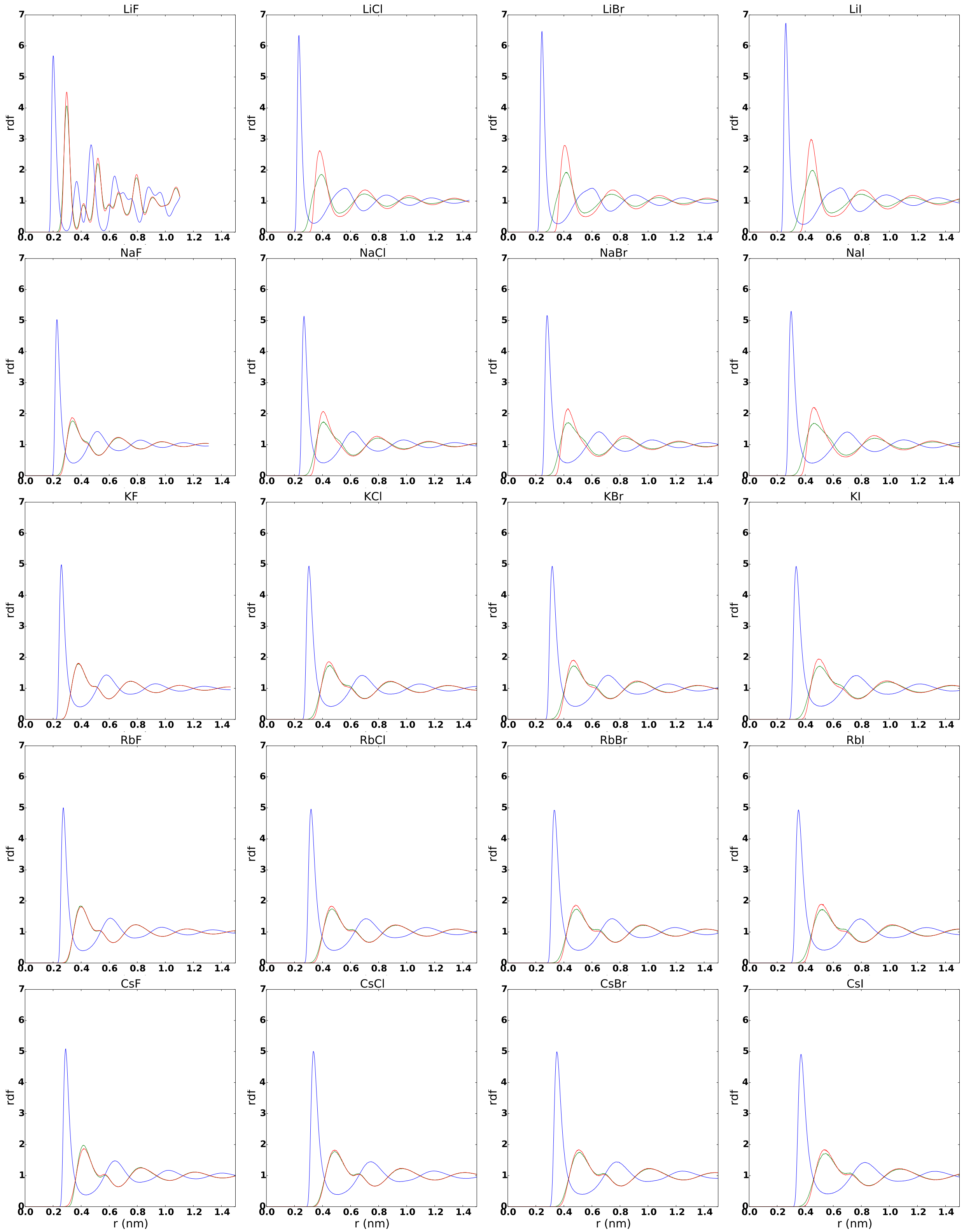

Figure S2: Radial distribution functions for all alkali halide melts at $T_{m,exp}$ simulated with the non-polarisable JC force field. In dark blue $g(r)_{+-}$, in green $g(r)_{++}$ and in red $g(r)_{--}$.

Interionic distances and coordination numbers

Table S1: Interionic distances *r* (in pm) and coordination numbers *N* of the cation-anion, cation-cation and anion-anion evaluated from computed radial distribution functions at $T_{m,exp}$ and 100 K above using the WBK force field. The uncertainty in the interionic distance should be approx. ± 2 pm, and in the CN in the order of ± 0.5.

Salt IJ	T/K	r_{IJ}	N_{IJ}	r_{II}	N_{II}	r_{JJ}	N_{JJ}
LiF	1118.15	186	5.3	280	14.9	284	15
	1218.15	184	5.2	282	14.6	284	14.9
LiCl	878.15	238	5.2	352	14.7	358	14.8
	978.15	236	5	352	14.1	362	14.1
LiBr	823.15	252	5	374	14.4	386	14.5
	923.15	252	4.9	372	13.9	388	14
LiI	722.15	276	5.1	392	13.8	422	14.2
	822.15	274	4.9	392	13.3	426	14
NaF	1266.15	216	5.1	326	14.6	332	14.8
	1366.15	214	5	326	14.2	334	14.5
NaCl	1074.15	264	5.3	392	15.2	398	15.2
	1174.15	264	5.1	396	14.5	404	14.7
NaBr	1020.15	280	5.3	414	15	420	15.2
	1120.15	280	5.1	416	14.7	426	14.5
NaI	934.15	304	5.3	436	15.3	454	15.2
	1034.15	304	5.2	444	14.6	458	14.7
KF	1131.15	246	4.8	378	13.8	382	13.8
	1231.15	244	4.8	380	13.3	384	13.7
KCl	1043.15	296	5.4	438	15.4	446	15.7
	1143.15	296	5.2	438	15.2	452	15.1

Continued on next page

Table S1 – continued

Salt IJ	T/K	r_{IJ}	N_{IJ}	r_{II}	N_{II}	r_{JJ}	N_{JJ}
KBr	1007.15	312	5.5	456	15.8	466	15.8
	1107.15	312	5.3	458	15	470	15.4
KI	954.15	336	5.6	484	16.3	494	16.4
	1054.15	334	5.4	488	15.4	502	15.5
RbF	1068.15	258	4.7	400	13.5	406	13.4
	1168.15	256	4.6	400	12.9	406	13
RbCl	991.15	310	5.4	456	15.8	464	15.9
	1091.15	310	5.3	460	14.9	470	15
RbBr	966.15	326	5.6	470	16.2	488	16.1
	1066.15	326	5.3	480	15.4	490	15.6
RbI	920.15	350	5.7	502	16.4	516	16.4
	1020.15	348	5.5	510	15.8	520	15.7
CsF	955.15	278	4.8	424	13.7	422	13.8
	1055.15	276	4.7	424	13.3	428	13.3
CsCl	918.15	328	5.5	478	16	488	16
	1018.15	326	5.3	482	15.3	488	15.6
CsBr	909.15	342	5.6	496	16.3	508	16.4
	1009.15	342	5.4	502	15.6	514	15.8
CsI	899.15	366	5.7	526	16.7	542	16.5
	999.15	366	5.5	530	15.9	546	15.8

Table S2: Interionic distances r (in pm) and coordination numbers N of the cation-anion, cation-cation and anion-anion evaluated from computed radial distribution functions at $T_{m,exp}$ and 100 K above using the JC force field. The uncertainty in the interionic distance should be approx. ± 2 pm, and in the CN in the order of ± 0.5. (*) Note: LiF at $T_{m,exp}$ is a solid.

Salt IJ	T/K	r_{IJ}	N_{IJ}	r_{II}	N_{II}	r_{JJ}	N_{JJ}
LiF	1118.15	200*	5.7*	296*	11*	296*	11.1*
	1218.15	194	4.7	294	14.1	296	13.7
LiCl	878.15	230	3.9	390	11.4	378	11.7
	978.15	230	3.9	392	11.4	378	11.6
LiBr	823.15	242	3.8	414	10.9	406	11.4
	923.15	242	3.8	416	10.7	406	11.2
LiI	722.15	260	3.7	448	10.4	440	11.1
	822.15	260	3.6	446	10.2	440	11.1
NaF	1266.15	226	5.2	336	15.4	336	15.4
	1366.15	226	5.1	340	15	338	15
NaCl	1074.15	266	4.9	404	14.5	404	14.3
	1174.15	266	4.8	410	14.1	406	14
NaBr	1020.15	280	4.8	426	14.3	428	13.9
	1120.15	280	4.6	430	13.8	430	13.6
NaI	934.15	298	4.5	464	13.5	460	13.3
	1034.15	298	4.5	466	13	464	12.7
KF	1131.15	258	5.5	380	16.3	380	16.1
	1231.15	258	5.3	382	15.7	382	15.7
KCl	1043.15	302	5.4	450	16	444	15.8
	1143.15	300	5.2	452	15.3	448	15.3
KBr	1007.15	316	5.3	468	15.8	468	15.7

Continued on next page

Table S2 – continued

Salt IJ	T/K	r_{IJ}	N_{IJ}	r_{II}	N_{II}	r_{JJ}	N_{JJ}
	1107.15	314	5.2	472	15.3	470	15.2
KI	954.15	334	5.3	500	15.3	496	15.1
	1054.15	334	5.1	506	14.7	500	14.4
RbF	1068.15	272	5.6	396	16.5	398	16.5
	1168.15	272	5.4	400	15.9	402	16.2
RbCl	991.15	316	5.5	464	16.4	462	16.4
	1091.15	316	5.4	472	16	466	15.8
RbBr	966.15	332	5.5	486	16.4	486	16.3
	1066.15	330	5.4	494	15.8	488	15.9
RbI	920.15	350	5.4	518	16.2	516	16.1
	1020.15	350	5.3	526	15.5	518	15.4
CsF	955.15	288	5.7	416	17.1	420	17.1
	1055.15	288	5.6	418	16.4	420	16.6
CsCl	918.15	334	5.8	484	17.1	484	17.2
	1018.15	334	5.6	490	16.6	490	16.6
CsBr	909.15	350	5.7	510	17.1	506	16.9
	1009.15	348	5.6	510	16.3	510	16.4
CsI	899.15	368	5.6	544	16.8	538	16.6
	999.15	368	5.4	550	15.9	544	15.9

Table S3: Interionic distances r (in pm) and coordination numbers N of the cation-anion, cation-cation and anion-anion from experiments. For neutron scattering data (N) both the cation-cation and the anion-anion distance is given. For X-ray diffraction data (X) just one like-like distance is given, which reflects more the anion-anion interaction. Exp.: Experimental technique, Orig. ref.: original reference, Int. ref.: reference that interpreted the data from the original paper.

Salt IJ	T/K	r_{IJ}	N_{IJ}	r_{II}	N_{II}	r_{JJ}	N_{JJ}	Exp.	Orig. ref.	Int. ref.
LiF	1148	185	3			302	8	X	[1]	
LiF	1133	195/200	3.7			300	8	X	[9]	[10] / [11]
LiCl	923	240	4			386	12	X	[12]	
LiCl		247	4			385	12	X	[4]	
LiCl	893	255	4.1			390	9	X	[13]	[11]
LiCl	958	230	5.5	370	14	370	14	N	[6,14]	
LiCl		245	3.5	380	8.3	380	8.3	N	[4]	
LiBr		268	5.2			412	12.8	X	[4]	
LiBr		265	3.8			400		X	[2]	
LiI		285	5.6			445	11.3	X	[4]	
NaF	1273	230	4.1			344/350	9	X	[9]	[10] / [15]
NaCl	1083	277	3.7			415		X	[7]	[15]
NaCl	1093	280/288	4.7			420	9	X	[13]	[10] / [11,15]
NaCl	1148	272	5.8	389	13	390	13.3	N	[16]	[10]
NaCl	1148	278	4.0	396		391		N	[16]	[8]
NaBr		305	3.5			456	11.7	X	[5]	
NaI		315	4			480	8.9	X	[4]	
NaI		315	4					X	[5]	
NaI	973	310				460		X	[3]	
KF	1143	265/270	4.9			386	9	X	[9]	[11,15] / [10]
KCl		305	4.1			435		X	[17]	

Continued on next page

Table S3 – continued

Salt IJ	T/K	r_{IJ}	N_{IJ}	r_{II}	N_{II}	r_{JJ}	N_{JJ}	Exp.	Orig. ref.	Int. ref.
KCl		310	3.7			400-500		X	4	15
KCl	1083	310/320	5.2			440	10	X	13	10 /11,15
KCl		314	5.8			430		X	18	11
KCl	1073	306	6.1	484	12/15.9	482	12.3/16.2	N	19	
KCl		310	3.5	470	7.4	470	7.4	N	4	
KBr	1023	318	3.5			465		X	15	
KBr		335	4.9					X	5	
KBr	1025	321	3.78			507	8.79	EXAFS	20	10
KI		352	4			490	7.15	X	5	
RbF										
RbCl		330	4.2					X	21	10
RbCl	1023	318	6.9	486	13	480	14	N	22	10
RbBr		340	4.1			472	7.35	X	5	
RbI		365	4.6			515	7.6	X	5	
RbI	973	360				500		X	3	
CsF										
CsCl		353	4.6			487	7.1	X	4	
CsCl	973	338		385		385		N	23	10
CsCl	968	340	5.8	495	15.4	485	16.3	N	24	10
CsCl	973	338	3/5.9	385		385		N	19	
CsBr		355	4.6			540	8.3	X	4	
CsBr		366	4.65					X	5	
CsBr		355	4.7	520	7.9	520	7.9	N	4	
CsI		385	4.5			550	7.2	X	4	

Continued on next page

Table S3 – continued

Salt IJ	T/K	r_{IJ}	N_{IJ}	r_{II}	N_{II}	r_{JJ}	N_{JJ}	Exp.	Orig. ref.	Int. ref.
CsI		385	4.25					X	5	

Table S4: Interionic distances *r* (in pm) and coordination numbers *N* of the cation-anion, cation-cation and anion-anion from simulations taken from literature. *Only like-like values are reported, not whether cations or anions.

Salt IJ	T/K	r_{IJ}	N_{IJ}	r_{II}	N_{II}	r_{JJ}	N_{JJ}	Method.	Ref.
LiF	1173	180	4.2					MC	25
LiCl	883	230	4.9	365	13.2	365	13.6	MC	26
LiCl	900	225	4.05	387	11.81	376	11.86	MC	27
LiCl	1096	221	4.05	376	12.26	369	11.95	MD	28
LiCl	1050	220	4.1	370	13.2	370	12.7	MD	29
LiCl	918	220	4.2	370	12.6	370	12.5	MD	29
LiCl	923	220	4.0					MC	25
LiCl	923	211		368		366		FPMD	30
LiCl	1073	240	4.1			410	11.1	MC	31
LiBr	923	240	3.8					MC	25
LiBr	1000	240	4.27					MC	2,32
LiI	742	260	4.3	445	14.1	445	14.1	MC	26
LiI	800	270	4.8	420	13.0	420	13.4	MC	10
LiI	1453	270	4.5	450	12.4	440	12.4	MC	10
LiI	773	260	4.2					MC	25
LiI	800	265	3.9	435		425		MD	33
NaF	1323	210	4.9					MC	25
NaCl	1074	270	5.2	425	13.9	425	14.7	MC	26

Continued on next page

Table S4 – continued

Salt IJ	T/K	r_{IJ}	N_{IJ}	r_{II}	N_{II}	r_{JJ}	N_{JJ}	Method	Ref.
NaCl	1080	261	4.76	417	13.59	405	13.54	MD	[27]
NaCl	1123	255	5.0					MC	[25]
NaCl	1079	280		420		390		DFTB-MD	[34]
NaCl	1528	260		400		410		MD	[35]
NaBr	1073	270	5.2					MC	[25]
NaI	973	290	4.7					MC	[25]
NaI	996	300		450		470		MD	[36]
KF	1173	260	5.3					MC	[25]
KCl	1045	294	5.3	445*	15.4*	445*	15.4*	MC	[37]
KCl	1306	293	5.2	461*	14.8*	461*	14.8*	MC	[37]
KCl	1053	296	5.18	458	14.57	458	14.28	MD	[27]
KCl	1096	294	5.13	463	14.6	436	15.5	MD	[28]
KCl	1043	300	5.2	450	15.5	440	15.6	MD	[29]
KCl	1073	300	5.8					MC	[25]
KCl	1073	292		461		453		FPMD	[30]
KCl	1061	310		480		420		DFTB-MD	[34]
KCl	1173	295	4.7	450*		450*		MD	[17]
KCl	1173	295	5.1	425*		425*		MD	[17]
KBr	1007	320	5.5	480	15.0	480	15.0	MC	[26]
KBr	1100	327	3.64			500	8.79	MD	[20]
KBr	1073	310	5.9					MC	[25]
KI	954	345	5.9	490	16.0	490	16.6	MC	[26]
KI	973	330	5.3					MC	[25]

Continued on next page

Table S4 – continued

Salt IJ	T/K	r_{IJ}	N_{IJ}	r_{II}	N_{II}	r_{JJ}	N_{JJ}	Method	Ref.
KI	1299	330	6					MD	[38]
RbF	1155	260		400		400		MD	[39]
RbF	1073	270	6.2					MC	[25]
RbCl	995	320	5.8	460	16.5	460	16.4	MC	[26]
RbCl	1359	310		480		450		MD	[39]
RbCl	1000	312	5.41	467	15.66	474	15.71	MD	[27]
RbCl	1023	320	5.7					MC	[25]
RbBr	1365	330		490		480		MD	[39]
RbBr	1023	330	5.9					MC	[25]
RbI	1341	350		530		530		MD	[39]
RbI	973	360	5.5					MC	[25]
CsF	976	290	5.4	440	16.9	440	16.8	MC	[26]
CsF	962	270		420		410		MD	[40]
CsF	1023	290	5.7					MC	[25]
CsCl	996	330		470		460		MD	[40]
CsCl	900	330	5.7	476	16.26	490	16.34	MD	[27]
CsCl	973	330	5.8					MC	[25]
CsBr	942	350		480		500		MD	[40]
CsBr	973	340	6.1					MC	[25]
CsI	871	370		520		520		MD	[40]
CsI	923	360	5.7					MC	[25]

Lifetimes and thermodynamic analysis

Table S5: Lifetimes (ps) and activation thermodynamics ($\Delta^{\ddagger}G$, $\Delta^{\ddagger}H$ and $T\Delta^{\ddagger}S$ in kJ/mol) for all pure alkali halide melts using the WBK force field.

Salt IJ	T/K	τ	$\Delta^{\ddagger}G$	$\Delta^{\ddagger}H$	$T\Delta^{\ddagger}S$
LiF	1118.15	1.84	34.93	16.0	-19.8
	1218.15	1.47	36.63		
LiCl	878.15	3.81	30.98	14.4	-17.5
	978.15	2.79	32.87		
LiBr	823.15	5.07	30.57	12.5	-19.2
	923.15	3.71	32.76		
LiI	722.15	7.46	28.34	12.4	-17.1
	822.15	5.10	30.56		
NaF	1266.15	2.29	43.19	15.8	-28.5
	1366.15	1.91	45.36		
NaCl	1074.15	4.07	40.28	15.5	-26.0
	1174.15	3.21	42.60		
NaBr	1020.15	5.47	40.35	15.7	-25.9
	1120.15	4.23	42.77		
NaI	934.15	7.18	38.36	13.9	-25.7
	1034.15	5.45	40.98		
KF	1131.15	2.97	39.95	11.9	-29.3
	1231.15	2.46	42.43		
KCl	1043.15	5.18	40.97		

Continued on next page

Table S5 – continued

Salt IJ	T/K	τ	$\Delta^{\ddagger}G$	$\Delta^{\ddagger}H$	$T\Delta^{\ddagger}S$
				15.6	-26.6
	1143.15	4.04	43.40		
KBr	1007.15	6.96	41.73		
				15.8	-27.2
	1107.15	5.33	44.30		
KI	954.15	8.76	40.94		
				16.3	-26.0
	1054.15	6.53	43.52		
RbF	1068.15	3.78	39.36		
				10.6	-30.1
	1168.15	3.12	42.06		
RbCl	991.15	7.06	41.06		
				14.5	-27.9
	1091.15	5.45	43.73		
RbBr	966.15	9.34	42.06		
				16.4	-27.0
	1066.15	6.99	44.72		
RbI	920.15	11.77	41.46		
				15.5	-27.4
	1020.15	8.71	44.28		
CsF	955.15	5.86	37.79		
				11.4	-27.7
	1055.15	4.62	40.55		
CsCl	918.15	10.23	40.28		
				16.7	-24.9
	1018.15	7.44	42.85		
CsBr	909.15	12.61	41.39		
				15.6	-27.2
	1009.15	9.26	44.23		
CsI	899.15	14.09	41.69		
				15.2	-28.0

Continued on next page

Table S5 – continued

Salt IJ	T/K	τ	$\Delta^{\ddagger}G$	$\Delta^{\ddagger}H$	$T\Delta^{\ddagger}S$
	999.15	10.35	44.64		

Table S6: Lifetimes (ps) and activation thermodynamics ($\Delta^{\ddagger}G$, $\Delta^{\ddagger}H$ and $T\Delta^{\ddagger}S$ in kJ/mol) for all pure alkali halide melts using the JC force field. * LiF is a solid at the experimental melting point and was therefore not used in the evaluation of the lifetimes and activation thermodynamics.

Salt IJ	T/K	τ	$\Delta^{\ddagger}G$	$\Delta^{\ddagger}H$	$T\Delta^{\ddagger}S$
LiF	1118.15	*	*	*	*
	1218.15	3.94	46.65		
LiCl	878.15	11.21	38.87	26.2	-13.4
	978.15	6.98	40.32		
LiBr	823.15	16.76	38.74	25.8	-13.8
	923.15	9.94	40.32		
LiI	722.15	28.15	36.32	24.4	-12.7
	822.15	15.07	37.96		
NaF	1266.15	4.59	50.49	24.8	-26.7
	1366.15	3.58	52.52		
NaCl	1074.15	6.52	44.50	19.9	-25.7
	1174.15	4.93	46.79		
NaBr	1020.15	8.35	43.92	16.6	-28.7
	1120.15	6.38	46.60		
NaI	934.15	10.34	41.20	14.0	-28.7
	1034.15	7.85	44.11		

Continued on next page

Table S6 – continued

Salt IJ	T/K	τ	$\Delta^\ddagger G$	$\Delta^\ddagger H$	$T\Delta^\ddagger S$
KF	1131.15	6.87	47.85	24.1	-24.8
	1231.15	5.13	49.95		
KCl	1043.15	8.41	45.18	20.5	-25.9
	1143.15	6.25	47.55		
KBr	1007.15	10.97	45.55	20.5	-26.3
	1107.15	8.00	48.04		
KI	954.15	12.57	43.80	18.2	-27.0
	1054.15	9.16	46.49		
RbF	1068.15	10.33	48.29	25.9	-23.5
	1168.15	7.36	50.39		
RbCl	991.15	12.50	45.77	21.8	-25.2
	1091.15	8.91	48.19		
RbBr	966.15	15.76	46.27	20.9	-26.7
	1066.15	11.19	48.89		
RbI	920.15	17.78	44.61	18.5	-27.5
	1020.15	12.65	47.45		
CsF	955.15	19.12	47.18	29.6	-18.5
	1055.15	12.15	49.02		
CsCl	918.15	19.20	45.09	23.4	-22.8
	1018.15	12.80	47.44		
CsBr	909.15	22.79	45.87		

Continued on next page

Table S6 – continued

Salt IJ	T/K	τ	$\Delta^\ddagger G$	$\Delta^\ddagger H$	$T\Delta^\ddagger S$
	1009.15	15.32	48.46	22.3	-24.8
CsI	899.15	22.27	45.11	20.6	-25.9
	999.15	15.21	47.84		

References

(1) Vaslow, F.; Narten, A. *J. Chem. Phys.* **1973**, *59*, 4949–4954.

(2) Ohno, H.; Furukawa, K.; Igarashi, K.; Mochinaga, J. *J. Chem. Soc. Far. Trans.* **1982**, *78*, 1555–1560.

(3) Tahara, S.; Ohara, K.; Shimakura, H.; Fukami, T. *EPJ Web of Conferences* **2017**, *151*, 03006.

(4) Levy, H. A.; Agron, P. A.; Bredig, M. A.; Danford, M. D. *Ann. NY Acad. Sci.* **1960**, *79*, 762–780.

(5) Antonov, B. *J. Struct. Chem.* **1975**, *16*, 474–476.

(6) McGreevy, R.; Howe, M. *J. Phys.: Condens. Matter* **1989**, *1*, 9957.

(7) Ohno, H.; Furukawa, K. *J. Chem. Soc. Far. Trans.* **1981**, *77*, 1981–1985.

(8) Biggin, S.; Enderby, J. E. *J. Phys. C: Solid State* **1982**, *15*, L305.

(9) Zarzycki, J. *J. Phys. Phys. Appl.* **1957**, *18*, 65–69.

(10) Marcus, Y. *Ionic Liquid Properties - From Molten Salts to RTILs*; Springer: Switzerland, 2016.

(11) Furukawa, K. *Discuss. Faraday Soc.* **1961**, *32*, 53–62.

(12) Ohno, H.; Yoroki, M.; Furukawa, K.; Takagi, Y.; Nakamura, T. *J. Chem. Soc. Far. Trans.* **1978**, *74*, 1861–1870.

(13) Zarzycki, J. *J. Phys. Phys. Appl.* **1958**, *19*, 13–19.

(14) Howe, M.; McGreevy, R. *Philos. Mag. B* **1988**, *58*, 485–495.

(15) Ohno, H.; Furukawa, K. *J. Chem. Soc. Far. Trans.* **1983**, *79*, 463–471.

(16) Edwards, F. G.; Enderby, J. E.; Howe, R. A.; Page, D. I. *J. Phys. C: Solid State* **1975**, *8*, 3483.

(17) Takagi, R.; Ohno, H.; Furukawa, K. *J. Chem. Soc., Faraday Trans. 1* **1979**, *75*, 1477–1486.

(18) Lark, K.; Miller, E. *Phys. Rev.* **1937**, *51*, 61.

(19) Derrien, J.; Dupuy, J. *J. Phys. - Paris* **1975**, *36*, 191–198.

(20) Di Cicco, A.; Rosolen, M. J.; Marassi, R.; Tossici, R.; Filipponi, A.; Rybicki, J. *J. Phys.: Condens. Matter* **1996**, *8*, 10779.

(21) Levy, H. A.; Danford, M. D. *Diffraction studies of the structure of molten salts. In: Blander M (ed) Molten salt chemistry*; Interscience: New York, 1964.

(22) Mitchell, E.; Poncet, P.; Stewart, R. *Philos. Mag.* **1976**, *34*, 721–732.

(23) Eisenberg, S.; Jal, J.-F.; Dupuy, J.; Chieux, P.; Knoll, W. *Phil. Mag. A* **1982**, *46*, 195–209.

(24) Locke, J.; Messoloras, S.; Stewart, R.; McGreevy, R.; Mitchell, E. *Philos. Mag. B* **1985**, *51*, 301–315.

(25) Baranyai, A.; Ruff, I.; McGreevy, R. *J. Phys. C Solid State* **1986**, *19*, 453.

(26) Lewis, J. W.; Singer, K.; Woodcock, L. V. *J. Chem. Soc. Farad. T. 2* **1975**, *71*, 301–312.

(27) Wang, J.; Sun, Z.; Lu, G.; Yu, J. *J. Phys. Chem. B* **2014**, *118*, 10196 – 10206.

(28) Lantelme, F.; Turq, P. *J. Chem. Phys.* **1982**, *77*, 3177–3187.

(29) Caccamo, C.; Dixon, M. *J. Phys. C: Solid State* **1980**, *13*, 1887.

(30) Chen, C.-F.; Cheng, Y.-C.; Hong, C.-W. *CMES-Comp. Model. Eng.* **2015**, *109*, 263–283.

(31) Krogh-Moe, J.; Østvold, T.; Førland, T. *Acta Chem. Scand.* **1969**, *23*, 2421–2429.

(32) Lantelme, F.; Turq, P.; Schofield, P. *J. Chem. Phys.* **1977**, *67*, 3869–3877.

(33) Tabacchi, G.; Mundy, C. J.; Hutter, J.; Parrinello, M. *J. Chem. Phys.* **2002**, *117*, 1416–1433.

(34) Hazebroucq, S.; Picard, G. S.; Adamo, C.; Heine, T.; Gemming, S.; Seifert, G. *J. Chem. Phys.* **2005**, *123*, 134510.

(35) Galamba, N.; Costa Cabral, B. *J. Chem. Phys.* **2007**, *126*, 124502.

(36) Galamba, N.; Costa Cabral, B. *J. Chem. Phys.* **2007**, *127*, 094506.

(37) Woodcock, L.; Singer, K. *T. Faraday Soc.* **1971**, *67*, 12–30.

(38) Aguado, A.; Wilson, M.; Madden, P. A. *J. Chem. Phys.* **2001**, *115*, 8603–8611.

(39) Dixon, M.; Sangster, M. *J. Phys. C Solid State* **1976**, *9*, 3381.

(40) Dixon, M.; Sangster, M. *J. Phys. C Solid State* **1977**, *10*, 3015.