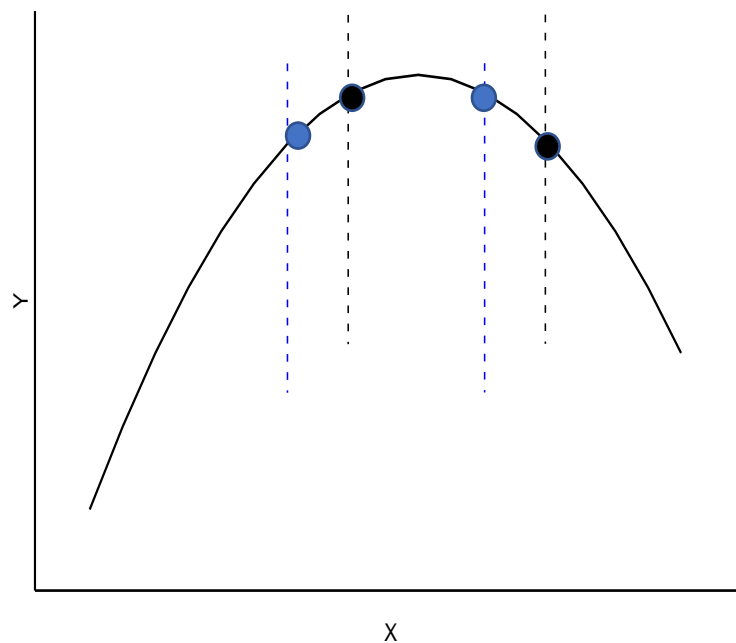


Notes on the experimental determination of the TMD:

1) In all the salts measured with the Hare and Sorensen method (i.e., NaI, MgBr<sub>2</sub>, CsI, and NaF), marked with asterisks in the Table below, the maximum is clearly observed in the raw data as a diminution of the density as the temperature decreases below the TMD.

2) For the remaining salts, the higher volume of the solution employed to perform the experiments leads to a somehow higher probability of freezing. For that reason, and provided the freezing used to happen close to the TMD, in most of the experiments we stopped the cooling down of the solutions after observing the liquid expansion. In this way, we ensure that the TMD has been overcome at the time that the undesirable freezing was avoided. In case of freezing events, the whole systems should be dismantled and recalibrated.

Because of the way we measured, it might be confusing that continuously increasing temperatures are observed in the tables below for some solutions. However, it can be easily observed that the TMD occurs before the last recorded temperature. Finally, some didactical graph might be of utility for clarifying this point. In the following figure we have sketched two different intervals of the same wide enclosing the single maximum of a parabola. If these intervals stand for the length of the measurements, depending on the relative position of the interval with respect to this maximum, an increasing (blue dots in the figure) or decreasing (black dots) trend would be obtained. Even a roughly constant values could be obtained for sufficiently centered intervals.



Experimental densities at room pressure

FLUORIDES

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NaF*		KF		CsF	
T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$
298.15	1037.649298	274.15	1048.8864	274.15	1127.2177
297.15	1038.007157	273.15	1048.9856	273.15	1127.3193
296.15	1038.358641	272.65	1049.0377	272.65	1127.3701
295.15	1038.703511	272.15	1049.0833	272.15	1127.4162
294.15	1039.041527			271.65	1127.4695
293.15	1039.372446	271.65	1049.1253	271.15	1127.5145
292.15	1039.696029	271.15	1049.1644	270.65	1127.5548
291.15	1040.012036	270.65	1049.2029	270.15	1127.5916
290.15	1040.320225	270.15	1049.2384	269.65	1127.6290
289.15	1040.620355	269.65	1049.2703	269.15	1127.6623
288.15	1040.912187			268.65	1127.6944

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287.15	1041.195479	269.15	1049.3007	268.15	1127.7229
286.15	1041.469992	268.65	1049.3249	267.65	1127.7498
285.15	1041.735484	268.15	1049.3460	267.15	1127.7743
284.15	1041.991714	267.65	1049.3664	266.65	1127.7941
283.15	1042.238443	267.15	1049.3825	266.15	1127.8108
282.15	1042.475429	266.65	1049.3957	265.65	1127.8265
281.15	1042.702432	266.15	1049.4066	265.15	1127.8361
280.15	1042.919211	265.65	1049.4132	264.65	1127.8470
279.15	1043.125525			264.15	1127.8550
278.15	1043.321135	265.15	1049.4170	263.65	1127.8594
277.15	1043.505799	264.65	1049.4179	263.15	1127.8603
276.15	1043.679277	264.15	1049.4129		
275.15	1043.841328	263.65	1049.4044		
274.15	1043.991711	263.15	1049.3916		
273.15	1044.130186				
272.15	1044.256513				
271.15	1044.370449				
270.15	1044.471756				
269.15	1044.560193				
268.15	1044.635518				

267.15 1044.697491  
266.15 1044.745871  
265.15 1044.780419  
264.15 1044.800892  
263.15 1044.807052  
262.15 1044.798656  
261.15 1044.775464  
260.15 1044.737237  
259.15 1044.683732  
258.15 1044.61471  
257.15 1044.52993

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CHLORIDES

RbCl		CsCl	
T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$
274.15	1086.6623	278.15	1123.7811
273.65	1086.7114	277.15	1123.9311
273.15	1086.7617		
272.65	1086.8115	276.15	1124.0683
272.15	1086.8589	275.15	1124.1978
271.65	1086.9093		
271.15	1086.9383	274.15	1124.3128
270.65	1086.9765	273.65	1124.3685
270.15	1087.0095	273.15	1124.4220
269.65	1087.0403	272.65	1124.4743
269.15	1087.0693	272.15	1124.5248
268.65	1087.0954	271.65	1124.5716
268.15	1087.1187	271.15	1124.6150

267.65	1087.1373		
267.15	1087.1548	270.65	1124.6534
266.65	1087.1671	270.15	1124.6883
266.15	1087.1776	269.65	1124.7232
265.65	1087.1843	269.15	1124.7521
265.15	1087.1879	268.65	1124.7794
264.65	1087.1859	268.15	1124.8034
264.15	1087.1861	267.65	1124.8228
		267.15	1124.8390
		266.65	1124.8487
		266.15	1124.8520
		265.65	1124.8552

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BROMIDES

LiBr		NaBr		KBr		CsBr		MgBr <sub>2</sub> *	
T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$
276.65	1060.1003	274.15	1079.0216	275.15	1082.788224	275.15	1160.6610	278.15	1144.4164
276.15	1060.1392	273.15	1079.1565	274.15	1082.911031	274.15	1160.8166	277.15	1144.6273
275.65	1060.1771			273.65	1082.972419	273.15	1160.9692	276.15	1144.8314
275.15	1060.2118	272.15	1079.2817					275.15	1145.0284
274.65	1060.2463	271.15	1079.4040	273.15	1083.028147	272.65	1161.0407	274.15	1145.2177
274.15	1060.2759	270.65	1079.4594	272.65	1083.076392	272.15	1161.0973	273.15	1145.3990
273.65	1060.3033			272.15	1083.126942	271.65	1161.1534	272.15	1145.5717
273.15	1060.3264	270.15	1079.5121	271.65	1083.175773	271.15	1161.2064	271.15	1145.7355
272.65	1060.3510	269.65	1079.5721	271.15	1083.220591			270.15	1145.8900
272.15	1060.3679			270.65	1083.260851	270.65	1161.2589	269.15	1146.0347
271.65	1060.3820	269.15	1079.6265	270.15	1083.301686	270.15	1161.3051	268.15	1146.1691
271.15	1060.3972	268.65	1079.6770	269.65	1083.336804	269.65	1161.3513	267.15	1146.2929
270.65	1060.4080	268.15	1079.7235			269.15	1161.3957	266.15	1146.4056
270.15	1060.4133	267.65	1079.7677	269.15	1083.375928	268.65	1161.4383	265.15	1146.5068

269.65	1060.4174	267.15	1079.8120	268.65	1083.404202	268.15	1161.4760	264.15	1146.5961
269.15	1060.4177	266.65	1079.8488	268.15	1083.432455	267.65	1161.5112	263.15	1146.6730
268.65	1060.4130	266.15	1079.8827	267.65	1083.458991	267.15	1161.5415	262.15	1146.7371
268.15	1060.4100	265.65	1079.9093	267.15	1083.483812	266.65	1161.5688	261.15	1146.7880
		265.15	1079.9370	266.65	1083.50291	266.15	1161.5905	260.15	1146.8252
		264.65	1079.9623	266.15	1083.519722	265.65	1161.6079	259.15	1146.8483
		264.15	1079.9866	265.65	1083.529092	265.15	1161.6224	258.15	1146.8568
		263.65	1080.3962	265.15	1083.541898	264.65	1161.6342	257.15	1146.8504
				264.65	1083.548978	264.15	1161.6400	256.15	1146.8287
		263.15	1080.0252	264.15	1083.555488	263.65	1161.6439	255.15	1146.7911
		262.65	1080.0374	263.65	1083.555702	263.15	1161.6448	254.15	1146.7372
		262.15	1080.0456	263.15	1083.556489			253.15	1146.6667
		261.65	1080.0487						
		261.15	1080.0489						

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IODIDES



LiI		NaI*		KI		CsI*	
T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$
278.15	1095.5491	278.15	1110.9996	276.15	1117.6654	278.15	1191.8337
277.15	1095.6815	277.15	1111.2459	275.15	1117.8220	277.15	1192.0642
		276.15	1111.4834	274.65	1117.9096	276.15	1192.2827
276.15	1095.8093	275.15	1111.7116	274.15	1117.9648	275.15	1192.4885
275.65	1095.8710	274.15	1111.9302	273.65	1118.0356	274.15	1192.6813
275.15	1095.9292	273.15	1112.1386	273.15	1118.1104	273.15	1192.8605
274.65	1095.9851	272.15	1112.3366	272.65	1118.1818	272.15	1193.0257
274.15	1096.0352	271.15	1112.5236			271.15	1193.1762
273.65	1096.0841	270.15	1112.6993	272.15	1118.2468	270.15	1193.3116
		269.15	1112.8631	271.65	1118.3130	269.15	1193.4315
273.15	1096.1290	268.15	1113.0147	271.15	1118.3813	268.15	1193.5352
272.65	1096.1686	267.15	1113.1537	270.65	1118.4441	267.15	1193.6222
272.15	1096.2082	266.15	1113.2796			266.15	1193.6922
271.65	1096.2449	265.15	1113.3919	270.15	1118.5018	265.15	1193.7445

271.15	1096.2786	264.15	1113.4904	269.65	1118.5637	264.15	1193.7786
270.65	1096.3089	263.15	1113.5744	269.15	1118.6141	263.15	1193.7941
270.15	1096.3358	262.15	1113.6437	268.65	1118.6670	262.15	1193.7905
269.65	1096.3609	261.15	1113.6978			261.15	1193.7671
269.15	1096.3819	260.15	1113.7362	268.15	1118.7116	260.15	1193.7236
268.65	1096.4006	259.15	1113.7586	267.65	1118.7347	259.15	1193.6594
268.15	1096.4159	258.15	1113.7644	267.15	1118.7748	258.15	1193.5740
267.65	1096.4271	257.15	1113.7533	266.65	1118.8072	257.15	1193.4669
267.15	1096.4378	256.15	1113.7249	266.15	1118.8379		
266.65	1096.4438	255.15	1113.6787	265.65	1118.8779		
266.15	1096.4469	254.15	1113.6143	265.15	1118.9161		
265.65	1096.4466			264.65	1118.9367		
265.15	1096.4410			264.15	1118.9542		
				263.65	1118.9655		
				263.15	1118.9827		
				262.65	1118.9935		
				262.15	1119.0031		
				261.65	1119.0093		
				261.15	1119.0148		

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Molecular Dynamics results for densities at room pressure

FLUORIDES

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NaF		KF		CsF	
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T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$
-----					
250	1049.08	250	1052.73	250.15	1128.51
255	1049.44	255	1053.40	255.15	1129.39
260	1049.37	260	1053.48	260.15	1130.07
265	1049.09	265	1053.41	265.15	1130.15
270	1048.44	270	1053.17	270.15	1130.02
275	1047.43	275	1052.39	275.15	1129.42
280	1046.32	280	1051.59	280.15	1128.59

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CHLORIDES

RbCl		CsCl	
T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$
245	1077.62	245	1117.43
255	1081.20	255	1120.90
260	1081.92	265	1122.55
265	1082.31	270	1122.80
270	1082.67	275	1122.55
275	1082.26	285	1121.12
280	1081.63	290	1119.86
290	1079.72	298.15	1117.49
298.15	1077.29	305	1115.01

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BROMIDES

LiBr		NaBr		KBr		CsBr		MgBr <sub>2</sub>	
T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$
255.15	1058.02	242	1076.615	242	1078.1	245	1151.07	282	1144.02
260.15	1059	247	1079.05	247	1080.41	255	1154.92	272	1145.11
265.15	1059.73	252	1079.84	252	1081.95	265	1156.99	262	1145.45
270.15	1060.08	257	1080.23	257	1082.89	270	1157.18	252	1144.41
275.15	1060.01	262	1079.84	262	1083.42	275	1157	242	1141.48
280.15	1059.59	267	1079.47	267	1083.71	285	1155.65		
285.15	1058.69	272	1078.64	272	1083.54	298.15	1152.03		
290.15	1057.75	278	1077.66	278	1082.85	305	1149.43		
		282	1078.12	282	1082.14				
		287	1079.23	287	1081.18				
		292	1079.95	292	1079.82				
		297	1080.04	297	1078.13				
		302	1076.63						

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IODIDES

LiI		NaI		KI		CsI	
T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$	T(K)	$\rho(\text{kg/m}^3)$
250	1089.79	240	1108.93	240	1110.23	250	1185.32
260	1092.76	250	1112.27	250	1114.56	260	1188.50
265	1093.49	255	1113.40	255	1116.05	265	1189.25
270	1093.88	260	1113.96	260	1117.02	270	1189.58
275	1093.84	265	1114.36	265	1117.51	275	1189.51
280	1093.49	270	1114.19	270	1117.53	280	1188.69
285	1092.90	280	1112.65	280	1116.06	285	1187.74
290	1091.88	285	1111.50	290	1114.04	298.15	1184.10
298.15	1089.77	298.15	1107.21	298.15	1111.49		