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Systematically improved melting point prediction: a detailed physical simulation model is required - Supporting Information

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Computational methods - Additional details

For determining the melting points we choose the so-called liquid-solid direct coexistence method using Molecular Dynamics (MD) simulations. Other applicable methods are e.g. free energy calculations or the Hamiltonian Gibbs-Duhem integration.[1,2] These different methods were tested by Aragones et al. on alkali halides, and shown to give consistent results. However, as observed by Zhang et al.[3] for systems consisting of larger molecules, such as e.g. ionic liquids, direct methods can by inappropriate due to the slow dynamics of these molecules. Regarding the liquid-solid coexistence method, a starting configuration has to be set up where the solid crystal is in direct contact with its melt, where the z-axis was chosen to be perpendicular to the liquid-solid interface. In a next step the liquid-solid coexistence box is simulated using NPT simulations with semiisotropic pressure coupling at 1 bar at different temperatures. Depending on the temperature, the system evolves either to become a crystal or a melt. The different salts (boxes with 4000

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*To whom correspondence should be addressed ions) are simulated in a wide range of temperatures around the experimental melting point with a step size of 25 K, as the exact melting point given by the force field is not known. The force field's melting point is then determined by the average of the highest temperature where the salt is still a solid and the lowest temperature where the salt is a melt. In order to evaluate the final phase (i.e. solid or liquid) of the simulated salt boxes that were run for 5 ns at each temperature, both diffusion coefficients and radial distribution functions were evaluated for the last 100 ps (for figures see below). Using the diffusion coefficients it was determined whether the salt was liquid or solid (which was also confirmed visually at the phase transition temperature by looking at the final coordinate file), while the radial distribution function allowed us in addition to investigate the solid's crystallinity (i.e. whether the crystal structure was stable). For both the WBK and JC model it was observed that in certain cases (i.e. for some salts at a temperature close to the phase transition point) a box would be still partially solid and liquid at the same time after 5 ns of simulation, while 25 K higher or lower the simulation box was either completely liquid or solid. This indicates that this temperature is very close to the solid-liquid coexistence point, and that a complete conversion to either solid or liquid might take a significantly longer time than 5 ns or might even not be obtained (this would correspond to the case where the liquid and the solid phase have an equal chemical potential which defines the melting point).

The MD simulations were performed using the GROMACS simulation software (version 4.6.7), using tabulated Coulomb (coulomb-type: PME-User) and Van der Waals potentials (vdw-type: User) using tables with a spacing of 0.5 pm and double precision. The integration step size was 1 fs, and the cutoff length for the Coulomb and van der Waals interactions was equal to half of the box size at room temperature. A dispersion correction for energy and pressure was applied after the cutoff. For the polarisable force field, the convergence tolerance for the shell minimisation was set to 0.1 kJ/(mol nm).[4] All simulations were performed using periodic boundary conditions. The results were obtained by running constant pressure simulations (NPT simulations) using the Berendsen semiisotropic pressure coupling (τ_P 10),[5] and for the temperature coupling the velocity rescaling thermostat (τ_T 0.1).[6]

For the evaluation of the melting points of alkali halides with an fcc structure at high temperature (i.e. all alkali halides besides CsBr and CsI), we employed our polarisable force field (called WBK, Wang-Buckingham)[7] and a non-polarisable force field (JC, Joung & Cheatham).[8] Our results are compared to literature results from Aragones et al.[2] that tested three force fields for NaCl (JC, Smith-Dang (SD),[9,10] and Tosi-Fumi (TF[11])). The TF parameters were also applied for eleven alkali halides in total (LiF, LiCl, NaF, NaCl, NaBr, KF, KCl, KBr, RbF, RbCl and RbBr). Joung & Cheatham presented three sets of ion-specific parameters for the AHs, which are compatible with the water models TIP3P, TIP4P$_{EW}$ and SPC/E. While Aragones et al. tested the SPC/E-compatible set for NaCl, we choose here to test the TIP3P-compatible set. The different ion-specific parameters of JC and SD that are directly comparable as they use the same physical model and the same combing rules are summarised in Table Table S1.

Table S1: TIP3P- and SPC/E-compatible NaCl parameters from JC,[8] and in addition the SD parameters.[9,10]

Force field	Water model	Ion	σ (Å)	ε (kcal/mol)
JC	TIP3P	Na^+	2.439	0.0874393
JC	SPC/E	Na^+	2.160	0.3526418
SD	SPC/E	Na^+	2.350	0.1300
JC	TIP3P	Cl^-	4.478	0.0355910
JC	SPC/E	Cl^-	4.830	0.0127850
SD	SPC/E	Cl^-	4.400	0.1000

There are several differences that distinguish the applied force fields: (i) the WBK, JC and SD force field use ion-specific parameters, whereas the TF model uses salt-specific parameters; (ii) the WBK model is polarisable using a core-shell model, while the JC, SD and TF model are non-polarisable; (iii) the WBK model uses distributed charges, while the JC, SD and TF model use point charges; (iv) the van der Waals interactions are modelled differently: WBK uses a modified Buckingham potential that has no singularity and has in general a softer repulsive part,[12] JC and SD use a classical 12-6 Lennard-Jones (LJ) potential, and the TF model employs a Buckingham potential that is extended by a r^{-8} term. (v) JC and SD use the Loretz-Berthelot combining rules, TF has no combining rules as the parameters are salt-specific, and WBK uses combing rules introduced by Hogervorst.[13]

Melting point temperatures

The melting points for the WBK and JC (TIP3P) model were determined using the liquid-solid coexistence method. The simulations were run for 5 ns, and the diffusion coefficient was then evaluated for the whole simulation box for the last 100 ps of the simulation (see figures below). The phase of the simulation boxes was determined, i.e. to be either solid or liquid. Solid boxes have a diffusion coefficient that is equal to zero, while boxes that contain liquid have a value larger than zero. As mentioned above in certain cases the simulation box was still partially liquid and solid after a simulation time of 5 ns, indicating a temperature very close to the phase transition point. 25 K higher or lower than that, the simulation boxes were either completely liquid or solid (besides one single case, i.e. LiCl using the JC (TIP3P-compatible) model, where for three temperatures close to the phase transition point liquid-solid boxes were observed after 5 ns; at higher or lower temperatures the boxes were also completely solid or liquid after 5 ns of simulation). The melting point was determined by calculating the average between the highest temperature where the simulation box is completely solid and the lowest temperatures where the simulation box is completely liquid.

Table S2: Melting point temperatures in K. The error is estimated to be approx. 25 K for the WBK and JC (TIP3P) model. Experimental data is taken from the book Alkali Halides, A Handbook of Physical Properties (p. 70, ref b).[14] The T_m values for TF, JC (SPC/E) and SD are taken from Aragones et al.[2] The residual mean square deviation (RMSD) and the mean signed error (MSE) value are given. *Value taken from the text (in the table the value 1286 K is given.)

Salt	Experiment	WBK	JC (TIP3P)	TF[2]	JC (SPC/E)[2]	SD[2]
LiF	1121.15	1155	1630	1010		
LiCl	883.15	1053	990	780		
LiBr	825.15	998	1060			
LiI	742.15	909	959			
NaF	1269.15	1178	1516	611		
NaCl	1074.15	1074	1324	1082	1285*	1327
NaBr	1020.15	1045	1270	1022		
NaI	933.15	971	1134			
KF	1131.15	1081	1368	859		
KCl	1044.15	1018	1230	1039		
KBr	1007.15	994	1207	1043		
KI	954.15	929	1129			
RbF	1106.15	1018	1343	996		
RbCl	988.15	991	1191	1092		
RbBr	955.15	953	1178	1047		
RbI	915.15	907	1107			
CsF	976.15	1005	1330			
CsCl	918.15	968	1155			
RMSD		79	250	226		
MSE		21	237	-93		

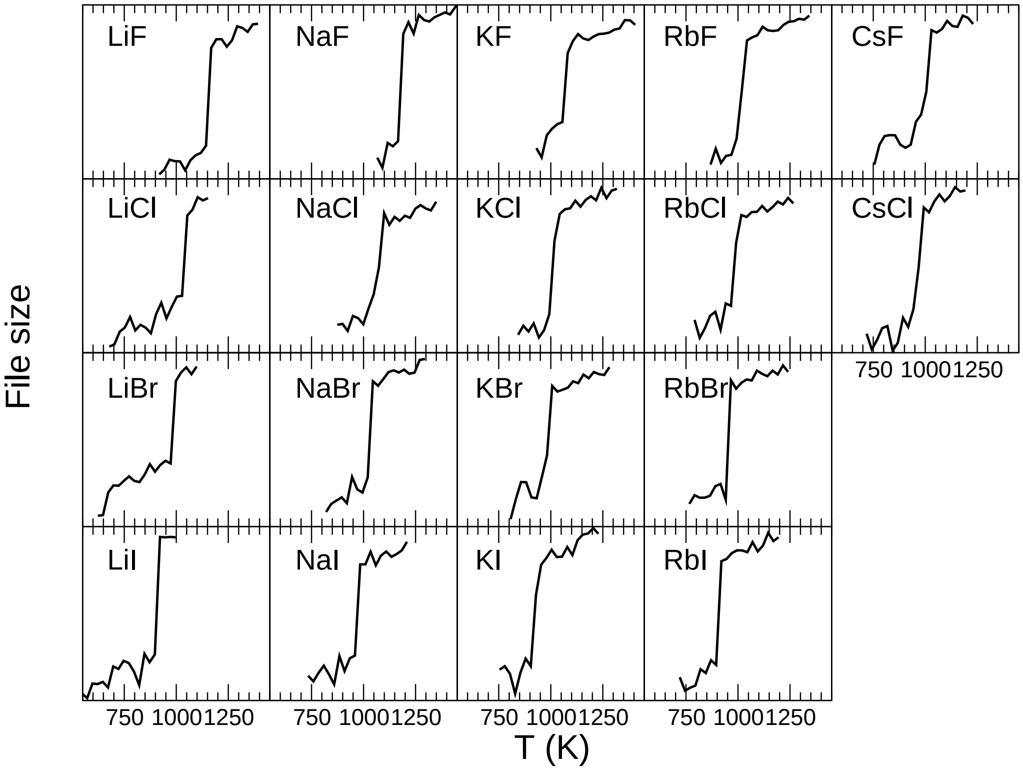
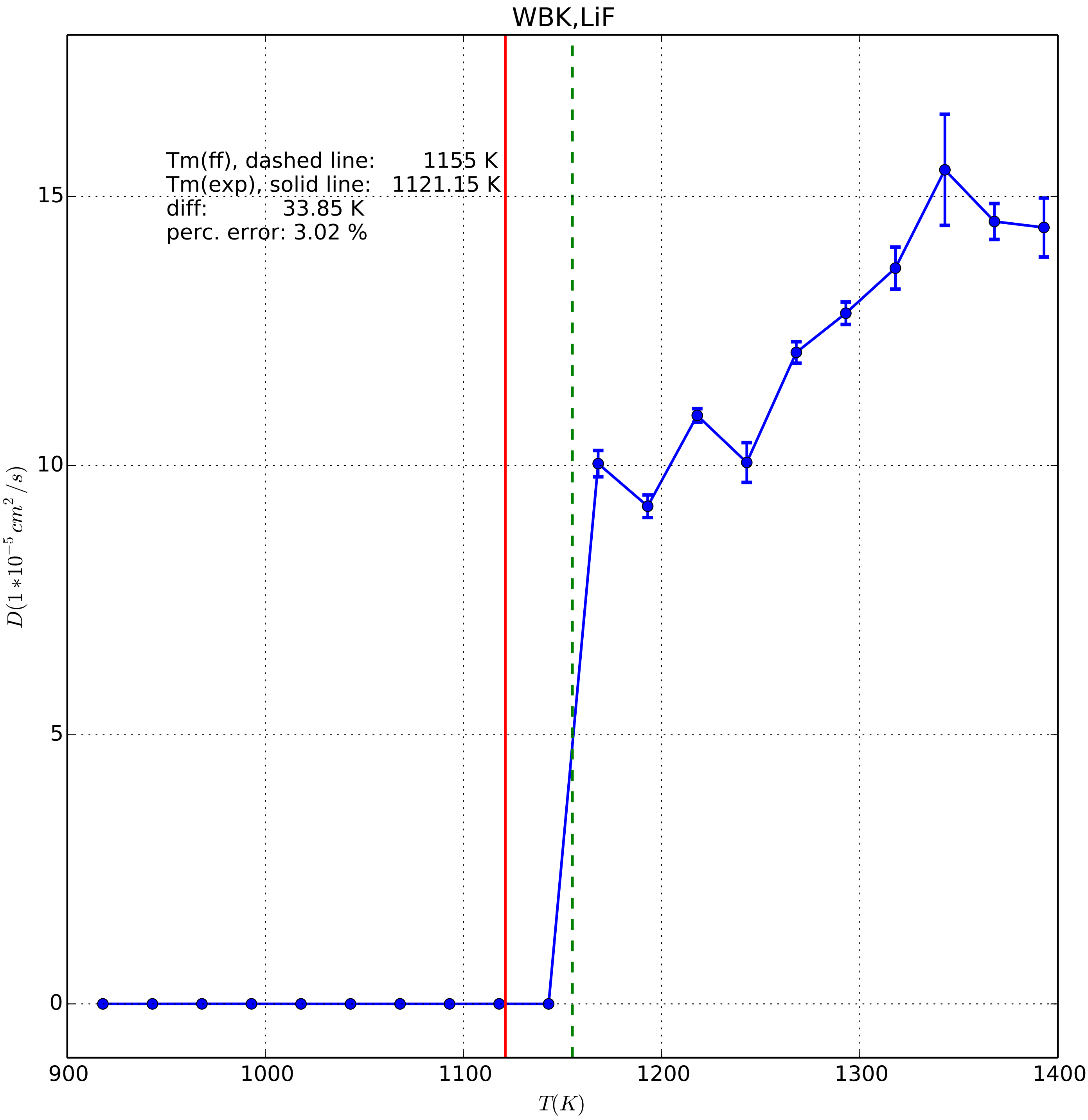
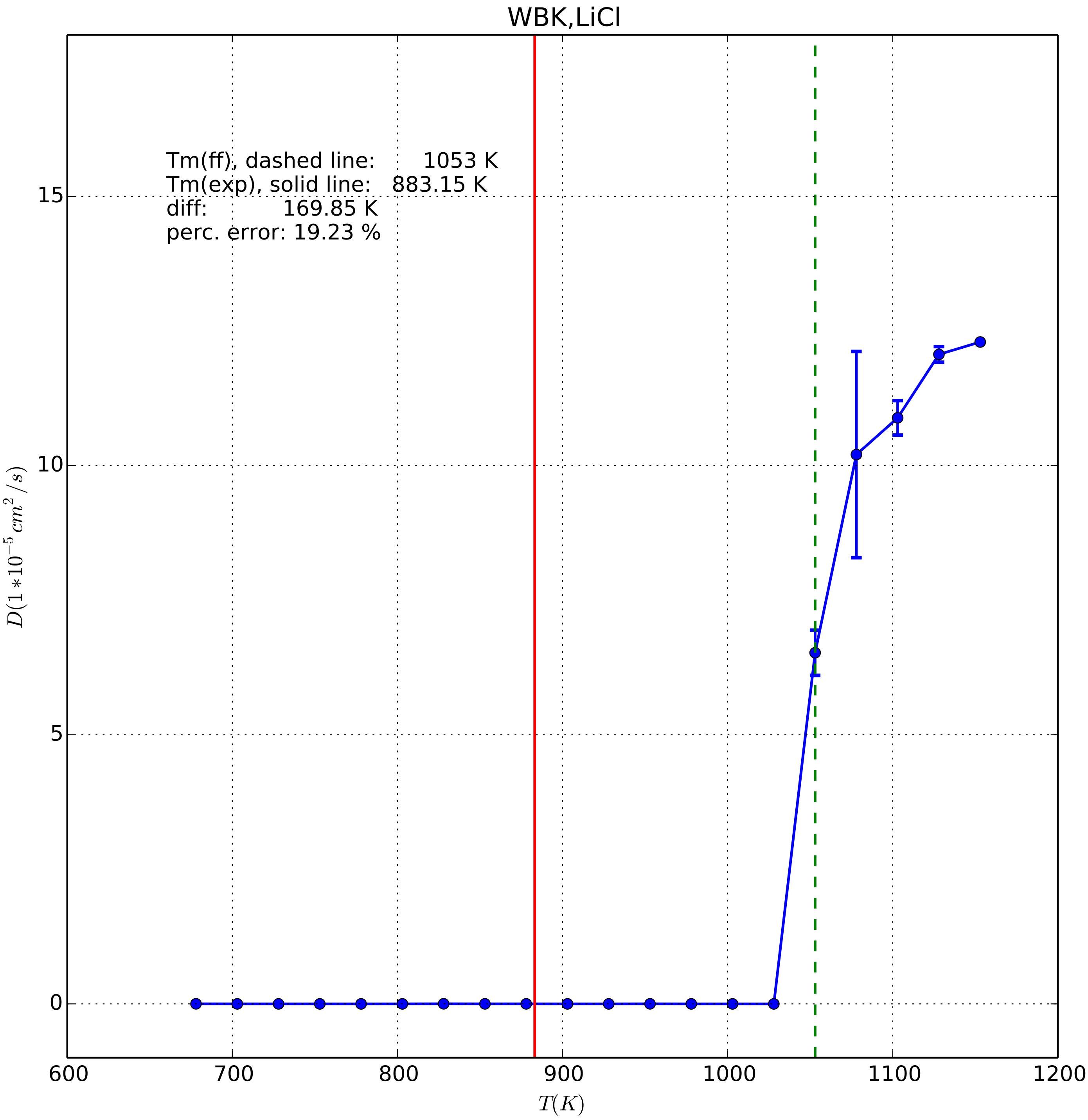


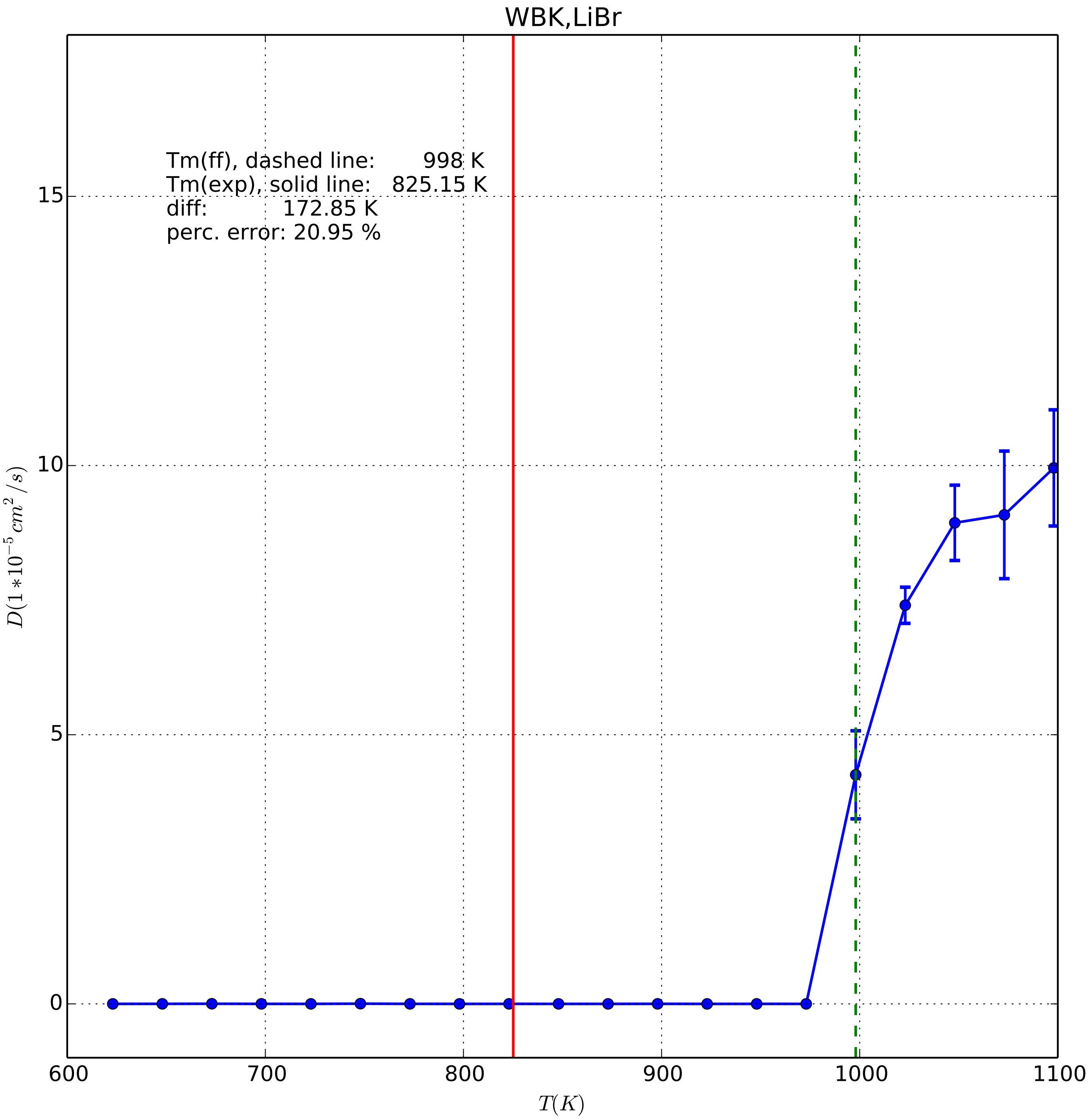
Figure S1: Filesize at the end of the co-existence simulations for the WBK force field for alkali-halides. The jump in file size indicates the melting point[15] and the T$_m$ correspond to those in Table Table S2.

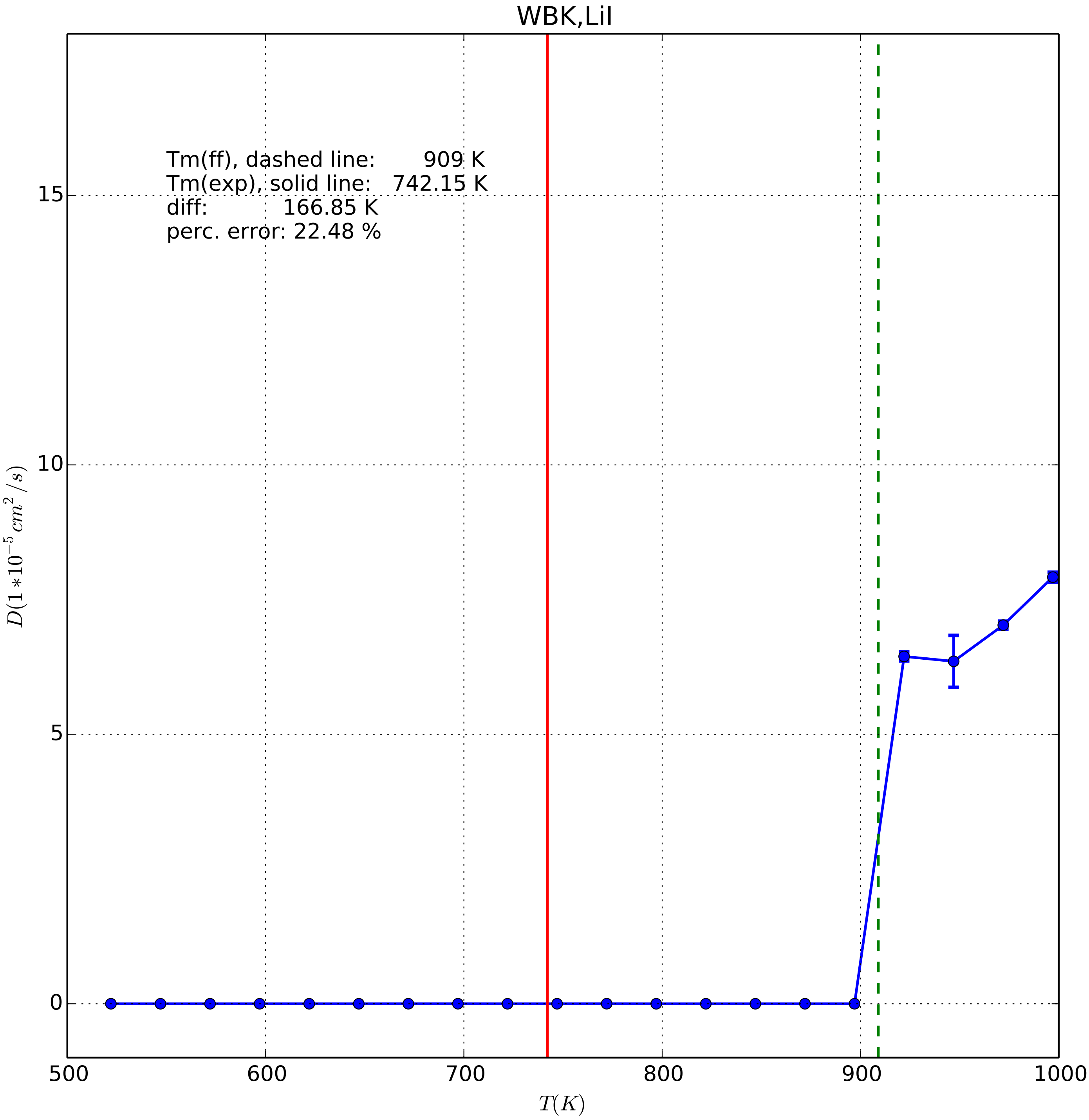
Diffusion coefficients and radial distribution functions

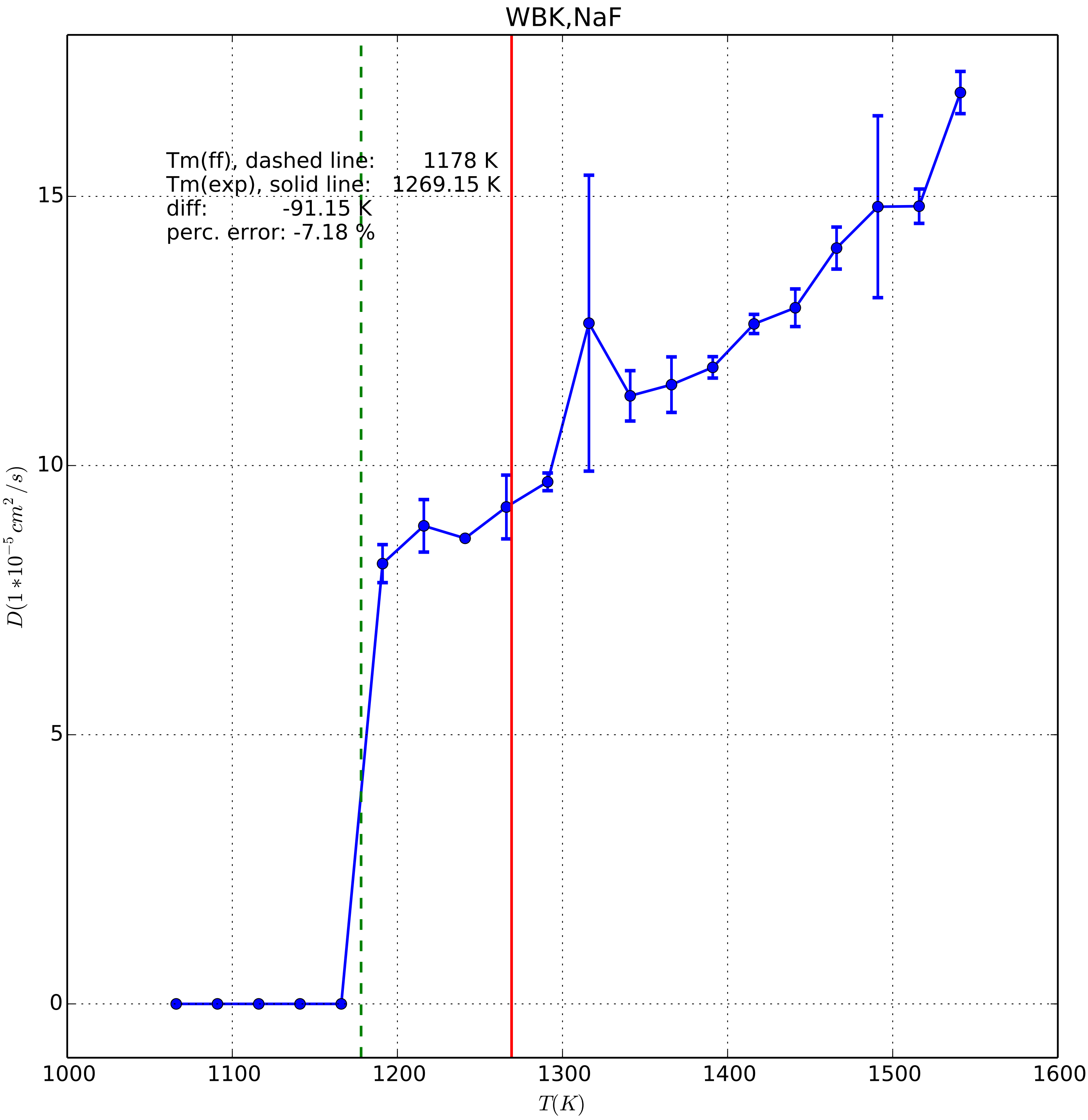


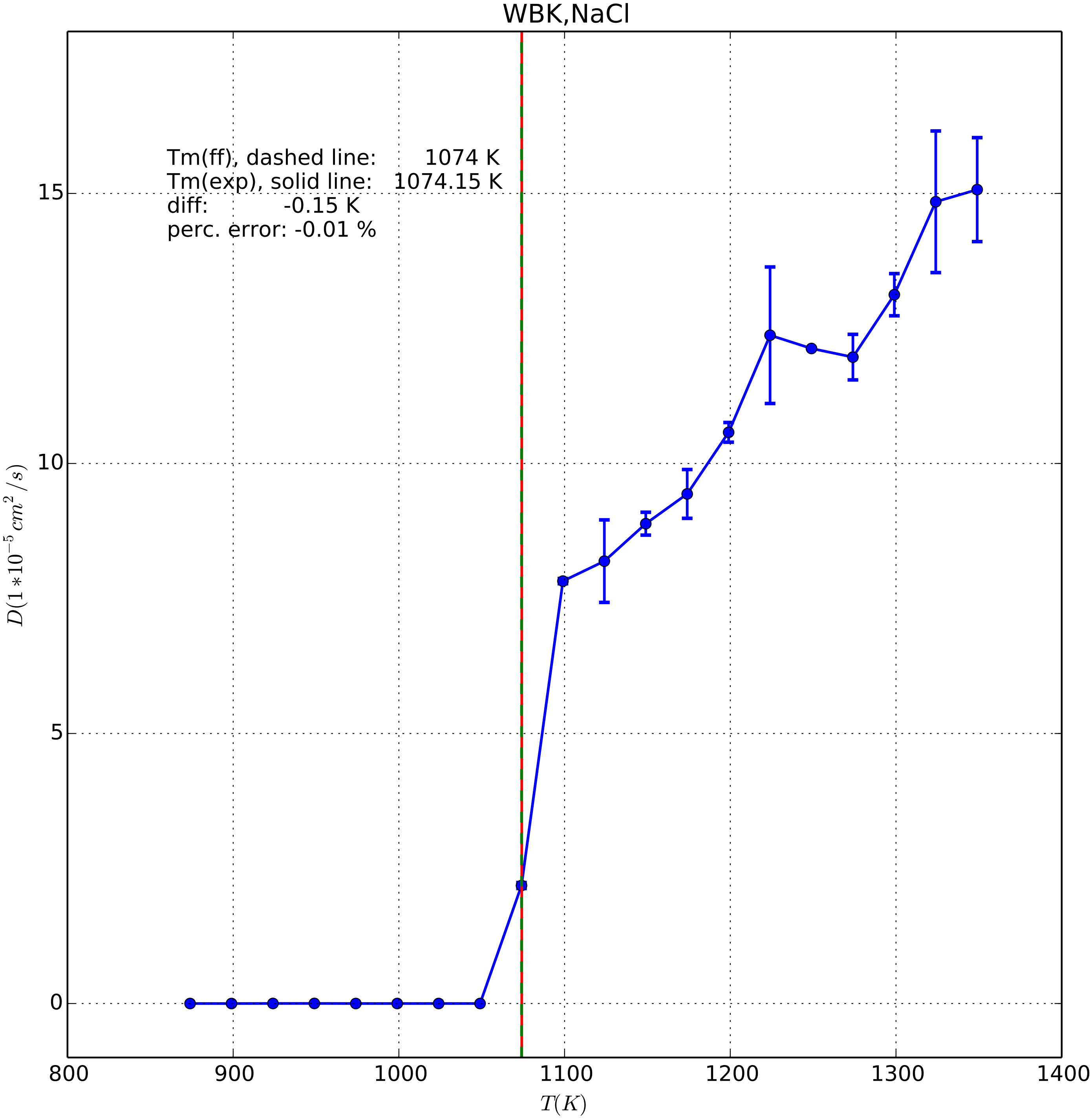
WBK,LiF
Tm(ff), dashed line: 1155 K
Tm(exp), solid line: 1121.15 K
diff: 33.85 K
perc. error: 3.02 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
900
1000
1100
1200
1300
1400
$T(K)$

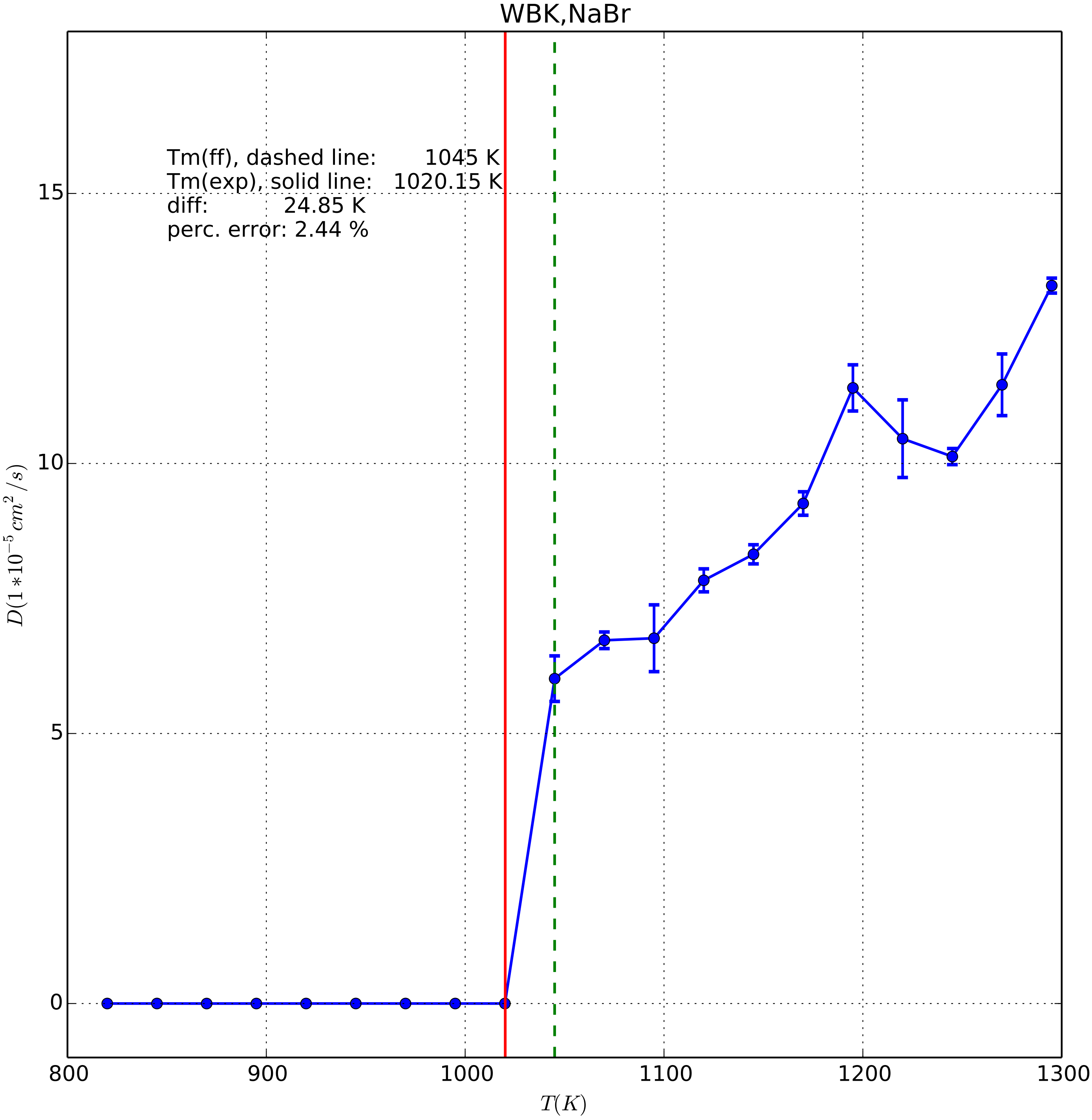

WBK,LiCl
Tm(ff), dashed line: 1053 K
Tm(exp), solid line: 883.15 K
diff: 169.85 K
perc. error: 19.23 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
600
700
800
900
1000
1100
1200
$T(K)$

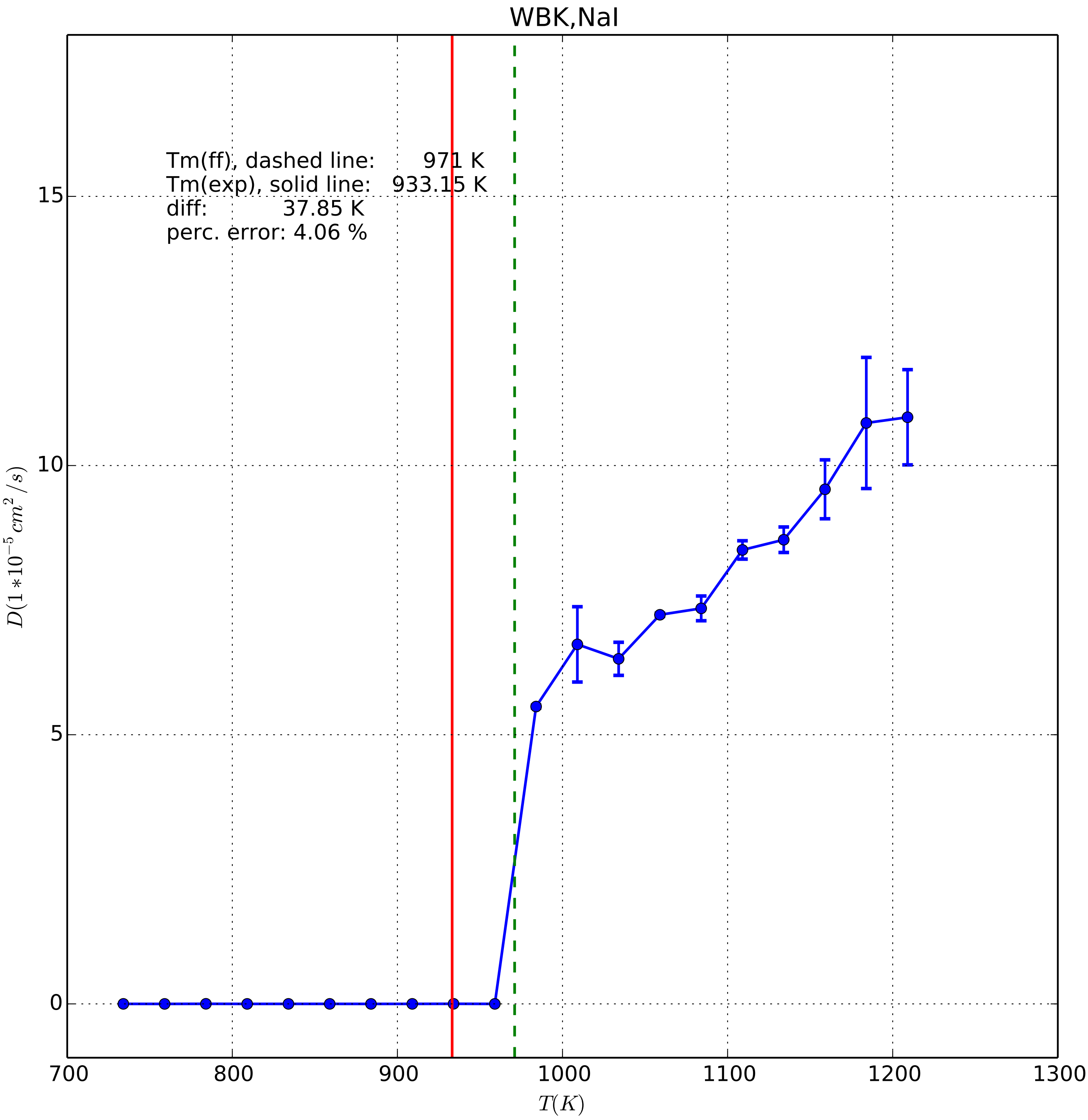

WBK,LiBr
Tm(ff), dashed line: 998 K
Tm(exp), solid line: 825.15 K
diff: 172.85 K
perc. error: 20.95 %
$D(1*10^{-5}cm^2/s)$
15
10
5
0
600
700
800
900
1000
1100
$T(K)$

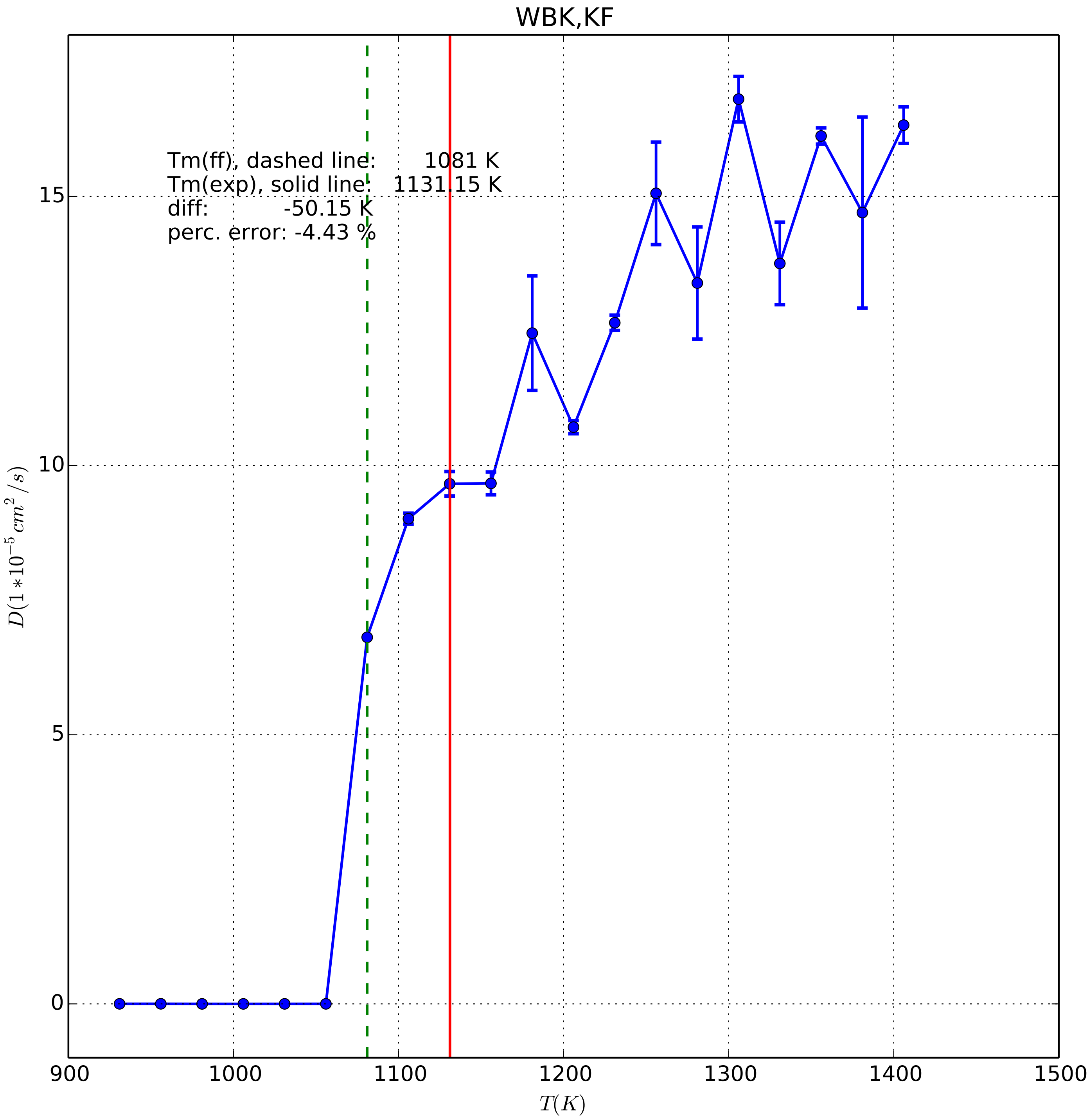

WBK,LiI
Tm(ff), dashed line: 909 K
Tm(exp), solid line: 742.15 K
diff: 166.85 K
perc. error: 22.48 %
$D(1*10^{-5}cm^2/s)$
15
10
5
0
500
600
700
800
900
1000
$T(K)$

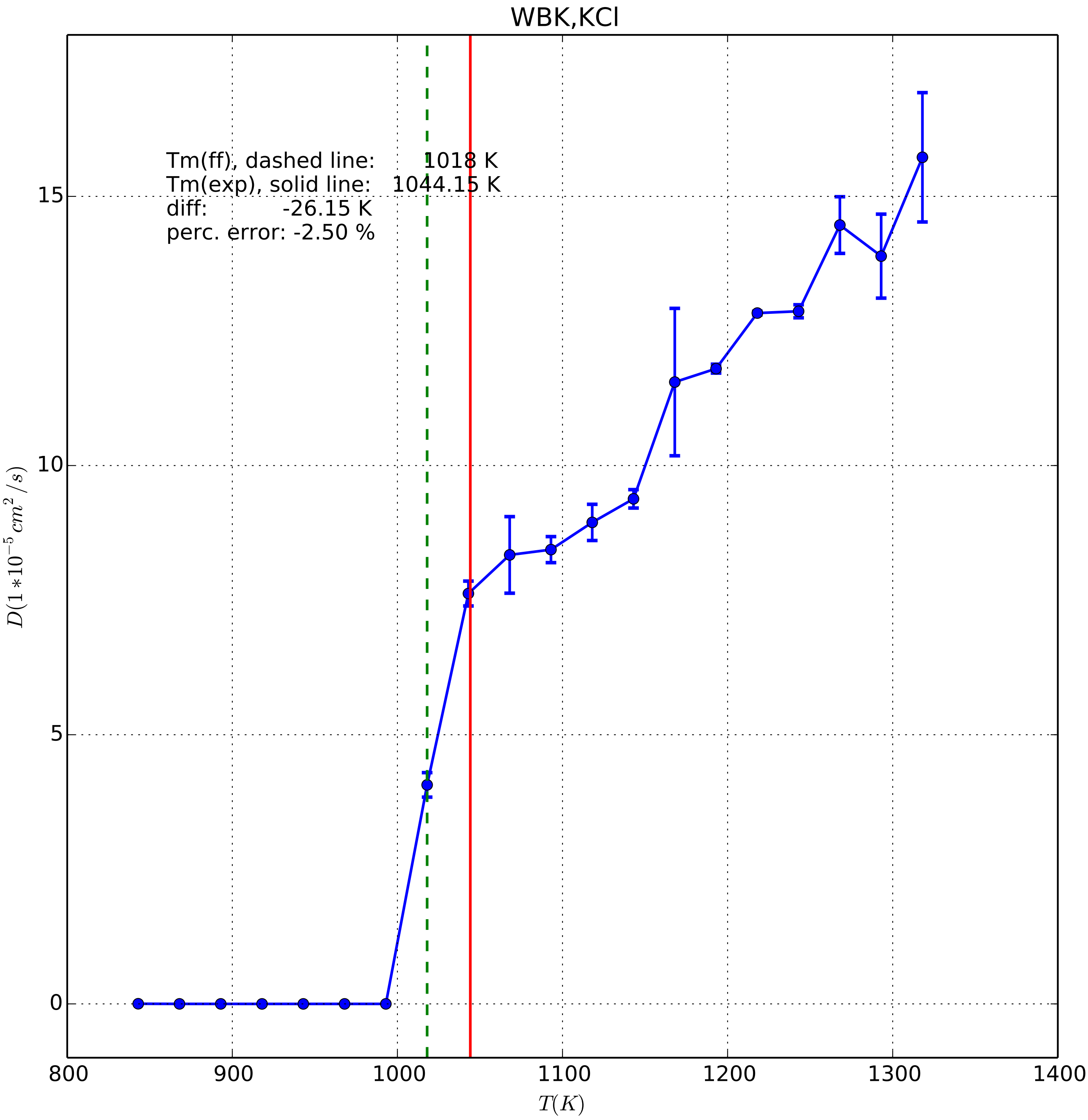

WBK,NaF
Tm(ff), dashed line: 1178 K
Tm(exp), solid line: 1269.15 K
diff: -91.15 K
perc. error: -7.18 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
1000
1100
1200
1300
1400
1500
1600
$T(K)$

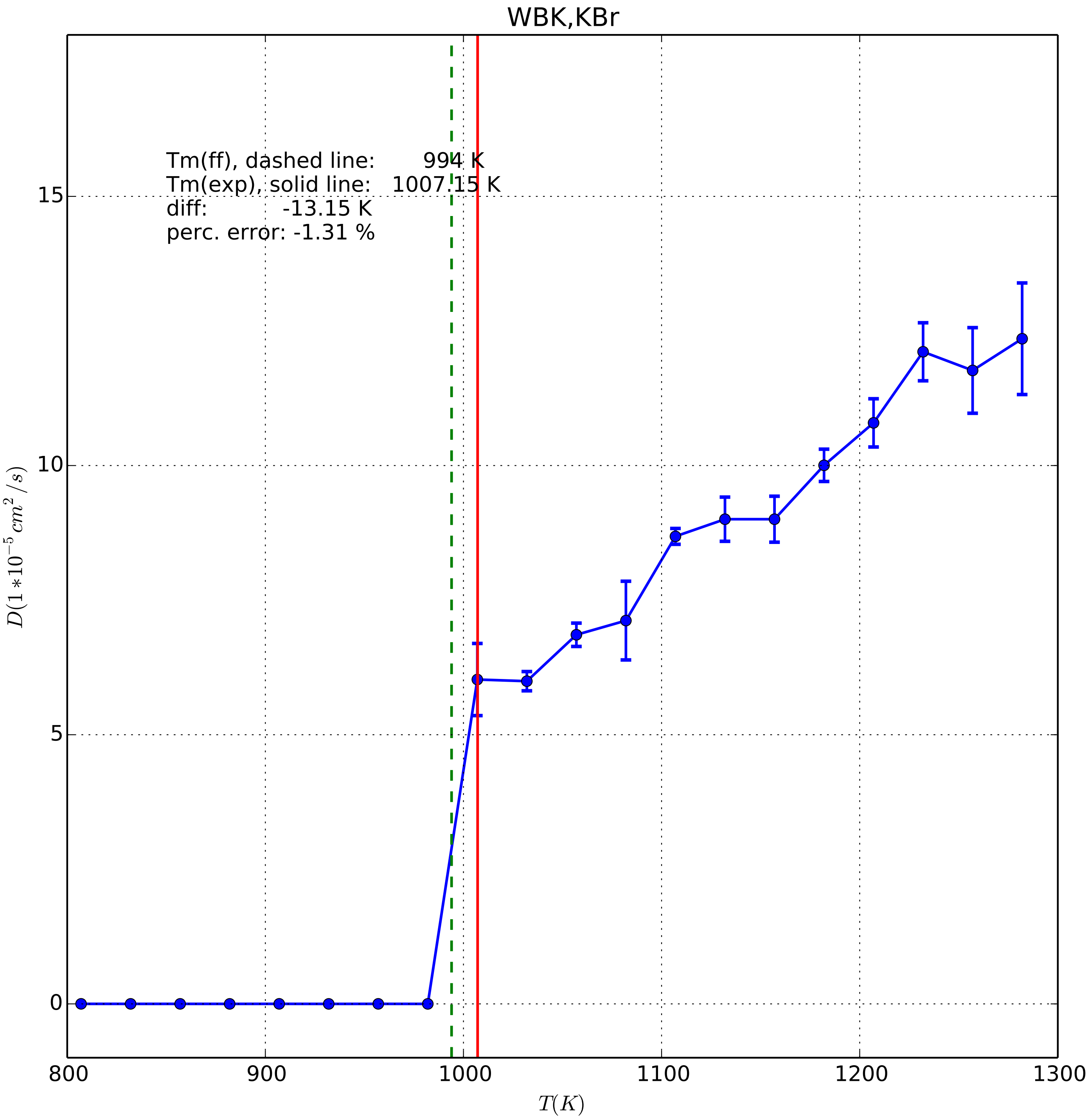

WBK,NaCl
Tm(ff), dashed line: 1074 K
Tm(exp), solid line: 1074.15 K
diff: -0.15 K
perc. error: -0.01 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
800
900
1000
1100
1200
1300
1400
$T(K)$

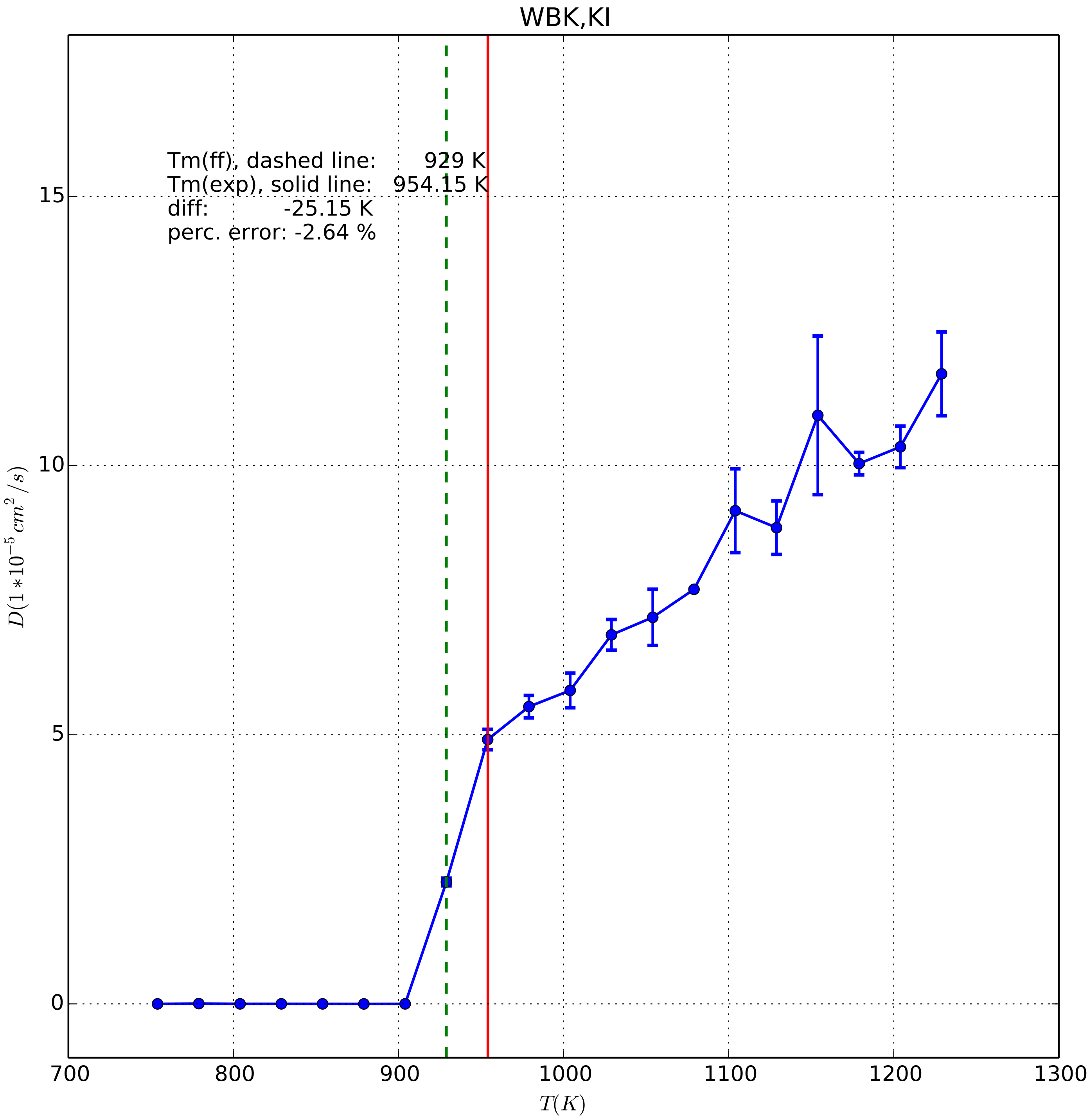

WBK,NaBr
Tm(ff), dashed line: 1045 K
Tm(exp), solid line: 1020.15 K
diff: 24.85 K
perc. error: 2.44 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
800
900
1000
1100
1200
1300
$T(K)$

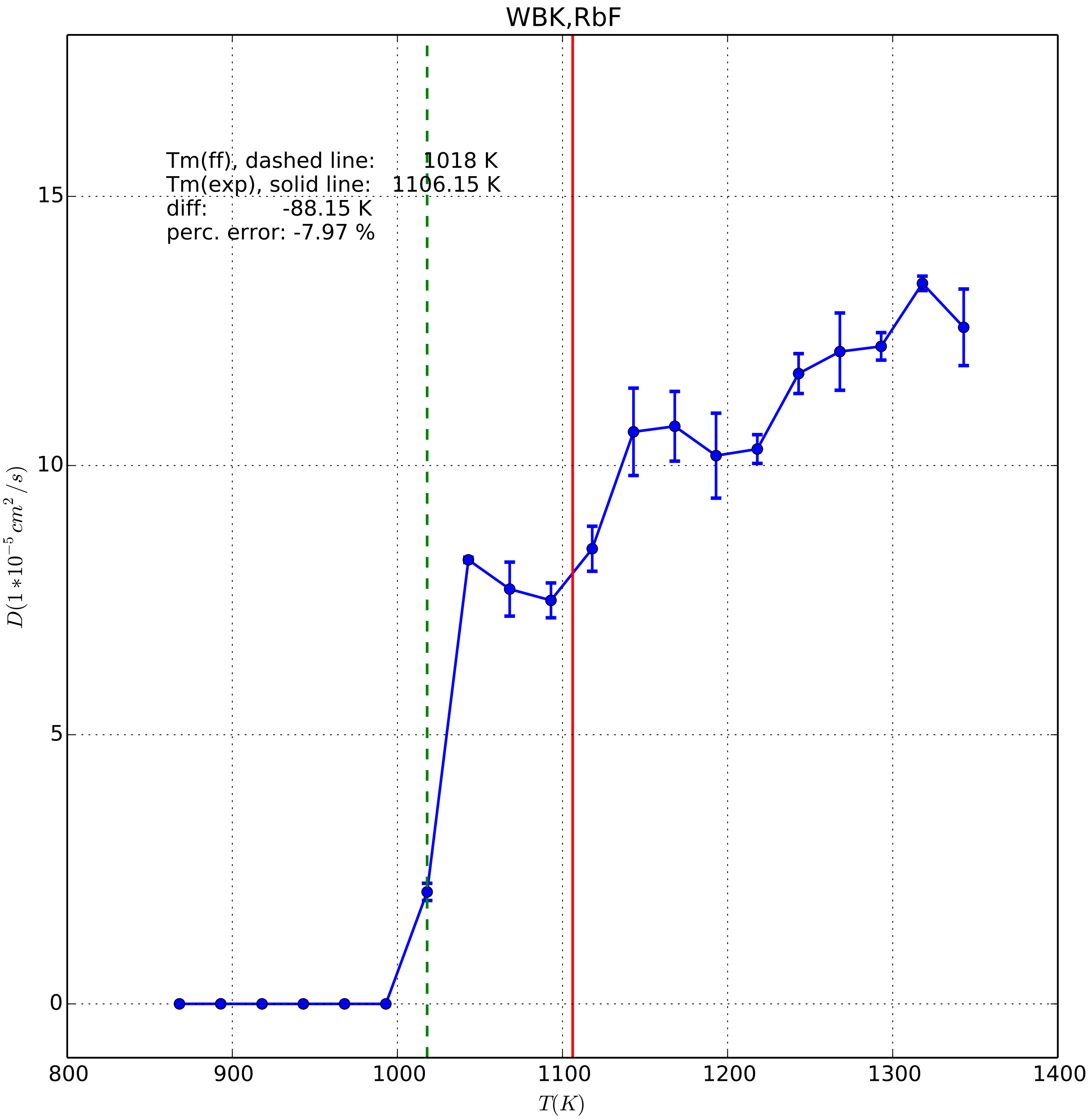

WBK,NaI
Tm(ff), dashed line: 971 K
Tm(exp), solid line: 933.15 K
diff: 37.85 K
perc. error: 4.06 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
700
800
900
1000
1100
1200
1300
$T(K)$

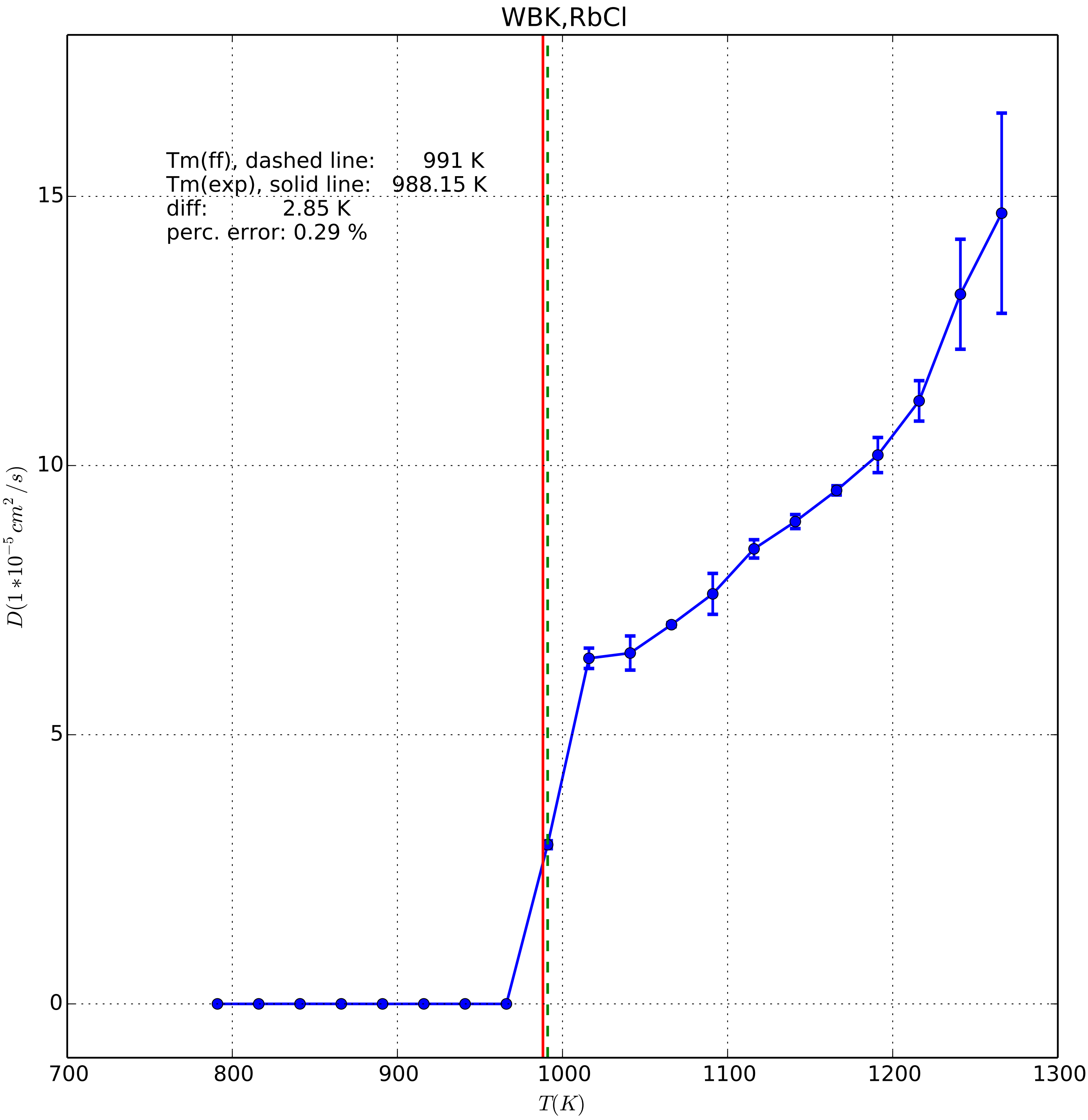

WBK,KF
Tm(ff), dashed line: 1081 K
Tm(exp), solid line: 1131.15 K
diff: -50.15 K
perc. error: -4.43 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
900
1000
1100
1200
1300
1400
1500
$T(K)$


WBK,KCl
Tm(ff), dashed line: 1018 K
Tm(exp), solid line: 1044.15 K
diff: -26.15 K
perc. error: -2.50 %
$D(1*10^{-5}cm^2/s)$
$T(K)$
0
5
10
15
800
900
1000
1100
1200
1300
1400

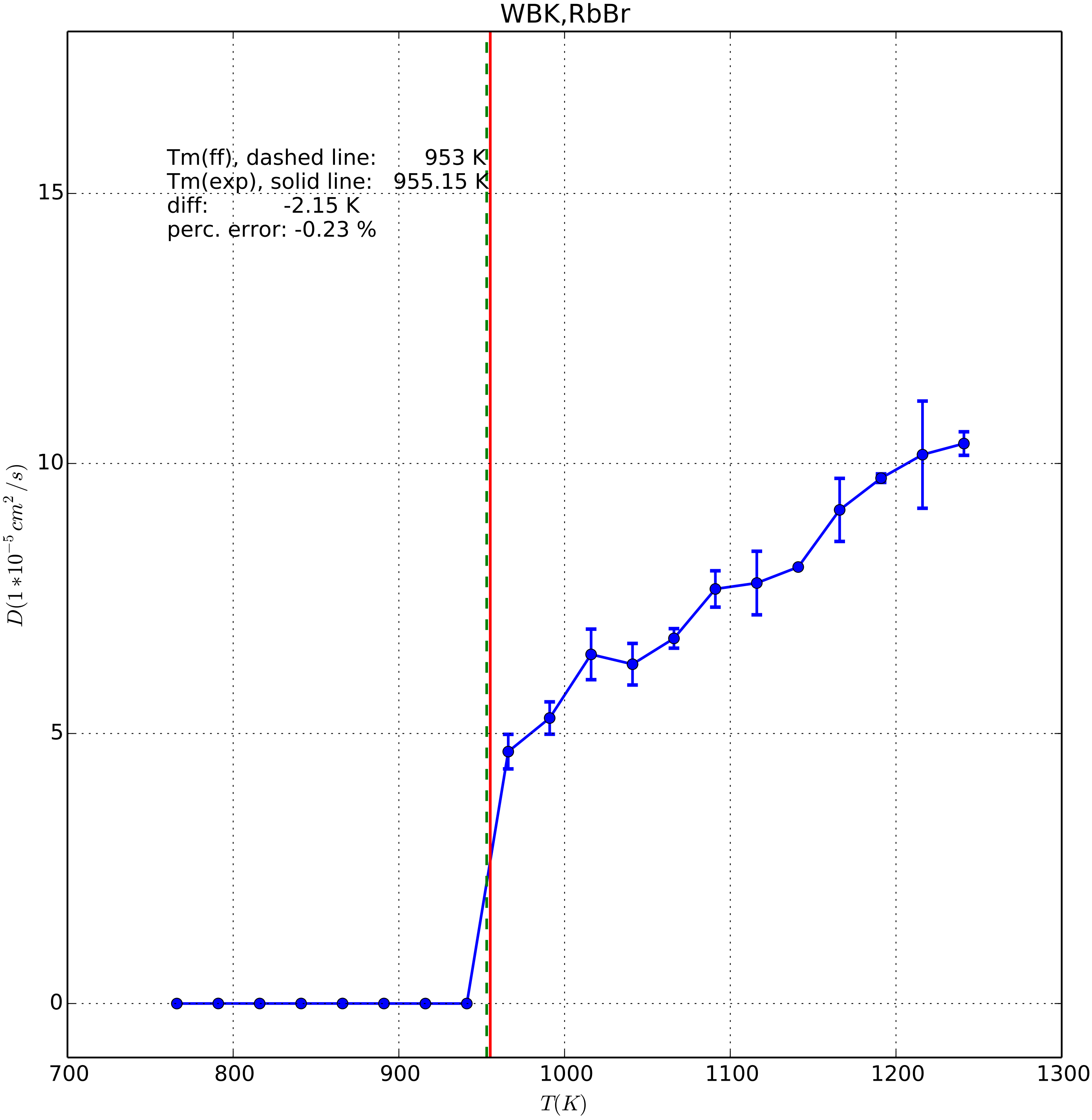

WBK,KBr
Tm(ff), dashed line: 994 K
Tm(exp), solid line: 1007.15 K
diff: -13.15 K
perc. error: -1.31 %
$D(1*10^{-5}cm^2/s)$
15
10
5
0
800
900
1000
1100
1200
1300
$T(K)$

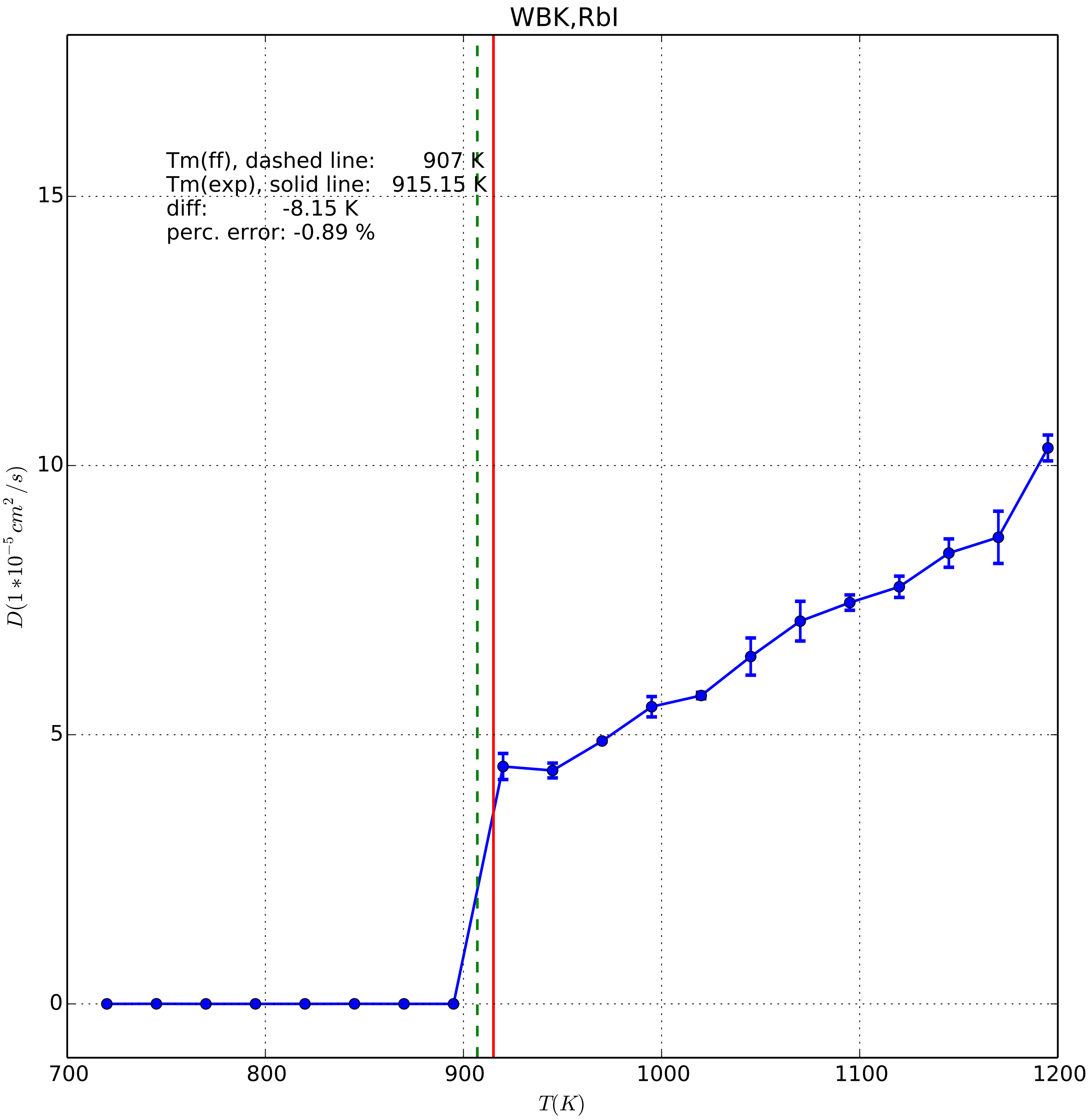

WBK,KI
Tm(ff), dashed line: 929 K
Tm(exp), solid line: 954.15 K
diff: -25.15 K
perc. error: -2.64 %
$D(1*10^{-5}cm^2/s)$
15
10
5
0
700
800
900
1000
1100
1200
1300
$T(K)$

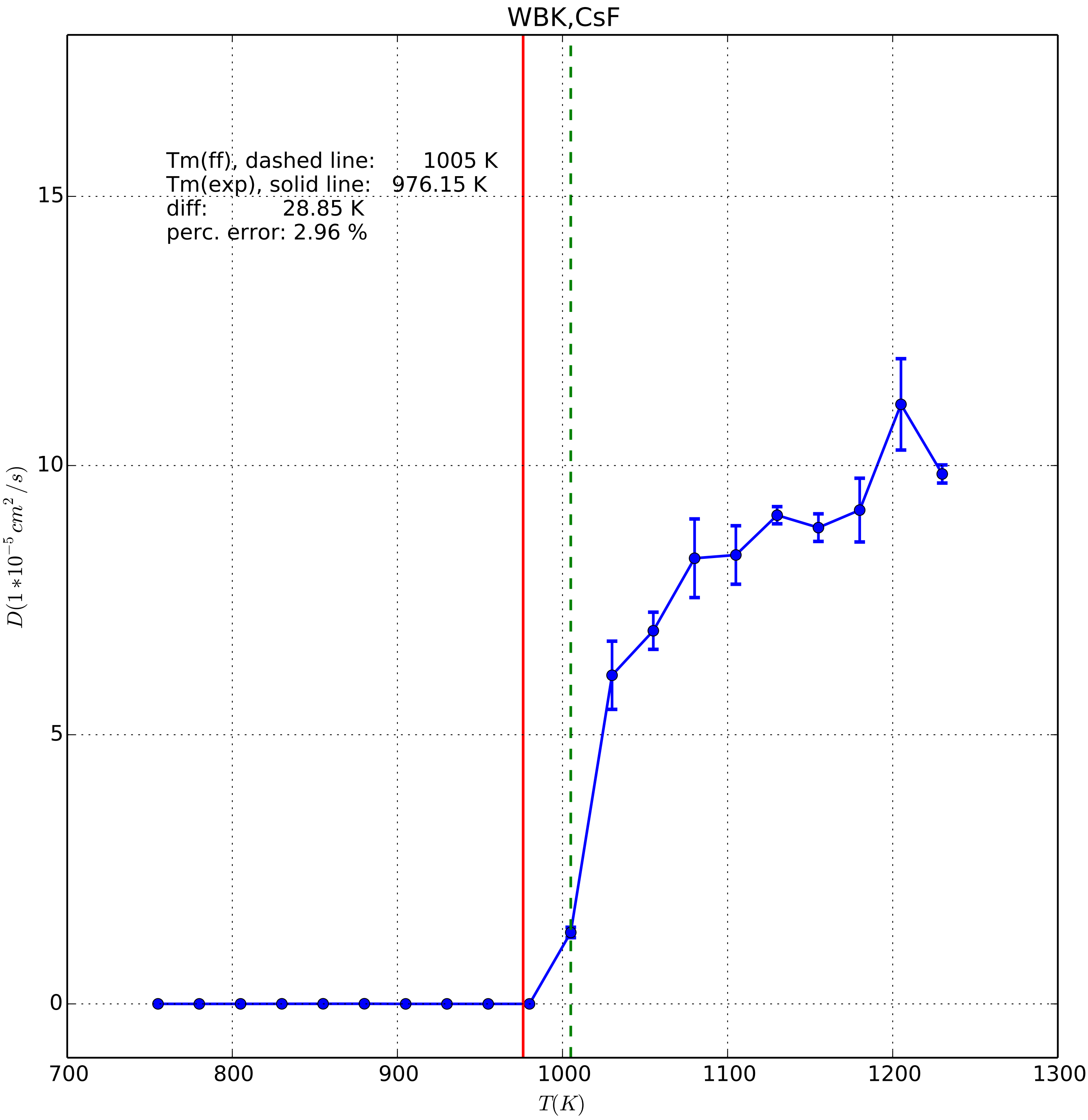

WBK,RbF
Tm(ff), dashed line: 1018 K
Tm(exp), solid line: 1106.15 K
diff: -88.15 K
perc. error: -7.97 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
800
900
1000
1100
1200
1300
1400
$T(K)$

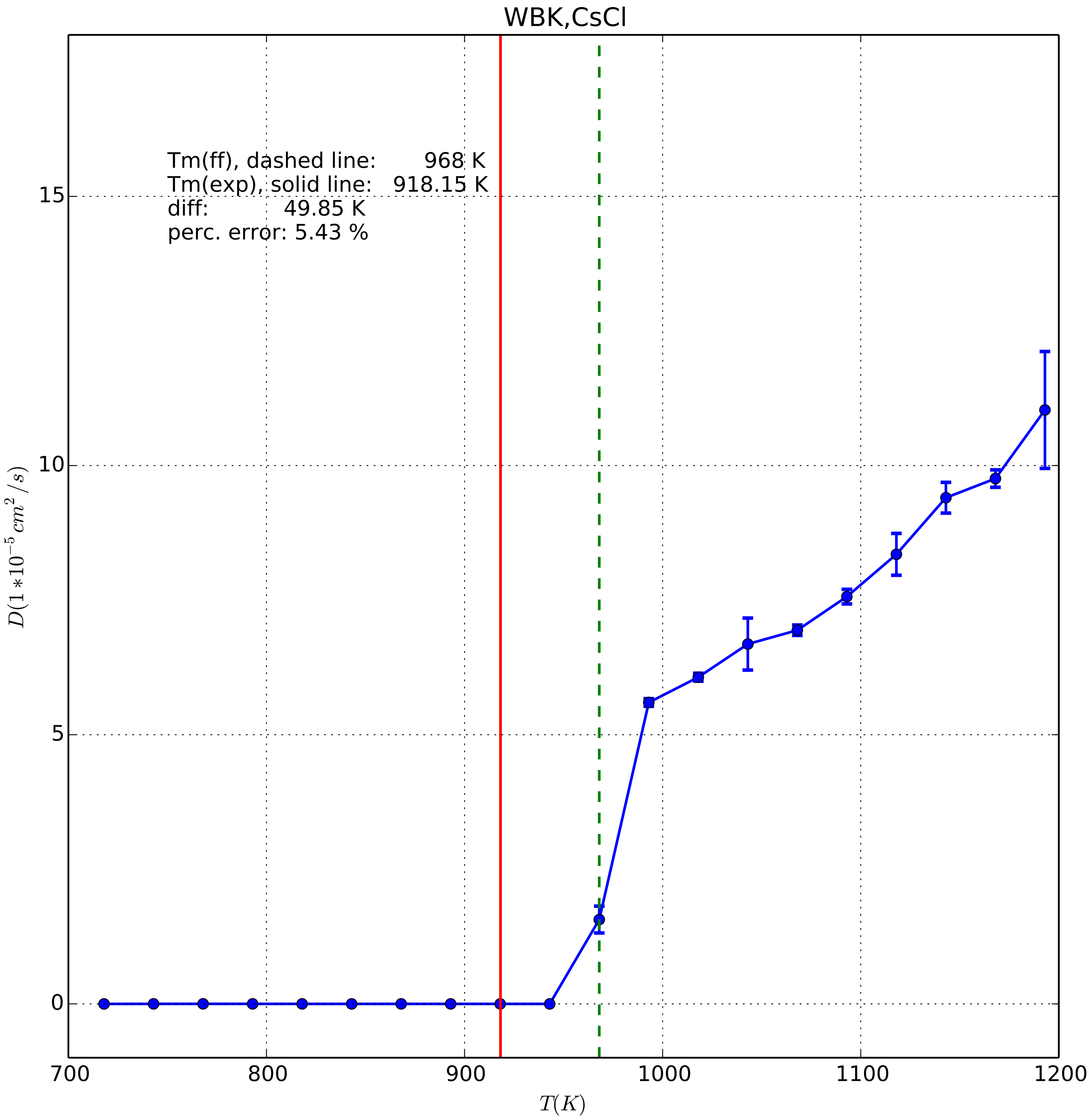


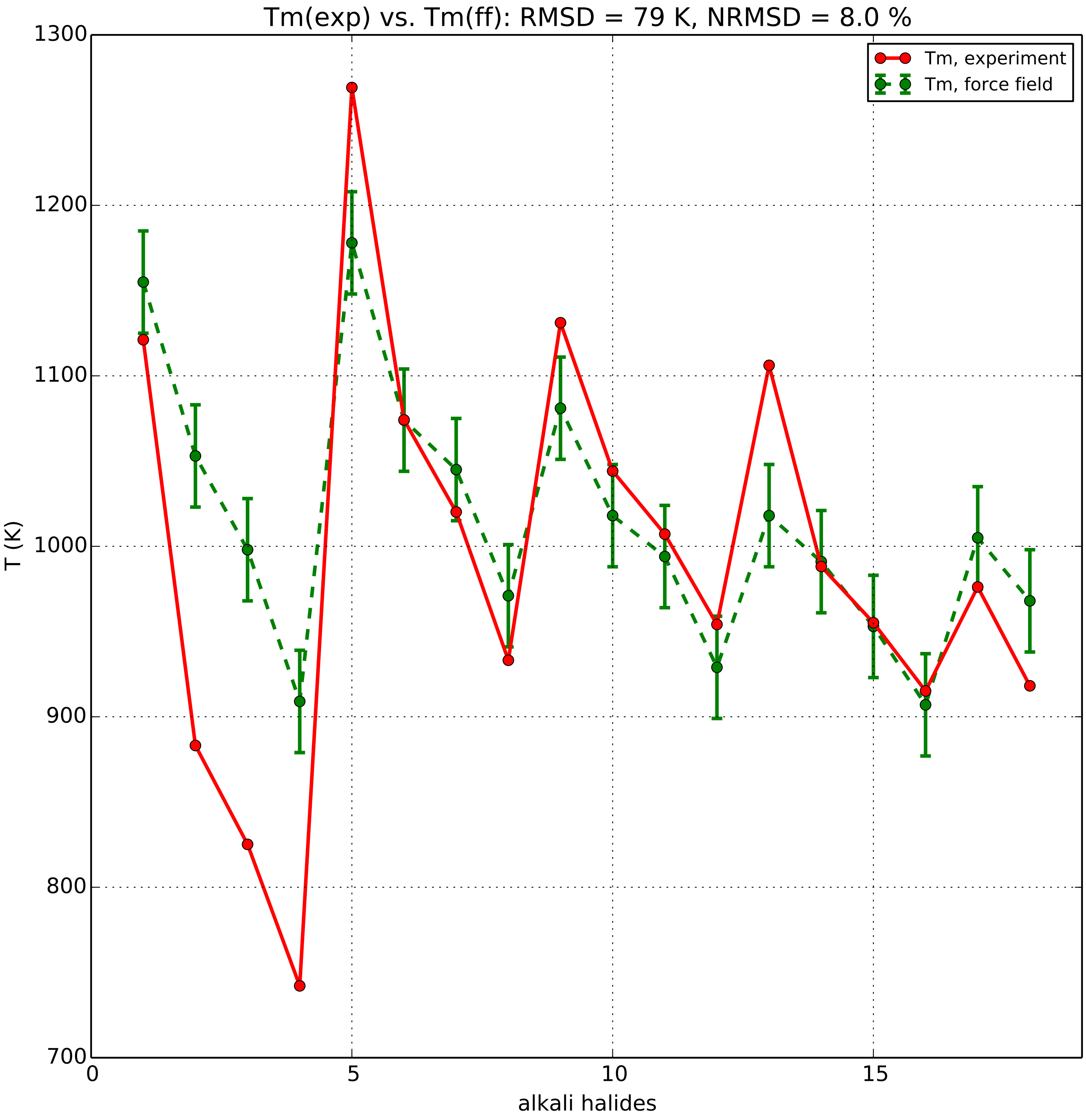
WBK,RbCl
Tm(ff), dashed line: 991 K
Tm(exp), solid line: 988.15 K
diff: 2.85 K
perc. error: 0.29 %
$D(1*10^{-5}cm^2/s)$
$T(K)$
0
5
10
15
700
800
900
1000
1100
1200
1300

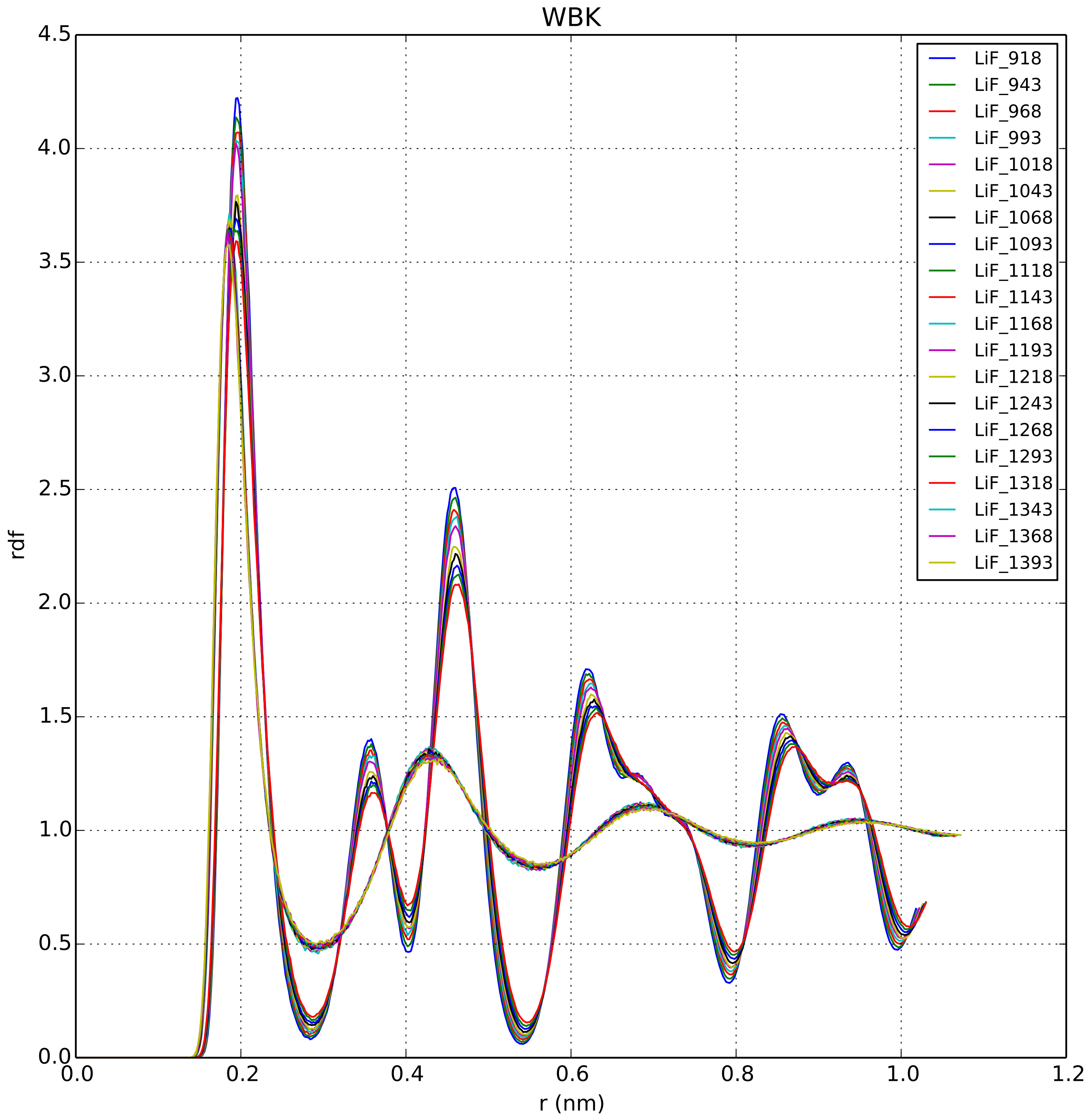

WBK,RbBr
Tm(ff), dashed line: 953 K
Tm(exp), solid line: 955.15 K
diff: -2.15 K
perc. error: -0.23 %
15
10
5
0
$D(1*10^{-5}cm^2/s)$
700
800
900
1000
1100
1200
1300
$T(K)$


WBK,RbI
Tm(ff), dashed line: 907 K
Tm(exp), solid line: 915.15 K
diff: -8.15 K
perc. error: -0.89 %
15
10
5
0
700
800
900
1000
1100
1200
$D(1*10^{-5}cm^2/s)$
$T(K)$


WBK,CsF
Tm(ff), dashed line: 1005 K
Tm(exp), solid line: 976.15 K
diff: 28.85 K
perc. error: 2.96 %
$D(1*10^{-5}cm^2/s)$
15
10
5
0
700
800
900
1000
1100
1200
1300
$T(K)$


WBK,CsCl
Tm(ff), dashed line: 968 K
Tm(exp), solid line: 918.15 K
diff: 49.85 K
perc. error: 5.43 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
700
800
900
1000
1100
1200
$T(K)$


Tm(exp) vs. Tm(ff): RMSD = 79 K, NRMSD = 8.0 %
Tm, experiment
Tm, force field
T (K)
1300
1200
1100
1000
900
800
700
0
5
10
15
alkali halides


WBK
rdf
r (nm)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
0.0
0.2
0.4
0.6
0.8
1.0
1.2
LiF_918
LiF_943
LiF_968
LiF_993
LiF_1018
LiF_1043
LiF_1068
LiF_1093
LiF_1118
LiF_1143
LiF_1168
LiF_1193
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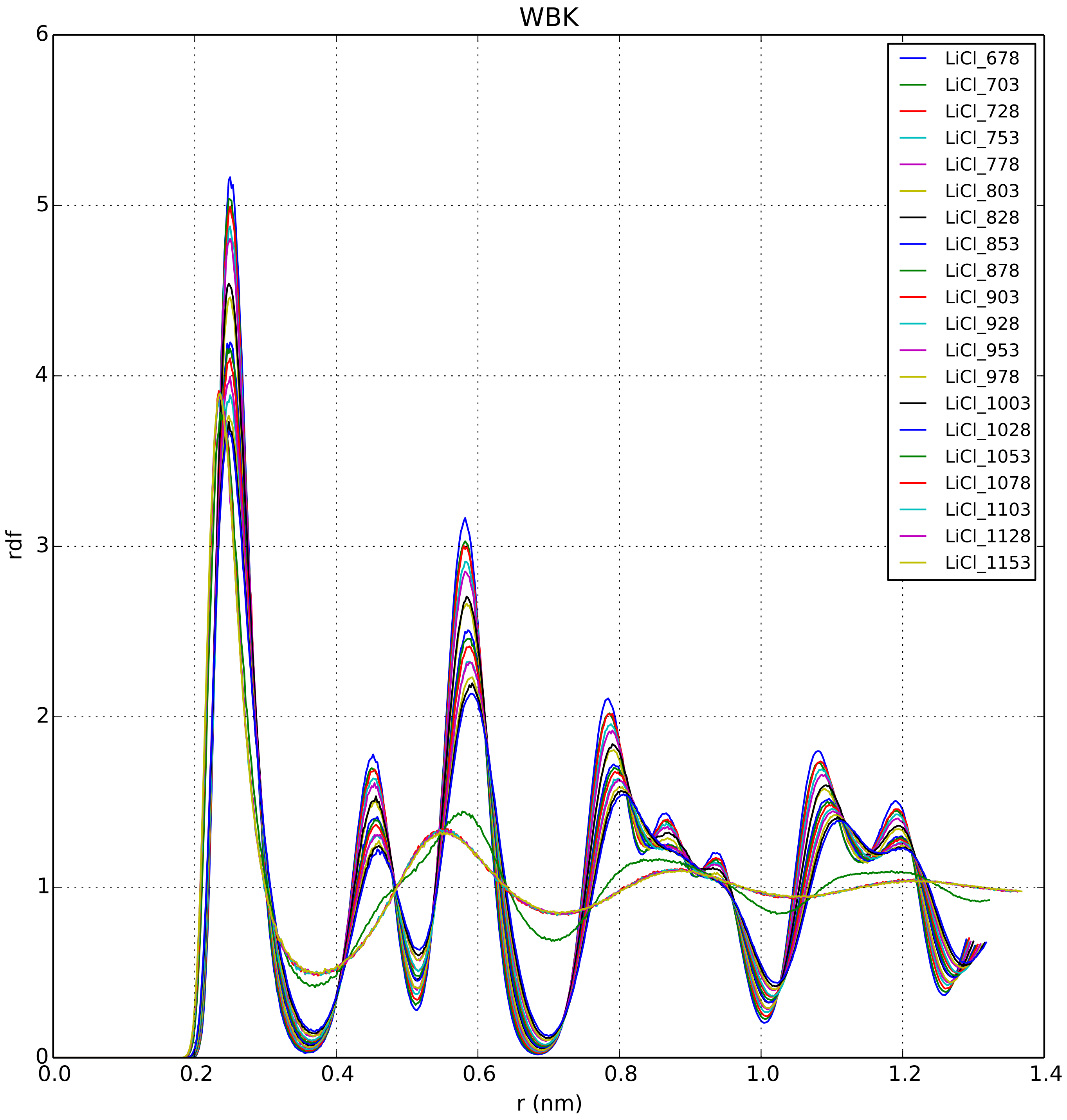
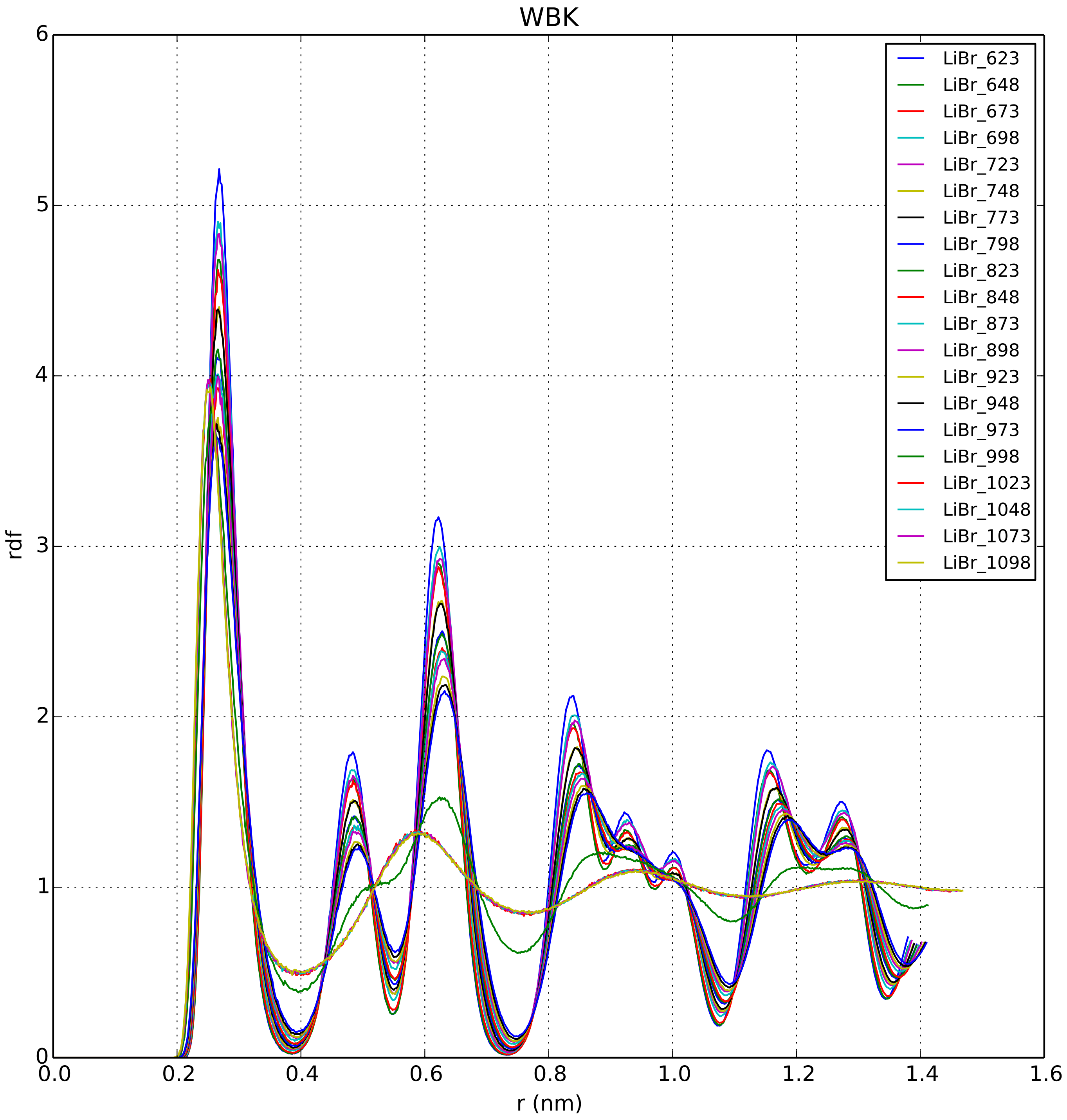
LiF_1368
LiF_1393


WBK
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
LiCl_678
LiCl_703
LiCl_728
LiCl_753
LiCl_778
LiCl_803
LiCl_828
LiCl_853
LiCl_878
LiCl_903
LiCl_928
LiCl_953
LiCl_978
LiCl_1003
LiCl_1028
LiCl_1053
LiCl_1078
LiCl_1103
LiCl_1128
LiCl_1153


WBK
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
LiBr_623
LiBr_648
LiBr_673
LiBr_698
LiBr_723
LiBr_748
LiBr_773
LiBr_798
LiBr_823
LiBr_848
LiBr_873
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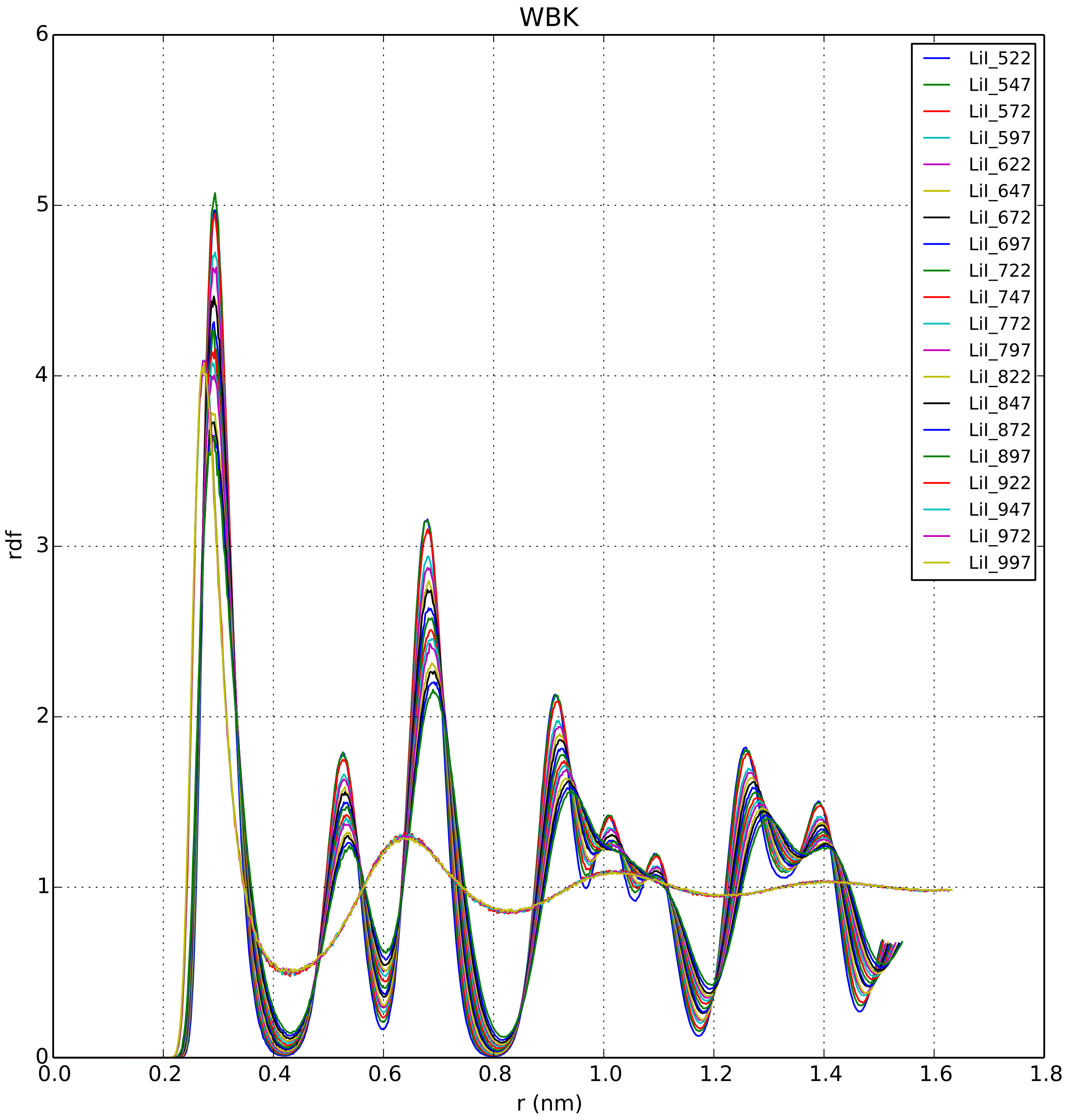
LiBr_1073
LiBr_1098


WBK
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
LiI_522
LiI_547
LiI_572
LiI_597
LiI_622
LiI_647
LiI_672
LiI_697
LiI_722
LiI_747
LiI_772
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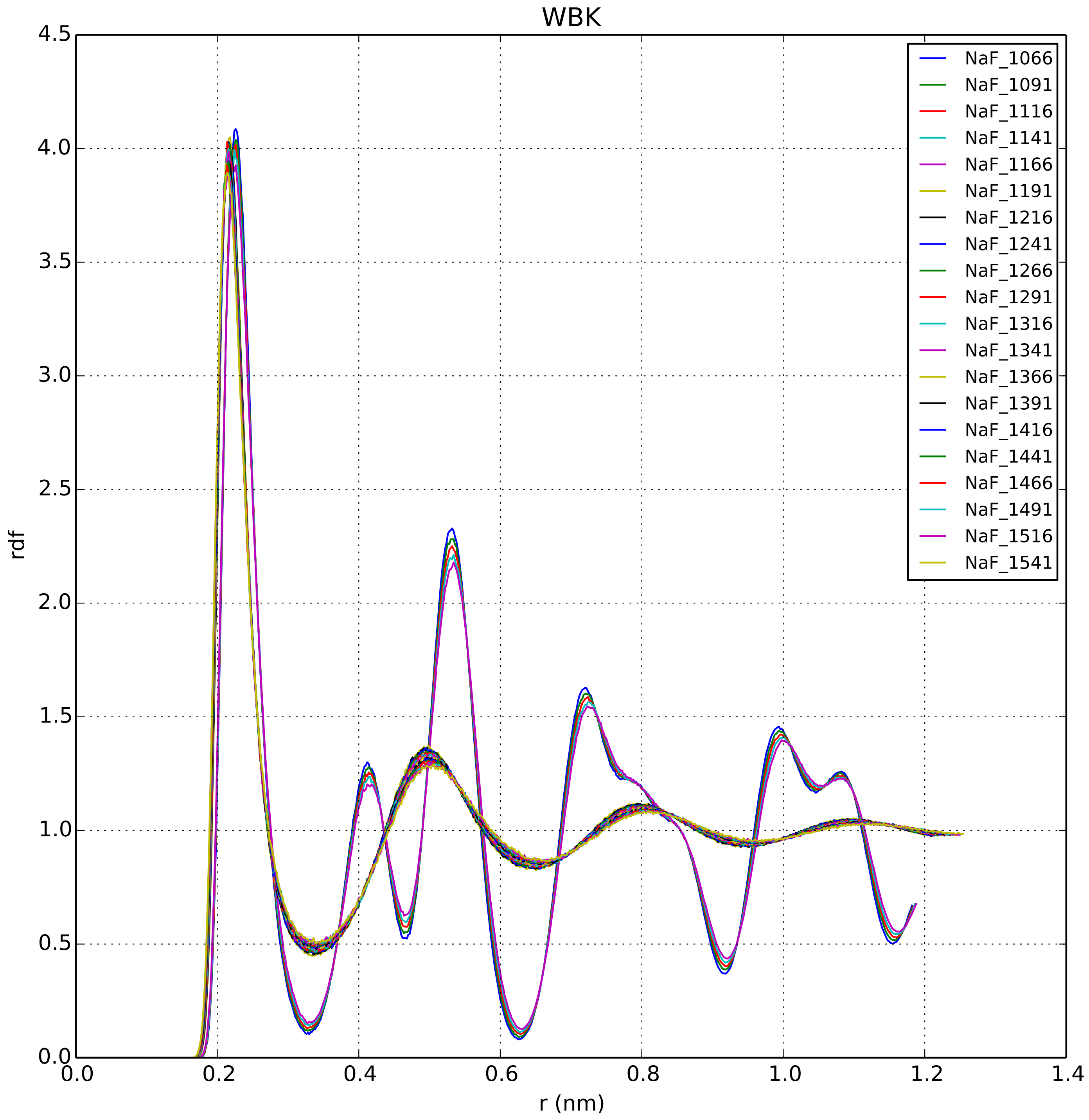
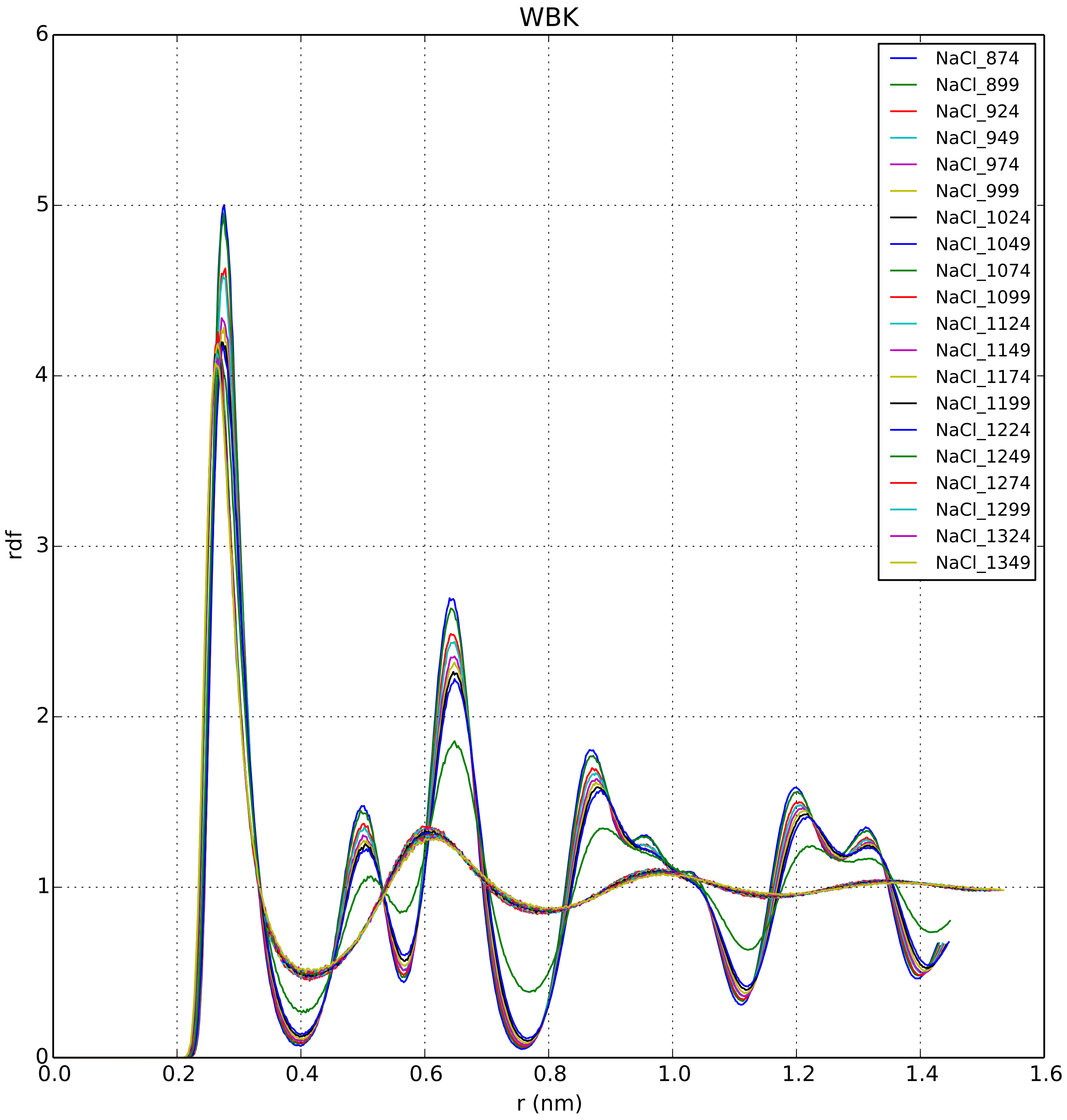
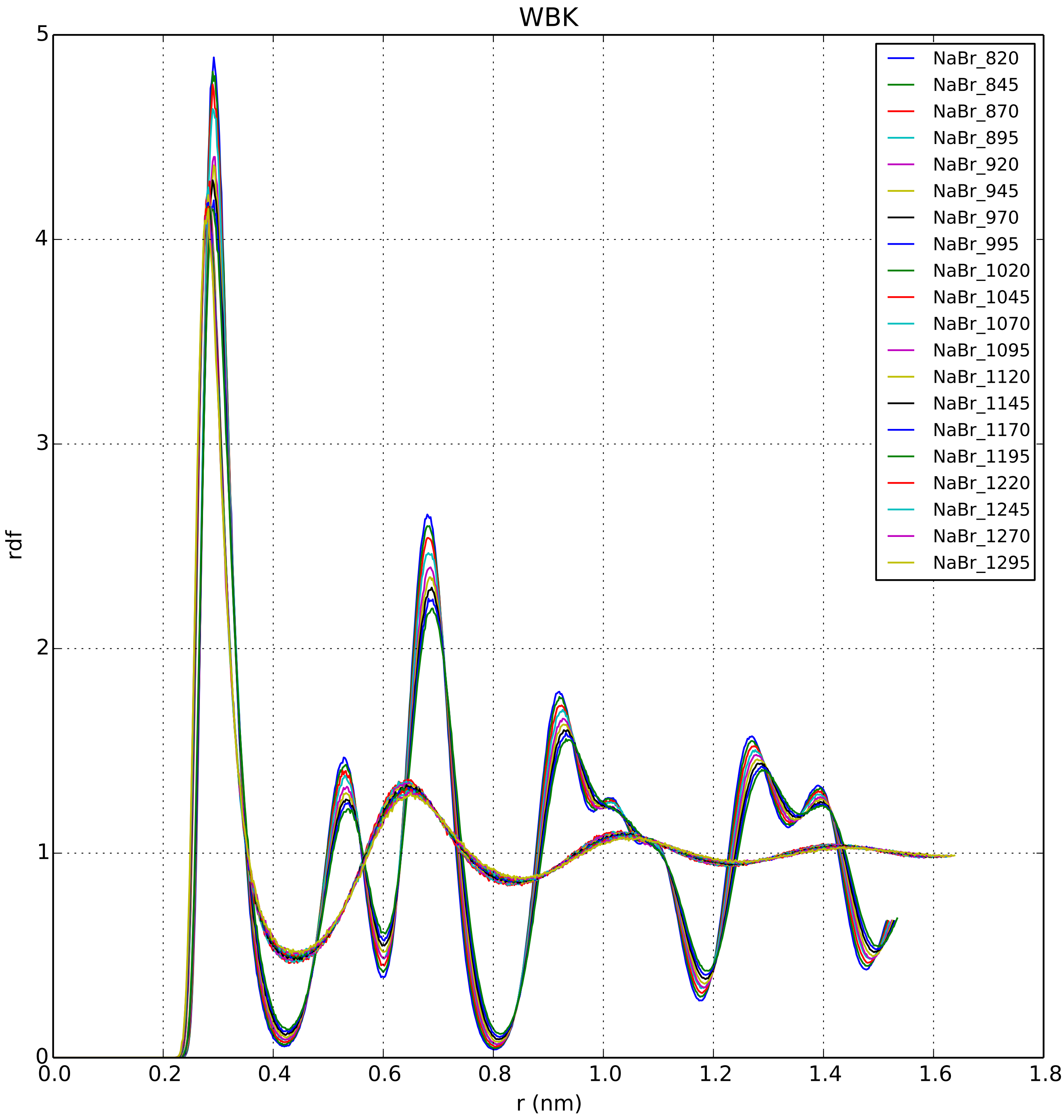
LiI_947
LiI_972
LiI_997


WBK
rdf
r (nm)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
NaF_1066
NaF_1091
NaF_1116
NaF_1141
NaF_1166
NaF_1191
NaF_1216
NaF_1241
NaF_1266
NaF_1291
NaF_1316
NaF_1341
NaF_1366
NaF_1391
NaF_1416
NaF_1441
NaF_1466
NaF_1491
NaF_1516
NaF_1541


WBK
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
NaCl_874
NaCl_899
NaCl_924
NaCl_949
NaCl_974
NaCl_999
NaCl_1024
NaCl_1049
NaCl_1074
NaCl_1099
NaCl_1124
NaCl_1149
NaCl_1174
NaCl_1199
NaCl_1224
NaCl_1249
NaCl_1274
NaCl_1299
NaCl_1324
NaCl_1349


WBK
rdf
r (nm)
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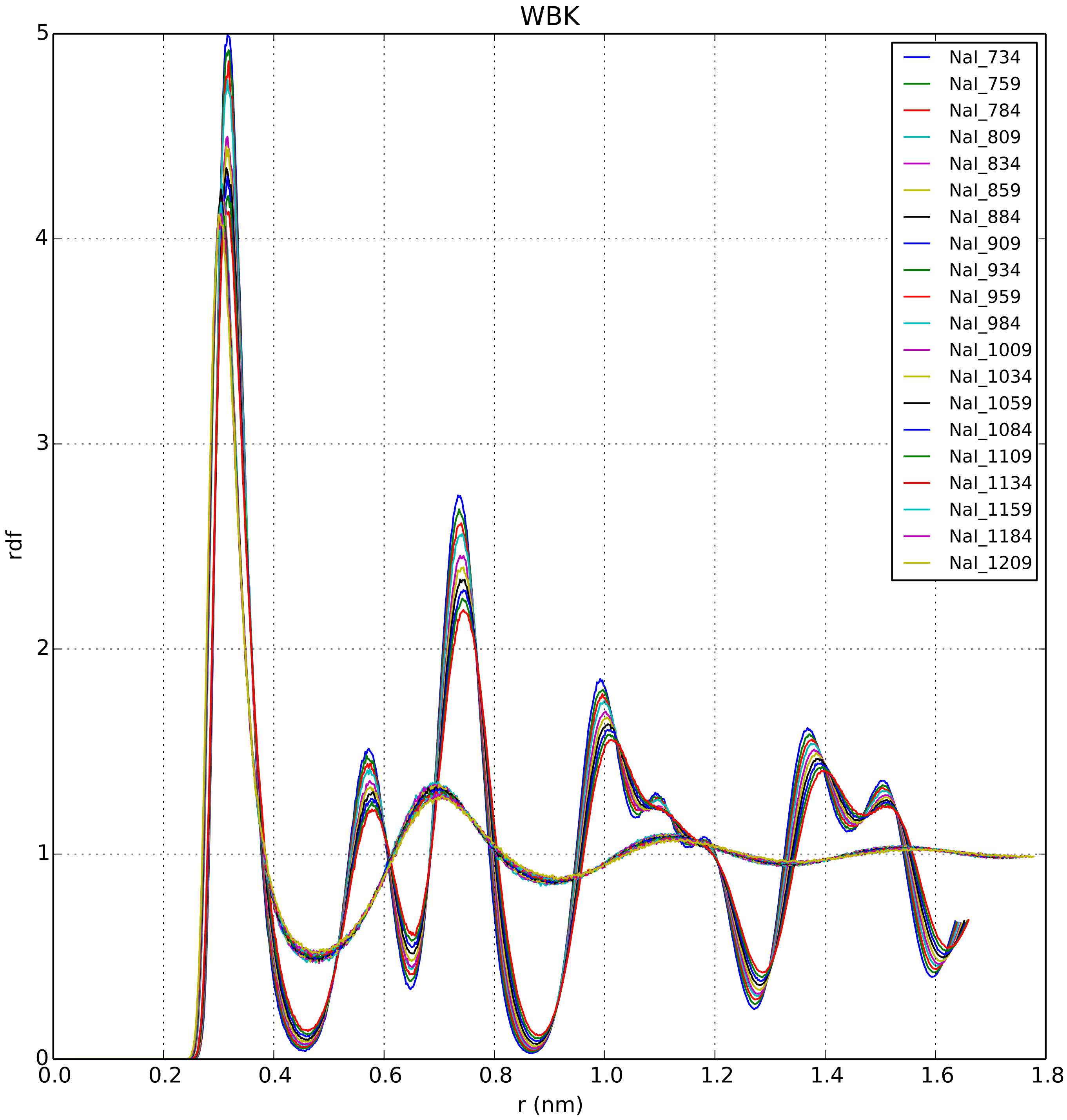
3
4
5
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
NaBr_820
NaBr_845
NaBr_870
NaBr_895
NaBr_920
NaBr_945
NaBr_970
NaBr_995
NaBr_1020
NaBr_1045
NaBr_1070
NaBr_1095
NaBr_1120
NaBr_1145
NaBr_1170
NaBr_1195
NaBr_1220
NaBr_1245
NaBr_1270
NaBr_1295


WBK
rdf
r (nm)
0
1
2
3
4
5
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
NaI_734
NaI_759
NaI_784
NaI_809
NaI_834
NaI_859
NaI_884
NaI_909
NaI_934
NaI_959
NaI_984
NaI_1009
NaI_1034
NaI_1059
NaI_1084
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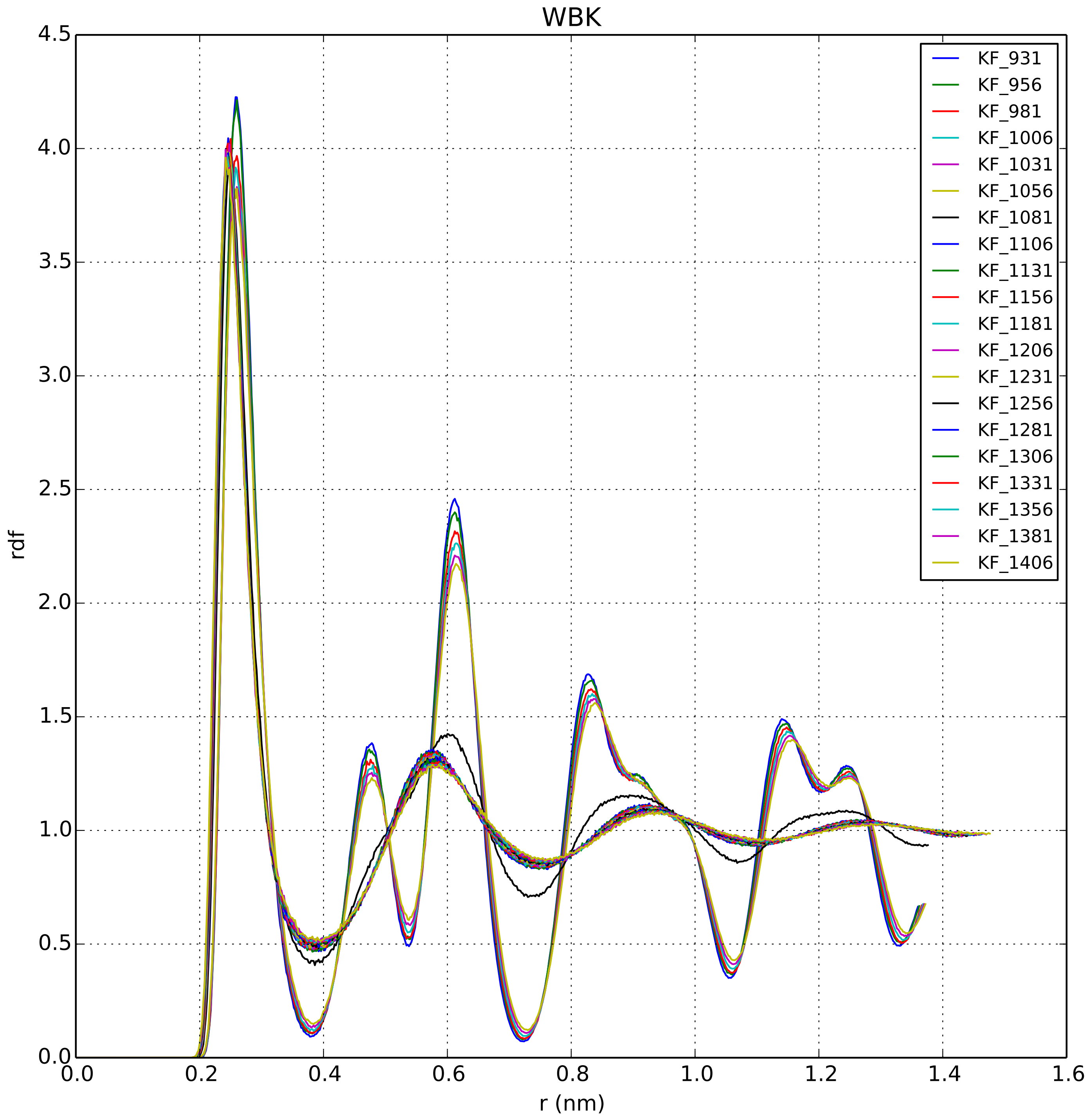
NaI_1159
NaI_1184
NaI_1209


WBK
rdf
r (nm)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
KF_931
KF_956
KF_981
KF_1006
KF_1031
KF_1056
KF_1081
KF_1106
KF_1131
KF_1156
KF_1181
KF_1206
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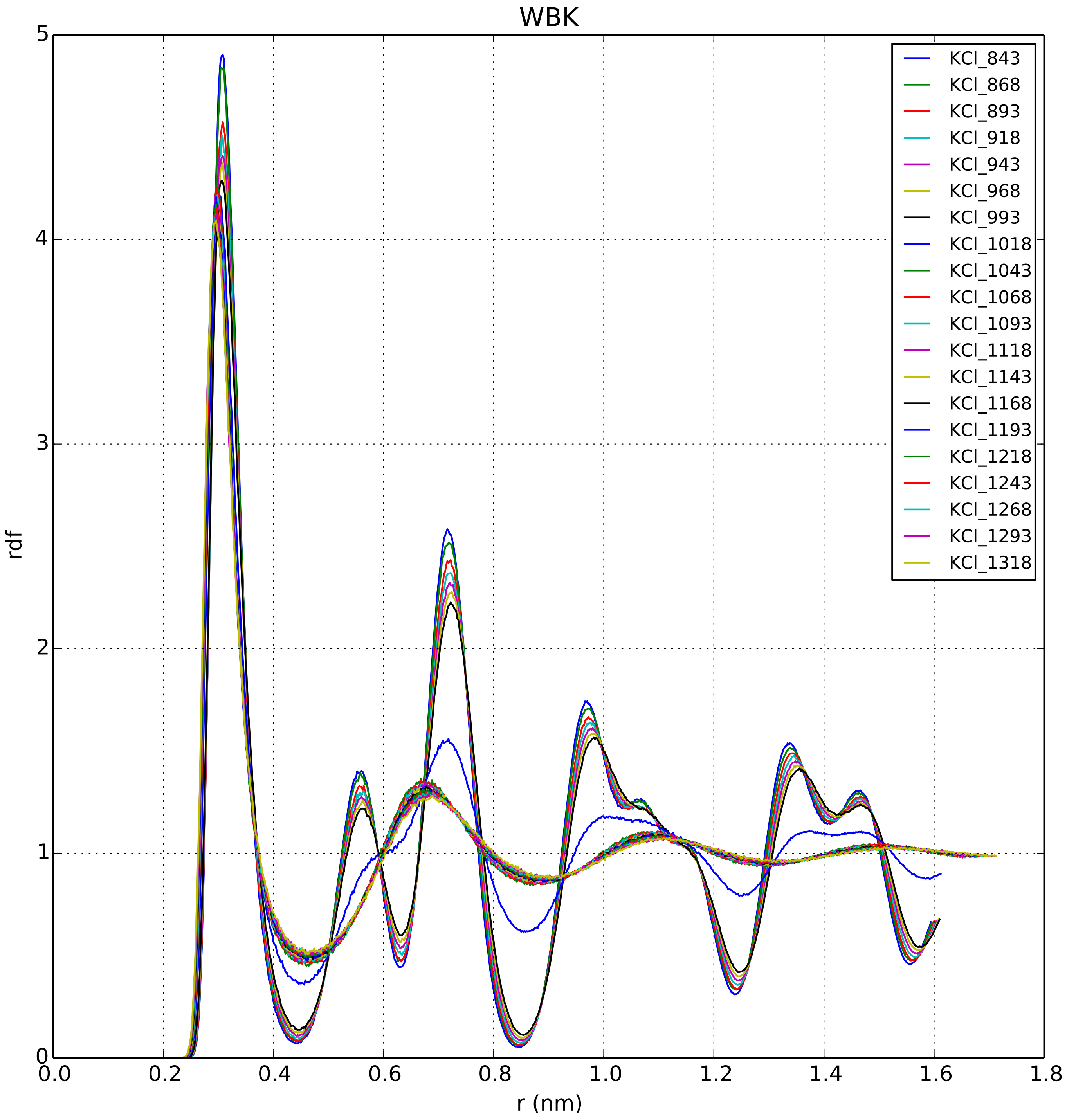
KF_1356
KF_1381
KF_1406


WBK
rdf
r (nm)
0
1
2
3
4
5
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
KCl_843
KCl_868
KCl_893
KCl_918
KCl_943
KCl_968
KCl_993
KCl_1018
KCl_1043
KCl_1068
KCl_1093
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KCl_1193
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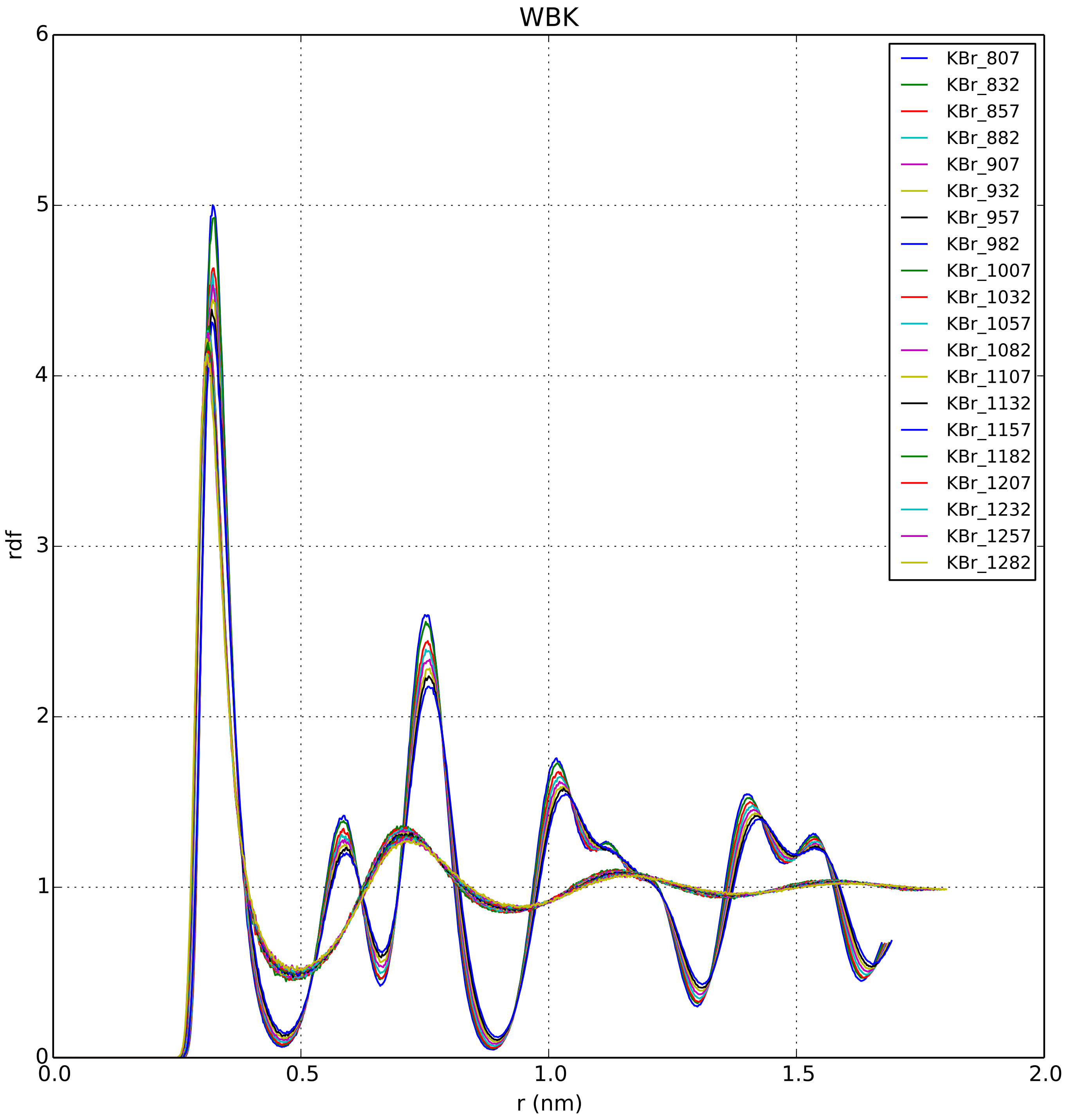
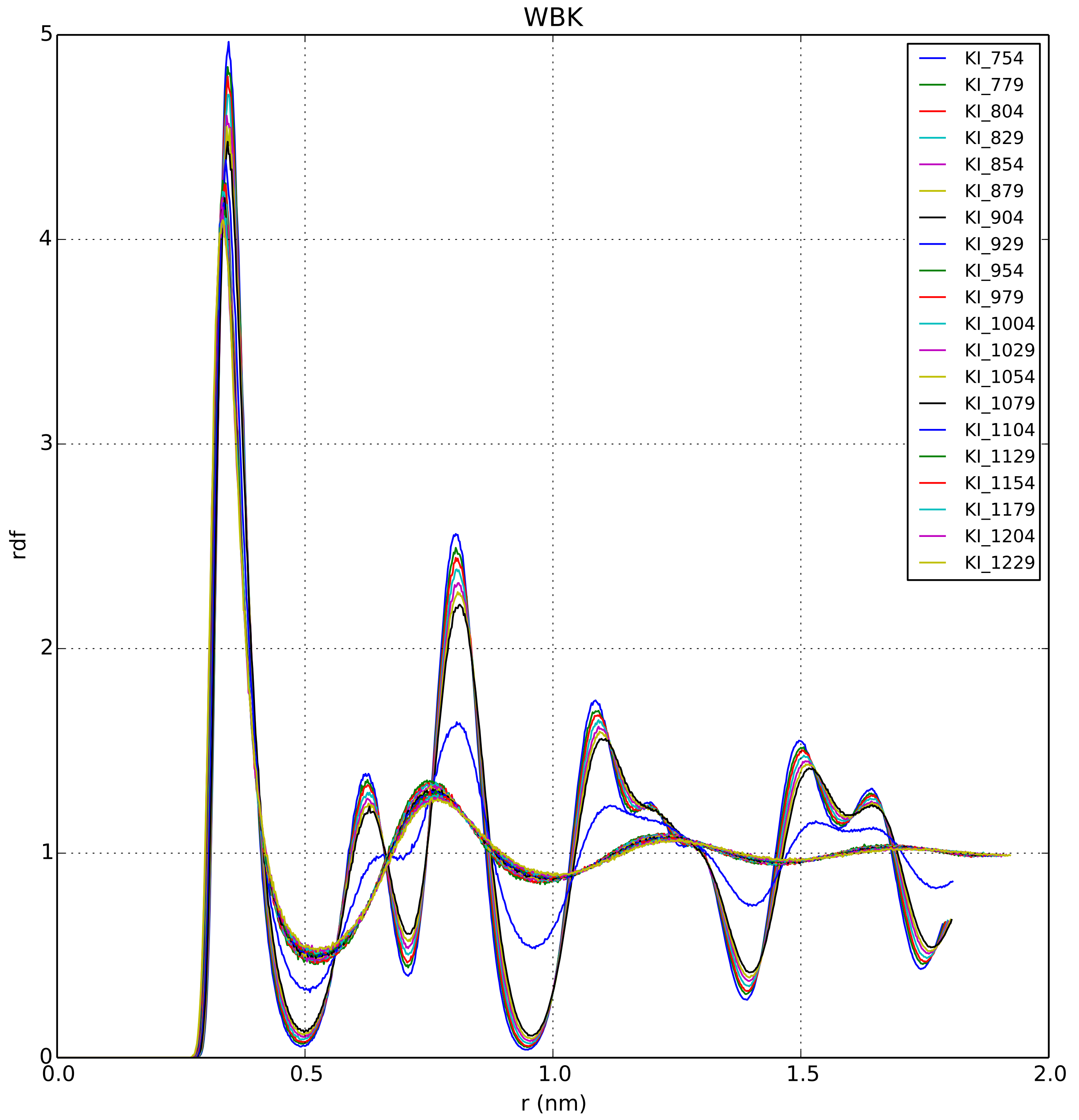
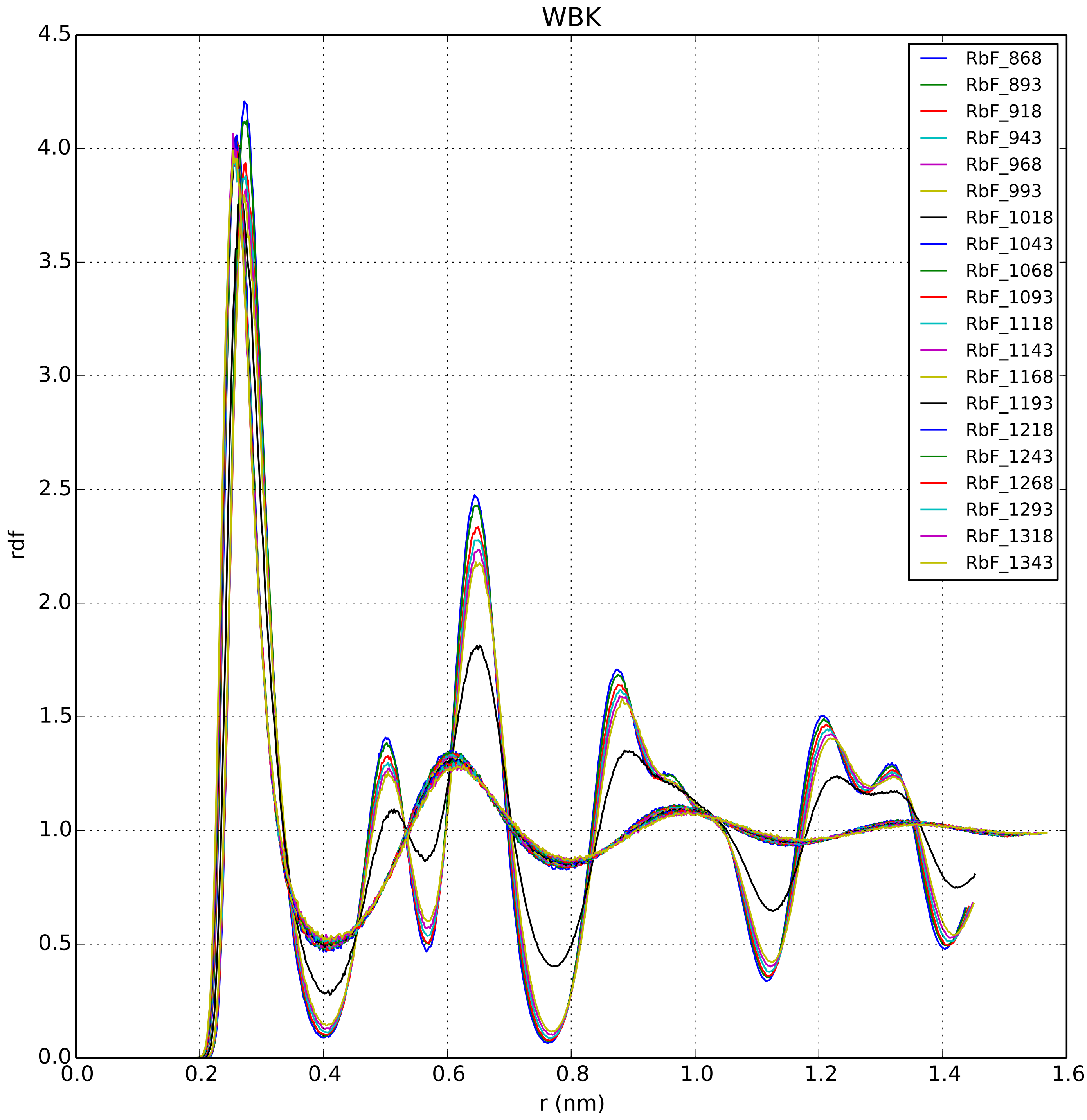
KCl_1293
KCl_1318


WBK
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.5
1.0
1.5
2.0
KBr_807
KBr_832
KBr_857
KBr_882
KBr_907
KBr_932
KBr_957
KBr_982
KBr_1007
KBr_1032
KBr_1057
KBr_1082
KBr_1107
KBr_1132
KBr_1157
KBr_1182
KBr_1207
KBr_1232
KBr_1257
KBr_1282


WBK
rdf
r (nm)
0.0
0.5
1.0
1.5
2.0
0
1
2
3
4
5
KI_754
KI_779
KI_804
KI_829
KI_854
KI_879
KI_904
KI_929
KI_954
KI_979
KI_1004
KI_1029
KI_1054
KI_1079
KI_1104
KI_1129
KI_1154
KI_1179
KI_1204
KI_1229


WBK
rdf
r (nm)
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
4.0
4.5
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
RbF_868
RbF_893
RbF_918
RbF_943
RbF_968
RbF_993
RbF_1018
RbF_1043
RbF_1068
RbF_1093
RbF_1118
RbF_1143
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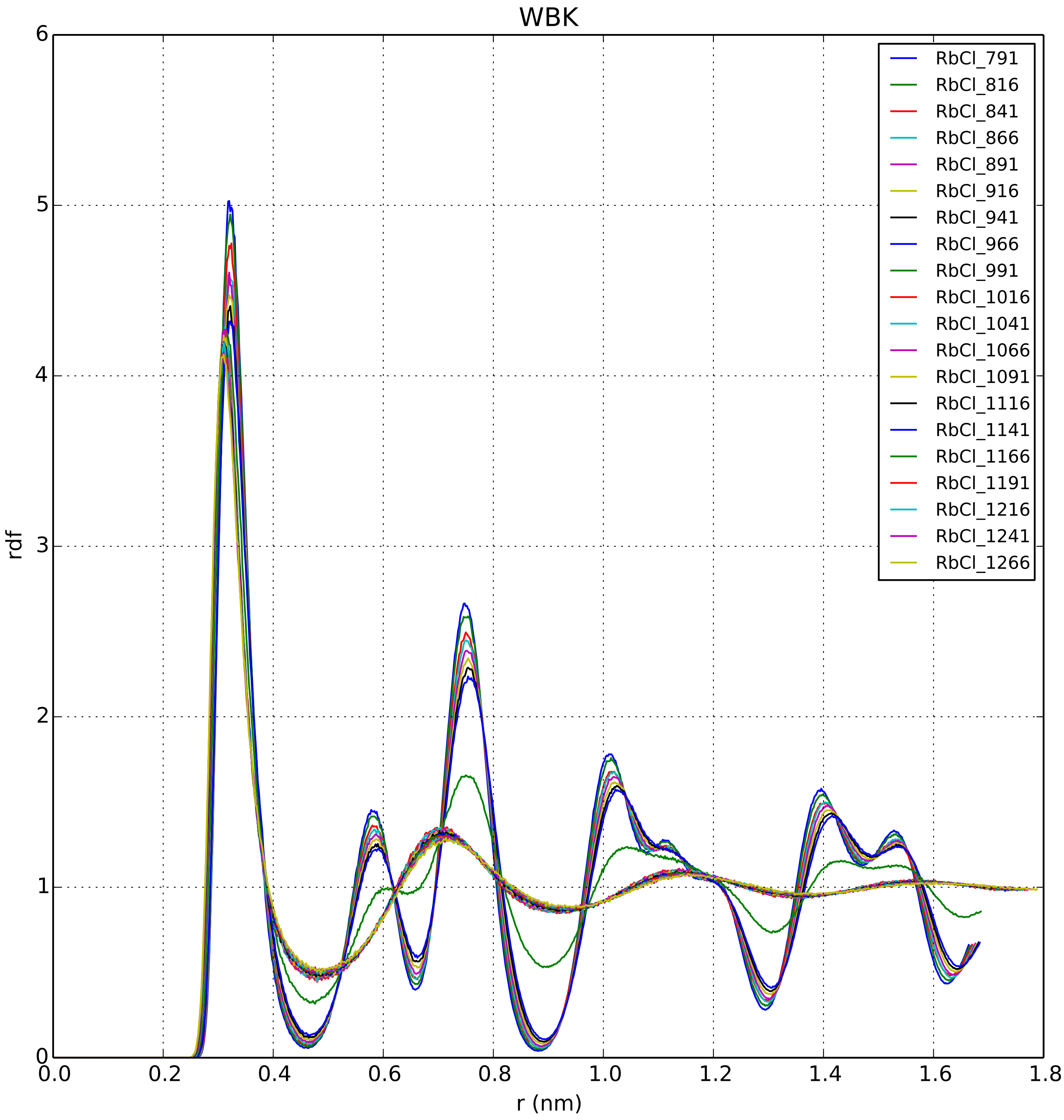
RbF_1193
RbF_1218
RbF_1243
RbF_1268
RbF_1293
RbF_1318
RbF_1343


WBK
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
RbCl_791
RbCl_816
RbCl_841
RbCl_866
RbCl_891
RbCl_916
RbCl_941
RbCl_966
RbCl_991
RbCl_1016
RbCl_1041
RbCl_1066
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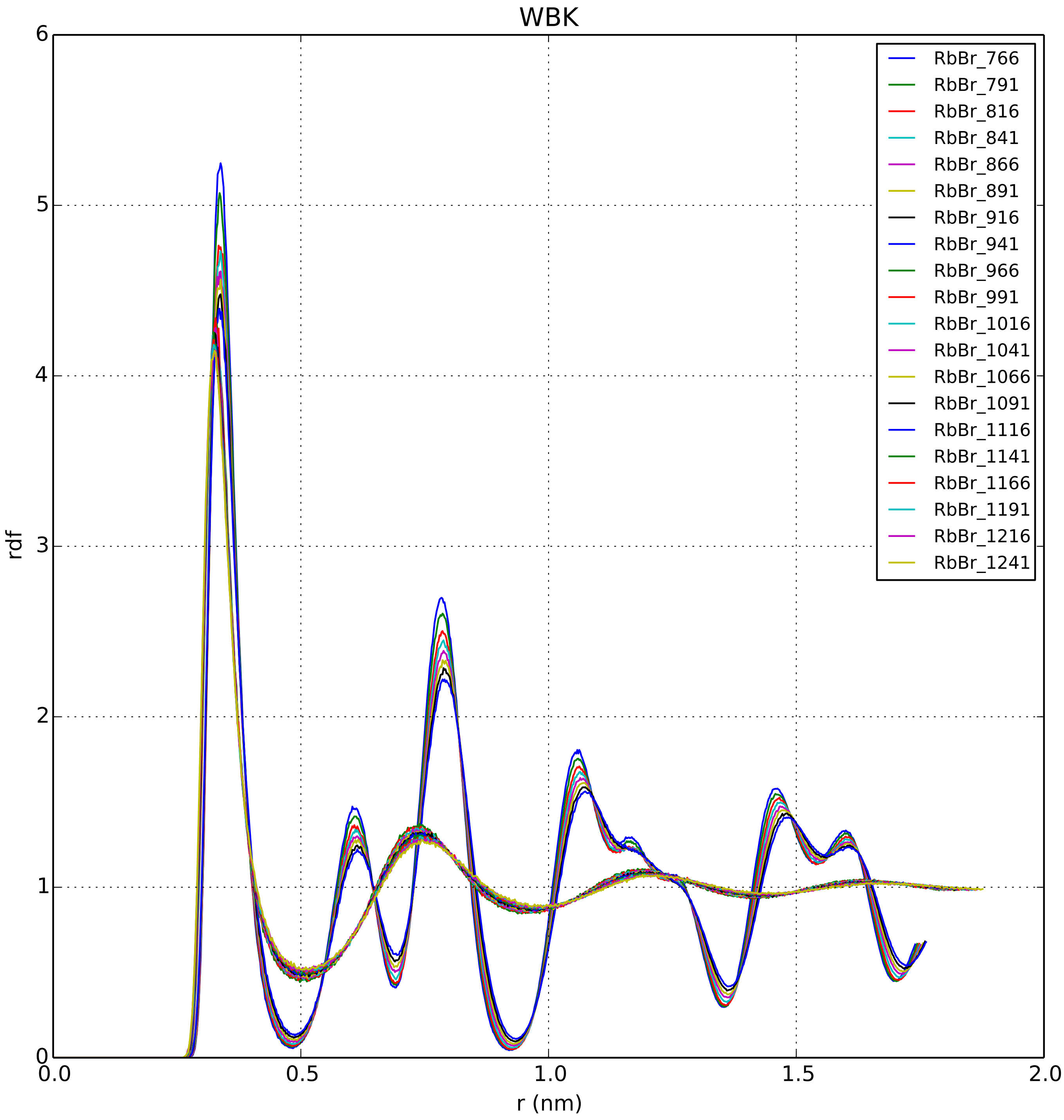
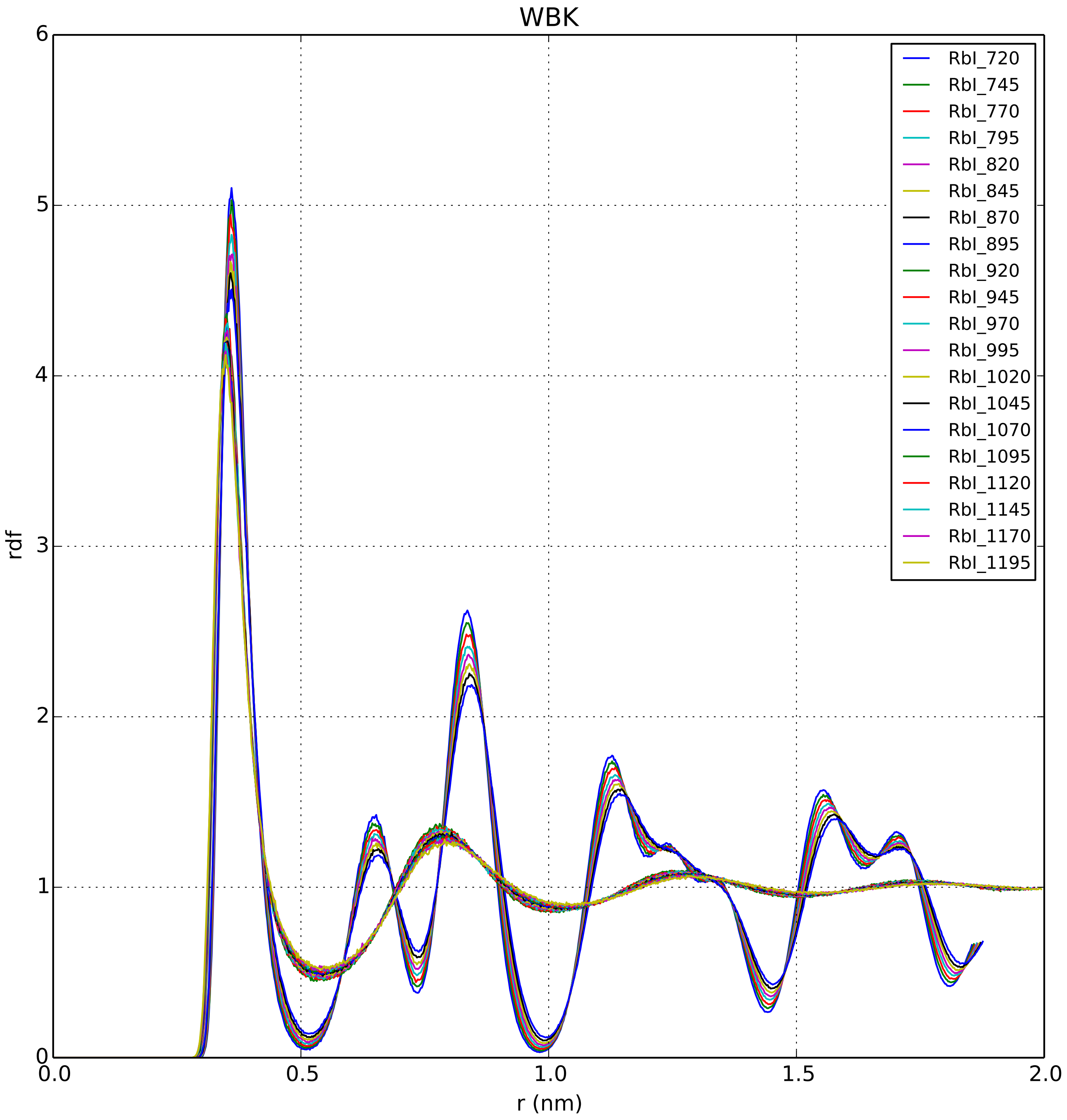
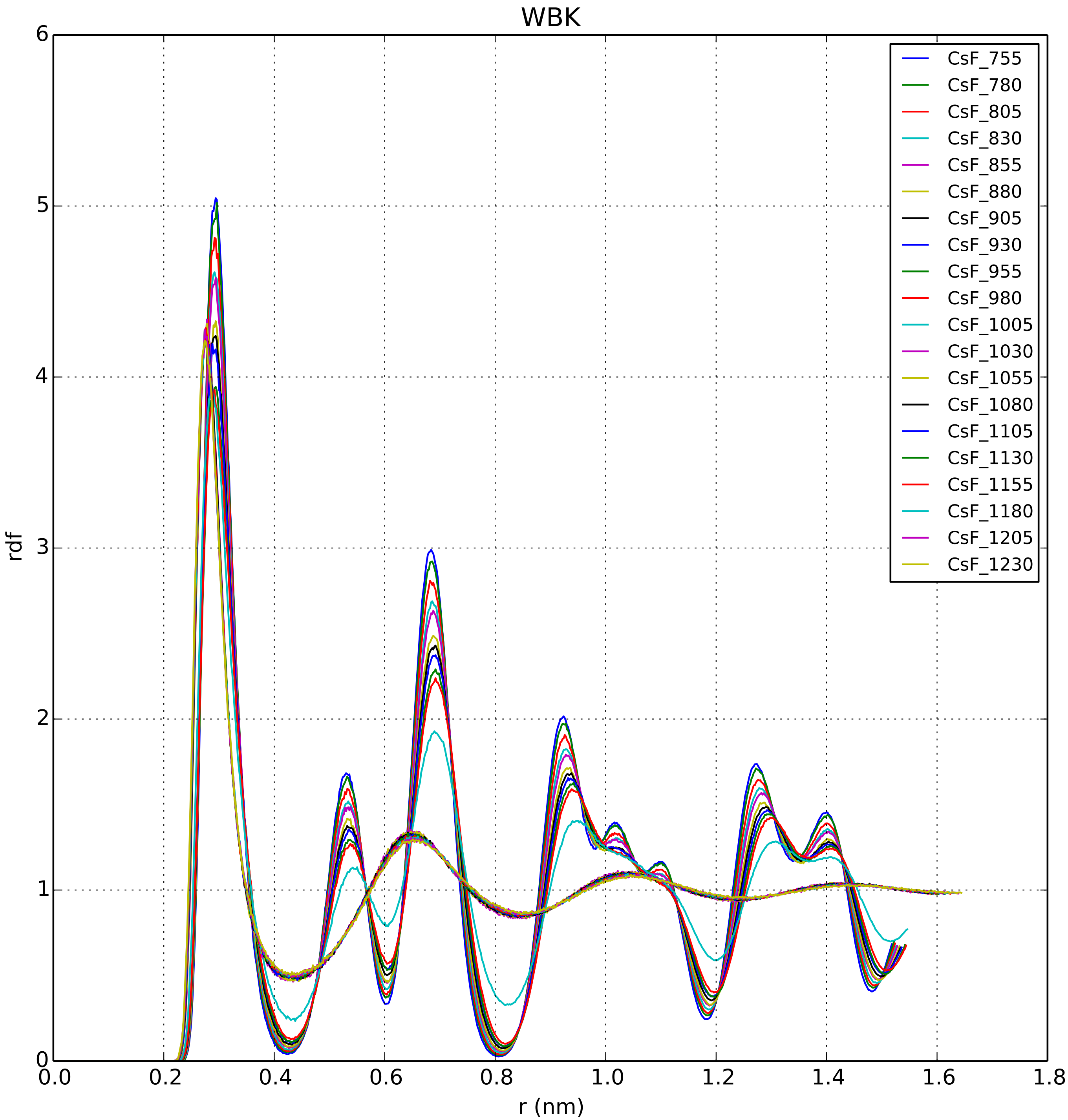
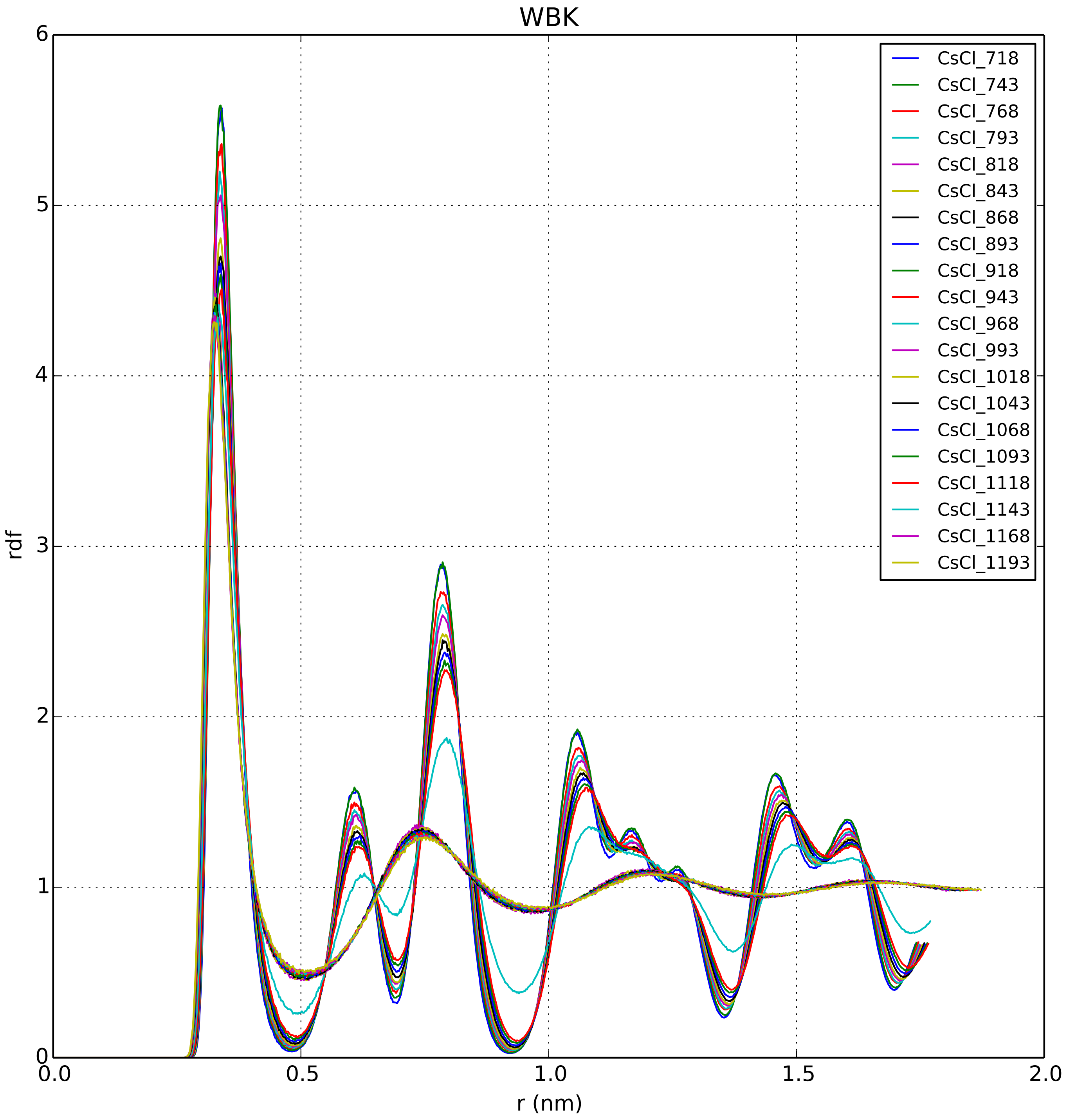
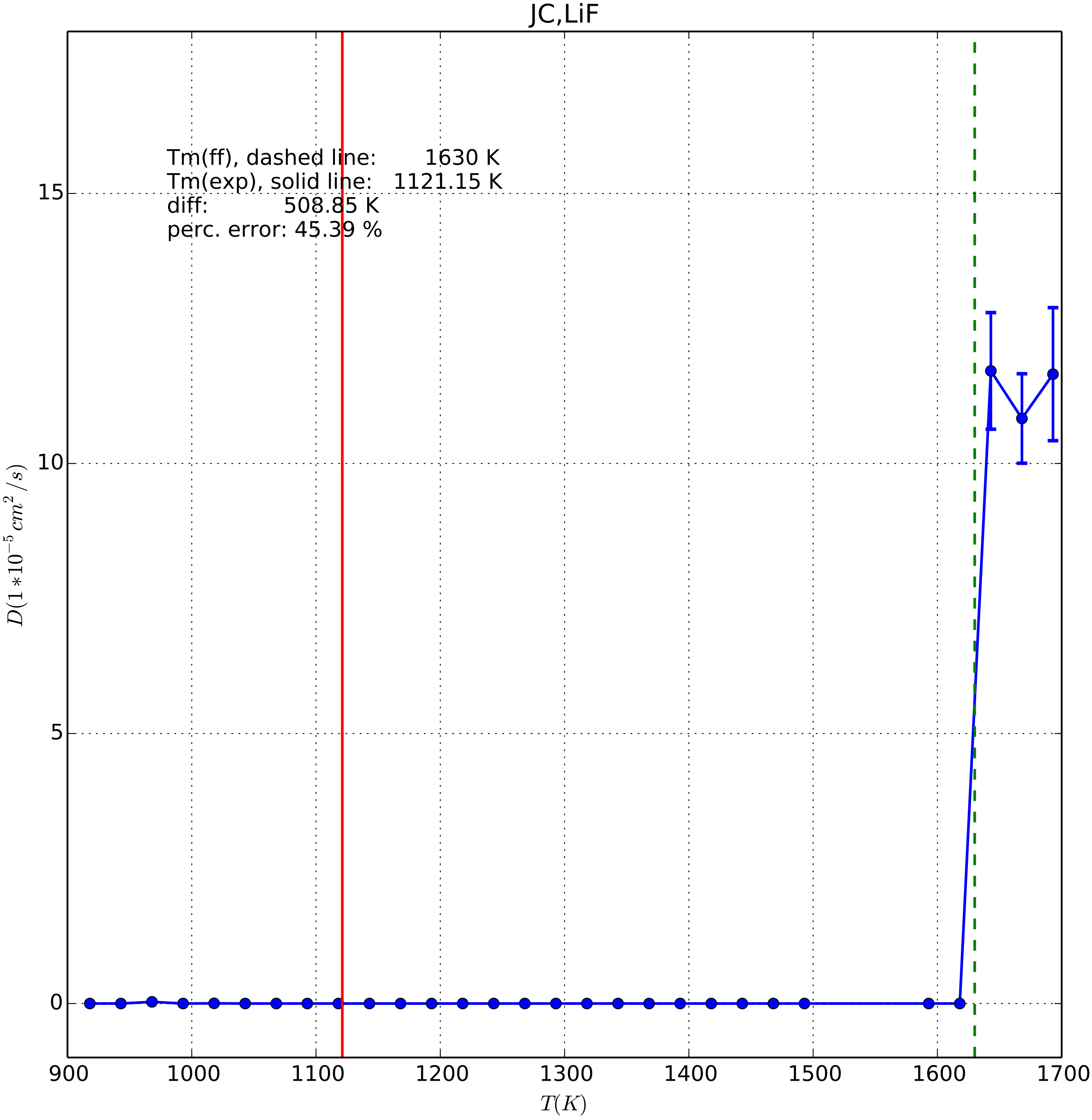
RbCl_1116
RbCl_1141
RbCl_1166
RbCl_1191
RbCl_1216
RbCl_1241
RbCl_1266

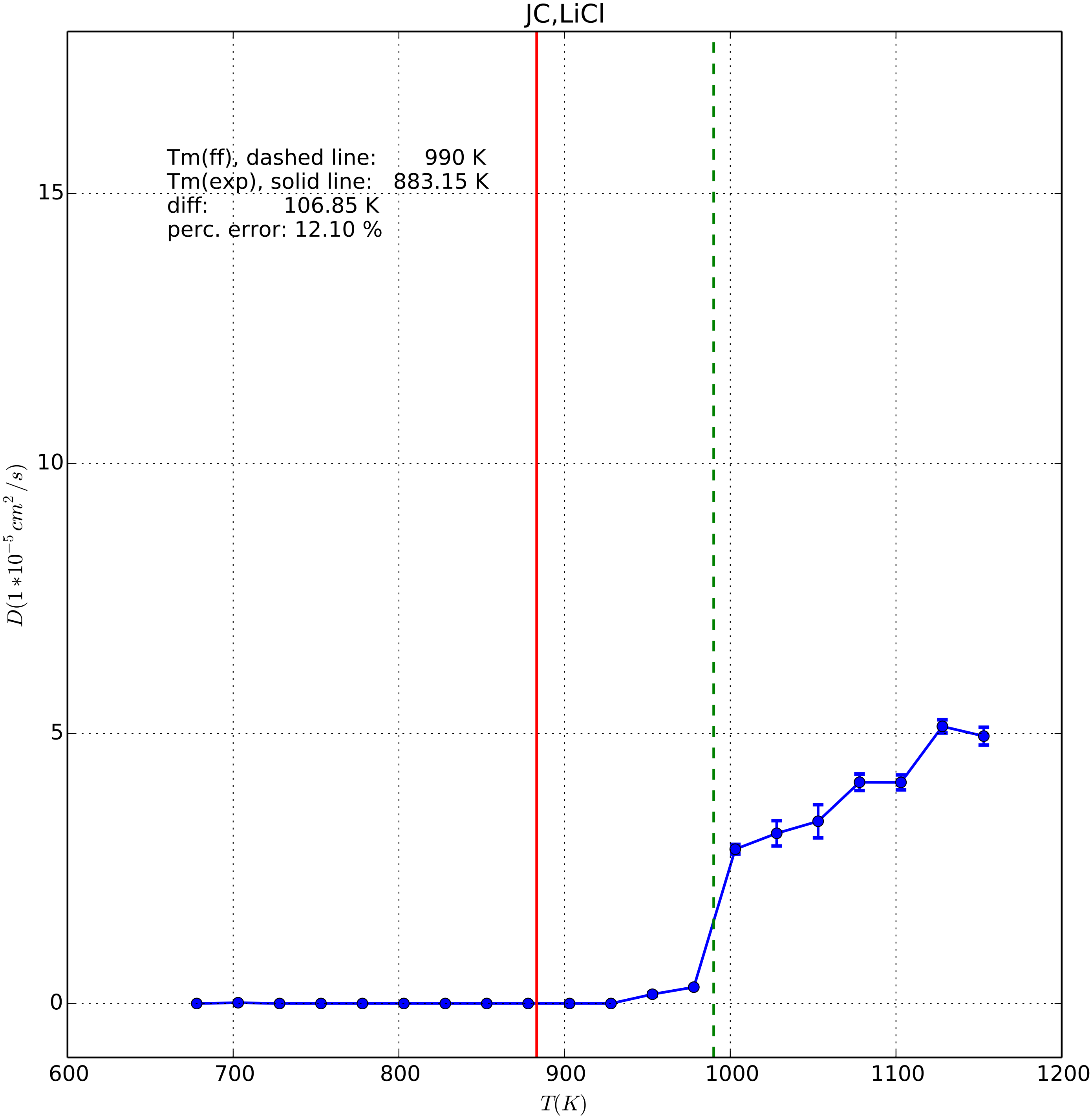

WBK
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.5
1.0
1.5
2.0
RbBr_766
RbBr_791
RbBr_816
RbBr_841
RbBr_866
RbBr_891
RbBr_916
RbBr_941
RbBr_966
RbBr_991
RbBr_1016
RbBr_1041
RbBr_1066
RbBr_1091
RbBr_1116
RbBr_1141
RbBr_1166
RbBr_1191
RbBr_1216
RbBr_1241


WBK
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.5
1.0
1.5
2.0
RbI_720
RbI_745
RbI_770
RbI_795
RbI_820
RbI_845
RbI_870
RbI_895
RbI_920
RbI_945
RbI_970
RbI_995
RbI_1020
RbI_1045
RbI_1070
RbI_1095
RbI_1120
RbI_1145
RbI_1170
RbI_1195

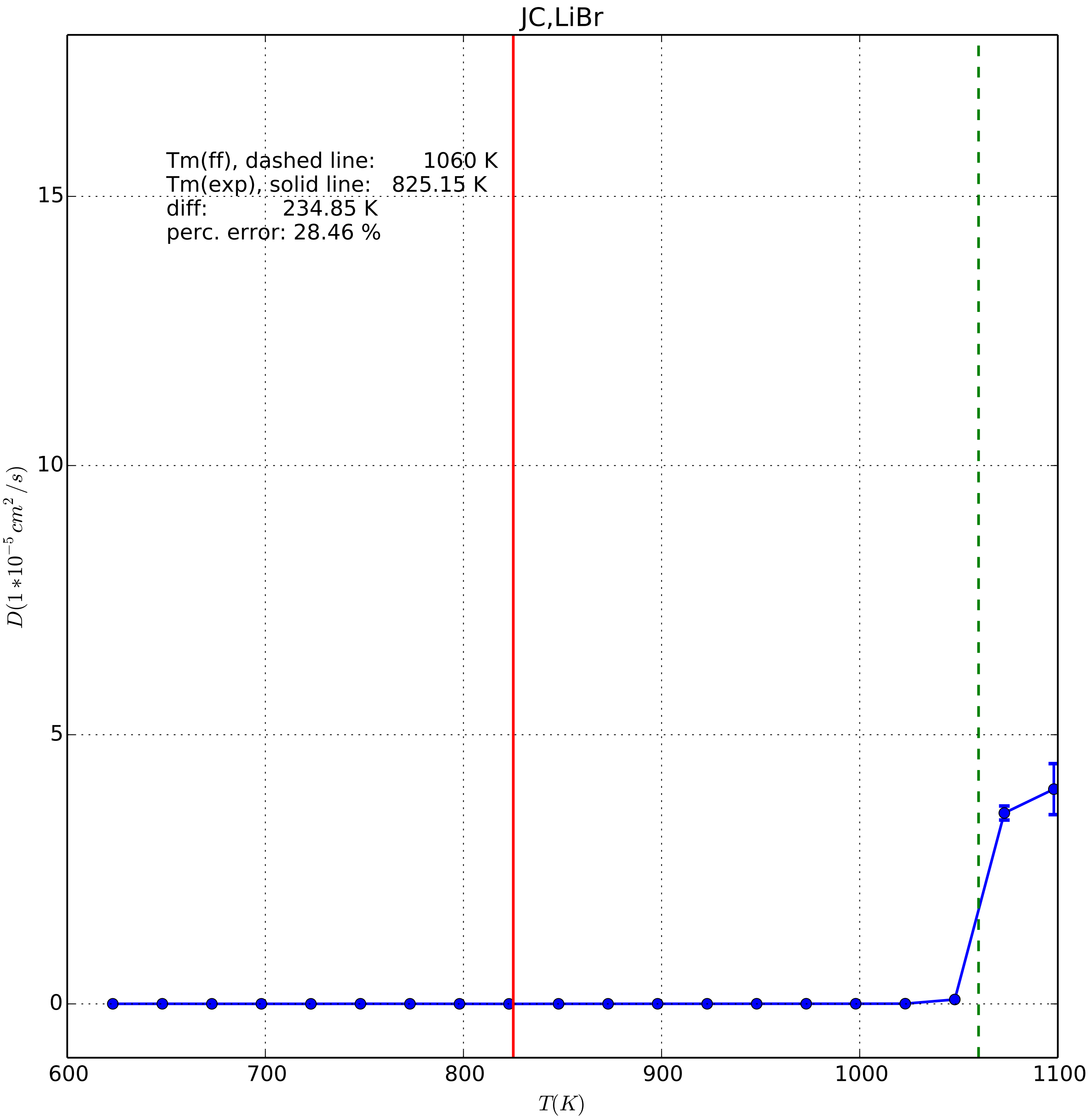

WBK
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
CsF_755
CsF_780
CsF_805
CsF_830
CsF_855
CsF_880
CsF_905
CsF_930
CsF_955
CsF_980
CsF_1005
CsF_1030
CsF_1055
CsF_1080
CsF_1105
CsF_1130
CsF_1155
CsF_1180
CsF_1205
CsF_1230

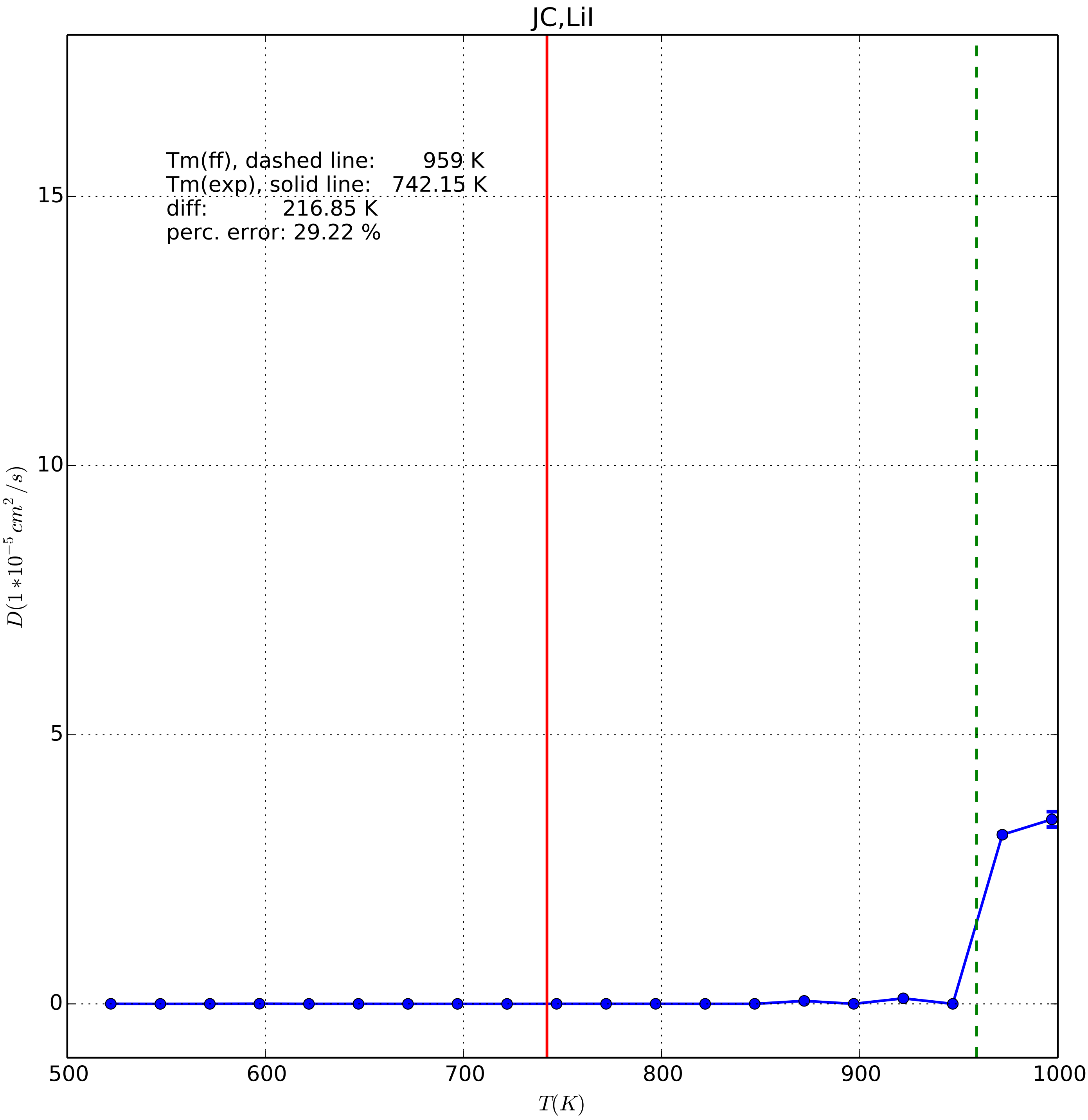

WBK
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.5
1.0
1.5
2.0
CsCl_718
CsCl_743
CsCl_768
CsCl_793
CsCl_818
CsCl_843
CsCl_868
CsCl_893
CsCl_918
CsCl_943
CsCl_968
CsCl_993
CsCl_1018
CsCl_1043
CsCl_1068
CsCl_1093
CsCl_1118
CsCl_1143
CsCl_1168
CsCl_1193

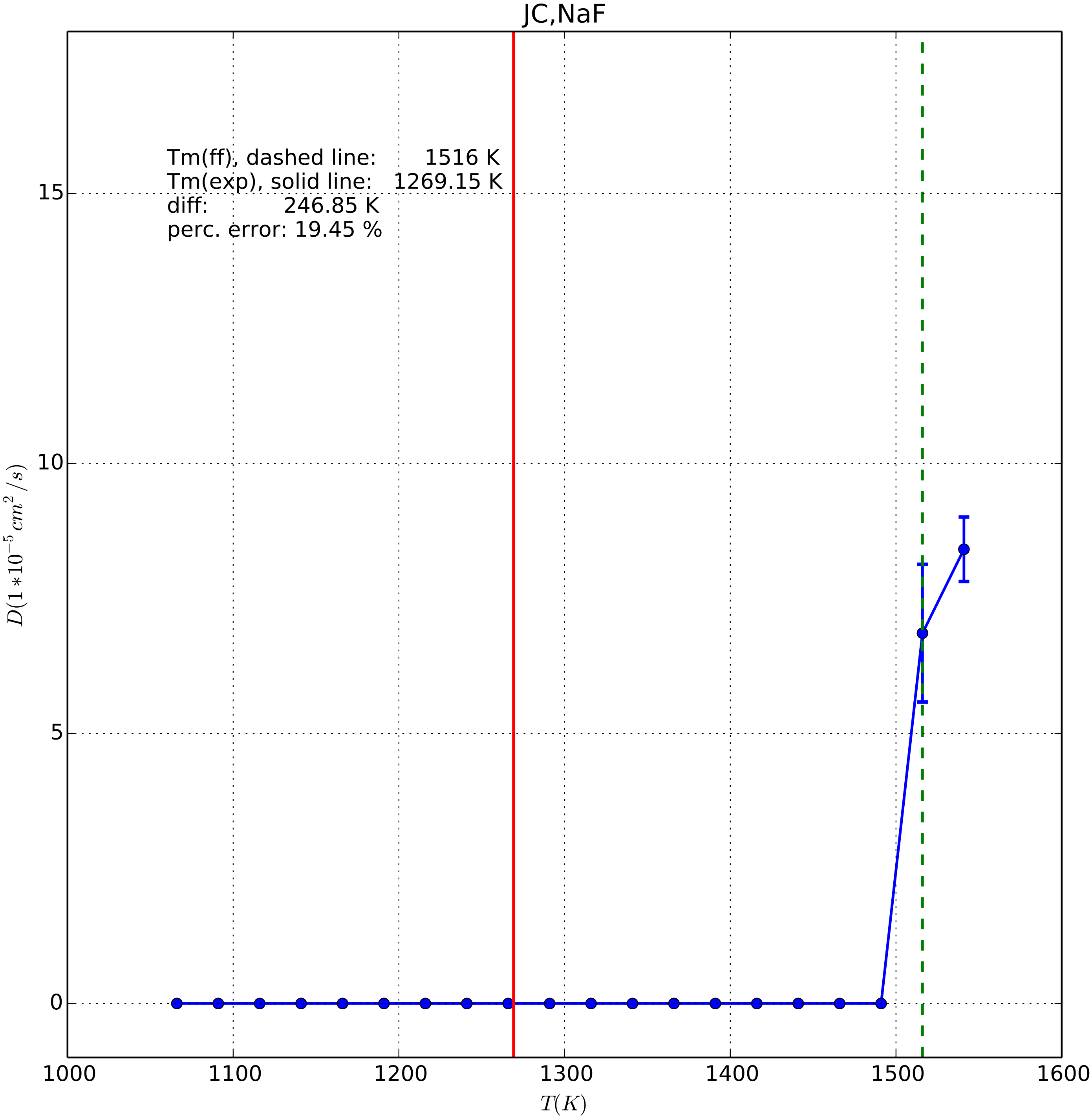

JC,LiF
Tm(ff), dashed line: 1630 K
Tm(exp), solid line: 1121.15 K
diff: 508.85 K
perc. error: 45.39 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
900
1000
1100
1200
1300
1400
1500
1600
1700
$T(K)$

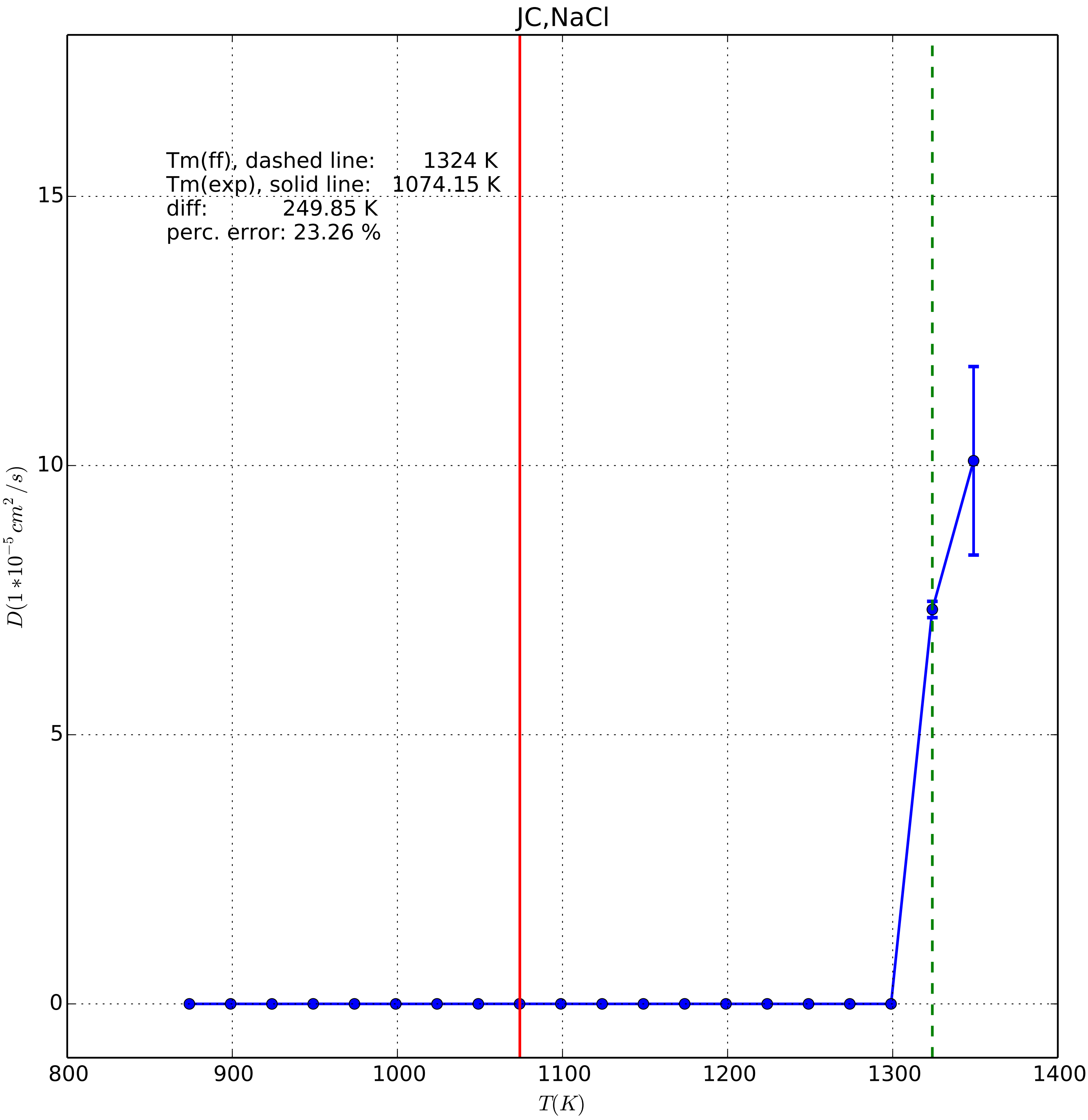


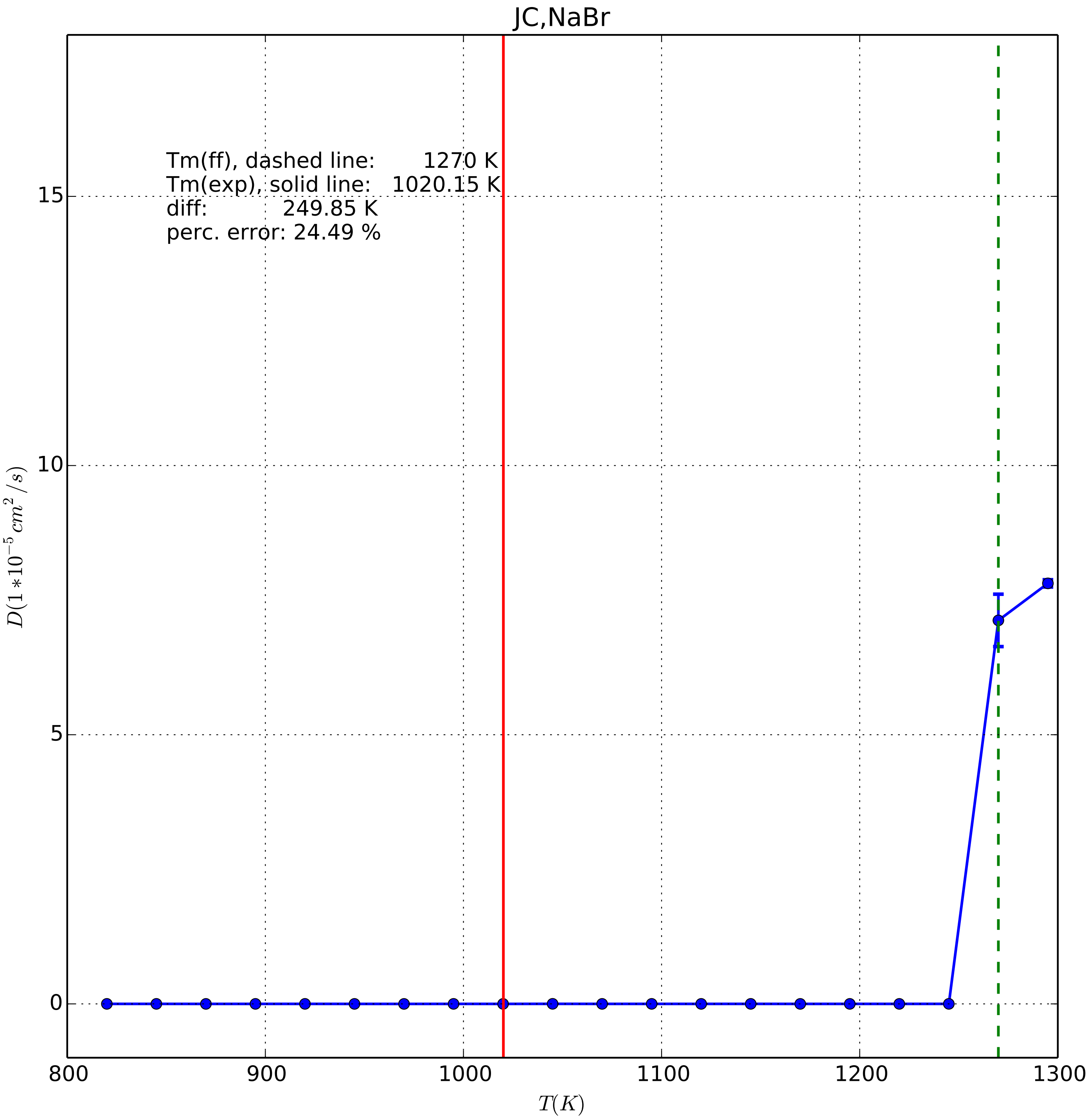
JC,LiCl
Tm(ff), dashed line: 990 K
Tm(exp), solid line: 883.15 K
diff: 106.85 K
perc. error: 12.10 %
15
10
5
0
600
700
800
900
1000
1100
1200
$D(1*10^{-5}cm^2/s)$
$T(K)$

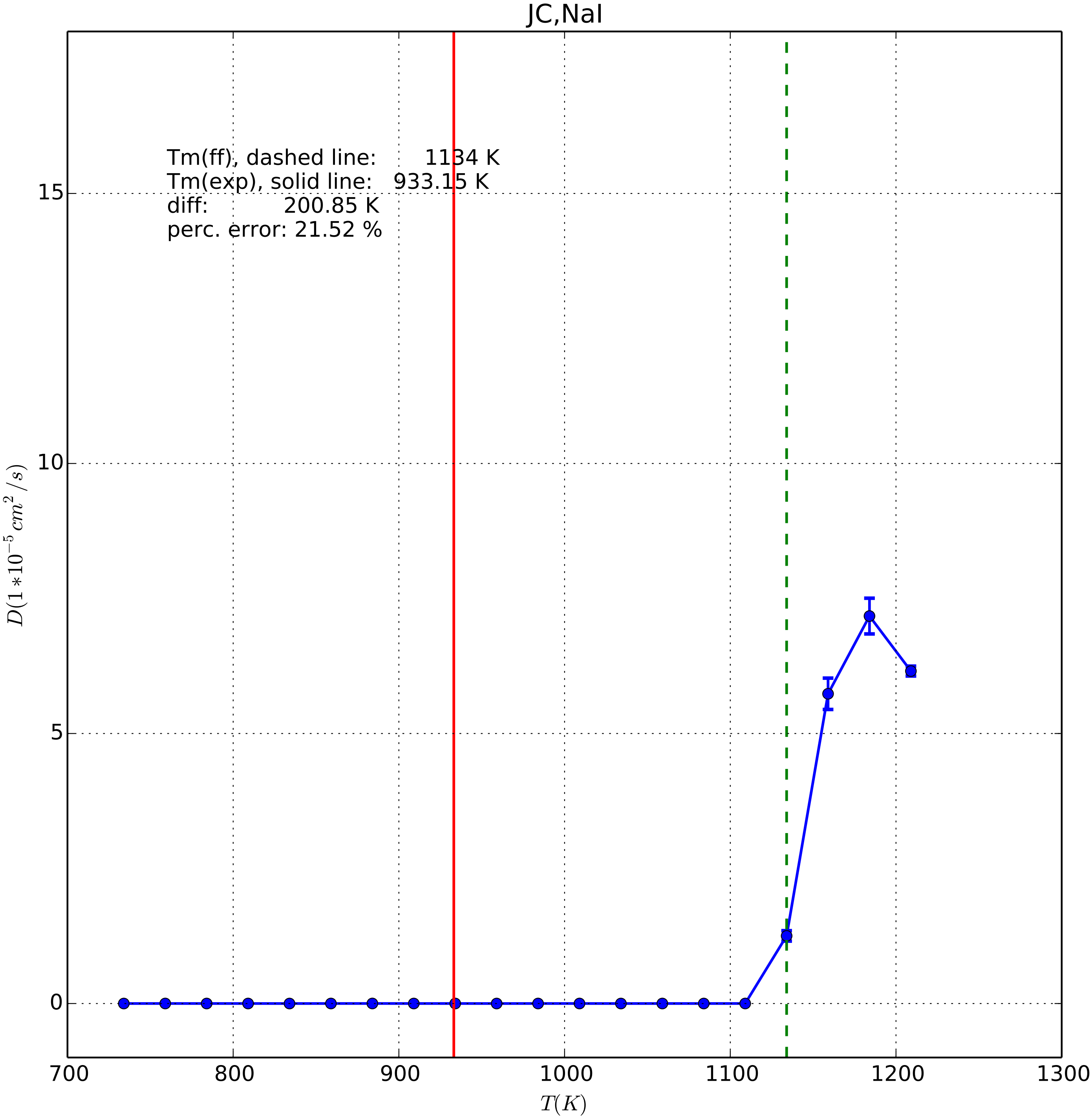

JC,LiBr
Tm(ff), dashed line: 1060 K
Tm(exp), solid line: 825.15 K
diff: 234.85 K
perc. error: 28.46 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
600
700
800
900
1000
1100
$T(K)$

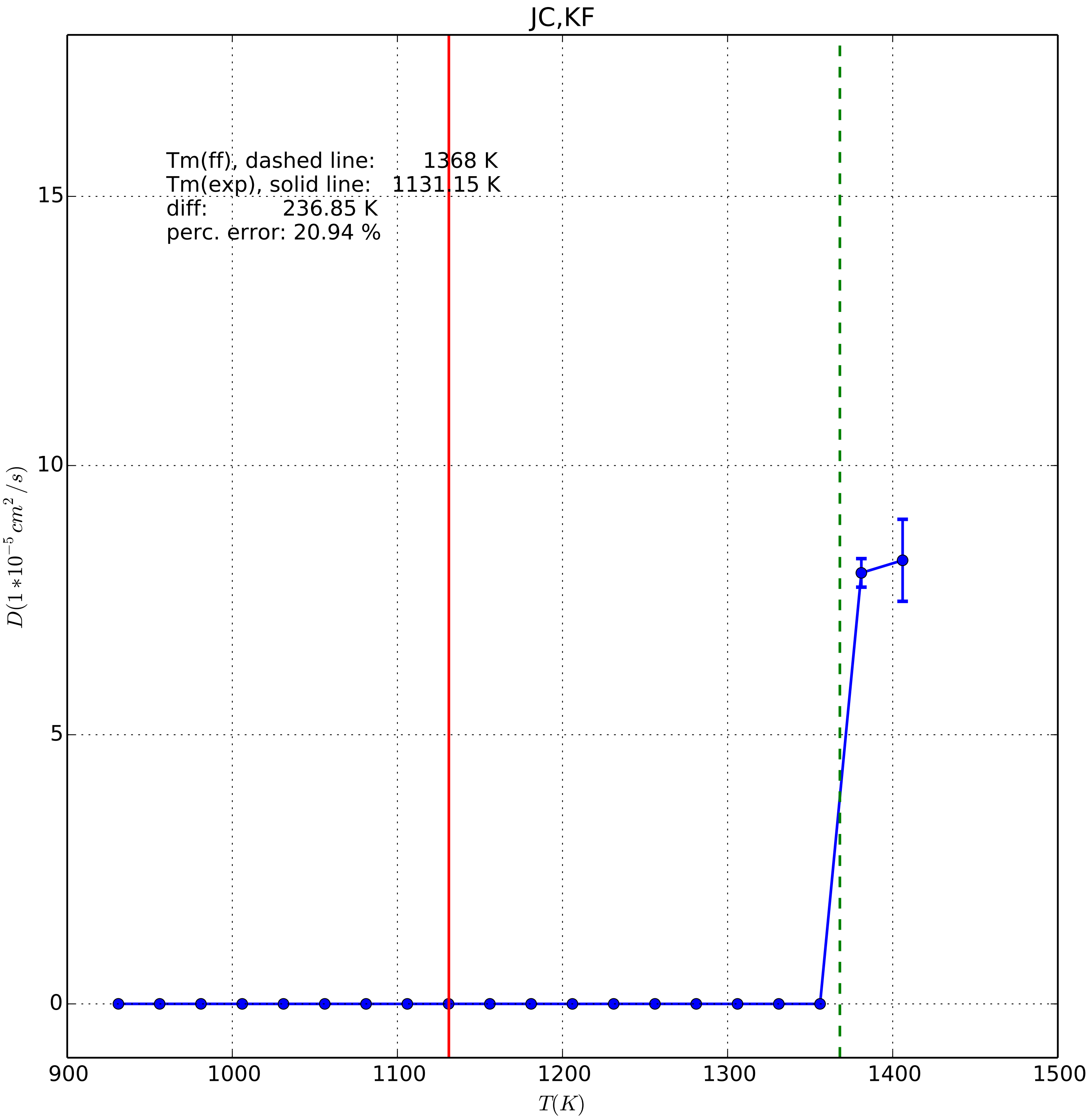

JC,LiI
Tm(ff), dashed line: 959 K
Tm(exp), solid line: 742.15 K
diff: 216.85 K
perc. error: 29.22 %
15
10
5
0
$D(1*10^{-5}cm^2/s)$
500
600
700
800
900
1000
$T(K)$

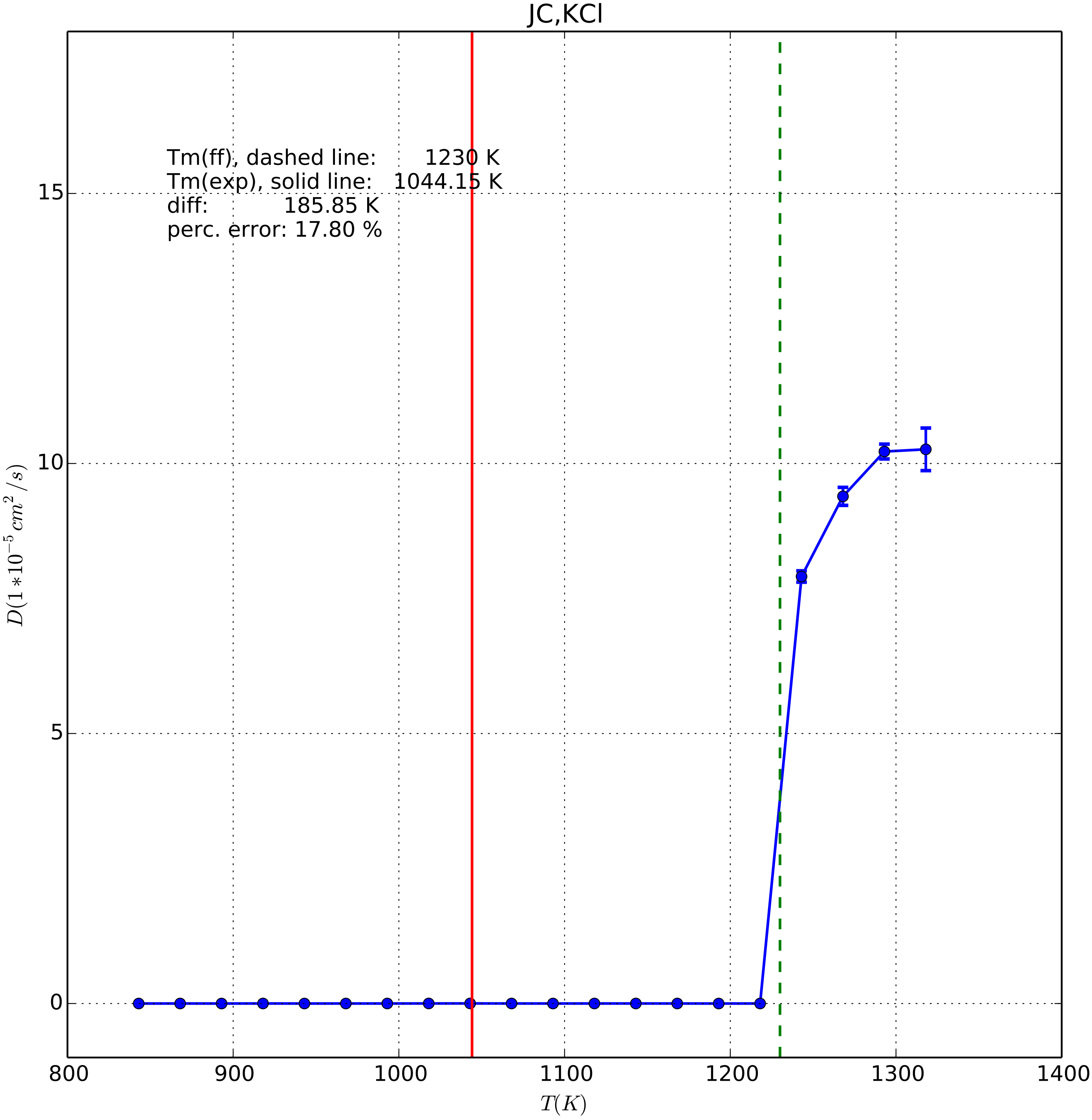

JC,NaF
Tm(ff), dashed line: 1516 K
Tm(exp), solid line: 1269.15 K
diff: 246.85 K
perc. error: 19.45 %
$D(1*10^{-5}cm^2/s)$
15
10
5
0
1000
1100
1200
1300
1400
1500
1600
$T(K)$

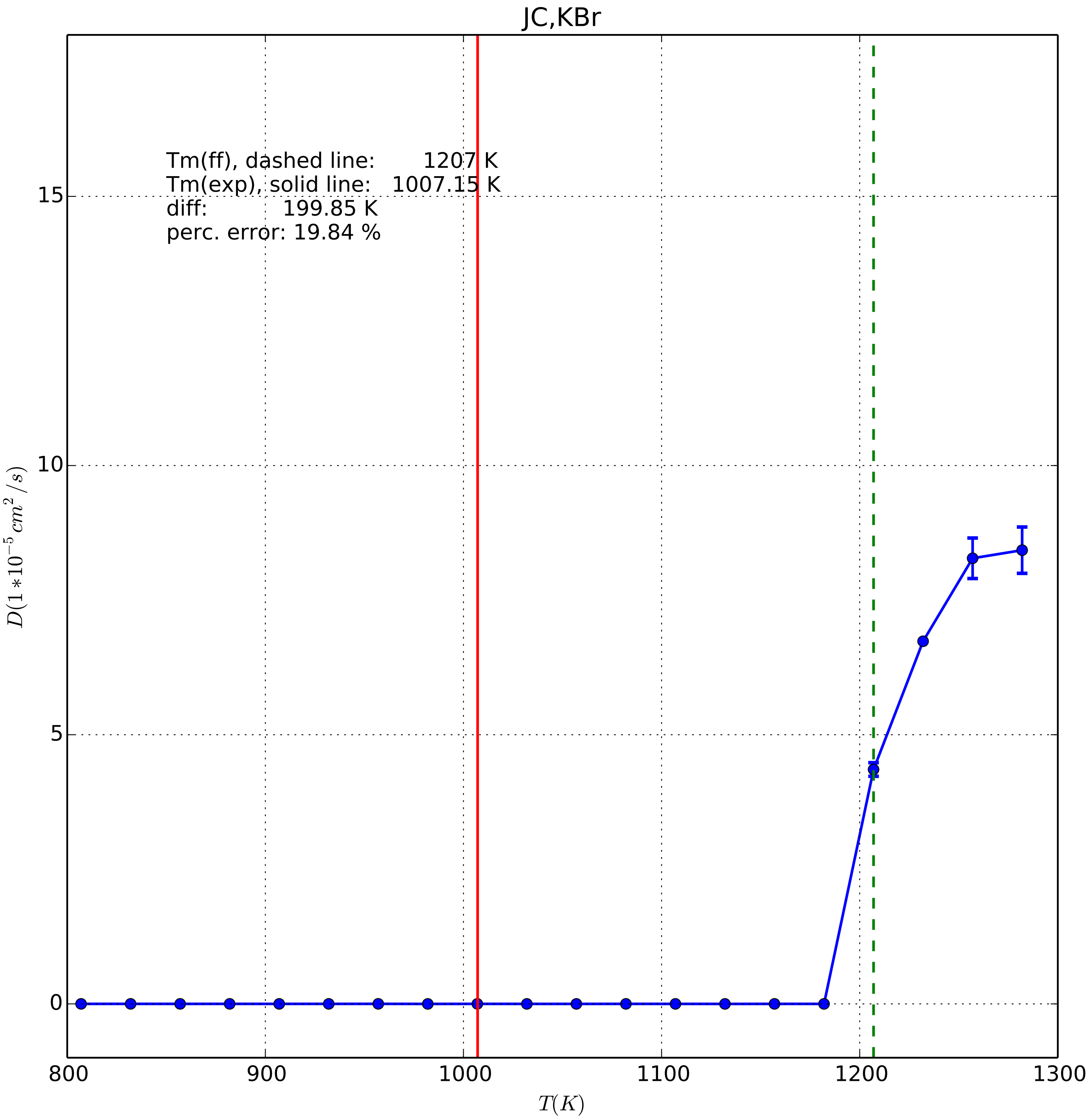

JC,NaCl
Tm(ff), dashed line: 1324 K
Tm(exp), solid line: 1074.15 K
diff: 249.85 K
perc. error: 23.26 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
800
900
1000
1100
1200
1300
1400
$T(K)$

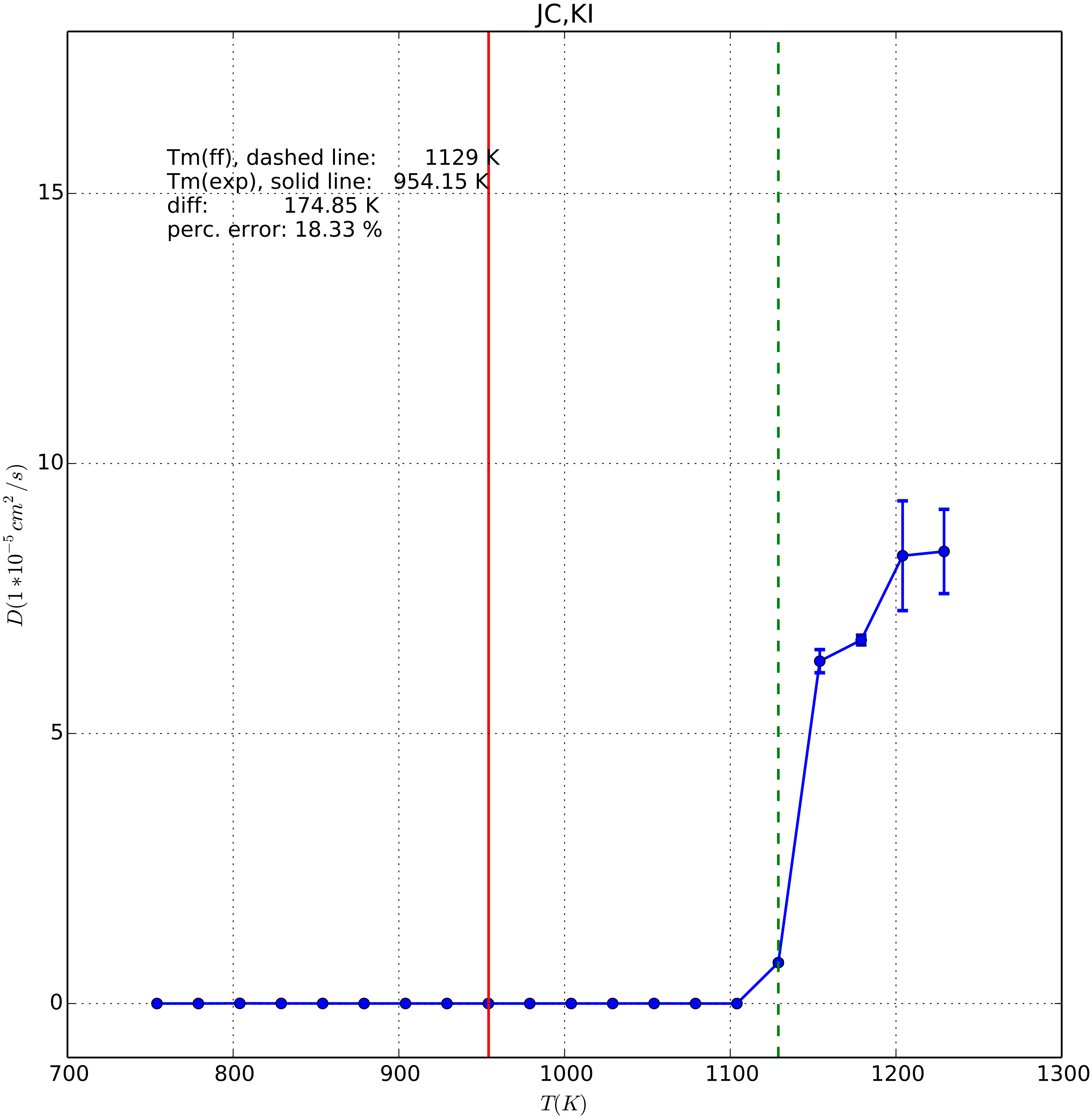

JC,NaBr
Tm(ff), dashed line: 1270 K
Tm(exp), solid line: 1020.15 K
diff: 249.85 K
perc. error: 24.49 %
$D(1*10^{-5}cm^2/s)$
$T(K)$
0
5
10
15
800
900
1000
1100
1200
1300

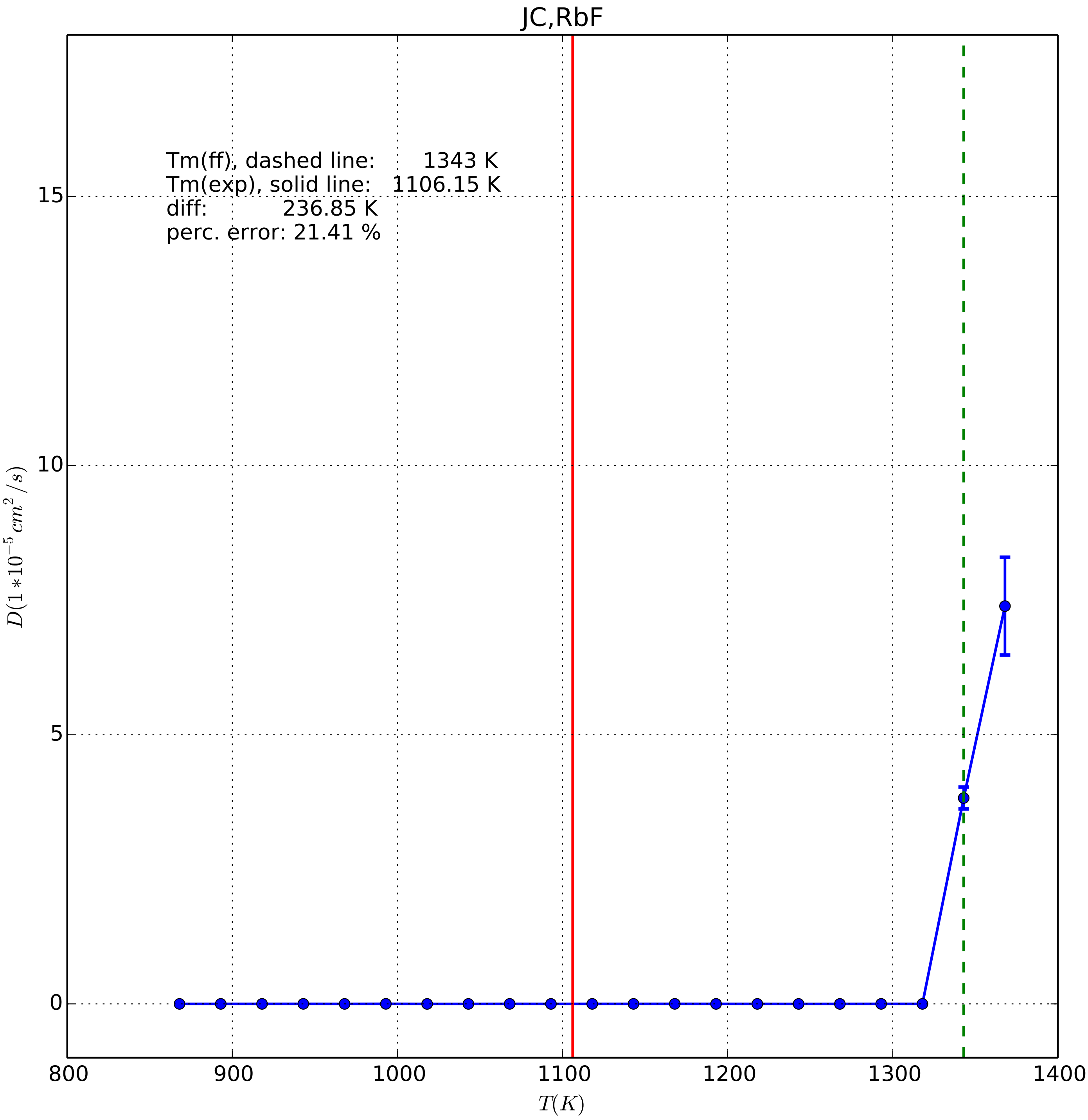

JC,NaI
Tm(ff), dashed line: 1134 K
Tm(exp), solid line: 933.15 K
diff: 200.85 K
perc. error: 21.52 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
700
800
900
1000
1100
1200
1300
$T(K)$

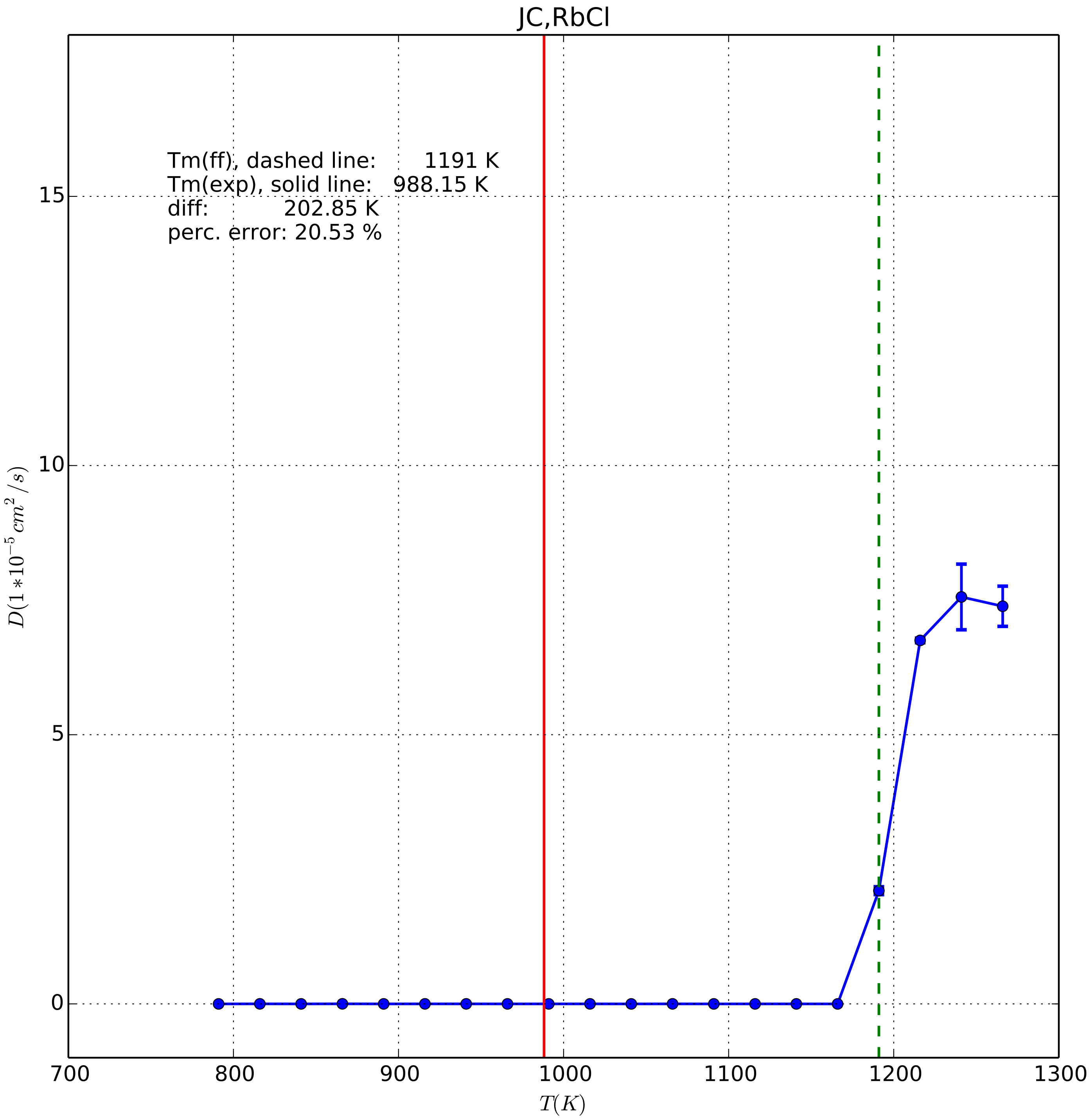

JC,KF
Tm(ff), dashed line: 1368 K
Tm(exp), solid line: 1131.15 K
diff: 236.85 K
perc. error: 20.94 %
$D(1*10^{-5}cm^2/s)$
$T(K)$
0
5
10
15
900
1000
1100
1200
1300
1400
1500

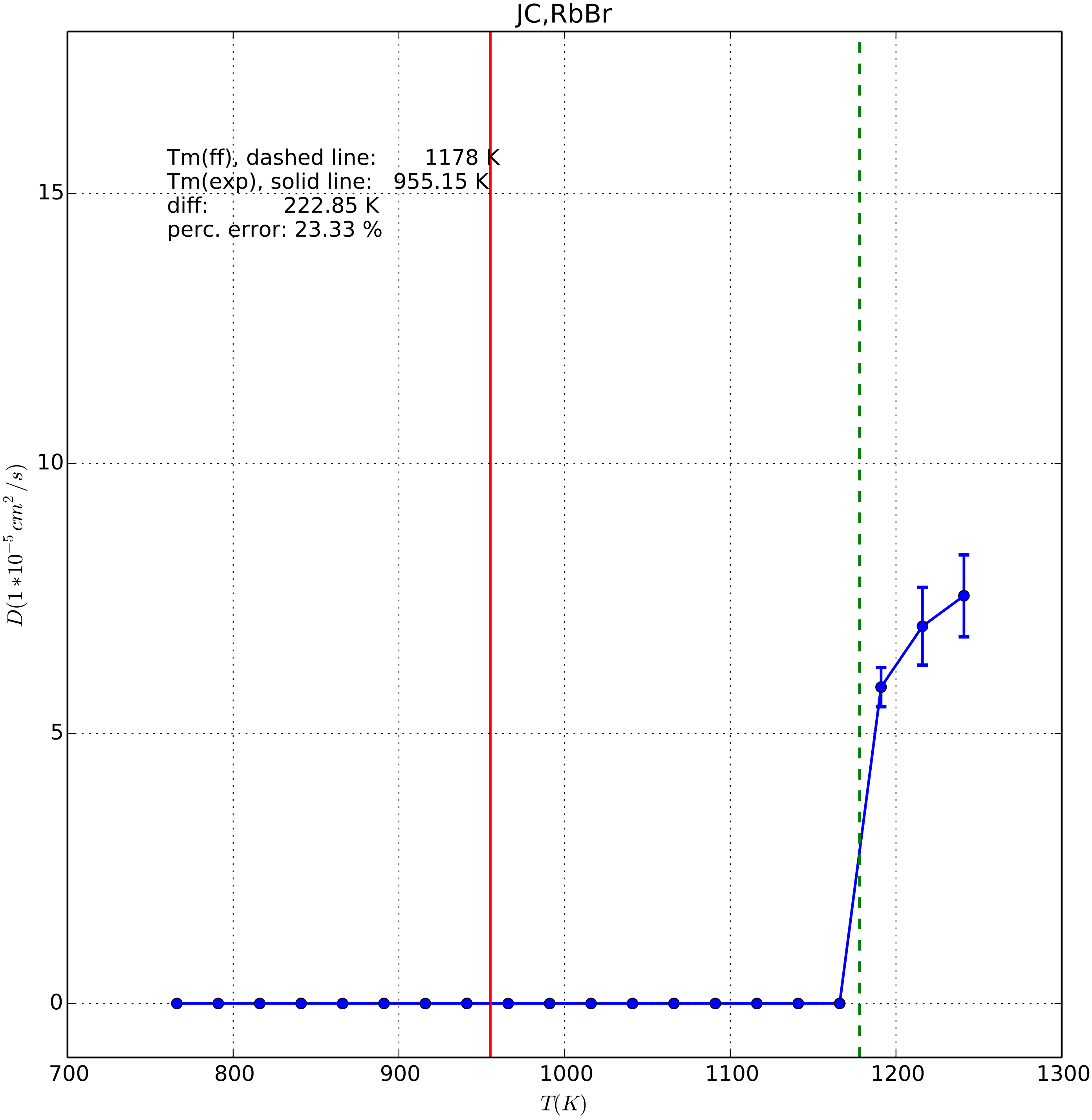

JC,KCl
Tm(ff), dashed line: 1230 K
Tm(exp), solid line: 1044.15 K
diff: 185.85 K
perc. error: 17.80 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
800
900
1000
1100
1200
1300
1400
$T(K)$

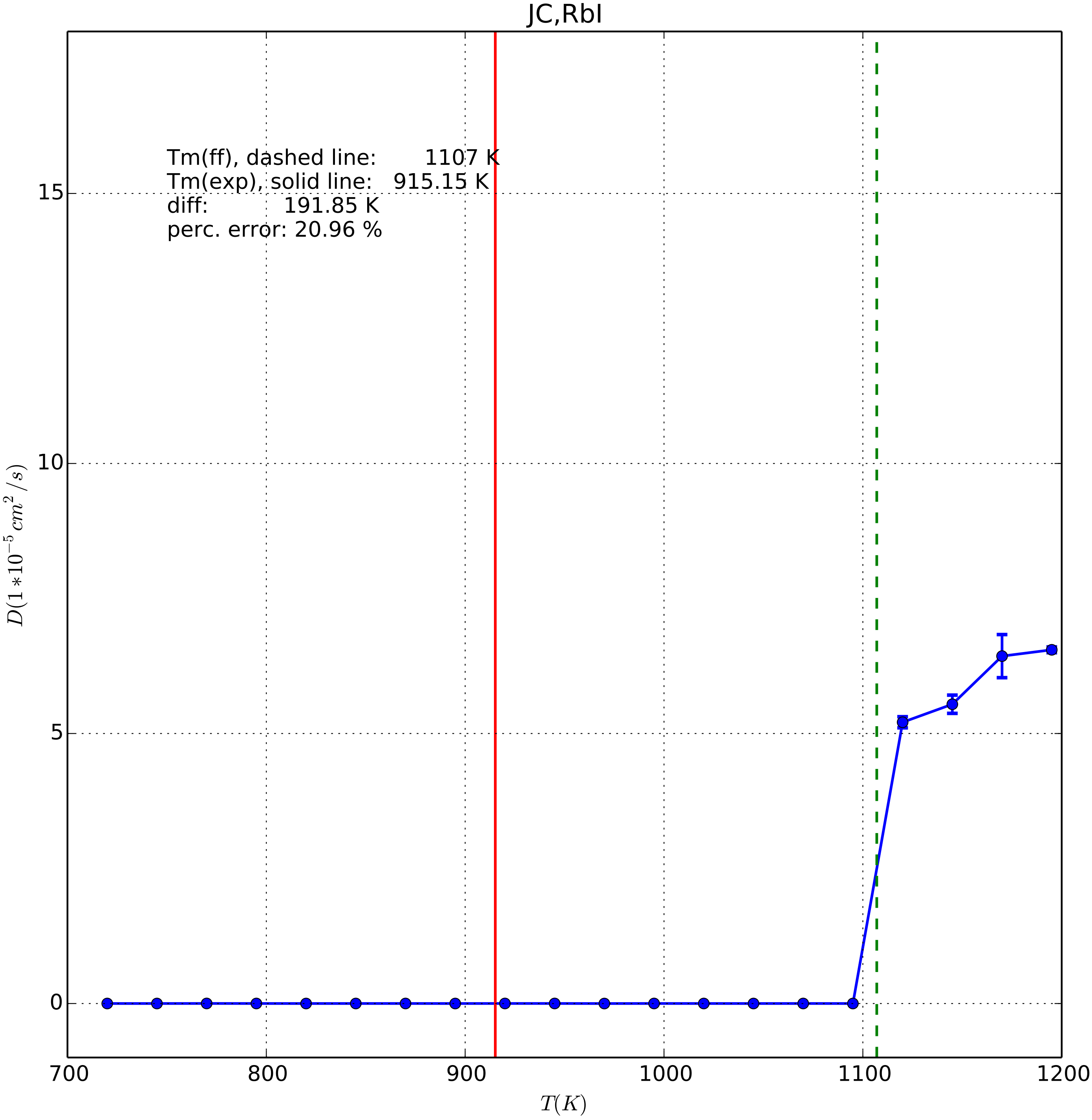

JC,KBr
Tm(ff), dashed line: 1207 K
Tm(exp), solid line: 1007.15 K
diff: 199.85 K
perc. error: 19.84 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
800
900
1000
1100
1200
1300
$T(K)$

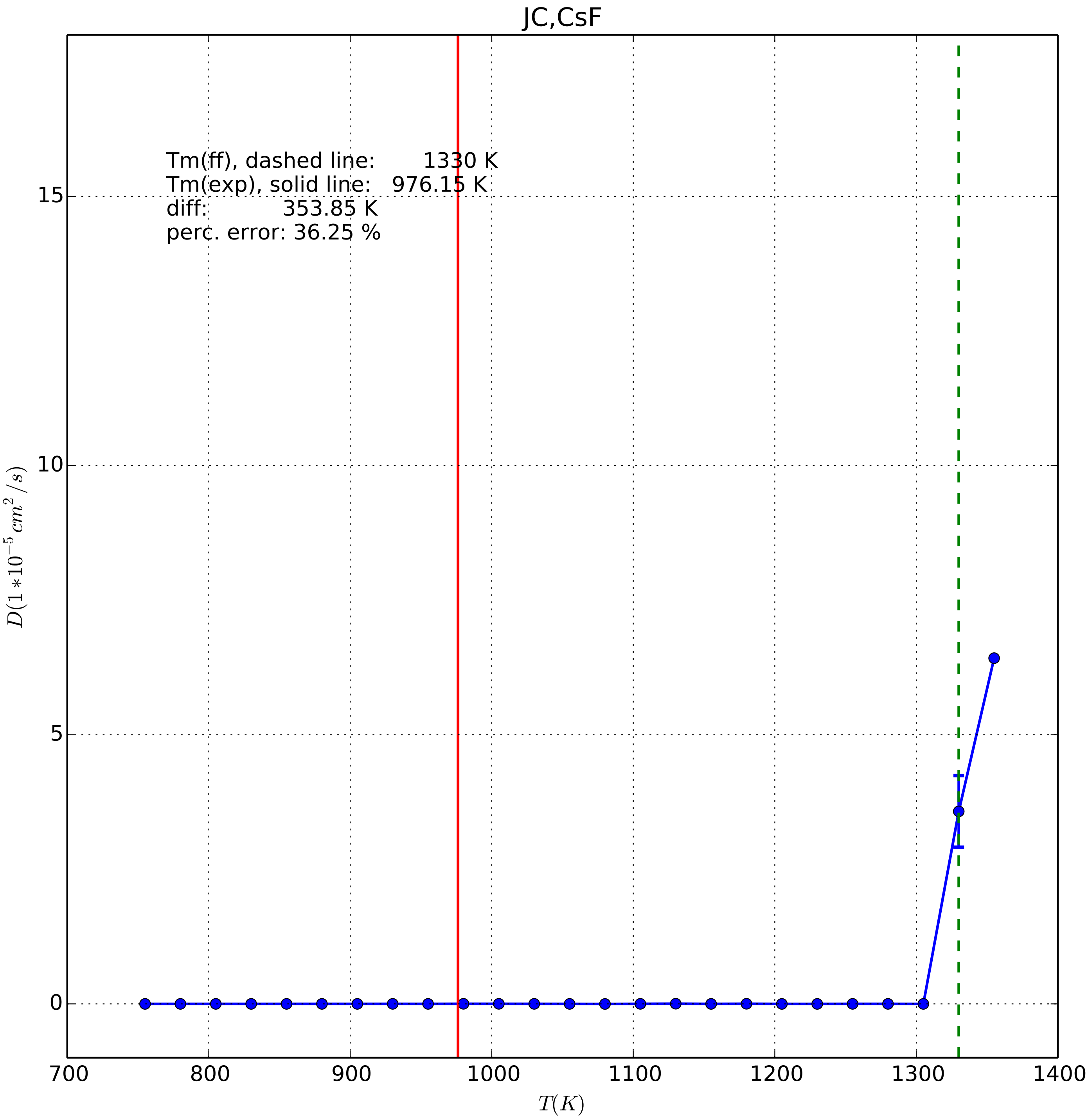

JC,KI
Tm(ff), dashed line: 1129 K
Tm(exp), solid line: 954.15 K
diff: 174.85 K
perc. error: 18.33 %
$D(1*10^{-5}cm^2/s)$
$T(K)$
0
5
10
15
700
800
900
1000
1100
1200
1300

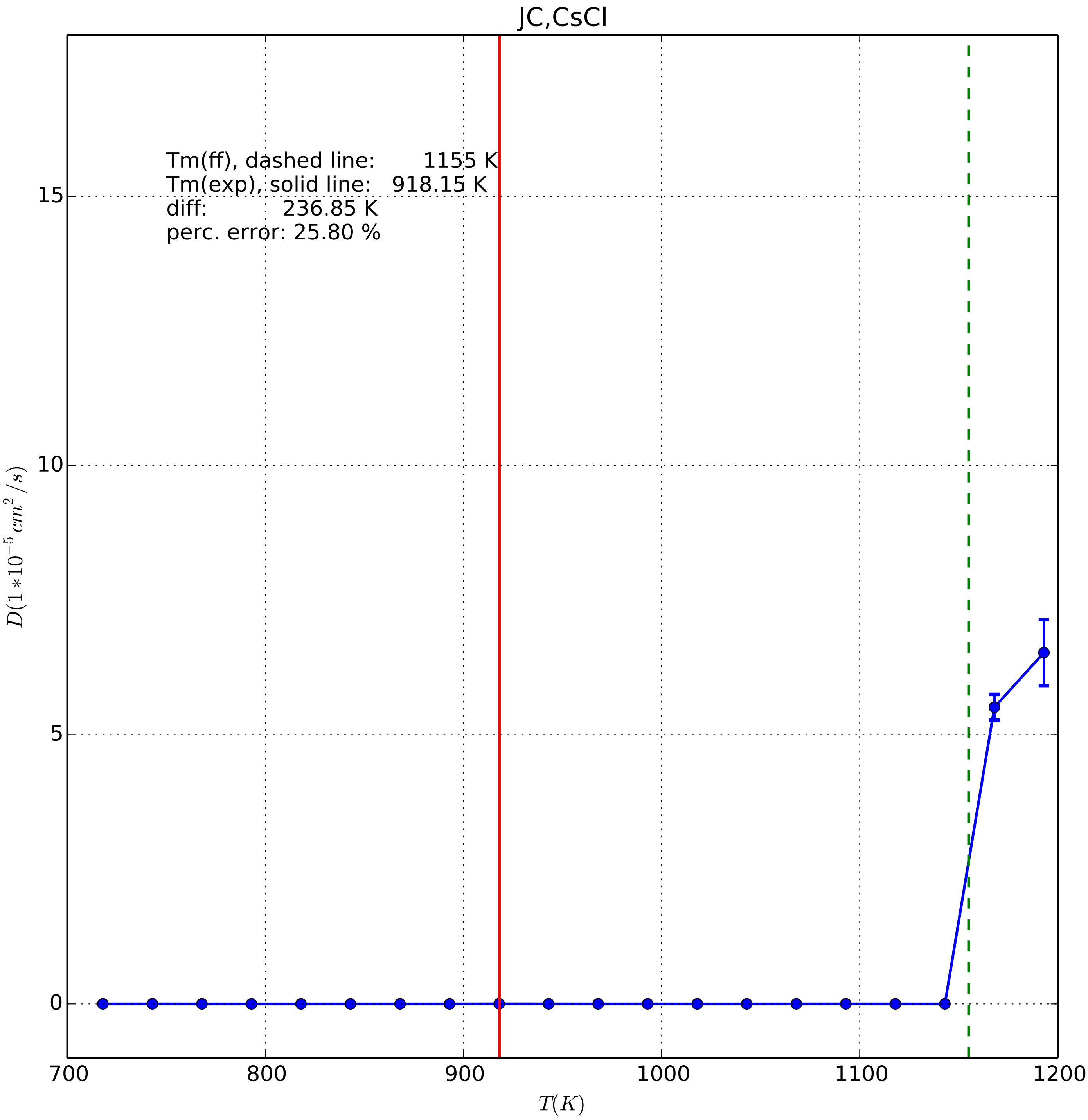

JC,RbF
Tm(ff), dashed line: 1343 K
Tm(exp), solid line: 1106.15 K
diff: 236.85 K
perc. error: 21.41 %
15
10
5
0
$D(1*10^{-5}cm^2/s)$
800
900
1000
1100
1200
1300
1400
$T(K)$

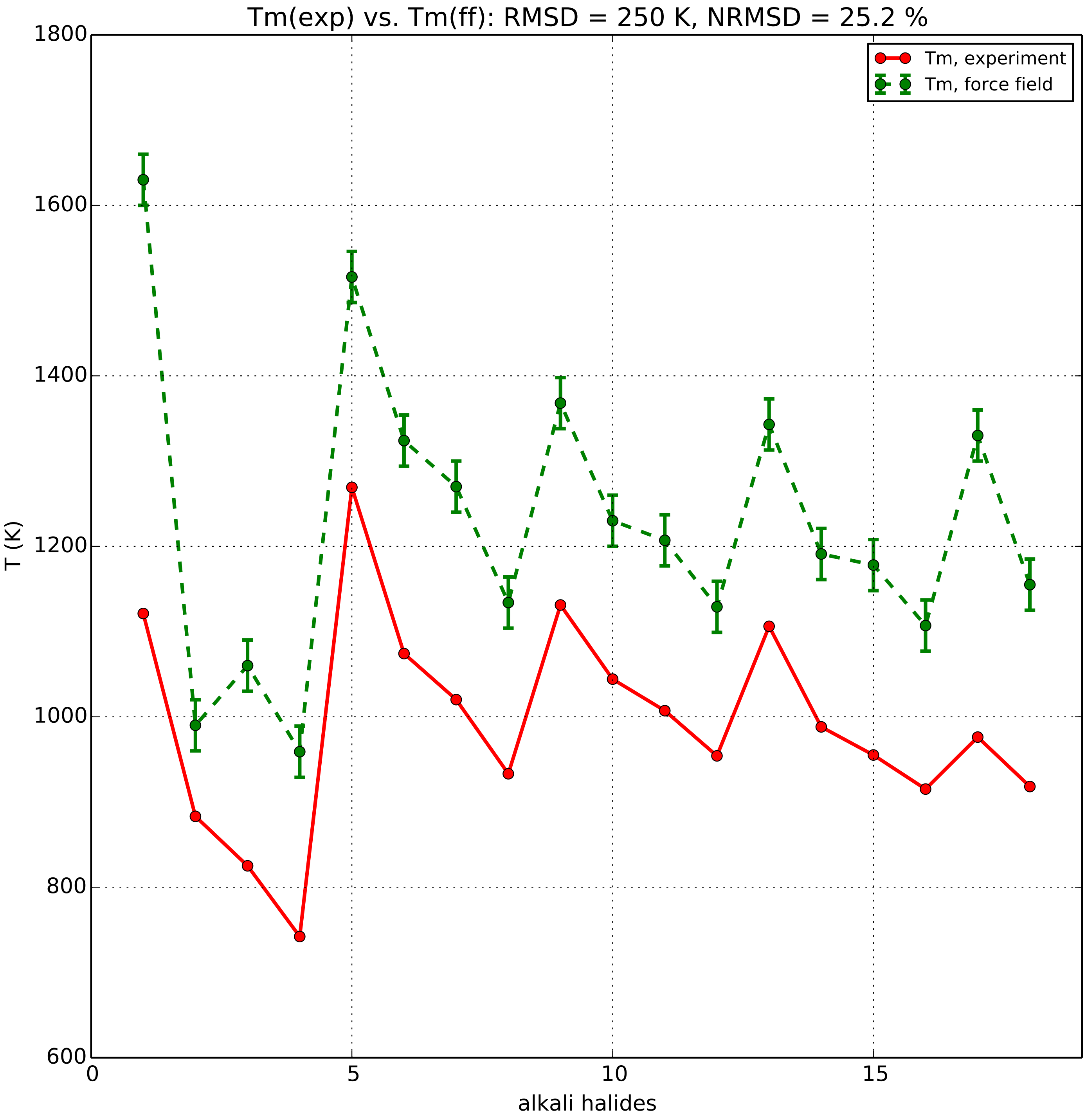

JC,RbCl
Tm(ff), dashed line: 1191 K
Tm(exp), solid line: 988.15 K
diff: 202.85 K
perc. error: 20.53 %
$D(1*10^{-5}cm^2/s)$
15
10
5
0
700
800
900
1000
1100
1200
1300
$T(K)$

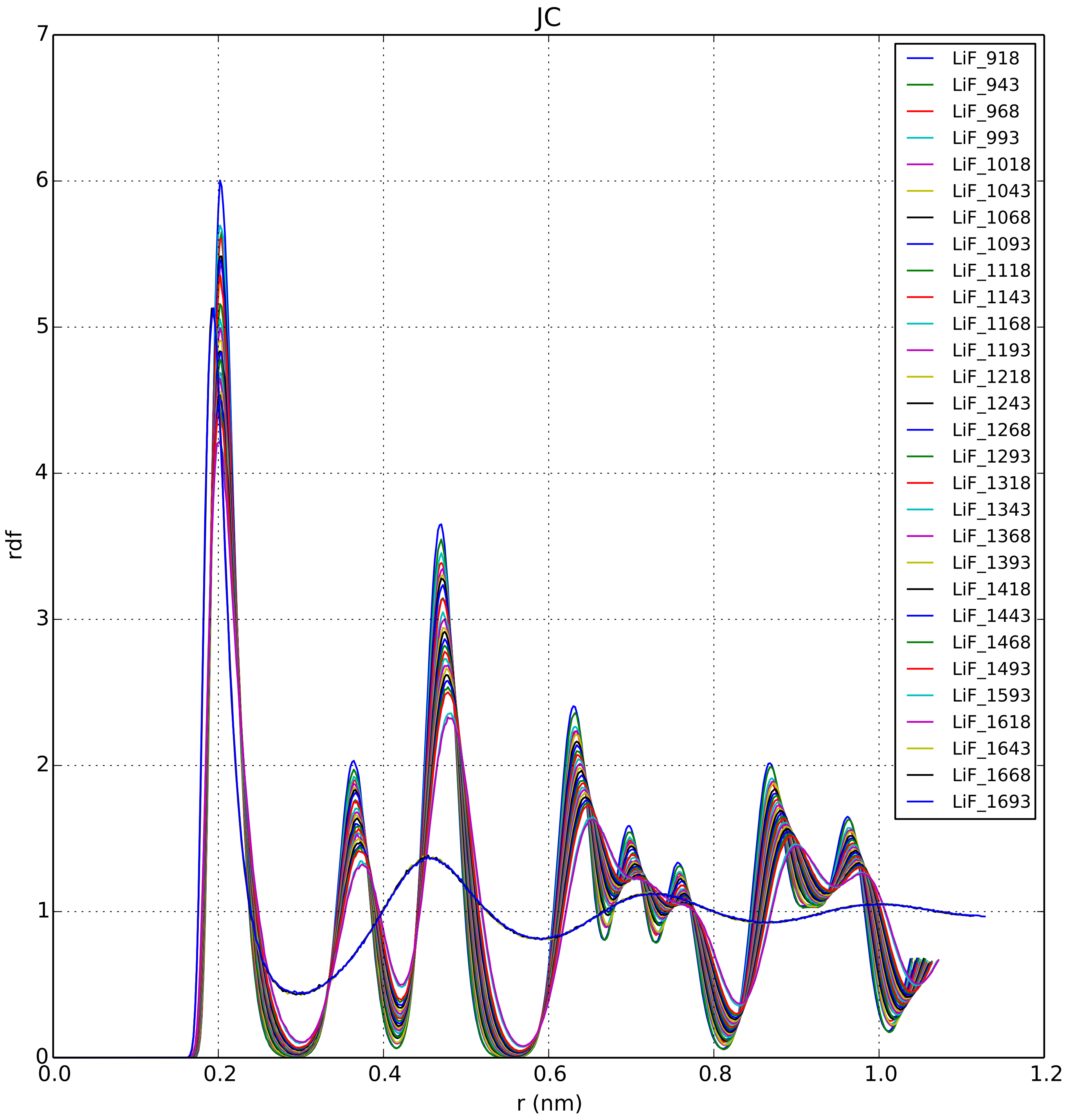

JC,RbBr
Tm(ff), dashed line: 1178 K
Tm(exp), solid line: 955.15 K
diff: 222.85 K
perc. error: 23.33 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
700
800
900
1000
1100
1200
1300
$T(K)$


JC,RbI
Tm(ff), dashed line: 1107 K
Tm(exp), solid line: 915.15 K
diff: 191.85 K
perc. error: 20.96 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
700
800
900
1000
1100
1200
$T(K)$


JC,CsF
Tm(ff), dashed line: 1330 K
Tm(exp), solid line: 976.15 K
diff: 353.85 K
perc. error: 36.25 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
700
800
900
1000
1100
1200
1300
1400
$T(K)$

JC,CsCl
Tm(ff), dashed line: 1155 K
Tm(exp), solid line: 918.15 K
diff: 236.85 K
perc. error: 25.80 %
$D(1*10^{-5}cm^2/s)$
0
5
10
15
700
800
900
1000
1100
1200
$T(K)$


Tm(exp) vs. Tm(ff): RMSD = 250 K, NRMSD = 25.2 %
Tm, experiment
Tm, force field
T (K)
1800
1600
1400
1200
1000
800
600
0
5
10
15
alkali halides


JC
rdf
r (nm)
0
1
2
3
4
5
6
7
0.0
0.2
0.4
0.6
0.8
1.0
1.2
LiF_918
LiF_943
LiF_968
LiF_993
LiF_1018
LiF_1043
LiF_1068
LiF_1093
LiF_1118
LiF_1143
LiF_1168
LiF_1193
LiF_1218
LiF_1243
LiF_1268
LiF_1293
LiF_1318
LiF_1343
LiF_1368
LiF_1393
LiF_1418
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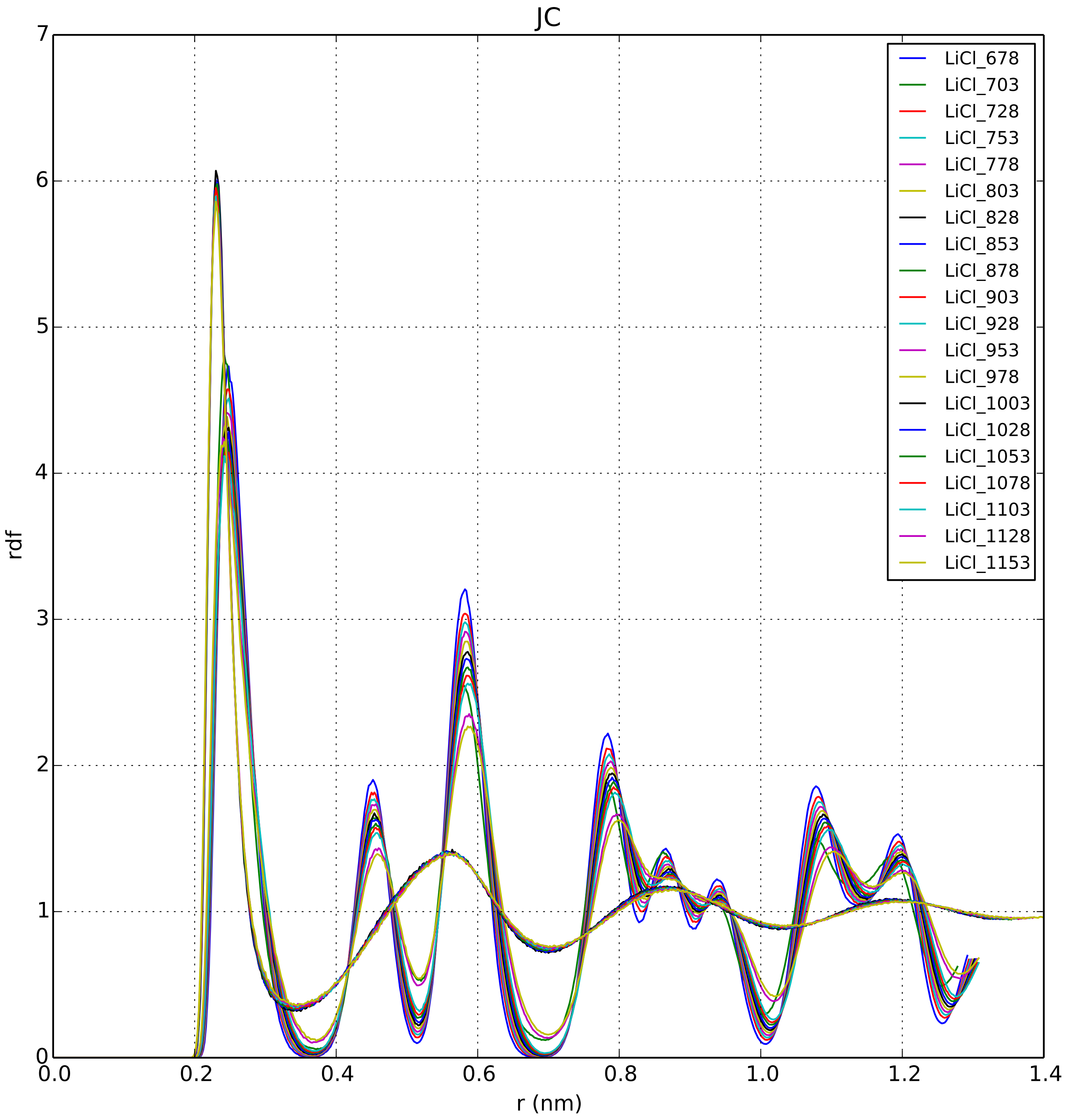
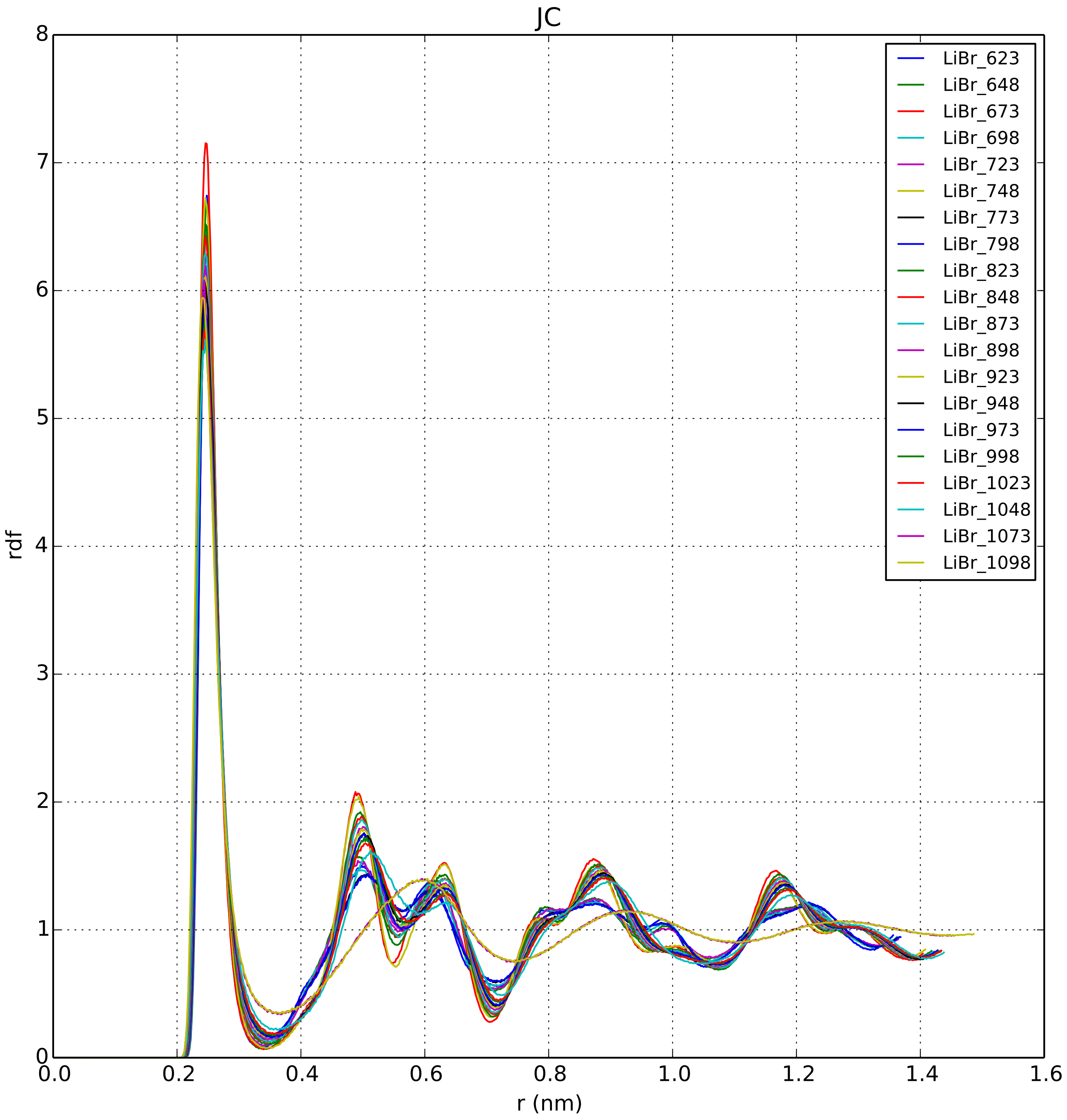
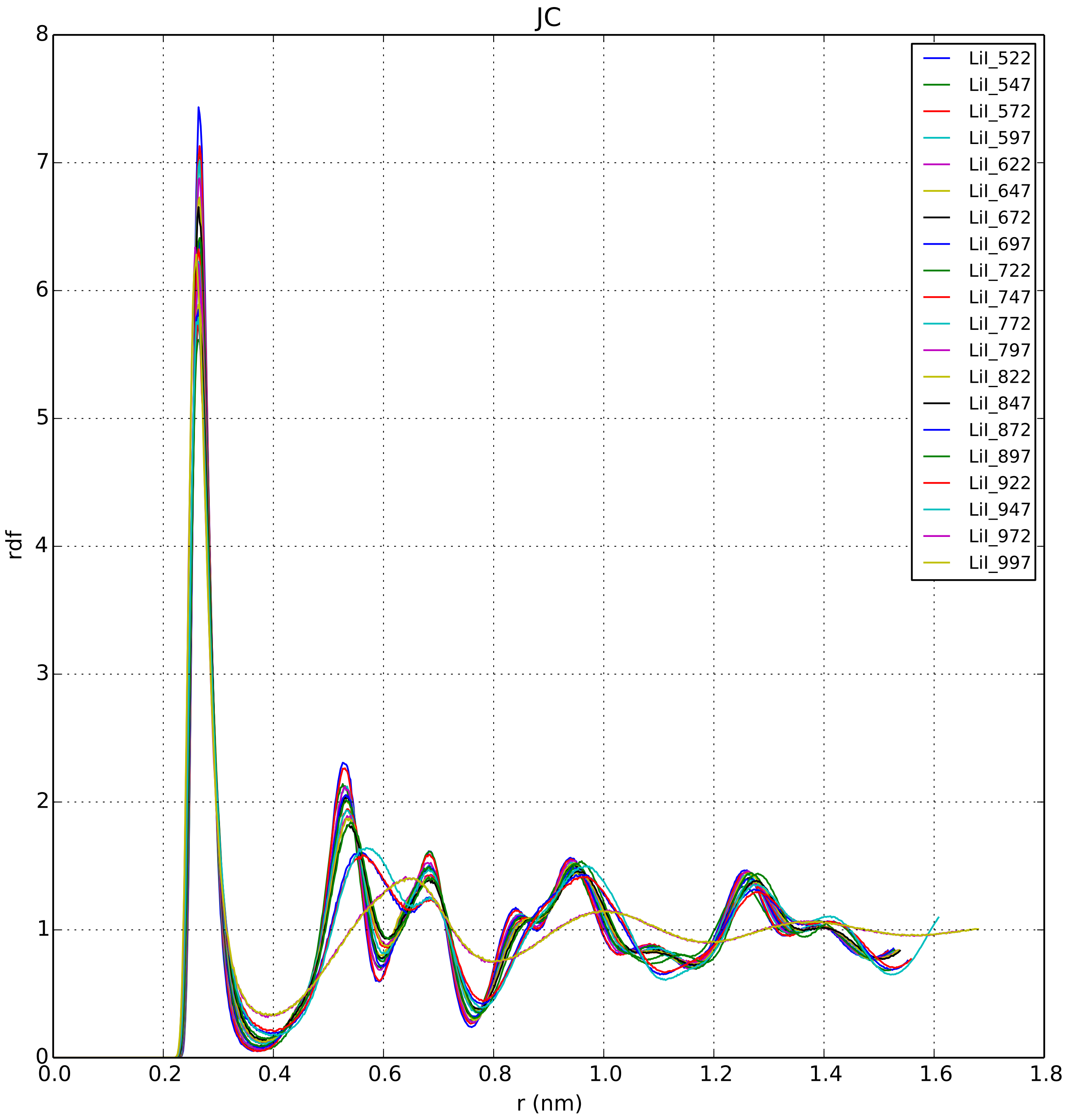
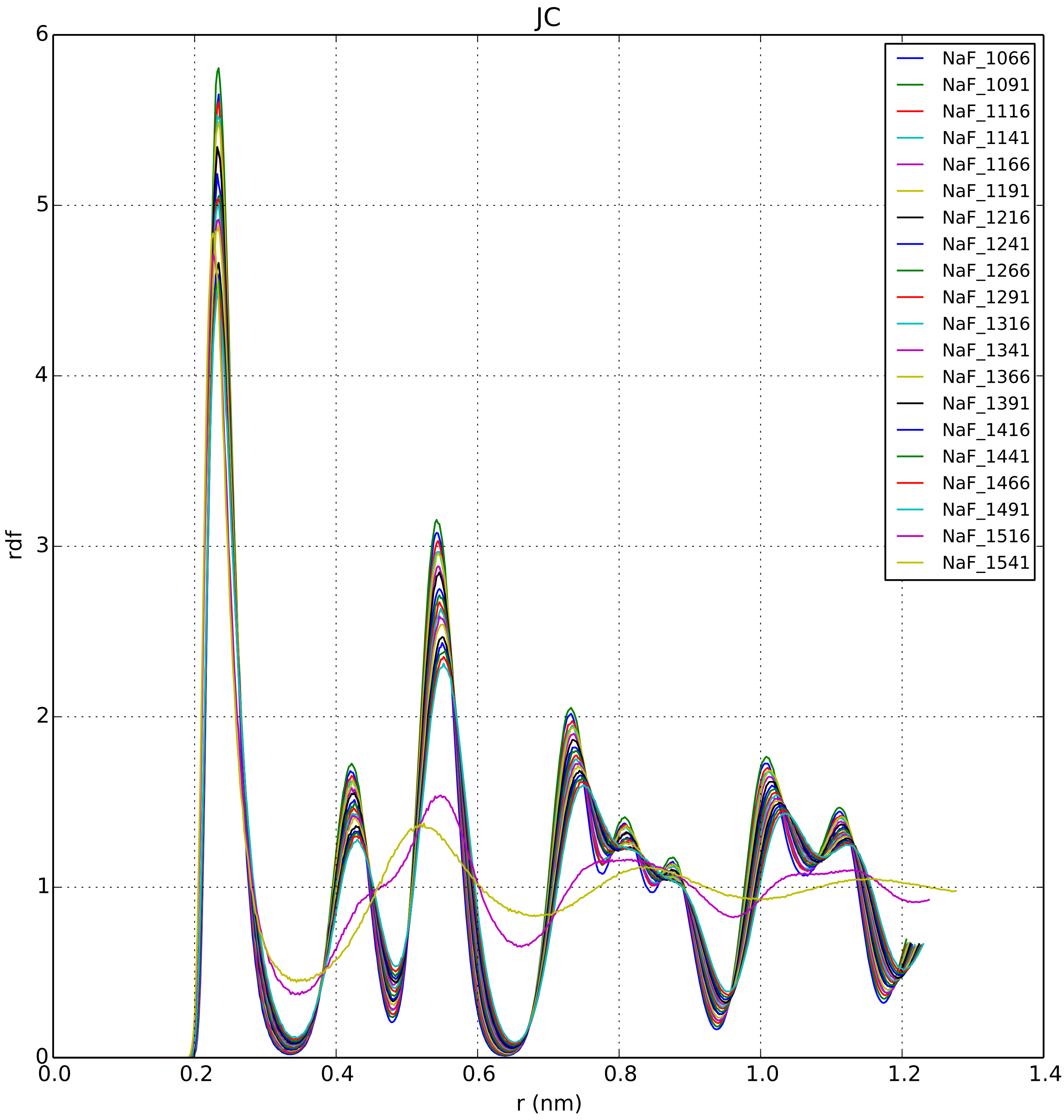
LiF_1643
LiF_1668
LiF_1693


JC
rdf
r (nm)
0
1
2
3
4
5
6
7
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
LiCl_678
LiCl_703
LiCl_728
LiCl_753
LiCl_778
LiCl_803
LiCl_828
LiCl_853
LiCl_878
LiCl_903
LiCl_928
LiCl_953
LiCl_978
LiCl_1003
LiCl_1028
LiCl_1053
LiCl_1078
LiCl_1103
LiCl_1128
LiCl_1153


JC
rdf
r (nm)
0
1
2
3
4
5
6
7
8
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
LiBr_623
LiBr_648
LiBr_673
LiBr_698
LiBr_723
LiBr_748
LiBr_773
LiBr_798
LiBr_823
LiBr_848
LiBr_873
LiBr_898
LiBr_923
LiBr_948
LiBr_973
LiBr_998
LiBr_1023
LiBr_1048
LiBr_1073
LiBr_1098


JC
rdf
r (nm)
0
1
2
3
4
5
6
7
8
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
LiI_522
LiI_547
LiI_572
LiI_597
LiI_622
LiI_647
LiI_672
LiI_697
LiI_722
LiI_747
LiI_772
LiI_797
LiI_822
LiI_847
LiI_872
LiI_897
LiI_922
LiI_947
LiI_972
LiI_997


JC
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
NaF_1066
NaF_1091
NaF_1116
NaF_1141
NaF_1166
NaF_1191
NaF_1216
NaF_1241
NaF_1266
NaF_1291
NaF_1316
NaF_1341
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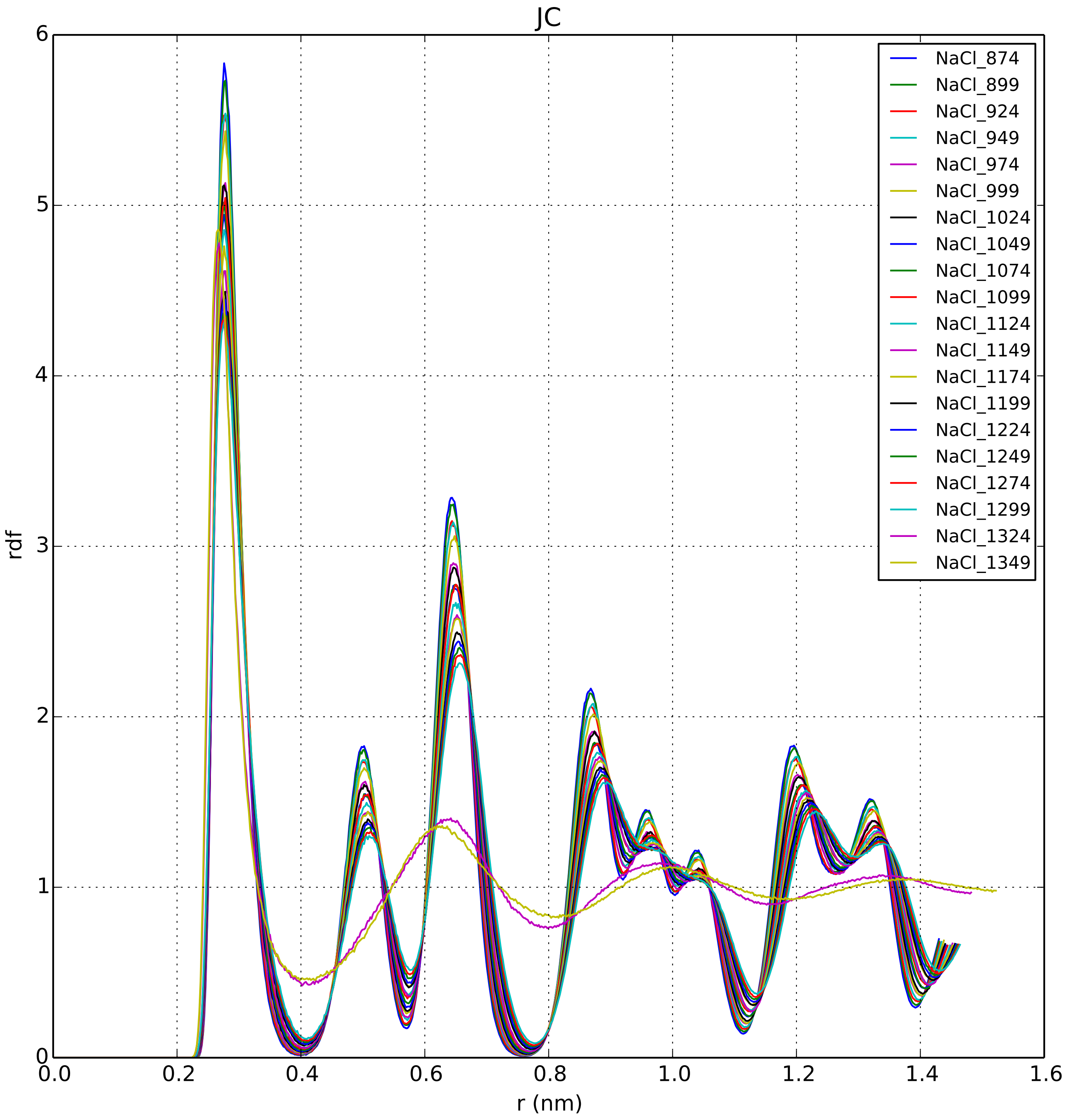
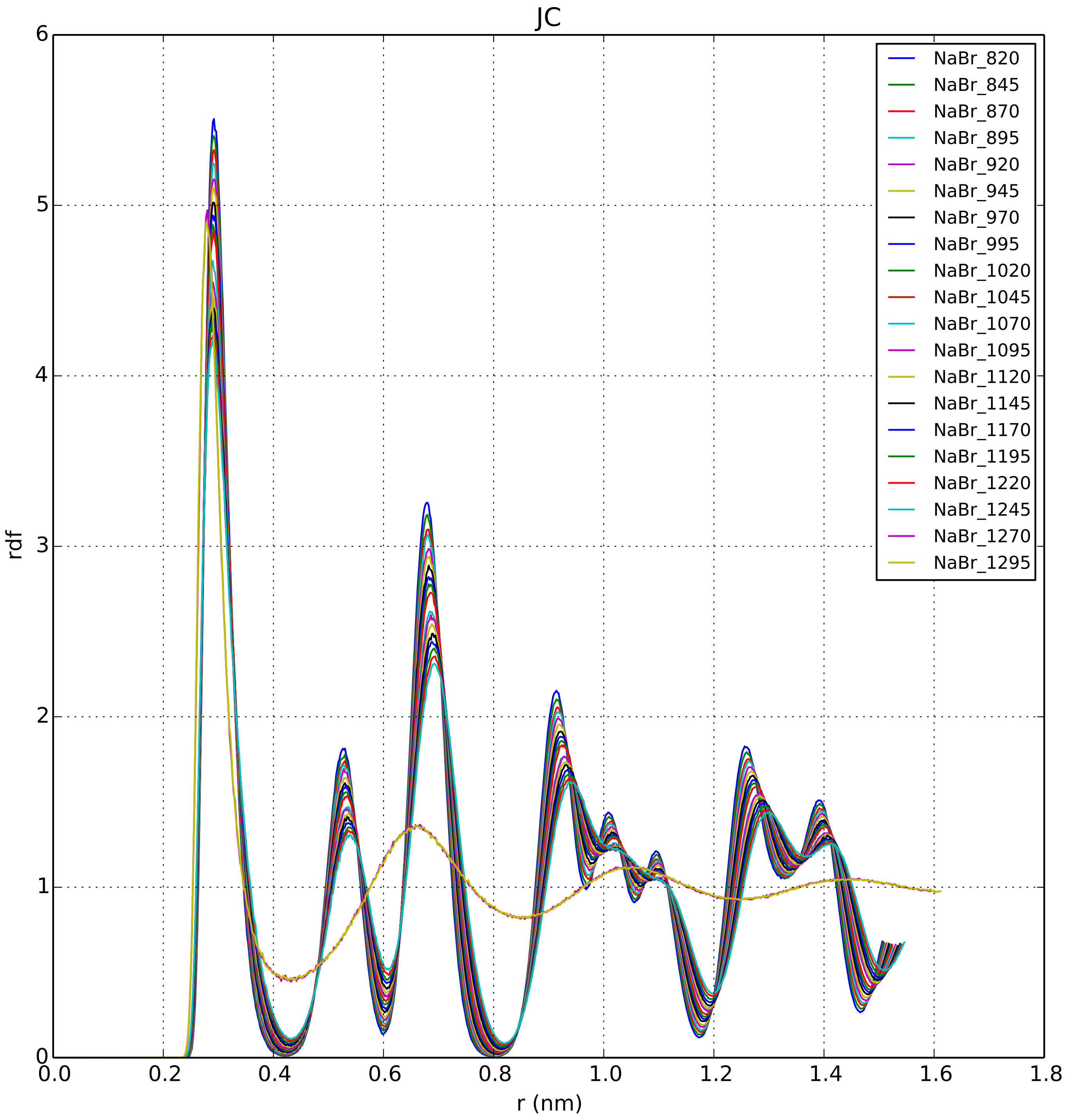
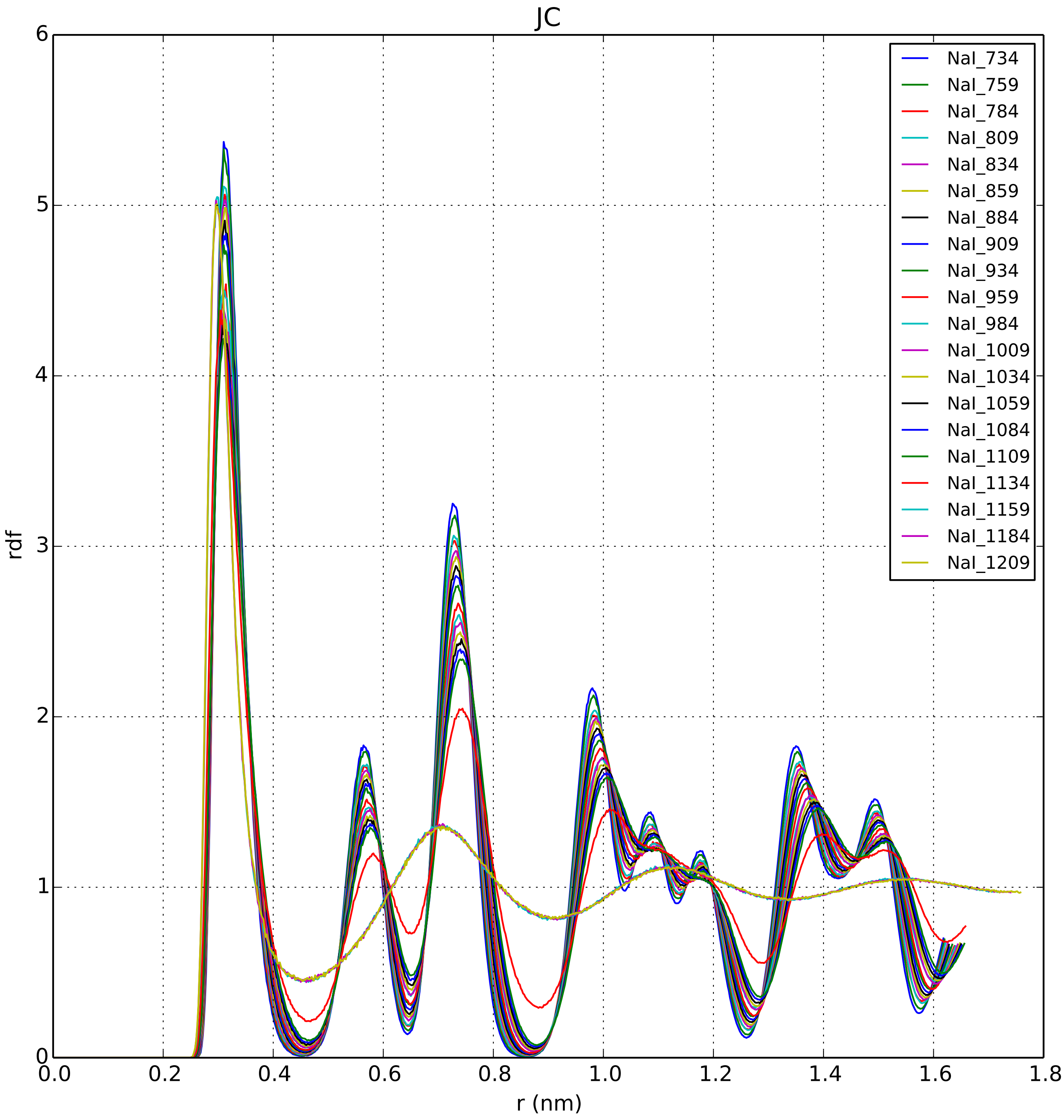
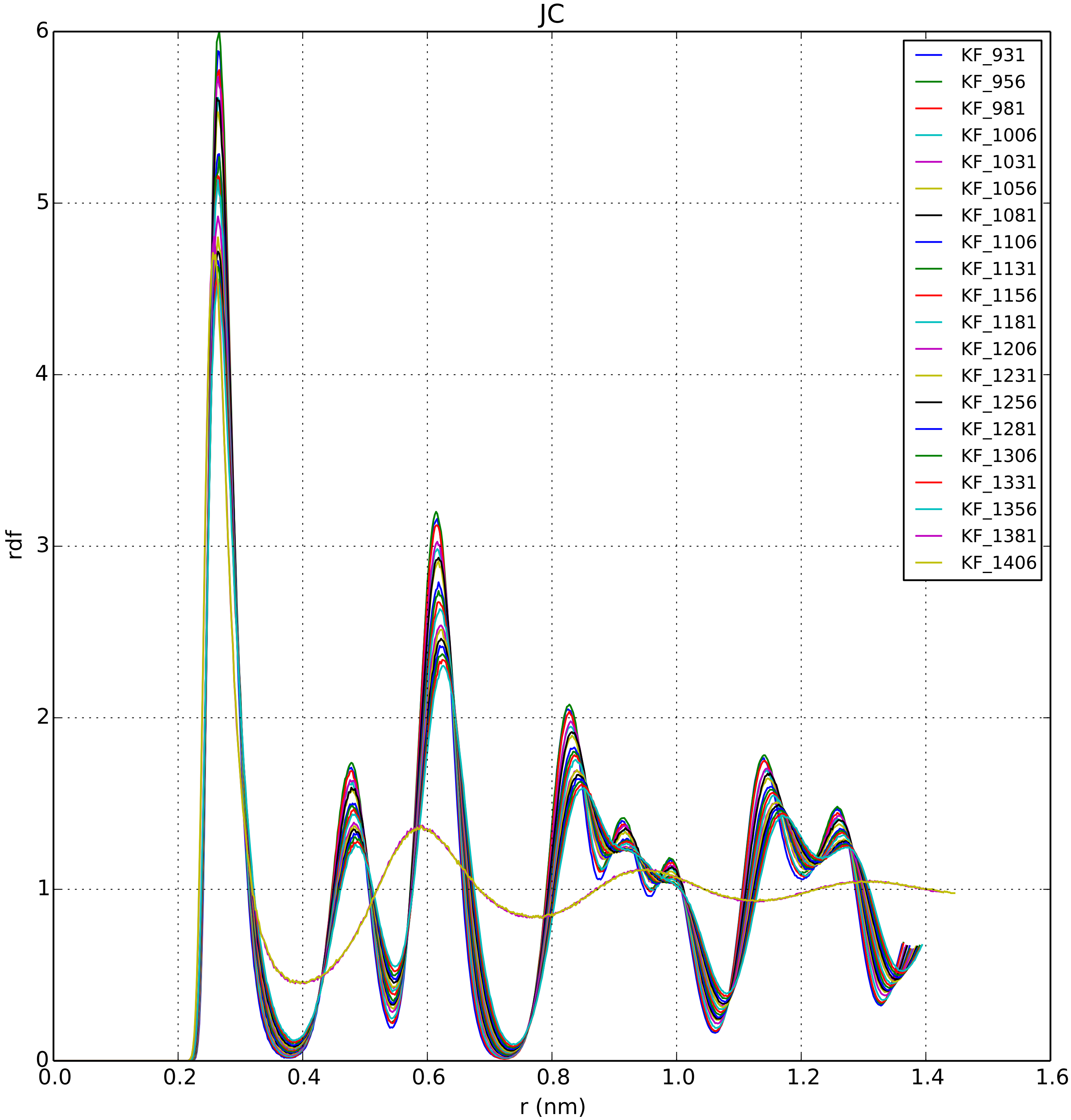
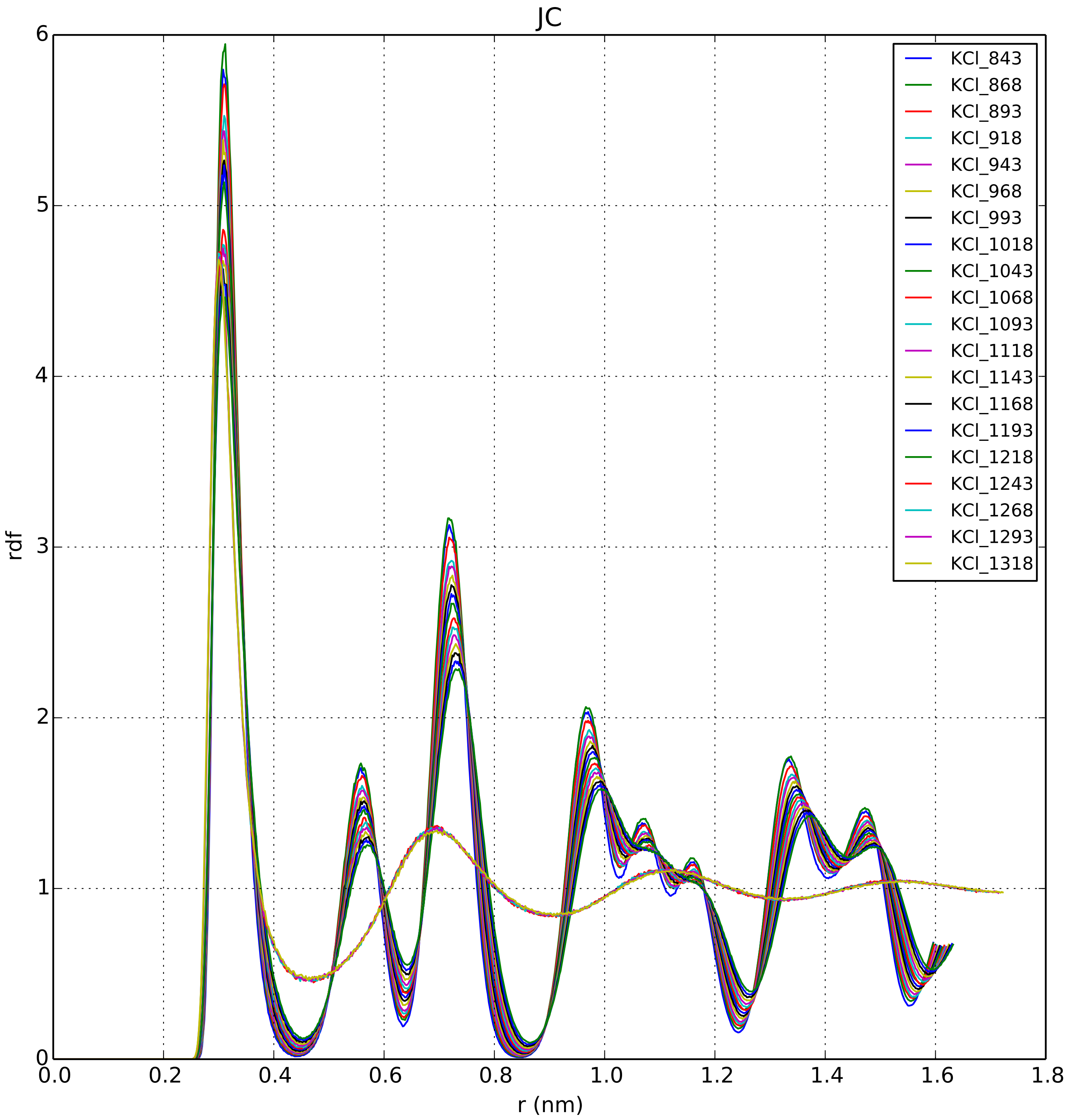
NaF_1491
NaF_1516
NaF_1541


JC
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
NaCl_874
NaCl_899
NaCl_924
NaCl_949
NaCl_974
NaCl_999
NaCl_1024
NaCl_1049
NaCl_1074
NaCl_1099
NaCl_1124
NaCl_1149
NaCl_1174
NaCl_1199
NaCl_1224
NaCl_1249
NaCl_1274
NaCl_1299
NaCl_1324
NaCl_1349


JC
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
NaBr_820
NaBr_845
NaBr_870
NaBr_895
NaBr_920
NaBr_945
NaBr_970
NaBr_995
NaBr_1020
NaBr_1045
NaBr_1070
NaBr_1095
NaBr_1120
NaBr_1145
NaBr_1170
NaBr_1195
NaBr_1220
NaBr_1245
NaBr_1270
NaBr_1295


JC
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
NaI_734
NaI_759
NaI_784
NaI_809
NaI_834
NaI_859
NaI_884
NaI_909
NaI_934
NaI_959
NaI_984
NaI_1009
NaI_1034
NaI_1059
NaI_1084
NaI_1109
NaI_1134
NaI_1159
NaI_1184
NaI_1209


JC
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
KF_931
KF_956
KF_981
KF_1006
KF_1031
KF_1056
KF_1081
KF_1106
KF_1131
KF_1156
KF_1181
KF_1206
KF_1231
KF_1256
KF_1281
KF_1306
KF_1331
KF_1356
KF_1381
KF_1406


JC
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
KCl_843
KCl_868
KCl_893
KCl_918
KCl_943
KCl_968
KCl_993
KCl_1018
KCl_1043
KCl_1068
KCl_1093
KCl_1118
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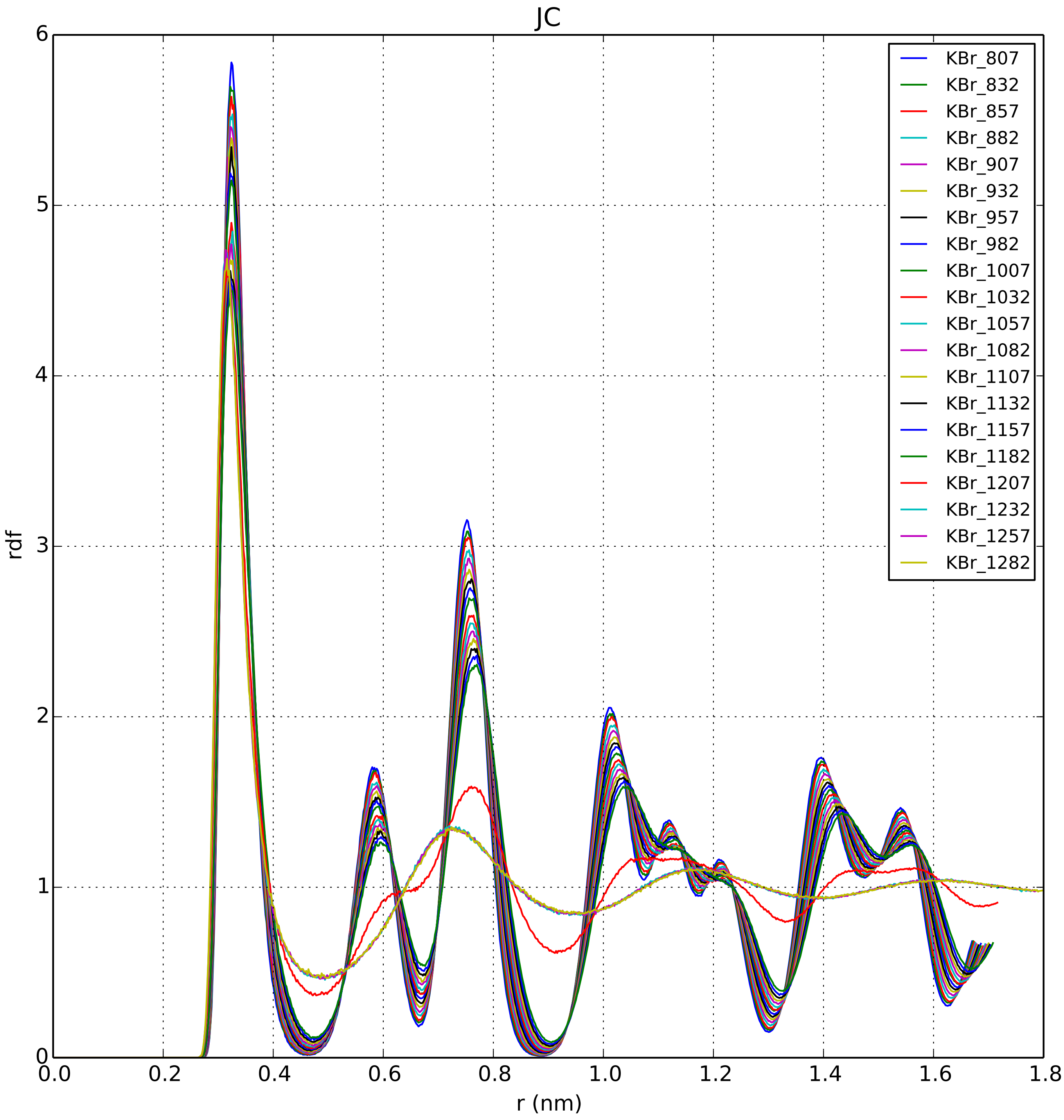
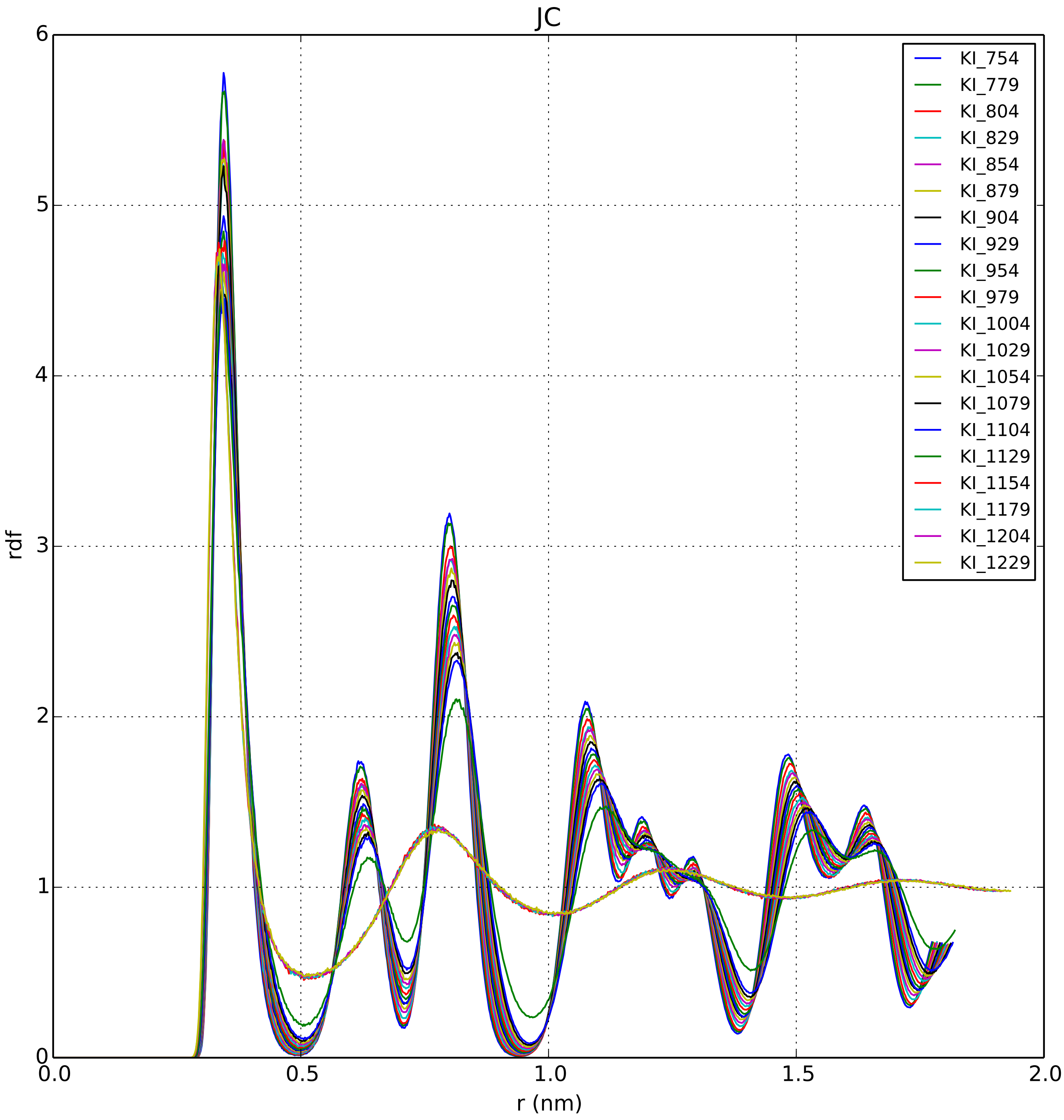
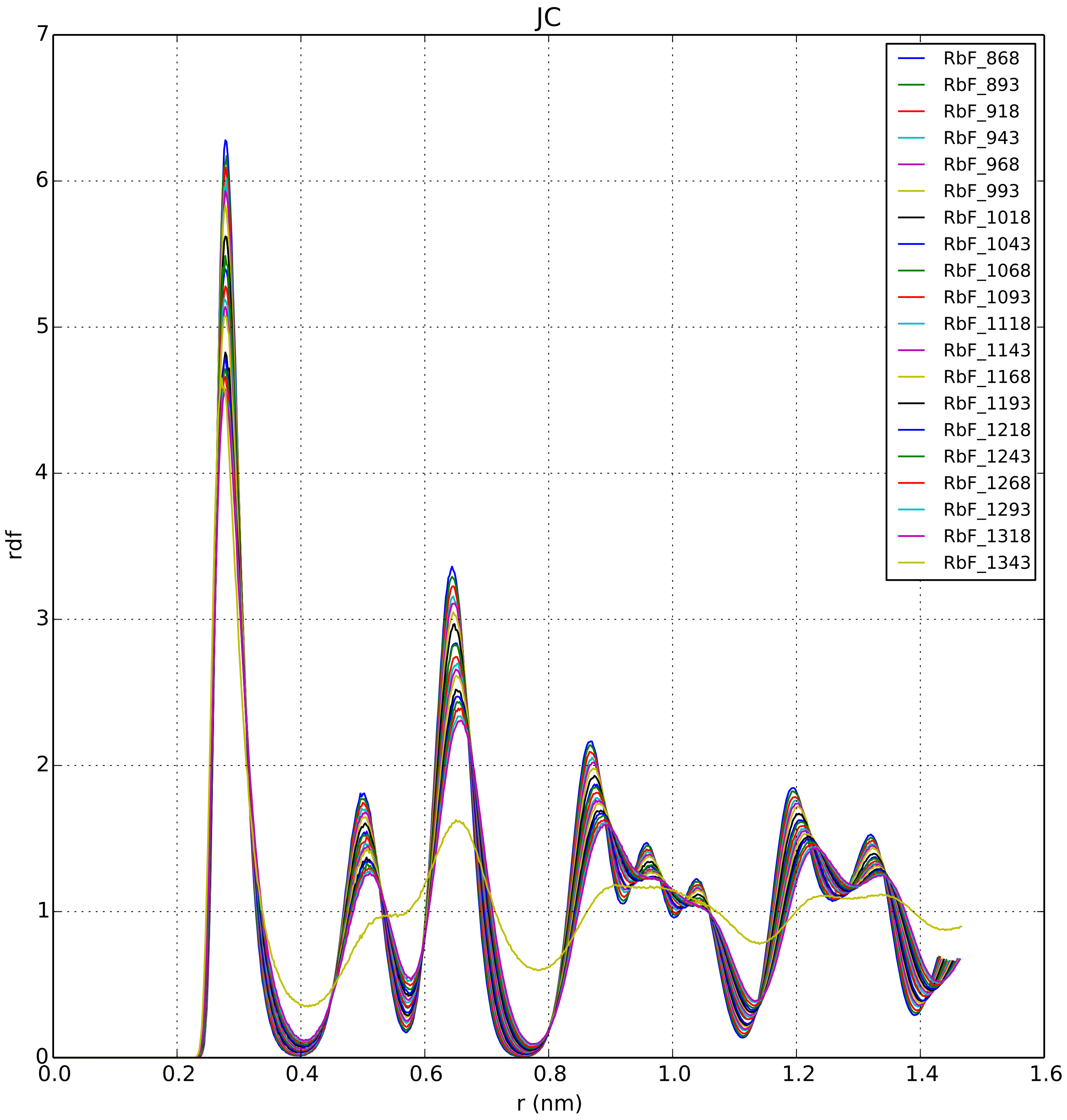
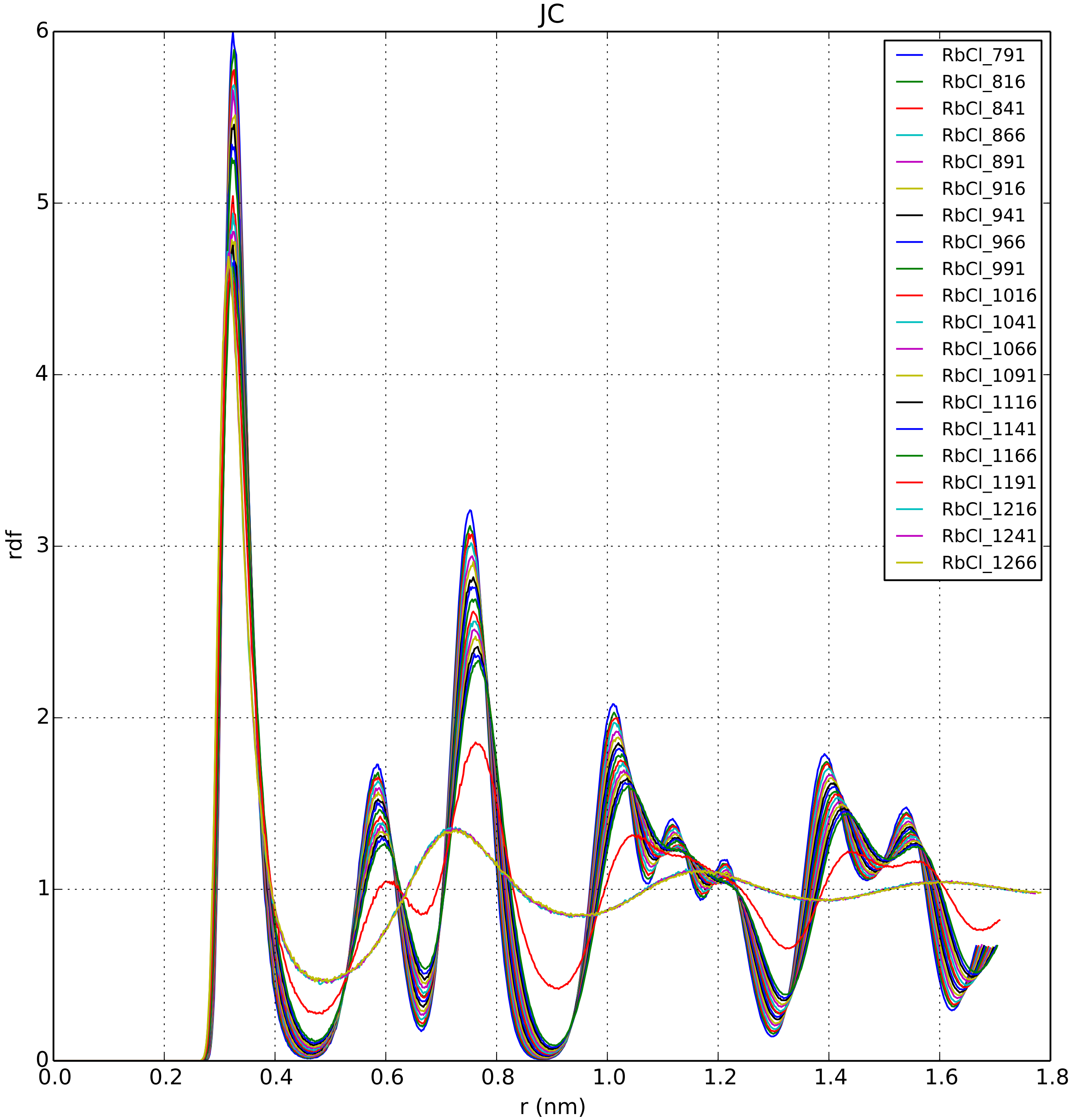
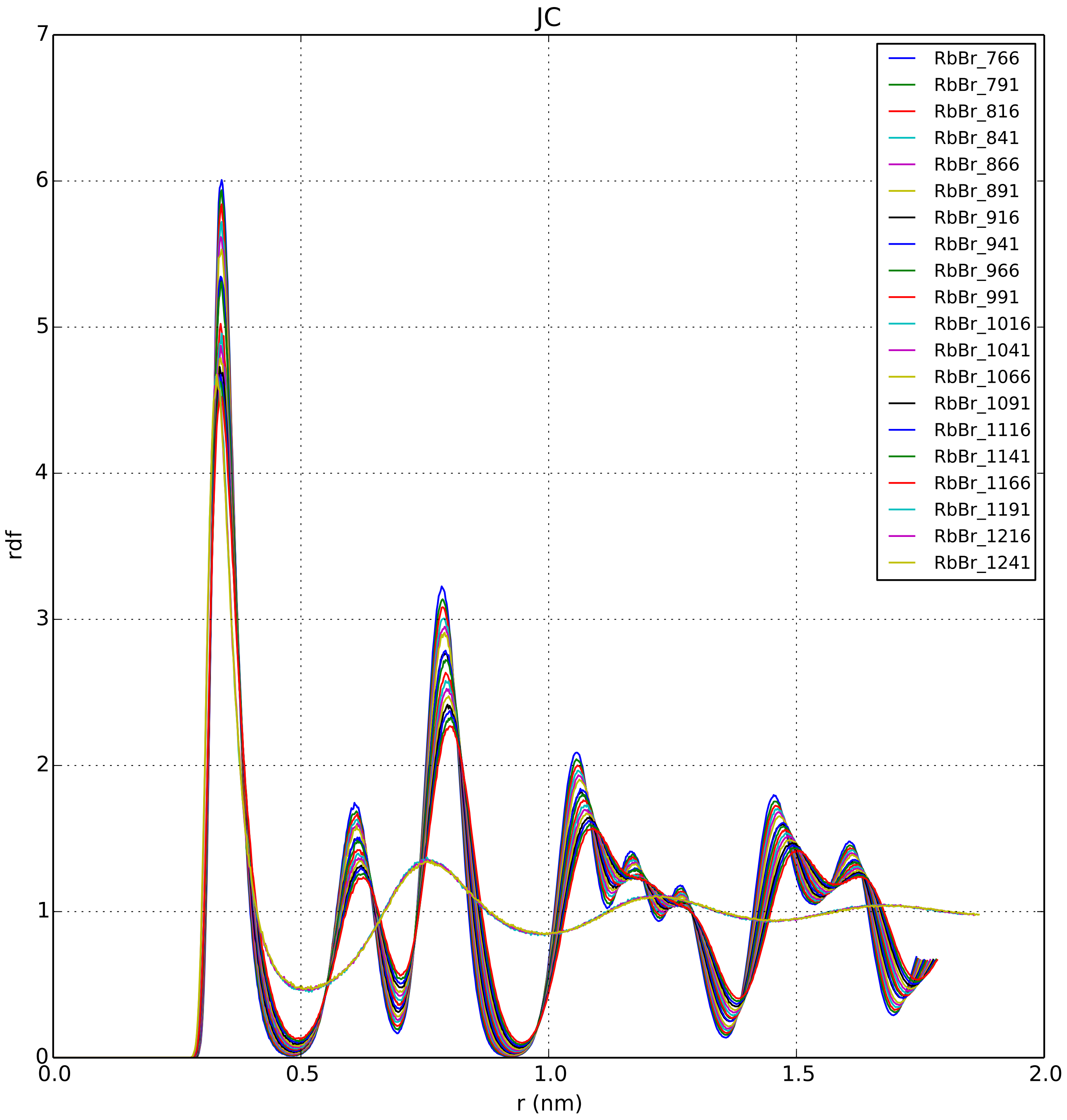
KCl_1268
KCl_1293
KCl_1318

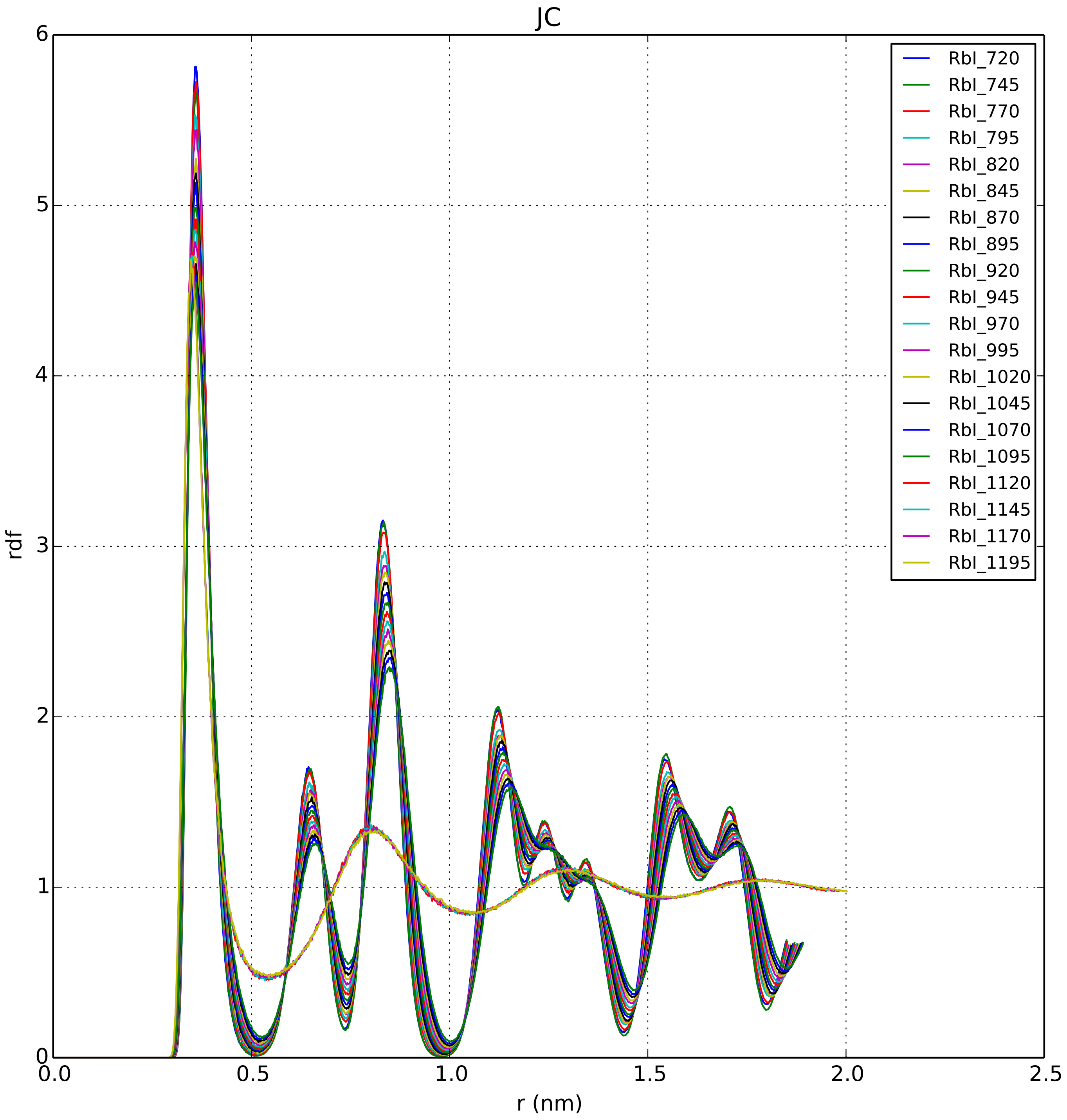

JC
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
KBr_807
KBr_832
KBr_857
KBr_882
KBr_907
KBr_932
KBr_957
KBr_982
KBr_1007
KBr_1032
KBr_1057
KBr_1082
KBr_1107
KBr_1132
KBr_1157
KBr_1182
KBr_1207
KBr_1232
KBr_1257
KBr_1282

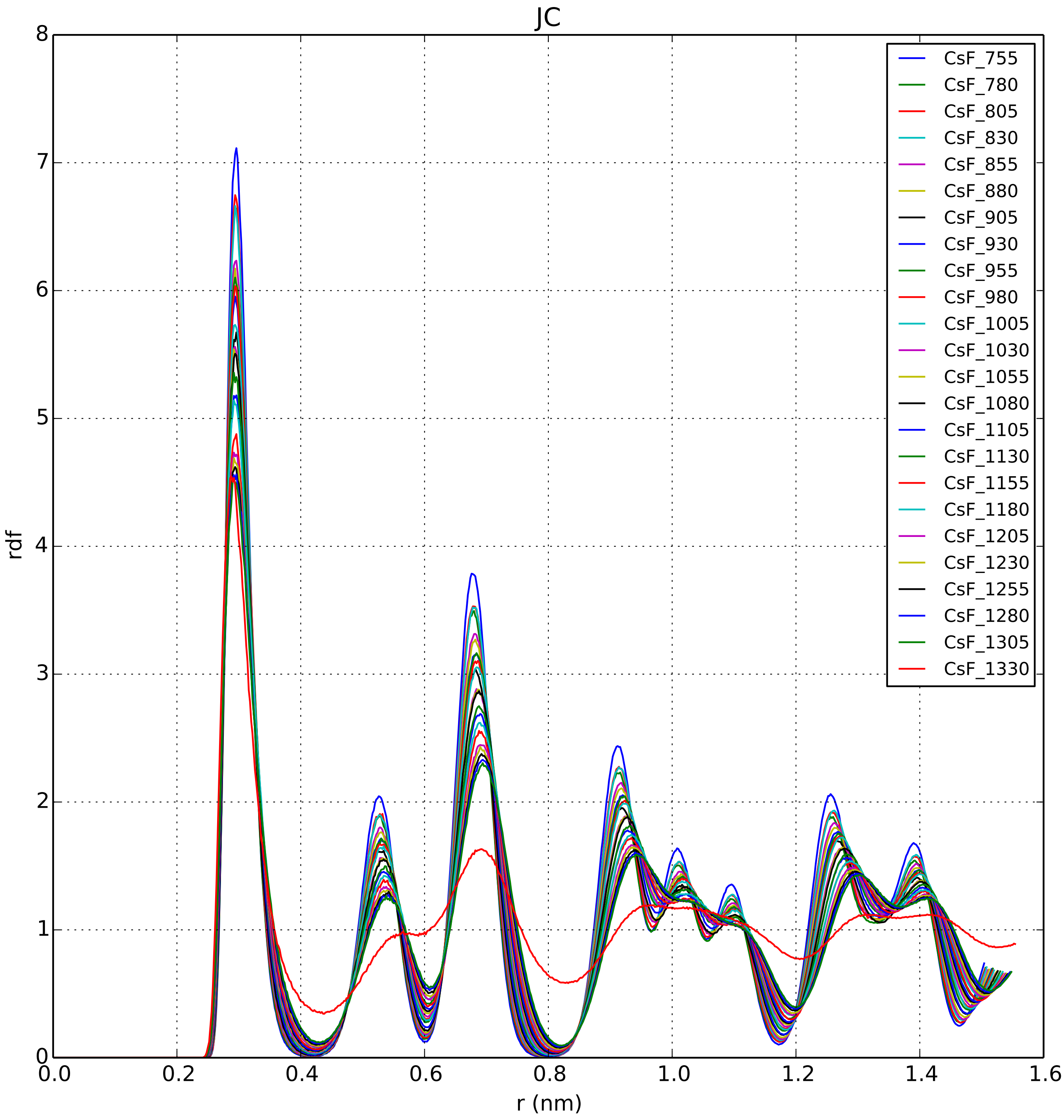

JC
rdf
r (nm)
0
1
2
3
4
5
6
0.0
0.5
1.0
1.5
2.0
KI_754
KI_779
KI_804
KI_829
KI_854
KI_879
KI_904
KI_929
KI_954
KI_979
KI_1004
KI_1029
KI_1054
KI_1079
KI_1104
KI_1129
KI_1154
KI_1179
KI_1204
KI_1229


JC
rdf
r (nm)
0
1
2
3
4
5
6
7
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
RbF_868
RbF_893
RbF_918
RbF_943
RbF_968
RbF_993
RbF_1018
RbF_1043
RbF_1068
RbF_1093
RbF_1118
RbF_1143
RbF_1168
RbF_1193
RbF_1218
RbF_1243
RbF_1268
RbF_1293
RbF_1318
RbF_1343


JC
rdf
r (nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
0
1
2
3
4
5
6
RbCl_791
RbCl_816
RbCl_841
RbCl_866
RbCl_891
RbCl_916
RbCl_941
RbCl_966
RbCl_991
RbCl_1016
RbCl_1041
RbCl_1066
RbCl_1091
RbCl_1116
RbCl_1141
RbCl_1166
RbCl_1191
RbCl_1216
RbCl_1241
RbCl_1266


JC
rdf
r (nm)
0
1
2
3
4
5
6
7
0.0
0.5
1.0
1.5
2.0
RbBr_766
RbBr_791
RbBr_816
RbBr_841
RbBr_866
RbBr_891
RbBr_916
RbBr_941
RbBr_966
RbBr_991
RbBr_1016
RbBr_1041
RbBr_1066
RbBr_1091
RbBr_1116
RbBr_1141
RbBr_1166
RbBr_1191
RbBr_1216
RbBr_1241


JC
rdf
r (nm)
0.0
0.5
1.0
1.5
2.0
2.5
0
1
2
3
4
5
6
RbI_720
RbI_745
RbI_770
RbI_795
RbI_820
RbI_845
RbI_870
RbI_895
RbI_920
RbI_945
RbI_970
RbI_995
RbI_1020
RbI_1045
RbI_1070
RbI_1095
RbI_1120
RbI_1145
RbI_1170
RbI_1195


JC
rdf
r (nm)
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
1
2
3
4
5
6
7
8
CsF_755
CsF_780
CsF_805
CsF_830
CsF_855
CsF_880
CsF_905
CsF_930
CsF_955
CsF_980
CsF_1005
CsF_1030
CsF_1055
CsF_1080
CsF_1105
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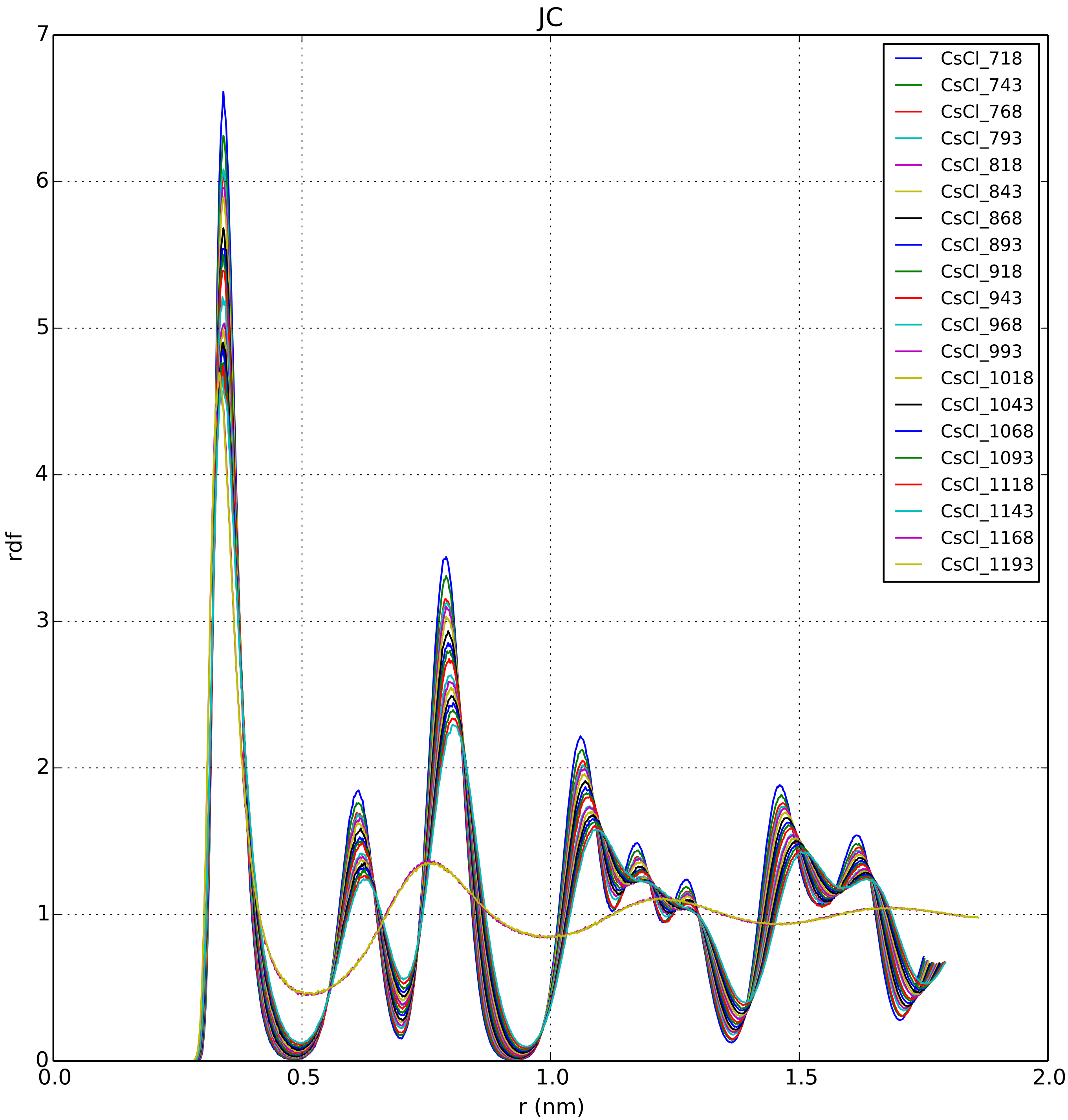
CsF_1280
CsF_1305
CsF_1330


JC
rdf
r (nm)
0.0
0.5
1.0
1.5
2.0
0
1
2
3
4
5
6
7
CsCl_718
CsCl_743
CsCl_768
CsCl_793
CsCl_818
CsCl_843
CsCl_868
CsCl_893
CsCl_918
CsCl_943
CsCl_968
CsCl_993
CsCl_1018
CsCl_1043
CsCl_1068
CsCl_1093
CsCl_1118
CsCl_1143
CsCl_1168
CsCl_1193

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