Pandat 2026

Database Manual

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Database Manuals

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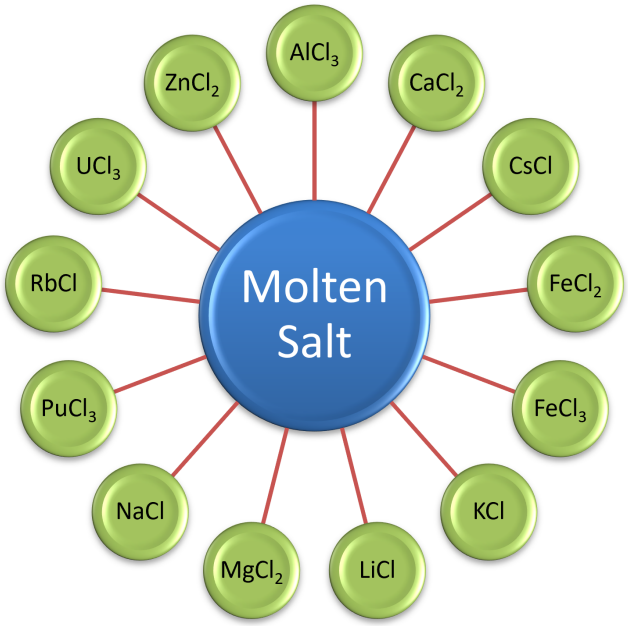
PanMoltenSalt

Thermodynamic Database

Database for Multi-Component Chloride-based Molten Salt systems



PANDAT™
SOFTWARE

Thermodynamic database

Components (14)

A total of 14 components are included in the database as listed here:

Major alloying chlorides: $AlCl_3$, $BaCl_2$, $CaCl_2$, CsCl, $FeCl_2$, $FeCl_3$, KCl, LiCl, $MgCl_2$, NaCl, $PuCl_3$, RbCl, UCl_3, and $ZnCl_2$

Suggested Composition Range

The suggested composition range for metal elements is listed in Table 1.1.

Table 1.1: Suggested composition range

Components	Composition Range (wt.%)
KCl,NaCl,$MgCl_2$,$CaCl_2$,$AlCl_3$ LiCl,RbCl,$ZnCl_2$	0-100
$BaCl_2$,CsCl,$FeCl_2$,$FeCl_3$	0-50
$PuCl_3$,UCl_3	0-25

Phases

There are **55** phases available in the current molten salt database. Table 1.2 lists all the phases for molten salt systems with lattice size and components in detail.

Table 1.2: Phase Information

Name	Lattice Size	Constituent
AlCl3	(1)	(AlCl3)
BaCl2_Alpha	(1)	(BaCl2)
BaCl2_Beta	(1)	(BaCl2)
CaAlCl5	(1)(1)	(CaCl2)(AlCl3)
CaBaCl4	(1)(1)	(CaCl2)(BaCl2)

Name	Lattice Size	Constituent
CaCl2	(1)	(CaCl2,MgCl2,UCl3)
CaCl2_LT	(1)	(CaCl2)
CaFeCl5	(1)(1)	(CaCl2)(FeCl3)
Cs2FeCl4	(2)(1)	(CsCl)(FeCl2)
CsCl	(1)	(CsCl)
FCC	(1)	(CsCl,FeCl2,FeCl3,LiCl,NaCl,KCl,MgCl2,CaCl2,RbCl)
FeAl2Cl8	(1)(2)	(FeCl2)(AlCl3)
FeCl3	(1)	(FeCl3)
Gas	(1)	(AlCl3,Al2Cl6,BaCl2,CaCl2,FeCl2,FeCl3,Fe2Cl6,KCl, LiCl,MgCl2,NaCl,ZnCl2,Zn2Cl4,NaAlCl4,KAlCl4, Na2Al2Cl8,K2Al2Cl8)
K2BaCl4	(2)(1)	(KCl)(BaCl2)
K2FeCl4	(2)(1)	(KCl)(FeCl2)
K2MgCl4	(2)(1)	(KCl,LiCl,NaCl,RbCl)(MgCl2)
K3Mg2Cl7	(3)(2)	(KCl)(MgCl2)
K5Zn4Cl13	(5)(4)	(KCl)(ZnCl2)
KAlCl4	(1)(1)	(KCl)(AlCl3)
KCaCl3_HT	(1)(1)	(KCl)(CaCl2)
KFeCl3	(1)(1)	(KCl)(FeCl2)
KFeCl4_L	(1)(1)	(KCl)(FeCl3)
KZn2Cl5	(1)(2)	(KCl)(ZnCl2)
Li2FeCl4	(2)(1)	(LiCl)(FeCl2)
Li2FeCl4_H	(2)(1)	(LiCl)(FeCl2)
Li6FeCl8	(6)(1)	(LiCl)(FeCl2)
LiAlCl4	(1)(1)	(LiCl)(AlCl3)
LiCs2Cl3	(1)(2)	(LiCl)(CsCl)
LiKMgCl4	(1)(1)(1)	(LiCl)(KCl)(MgCl2)

Name	Lattice Size	Constituent
LiRbCl2	(1)(1)	(LiCl)(RbCl)
Liquid	(1)	(AlCl3,Al2Cl6,BaCl2,CsCl,FeCl2,FeCl3,LiCl,NaCl, KCl,MgCl2,CaCl2,RbCl,UCl3,PuCl3,ZnCl2,CaAl2Cl8, MgAl2Cl8,Cs2FeCl4,FeAl2Cl8,CaFe2Cl8,KFeCl4, LiFeCl4,MgFe2Cl8,NaFeCl4,KAlCl4,K2MgCl4, KMgCl3,K2ZnCl4,LiAlCl4,NaAlCl4,NaMgCl3, Na2MgCl4,Na2ZnCl4)
M2BaCl4	(2)(1)	(CsCl,RbCl)(BaCl2)
M2ZnCl4	(2)(1)	(KCl,NaCl)(ZnCl2)
MCl2	(1)	(FeCl2,LiCl,MgCl2,FeCl3)
MCl3	(1)	(UCl3,PuCl3,CaCl2)
MFeCl4	(1)(1)	(KCl,LiCl)(FeCl3)
MgAl2Cl8	(1)(2)	(MgCl2)(AlCl3)
MgBa2Cl6	(1)(2)	(MgCl2)(BaCl2)
MgFe2Cl8	(1)(2)	(MgCl2)(FeCl3)
Na2MgCl4	(2)(1)	(NaCl)(FeCl2,MgCl2)
NaAlCl4	(1)(1)	(NaCl)(AlCl3)
NaFeCl4	(1)(1)	(NaCl)(FeCl3)
Perovskite_c	(1)(1)	(CsCl,KCl,RbCl)(BaCl2,CaCl2)
Perovskite_h	(1)(1)	(CsCl,RbCl)(FeCl2,MgCl2)
Perovskite_o	(1)(1)	(KCl,LiCl,NaCl)(CaCl2,MgCl2)
Rb2PuCl5	(2)(1)	(RbCl)(PuCl3)
Rb2UCl5	(2)(1)	(RbCl)(UCl3)
Rb3PuCl6_alpha	(3)(1)	(RbCl)(PuCl3)
Rb3PuCl6_beta	(3)(1)	(RbCl)(PuCl3)
Rb3UCl6	(3)(1)	(RbCl)(UCl3)

Name	Lattice Size	Constituent
RbPu2Cl7_alpha	(1)(2)	(RbCl)(PuCl3)
RbPu2Cl7_beta	(1)(2)	(RbCl)(PuCl3)
RbUCl4	(1)(1)	(RbCl)(UCl3)
ZnCl2	(1)	(ZnCl2)

Sub-System Information

Complete thermodynamic descriptions are developed for the assessed **57** binary systems and **4** ternary systems as listed in Table 1.3 and Table 1.4.

Table 1.3: Current Status of Binary Systems

	BaCl2	CaCl2	CsCl	FeCl2	FeCl3	LiCl	KCl	MgCl2	NaCl	PuCl3	RbCl	UCl3	ZnCl2
AlCl3		■		■		■	■	■	■				■
BaCl2		■	■			■	■	■	■		■		
CaCl2			■	■	■	■	■	■	■	■	■	■	■
CsCl							■		■		■		
FeCl2							■	■					
FeCl3						■	■	■	■				
LiCl							■	■	■	■	■	■	■
KCl								■	■		■		■
MgCl2									■		■		■
NaCl											■		■
PuCl3											■		
RbCl												■	
UCl3													

Table 1.4: Current Status of Ternary Systems

BaCl2-CaCl2-KCl	BaCl2-CaCl2-NaCl	BaCl2-MgCl2-NaCl	KCl-NaCl-ZnCl2

Database Validation

Figure 1.1 shows the calculated NaCl-$AlCl_3$ binary system, which is in accord with the experimental data. Figure 1.2 and Figure 1.3 show the calculated liquidus lines through different isopleths and liquidus projection for KCl-NaCl-$ZnCl_2$ ternary system.

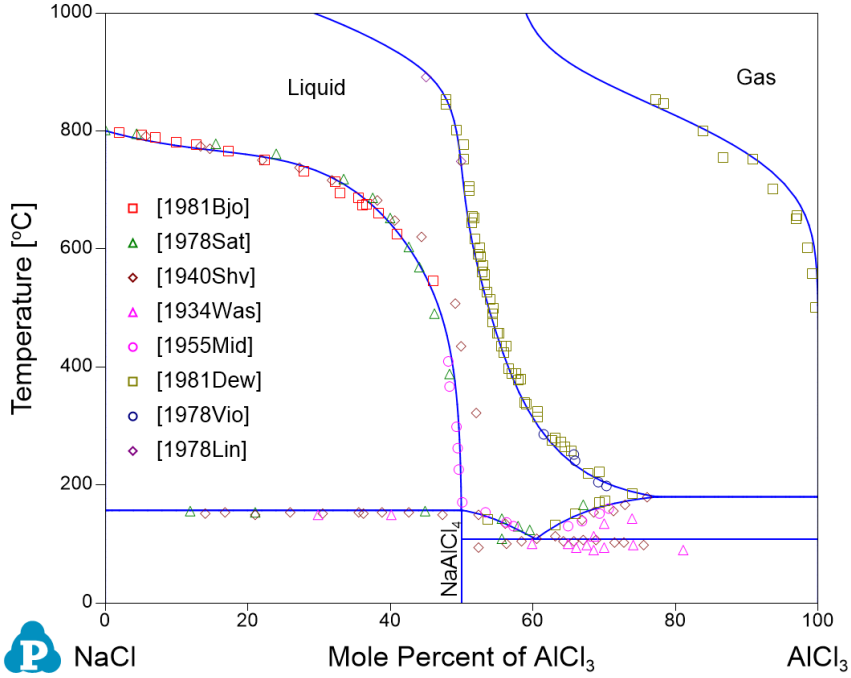


Figure 1.1: Calculated NaCl-$AlCl_3$ binary system compared with the experimental data [1934Was, 1940Shv, 1955Mid, 1978Lin, 1978Sat, 1978Vlo, 1981Bjo, 1981Dew].

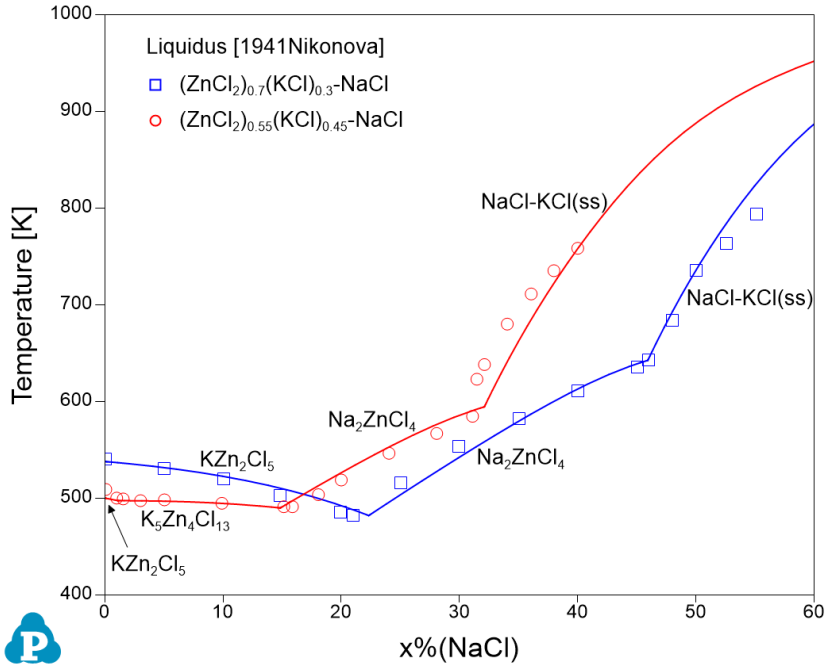


Figure 1.2: Calculated Liquidus lines through ternary isopleths compared with the experimental data [1941Nik].

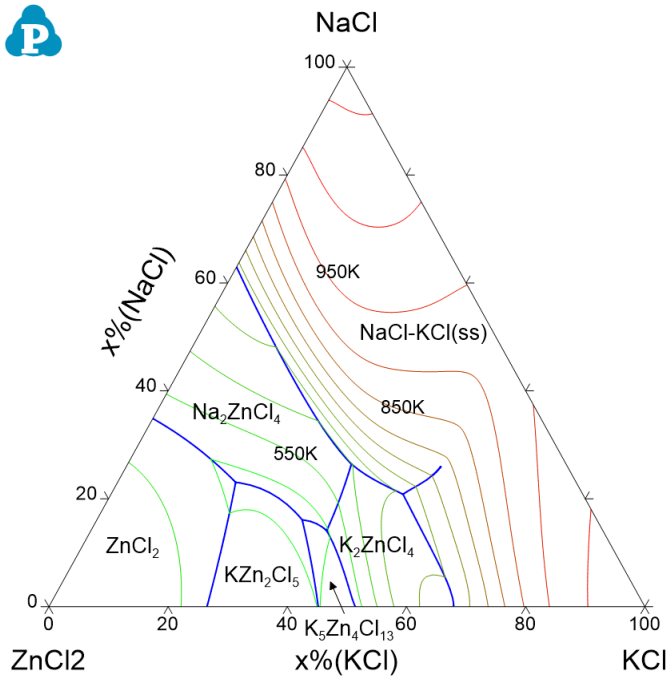


Figure 1.3: Calculated Liquidus projection of KCl-NaCl-$ZnCl_2$ ternary system.

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