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FORSCHUNGSZENTRUM

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Database development for the HotVeGas project

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HOTVEGAS
Hochtemperaturvergasung und Gasreinigung

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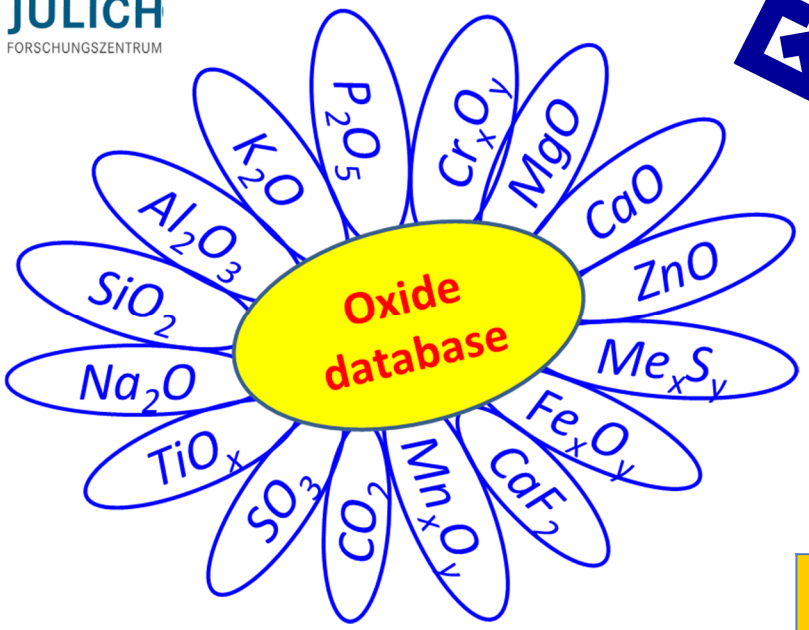
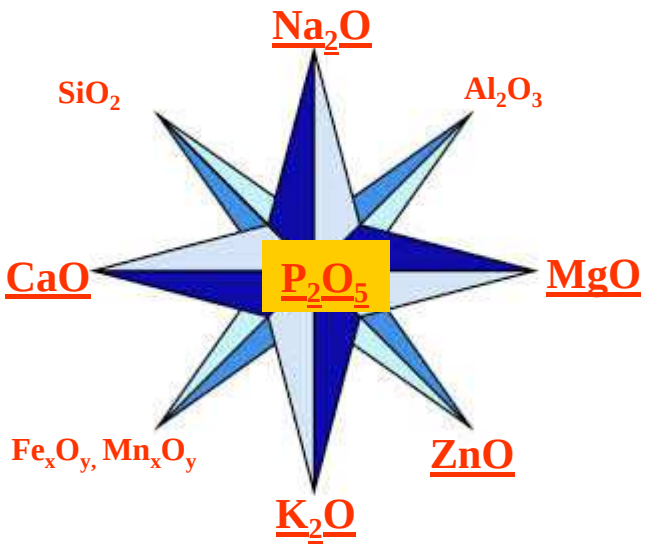
Oxide system





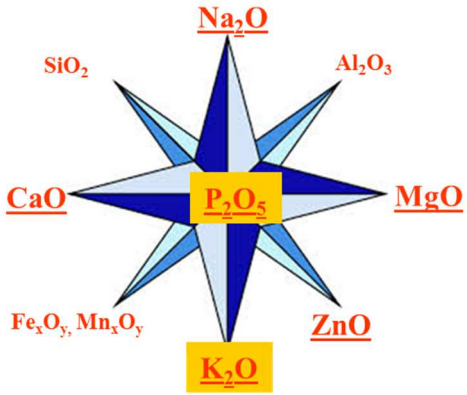
Oxide database	Slag atlas (12.0) March 2017
Binary systems	130
Ternary systems	110
Quaternaries	7
Slag components	166
Solid solution phases	104
Stoichiometric compounds	661

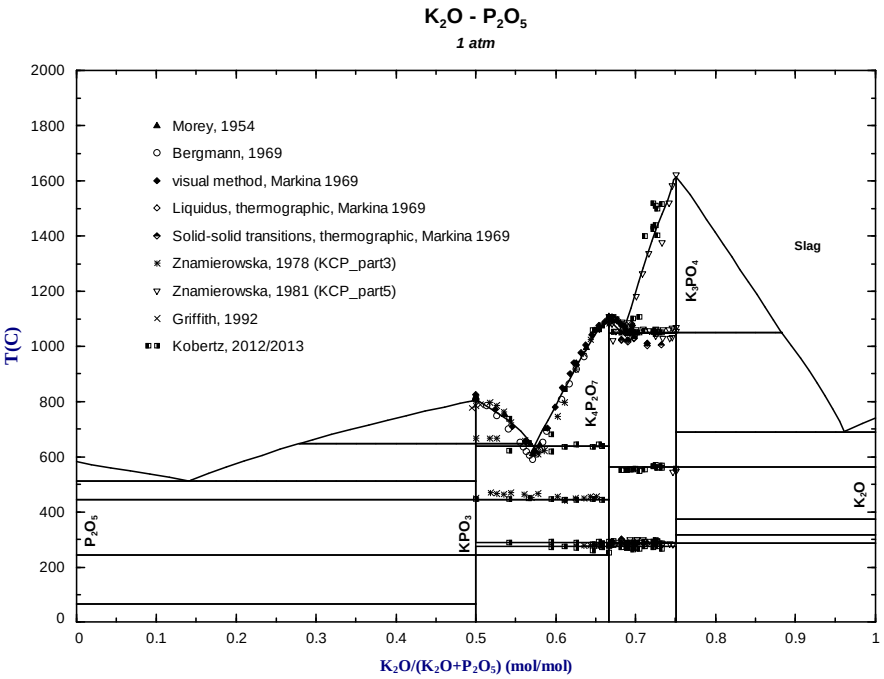
HOTVEGAS
Hochtemperaturvergasung und Gasreinigung

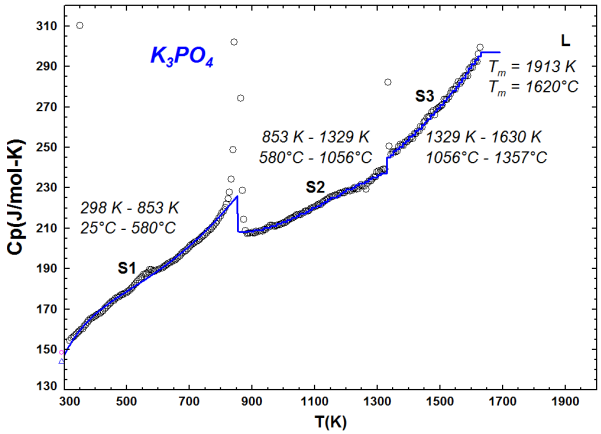
Data revision: K_2O-P_2O_5

Revision of the binary data on the alkali-phosphor oxides systems due to new experimental information:

- Cp (DSC), ΔH_{tr} of pure AlkPOx along with phase equilibria (DTA/TG)
- properties from literature: ΔH_{mix} of liquid, Q-species
- Structure units distribution is a basis of viscosity modelling







Data revision: Na_2O-P_2O_5

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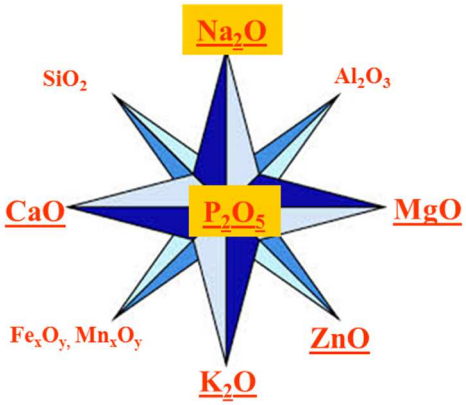
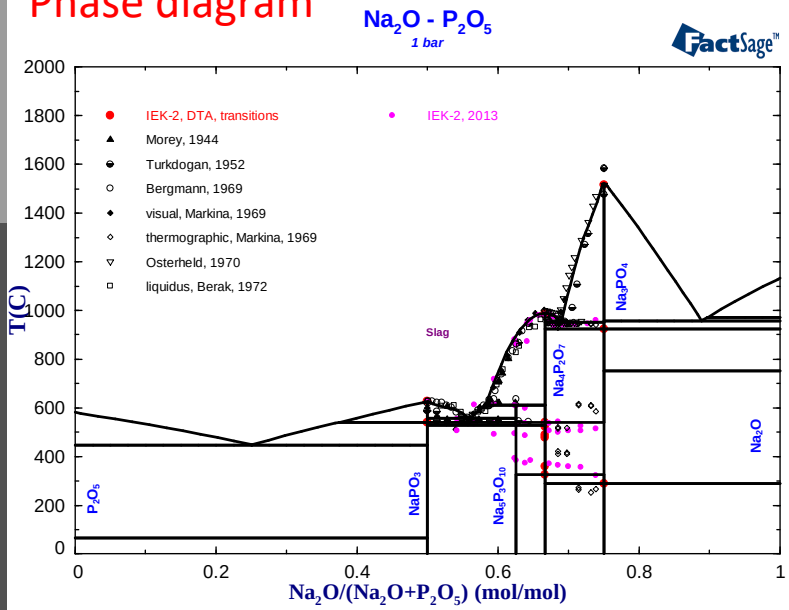
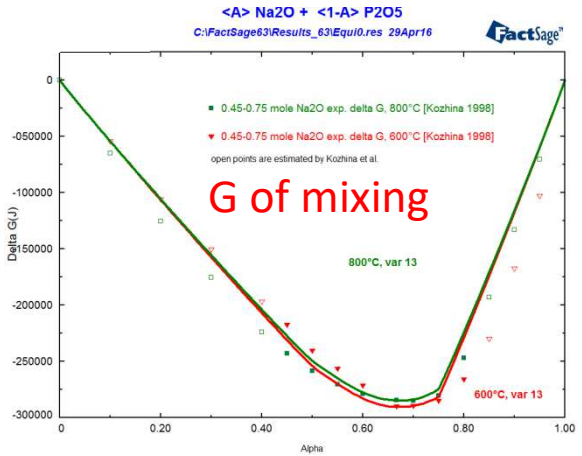
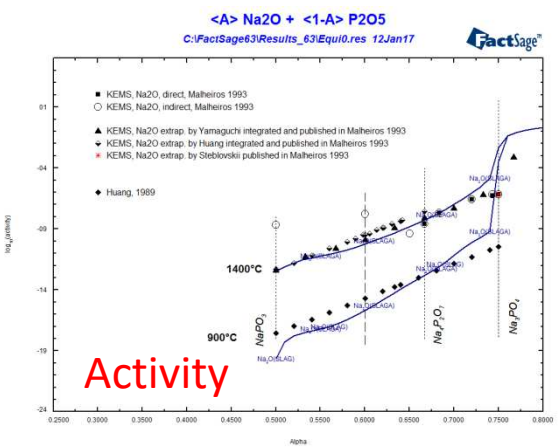
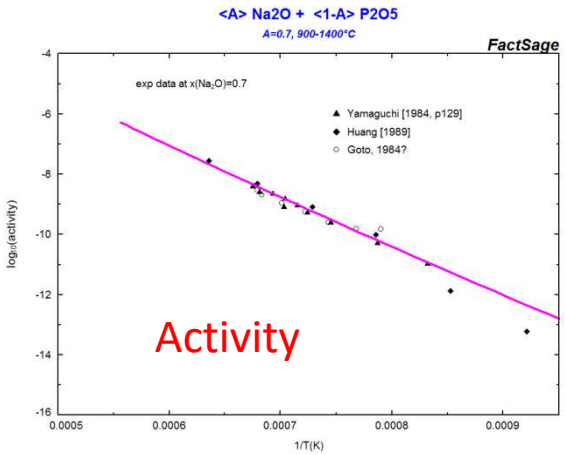


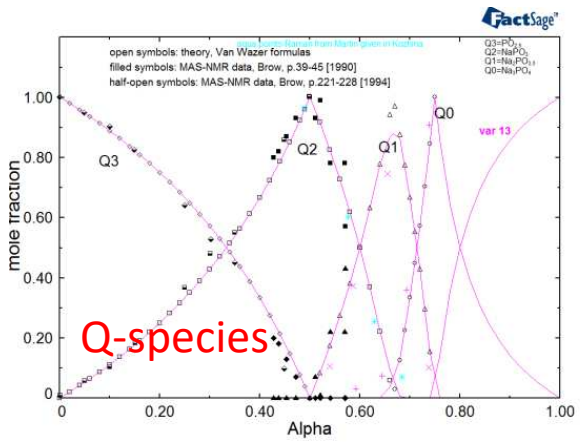
Phase diagram





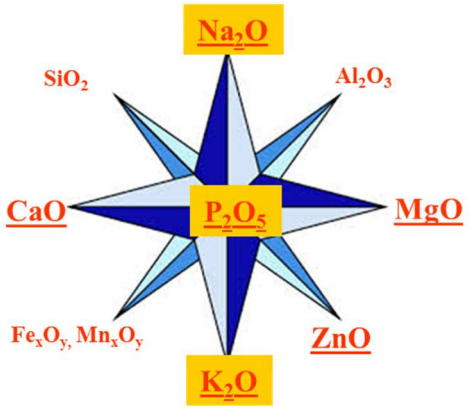






Q-species

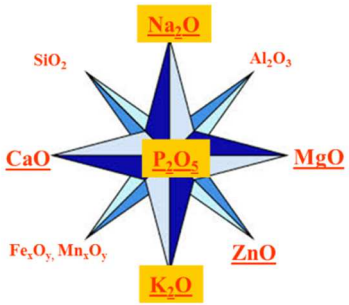
Description of the system

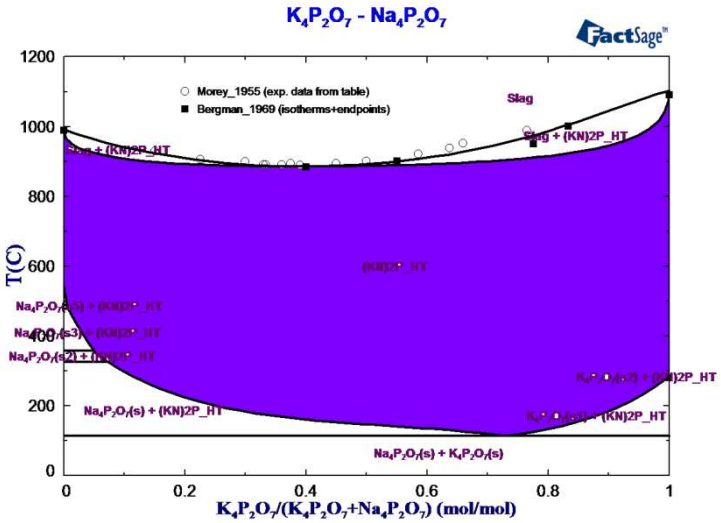


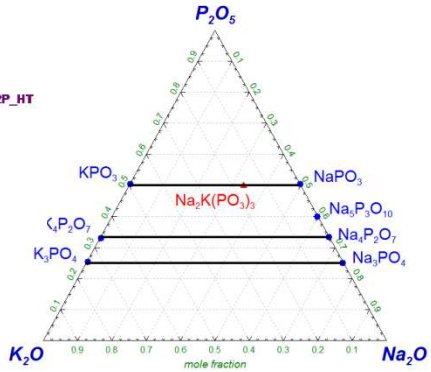
Phase	Model	Description
Liquid	Modified associate species	Alk_2O, P_2O_5 Alk_2O:P_2O_5=1:1 $AlkPO_3$ Alk_2O:P_2O_5=2:1 $Alk_4P_2O_7$*1/3 Alk_2O:P_2O_5=3:1 Alk_3PO_4*1/2
KP_H, KPO_3(HT)-$NaPO_3$(HT)	Sublattice model	$(\underline{K^{1+}}, Na^{1+})(P^{5+})(O^{2-})_3$
NP_H, $NaPO_3$(HT)-KPO_3(HT)	Sublattice model	$(K^{1+}, \underline{Na^{1+}})(P^{5+})(O^{2-})_3$
KN2P, $Na_4P_2O_7$(HT)-$K_4P_2O_7$(HT)	Sublattice model	$(K_2O, Na_2O)_2(P_2O_5)$
N3PH, Na_2PO_4-K_3PO_4, ht-phase	Sublattice model	$(Na_2O,K_2O)_2(P_2O_5)(Na_2O)$: $2N3P+K_4Na_2P_2O_8$
K3PH, K_2PO_4-Na_3PO_4, ht-phase	Sublattice model	$(K_2O)_2(P_2O_5)(K_2O, Na_2O)$: $2K3P+K_4Na_2P_2O_8$

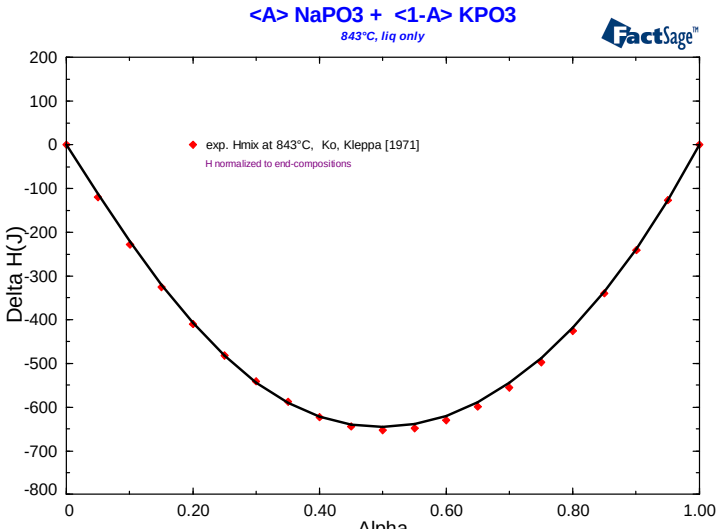
The system K_2O-Na_2O-P_2O_5

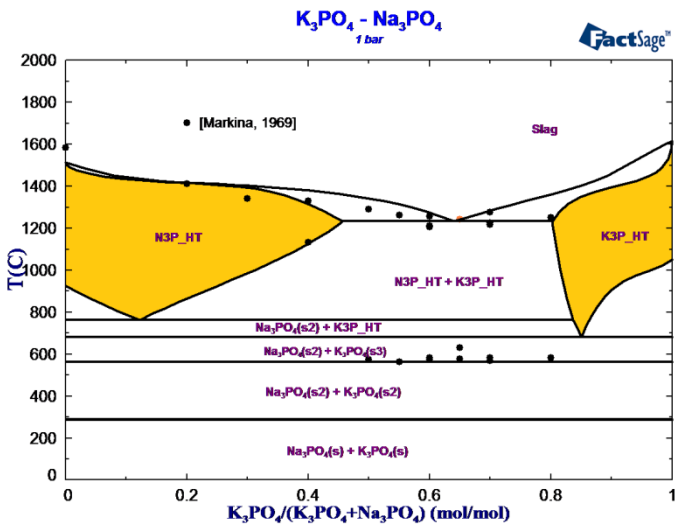
Quasi-binary sections

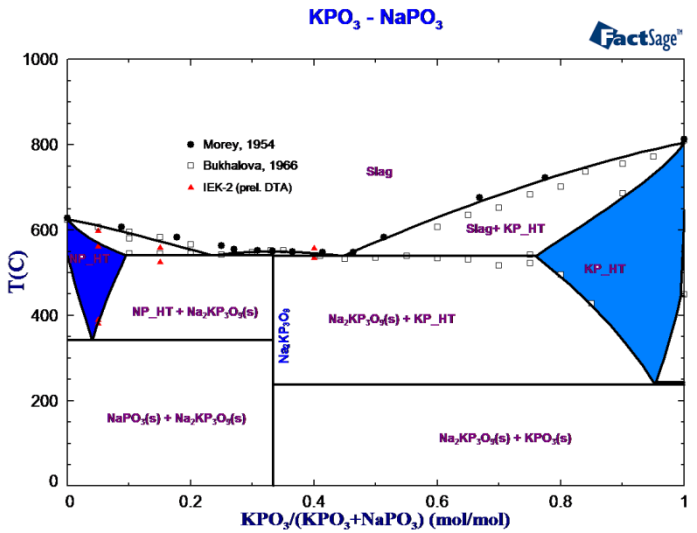






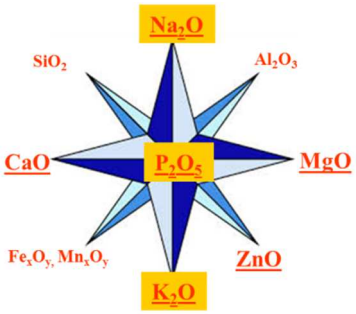


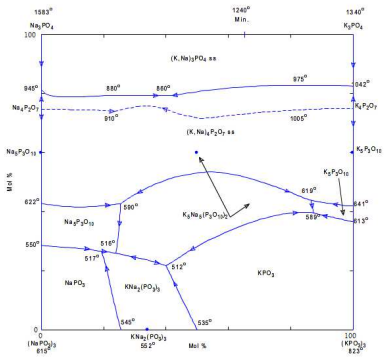




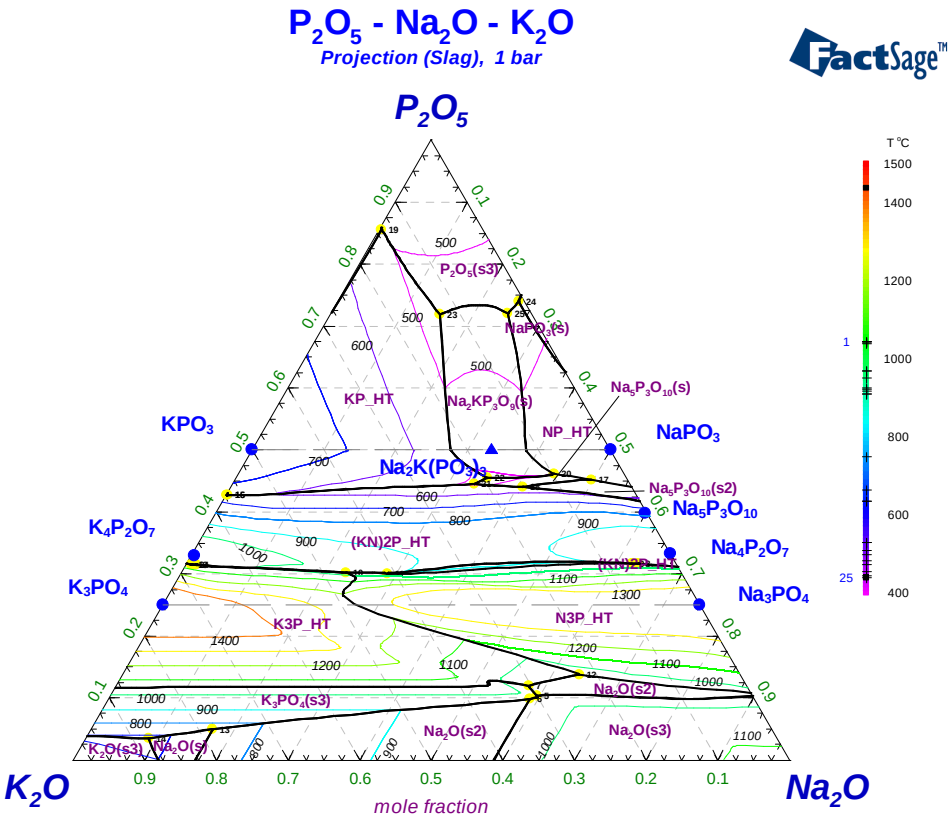
The system K_2O-Na_2O-P_2O_5

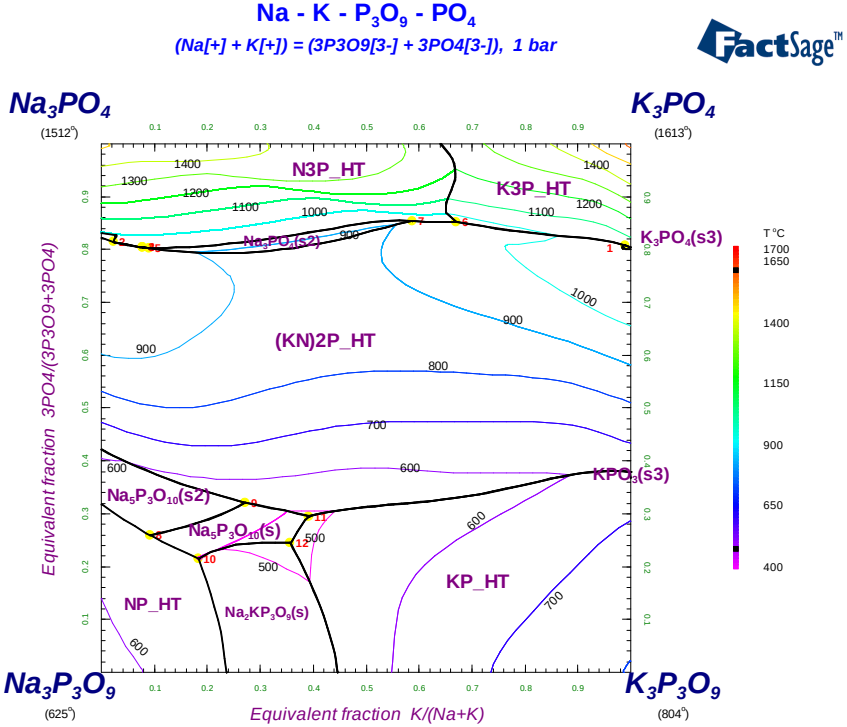
Liquidus surface





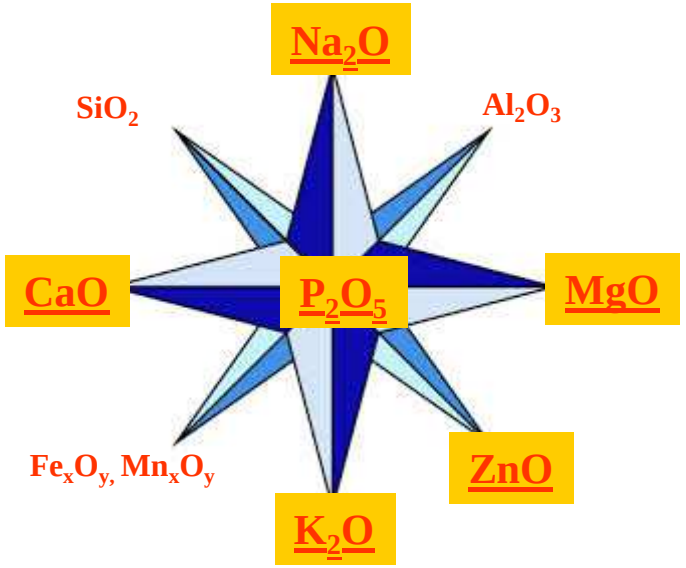
I.B.Markina,N.K. Voskresenskaya, *Zh. Neorg. Khim.*, **14** [8] 2263-2269 (1969); *Russ. J. Inorg. Chem. (Engl. Transl.)*, **14** [8] 1188-1192 (1969).

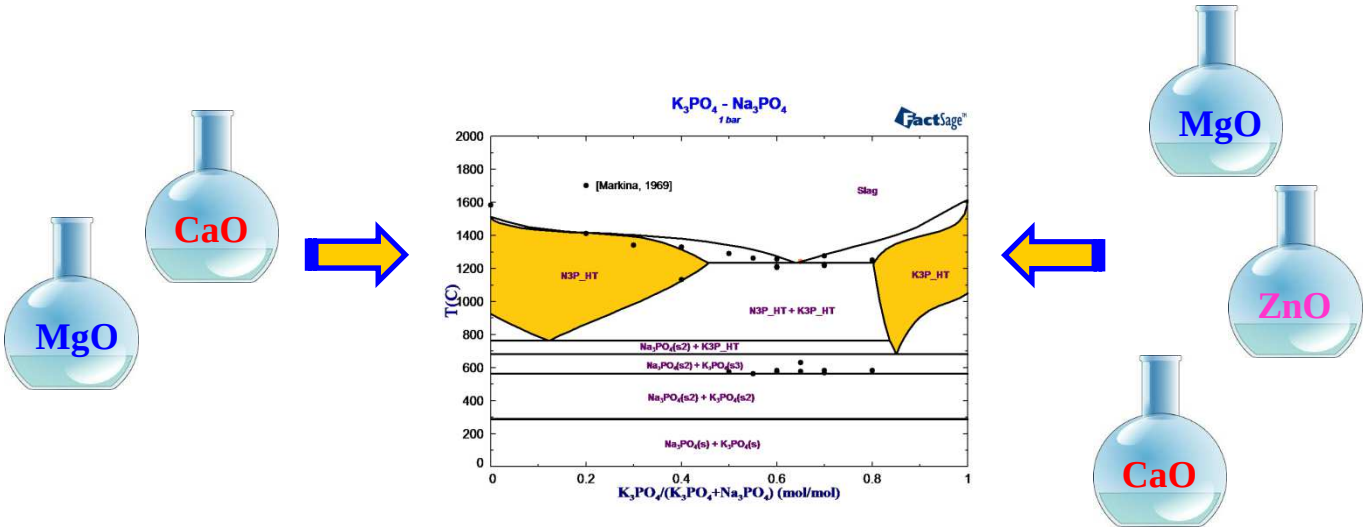




Oxide system

After re-assessment of the binary systems all ternary systems have to be considered taking into account the solubility in solid state





- Na_2O-K_2O-P_2O_5
- K_2O-CaO-P_2O_5
- K_2O-MgO-P_2O_5
- K_2O-ZnO-P_2O_5
- Na_2O-CaO-P_2O_5
- Na_2O-MgO-P_2O_5
- Na_2O-ZnO-P_2O
- Al_2O_3-Na_2O-P_2O
- Al_2O_3-K_2O-P_2O

Description of the system

The species with composition $KCa(PO_3)_3$ in the non-ideal associate solution were added in order to describe the liquid phase

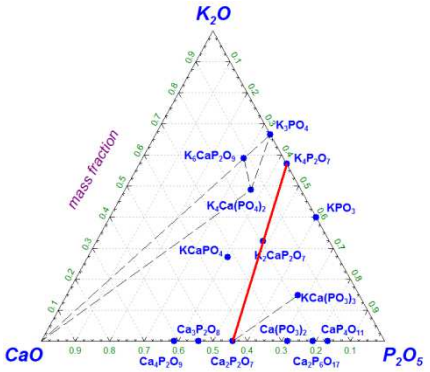
Name	Composition	Tm, calc. (exp.), °C	Liquid species
CKP	$K_2CaP_2O_7$	1149 (1143)	
C2KP3	$KCa(PO_3)_3$	850 (850)	$KCaP_3O_9$/2.5
C2KP	$KCaPO_4$	1559 (1560)	
	*$K_6CaP_2O_9$	1745 (1750)	
	*$K_4CaP_2O_8$	1647 (1645)	
* - solid solution component			

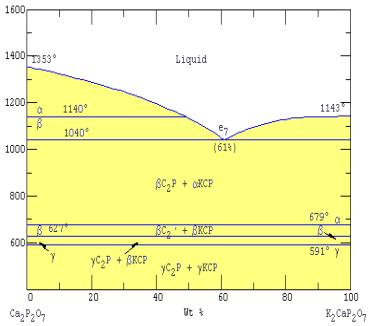
$(\underline{K_2})_2(\underline{K_2}, Ca, K_2CaO, Na_2, Mg, K_2MgO)_1 (PO_4)_2$

solid solutions for HT, MT, LT modifications

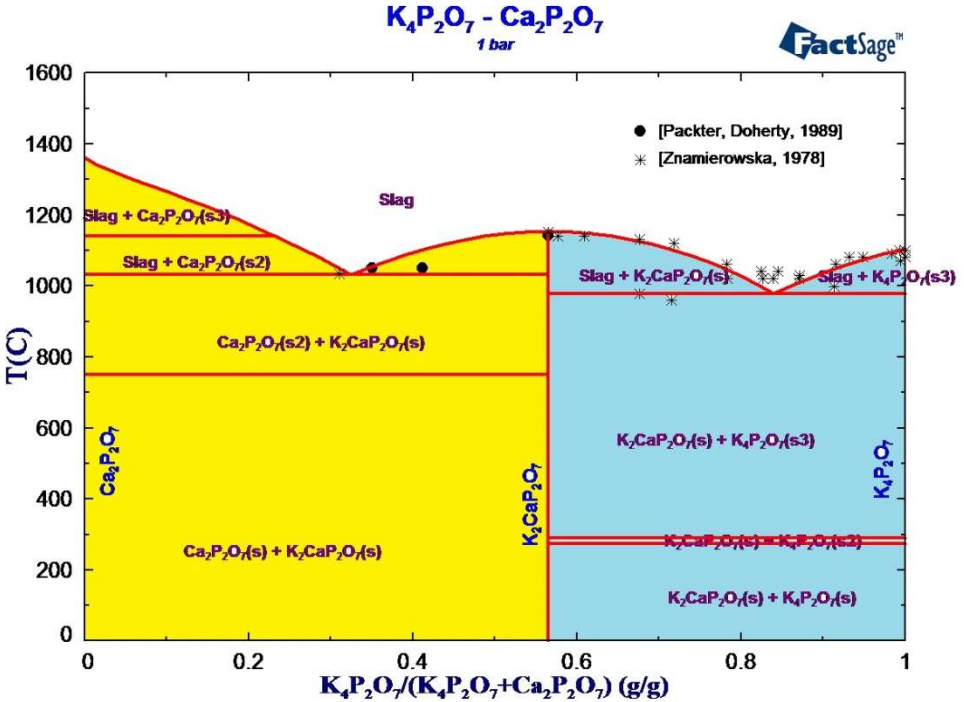
$(\underline{K_2O})_2(P_2O_5)(\underline{K_2O}, CaO, K_2CaO_2, Na_2O, MgO, K_2MgO_2)$

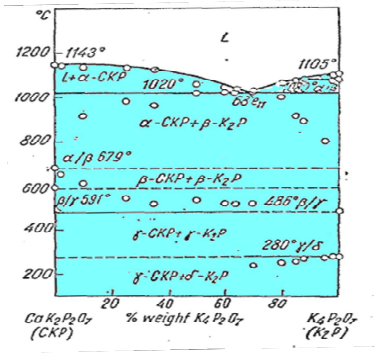
Quasi-binary section $K_4P_2O_7$-$Ca_2P_2O_7$





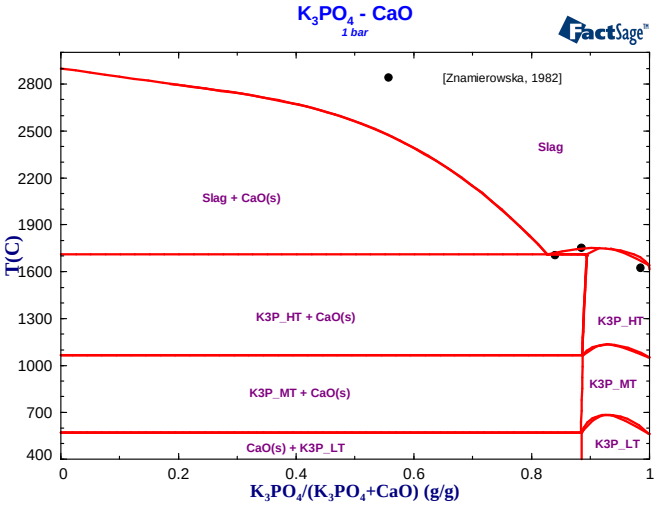
T. Znamierowska, Pol. J. Chem., 52 [6] 1127-1134 (1978).

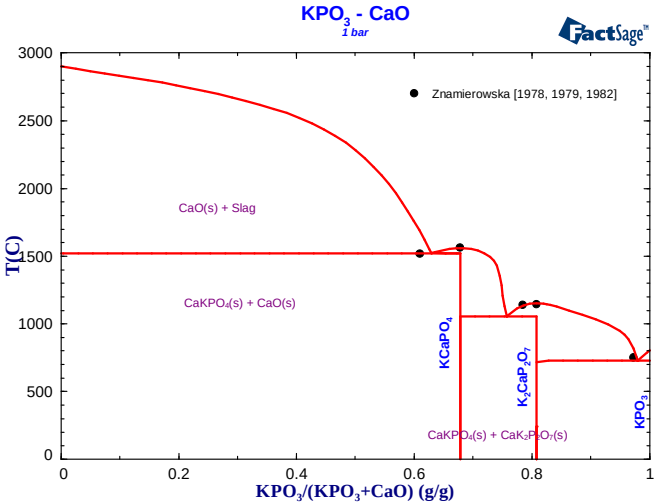


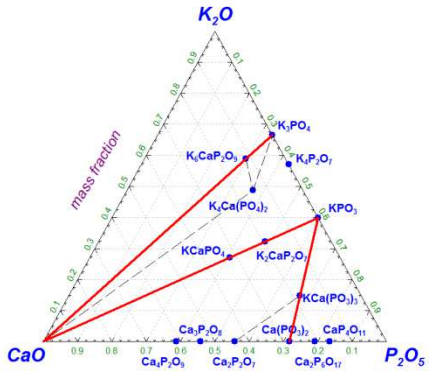


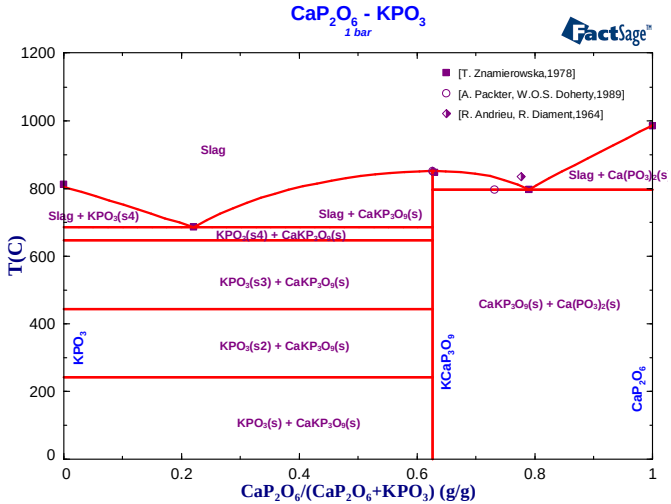
Znamierowska, Pol. J. Chem., 52 [10] 1889-1895 (1978)

Sections CaO-K3P, CaO-KP, CP-KP

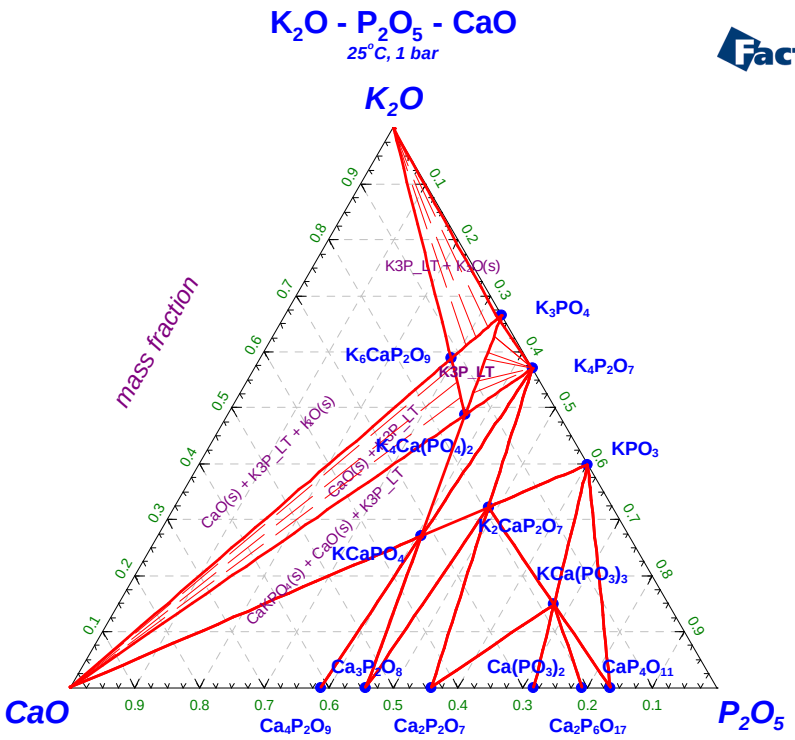


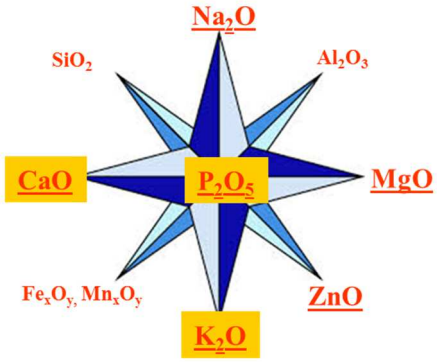


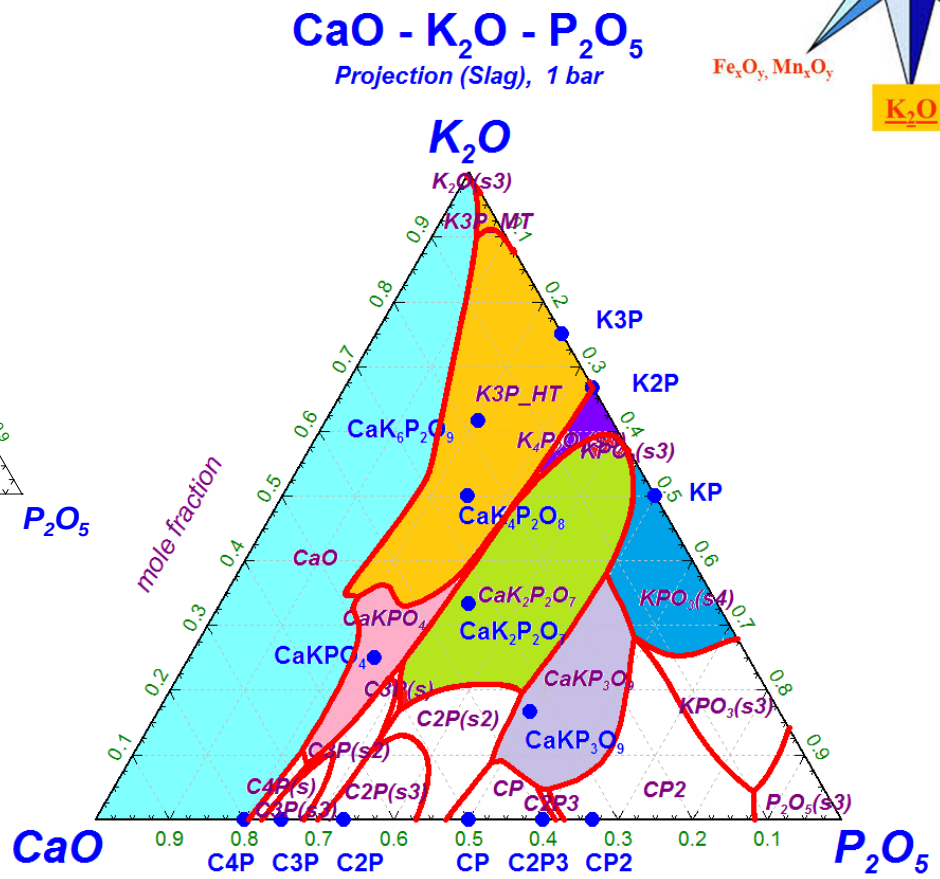




Sub-solidus equilibria and liquidus surface







Description of the system

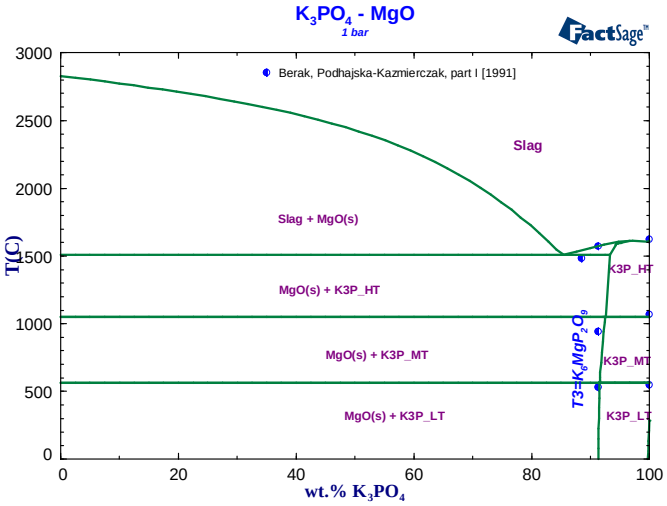
Name	Composition	Tm, calc. (exp.), °C	Liquid species
R	$KMgPO_4$	1520 (1520)	$KMgPO_4$/1.5
J	$KMg_4(PO_4)_3$	1169 (1175)	
W	$K_4Mg_4P_6O_{21}$	790 (792)	
T1	$K_2MgP_2O_7$	733 (736)	
T2	*$K_4Mg(PO_4)_2$	1375 (1374)	
T3	*$K_6MgP_2O_9$	1570 (1570)	
B1	$KMg(PO_3)_3$	904 (906)	$KMgP_3O_9$/2.5
B2	$K_2Mg(PO_3)_4$	734 (730)	
* - solid solution component			

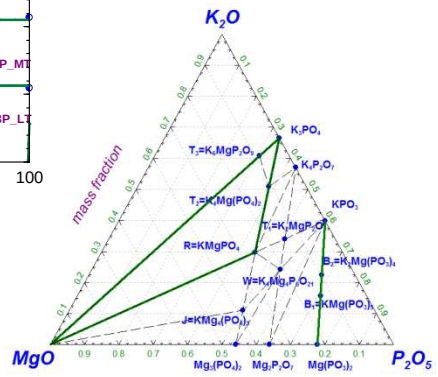
$(\underline{K_2})_2(\underline{K_2}, Ca, K_2CaO, Na_2, Mg, K_2MgO)_1 (PO_4)_2$

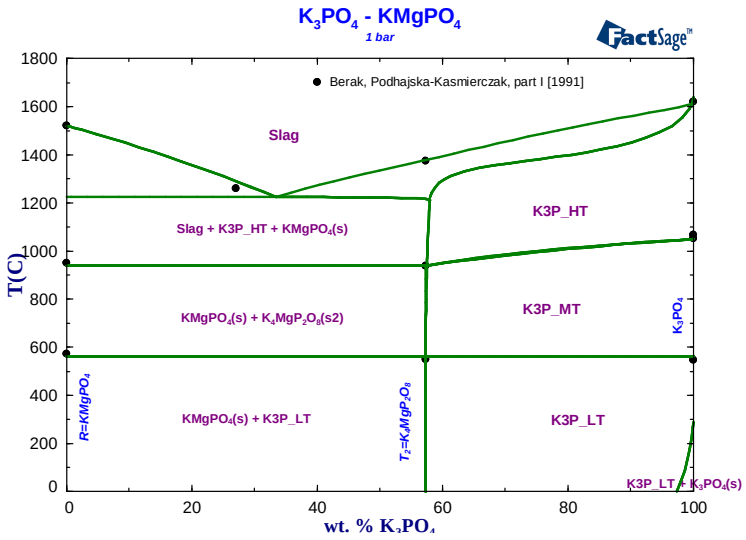
solid solutions for HT, MT, LT modifications

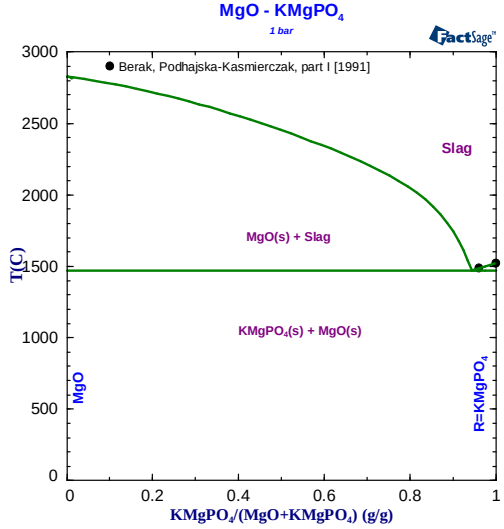
$(\underline{K_2O})_2(P_2O_5)(\underline{K_2O}, CaO, K_2CaO_2, Na_2O, MgO, K_2MgO_2)$

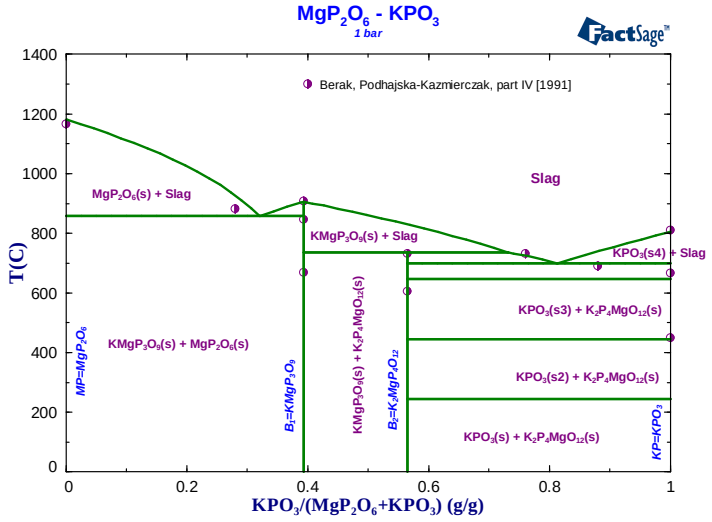
Quasi-binary sections



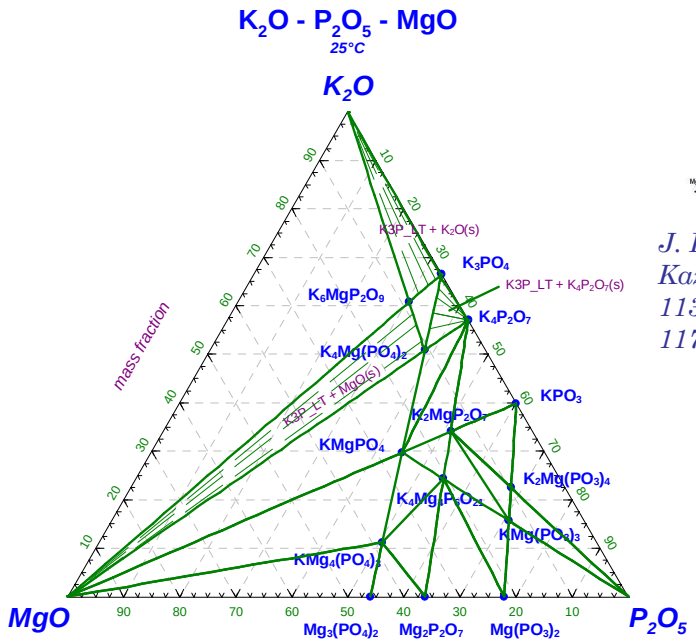




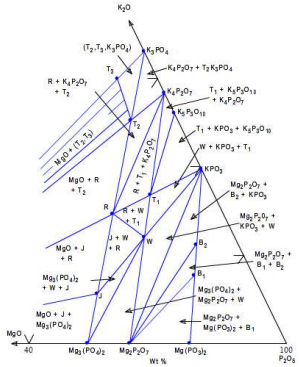




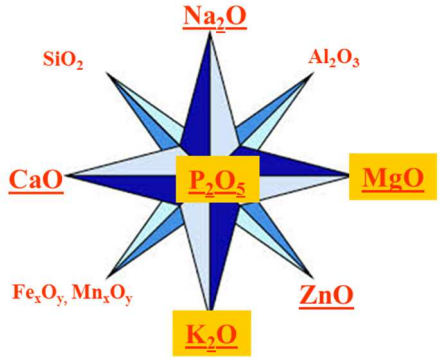
Sub-solidus equilibria and liquidus surface

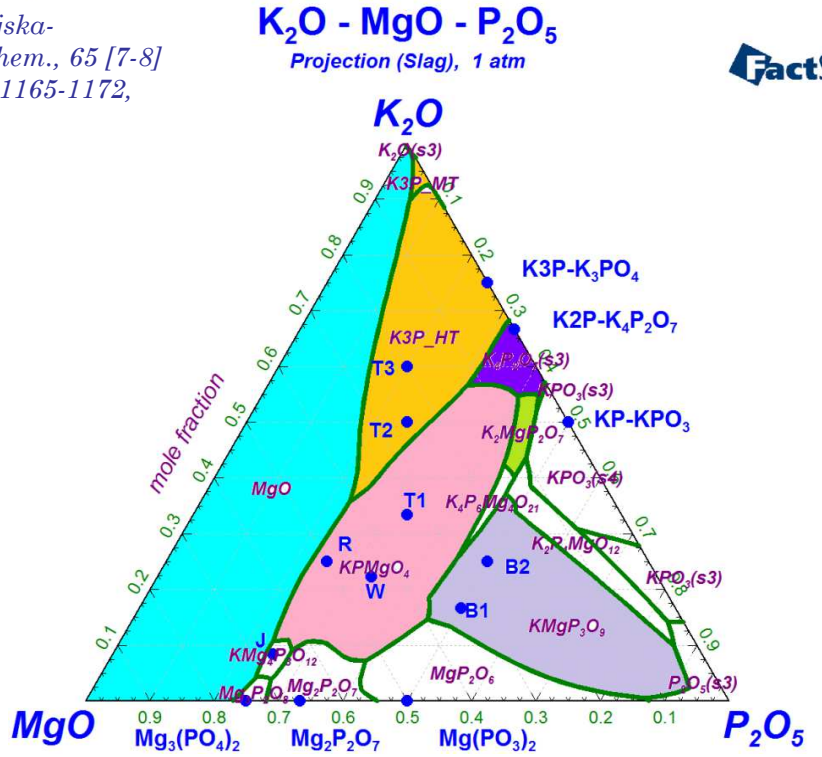


Solid state compatibility observed at room temperature



J. Berak and T. Podhajska-Kazmierczak, Pol. J. Chem., 65 [7-8] 1137-1149, 1151-1163, 1165-1172, 1173-1184 (1991)



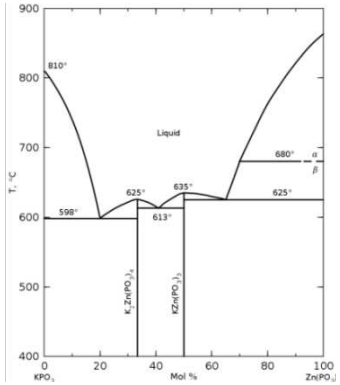


Description of the system

The species with composition D in the non-ideal associate solution were added in order to describe the liquid phase.

Name	Composition	Tm, calc. (exp.), °C	Liquid species
A	$K_2Zn(PO_3)_4$	625 (625)	
B	$KZn_4(PO_3)_3$	964 (965)	
C	$KZn(PO_3)_3$	632 (632)	
D	$KZnPO_4$	1346 (≈1354)	$KZnPO_4$/1.5
E	$K_2ZnP_2O_7$	683 (683)	
F	$K_2Zn_3(P_2O_7)_2$	800 (800)	

Quasi-binary section KPO_3-ZnP_2O_6



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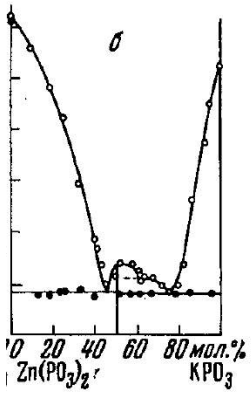
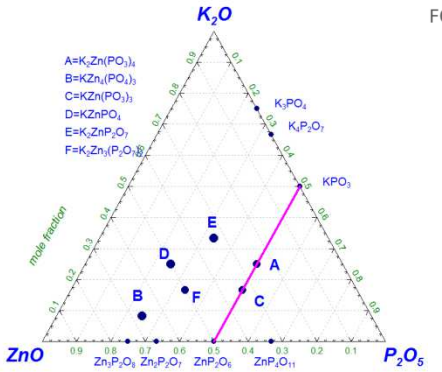
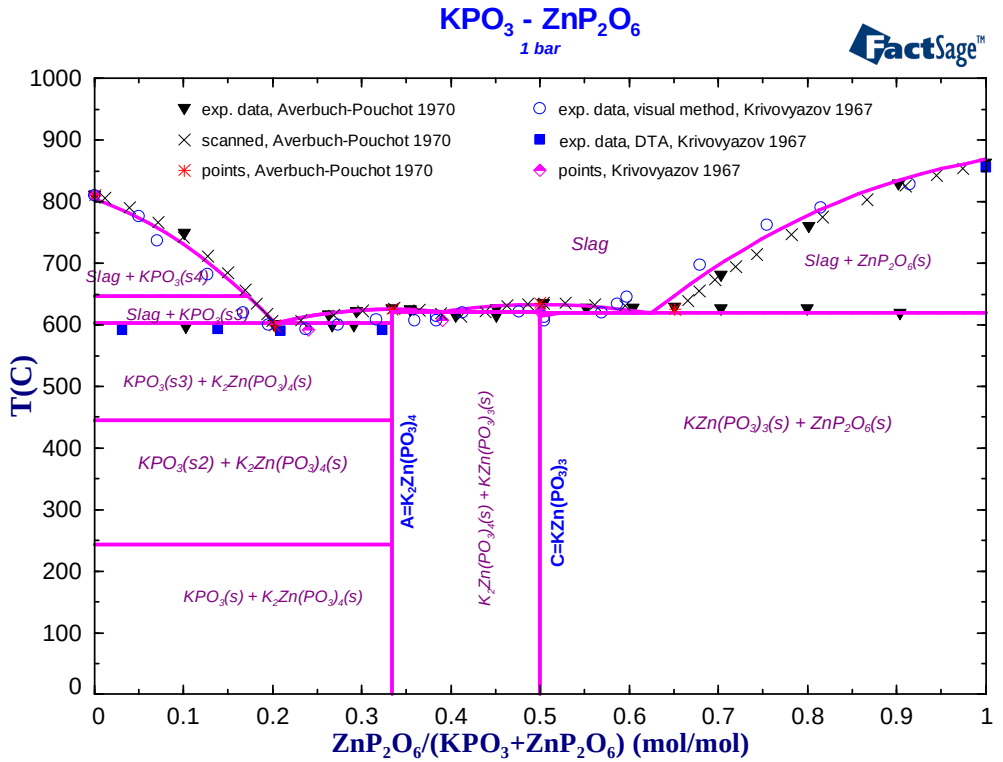
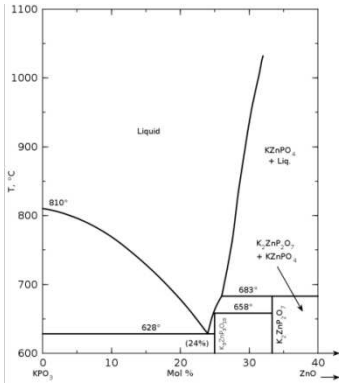


E.L. Krivovjasov, K.K. Palkina, N.K. Voskresenskaja, Dokl. Akad. Nauk, UdSSR, Chem., 174 [3] 610-613 (1967)





Sections KPO_3-ZnO and B-ZnO



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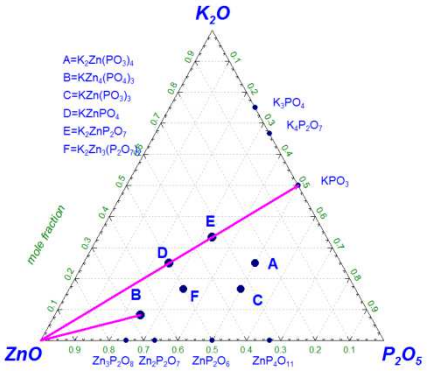
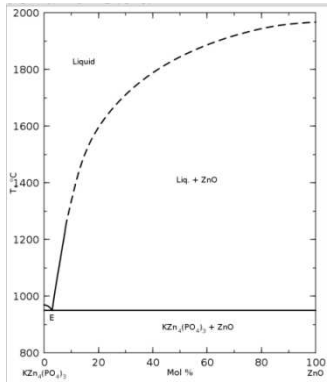
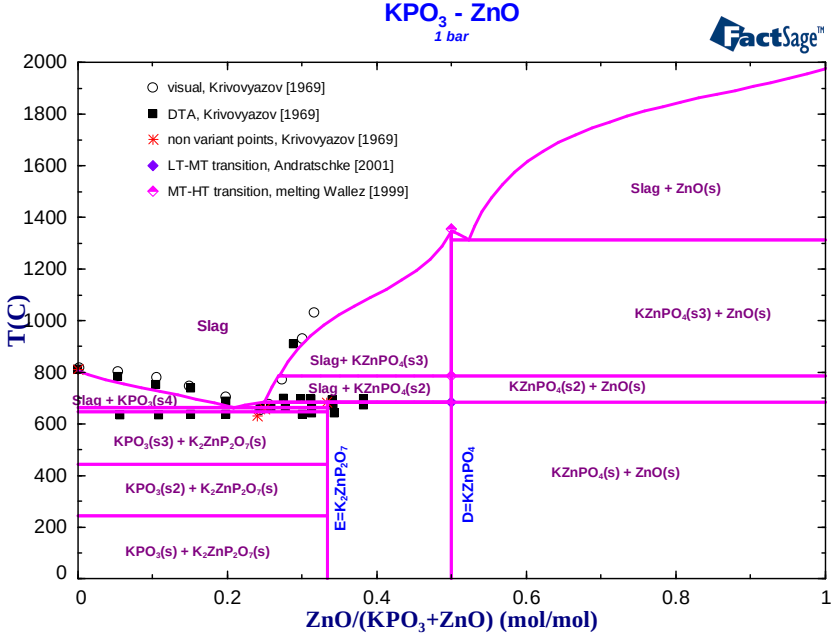
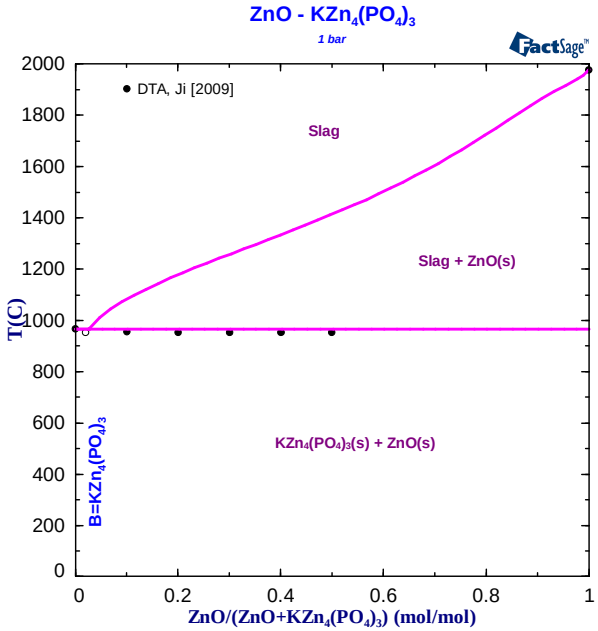




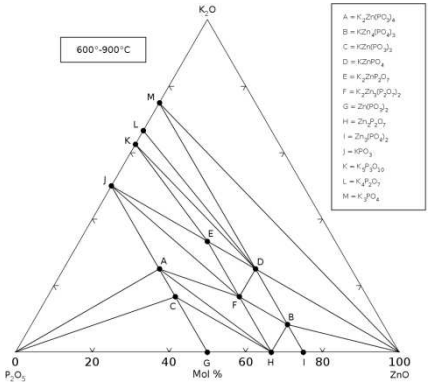
*L. N. Ji, J. B. Li, J. Luo, J. K. Liang, Y. H. Liu, J. Y. Zhang, and G. H. Rao, J. Alloys Compd., **470** [1-2] 336-339 (2009).*

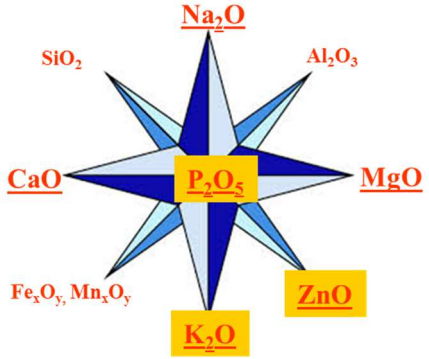


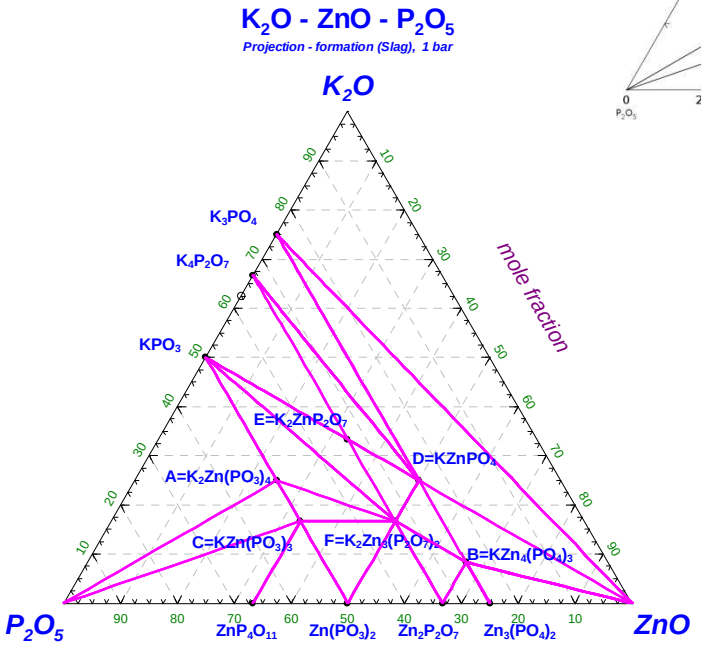


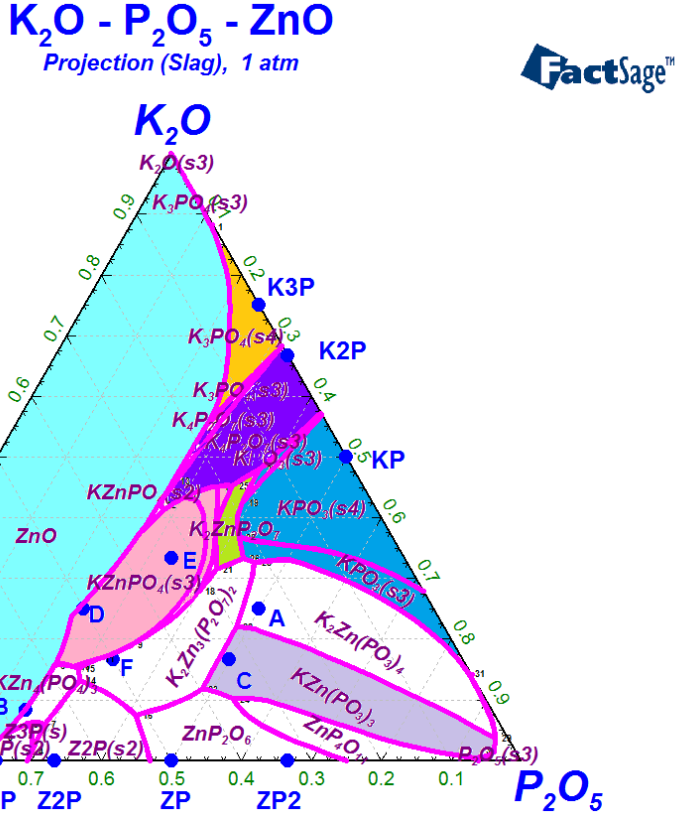
Sub-solidus and liquidus surface

L. N. Ji, J. B. Li, J. Luo, J. K. Liang, Y. H. Liu, J. Y. Zhang, and G. H. Rao, J. Alloys Compd., 470 [1-2] 336-339 (2009).









Description of the system

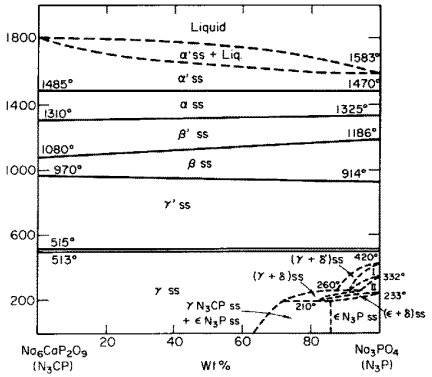
Name	Composition	Tm, calc. (exp.), °C	Liquid species
CNP	$Na_2CaP_2O_7$	835 (814)	
C2NP	$NaCaPO_4$	1830 (1830)	$NaCaPO_4$/1.5
CN2P	$Na_4CaP_2O_8$	1756 (1750)	$Na_4CaP_2O_8$/3.5
CN2P3	$Na_4CaP_6O_{18}$	734 (733)	
	*$Na_6CaP_2O_9$	1800 (1800)	
* - solid solution component			

$(\underline{Na_2}, K_2, Zn)_2(\underline{Na_2}, Na_2CaO, Mg, Na_2MgO)_1 (PO_4)_2$

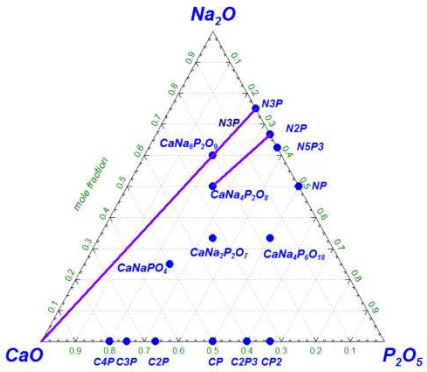
solid solutions for HT, MT, LT modifications

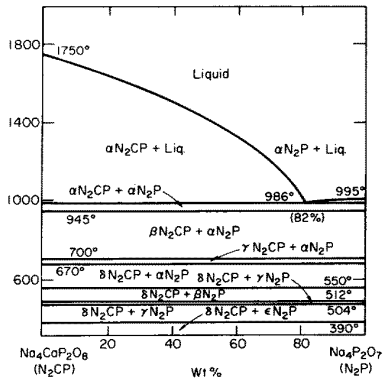
$(\underline{Na_2O}, K_2O, ZnO)_2(P_2O_5)(\underline{Na_2O}, Na_2CaO_2, MgO, Na_2MgO_2)$

Sections CaO-N3P and N2P-CN2P

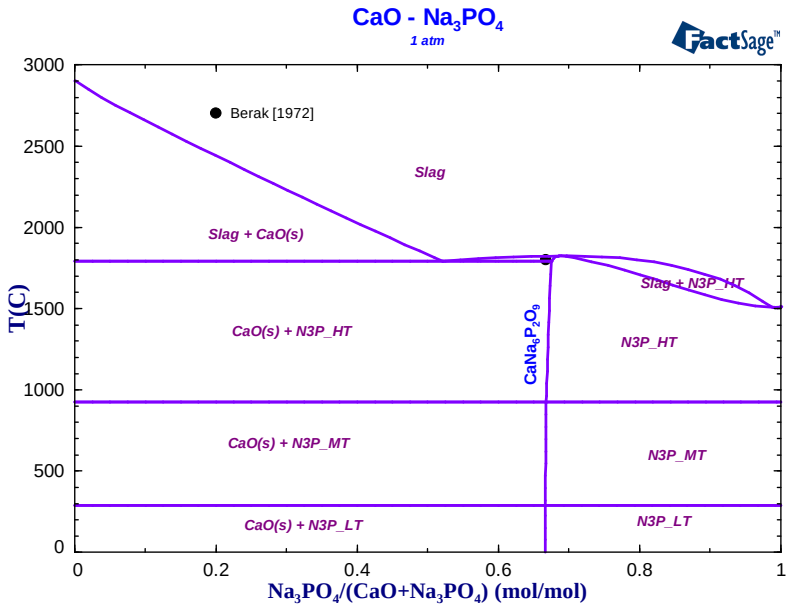


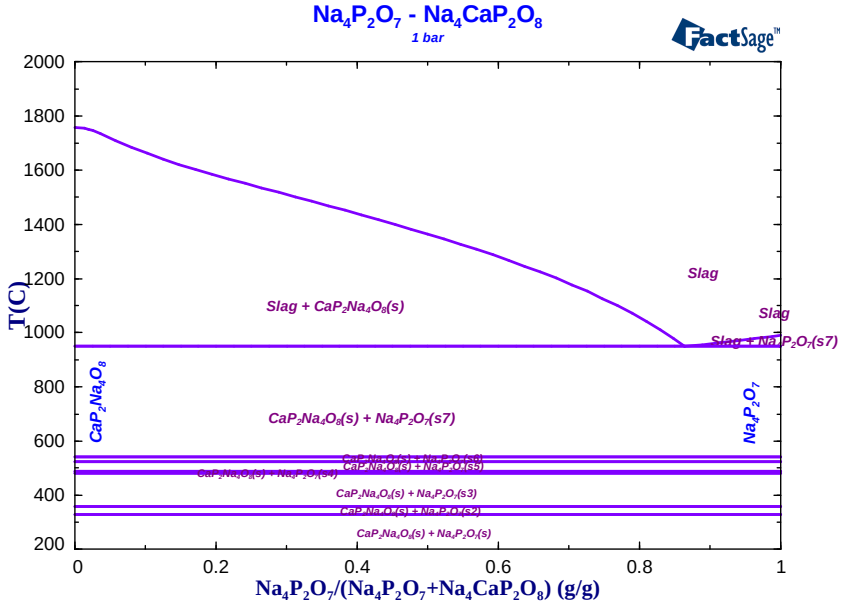
J. Berak and T. Znamierowska, Rocz. Chem., 46 [10] 1697-1708 (1972).



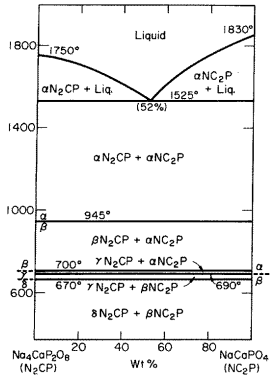


J. Berak and T. Znamierowska, Rocz. Chem., 46 [10] 1697-1708 (1972).





Quasi-binary sections



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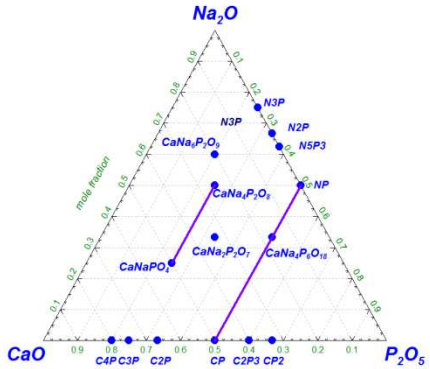

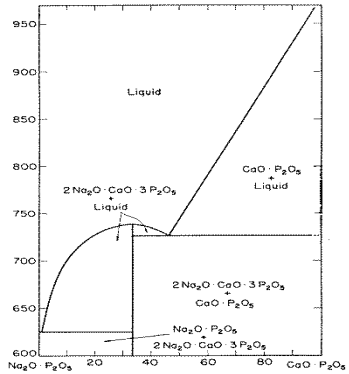

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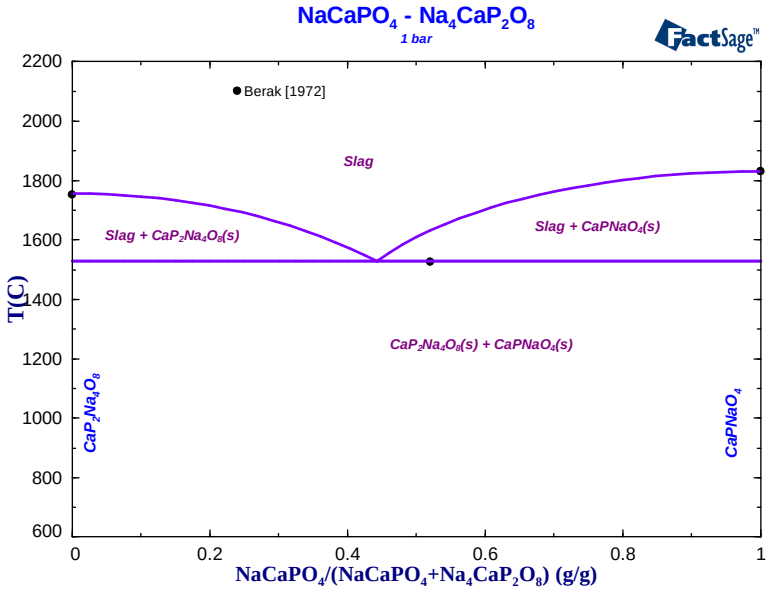
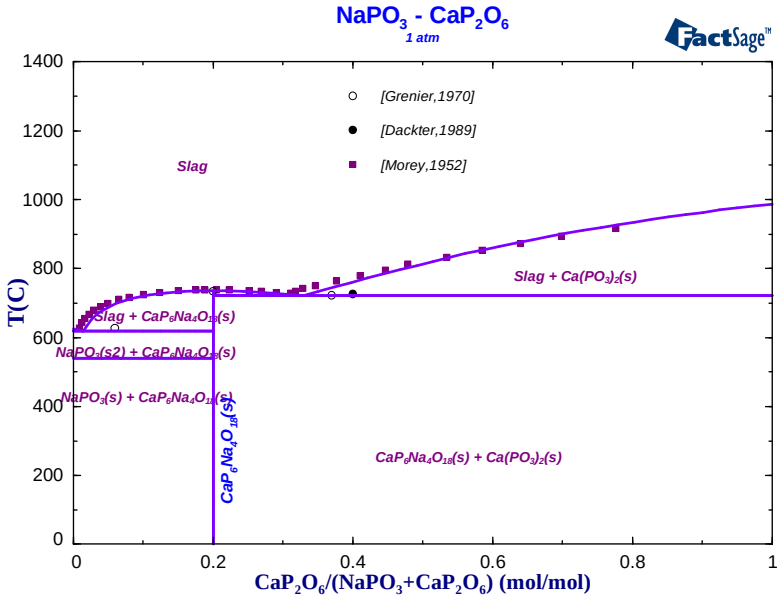
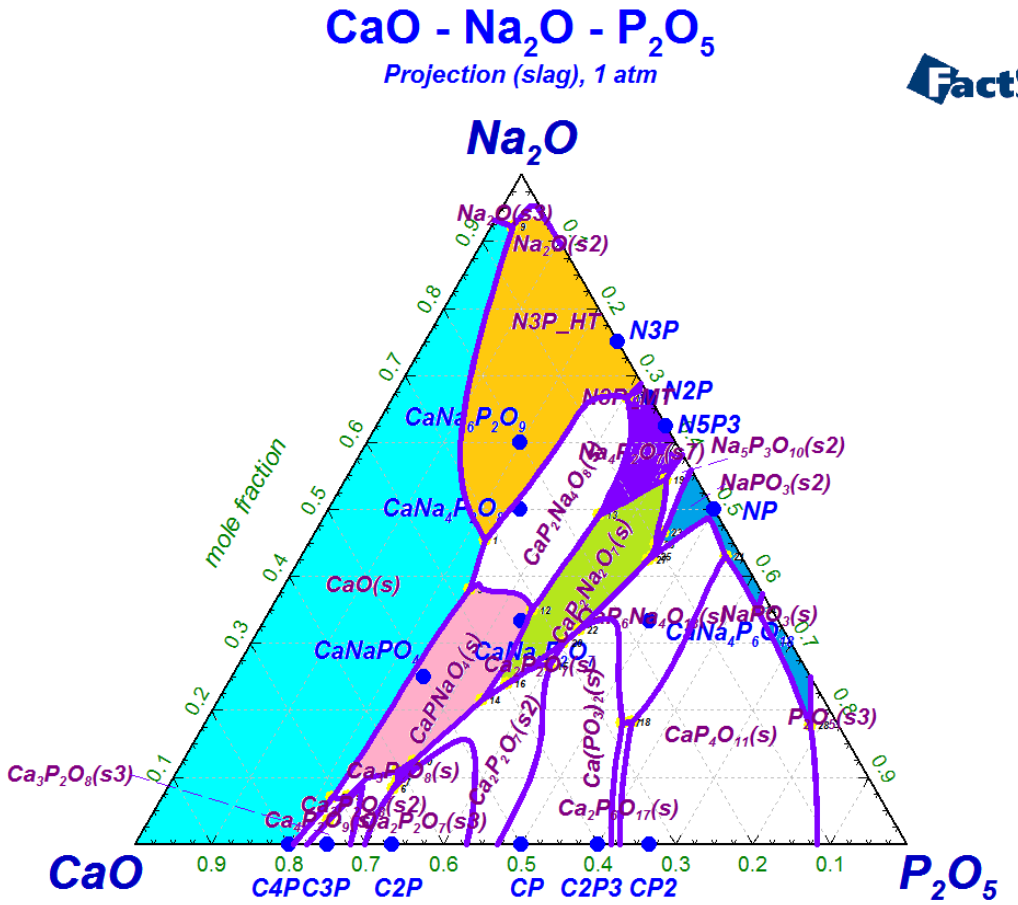
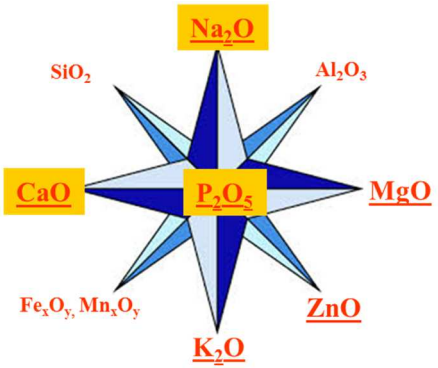




Liquidus surface





Description of the system

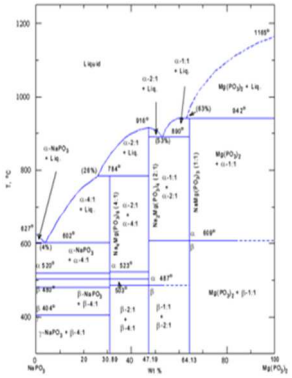
Name	Composition	Tm, calc. (exp.), °C	Liquid species
R	$NaMgPO_4$	968 (960)	
T2	*$Na_4Mg(PO_4)_2$	1662 (1655)	$Na_4Mg(PO_4)_2$/3.5
T3	*$Na_6MgP_2O_9$	1665 (1665)	
B1	$NaMg(PO_3)_3$	941 (942)	
B2	$Na_2Mg(PO_3)_4$	916 (916)	
B3	$Na_4Mg(PO_3)_6$	785 (784)	
F1	$Na_8Mg_6(P_2O_7)_5$	807 (808)	$Na_8Mg_6(P_2O_7)_5$/12
J	$NaMg_4(PO_4)_3$	1159 (1155)	
* - solid solution component			

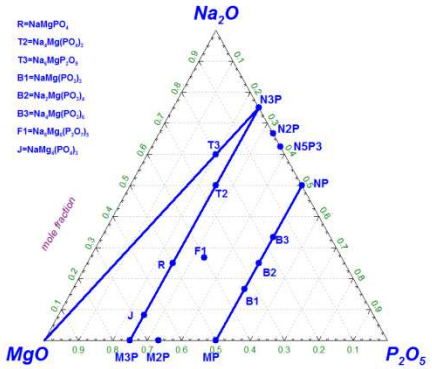
$(\underline{Na_2}, K_2, Zn)_2(\underline{Na_2}, Na_2CaO, Mg, Na_2MgO)_1 (PO_4)_2$

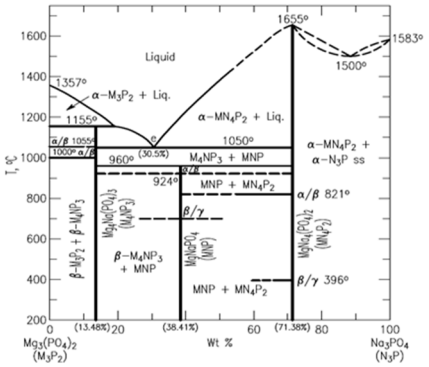
solid solutions for HT, MT, LT modifications

$(\underline{Na_2O}, K_2O, ZnO)_2(P_2O_5)(\underline{Na_2O}, Na_2CaO_2, MgO, Na_2MgO_2)$

Sections NP-MP, N3P-MgO, N3P-M3P







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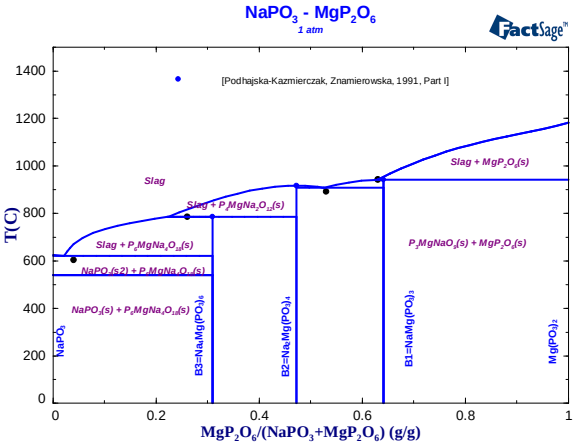
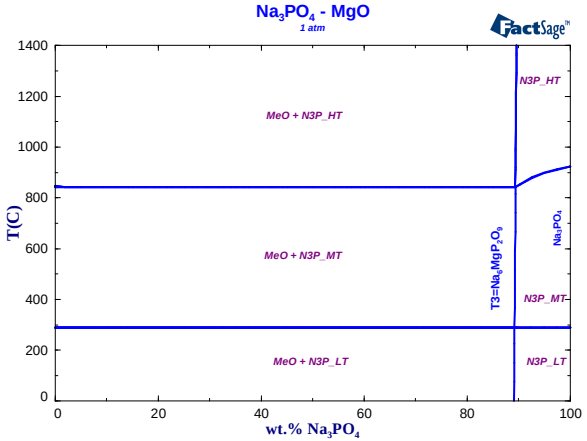
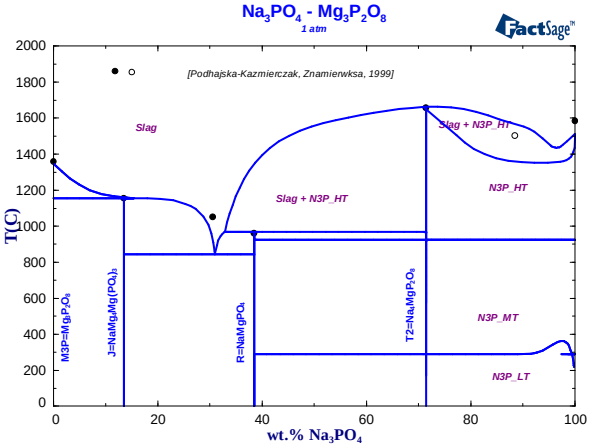
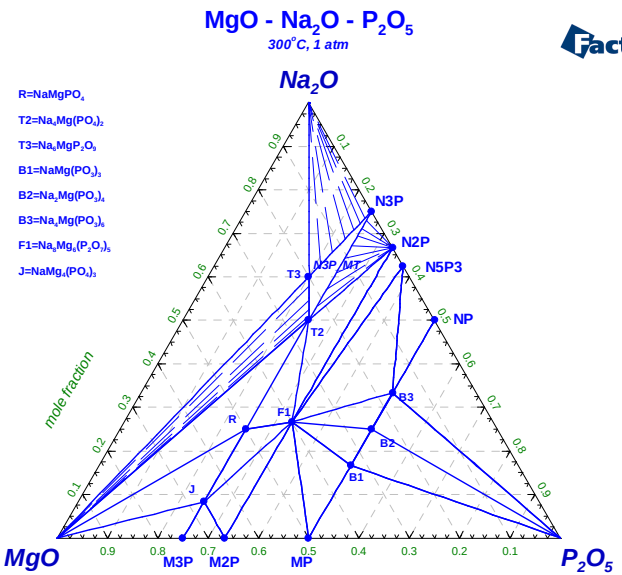
T.Podhajska-Kazmierczak, T.Znamierowska, Pol. J. Chem., 73 [2] 279-286 (1999).

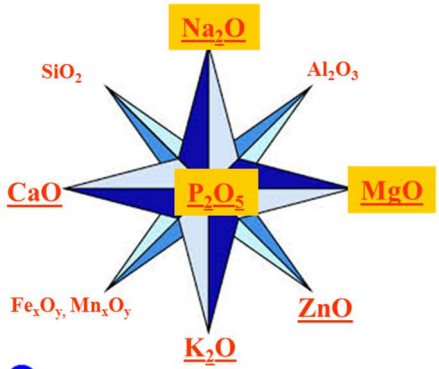


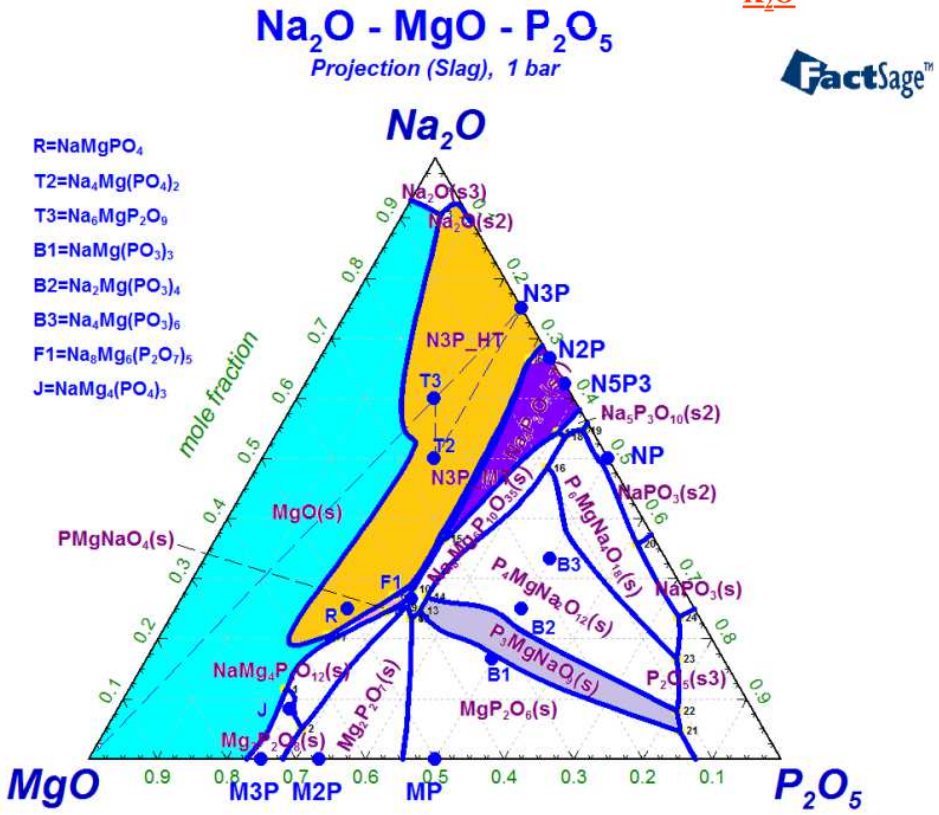




Sub-solidus and liquidus surface







Description of the system

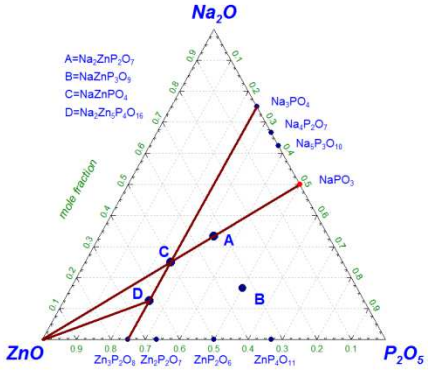
Name	Composition	Tm, calc. (exp.), °C	Liquid species
A	$Na_2ZnP_2O_7$	783 (782)	$Na_2ZnP_2O_7$*2.5
B	$NaZnP_3O_9$	720 (720)	
C	$NaZnPO_4$	1009 (1007)	
D	$Na_2Zn_5(PO_4)_4$	886 (888)	$Na_2Zn_5(PO_4)_4$*5.5

$(\underline{Na_2}, K_2, Zn)_2(\underline{Na_2}, Na_2CaO, Mg, Na_2MgO)_1 (PO_4)_2$

solid solution N3P-Z3P for HT modification

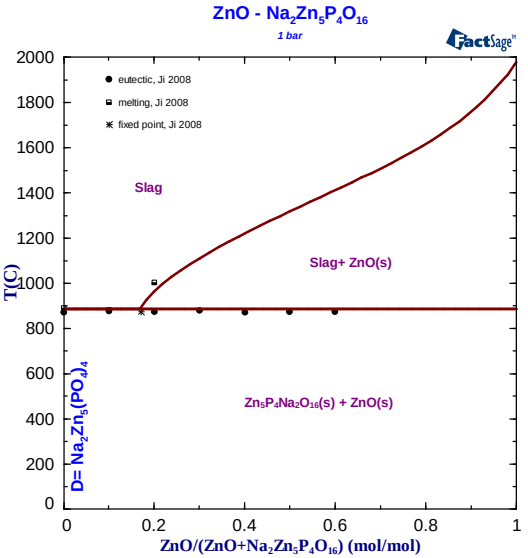
$(\underline{Na_2O}, K_2O, ZnO)_2(P_2O_5)(\underline{Na_2O}, Na_2CaO_2, MgO, Na_2MgO_2)$

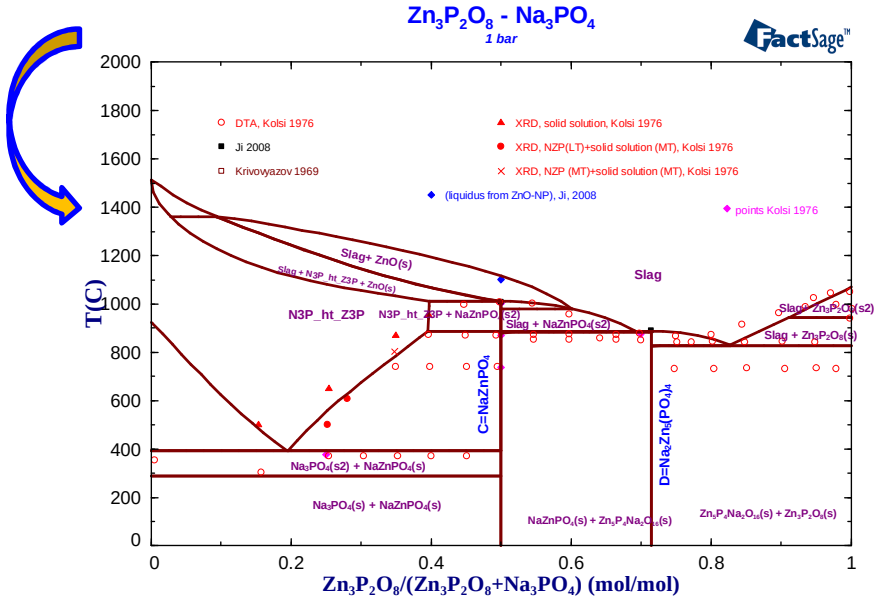
Sections N3P-Z3P, ZnO-D, ZnO-NP-ZP

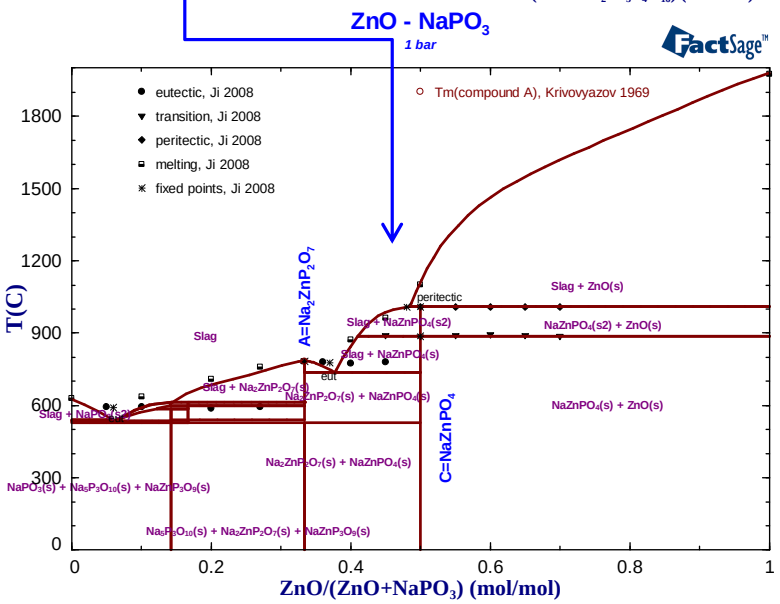


Compound $NaZnPO_4$ was modelled taking into account the enthalpy of formation (exp)

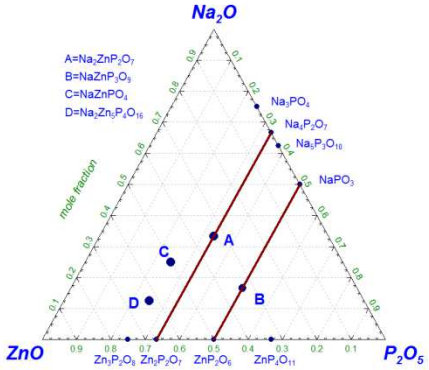
$(Na_2O, ZnO)_2(P_2O_5)(Na_2O)$

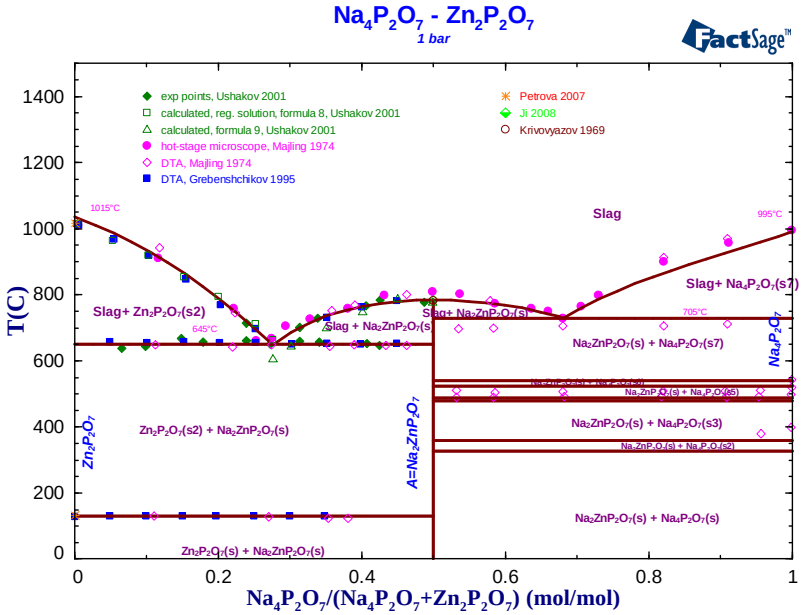


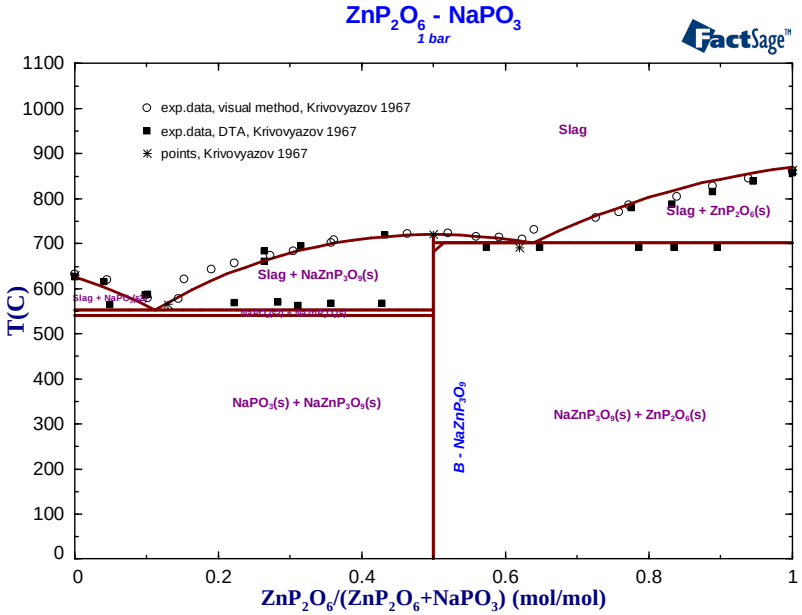




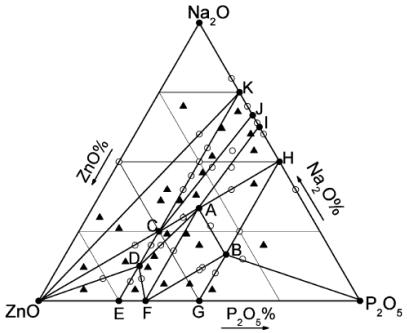
Quasi-binary sections N2P-Z2P and NP-ZP







Sub-solidus equilibria and liquidus surface



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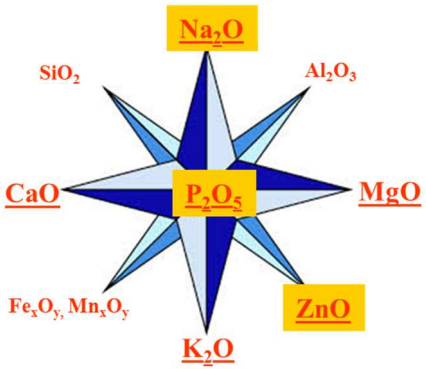
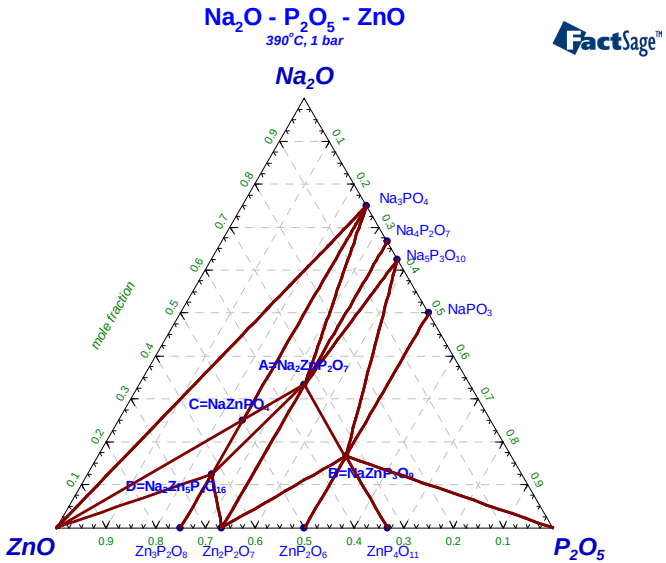
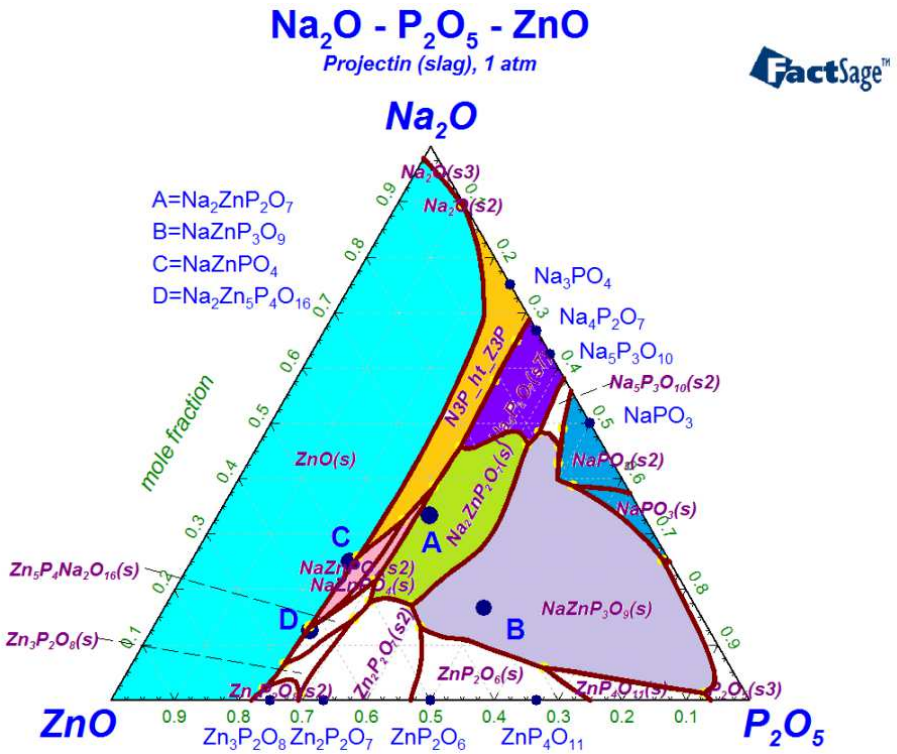
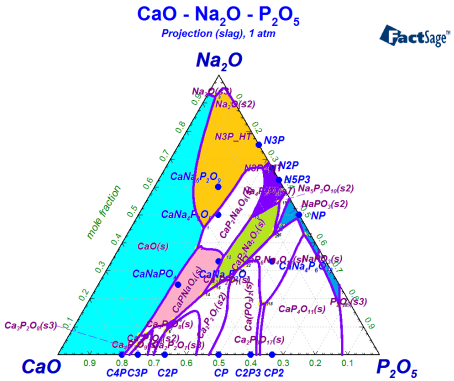
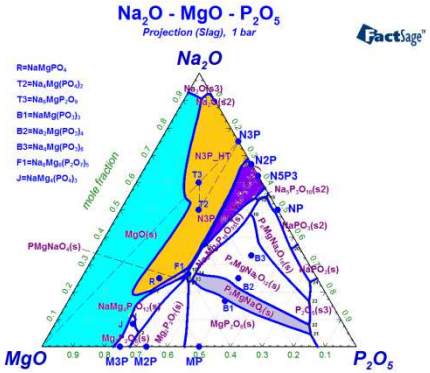


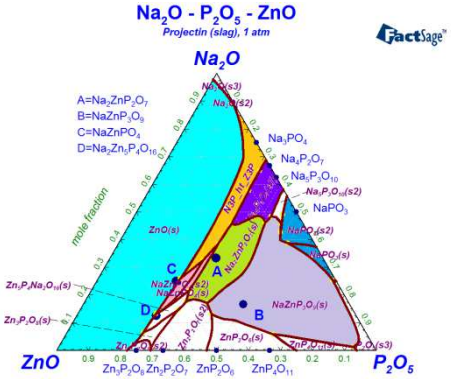


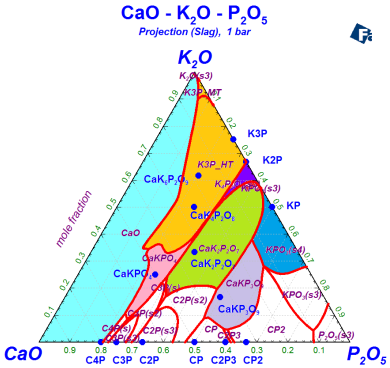


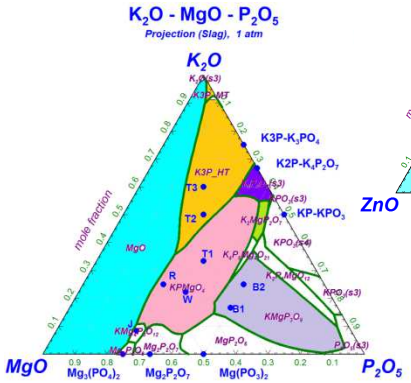
Systems Alk_2O-MeO-P_2O_5

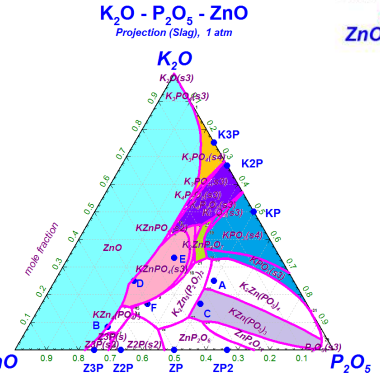


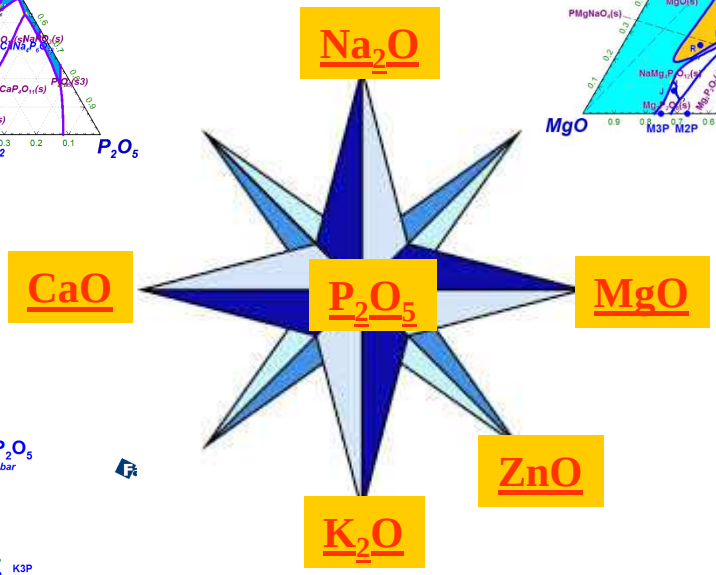












Conclusions

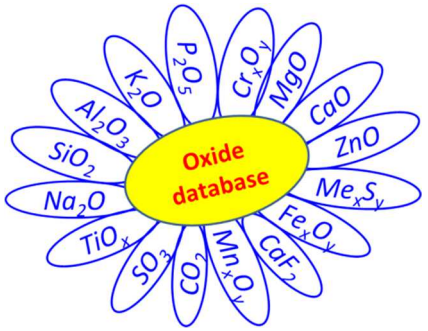
- Binary systems Alk_2O-P_2O_5 (Alk=Na, K) have been re-assessed taking into account the new experimental data
- All phases (slag, solid solutions based on $AlkPO_x$) in the ternary system with both alkalis have been added into the dataset
- All ternary compounds in the ternary systems Alk_2O-MeO-P_2O_5 (Alk=Na, K; Me=Ca, Mg, Zn) have been considered. The thermodynamic dataset including solubilities between Alk_3PO_4-$Alk_4Me(PO_4)_2$-$Alk_6MeP_2O_9$ allows the description the phase equilibria in the different sections
- The liquid phase in all subsystems was evaluated using non-ideal associate species model (two cations per species). The corresponding ternary species have been added into the liquid
- All systems (7 ternaries) in the framework of the system Na_2O-K_2O-CaO-MgO-ZnO-P_2O_5 were assessed using experimental phase diagram information. The quasi-binary sections and liquidus surfaces in the systems Alk_2O-MeO-P_2O_5 have been calculated using the corresponding data

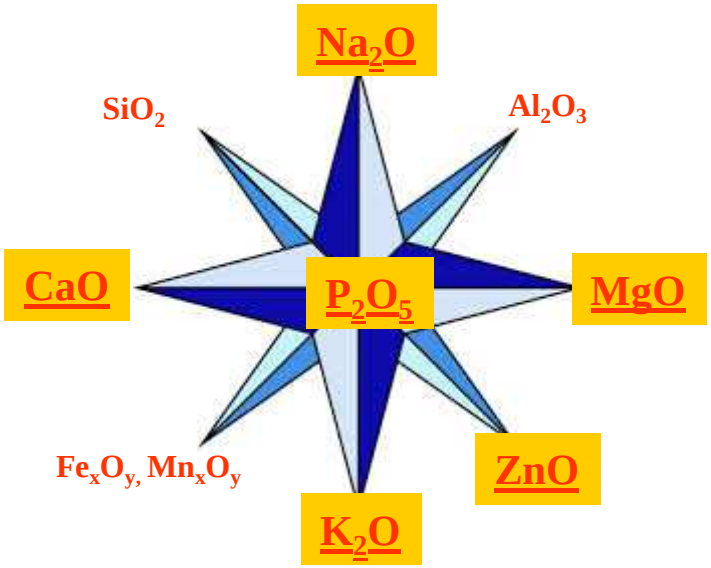
On behalf of all co-authors:

Thank you for your attention!

Vielen Dank für Ihre Aufmerksamkeit!

Благодарю за внимание!





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