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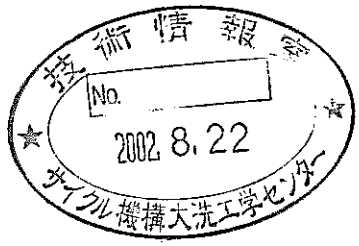

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Assessment of Thermochemical Data of Ternary Na-Fe Oxides and Calculation of the Na-Fe-O Phase Diagram

Jintao HUANG*, Tomohiro Furukawa* and Kazumi Aoto*

Abstract

In Na-Fe-O system, some ternary sodium-iron complex oxides have not been intensively investigated, so their thermodynamic data obtained separately seem not consistent to each other. Available thermodynamic databases sometimes lead to wrong conclusions. The Gibbs energies of formation of Na_3FeO_3 and Na_4FeO_3 were both evaluated based on the latest experiment results. Consistent sets of thermodynamic data tables were created for Thermo-Calc and MALT2 computer codes.

The modified thermodynamic database was applied to carry out ternary phase diagram calculations by Thermo-Calc code at different temperatures. Meanwhile, predominance diagram of Na-Fe-O at high temperatures were calculated too. The chemical stability of sodium iron complex oxides was quantitatively determined according to present calculation.

Compared to some early phase diagrams in the Na-Fe-O system, the new phase diagrams show better consistence with the experiment results obtained up to now. The fundamental information given in this study is of important significance for further studies related to Na-Fe-O system.

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Na-Fe-O系熱化学データベースの整合と状態図の計算

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要　旨

Na-Fe-O系化合物の中でいくつかのNaFe複合酸化物に関する研究はこれまで詳細に実施されておらず、個々に得られたそれらの熱力学データは互いに矛盾が生じているように思われる。このため利用可能な熱力学データベースは時には誤った結果を導く。これまでに報告されている Na-Fe-O 三元系平衡状態図は必ずしも正しい結果を示しているとはいえない。そこで、信頼性のあるデータを得るために蒸気圧測定実験分析を実施した。Na_3FeO_3 と Na_4FeO_3 の生成ギブスエネルギーを評価し、その実験結果に基づいて Thermo-Calc フォーマットと互換性のある熱力学ユーザーデータベースを構築した。

各相の安定条件を定量的に示すために、Na-O雰囲気におけるNaFe複合酸化物の化学ポテンシャル図を 400、600、800 および 1000K に対してそれぞれ作成した。室温から 1000K までの範囲で新たに作成した Na-Fe-O 系平衡状態図は、実験結果と矛盾のない結果が得られた。

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Assessment of Thermochemical Data of Ternary Na-Fe Oxides and Calculation of the Na-Fe-O Phase Diagram

1. Introduction

Early phase diagram study on the Na-Fe-O system had been done by Dai et al[1-2]. Some isothermal phase diagrams of FeO(s)-Na_2O(s), FeO(s)-$Na_2Fe_2O_4$(s) and Fe_3O_4(s)-$Na_2Fe_2O_4$(s) were given. Lindemer constructed ternary Na-Fe-O phase diagram (Fig.1) by combing existed experimental results and estimated thermodynamic data of some possible ternary Na-Fe oxides[3]. His work correctly predicted the formation of Na(l)-Fe(s)-Na_4FeO_3(s) at high temperatures though stability of ternary Na-Fe oxides involved had not been confirmed. Recent phase diagrams given by Seetharaman[4] and Sridharan[5-6] were both based on their original experimental results. In their research, Even though high order complex oxides, such as $Na_3Fe_5O_9$(s), $Na_4Fe_6O_{11}$(s), $Na_4Fe_2O_7$(s) as well as Na_2FeO_2(s) were not included, however, large discrepancy still exists among their phase diagrams. For example, Sridharan et. al. suggested that there exist two-phase lines Na_4FeO_3(s)-Na_3FeO_3(s) and Na_3FeO_3(s)-$NaFeO_2$(s) in 500-650°C as shown in Fig. 2 while Seetharaman reported Na_4FeO_3(s)-$NaFeO_2$(s) and Na_4FeO_3(s)-Na_2O(s) two-phase lines as shown in Fig. 3. By using currently available databases MALT2[7] and KTH's user database[8], the Na-Fe-O phase diagram are calculated again by the present authors. For comparison with our experiment, typical results at 650K are given in Fig. 4 and Fig. 5, respectively. However, neither of them could predict the coexistence of Na_4FeO_3(s)-Na_3FeO_3(s) that was observed in recent investigation by high temperature mass spectrometry[9] as well as thermal analysis and Raman analysis in the present laboratory.

To solve this discrepancy and construct correct Na-Fe-O phase diagram of better consistency with experiment results, the authors once again evaluated thermodynamic data of some sodium iron complex oxides. By reviewing thermodynamic data in literatures together with new experimental data obtained in the present laboratory, a modified user database was created. Thus, new ternary phase diagrams and chemical potential diagrams in the Na-Fe-O system were constructed from room temperature to 1000K by using the Thermo-Calc code. Stability of the ternary oxides was quantitatively discussed.

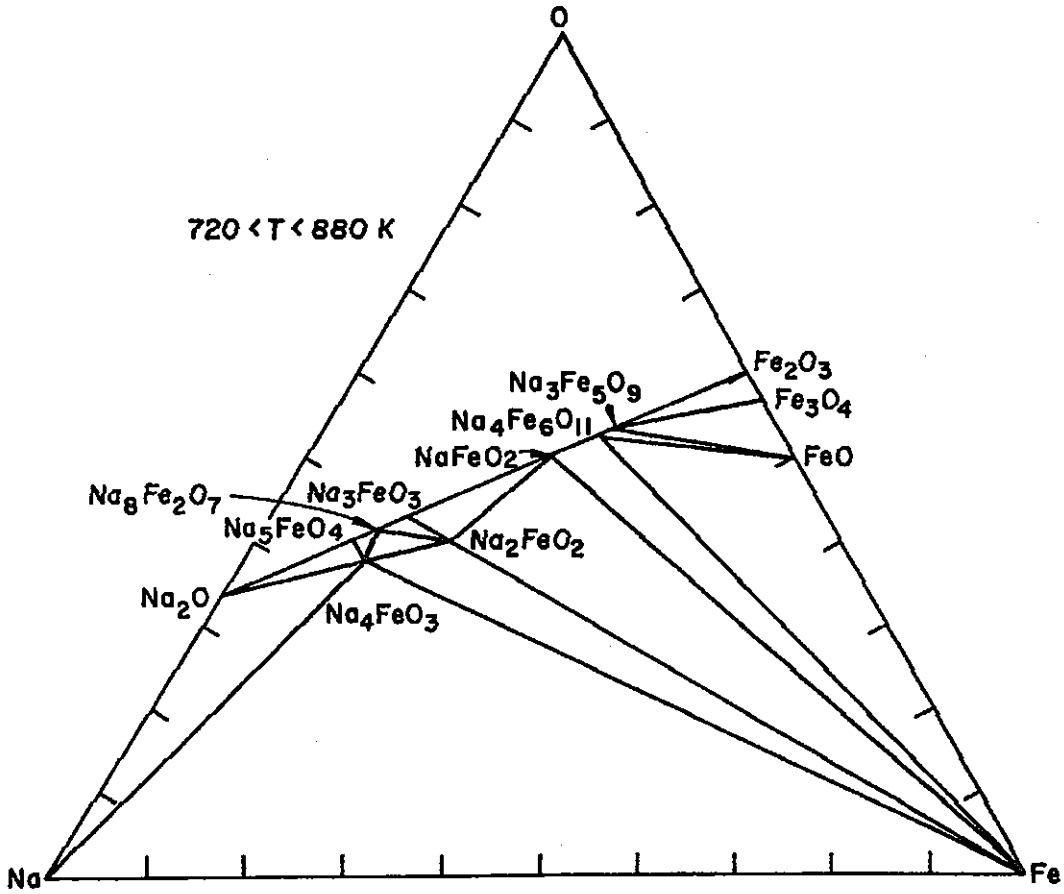

Fig. 1: Na-Fe-O equilibrium diagram for 720<T<880K by Lindemer

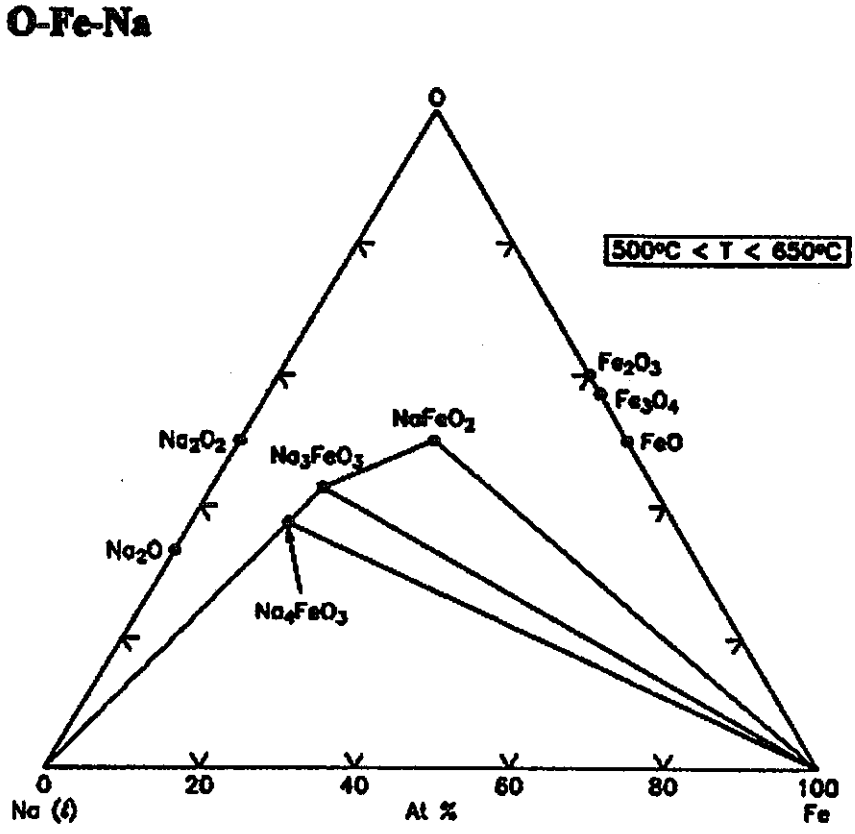

Fig. 2: Ternary phase fields of Na-Fe-O system at 773-923K by Sridharan

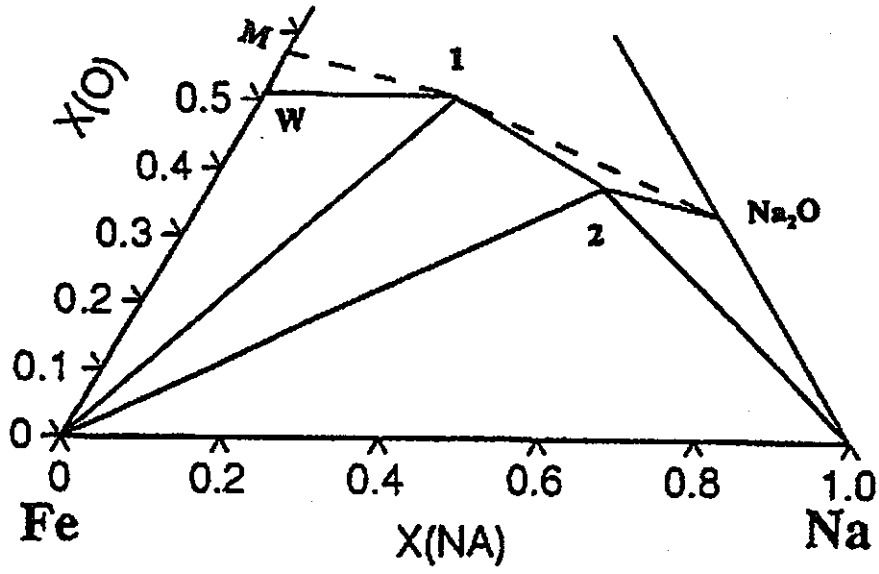

Fig. 3: Calculated isothermal section at 853K by Seetharaman. Compounds shown in the diagram are 1-$NaFeO_2$, 2-Na_4FeO_3, M-Magnetite and W-Wustite.

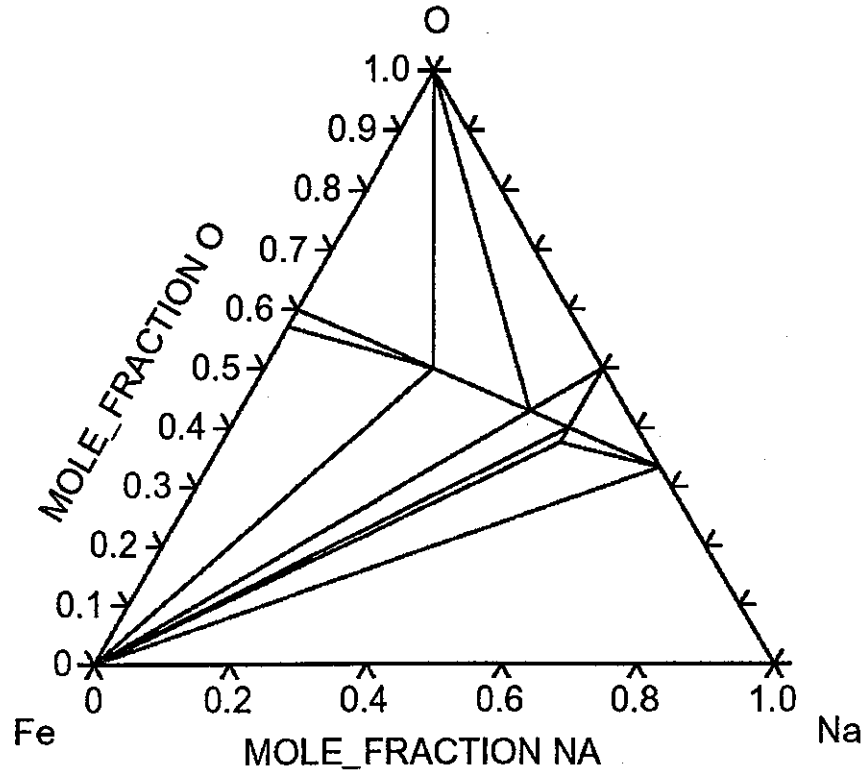

Fig. 4: Na-Fe-O phase diagram at 650K produced by using MALT2 database

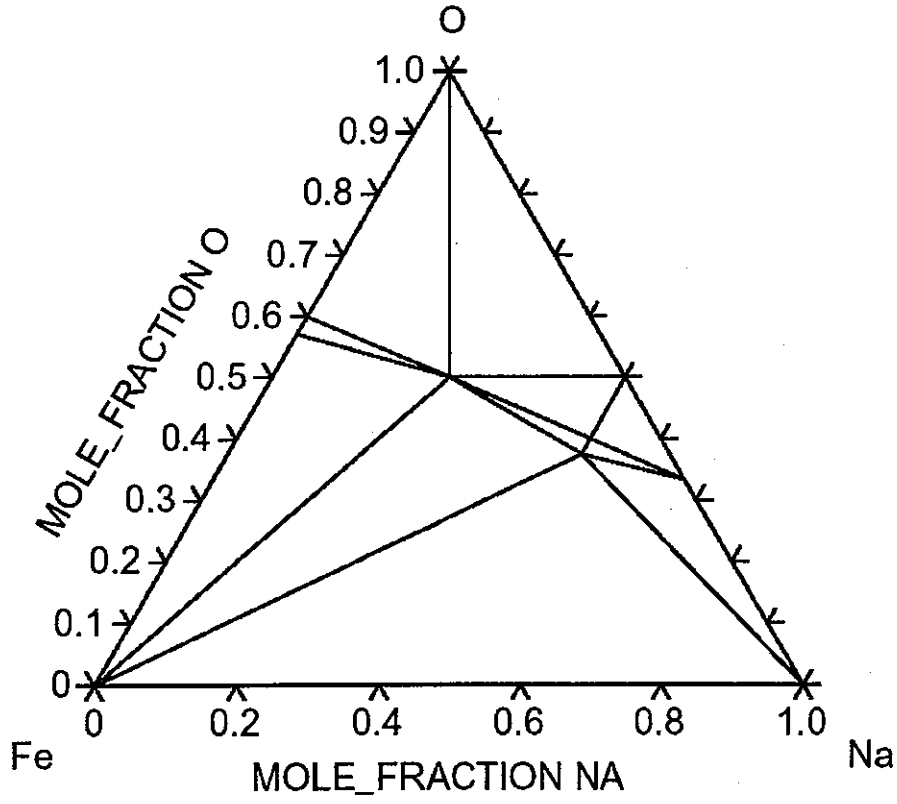

Fig. 5: Na-Fe-O phase diagram at 650K produced by KTH's user database

2. Thermodynamic aspects

Thermodynamic basis of equilibrium calculation and the construction of phase diagram by the Thermo-Calc can be found in literature[10] as well as the User's guide. Present study employed TERN-module to create ternary phase diagram of the Na-Fe-O system. POLY-module was used to generate potential diagrams. BIN-module is not adapted because the calculation needs to run in extremely low oxygen potentials. The assessed SSUB database provided by SGTE is employed as the main database for the calculation. It is assumed that all the condensed phases stay in their standard states and their mutual solubility has to be neglected for simplicity. A user database was built up for the calculation. Thermodynamic data source and assessment of literatures and experimental results are given in detail.

2.1 **Binary system in Na-Fe-O**

Na-O system

A schematic binary Na-O phase diagram can be found in literature[11]. The three binary oxides in the system, $Na_2O(s)$, $Na_2O_2(s)$ and $NaO_2(s)$, were taken into account in the present calculation but no solutions were included for lack of information.

Fe-O system

This system is extensively investigated so that original data given in the SSUB database were utilized for the calculation, in which the three well known solid solutions, Hematite, Magnetite and Wustite were included. Further discussion in this part is no longer necessary.

Na-Fe system

No further treatment was done for this binary system because no compounds were found and only very limited solutions were reported.

2.2 Ternary Na-Fe oxides

$NaFeO_2$(s)

Data assessed by SGTE was used.

Na_4FeO_3(s)

This compound has been studied so many times that thermodynamic evaluation are possible. Among the existing a few data of Na_4FeO_3(s), Bhat and Borgstede's result[12] seems more reliable because it is quite consistent with experimental data given by Gross[13] and Shaiu[14]. Therefore, the following expression is employed in the present study.

$$\Delta_f G°(Na_4FeO_3) = -1212202 + 351.10 \times T. \quad \text{----------(1)}$$

Since experimental data, such as heat capacities, enthalpy increments and Gibbs energy functions of Na_4FeO_3(s) are not available, estimated data have to be used. So, Lindemer's estimation of entropy $S°(298)$=208.9 J/molK was employed. Heat capacity Cp(T) was roughly summed from its corresponding simple oxides. $\Delta_f H°(298)$ was calculated according to the following formula.

$$\Delta_f H°(298) = \Delta_f G°(298) + T\Delta_f S° \quad \text{----------(2)}$$

$$Cp(T) = 212.49 + 0.03.83T - 3.28E+06/T^2 \quad \text{----------(3)}$$

Thermal analysis on this compound by DSC carried out in the present laboratory shows that the melting point is around 1008±15K. No other phase transitions were found up to its melting point. Property of its liquid phase is not determined so the whole calculation was done below its melting point.

Then the whole thermodynamic table of Na_4FeO_3 is built up in Table 1.

Table 1: Thermodynamic table of Na_4FeO_3(s) evaluated by JNC

T	Cp	S°	H°-H°(T$_o$)	(gef)	Δ_fH°	Δ_fG°
K	J/K.mol	J/K.mol	kJ/mol	J/K.mol	kJ/mol	kJ/mol
298.15	186.969	208.9	0	-208.9	-1206.13	-1107.52
300	187.494	210.058	0.346	-208.904	-1206.12	-1106.91
400	207.289	267.037	20.2	-216.538	-1215.81	-1073.13
500	218.509	314.589	41.531	-231.528	-1214.36	-1037.6
600	226.354	355.155	63.792	-248.835	-1212.03	-1002.46
700	232.605	390.531	86.749	-266.604	-1209.14	-967.75
800	238.007	421.951	110.285	-284.095	-1205.92	-933.481
900	242.915	450.271	134.334	-301.011	-1202.58	-899.625
1000	247.516	476.105	158.858	-317.247	-1199.265	-866.119

Na_3FeO_3(s)

Experimental measurement on this compound was very scarce. The latest vapor mass spectrometric study[9] by the present authors provided Gibbs energy of formation, as expressed in the following,

$$\Delta_f G°(Na_3FeO_3) = -1168629 + 338.34 \times T \quad \text{----------(4)}$$

The expression should be valid until about 1000K because no phase transition was observed till 1033K in our thermal analysis. Similar treatments were made to estimate $S°(298)$, Cp(T) and $\Delta_f H°(298)$ of Na_3FeO_3(s) as expressed above, i.e.,

Δ_fG°(Na_3FeO_3) at 298.15K = −1068.29 kJ/mol.

Using Cp(T) and S(298.15) given by MALT2, Δ_fH°(Na_3FeO_3) at 298.15K can be determined.

$$Cp(T) = 181.69 + 33.39\times10^{-3}\,T - 29.67\times 10^5/T^2, \quad \text{----------(5)}$$

S(298.15) = 172 J/molK

Δ_fH°(Na_3FeO_3) = Δ_fG°(Na_3FeO_3)+TΔ_fS°(Na_3FeO_3)

Δ_fH°(Na_3FeO_3) at 298.15K = −1162.640 kJ/mol.

Then the whole thermodynamic table of Na_3FeO_3 is built up in Table 2.

Table 2: Thermodynamic table of Na_3FeO_3(s) evaluated by JNC

T	Cp	S°	H°-H°(T$_o$)	(gef)	Δ_fH°	Δ_fG°
C	J/C.mol	J/C.mol	kJ/mol	J/C.mol	kJ/mol	kJ/mol
298.15	158.268	172	0	-172	-1162.64	-1068.29
300	158.74	172.98	0.293	-172.003	-1162.63	-1067.71
400	176.502	221.377	17.158	-178.481	-1169.69	-1035.56
500	186.517	261.921	35.346	-191.228	-1168.28	-1002.17
600	193.482	296.573	54.363	-205.968	-1166.16	-969.139
700	199.008	326.826	73.996	-221.118	-1163.64	-936.497
800	203.766	353.717	94.139	-236.043	-1160.9	-904.234
900	208.078	377.969	114.734	-250.487	-1158.12	-872.319
1000	212.113	400.103	135.746	-264.358	-1155.47	-840.707

Na_5FeO_4(s)

Thermal analysis in the present laboratory shows that there are no phase transitions for this compound from room temperature to 1073K. Up to date, experimentally measured results of $\Delta_f G°(Na_5FeO_4)$ have been seldom reported in publications. Thermodynamic data for this compound were all taken from estimation as discussed above. The whole thermodynamic table of Na_3FeO_3 is built up in Table 3.

Table 3: Thermodynamic table of Na_5FeO_4(s) evaluated by JNC

T	Cp	S°	H°-H°(T$_o$)	(gef)	Δ_fH°	Δ_fG°
K	J/K.mol	J/K.mol	kJ/mol	J/K.mol	kJ/mol	kJ/mol
298.15	226.859	246.3	0	-246.3	-1596	-1462.7
300	227.564	247.705	0.42	-246.304	-1596	-1461.87
371	248.118	298.343	17.371	-251.52	-1595.58	-1430.17
371	248.118	298.343	17.371	-251.52	-1608.57	-1430.17
400	254.038	317.244	24.655	-255.606	-1608.4	-1416.23
500	268.88	375.649	50.857	-273.936	-1606.71	-1368.36
600	279.143	425.624	78.283	-295.153	-1603.84	-1320.94
700	287.244	469.282	106.615	-316.976	-1600.17	-1274.07
800	294.193	508.102	135.694	-338.485	-1595.99	-1227.77
900	300.472	543.12	165.431	-359.308	-1591.55	-1182
1000	306.335	575.084	195.774	-379.31	-1587.06	-1136.74

Na_2FeO_2(s) and other higher order oxides

Since experimental and theoretic attempts to look for stability of formation of Na_2FeO_2(s) failed[5-6,9], it is reasonable to exclude Na_2FeO_2(s) from the present calculation. Though some higher order Na-Fe oxides, such as $Na_3Fe_5O_9$, $Na_4Fe_6O_{11}$, $Na_8Fe_2O_7$, $Na_{10}Fe_{16}O_{29}$ and $Na_{34}Fe_8O_{29}$ had been reported[3], it seems they need more experimental evidence. So, these higher order compounds are not considered for simplicity.

A summary of thermodynamic data of the ternary Na-Fe oxides used for the present calculation is listed in Table 4.

Table 4: Summary of ternary oxides data used for the calculation

Ternary compounds		$NaFeO_2$(s)	Na_4FeO_3(s)	Na_3FeO_3(s)	Na_5FeO_4(s)
$\Delta_f G°$(298.15), kJ/mol		-639.98	-1107.521	-1068.29	-1462.7
$\Delta_f H°$(298.15), kJ/mol		-698.18	-1206.130	-1162.64	-1596.0
$S°$(298.15), J/mol·K		88.3	208.9	172.0	246.3
$Cp(T) = a+b\times10^{-2}T-c\times10^{6}/T^2$ J/mol·K, (298.15-1000K)	a	100.77	212.49	181.69	262.61
	b	1.86	3.83	3.339	4.818
	c	1.479	3.28	2.967	4.455
$G(T) = -g1\times10^{6}+g2\times10^{3}T-g3\times10^{2}T\times\ln(T)-g4\times10^{-2}T^2+g5\times10^{6}/T$ J/mol·K, (298.15-1000K)	g1	0.723394	1.282201	1.228246	1.691381
	g2	0.455159	1.244166	1.071530	1.551917
	g3	0.8055	2.1249	1.8169	2.6260
	g4	0.6653	1.9155	1.6695	2.4000
	g5	0.0000	1.6420	1.4835	2.2280

2.3 Data source prepared for Thermo-Calc code

To use thermal-calc code for calculation, thermo-calc compatible format has to be created. To meet this requirement, thermodynamic data of the ternary Na-Fe oxides have been changed as shown in the following.

FE1NA3O3

CONSTITUENTS: FE1NA3O3

G(FE1NA3O3,FE1NA3O3;0)-H298(BCC(A2),FE;0)- 3 H298(BCC(A2),NA;0)-
3 H298(1/2_MOLE_O2(G),O;0) = -1228246+1071.5301*T-181.69*T*LN(T)
-.016695*T**2+1483500*T**(-1) ----------(6)

FE1NA4O3

CONSTITUENTS: FE1NA4O3

G(FE1NA4O3,FE1NA4O3;0)-H298(BCC(A2),FE;0)- 4 H298(BCC(A2),NA;0)-
3 H298(1/2_MOLE_O2(G),O;0) = -1282201.24+1244.166*T-212.49*T*LN(T)
-.019155*T**2+1642000*T**(-1) ----------(7)

FE1NA5O4

CONSTITUENTS: FE1NA5O4

G(FE1NA5O4,FE1NA5O4;0)-H298(BCC,FE;0)- 5 H298(BCC,NA;0)
- 4 H298(O2(G),O;0) = -1691380.76+1551.97884*T-262.61*T*LN(T) -.02409*T**2
+2227500*T**(-1) ----------(8)

User database "HJT.TDB" for POLY-module and "H-TER.TDB" for TERN-module are given in the appendix part. Example executable files with macro commands are printed out in appendix too. Although some error may arise during the mathematic treatments during the data format transformation, final data generated from the Thermo-Calc code are given in Table 5-7 for comparison with the data source. It is clear that the outputs from Thermo-Calc are almost identical to the input source data as listed in Table 1-4 .

Table 5: Thermodynamic table of Na_3FeO_3 generated by Thermo-Calc

T	Cp	H	S	G
(K)	(Joule/K)	(Joule)	(Joule/K)	(Joule)
298.15	158.3	-1162640	172.0	-1213920
300	158.7	-1162350	173.0	-1214240
400	176.5	-1145480	221.4	-1234030
500	186.5	-1127290	261.9	-1258250
600	193.5	-1108280	296.6	-1286220
700	199.0	-1088640	326.8	-1317420
800	203.8	-1068500	353.7	-1351470
900	208.1	-1047910	378.0	-1388080
1000	212.1	-1026890	400.1	-1427000

Table 6: Thermodynamic table of Na_4FeO_3 generated by Thermo-Calc

T	Cp	H	S	G
(K)	(Joule/K)	(Joule)	(Joule/K)	(Joule)
298.15	187.0	-1206130	208.9	-1268410
300	187.5	-1205780	210.1	-1268800
400	207.3	-1185930	267.0	-1292750
500	218.5	-1164600	314.6	-1321890
600	226.4	-1142340	355.2	-1355430
700	232.6	-1119380	390.5	-1392750
800	238.0	-1095850	422.0	-1433410
900	242.9	-1071800	450.3	-1477040
1000	247.5	-1047270	476.1	-1523380

Table 7: Thermodynamic table of Na_5FeO_4 generated by Thermo-Calc

T	Cp	H	S	G
(K)	(Joule/K)	(Joule)	(Joule/K)	(Joule)
298.15	226.9	-1596000	246.3	-1669430
300	227.6	-1595580	247.7	-1669890
400	254.0	-1571340	317.2	-1698240
500	268.9	-1545140	375.6	-1732970
600	279.1	-1517720	425.6	-1773090
700	287.2	-1489390	469.3	-1817880
800	294.2	-1460310	508.1	-1866790
900	300.5	-1430570	543.1	-1919380
1000	306.3	-1400230	575.1	-1975310

3. Calculation results and discussion

By means of Thermo-Calc code, new chemical potential diagram and ternary Na-Fe-O phase diagram were constructed up to about 1000K, just below the melting point of $Na_4FeO_3(s)$. Comparison with experimental results and existing phase diagram were discussed too.

3.1 Chemical potential diagram

Predominance diagrams on coordinates of $\log P(O_2)$ versus $\log P(Na)$ were shown in Fig. 6-9. It expresses relationships among the main ternary Na-Fe oxides together with stable conditions. As indicted in Fig.7, some main equilibrium reactions are suggested as the following,

① $1/2Fe_2O_3(s) + Na(g) + 1/4O_2(g) = NaFeO_2(s)$ ----------(9)

② $1/3Fe_3O_4(s) + Na(g) + 1/3O_2(g) = NaFeO_2(s)$ ----------(10)

③ $Fe(s) + Na(g) + O_2(g) = NaFeO_2(s)$ ----------(11)

④ $NaFeO_2(s) + 1/2O_2(g) + 2Na(g) = Na_3FeO_3(s)$ ----------(12)

⑤ $Na_3FeO_3(s) + 1/2O_2(g) + 2Na(g) = Na_5FeO_4(s)$ ----------(13)

⑥ $Fe(s) + 3Na(g) + 3/2O_2(g) = Na_3FeO_3(s)$ ----------(14)

⑦ $Na_3FeO_3(s) + Na(g) = Na_4FeO_3(s)$ ----------(15)

⑧ $Na_4FeO_3(s) + Na(g) + O_2(g) = Na_5FeO_4(s)$ ----------(16)

⑨ $Fe(s) + 4Na(g) + 3/2O_2(g) = Na_4FeO_3(s)$ ----------(17)

⑩ $2Na(liq) + O_2(g) = Na_2O(s)$ ----------(18)

It should be noted that the phase $Na_4FeO_3(s)$ only exists at low oxygen potentials compared to other ternary oxides. The calculated highest oxygen potential that $Na_4FeO_3(s)$ can exist at 800K is as low as about –536kJ/mol. On the other hand, stable area for $NaFeO_2(s)$, $Na_3FeO_3(s)$ and $Na_5FeO_4(s)$ may be relatively very wide as shown in Fig. 6-9. Another character is that $Na_4FeO_3(s)$ can coexist with $Na_3FeO_3(s)$ at proper conditions in the whole temperature range of the calculation. It agrees well with the vapor pressure measurement and thermal analysis experiments carried out by the present authors[9].

Potential diagram at 650K derived from MALT2 database is given in Fig. 10 for comparison with experimental results. It should be noticed that Na_4FeO_3(s) phase area and Na_3FeO_3(s) are separated by Na_5FeO_4(s). It means that the two phases Na_3FeO_3(s) and Na_4FeO_3(s) cannot coexist at this condition. Apparently, it is contrast to experiment results. From the thermodynamic assessment in previous study, it is found that both MALT2 database and JNC's database give similar Gibbs energies for Na_4FeO_3(s) and Na_3FeO_3(s) [See Fig.27 in Ref 9]. It indicates that the Na-Fe-O phase diagram is thermodynamically very sensitive to the relative values of these ternary oxides. It is interesting to compare MALT2's data and the data used in the present study in detail. First, data of Na_5FeO_4(s) is completely the same in both databases. However, $\Delta_fH°$ and $\Delta_fG°$ of Na_4FeO_3(s) and Na_3FeO_3(s) used by MALT2 (Table 8-9) are about 0.7% positive compared with data by JNC (Table 1-2). Usually, an experiment error of a few kJ/mol seems quite reasonable. It reflects the difficulty of construction of Na-Fe-O phase diagram. This might be the main reason why there exists large discrepancy in the Na-Fe-O phase diagrams published by some frontiers. Fortunately, thermodynamic evaluations of Na_3FeO_3(s) in the present study were directly based on the reaction $Na_4FeO_3(s)=Na_3FeO_3(s)+Na(g)$. Thus, the thermodynamic relationship between these two phases is correctly reflected so that the user database can be considered as self-consistent. That is why JNC's calculated phase diagram seems quite consistent with the experiment results for the time being.

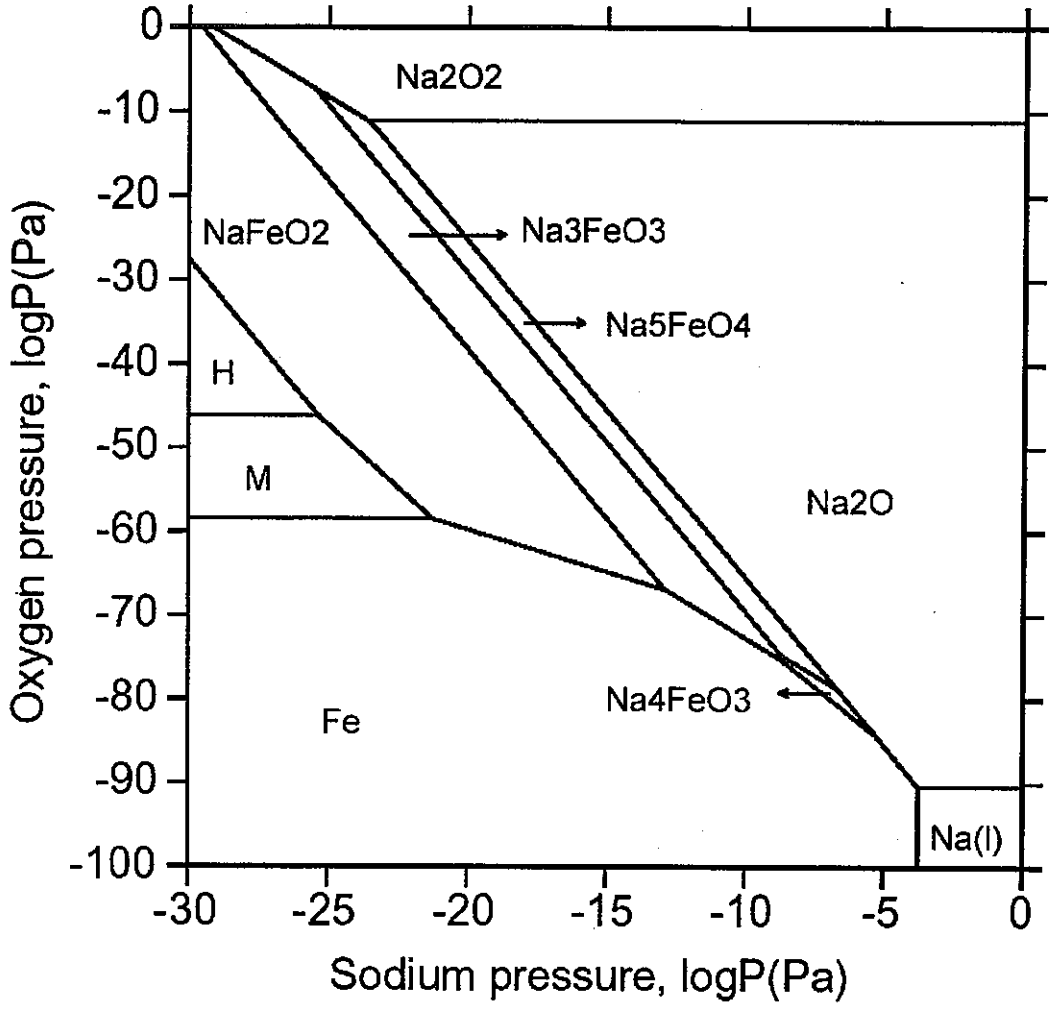

Fig. 6: Chemical potential diagram at 400K

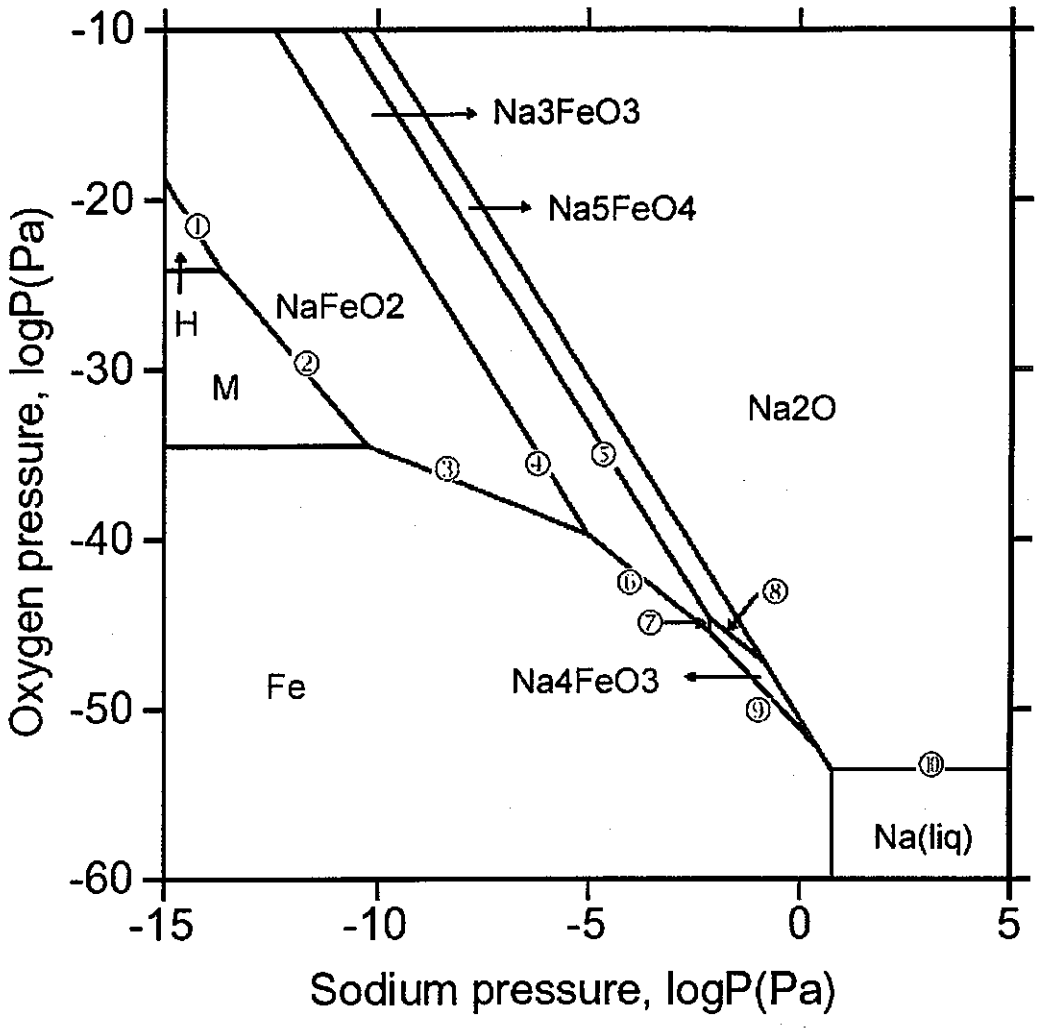

Fig. 7: Chemical potential diagram at 600K

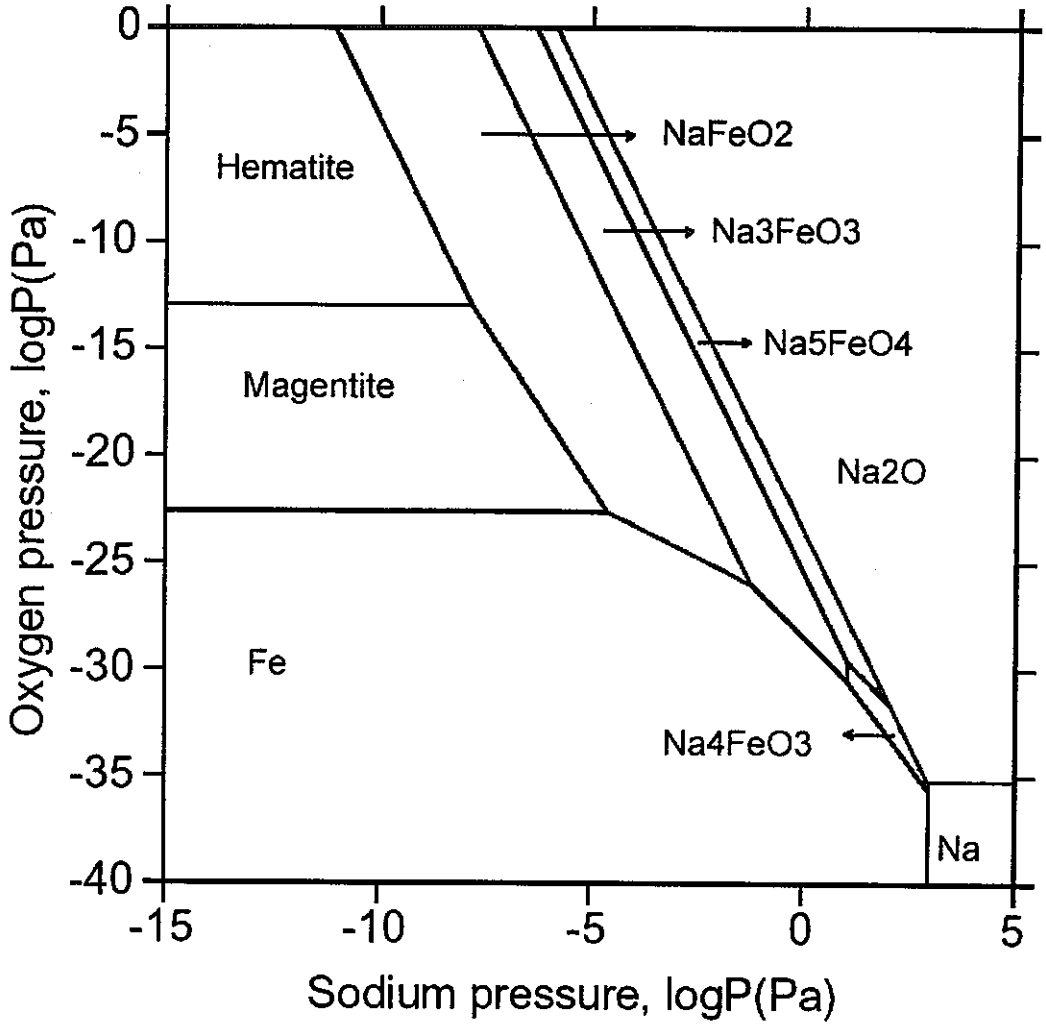

Fig. 8: Chemical potential diagram at 800K

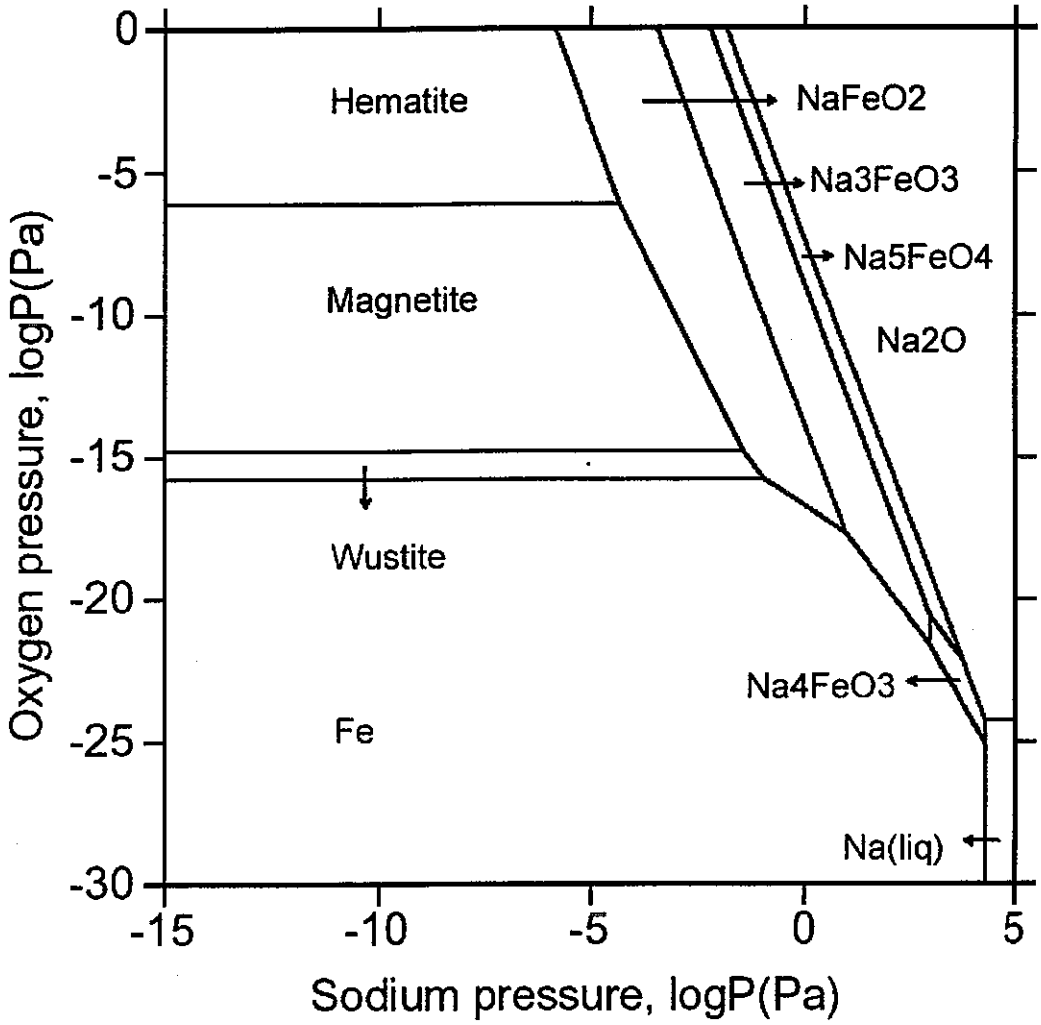

Fig. 9: Chemical potential diagram at 1000K

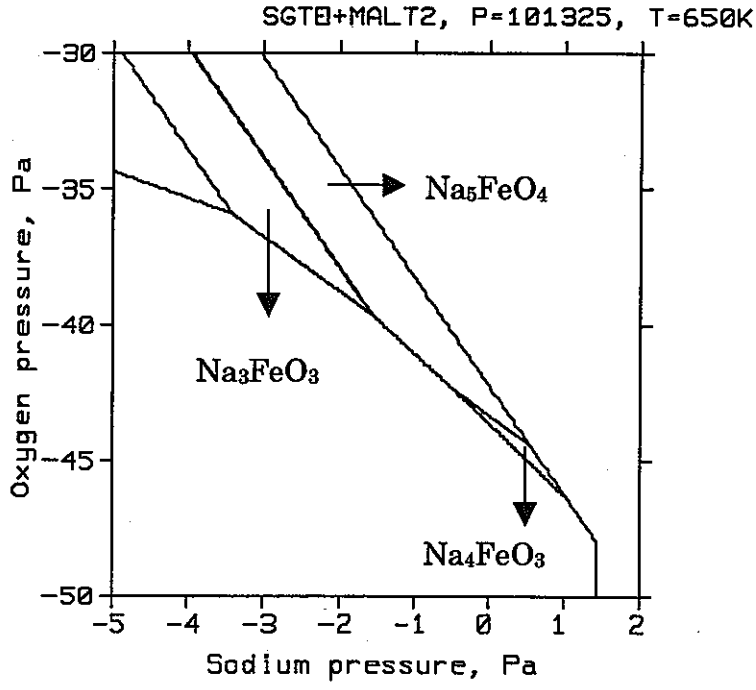

Fig. 10: Na-Fe-O predominance diagram at 650K by using MALT2 database

Table 8: Thermodynamic data of Na_3FeO_3(s) given by MALT2

T	Cp	S°	H°-H°(T$_o$)	(gef)	Δ_fH°	Δ_fG°
K	J/C.mol	J/C.mol	kJ/mol	J/C.mol	kJ/mol	kJ/mol
298.15	158.268	172	0	-172	-1155	-1060.6
300	158.74	172.98	0.293	-172.003	-1154.99	-1060.02
400	176.502	221.377	17.158	-178.481	-1162.05	-1027.87
500	186.517	261.921	35.346	-191.228	-1160.64	-994.481
600	193.482	296.573	54.363	-205.968	-1158.52	-961.449
700	199.008	326.826	73.996	-221.118	-1156	-928.807
800	203.766	353.717	94.139	-236.043	-1153.26	-896.544
900	208.078	377.969	114.734	-250.487	-1150.48	-864.629
1000	212.113	400.103	135.746	-264.358	-1147.83	-833.017

Table 9: Thermodynamic data of $Na_4FeO_3(s)$ given by MALT2

T	Cp	S°	$H^\circ-H^\circ(T_o)$	(gef)	Δ_fH°	Δ_fG°
K	J/C.mol	J/C.mol	kJ/mol	J/C.mol	kJ/mol	kJ/mol
298.15	186.969	208.9	0	-208.9	-1200	-1101.4
300	187.494	210.058	0.346	-208.904	-1199.99	-1100.79
400	207.289	267.037	20.2	-216.538	-1209.68	-1067.01
500	218.509	314.589	41.531	-231.528	-1208.23	-1031.48
600	226.354	355.155	63.792	-248.835	-1205.9	-996.337
700	232.605	390.531	86.749	-266.604	-1203.01	-961.629
800	238.007	421.951	110.285	-284.095	-1199.79	-927.36
900	242.915	450.271	134.334	-301.011	-1196.45	-893.504
1000	247.516	476.105	158.858	-317.247	-1193.17	-860.019

3.2 Isothermal sections of the Na-Fe-O system

Isothermal sections of the ternary phase diagram in the Na-Fe-O system at different temperature were constructed. According to the calculation, 4 typical phase diagrams were found in the Na-Fe-O system from room temperature to about 1000K as shown in Fig. 11-14. It suggests that Na(l), Fe(s) and $Na_4FeO_3(s)$ coexist over 695K and Na(liq)-Na_2O(s)-Fe(s) is more stable at lower temperatures.

From Fig. 13-14, it can be seen that the new ternary phase diagrams are very consistent with the schematic diagram (Fig. 1) drawn by Sridharan et al[5-6]. The characteristic three-phase areas in the system at high temperature, i.e., Na(l)-Na_4FeO_3(s)-Fe(s),Na_4FeO_3(s)-Na_3FeO_3(s)-Fe(s) and Na_3FeO_3(s)-$NaFeO_2$(s)-Fe(s) can all be found in both studies. It indicates that the present theoretic study agree well with their experimental results

Due to the importance in nuclear industry, special attention was paid to low oxygen potentials. $Na_4FeO_3(s)$ is considered as one of the main corrosion products in the sodium-leak incident of the MONJU FBR. From this calculation, the transition temperature is 695K that is a little lower than 723K reported by Bhat and Borgendete[12]. It was a pity that there were only two points at the low temperature side of their measurements. It might be not sufficient to determine the transition temperature precisely. Consider a 25K step in their measurements, the present

calculation result agree quite well with their experiments. From the Ellingham diagram given by Lindemer (Fig. 15). The transition temperature might be around 650K. It should be noted that Sridharan et al. found the transition temperature might be about 629K[5]. So, the temperature obtained by different methods scattered from 629K to 723K. The present calculation and Lindemer's estimation did not considered solid solutions in the Na-Fe-O system, but solid solutions might have affected the transition temperature greatly in experimental measurements. Therefore, possible reason can be attributed to the influences from solid solutions.

The new phase diagram also shows that the triangle Na_4FeO_3(s)-Na_3FeO_3(s)-Na_5FeO_4(s) is stable from room temperature to 1000K. From the phase diagram given by Seetharaman et al[4], however, coexistence of a tentative three-phase Na_2O(s)-Na_4FeO_3(s)-$NaFeO_2$(s) was once suggested(Fig. 3). Although the present study suggests that Na_4FeO_3(s)-Na_3FeO_3(s)-Na_5FeO_4(s) is thermodynamically more favorable in the whole temperature range below 1000K, further experimental confirmation is in need to judge the two predictions.

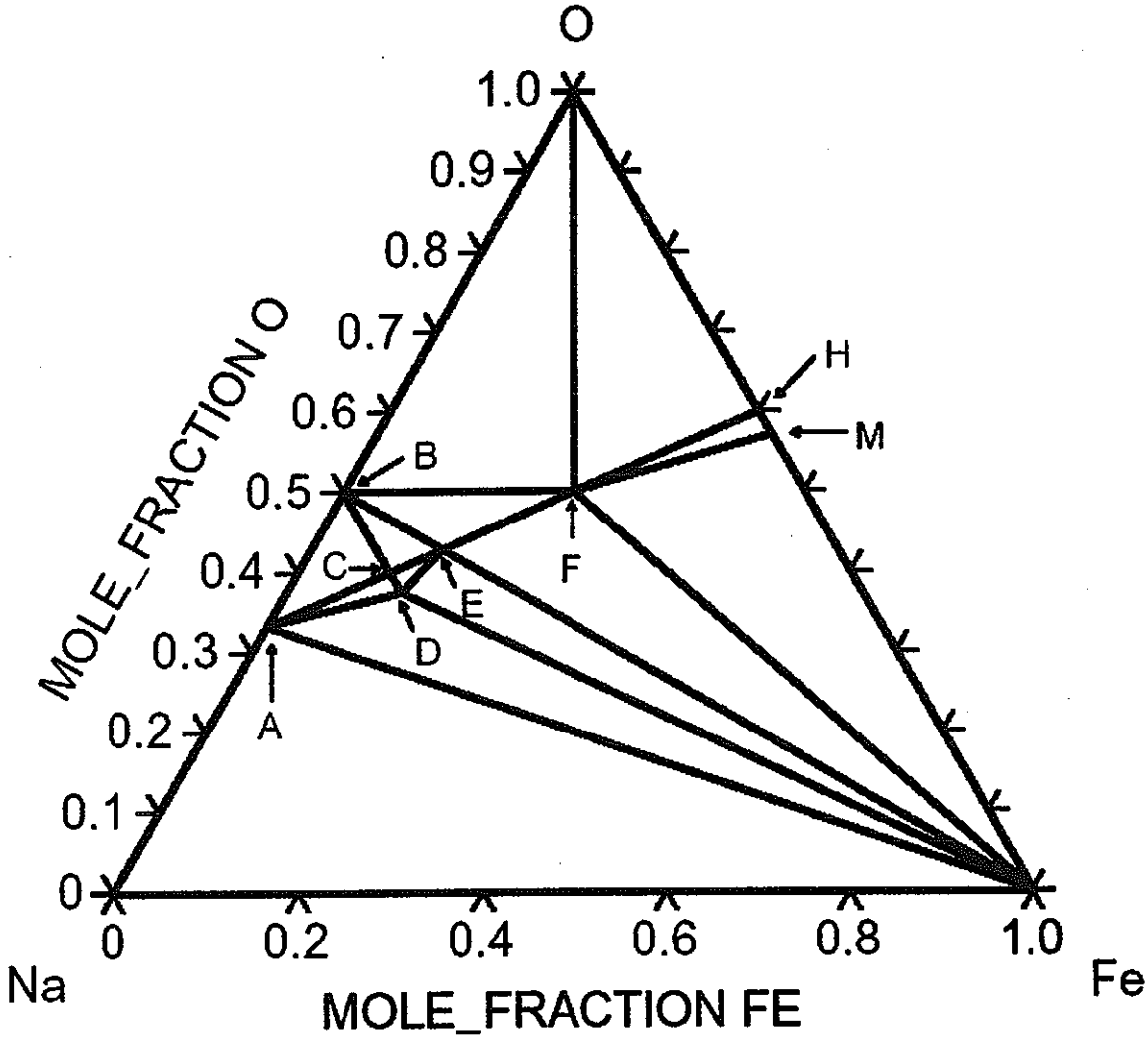

Fig. 11: Isothermal cross section at 298-535K. (A-Na_2O, B-Na_2O_2, C-Na_5FeO_4, D-Na_4FeO_3, E-Na_3FeO_3, F-$NaFeO_2$, H-Hematite, M-Magnetite)

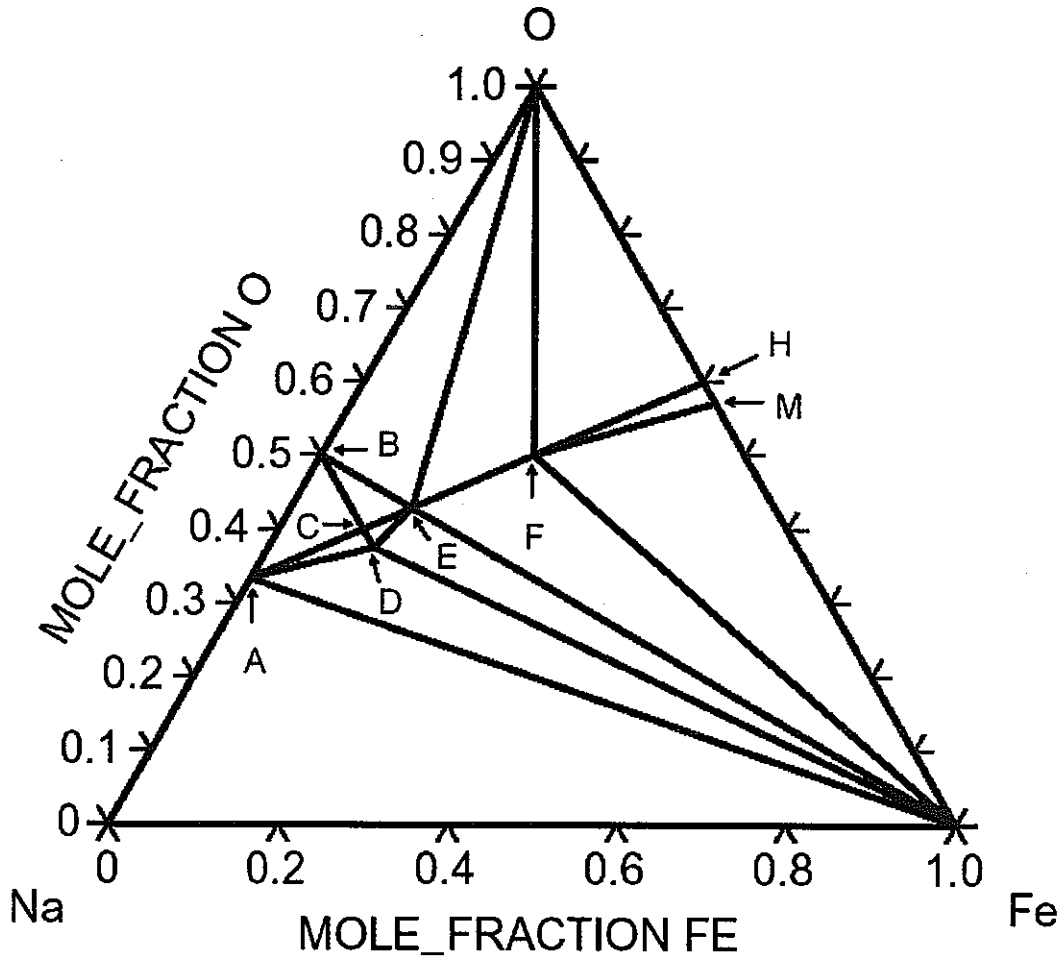

Fig. 12: Isothermal cross section at 536-694K. (A-Na_2O, B-Na_2O_2, C-Na_5FeO_4, D-Na_4FeO_3, E-Na_3FeO_3, F-$NaFeO_2$, H-Hematite, M-Magnetite)

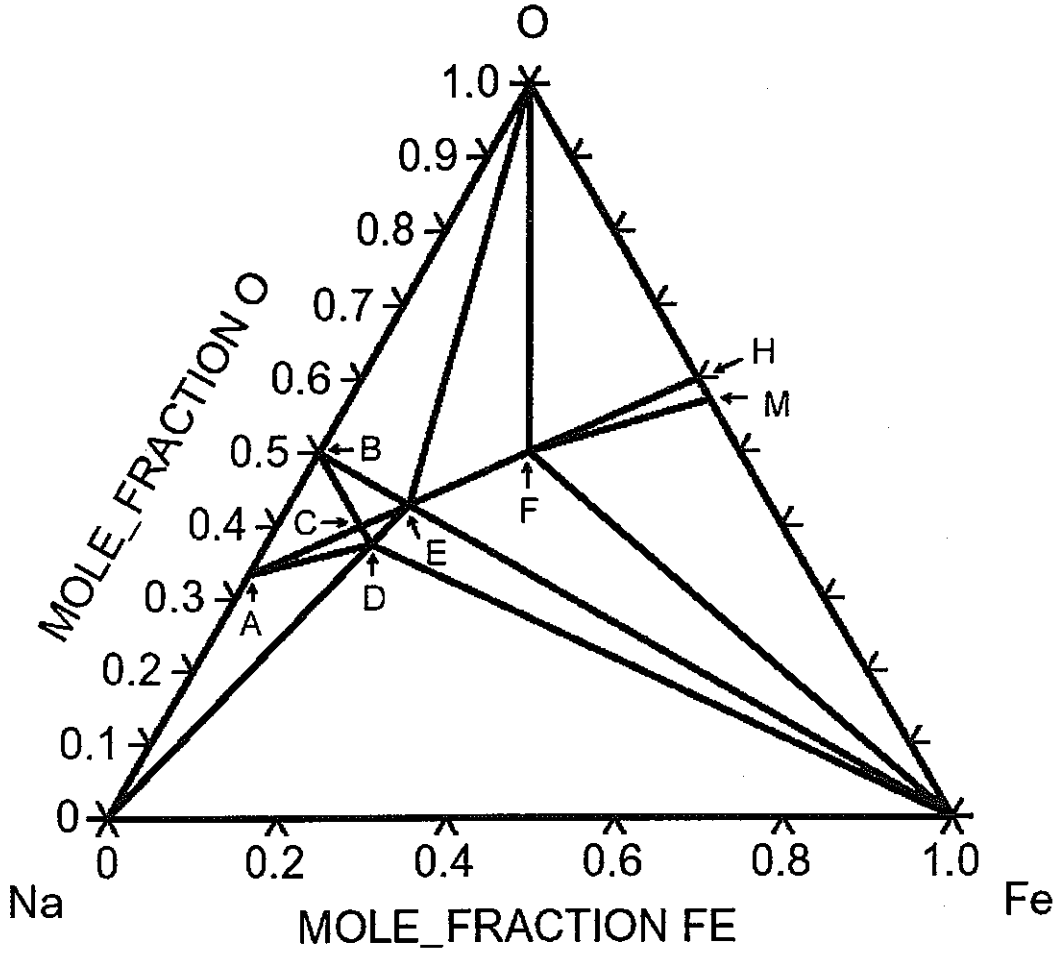

Fig. 13: Isothermal cross section at 695-838K. (A-Na_2O, B-Na_2O_2, C-Na_5FeO_4, D-Na_4FeO_3, E-Na_3FeO_3, F-$NaFeO_2$, H-Hematite, M-Magnetite)

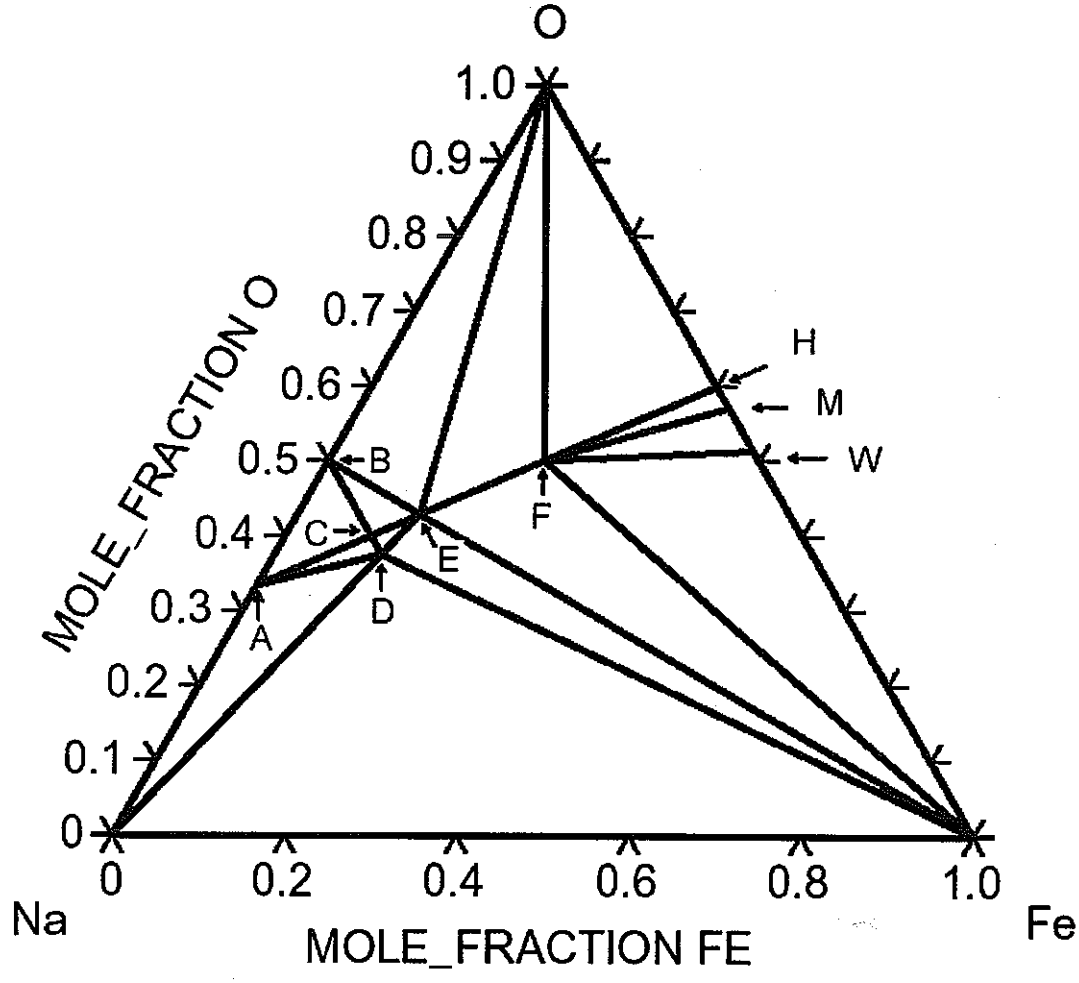

Fig. 14: Isothermal cross section at 839-1008K. (A-Na_2O, B-Na_2O_2, C-Na_5FeO_4, D-Na_4FeO_3, E-Na_3FeO_3, F-$NaFeO_2$, H-Hematite, M-Magnetite, W-Wustite)

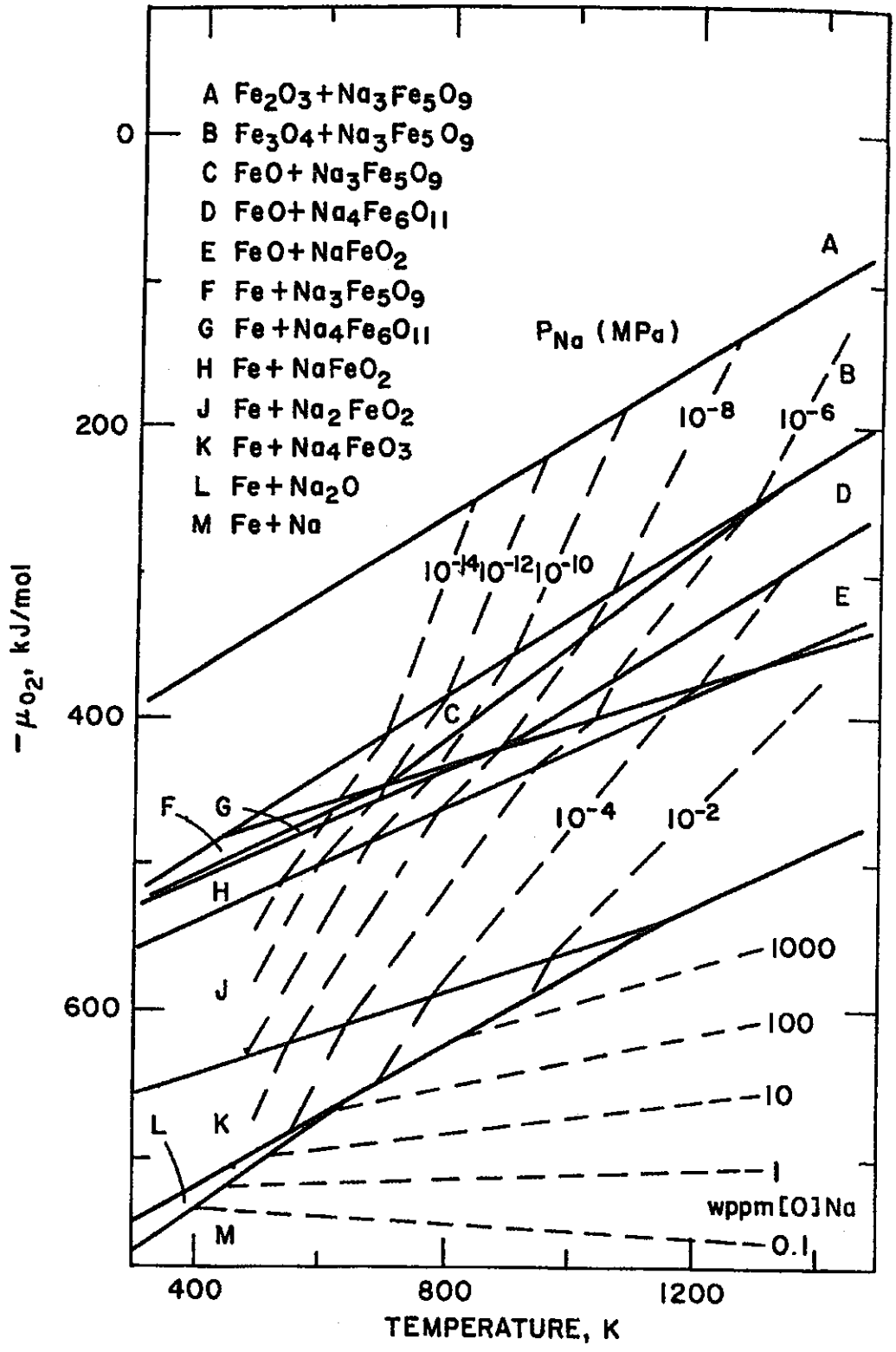

Fig. 15: Ellingham diagram for the Na-Fe-O system by Lindemer

Conclusion

Ternary phase diagrams of the Na-Fe-O system are far from complete due to lack of experimental data. By reviewing literature data together with recent DSC and vapor pressure measurements by the present authors, thermodynamic data of main ternary Na-Fe oxides Na_4FeO_3(s), Na_3FeO_3(s) and Na_5FeO_4(s) have been evaluated. New ternary phase diagrams of the Na-Fe-O system and chemical potentials diagrams have been constructed from room temperature to 1000K. Stability of the ternary oxides was quantitatively discussed.

References

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Appendix User database and log files for calculation

File No.1: Log file for potential diagram calculation of Na-Fe-O at 650K

```
@@LOGFILE GENERATED ON PC/WINDOWS NT      DATE 2001-12-27
@@Draw predominance phase diagram NA-FE-O at 650K
@@Using Huang's data of Na3FeO3 and Na4FeO3 together with MALT2's Na5FeO4
GO DATA
SW SSUB
DEF-SYS
NA FE O
GET
GO GIBBS
ENT-SP
FE1NA3O3
FE1NA3O3
ENT-PH
FE1NA3O3

1
FE1NA3O3

NO
YES
ENT-PARA
G(FE1NA3O3,FE1NA3O3;0)
298.15
-1228246+1071.5301*T-181.69*T*LN(T)-0.016695*T*T+1483500*T**(-1)

1500
N
ENT-SP
FE1NA4O3
FE1NA4O3
ENT-PH
FE1NA4O3

1
FE1NA4O3

NO
YES
ENT-PARA
G(FE1NA4O3,FE1NA4O3;0)
298.15
-1282201.237+1244.166*T-212.49*T*LN(T)-0.019155*T*T+1642000*T**(-1)

1500
N
ENT-SP
FE1NA5O4
FE1NA5O4
ENT-PH
FE1NA5O4
```

```
1
FE1NA5O4

NO
YES
ENT-PARA
G(FE1NA5O4,FE1NA5O4;0)
298.15
-1691381.13+1551.917*T-262.6*T*LN(T)-0.024*T*T+2228000*T**(-1)

1500
N
L-D
SCREEN

GO TAB
TAB-SUB
FE1NA3O3

101325
298.15
1500
100
SCREEN
TAB-SUB
FE1NA4O3

101325
298.15
1500
100
SCREEN
TAB-SUB
FE1NA5O4

101325
298.15
1500
100
SCREEN
go pol-3
s-c T=650,P=101325,N=1, lnacr(na,gas)=-50,lnacr(o2,gas)=-200
l-c
s-n-l
20000
1E-06
1E-30
Y
c-e

s-a-v
1
lnacr(na,gas)
-50
5

s-a-v
```

```
2
lnacr(o2,gas)
-200
5

map
post
set-title
SGTE+Huang, P=101325, T=650K
s-p-o
No, No, No, No, Yes,,,
ent
fun
lgPNa
log10(acr(na,gas)*101325)

ent
fun
lgPO2
log10(acr(o2,gas)*101325)

s-l-c-o
N
s-d-a
x
lgPNa
s-d-a
y
lgPO2
s-s-s
x,n
-15
5
s-s-s
y,n
-50
10
s-t
s-a-t-s
x
n
Sodium pressure, Pa
s-a-t-s
y
n
Oxygen pressure, Pa
s-c-t
UPPER_RIGHT
SGTE+Huang, P=101325, T=650K
plot
SCREEN
GO SYS
SET-INTER
---------- END of FILE No. 1 ----------
```

File No.2: Log file for Na-Fe-O phase diagram calculation at 650K

```
@@LOGFILE GENERATED ON PC/WINDOWS NT      DATE 2001-12-27
@@Draw NA-FE-O phase diagram at 650K
@@Using Huang's data of Na3FeO3 and Na4FeO3 together with MALT2's Na5FeO4
go data
sw SSUB
def-sys
na fe o
get
GO GIBBS
ENT-SP
FE1NA3O3
FE1NA3O3
ENT-PH
FE1NA3O3

1
FE1NA3O3

NO
YES
ENT-PARA
G(FE1NA3O3,FE1NA3O3;0)
298.15
-1228246+1071.5301*T-181.69*T*LN(T)-0.016695*T*T+1483500*T**(-1)

1500
N
ENT-SP
FE1NA4O3
FE1NA4O3
ENT-PH
FE1NA4O3

1
FE1NA4O3

NO
YES
ENT-PARA
G(FE1NA4O3,FE1NA4O3;0)
298.15
-1282201.237+1244.166*T-212.49*T*LN(T)-0.019155*T*T+1642000*T**(-1)

1500
N
ENT-SP
FE1NA5O4
FE1NA5O4
ENT-PH
FE1NA5O4

1
FE1NA5O4

NO
YES
```

```
ENT-PARA
G(FE1NA5O4,FE1NA5O4;0)
298.15
-1681381.13+1551.917*T-262.6*T*LN(T)-0.024*T*T+2228000*T**(-1)

1500
N
L-D
SCREEN

GO TAB
TAB-SUB
FE1NA3O3

101325
298.15
1500
100
SCREEN
TAB-SUB
FE1NA4O3

101325
298.15
1500
100
SCREEN
TAB-SUB
FE1NA5O4

101325
298.15
1500
100
SCREEN
go pol-3
s-n-l
20000
1E-06
1E-30
Y
s-c T=650, P=101325, n=1, x(na)=0.2, x(o)=0.5
L-C
c-e
ADD
add

S-A-V
1
X(NA)
0
1
.025
S-A-V
2
X(O)
0
1
.025
MAP
```

POST
S-D-T
Y
Y
Y
s-c-t
UPPER_RIGHT
T=650K, SGTE+Huang
PLOT
SCREEN
GO SYS
SET-INTER
EXIT

---------- END of FILE No. 2 ----------

File No.3: User database created for the Na-Fe-O-H system

```
$ Database file written 2002- 3-15
$
 ELEMENT /-   ELECTRON_GAS              0.0000E+00   0.0000E+00   0.0000E+00!
 ELEMENT VA   VACUUM                    0.0000E+00   0.0000E+00   0.0000E+00!
 ELEMENT FE   BCC(A2)                   5.5847E+01   0.0000E+00   6.5200E+00!
 ELEMENT H    1/2_MOLE_H2(G)            1.0079E+00   0.0000E+00   1.5603E+01!
 ELEMENT NA   BCC(A2)                   2.2990E+01   0.0000E+00   1.2260E+01!
 ELEMENT O    1/2_MOLE_O2(G)            1.5999E+01   0.0000E+00   2.4502E+01!

 SPECIES FE0.947O1                     FE0.947O1!
 SPECIES FE1H1O1                        FE1H1O1!
 SPECIES FE1H1O2                        FE1H1O2!
 SPECIES FE1H2O2                        FE1H2O2!
 SPECIES FE1H3O3                        FE1H3O3!
 SPECIES FE1NA1O2                       FE1NA1O2!
 SPECIES FE1O1                         FE1O1!
 SPECIES FE1O2                         FE1O2!
 SPECIES FE2H2O4                        FE2H2O4!
 SPECIES FE2O3                         FE2O3!
 SPECIES FE3O4                         FE3O4!
 SPECIES H1NA1                          H1NA1!
 SPECIES H1NA1O1                        H1NA1O1!
 SPECIES H1O1                          H1O1!
 SPECIES H1O2                          H1O2!
 SPECIES H2                            H2!
 SPECIES H2NA2O2                        H2NA2O2!
 SPECIES H2O1                          H2O1!
 SPECIES H2O2                          H2O2!
 SPECIES NA1O1                          NA1O1!
 SPECIES NA1O2                          NA1O2!
 SPECIES NA2                           NA2!
 SPECIES NA2O1                          NA2O1!
 SPECIES NA2O2                          NA2O2!
 SPECIES FE1NA3O3                       FE1NA3O3!
 SPECIES FE1NA4O3                       FE1NA4O3!
 SPECIES FE1NA5O4                       FE1NA5O4!
 SPECIES O2                            O2!
 SPECIES O3                            O3!

 FUNCTION F9454T       2.98150E+02   +405563.032+35.536443*T-32.8261*T*LN(T)
     +.00908265*T**2-1.34845667E-06*T**3+108791.4*T**(-1);  9.00000E+02   Y
      +414134.539-53.8401478*T-19.84276*T*LN(T)+6.959445E-05*T**2
     -1.30682983E-07*T**3-976411.5*T**(-1);  2.40000E+03   Y
      +410389.799-49.3269727*T-20.12513*T*LN(T)-5.66549E-04*T**2
     -5.290265E-08*T**3+887592*T**(-1);  5.50000E+03   Y
      +521855.538-375.147472*T+18.70844*T*LN(T)-.00634452*T**2
     +1.038655E-07*T**3-55487750*T**(-1);  1.00000E+04   N !
 FUNCTION F9508T       2.98150E+02   +249732.775+18.778107*T-37.98559*T*LN(T)
     +4.2210085E-04*T**2-2.25378667E-07*T**3+22271.26*T**(-1);  1.50000E+03
     Y
      +262903.037-60.5714542*T-27.43354*T*LN(T)-.0034932425*T**2
     +6.87334333E-08*T**3-3102568*T**(-1);  3.90000E+03   Y
      +253484.995-64.1799486*T-26.40668*T*LN(T)-.0045433265*T**2
     +1.32989417E-07*T**3+6792160*T**(-1);  6.00000E+03   N !
```

```
FUNCTION F9513T      2.98150E+02  +65439.2659-1.53488826*T-37.66195*T*LN(T)
    -.018843285*T**2+3.34079333E-06*T**3+208386.8*T**(-1);  7.00000E+02  Y
     +55703.5103+130.7305*T-57.76235*T*LN(T)-9.1828E-05*T**2
    +3.27092E-09*T**3+1105839*T**(-1);  6.00000E+03  N!
FUNCTION F12299T     2.98150E+02  +101202.044-12.9290068*T-21.02539*T*LN(T)
    +1.9194285E-04*T**2-2.37558167E-08*T**3+6714.165*T**(-1);  2.70000E+03
    Y
     +123818.458-80.8203215*T-13.00233*T*LN(T)-6.87485E-04*T**2
    -3.3153E-08*T**3-10435685*T**(-1);  5.50000E+03  Y
     +200317.377-314.322311*T+14.94379*T*LN(T)-.0049580625*T**2
    +8.45444167E-08*T**3-45680820*T**(-1);  9.60000E+03  Y
     -248549.945+382.618817*T-61.81729*T*LN(T)+8.73722E-04*T**2
    +1.54938383E-09*T**3+4.4661115E+08*T**(-1);  1.00000E+04  N!
FUNCTION F12307T     2.98150E+02  +95770.8472-1.68140505*T-33.33245*T*LN(T)
    -.00550342*T**2+7.49651167E-07*T**3+50626.15*T**(-1);  1.10000E+03  Y
     +92178.4123+47.1275967*T-40.64359*T*LN(T)+3.6413025E-04*T**2
    -7.7445E-08*T**3+297128.85*T**(-1);  3.10000E+03  Y
     +55380.3166+104.324159*T-46.25103*T*LN(T)-.0010187635*T**2
    +8.13418167E-08*T**3+24455830*T**(-1);  5.80000E+03  Y
     -132699.87+582.456962*T-102.3352*T*LN(T)+.00638169*T**2
    -1.00839067E-07*T**3+1.4234635E+08*T**(-1);  6.00000E+03  N!
FUNCTION F12339T     2.98150E+02  +131697.685+6.55101085*T-35.05636*T*LN(T)
    -.0039954535*T**2+5.82776667E-07*T**3-20127.66*T**(-1);  8.00000E+02  Y
     +123510.411+75.1001481*T-44.47351*T*LN(T)-5.345085E-04*T**2
    +6.400745E-07*T**3+1150765*T**(-1);  1.50000E+03  Y
     +79657.0271+417.408691*T-91.76357*T*LN(T)+.022097085*T**2
    -1.3875195E-06*T**3+8765605*T**(-1);  3.10000E+03  Y
     +841444.171-2436.16812*T+261.4099*T*LN(T)-.0509968*T**2
    +1.46319E-06*T**3-3.005069E+08*T**(-1);  4.80000E+03  Y
     -471200.866+911.74126*T-131.5149*T*LN(T)+.0011608825*T**2
    +1.68225167E-07*T**3+5.200375E+08*T**(-1);  6.00000E+03  N!
FUNCTION F12353T     2.98150E+02  -36208.3602+139.991847*T-60.99434*T*LN(T)
    -7.94846E-04*T**2+8.105565E-08*T**3+208188.85*T**(-1);  1.80000E+03  Y
     -37169.2598+149.534408*T-62.35718*T*LN(T)+8.054565E-08*T**2
    -9.43098333E-12*T**3+332214.75*T**(-1);  6.00000E+03  N!
FUNCTION F12365T     2.98150E+02  -149425.429+215.299821*T-74.07082*T*LN(T)
    -.007371005*T**2+1.12289333E-06*T**3+417484.75*T**(-1);  1.00000E+03  Y
     -154321.431+275.560967*T-83.0616*T*LN(T)-1.560291E-05*T**2
    +5.18616333E-10*T**3+925422*T**(-1);  6.00000E+03  N!
FUNCTION F12657T     2.98150E+02  +243206.494-20.8612582*T-21.01555*T*LN(T)
    +1.2687055E-04*T**2-1.23131283E-08*T**3-42897.09*T**(-1);  2.95000E+03
    Y
     +252301.423-52.0847281*T-17.21188*T*LN(T)-5.413565E-04*T**2
    +7.64520667E-09*T**3-3973170.5*T**(-1);  6.00000E+03  N!
FUNCTION F12999T     2.98150E+02  -6960.6927-51.1831467*T-22.25862*T*LN(T)
    -.01023867*T**2+1.339947E-06*T**3-76749.55*T**(-1);  9.00000E+02  Y
     -13136.0174+24.7432966*T-33.55726*T*LN(T)-.0012348985*T**2
    +1.66943333E-08*T**3+539886*T**(-1);  3.70000E+03  Y
     +14154.6459-51.485458*T-24.47978*T*LN(T)-.002634759*T**2
    +6.01544333E-08*T**3-15120935*T**(-1);  9.60000E+03  Y
     -314316.629+515.068037*T-87.56143*T*LN(T)+.0025787245*T**2
    -1.878765E-08*T**3+2.9052515E+08*T**(-1);  1.85000E+04  Y
     -108797.175+288.483019*T-63.737*T*LN(T)+.0014375*T**2-9E-09*T**3
    +.25153895*T**(-1);  2.00000E+04  N!
FUNCTION F13287T     2.98150E+02  +130696.944-37.9096643*T-27.58118*T*LN(T)
    -.02763076*T**2+4.60539333E-06*T**3+99530.45*T**(-1);  7.00000E+02  Y
     +114760.623+176.626737*T-60.10286*T*LN(T)+.00206456*T**2
    -5.17486667E-07*T**3+1572175*T**(-1);  1.30000E+03  Y
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      +49468.3956+710.09482*T-134.3696*T*LN(T)+.039707355*T**2
     -4.10457667E-06*T**3+12362250*T**(-1);  2.10000E+03  Y
      +866367.075-3566.80563*T+421.2001*T*LN(T)-.1284109*T**2
     +5.44768833E-06*T**3-2.1304835E+08*T**(-1);  2.80000E+03  Y
      +409416.383-1950.70834*T+223.4437*T*LN(T)-.0922361*T**2
     +4.306855E-06*T**3-21589870*T**(-1);  3.50000E+03  Y
      -1866338.6+6101.13383*T-764.8435*T*LN(T)+.09852775*T**2
     -2.59784667E-06*T**3+9.610855E+08*T**(-1);  4.90000E+03  Y
      +97590.043+890.798361*T-149.9608*T*LN(T)+.01283575*T**2
     -3.555105E-07*T**3-2.1699975E+08*T**(-1);  6.00000E+03  N !
FUNCTION F9499T       2.98150E+02  -723393.955+455.159127*T-80.54995*T*LN(T)
     -.00665277*T**2;  1.62000E+03  Y
      -778785.906+810.911031*T-125.52*T*LN(T);  2.00000E+03  N !
FUNCTION F9596T       2.98150E+02  -845288.29+691.537822*T-113.6403*T*LN(T)
     -.02191314*T**2-9.37486833E-10*T**3+813718.5*T**(-1);  1.00000E+03  N !
FUNCTION F9618T       2.98150E+02  -1145033.85+522.516651*T-91.5501*T*LN(T)
     -.1009995*T**2;  9.00000E+02  Y
      -1172889.17+1291.43857*T-213.4*T*LN(T);  1.87000E+03  Y
      -1149387.01+1184.18711*T-200.832*T*LN(T);  2.00000E+03  N !
FUNCTION F9449T       2.98150E+02  +1225.73315+124.13367*T-23.5143*T*LN(T)
     -.00439752*T**2-5.89269E-08*T**3+77358.5*T**(-1);  1.18480E+03  Y
      -1249.64059+133.270634*T-24.6643*T*LN(T)-.00375752*T**2
     -5.89269E-08*T**3+77358.5*T**(-1);  1.66750E+03  Y
      -613.084238+125.483902*T-23.5143*T*LN(T)-.00439752*T**2
     -5.89269E-08*T**3+77358.5*T**(-1);  1.81100E+03  Y
      -25628.1275+299.878719*T-46*T*LN(T);  6.00000E+03  N !
FUNCTION F9598T       2.98150E+02  -861152.96+602.345147*T-98.2801*T*LN(T)
     -.0389099*T**2+742500*T**(-1);  9.50000E+02  Y
      -874177.523+938.642928*T-150.6*T*LN(T);  1.05000E+03  Y
      -859410.428+803.714268*T-132.67*T*LN(T)-.003682*T**2;  1.75000E+03  N !
FUNCTION F12317T      2.98150E+02  -280135.425+293.555037*T-59.2651*T*LN(T)
     -.02131225*T**2+2.00263E-07*T**3-12159.79*T**(-1);  8.25000E+02  N !
FUNCTION F12347T      2.98150E+02  -430663.482+146.385926*T-27.21985*T*LN(T)
     -.076745*T**2+1.60958483E-05*T**3-209099.6*T**(-1);  6.00000E+02  Y
      -450304.11+485.311402*T-80.99387*T*LN(T)-.01093656*T**2
     +9.42725E-07*T**3+1147232*T**(-1);  1.02320E+03  Y
      -446703.464+489.879062*T-82.56287*T*LN(T)-.00617663*T**2;  1.24320E+03
      Y
      -446703.464+489.879062*T-82.56287*T*LN(T)-.00617663*T**2;  1.40520E+03
      Y
      -465473.746+654.281075*T-104.6*T*LN(T);  3.50000E+03  N !
FUNCTION F12361T      2.98150E+02  -541543.978+450.653631*T-77.90817*T*LN(T)
     -.035690775*T**2+4.83677333E-06*T**3+326469.15*T**(-1);  7.85000E+02  Y
      -551412.743+676.599499*T-113.5956*T*LN(T);  9.48000E+02  Y
      -554784.21+704.532725*T-117.152*T*LN(T);  3.50000E+03  N !
FUNCTION F12295T      2.00000E+02  -11989.4322+260.548717*T-51.03936*T*LN(T)
     +.07230665*T**2-4.36382833E-05*T**3+132153.75*T**(-1);  3.70800E+02  Y
      -10997.4282+199.589766*T-38.11988*T*LN(T)+.009745855*T**2
     -1.70664E-06*T**3+34342.48*T**(-1);  2.30000E+03  N !
FUNCTION F9447T       2.98150E+02  -278864.086+270.768206*T-48.79*T*LN(T)
     -.004185045*T**2+140000*T**(-1);  1.64400E+03  N !
FUNCTION UN_ASS       2.98150E+02  0.0 ;  3.00000E+02  N !
FUNCTION F9468T       2.98150E+02  +87159.2063+143.413995*T-59.02225*T*LN(T)
     +.00594678*T**2-1.55698683E-06*T**3+200864.85*T**(-1);  1.00000E+03  Y
      +96842.7077+22.7910378*T-41.09489*T*LN(T)-.00802325*T**2
     +4.10391E-07*T**3-694843*T**(-1);  3.00000E+03  Y
      +46261.1872+261.212868*T-71.58472*T*LN(T)+1.263785E-04*T**2
     +4.43522833E-09*T**3+15110770*T**(-1);  6.00000E+03  N !
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FUNCTION F9475T      2.98150E+02  -345.4458+62.8061583*T-48.74703*T*LN(T)
    -.022327*T**2+3.54829E-06*T**3+275025.5*T**(-1);  7.00000E+02  Y
     -9219.01892+186.198586*T-67.58338*T*LN(T)-.0042074325*T**2
    +2.18605833E-07*T**3+1073919*T**(-1);  2.90000E+03  Y
     -31864.0115+297.240975*T-81.88218*T*LN(T)-1.563072E-04*T**2
    +3.72014167E-09*T**3+7985695*T**(-1);  6.00000E+03  N!
FUNCTION F9482T      2.98150E+02  -335829.162+364.49668*T-96.60458*T*LN(T)
    +.0025303465*T**2-1.12857533E-06*T**3+499940.1*T**(-1);  1.20000E+03  Y
     -331017.442+286.133981*T-84.72734*T*LN(T)-.00730903*T**2
    +2.32372333E-07*T**3+485360.7*T**(-1);  5.50000E+03  Y
     -480847.001+716.769004*T-136.0473*T*LN(T)+3.980251E-04*T**2
    +1.84211E-08*T**3+81654150*T**(-1);  6.00000E+03  N!
FUNCTION F9878T      2.98150E+02  +211801.621+24.4989821*T-20.78611*T*LN(T);
     6.00000E+03  N!
FUNCTION F10057T     2.98150E+02  +132553.465-16.1455876*T-24.82785*T*LN(T)
    -.010652725*T**2+1.5821195E-06*T**3+2238.863*T**(-1);  8.00000E+02  Y
     +129256.792+35.5334784*T-32.81208*T*LN(T)-.0026811235*T**2
    +1.59482667E-07*T**3+223972.1*T**(-1);  2.50000E+03  Y
     +52224.6946+343.223031*T-71.12485*T*LN(T)+.00541529*T**2
    -1.38711217E-07*T**3+28391720*T**(-1);  5.80000E+03  Y
     +307909.677-276.144986*T+1.091352*T*LN(T)-.003663472*T**2
    +7.54038833E-08*T**3-1.4180265E+08*T**(-1);  6.00000E+03  N!
FUNCTION F10067T     2.98150E+02  -202543.241+122.373896*T-51.97142*T*LN(T)
    -.001140696*T**2-1.29730167E-07*T**3+192408.95*T**(-1);  1.50000E+03  Y
     -213936.602+173.046309*T-58.19573*T*LN(T)-6.575535E-04*T**2
    +1.92051E-08*T**3+3304368.5*T**(-1);  6.00000E+03  N!
FUNCTION F10091T     2.98150E+02  +30698.6896+15.9096457*T-29.97699*T*LN(T)
    +.001713168*T**2-6.799205E-07*T**3-25503.82*T**(-1);  1.00000E+03  Y
     +31735.5125-12.6866354*T-25.42186*T*LN(T)-.003149545*T**2
    +1.34404917E-07*T**3+116618.65*T**(-1);  3.00000E+03  Y
     +41016.0781-20.734325*T-24.94216*T*LN(T)-.0023107985*T**2
    +5.91863E-08*T**3-6415210*T**(-1);  8.60000E+03  Y
     -154907.953+370.326117*T-69.24542*T*LN(T)+.0019361405*T**2
    -1.47539017E-08*T**3+1.4391015E+08*T**(-1);  1.80000E+04  Y
     +326722.277-65.0792735*T-24.2768*T*LN(T)+6.42189E-05*T**2
    -1.30298483E-10*T**3-8.292415E+08*T**(-1);  2.00000E+04  N!
FUNCTION F10161T     2.98150E+02  +1075.64085-55.2420473*T-24.45435*T*LN(T)
    -.018507875*T**2+2.36297E-06*T**3-29469.05*T**(-1);  8.00000E+02  Y
     -7932.99186+54.201624*T-40.775*T*LN(T)-.00501027*T**2
    +2.122915E-07*T**3+925845*T**(-1);  3.60000E+03  Y
     -67875.8963+275.406717*T-68.1173*T*LN(T)+6.12331E-04*T**2
    -6.573855E-09*T**3+26048030*T**(-1);  6.00000E+03  N!
FUNCTION F10262T     2.98150E+02  -9522.9741+78.5273879*T-31.35707*T*LN(T)
    +.0027589925*T**2-7.46390667E-07*T**3+56582.3*T**(-1);  1.00000E+03  Y
     +180.108664-15.6128256*T-17.84857*T*LN(T)-.00584168*T**2
    +3.14618667E-07*T**3-1280036*T**(-1);  2.10000E+03  Y
     -18840.1663+92.3120255*T-32.05082*T*LN(T)-.0010728235*T**2
    +1.14281783E-08*T**3+3561002.5*T**(-1);  6.00000E+03  N!
FUNCTION F10359T     2.98150E+02  -626086.99+435.314719*T-111.5671*T*LN(T)
    -.0029656875*T**2-1.48530817E-07*T**3+494445.4*T**(-1);  1.60000E+03  Y
     -650929.035+547.724419*T-125.5184*T*LN(T)-.001162834*T**2
    +3.34162833E-08*T**3+7395070*T**(-1);  6.00000E+03  N!
FUNCTION F10378T     2.98150E+02  -250423.434+4.45470381*T-28.40916*T*LN(T)
    -.00623741*T**2-6.01526167E-08*T**3-64163.45*T**(-1);  1.10000E+03  Y
     -256145.88+30.1894688*T-31.43044*T*LN(T)-.007055445*T**2
    +3.05535833E-07*T**3+1246309.5*T**(-1);  2.80000E+03  Y
     -268423.418+116.690198*T-42.96842*T*LN(T)-.003069987*T**2
    +6.97594167E-08*T**3+2458230.5*T**(-1);  8.40000E+03  Y
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      -489068.882+553.259882*T-92.4077*T*LN(T)+.0016703495*T**2
     -1.32333233E-08*T**3+1.765625E+08*T**(-1);  1.80000E+04  Y
      -165728.771+239.645644*T-59.77872*T*LN(T)+2.213599E-04*T**2
     -1.2921095E-09*T**3-4.1931655E+08*T**(-1);  2.00000E+04  N !
 FUNCTION F10402T      2.98150E+02  -147258.971-37.1497204*T-26.10636*T*LN(T)
     -.036948065*T**2+6.659505E-06*T**3+65357.65*T**(-1);  7.00000E+02  Y
      -156470.506+120.191296*T-50.94271*T*LN(T)-.007931945*T**2
     +4.29733833E-07*T**3+684985.5*T**(-1);  1.50000E+03  N !
 FUNCTION F9473T       2.98150E+02  -587814.047+492.306083*T-80.19297*T*LN(T)
     -.01425421*T**2+2.42746667E-10*T**3+631693.5*T**(-1);  1.50000E+03  N !
 FUNCTION F9480T       2.98150E+02  -596587.698+555.75785*T-95.10392*T*LN(T)
     -.01424189*T**2+2.848015E-10*T**3+293151.4*T**(-1);  1.50000E+03  N !
 FUNCTION F9487T       2.98150E+02  -905596.077+1011.40452*T-162.4986*T*LN(T)
     -.00593129*T**2+1.74291167E-10*T**3+2179458*T**(-1);  1.50000E+03  N !
 FUNCTION F9570T       2.98150E+02  -1170358.1+1058.12928*T-175.728*T*LN(T);
     4.00000E+02  N !
 FUNCTION F10063T      2.98150E+02  -424509.968-80.2436771*T+7.885218*T*LN(T)
     -.07904065*T**2-2.43202E-08*T**3-901387.5*T**(-1);  5.72000E+02  Y
      -455494.079+522.040451*T-86*T*LN(T);  5.96000E+02  Y
      -451655.377+493.733782*T-82.28156*T*LN(T)-5.98098E-04*T**2
     +4.85977167E-11*T**3-546813.5*T**(-1);  3.00000E+03  N !
 FUNCTION F10053T      2.98150E+02  -68963.4802+183.619749*T-31.40199*T*LN(T)
     -.017664615*T**2-1.24852417E-09*T**3+246069.55*T**(-1);  9.11000E+02  Y
      -76169.9259+343.357419*T-56*T*LN(T)-2.210761E-15*T**2
     +2.674945E-19*T**3-2.818468E-07*T**(-1);  1.20000E+03  N !
 FUNCTION F10373T      2.98150E+02  -332319.672+1078.59563*T-186.8669*T*LN(T)
     +.2320948*T**2-9.14296167E-05*T**3+978019*T**(-1);  5.00000E+02  Y
      -62418.8793-3288.18729*T+495.1304*T*LN(T)-.504926*T**2
     +4.917665E-05*T**3-18523425*T**(-1);  5.40000E+02  Y
      -8528143.9+142414.45*T-22596.19*T*LN(T)+27.48508*T**2
     -.00631160667*T**3+5.63356E+08*T**(-1);  6.00000E+02  Y
      -331037.282+741.178606*T-117.41*T*LN(T);  6.01000E+02  N !
 FUNCTION F10406T      2.98150E+02  -214494.862+488.664598*T-89.3284*T*LN(T);
     1.50000E+03  N !

 TYPE_DEFINITION % SEQ *!
 DEFINE_SYSTEM_DEFAULT ELEMENT 2 !
 DEFAULT_COMMAND DEF_SYS_ELEMENT VA !


 PHASE GAS:G % 1 1.0 !
    CONSTITUENT GAS:G :FE,FE1H1O1,FE1H1O2,FE1H2O2,FE1O1,FE1O2,H,H1NA1,

H1NA1O1,H1O1,H1O2,H2,H2NA2O2,H2O1,H2O2,NA,NA1O1,NA2,NA2O1,NA2O2,O,O2,
O3
    : !

   PARAMETER G(GAS,FE;0)  2.98150E+02  +F9454T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF4363 !
   PARAMETER G(GAS,FE1H1O1;0)  2.98150E+02  +F9468T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF4366 !
   PARAMETER G(GAS,FE1H1O2;0)  2.98150E+02  +F9475T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF4368 !
   PARAMETER G(GAS,FE1H2O2;0)  2.98150E+02  +F9482T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF4370 !
   PARAMETER G(GAS,FE1O1;0)  2.98150E+02  +F9508T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF4386 !
   PARAMETER G(GAS,FE1O2;0)  2.98150E+02  +F9513T#+R#*T*LN(1E-05*P);
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```
 6.00000E+03    N REF4387 !
  PARAMETER G(GAS,H;0)  2.98150E+02  +F9878T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF4629 !
  PARAMETER G(GAS,H1NA1;0)  2.98150E+02  +F10057T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF4675 !
  PARAMETER G(GAS,H1NA1O1;0)  2.98150E+02  +F10067T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF4677 !
  PARAMETER G(GAS,H1O1;0)  2.98150E+02  +F10091T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF4682 !
  PARAMETER G(GAS,H1O2;0)  2.98150E+02  +F10161T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF4695 !
  PARAMETER G(GAS,H2;0)  2.98150E+02  +F10262T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF4716 !
  PARAMETER G(GAS,H2NA2O2;0)  2.98150E+02  +F10359T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF4744 !
  PARAMETER G(GAS,H2O1;0)  2.98150E+02  +F10378T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF4752 !
  PARAMETER G(GAS,H2O2;0)  2.98150E+02  +F10402T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF4756 !
  PARAMETER G(GAS,NA;0)  2.98150E+02  +F12299T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF5621 !
  PARAMETER G(GAS,NA1O1;0)  2.98150E+02  +F12307T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF5623 !
  PARAMETER G(GAS,NA2;0)  2.98150E+02  +F12339T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF5641 !
  PARAMETER G(GAS,NA2O1;0)  2.98150E+02  +F12353T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF5645 !
  PARAMETER G(GAS,NA2O2;0)  2.98150E+02  +F12365T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF5649 !
  PARAMETER G(GAS,O;0)  2.98150E+02  +F12657T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF5811 !
  PARAMETER G(GAS,O2;0)  2.98150E+02  +F12999T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF5888 !
  PARAMETER G(GAS,O3;0)  2.98150E+02  +F13287T#+R#*T*LN(1E-05*P);
 6.00000E+03    N REF5974 !


PHASE FE1H1O2_S  %  1  1.0  !
   CONSTITUENT FE1H1O2_S  :FE1H1O2 :  !

  PARAMETER G(FE1H1O2_S,FE1H1O2;0)  2.98150E+02  +F9473T#;    6.00000E+03
 N REF4367 !


PHASE FE1H2O2_S  %  1  1.0  !
   CONSTITUENT FE1H2O2_S  :FE1H2O2 :  !

  PARAMETER G(FE1H2O2_S,FE1H2O2;0)  2.98150E+02  +F9480T#;    6.00000E+03
 N REF4369 !


PHASE FE1H3O3_S  %  1  1.0  !
   CONSTITUENT FE1H3O3_S  :FE1H3O3 :  !

  PARAMETER G(FE1H3O3_S,FE1H3O3;0)  2.98150E+02  +F9487T#;    6.00000E+03
 N REF4371 !
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```
 PHASE FE1NA1O2_L  %  1  1.0  !
    CONSTITUENT FE1NA1O2_L  :FE1NA1O2 :  !

   PARAMETER G(FE1NA1O2_L,FE1NA1O2;0)  2.98150E+02  +F9499T#+49371
  -30.4759259*T;    6.00000E+03    N REF4380 !


 PHASE FE1NA1O2_S  %  1  1.0  !
    CONSTITUENT FE1NA1O2_S  :FE1NA1O2 :  !

   PARAMETER G(FE1NA1O2_S,FE1NA1O2;0)  2.98150E+02  +F9499T#;
6.00000E+03
   N REF4380 !


 PHASE FE2H2O4_S  %  1  1.0  !
    CONSTITUENT FE2H2O4_S  :FE2H2O4 :  !

   PARAMETER G(FE2H2O4_S,FE2H2O4;0)  2.98150E+02  +F9570T#;    6.00000E+03
  N REF4431 !


 PHASE FE2O3_GAMMA  %  1  1.0  !
    CONSTITUENT FE2O3_GAMMA  :FE2O3 :  !

   PARAMETER G(FE2O3_GAMMA,FE2O3;0)  2.98150E+02  +F9596T#;
6.00000E+03
  N REF4450 !


 PHASE FE3O4_L  %  1  1.0  !
    CONSTITUENT FE3O4_L  :FE3O4 :  !

   PARAMETER G(FE3O4_L,FE3O4;0)  2.98150E+02  +F9618T#+138072-73.8352941*T;
   6.00000E+03    N REF4470 !


 PHASE FE3O4_S  %  1  1.0  !
    CONSTITUENT FE3O4_S  :FE3O4 :  !

   PARAMETER G(FE3O4_S,FE3O4;0)  2.98150E+02  +F9618T#;    6.00000E+03    N
  REF4470 !


 PHASE FE_L  %  1  1.0  !
    CONSTITUENT FE_L  :FE :  !

   PARAMETER G(FE_L,FE;0)  2.98150E+02  +F9449T#+15644.6-8.97347268*T;
  6.00000E+03    N REF4361 !


 TYPE_DEFINITION & GES A_P_D FE_S MAGNETIC  -1.0     4.00000E-01 !
 PHASE FE_S  %&  1  1.0  !
    CONSTITUENT FE_S  :FE :  !

   PARAMETER G(FE_S,FE;0)  2.98150E+02  +F9449T#;    6.00000E+03    N
REF4361 !
   PARAMETER TC(FE_S,FE;0)  2.98150E+02  1043;  1.18480E+03  Y
```

```
 -201;  1.66750E+03  Y  1043;  1.81100E+03  Y  1E-05;  6.00000E+03  N
REF99 !
 PARAMETER BMAGN(FE_S,FE;0)  2.98150E+02  2.22;  1.18480E+03  Y
 -2.1;  1.66750E+03  Y  2.22;  1.81100E+03  Y  1E-05;  6.00000E+03  N
REF99 !


TYPE_DEFINITION ' GES A_P_D FE_S2 MAGNETIC  -3.0      2.80000E-01 !
PHASE FE_S2  %'  1  1.0  !
   CONSTITUENT FE_S2  :FE :  !

 PARAMETER G(FE_S2,FE;0)  2.98150E+02  +F9449T#+1012.8-.854827819*T;
6.00000E+03    N REF4361 !
 PARAMETER TC(FE_S2,FE;0)  2.98150E+02  1043;  1.18480E+03  Y
 -201;  1.66750E+03  Y  1043;  1.81100E+03  Y  1E-05;  6.00000E+03  N
REF99 !
 PARAMETER BMAGN(FE_S2,FE;0)  2.98150E+02  2.22;  1.18480E+03  Y
 -2.1;  1.66750E+03  Y  2.22;  1.81100E+03  Y  1E-05;  6.00000E+03  N
REF99 !


TYPE_DEFINITION ( GES A_P_D FE_S3 MAGNETIC  -1.0      4.00000E-01 !
PHASE FE_S3  %(  1  1.0  !
   CONSTITUENT FE_S3  :FE :  !

 PARAMETER G(FE_S3,FE;0)  2.98150E+02  +F9449T#+1838.6-1.3500602*T;
6.00000E+03    N REF4361 !
 PARAMETER TC(FE_S3,FE;0)  2.98150E+02  1043;  1.18480E+03  Y
 -201;  1.66750E+03  Y  1043;  1.81100E+03  Y  1E-05;  6.00000E+03  N
REF99 !
 PARAMETER BMAGN(FE_S3,FE;0)  2.98150E+02  2.22;  1.18480E+03  Y
 -2.1;  1.66750E+03  Y  2.22;  1.81100E+03  Y  1E-05;  6.00000E+03  N
REF99 !


PHASE H1NA1O1_L  %  1  1.0  !
   CONSTITUENT H1NA1O1_L  :H1NA1O1 :  !

 PARAMETER G(H1NA1O1_L,H1NA1O1;0)  2.98150E+02  +F10063T#+13650
-23.314521*T;    6.00000E+03    N REF4676 !


PHASE H1NA1O1_S  %  1  1.0  !
   CONSTITUENT H1NA1O1_S  :H1NA1O1 :  !

 PARAMETER G(H1NA1O1_S,H1NA1O1;0)  2.98150E+02  +F10063T#;
6.00000E+03
 N REF4676 !


PHASE H1NA1O1_S2  %  1  1.0  !
   CONSTITUENT H1NA1O1_S2  :H1NA1O1 :  !

 PARAMETER G(H1NA1O1_S2,H1NA1O1;0)  2.98150E+02  +F10063T#+5850
-10.2272727*T;    6.00000E+03    N REF4676 !


PHASE H1NA1_L  %  1  1.0  !
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```
    CONSTITUENT H1NA1_L  :H1NA1 :  !

   PARAMETER G(H1NA1_L,H1NA1;0)  2.98150E+02
+F10053T#+26000-28.5400659*T;
   6.00000E+03    N REF4674 !


 PHASE H1NA1_S  %  1  1.0  !
    CONSTITUENT H1NA1_S  :H1NA1 :  !

   PARAMETER G(H1NA1_S,H1NA1;0)  2.98150E+02  +F10053T#;  6.00000E+03  N
  REF4674 !


 PHASE H2O1_L  %  1  1.0  !
    CONSTITUENT H2O1_L  :H2O1 :  !

   PARAMETER G(H2O1_L,H2O1;0)  2.98150E+02  +F10373T#;  6.00000E+03  N
  REF4751 !


 PHASE H2O2_L  %  1  1.0  !
    CONSTITUENT H2O2_L  :H2O2 :  !

   PARAMETER G(H2O2_L,H2O2;0)  2.98150E+02  +F10406T#;  6.00000E+03  N
  REF4757 !


 PHASE HEMATITE  %  1  1.0  !
    CONSTITUENT HEMATITE  :FE2O3 :  !

   PARAMETER G(HEMATITE,FE2O3;0)  2.98150E+02  +F9598T#;  6.00000E+03
N
  REF4451 !


 PHASE NA1O2_S  %  1  1.0  !
    CONSTITUENT NA1O2_S  :NA1O2 :  !

   PARAMETER G(NA1O2_S,NA1O2;0)  2.98150E+02  +F12317T#;  6.00000E+03  N
  REF5625 !


 PHASE NA2O1_L  %  1  1.0  !
    CONSTITUENT NA2O1_L  :NA2O1 :  !

   PARAMETER G(NA2O1_L,NA2O1;0)  2.98150E+02
+F12347T#+61379.3-45.2527918*T;
    6.00000E+03    N REF5642 !


 PHASE NA2O1_S  %  1  1.0  !
    CONSTITUENT NA2O1_S  :NA2O1 :  !

   PARAMETER G(NA2O1_S,NA2O1;0)  2.98150E+02  +F12347T#;  6.00000E+03  N
  REF5642 !
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```
 PHASE NA2O1_S2  %  1  1.0  !
    CONSTITUENT NA2O1_S2  :NA2O1:  !

   PARAMETER G(NA2O1_S2,NA2O1;0)  2.98150E+02
+F12347T#+1757.3-1.71745504*T;
     6.00000E+03    N REF5642 !


 PHASE NA2O1_S3  %  1  1.0  !
    CONSTITUENT NA2O1_S3  :NA2O1:  !

   PARAMETER G(NA2O1_S3,NA2O1;0)  2.98150E+02  +F12347T#+13681.7
 -11.3091539*T;   6.00000E+03    N REF5642 !


 PHASE NA2O2_L  %  1  1.0  !
    CONSTITUENT NA2O2_L  :NA2O2:  !

   PARAMETER G(NA2O2_L,NA2O2;0)  2.98150E+02
+F12361T#+30250.3-33.1651184*T;
     6.00000E+03    N REF5647 !


 PHASE NA2O2_S  %  1  1.0  !
    CONSTITUENT NA2O2_S  :NA2O2:  !

   PARAMETER G(NA2O2_S,NA2O2;0)  2.98150E+02  +F12361T#;   6.00000E+03    N
  REF5647 !


 PHASE NA2O2_S2  %  1  1.0  !
    CONSTITUENT NA2O2_S2  :NA2O2:  !

   PARAMETER G(NA2O2_S2,NA2O2;0)  2.98150E+02
+F12361T#+5732.1-7.30203822*T;
     6.00000E+03    N REF5647 !


 PHASE NA_L  %  1  1.0  !
    CONSTITUENT NA_L  :NA:  !

   PARAMETER G(NA_L,NA;0)  2.98150E+02  +F12295T#+2597-7.00377562*T;
  6.00000E+03    N REF5619 !


 PHASE NA_S  %  1  1.0  !
    CONSTITUENT NA_S  :NA:  !

   PARAMETER G(NA_S,NA;0)  2.98150E+02  +F12295T#;   6.00000E+03    N
REF5619 !


 PHASE FE1NA3O3  %  1  1.0  !
    CONSTITUENT FE1NA3O3  :FE1NA3O3:  !

   PARAMETER G(FE1NA3O3,FE1NA3O3;0)  2.98150E+02  -1228246+1071.5301*T
  -181.69*T*LN(T)-.016695*T**2+1483500*T**(-1);  1.50000E+03  N REF99 !
```

```
PHASE FE1NA4O3  %  1  1.0  !
   CONSTITUENT FE1NA4O3  :FE1NA4O3 :  !

  PARAMETER G(FE1NA4O3,FE1NA4O3;0)  2.98150E+02  -1282201.24+1244.166*T
 -212.49*T*LN(T)-.019155*T**2+1642000*T**(-1);  1.50000E+03  N REF99 !


PHASE FE1NA5O4  %  1  1.0  !
   CONSTITUENT FE1NA5O4  :FE1NA5O4 :  !

  PARAMETER G(FE1NA5O4,FE1NA5O4;0)  2.98150E+02  -1691381.13+1551.917*T
 -262.6*T*LN(T)-.024*T**2+2228000*T**(-1);  1.50000E+03  N REF99 !


PHASE WUSTITE  %  1  1.0  !
   CONSTITUENT WUSTITE  :FE0.947O1 :  !

  PARAMETER G(WUSTITE,FE0.947O1;0)  2.98150E+02  +F9447T#;  6.00000E+03
 N REF4352 !

LIST_OF_REFERENCES
NUMBER  SOURCE
  REF4352  'Na3FeO3 and Na4FeO3 were defined by Dr. J. Huang
           Data were obtained by high temperature mass spectrometer
           Other data all from SGTE database'
 !
----------End of file No. 3----------
```

File No. 4: User database assessed for TERN-module calculation

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```
$ Database file written on 2002-3-14
$
DATABASE_INFO        '
This database is created by Dr. J. Huang based on vapor pressure '
measurement; Data of Na3FeO3 is original, Na4FeO3 is modified, '
Na5FeO4 from MALT2'
Note: when choosing starting elements,'
use (1)NA (2)FE and (3)O in order'
If no good, try other orders, Good luck'
 !

 ELEMENT /-   ELECTRON_GAS              0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT VA   VACUUM                    0.0000E+00  0.0000E+00  0.0000E+00!
 ELEMENT FE   BCC(A2)                   5.5847E+01  0.0000E+00  6.5200E+00!
 ELEMENT NA   BCC(A2)                   2.2990E+01  0.0000E+00  1.2260E+01!
 ELEMENT O    1/2_MOLE_O2(G)            1.5999E+01  0.0000E+00  2.4502E+01!

 SPECIES FE0.947O1                     FE0.947O1!
 SPECIES FE1NA1O2                       FE1NA1O2!
 SPECIES FE1O1                         FE1O1!
 SPECIES FE1O2                         FE1O2!
 SPECIES FE2O3                         FE2O3!
 SPECIES FE3O4                         FE3O4!
 SPECIES NA1O1                         NA1O1!
 SPECIES NA1O2                         NA1O2!
 SPECIES NA2                           NA2!
 SPECIES NA2O1                         NA2O1!
 SPECIES NA2O2                         NA2O2!
 SPECIES FE1NA3O3                       FE1NA3O3!
 SPECIES FE1NA4O3                       FE1NA4O3!
 SPECIES FE1NA5O4                       FE1NA5O4!
 SPECIES O2                            O2!
 SPECIES O3                            O3!


 FUNCTION F9454T      2.98150E+02  +405563.032+35.536443*T-32.8261*T*LN(T)
     +.00908265*T**2-1.34845667E-06*T**3+108791.4*T**(-1);  9.00000E+02  Y
      +414134.539-53.8401478*T-19.84276*T*LN(T)+6.959445E-05*T**2
     -1.30682983E-07*T**3-976411.5*T**(-1);  2.40000E+03  Y
      +410389.799-49.3269727*T-20.12513*T*LN(T)-5.66549E-04*T**2
     -5.290265E-08*T**3+887592*T**(-1);  5.50000E+03  Y
      +521855.538-375.147472*T+18.70844*T*LN(T)-.00634452*T**2
     +1.038655E-07*T**3-55487750*T**(-1);  1.00000E+04  N !
 FUNCTION F9508T      2.98150E+02  +249732.775+18.778107*T-37.98559*T*LN(T)
     +4.2210085E-04*T**2-2.25378667E-07*T**3+22271.26*T**(-1);  1.50000E+03
     Y
      +262903.037-60.5714542*T-27.43354*T*LN(T)-.0034932425*T**2
     +6.87334333E-08*T**3-3102568*T**(-1);  3.90000E+03  Y
      +253484.995-64.1799486*T-26.40668*T*LN(T)-.0045433265*T**2
     +1.32989417E-07*T**3+6792160*T**(-1);  6.00000E+03  N !
 FUNCTION F9513T      2.98150E+02  +65439.2659-1.53488826*T-37.66195*T*LN(T)
     -.018843285*T**2+3.34079333E-06*T**3+208386.8*T**(-1);  7.00000E+02  Y
```

```
     +55703.5103+130.7305*T-57.76235*T*LN(T)-9.1828E-05*T**2
    +3.27092E-09*T**3+1105839*T**(-1);  6.00000E+03  N !
FUNCTION F12299T     2.98150E+02  +101202.044-12.9290068*T-21.02539*T*LN(T)
    +1.9194285E-04*T**2-2.37558167E-08*T**3+6714.165*T**(-1);  2.70000E+03
    Y
     +123818.458-80.8203215*T-13.00233*T*LN(T)-6.87485E-04*T**2
    -3.3153E-08*T**3-10435685*T**(-1);  5.50000E+03  Y
     +200317.377-314.322311*T+14.94379*T*LN(T)-.0049580625*T**2
    +8.45444167E-08*T**3-45680820*T**(-1);  9.60000E+03  Y
     -248549.945+382.618817*T-61.81729*T*LN(T)+8.73722E-04*T**2
    +1.54938383E-09*T**3+4.4661115E+08*T**(-1);  1.00000E+04  N !
FUNCTION F12307T     2.98150E+02  +95770.8472-1.68140505*T-33.33245*T*LN(T)
    -.00550342*T**2+7.49651167E-07*T**3+50626.15*T**(-1);  1.10000E+03  Y
     +92178.4123+47.1275967*T-40.64359*T*LN(T)+3.6413025E-04*T**2
    -7.7445E-08*T**3+297128.85*T**(-1);  3.10000E+03  Y
     +55380.3166+104.324159*T-46.25103*T*LN(T)-.0010187635*T**2
    +8.13418167E-08*T**3+24455830*T**(-1);  5.80000E+03  Y
     -132699.87+582.456962*T-102.3352*T*LN(T)+.00638169*T**2
    -1.00839067E-07*T**3+1.4234635E+08*T**(-1);  6.00000E+03  N !
FUNCTION F12339T     2.98150E+02  +131697.685+6.55101085*T-35.05636*T*LN(T)
    -.0039954535*T**2+5.82776667E-07*T**3-20127.66*T**(-1);  8.00000E+02  Y
     +123510.411+75.1001481*T-44.47351*T*LN(T)-5.345085E-04*T**2
    +6.400745E-07*T**3+1150765*T**(-1);  1.50000E+03  Y
     +79657.0271+417.408691*T-91.76357*T*LN(T)+.022097085*T**2
    -1.3875195E-06*T**3+8765605*T**(-1);  3.10000E+03  Y
     +841444.171-2436.16812*T+261.4099*T*LN(T)-.0509968*T**2
    +1.46319E-06*T**3-3.005069E+08*T**(-1);  4.80000E+03  Y
     -471200.866+911.74126*T-131.5149*T*LN(T)+.0011608825*T**2
    +1.68225167E-07*T**3+5.200375E+08*T**(-1);  6.00000E+03  N !
FUNCTION F12353T     2.98150E+02  -36208.3602+139.991847*T-60.99434*T*LN(T)
    -7.94846E-04*T**2+8.105565E-08*T**3+208188.85*T**(-1);  1.80000E+03  Y
     -37169.2598+149.534408*T-62.35718*T*LN(T)+8.054565E-08*T**2
    -9.43098333E-12*T**3+332214.75*T**(-1);  6.00000E+03  N !
FUNCTION F12365T     2.98150E+02  -149425.429+215.299821*T-74.07082*T*LN(T)
    -.007371005*T**2+1.12289333E-06*T**3+417484.75*T**(-1);  1.00000E+03  Y
     -154321.431+275.560967*T-83.0616*T*LN(T)-1.560291E-05*T**2
    +5.18616333E-10*T**3+925422*T**(-1);  6.00000E+03  N !
FUNCTION F12657T     2.98150E+02  +243206.494-20.8612582*T-21.01555*T*LN(T)
    +1.2687055E-04*T**2-1.23131283E-08*T**3-42897.09*T**(-1);  2.95000E+03
    Y
     +252301.423-52.0847281*T-17.21188*T*LN(T)-5.413565E-04*T**2
    +7.64520667E-09*T**3-3973170.5*T**(-1);  6.00000E+03  N !
FUNCTION F12999T     2.98150E+02  -6960.6927-51.1831467*T-22.25862*T*LN(T)
    -.01023867*T**2+1.339947E-06*T**3-76749.55*T**(-1);  9.00000E+02  Y
     -13136.0174+24.7432966*T-33.55726*T*LN(T)-.0012348985*T**2
    +1.66943333E-08*T**3+539886*T**(-1);  3.70000E+03  Y
     +14154.6459-51.485458*T-24.47978*T*LN(T)-.002634759*T**2
    +6.01544333E-08*T**3-15120935*T**(-1);  9.60000E+03  Y
     -314316.629+515.068037*T-87.56143*T*LN(T)+.0025787245*T**2
    -1.878765E-08*T**3+2.9052515E+08*T**(-1);  1.85000E+04  Y
     -108797.175+288.483019*T-63.737*T*LN(T)+.0014375*T**2-9E-09*T**3
    +.25153895*T**(-1);  2.00000E+04  N !
FUNCTION F13287T     2.98150E+02  +130696.944-37.9096643*T-27.58118*T*LN(T)
    -.02763076*T**2+4.60539333E-06*T**3+99530.45*T**(-1);  7.00000E+02  Y
     +114760.623+176.626737*T-60.10286*T*LN(T)+.00206456*T**2
    -5.17486667E-07*T**3+1572175*T**(-1);  1.30000E+03  Y
     +49468.3956+710.09482*T-134.3696*T*LN(T)+.039707355*T**2
    -4.10457667E-06*T**3+12362250*T**(-1);  2.10000E+03  Y
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      +866367.075-3566.80563*T+421.2001*T*LN(T)-.1284109*T**2
     +5.44768833E-06*T**3-2.1304835E+08*T**(-1);  2.80000E+03  Y
      +409416.383-1950.70834*T+223.4437*T*LN(T)-.0922361*T**2
     +4.306855E-06*T**3-21589870*T**(-1);  3.50000E+03  Y
      -1866338.6+6101.13383*T-764.8435*T*LN(T)+.09852775*T**2
     -2.59784667E-06*T**3+9.610855E+08*T**(-1);  4.90000E+03  Y
      +97590.043+890.798361*T-149.9608*T*LN(T)+.01283575*T**2
     -3.555105E-07*T**3-2.1699975E+08*T**(-1);  6.00000E+03  N !
FUNCTION F9499T       2.98150E+02  -723393.955+455.159127*T-80.54995*T*LN(T)
    -.00665277*T**2;  1.62000E+03  Y
     -778785.906+810.911031*T-125.52*T*LN(T);  2.00000E+03  N !
FUNCTION F9596T       2.98150E+02  -845288.29+691.537822*T-113.6403*T*LN(T)
    -.02191314*T**2-9.37486833E-10*T**3+813718.5*T**(-1);  1.00000E+03  N !
FUNCTION F9618T       2.98150E+02  -1145033.85+522.516651*T-91.5501*T*LN(T)
    -.1009995*T**2;  9.00000E+02  Y
     -1172889.17+1291.43857*T-213.4*T*LN(T);  1.87000E+03  Y
     -1149387.01+1184.18711*T-200.832*T*LN(T);  2.00000E+03  N !
FUNCTION F9449T       2.98150E+02  +1225.73315+124.13367*T-23.5143*T*LN(T)
    -.00439752*T**2-5.89269E-08*T**3+77358.5*T**(-1);  1.18480E+03  Y
     -1249.64059+133.270634*T-24.6643*T*LN(T)-.00375752*T**2
    -5.89269E-08*T**3+77358.5*T**(-1);  1.66750E+03  Y
     -613.084238+125.483902*T-23.5143*T*LN(T)-.00439752*T**2
    -5.89269E-08*T**3+77358.5*T**(-1);  1.81100E+03  Y
     -25628.1275+299.878719*T-46*T*LN(T);  6.00000E+03  N !
FUNCTION F9598T       2.98150E+02  -861152.96+602.345147*T-98.2801*T*LN(T)
    -.0389099*T**2+742500*T**(-1);  9.50000E+02  Y
     -874177.523+938.642928*T-150.6*T*LN(T);  1.05000E+03  Y
     -859410.428+803.714268*T-132.67*T*LN(T)-.003682*T**2;  1.75000E+03  N !
FUNCTION F12317T      2.98150E+02  -280135.425+293.555037*T-59.2651*T*LN(T)
    -.02131225*T**2+2.00263E-07*T**3-12159.79*T**(-1);  8.25000E+02  N !
FUNCTION F12347T      2.98150E+02  -430663.482+146.385926*T-27.21985*T*LN(T)
    -.076745*T**2+1.60958483E-05*T**3-209099.6*T**(-1);  6.00000E+02  Y
     -450304.11+485.311402*T-80.99387*T*LN(T)-.01093656*T**2
    +9.42725E-07*T**3+1147232*T**(-1);  1.02320E+03  Y
     -446703.464+489.879062*T-82.56287*T*LN(T)-.00617663*T**2;  1.24320E+03
     Y
     -446703.464+489.879062*T-82.56287*T*LN(T)-.00617663*T**2;  1.40520E+03
     Y
     -465473.746+654.281075*T-104.6*T*LN(T);  3.50000E+03  N !
FUNCTION F12361T      2.98150E+02  -541543.978+450.653631*T-77.90817*T*LN(T)
    -.035690775*T**2+4.83677333E-06*T**3+326469.15*T**(-1);  7.85000E+02  Y
     -551412.743+676.599499*T-113.5956*T*LN(T);  9.48000E+02  Y
     -554784.21+704.532725*T-117.152*T*LN(T);  3.50000E+03  N !
FUNCTION F12295T      2.00000E+02  -11989.4322+260.548717*T-51.03936*T*LN(T)
    +.07230665*T**2-4.36382833E-05*T**3+132153.75*T**(-1);  3.70800E+02  Y
     -10997.4282+199.589766*T-38.11988*T*LN(T)+.009745855*T**2
    -1.70664E-06*T**3+34342.48*T**(-1);  2.30000E+03  N !
FUNCTION F9447T       2.98150E+02  -278864.086+270.768206*T-48.79*T*LN(T)
    -.004185045*T**2+140000*T**(-1);  1.64400E+03  N !
FUNCTION UN_ASS 298.15 0; 300 N !

TYPE_DEFINITION % SEQ *!
DEFINE_SYSTEM_DEFAULT ELEMENT 2 !
DEFAULT_COMMAND DEF_SYS_ELEMENT VA !


PHASE GAS:G %  1  1.0  !
   CONSTITUENT
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GAS:G :FE,FE1O1,FE1O2,NA,NA1O1,NA2,NA2O1,NA2O2,O,O2,O3 :  !

   PARAMETER G(GAS,FE;0)  2.98150E+02  +F9454T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF4363 !
   PARAMETER G(GAS,FE1O1;0)  2.98150E+02  +F9508T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF4386 !
   PARAMETER G(GAS,FE1O2;0)  2.98150E+02  +F9513T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF4387 !
   PARAMETER G(GAS,NA;0)  2.98150E+02  +F12299T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF5621 !
   PARAMETER G(GAS,NA1O1;0)  2.98150E+02  +F12307T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF5623 !
   PARAMETER G(GAS,NA2;0)  2.98150E+02  +F12339T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF5641 !
   PARAMETER G(GAS,NA2O1;0)  2.98150E+02  +F12353T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF5645 !
   PARAMETER G(GAS,NA2O2;0)  2.98150E+02  +F12365T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF5649 !
   PARAMETER G(GAS,O;0)  2.98150E+02  +F12657T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF5811 !
   PARAMETER G(GAS,O2;0)  2.98150E+02  +F12999T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF5888 !
   PARAMETER G(GAS,O3;0)  2.98150E+02  +F13287T#+R#*T*LN(1E-05*P);
  6.00000E+03    N REF5974 !


 PHASE FE1NA1O2_L  %  1  1.0  !
    CONSTITUENT FE1NA1O2_L  :FE1NA1O2 :  !

   PARAMETER G(FE1NA1O2_L,FE1NA1O2;0)  2.98150E+02  +F9499T#+49371
  -30.4759259*T;    6.00000E+03    N REF4380 !


 PHASE FE1NA1O2_S  %  1  1.0  !
    CONSTITUENT FE1NA1O2_S  :FE1NA1O2 :  !

   PARAMETER G(FE1NA1O2_S,FE1NA1O2;0)  2.98150E+02  +F9499T#;
6.00000E+03
   N REF4380 !


 PHASE FE2O3_GAMMA  %  1  1.0  !
    CONSTITUENT FE2O3_GAMMA  :FE2O3 :  !

   PARAMETER G(FE2O3_GAMMA,FE2O3;0)  2.98150E+02  +F9596T#;
6.00000E+03
  N REF4450 !


 PHASE FE3O4_L  %  1  1.0  !
    CONSTITUENT FE3O4_L  :FE3O4 :  !

   PARAMETER G(FE3O4_L,FE3O4;0)  2.98150E+02  +F9618T#+138072-73.8352941*T;
   6.00000E+03    N REF4470 !


 PHASE FE3O4_S  %  1  1.0  !
    CONSTITUENT FE3O4_S  :FE3O4 :  !
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   PARAMETER G(FE3O4_S,FE3O4;0)  2.98150E+02  +F9618T#;   6.00000E+03   N
  REF4470 !


 PHASE FE_L  %  1  1.0  !
    CONSTITUENT FE_L  :FE :  !

   PARAMETER G(FE_L,FE;0)  2.98150E+02  +F9449T#+15644.6-8.97347268*T;
  6.00000E+03   N REF4361 !


 TYPE_DEFINITION & GES A_P_D FE_S MAGNETIC  -1.0     4.00000E-01 !
 PHASE FE_S  %&  1  1.0  !
    CONSTITUENT FE_S  :FE :  !

   PARAMETER G(FE_S,FE;0)  2.98150E+02  +F9449T#;   6.00000E+03   N
REF4361 !
   PARAMETER TC(FE_S,FE;0)  2.98150E+02  1043;  1.18480E+03  Y
   -201;  1.66750E+03  Y  1043;  1.81100E+03  Y  1E-05;  6.00000E+03  N REF0 !
   PARAMETER BMAGN(FE_S,FE;0)  2.98150E+02  2.22;  1.18480E+03  Y
   -2.1;  1.66750E+03  Y  2.22;  1.81100E+03  Y  1E-05;  6.00000E+03  N REF0 !


 TYPE_DEFINITION ' GES A_P_D FE_S2 MAGNETIC  -3.0     2.80000E-01 !
 PHASE FE_S2  %'  1  1.0  !
    CONSTITUENT FE_S2  :FE :  !

   PARAMETER G(FE_S2,FE;0)  2.98150E+02  +F9449T#+1012.8-.854827819*T;
  6.00000E+03   N REF4361 !
   PARAMETER TC(FE_S2,FE;0)  2.98150E+02  1043;  1.18480E+03  Y
   -201;  1.66750E+03  Y  1043;  1.81100E+03  Y  1E-05;  6.00000E+03  N REF0 !
   PARAMETER BMAGN(FE_S2,FE;0)  2.98150E+02  2.22;  1.18480E+03  Y
   -2.1;  1.66750E+03  Y  2.22;  1.81100E+03  Y  1E-05;  6.00000E+03  N REF0 !


 TYPE_DEFINITION ( GES A_P_D FE_S3 MAGNETIC  -1.0     4.00000E-01 !
 PHASE FE_S3  %(  1  1.0  !
    CONSTITUENT FE_S3  :FE :  !

   PARAMETER G(FE_S3,FE;0)  2.98150E+02  +F9449T#+1838.6-1.3500602*T;
  6.00000E+03   N REF4361 !
   PARAMETER TC(FE_S3,FE;0)  2.98150E+02  1043;  1.18480E+03  Y
   -201;  1.66750E+03  Y  1043;  1.81100E+03  Y  1E-05;  6.00000E+03  N REF0 !
   PARAMETER BMAGN(FE_S3,FE;0)  2.98150E+02  2.22;  1.18480E+03  Y
   -2.1;  1.66750E+03  Y  2.22;  1.81100E+03  Y  1E-05;  6.00000E+03  N REF0 !


 PHASE HEMATITE  %  1  1.0  !
    CONSTITUENT HEMATITE  :FE2O3 :  !

   PARAMETER G(HEMATITE,FE2O3;0)  2.98150E+02  +F9598T#;   6.00000E+03
N
  REF4451 !


 PHASE NA1O2_S  %  1  1.0  !
    CONSTITUENT NA1O2_S  :NA1O2 :  !
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  PARAMETER G(NA1O2_S,NA1O2;0)  2.98150E+02  +F12317T#;  6.00000E+03  N
 REF5625 !


 PHASE NA2O1_L  %  1  1.0  !
   CONSTITUENT NA2O1_L  :NA2O1 :  !

  PARAMETER G(NA2O1_L,NA2O1;0)  2.98150E+02
+F12347T#+61379.3-45.2527918*T;
    6.00000E+03  N REF5642 !


 PHASE NA2O1_S  %  1  1.0  !
   CONSTITUENT NA2O1_S  :NA2O1 :  !

  PARAMETER G(NA2O1_S,NA2O1;0)  2.98150E+02  +F12347T#;  6.00000E+03  N
 REF5642 !


 PHASE NA2O1_S2  %  1  1.0  !
   CONSTITUENT NA2O1_S2  :NA2O1 :  !

  PARAMETER G(NA2O1_S2,NA2O1;0)  2.98150E+02
+F12347T#+1757.3-1.71745504*T;
    6.00000E+03  N REF5642 !


 PHASE NA2O1_S3  %  1  1.0  !
   CONSTITUENT NA2O1_S3  :NA2O1 :  !

  PARAMETER G(NA2O1_S3,NA2O1;0)  2.98150E+02  +F12347T#+13681.7
 -11.3091539*T;  6.00000E+03  N REF5642 !


 PHASE NA2O2_L  %  1  1.0  !
   CONSTITUENT NA2O2_L  :NA2O2 :  !

  PARAMETER G(NA2O2_L,NA2O2;0)  2.98150E+02
+F12361T#+30250.3-33.1651184*T;
    6.00000E+03  N REF5647 !


 PHASE NA2O2_S  %  1  1.0  !
   CONSTITUENT NA2O2_S  :NA2O2 :  !

  PARAMETER G(NA2O2_S,NA2O2;0)  2.98150E+02  +F12361T#;  6.00000E+03  N
 REF5647 !


 PHASE NA2O2_S2  %  1  1.0  !
   CONSTITUENT NA2O2_S2  :NA2O2 :  !

  PARAMETER G(NA2O2_S2,NA2O2;0)  2.98150E+02
+F12361T#+5732.1-7.30203822*T;
    6.00000E+03  N REF5647 !
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 PHASE NA_L  %  1  1.0  !
    CONSTITUENT NA_L  :NA :  !

   PARAMETER G(NA_L,NA;0)  2.98150E+02  +F12295T#+2597-7.00377562*T;
  6.00000E+03    N REF5619 !


 PHASE NA_S  %  1  1.0  !
    CONSTITUENT NA_S  :NA :  !

   PARAMETER G(NA_S,NA;0)  2.98150E+02  +F12295T#;    6.00000E+03    N
REF5619 !


 PHASE FE1NA3O3  %  1  1.0  !
    CONSTITUENT FE1NA3O3  :FE1NA3O3 :  !

   PARAMETER G(FE1NA3O3,FE1NA3O3;0)  2.98150E+02  -1228246+1071.5301*T
  -181.69*T*LN(T)-.016695*T**2+1483500*T**(-1);  1.50000E+03  N REF0 !


 PHASE FE1NA4O3  %  1  1.0  !
    CONSTITUENT FE1NA4O3  :FE1NA4O3 :  !

   PARAMETER G(FE1NA4O3,FE1NA4O3;0)  2.98150E+02  -1282201.24+1244.166*T
  -212.49*T*LN(T)-.019155*T**2+1642000*T**(-1);  1.50000E+03  N REF0 !


 PHASE FE1NA5O4  %  1  1.0  !
    CONSTITUENT FE1NA5O4  :FE1NA5O4 :  !

   PARAMETER G(FE1NA5O4,FE1NA5O4;0)  2.98150E+02  -1691381.13+1551.917*T
  -262.6*T*LN(T)-.024*T**2+2228000*T**(-1);  1.50000E+03  N REF0 !


 PHASE WUSTITE  %  1  1.0  !
    CONSTITUENT WUSTITE  :FE0.947O1 :  !

   PARAMETER G(WUSTITE,FE0.947O1;0)  2.98150E+02  +F9447T#;    6.00000E+03
  N REF4352 !

ASSESSED_SYSTEM FE-NA-O(;P3 *) !

 LIST_OF_REFERENCES
 NUMBER   SOURCE
   REF4363  'Ref4363: FE1<G> T.C.R.A.S Class: 1'
   REF4386  'Ref4386: FE1O1<G> T.C.R.A.S Class: 4'
   REF4387  'Ref4387: FE1O2<G> T.C.R.A.S Class: 6'
   REF5621  'Ref5621: NA1<G> T.C.R.A.S Class: 1'
   REF5623  'Ref5623: NA1O1<G> T.C.R.A.S Class: 4'
   REF5641  'Ref5641: NA2<G> T.C.R.A.S Class: 2'
   REF5645  'Ref5645: NA2O1<G> T.C.R.A.S Class: 6'
   REF5649  'Ref5649: NA2O2<G> T.C.R.A.S Class: 6'
   REF5811  'Ref5811: O1<G> JANAF 1982; ASSESSMENT DATED 3/77 SGTE'
   REF5888  'Ref5888: O2<G> T.C.R.A.S Class: 1'
   REF5974  'Ref5974: O3<G> T.C.R.A.S Class: 4'
   REF4380  'Ref4380: FE1NA1O2 THERMODATA 28/01/93 Condensed Standard State.'
   REF4450  'Ref4450: FE2O3<FE2O3_GAMMA> T.C.R.A.S Class: 6'
```

REF4470 'Ref4470: FE3O4 JANAF THERMOCHEMICAL TABLES SGTE Data sent by P. spencer 02/94. Data for liquid kept (source Janaf)'
REF4361 'Ref4361: FE1 S.G.T.E Data from SGTE Unary DB'
REF0 'Ref0: Defined by Dr. Jintao Huang from original experimental results by vapor pressure measurements, 2002'
REF4451 'Ref4451: FE2O3<HEMATITE> S.G.T.E. SGTE Data sent by Philip 02/94.'
REF5625 'Ref5625: NA1O2 JANAF THERMOCHEMICAL TABLES SGTE BY JANAF AT 6/63
Melts at 825 +- 10K.'
REF5642 'Ref5642: NA2O1 JANAF THERMOCHEMICAL TABLES SGTE TRANS GAMMA-BETA
AT 1023.2K,TRANS BETA-ALPHA AT 1243.2K.DECOMPOSITION AT PUBLISHED BY JANAF
AT 6/68. REVISED VALUE OF DH298 BY KUBA 1984.'
REF5647 'Ref5647: NA2O2 JANAF THERMOCHEMICAL TABLES SGTE BY JANAF AT 6/68 .'
REF5619 'Ref5619: NA1 S.G.T.E. Data from SGTE Unary DB'
REF4352 'Ref4352: FE0.947O1<WUSTITE> S.G.T.E. SGTE FE0.947O. Data from P. Spencer sent 02/94. Data from liquid kept from SGTE92.
Corrected Dec 1994. SL 0 0 1644.00 31338.2 NONE NONE
Cp 4 0.000 1.000 2.000 -2.000
6.819920E+01 0.000000E+00 0.000000E+00 0.000000E+00
Data for the liquid phase removed Dec.20 because solid decomposes below 1644 (comment frmo P.J. Spencer)'
!

---------- End of file No. 4 ----------