New Features of Update

Chapter 7 New Features of MALT for Windows Version 2

Of the MANUAL of MALT for Windows

Appendex 2 References which were mainly used in establishing MALT Database(Updated)

Appendex 2 Pourbaix diagram in CHD version 2

New Features of gem 2

Capter 7 New Features in MALT for Windows Version 2

7.1 Expansion of Database

Efforts have been made to collect as many compounds and species as possible. Particular efforts have been made on the following compounds and species:

1) High temperature compounds and gaseous species. In addition to double oxide compounds/species, double halides are also targeted to expand the availability of database.

2) Aqueous species are included from this version. Since the MALT database relies on the NBS chemical thermodynamic data, one strategy is adopted so as to be consistent with the MALT policies; that is, wherever the data are available in the NBS chemical thermodynamic data, such data are adopted first. The last compilation of the NBS data was made in 1982. Since then many data compilations have been made on the aqueous species. Some are made so as to be consistent with the NBS data, whereas others are made on the basis of CODATA recommended values and their consistent data. When such consistency is described, those data which are consistent with the NBS data are adopted in the MALT database.

As a result, numbers of stored compounds/species can be summarized as follows: Here, original and updated compounds are those stored in MALT for Windows version 1 which contained initially 4932 species. This means 6

Table 7.1 Number of compounds/species stored in MALT for Windows, original and updated in vers. 1, and newly added in vers.2

	original	updated	newly added	total
solid	2133	151	1397	3681
liquid	272	0	25	297
aqueous	0	0	1097	1097
gas	2305	65	58	2428
total	4710	216	2577	7503

compounds are deleted: 2 out of 6 is completely deleted because of inappropriateness, whereas 4 compounds are replaced by changing the compound stoichiomentric numbers, for example, from Sr3Fe2O6 to Sr1.5FeO3.

7.2 Special Treatments for Aqueous Species

Originally, the MALT database is designed for high temperature use. This implies that all compound data have the data at 298.15 K as well as the high temperature heat capacity. On the other hand, the thermodynamic properties concerning the aqueous species are mainly available at the standard temperature. Actually, in the NBS chemical thermodynamic data, many data are available only at 298.15 K and in many cases, there can be seen lack in the data of standard enthalpy for formation, the standard Gibbs energy for formation and the standard entropy. In the present compilation of the MALT database, the aqueous species are stored only when those three properties are available. Furthermore, even when the high temperature heat capacity is not available, such data are included in the database. Therefore, special care must be taken.

1) In the MALT main program, some functions are restricted for those species having no high temperature heat capacity. For keeping the simple database managing system, hypothetical zero heat capacity is set for those species but the valid temperature region is strictly confined only at 298.15 K. Thus, no extrapolation can be applied for such species

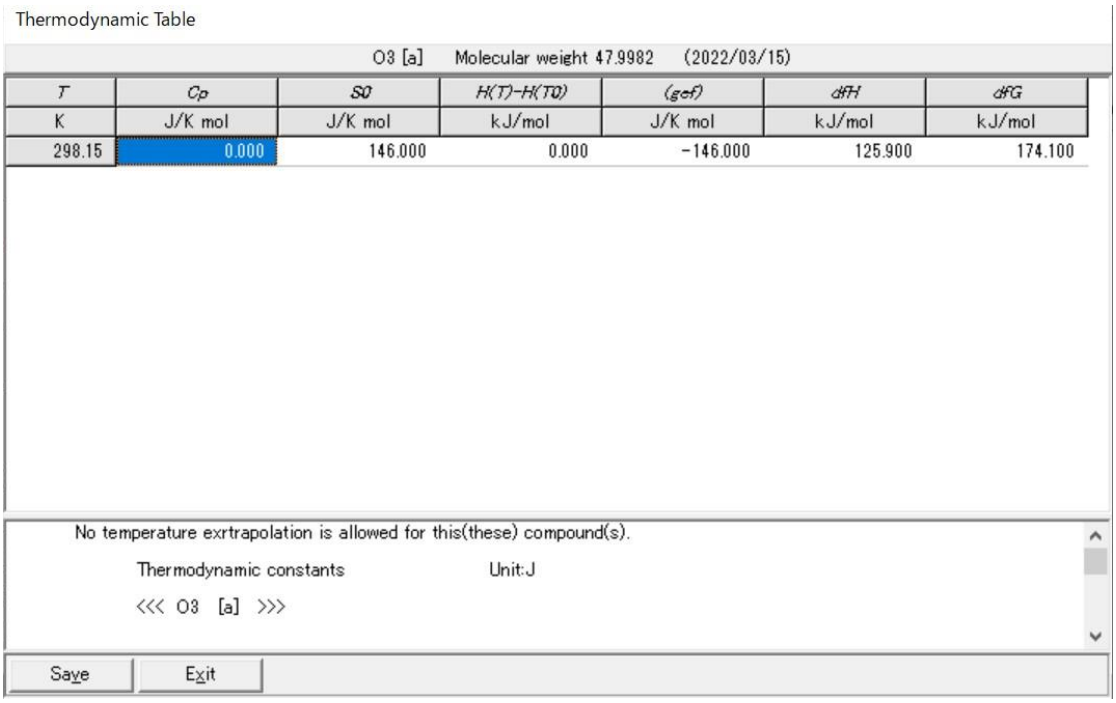

Fig. 7.1 Thermodynamic table for those aqueous species having no high temperature heat capacity. Special message is given in the comment column.

2) On the other hand, there is growing interest in utilizing the aqueous species at higher temperature particular in the mineralogy field. In order to meet such interest, the MALT database provide high temperature heat capacity values in the wider temperature region on the basis of recent advances in treatment of heat capacity for the aqueous species.

3) In the MALT related software, gem and CHD, special treatments are also adopted for those aqueous species having no heat capacities. Both gem and CHD have great advantages in handling many compounds involved in thermodynamic equilibrium. Therefore, always special warning will be made whenever those species having no high temperature heat capacity are involved in a targeted calculation in gem or CHD. Default setting is to exclude those species when calculations will be made other temperature than 298.15 K.

7.3 Handling UserDataBase

Some new functions of handling thermodynamic data are added for user database as well as the MALT database.

1) Read All Data from User DataBase: To assist the management of user database, this function is added. All compounds/species are retrieved so that any of those compounds can be edited in a systematical way using normal MALT data managing facilities.

2) Out of Target: Retrieval will be made for the MALT main database as well as the given user database in a special manner and this repeatedly will provide the same set of retrieved compounds. Even so, after retrieval, some of those compounds/species can be deleted out of such retrieved ones. For example, the menu of search Compounds/Delete Compounds provides such a procedure. Those compounds to be deleted from the retrieval table can be selected by using the compound table. In such a case, those deleted compounds/species can be stored in the file. In the next retrieval, those selected compounds listed in the file are automatically excluded. Any compounds in the MALT main database or in the user database can be selected as candidates for this exclusion. The list of Out Of Target can be edited by selecting the menu of Search Compounds/Out of Target.

Appendix 2. References which were mainly used in establishing MALT Database

1. Wagman, D. D. Evans, W. H., Parker, V. B., Schumm, R. H., Halow, I., Bailey, S. M., Churney, K. L., Nuttall, R. L.; The NBS tables of chemical thermodynamic properties, selected values for inorganic and C_1 and C_2 organic substances in SI units; J. Phys. *Chem. Ref. Data* Vol. **2**, Supplement No. 2, 1982.
2. JANAF Thermochemical Tables:
   (a) Stull, D. R., Prophet, H.; 2nd ed., 1971, NSRDS-NBS-37:
   (b) Chase, M. W., Jr., Curnutt, J. L., Hu, A. T., Prophet, H., Syverud, A. N., Walker, L. C.; *J. Phys. Chem. Ref. Data* **3**, 311, 1974:
   (c) Chase, M. W., Jr., Curnutt, J. L., Prophet, H., McDonald, R. A., Syverud, A. N.; *J. Phys. Chem. Ref. Data* **4**, 1, 1975:
   (d) Chase, M. W., Jr., Curnutt, J. L., McDonald, R. A., Syverud, A. N.; *J. Phys. Chem. Ref. Data* **7**, 793, 1978:
   (e) Chase, M. W., Jr., Curnutt, J. R., Downey, J. R., Jr., McDonald, R. A., Syverud, A. N., Valenzuela, E. A.; *J. Phys. Chem. Ref. Data* **11**, 695, 1982:
   (f) Chase, M. W., Jr., Davies, C. A., Downey, J. R., Jr., Frurip, D. J., McDonald, R. A., Syverud, A. N.; *J. Phys. Chem. Ref. Data* **14** Supplement No. 1, 1985.
3. Kubaschewski, O., Alcock, C. B.; Metallurgical Thermochemistry 5th ed.; 1979; Pergamon, Oxford.
4. Mills, K. C.; Thermodynamic Data for Inorganic Sulphides, Selenides and Tellurides; 1974; Butterworths, London.
5. Hultgren, R., Desai, P. D., Gleiser, M., Kelley, K. K.; Selected Values of the Thermodynamic Properties of the Elements; 1973; The American Society for Metals, Metals Park.
6. Barin, I., Knacke, O; Thermodynamic Properties of Inorganic Substances; 1973; Verlag Stahleisen, Berlin.
7. Barin, I., Knacke, O., Kubaschewski, O.; Thermodynamic Properties of Inorganic Substances Supplement; 1977; Verlag Stahleisen, Berlin.
8. Robie, R. A., Hemingway, B. S., Fisher, J. R.; Thermodynamic Properties of Minerals and Related Substances at 298.15 K and 1 Bars (10^5 Pascals) Pressure and at High Temperatures; 1978; US Government Printing Office, Washington.

9. Stull, D. R., Westrum, E. F., Jr., Sinke, G. C.; The Chemical Thermodynamics of Organic Compounds; 1969; John Wiley & sons, New York.
10. Stull, D. R., Sinke, G. C.; Thermodynamic Properties of the Elements; Advances in Chemistry Series 18; 1956; American Chemical Society, Washington.
11. Glushkov, V. P., Gurvich, L. V., Bergman, G. A., Veitz, I. V., Medvedev, V. A., Khachkuruzov, G. A., Yungman, V. A.; Thermodynamic Data for Individual Substances; High temperature Institute, State Institute of Applied Chemistry, National Academy of Sciences of the U. S. S. R., Moscow.
    Vol.1: The elements O, H, F, Cl, Br, I, He, Ne, Ar, Kr, Xe, Rn, S, N, and P and their compounds; 1978;
    Vol.2: The elements C, Si, Ge, Sn, and Pb and their compounds; 1979;
    Vol.3: The elements B, Al, Ga, In, Tl, Be, Mg, Ca, Sr, and Ba and their compounds; 1981;
    Vol.4: The elements Cr, Mo, W, V, Nb, Ta, Ti, Zr, Hf, Sc, Y, La, Th, U, Pu, Li, Na, K, Rb, and Cs and their compounds; 1982.
12. Atomic Energy Review Special issues.
    No. 1. Rand, M. H., Livey, D. T., Feshotte, P., Nowontny, H., Seifert, K., Ferro, R.; Plutonium: Physico-chemical Properties of its Compounds and Alloys; 1966; International Atomic Energy Agency, Vienna.
    No. 2. Lavrentev, V. I., Gerassimov, Ya. I., Feschotte, P., Livey, D. T., von Goldbeck, O., Nowontny, H., Seifert, K., Ferro, R., Dragoo, A. L.; Niobium: Physico-Chemical Properties of its Compounds and Alloys; 1968; International Atomic Energy Agency, Vienna.
    No. 3. Gerassimov, Ya. I., Lavrentev, V. I., von Goldbeck, O., Livey, D. T., Ferro, R., Dragoo, A. L.; Tantalum: Physico-Chemical Properties of its Compounds and Alloys; 1972; IAEA, Vienna.
    No. 4. Spencer, P. J., von Goldbeck, O., Ferro, R., Girgis, K., Dragoo, A. L.; Beryllium: Physico-Chemical Properties of its Compounds and Alloys; 1973; IAEA, Vienna.
    No. 5. Rand, M. H., von Goldbeck, O., Ferro, R., Girgis, K., Dragoo, A. L.; Thorium: Physico-Chemical Properties of its Compounds and Alloys; 1975; IAEA, Vienna.
    No. 6. Alcock, C. B., Jacob, K. T., Zador, S., Kubaschewski-von Goldbeck, Ortrud., Nowontny, H., Seifert, K., Kubaschewski, O.; Zirconium: Physico-Chemical Properties of its Compounds and Alloys; 1976; IAEA, Vienna.
    No. 7. Spencer, P. J., Kubaschewski-von Goldbeck, O., Ferro, R., Marazza, R., Girgis, K., Kubaschewski, O.; Hafnium: Physico-Chemical Properties of its Compounds and Alloys; 1981; IAEA,

Vienna.

No. 8. Brewer, L., Lamoreaux, R. H., Ferro, R., Marazza, R., Girgis, K.; Molybdenum: Physico-Chemical Properties of its Compounds and Alloys; 1980; IAEA, Vienna.

No. 9. Kubaschewski, O., Kubaschewski-von Goldbeck, Ortrud, Rogl, P., Franzen, K.L.; Titanium: Physico-chemical Properties of its Compounds and Alloys; 1983; IAEA, Vienna.

13. King, E. G., Mah, A. D., Pankratz, L. B.; Thermodynamic Properties of Copper and its Inorganic Compounds, INCRA monograph 2; 1973; International Copper Research Association, Inc.
14. Mah, A. D., Pankratz, L. B.; Contribution of the Data on Theoretical Metallurgy XVI. Thermodynamic Properties of Nickel and Its Inorganic Compounds; Bulletin of U. S. Bureau of Mines 668; 1976; U. S. Government Printing Office, Washington.
15. Pankratz, L. B.; Thermodynamic Properties of Elements and Oxides; Bulletin of U. S. Bureau of Mines 672; 1982; U. S. Government Printing Office, Washington: Pankratz, L. B., Stuve, J. M., Gokcen, N. A.; Thermodynamic Data for Mineral Technology, Bulletin of Bureau of Mines 677, 1984; U. S. Government Printing Office, Washington.
16. Chang, Y. Austin, Ashmad, Nazeer; Thermodynamic Data on Metal Carbonates and Related Oxides; 1982; The Metallurgical Society of AIME, Warrendale, Pa. US.
17. Chart, T. G.; *High Temp. - High Pressures*, **5**, 241-252, 1973.
18. Haas, J. L., Jr., Robinson, G. R., Jr., Hemingway, B. S.; Thermodynamic Tablations for Selected Phases in the System CaO-Al_2O_3-SiO_2-H_2O at 101,325 Pa (1 atm) between 273.15 and 1800 K; *J. Phys. Chem. Ref. Data* **10**(3), 575-669, 1981.
19. The Chemical Thermodynamics of Actinide Elements and Compounds;

Part 1: Oetting, F. L., Rand, M. H., Ackermann, R. J.; The Actinide Elements; 1976; IAEA, Vienna.

Part 2: Fluger, J., Oetting, F. L.; The Actinide Aqueous Ions; 1976; IAEA, Vienna.

Part 3: Cordfunke, E. H.P., O'Hare, P. A. G.; Miscellaneous Actinide Compounds; 1978; IAEA, Vienna.

Part 4: Gr nvold, F., Drowart, J., Westrum, E. F., Jr.; The Actinide Chalcogenides (Excluding Oxides); 1984; IAEA, Vienna.

Part 5: Chiotti, P., Akhachinskij, V. V., Ansara, I., Rand, M. H.; The Actinide Binary Alloys; 1981; IAEA, Vienna.

Part 6: Holley, C. E., Rand, M. H., Storms, E. K.; The Actinide Carbides; 1984; IAEA, Vienna.

Part 8: Fuger, J., Parker, V. B., Hubbard, W. N, Oetting, F. L.; The Actinide Halides; 1983; IAEA, Vienna.

Part 9: Flotow, H. E., Haschke, J. M.,Yamauchi, S.; The Actinide

Hydrides; 1984; IAEA, Vienna.

Part 13: Hildenbrand, D. L., Gurvich, L. V., Yungman, V. S.; The Gaseous Actinide Ions; 1985; IAEA, Vienna.

20. Kelley, K. K.; Contributions to the Data on Theoretical Metallurgy XIII. High-Temperature Heat-Content, Heat-Capacity, and Entropy Data for the Elements and Inorganic Compounds; Bulletin of U. S. Bureau of Mines 584; 1960; U. S. Government Printing Office, Washington.
21. Kubaschewski, O; *High Temp. - High Pressures* **4**, 1-12, 1972.
22. Cox, D, J. Pilcher, G.; Thermochemistry of Organic and Organometallic Compounds; 1970; Academic Press, London.
23. Martin, J. F.; Specialist Periodical Reports - Chemical Thermodynamics Vol. 1, pp 133-161; 1973; The Chemical Society, Burlington House, London, W1V 0BN.
24. Pedley, J. B., Naylor, R. D., Kirby, S. P.; Thermochemical Data of Organic Compounds 2nd ed.; 1986; Chapman and Hall, London.
25. Naumov, G. B., Ryzhenko, B. N., Khodakovsky, I. L.; Handbook of Thermodynamic Data; 1971; Moscow, Atomizdat; translated by Soleimani, G. J.; 1974; U. S. Geological Survey.
26. Barin, I.; Thermochemical Data of Pure Substances; 1989; VCH, Weinheim.
27. Domalski, Eugene S., Evans, William H., Hearing, Elizabeth D.; Heat Capacities and Entropies of Organic Compounds in the Condensed Phase, *J. Phys. Chem. Ref. Data* **13**, Supplement No.1, 1984.
28. Stephenson, R. M., Malanowski, S.; Handbook of the Thermodynamics of Organic Compounds; 1987; Elsevier, New York.
29. High Temperature Vaporization Behavior of Oxides:
    (1) Lamoreax, R. H., Hildenbrand, D. L.; I. Alkali Metal Binary Oxides, *J. Phys. Chem. Ref. Data* **13**(1), 151-173, 1984.
    (2) Lamoreax, R. H., Hildenbrand, D. L. Brewer, L.; II. Oxides of Be, Mg, Ca, Sr, Ba, B, Al, Ga, In, Tl, Si, Ge, Sn, Pb Zn, Cd, and Hg, *J. Phys. Chem. Ref. Data* **16**(3), 419-443, 1987.
30. Wilhoit, R. C., Zwolinski, B. J.; Physical and Thermodynamic Properties of Alphastic Alcohols; *J. Phys. Chem. Ref. Data* Vol. **2** Suppl. 1, 1973.
31. Cook, L. P., McMurdie, H. F. ed.;Phase Diagrams for Ceramists Vol. 7; 1989; The Am. Cera. Soc.
32. Pedley, J. B., Rylance, J.; Sussex -N.P.L. Computer Analysed Thermochemical Data: Organic and Organometallic Compounds; 1977; University of Sussex.
33. Cordfunke, E. H. P and Konings, R. J. M. ed.; Thermochemical Data for Reactor Materials and Fission Products; 1990; North-Holland, Amsterdam.
34. Gurvich, L. V., Veyts, I. V., Alcock, C. B.; Thermodynamic Properties of Individual Substances Fourth Ed. (See also 11);

Volume 1, O, H(D,T), F, Cl, Br, I, He, Ne, Ar, Kr, Xe, Rn, S, N, P and Their Compounds; 1989; Hemisphere, New York:

Volume 2, C, Si, Ge, Sn, Pb and Their Compounds; 1991; Hemisphere, New York.

35. Knacke, O., Kubaschewski, O., Hesselmann, K. ed. ; "Thermochemical Properties of Inorganic Substances," 2nd ed.; 1991; Springer-Verlag, Berlin, Verlag Stahleisen m.B.H. Dusseldorf.
36. Chase, M. W., Jr., J. Phys. Chem. Refer. Data Monongraph 9 NIST-JANAF Thermodynamical Tables Fourth Edition.1998.
37. Yokokawa H., DenkiKagaku Binran

101. Grønvold, F.; *J. Chem. Thermodyn.* **5**, 525-531, 1973.
102. Motzfeldt, K., Sanberg, B.; "Chemical Investigations Concerning Carbothermic Reduction of Alumina," pp. 411-428, in Light Metals 1979, Peterson, W. S. ed.; 1979; AIME, Warrendale, Pa.
103. Takahashi, Y., Kadokura, H., Yokokawa, H.; *J. Chem. Thermodyn.* **15**, 65-81, 1983.
104. Margrave, J. L., Houge, R. H., Fredin, L.; *Thermophysical Properties* **4** (Proceeding of The Fourth Japan Symposium on Thermophysical Properties) p 107, 1983.
105. Grønvold, F., Samuelsen, E. J.; *J. Phys. Chem. Solids* **36**, 249-256, 1975.
106. Grønvold, F., Sveen, A.; *J. Chem. Thermodyn.* **6**, 859-872, 1974.
107. Flotow, H. E., Osborne, D. W.; *J. Chem. Thermodyn.* **6**, 135-140, 1974.
108. Johnson, G. K.; *J. Chem. Thermodyn.* **16**, 295-300, 1984.
109. O'Hare, P. A. G., Hubbard, W. N., Johnson, G. K., Flotow, H. E.; *J. Chem. Thermodyn.* **16**, 45-59, 1984.
110. Skudlarski, K., Kapala, J.; *J. Chem. Thermodyn.* **16**, 91-100, 1984.
111. Loewenschuss, A., Maycus, Y.; *Chemical Review* **84**(2), 89-115, 1984.
112. Smith, J. F.; *Bull. Alloy Phase Diagrams* **2**(1), 42-48, 1981.
113. Pamidimukkala, K. M., Rogers, D., Skinner, G. B.; *J. Phys. Chem. Ref. Data* **11**(1), 83-99, 1982.
114. Chao, J., Zwolinski, B. J.; *J. Phys. Chem. Ref. Data* **7**(1), 363-377, 1978: Chen, S. S., Wilhoit, R. C. Zwolinski, B. J.; *J. Phys. Chem. Ref. Data* **6**(1), 105-112, 1977: Chao, J., Zwolinski, B. J.; *J. Phys. Chem. Ref. Data* **5**(2), 319-328, 1976: Chao, J., Rodgers, A. S., Wilhoit, R. C., Zwolinski, B. J.; *J. Phys. Chem. Ref. Data* **3**(1), 141-162, 1974: Chao, J., Wilhoit, R. C., Zwolinski, B. J.; *J. Phys. Chem. Ref. Data* **2**(2), 427-437, 1973: Chen, S. S., Wilhoit, R. C., Zwolinski, B. J.; *J. Phys. Chem. Ref. Data* **4**(4), 859-869, 1975: Chao, J., Zwolinski, B. J.; *J. Phys. Chem. Ref. Data* **4**(3), 251-261, 1975: Chen, S. S., Kudchadker, S. A., Zwolinski, B. J.; *J. Phys. Chem. Ref. Data* **4**(3), 251-261, 1975: Kudchadker, S. A., Kudchadker, A. P., Wilhoit, R. C., Zwolinski, B. J.;

J. Phys. Chem. Ref. Data **7**(2), 417-456, 1978: Kudchadker, S. A., Kudchadker, A. P., Wilhoit, R. C.; *J. Phys. Chem. Ref. Data* **8**(2), 519-526, 1979.

115. Tirtowidjojo, M., Pollard, R.; *J. Cryst. Growth* **77**, 200-209, 1986.
116. Brewer, L., Ebbinghaus, E. E.; *Thermochim. Acta* **129**, 49-55, 1988.
117. Leonov, A. I., Shvaiko-Shvaikovskii, V. E., Keler, E. K.; *Rus. J. Inorg. Chem.* **14**(3), 334-336, 1969.
118. Yokokawa, H., Sakai, N., Kawada, T., Dokiya, M.; *J. Am. Ceram. Soc.* **73**(3), 649-658, 1990.
119. Taylor, R. W., Schmalzried, H; *J. Phys. Chem.* **68**(9), 2444-2449, 1964.
120. Keneshea, F. J., Cubicciotti, D. D.; *J. Chem. Phys.* **40**, 177, 1964.
121. Yokokawa, H. Sakai, N., Kawada, T., Dokiya, M.; *Denki Kagaku* **58**, 561-563, 1990.
122. Yokokawa, H. Kawada, T., Dokiya, M.; *J. Am. Ceram. Soc*. **72**(11), 2104-2110, 1989.
123. Yokokawa, H. estimated and evaluated values during 1989-1991; Yokokawa,H., Sakai,N., Kawada,T., Dokiya, M., *J. Solid State Chem.* **94**(1),106-120, 1991.
124. Kellogg, H. H.; *Metal. Trans.* **20B**, 77, 1989.
125. Kuselev, A. I., Karnov, I. K.; Physicochemical modeling in geology; 1988; Academy Nauk SSSR, Siberian Branch.
126. Hubbard, W. N., Rawlins, P. L., Connick, P. A., Stedwell, R. E., Jr., O'Hare, P. A. G.; *J. Chem. Thermodyn*. **15**, 785-798, 1983; Ohlendorf, D., Flotow, H.; *J. Less-Common Metal* **73**, 25-32, 1980.
127. Wilhoit, R. C. Chao, J., Hall, K. R.; *J. Phys. Chem. Ref. Data* **14**(1), 1 (1985). Chao, J., Hall, K. R., Marsh, K. N., Wilhoit, R. C.; *J. Phys. Chem. Ref. Data* **15**(4), 1369-1436, 1986.
128. Lyman, J.; *J. Phys. Chem. Ref. Data* **18**(2), 799, 1989.
129. Pedley, J. B., Marshall, E. M.; *J. Phys. Chem. Ref. Data* **12**(14), 967, 1983.
130. Akila, R., Jacob, K. T., Shukla, A. K.; *Metal. Trans.* **18B**, 163, 1987: Dwivedi, R. K., Kay, D. A. R.; *Metal. Trans.* **15B**, 523, 1984: Fukatsu, N., Shidawara, N., Kozuka, Z.; *J. Electrochem. Soc*. **132**(9), 2258, 1985.
131. Takahashi, Y., Sakamoto, R., Kamimoto, M.; *Int. J. Thermophys.* **9**(6), 1081, 1988.
132. Robie, R. A., Russell-Robinson, S., Hemingway, B. S.; *Thermochim. Acta* **139**, 67, 1989.
133. Filippov., V. K., Kalinkin, A. M., Vasin, S. K.; *J. Chem. Thermodyn.* **19**, 185, 1987.
134. Abello, L., Chhor, K., Pommier, C.; *J. Chem. Thermodyn.* **19**, 797, 1987; *J. Chem. Thermodyn.* **17**, 1-23, 1985.
135. Cordfunke, E. H. P., Cluistra, R., van Miltenburg, J. C.; *J. Chem.*

Thermodyn. **17**, 1079, 1985.

136. Meisingset, K. K., Gr nvold, F.; *J. Chem. Thermodyn.* **18**, 159, 1986.
137. Beyer, R. P., Ferrante, M. J.; *J. Chem. Thermodyn.* **18**, 365, 1986.
138. O'Hare, P. A. G., Johnson, G. K.; *J. Chem. Thermodyn.* **17**, 593, 1985.
139. Levitskii, V. A., Balak, G. M.; *Rus. J. Phys. Chem.* **56**(5), 668, 1982: Levitskii, V. A., Klimenko, A. N., Marin, V. P., Chentsov, V. N., Men'shenin, Yu. V.; *Rus. J. Phys. Chem.* **58**(6), 1350-1354, 1984: Klimenko, A. N., Levitskii, V. A., Marin, V. P.; *Rus. J. Phys. Chem.* **60**(10), 2402-2409, 1986.
140. Lindemer, T. B., Besmann, T. M., Johnson, C. E.; *J. Nucl. Mater.* **100**, 178-226, 1981.
141. Yamaguchi, S., Kaneko, Y., Iguchi, Y.; *Trans. JIM,* **28**(12), 986-993, 1987: Seetharaman, W. D. S., Staffansson, L. -I.; *Metal. Trans.* **15B**, 319-327, 1984.
142. Yokokawa, H., Sakai, N., Kawada, T., Dokiya, M., Kato, S., Ota, K.; *Denki Kagaku* **58**(1), 57-62, 1990: Godshall, N. A., Raistrick, I. D., Huggins, R. A.; *Mater. Res. Bull.* **15**, 561, 1980: Takeshita, H., Ohmichi, T., Nasu, S., Watanabe, H., Sasayama, T., Maeda, A., Miyake, M., Sano, T.; *J. Nucl. Mater.* **78**, 281, 1978.
143. Hsu, H. S., Devan, J. H.; *J. Electrochem. Soc.* **133**, 2078, 1986.
144. Denielou, L., Petitet, J.-P., Tequi, C.; *J. Chem. Thermodyn.* **7**, 901-902, 1975.
145. Kohli, R., Lacom, W.; *Thermochim. Acta* **57**, 155-160, 1982; **81**, 327-333, 1984: O'Hare, P. A. G., Johnson, G. K.; *J. Chem. Thermodyn.* **17**, 391-400, 1985: Fredrickson, D. R., Johnson, G. K., O'Hare, P. A. G.; *J. Chem. Thermodyn*. **12**, 801-805, 1980: Venugopal, V., Iyer, V. S., Agarwal, R., Roy, K. N., Prasad, R., Sood, D. D.; *J. Chem. Thermodyn.* **19**, 1047-1051, 1987: Kim, K. Y., Johnson, G. K., Johnson, C. E., Flotow, H. E., Appelman, E. H., O'Hare, P. A. G., Phillips, B. A.; *J. Chem. Thermodyn.* **13**, 333-344, 1981: Kim, K. Y., Johnson, G. K., O'Hare, P. A. G., Phillips, B. A.; *J. Chem. Thermodyn.* **13**, 695-698, 1981: Brittain, R. D., Lau, K. H., Hildenbrand, D. L.; *J. Electrochem. Soc.* **134**, 2900-2904, 1987: Sirousse-zia, D.; *Thermochim. Acta* **19**, 244-246, 1977.
146. Konings, R. J. M., Cordfunke, E. H. P.; *Thermochim. Acta* **124**, 157-162, 1988: Crouch-Baker, S., Davies, P. K., Dickens, P. G.; *J. Chem. Thermodyn.* **16**, 273-279, 1984. Dickens, P. G., Neild, D. J.; *J. Less-Common Metals* **54**, 273-281, 1977.
147. Gvelesiani, G. G., Nadiradze, A. A., Abashidze, T. D.; *J. Chem. Thermodyn.* **19**, 461-466, 1987.
148. Knights, C. F., Phillips, B. A.; Special Publication No. 30. High Temperature Chemistry of Inorganic and Ceramic Materials; eds. Glasser, F. P, Potter, P. E.; 1977; The Chemical Society, London; 135-145.

149. Ito, Y., Maruyama, T., Yoshimura, M., Saito, Y.; *J. Mater. Sci. Letters* **8**, 456-458, 1989:

150. Katsura, T., Kitayama, K., Sugihara, T., Kimizuka, N.; *Bull. Chem. Soc. Japan* **48**, 1809-1811, 1975: Sugihara, T., Kimizuka, N., Katsura, T.; *Bull. Chem. Soc. Japan* **48**, 1806-1808, 1975: Kimizuka, N., Katsura, T.; *Bull. Chem. Soc. Japan* **47**, 1801-1802, 1974: Kitayama, K., Katsura, T.; *Bull. Chem. Soc. Japan* **49**, 998-1001, 1976: Kimizuka, N., Katsura, T.; *J. Solid State Chem.* **13**, 176-181, 1975; **15**, 151-157, 1975: Sekine, T., Katsura, T.; *J. Solid State Chem.* **17**, 49-54, 1976: Katsura, T., Sekine, T., Kitayama, K., Sugihara, T., Kimizuka, N.; *J. Solid State Chem.* **23**, 43-57, 1978: Kitayama, K., Nojiri, K., Sugihara, T., Katsura, T.; *J. Solid State Chem.* **56**, 1-11, 1985: Piekarczyk, W., Weppner, W., Rabenau, A.; *Mat. Res. Bull.* **13**, 1077-1083, 1978; *Z. Naturforsch.* **34a**, 430-436, 1979: Tretyakov, Yu, D., Kaul A. R., Portnoy, V. K.; *High Temp. Sci.* **9**, 61-70 1977.

151. Myers, C. E., Graves, D. T.; *J. Chem. Eng. Data* **22**(4), 436-439, 1977; 440-445, 1977: Bettonville, S., Goudiakas, J., Fuger, J.; *J. Chem. Thermodyn.* **19**, 595-604, 1987: Xiang-Yun, W., Zhu, J. T., Goudiakas, J., Fuger, J.; *J. Chem. Thermodyn.* **20**, 1195-1202, 1988: Petzel, T.; *J. Less-Common Metals* **108**, 241-247, 1985.

152. Cordefunke, E. H. P, Konings, R. J. M., Westrum, E. F., Jr.; *Thermochim. Acta* **128**, 31-38, 1988.

153. Johnson, G. K, Tasker, I. R., Howell, D. A.; *J. Chem. Thermodyn.* **19**, 617-632, 1987.

154. Kitayama, K.; *J. Solid State Chem.* **73**, 381-387, 1988: Kitayama, K.; *J. Solid State Chem.* **76**, 241-247, 1988: Kitayama, K.; *J. Solid State Chem.* **77**, 366-375, 1988: Seppänen, M., Kytö, M., Taskinen, P.; *Scand. J. Metall.* **8**, 199-204, 1979: Petrov, A. N., Cherepanov, V. A., Zuyev, A. Yu., Zhukovsky, V. M.; *J. Solid State Chem.* **77**, 1-14, 1988: Petrov, A. N., Kropanev, A. Yu, Zhukovsky, V. M.; *Rus. J. Phys. Chem.* **58**, 26, 1984: Cherepanov, V. A., Petrov, A. N., Grimova, L. Yu.; *Rus. J. Phys. Chem.* **59**, 1267, 1985.

155. Beyer, R. P., Johnson, E. A.; *J. Chem. Thermodyn.* **16**, 1025-1029, 1984: Chekhovskoy, V. Ya.; *J. Chem. Thermodyn.* **3**, 289-296, 1971: Furukawa, G. T., Douglas, T. B., Saba, W. G., Victor, A. C.; *J. Res. Natl. Bur. Stands.* **69A**, 423-438, 1965.

156. Rard, J. A.; *Chem. Rev.* **85**, 555-582, 1985.

157. Fegley, M. B. Jr.; *J. Am. Ceram. Soc.* **64**, C124, 1981: Kaufman, L.; *CALPHAD* **3**, 275-291, 1979: Moon, K. A., Kant, A., Croft, W. J.; *J. Am. Ceram. Soc.* **63**, 698, 1980.

158. Konings, R. J. M., Cordfunke, E. H. P., Shaviv, R., Westrum, E. F., Jr.; *Thermochim. Acta* **157**, 307-314, 1990.

159. Volkov, V. L.; *Rus. J. Inorg. Chem.* **23**, 98, 1978: Volkov, V. L.; *Rus. J. Inorg. Chem.* **24**, 583, 1979: Volkov, V. L.; *Rus. J. Phys. Chem.* **52**,

1411, 1978.

160. Vlach, K. C., You, Y.-Z., Chang, Y. A.; *Thermochim. Acta* **103**, 361-370, 1986: Schaefer, S. C., Gokcen, N. A.; *High Temp. Sci.* **24**, 63-69, 1987: Jacob, K. T., Kale, G. M., Iyengar, G. N. K.; *J. Mater. Sci.* **21**, 2753-2758, 1986.
161. Scolis, Yu, Ya., Levitskii, V. A., Lykova, L. N., Kalinina, T. A.; *J. Solid State Chem.* **38**, 10-18, 1981.
162. Warhus, U., Maier, J., Rabenau, A.; *J. Solid State Chem.* **72**, 113-125, 1988.
163. Asano, M., Kou, T.; *J. Chem. Thermodyn.* **20**, 1149-1156, 1988; **21**, 837-845, 1989; Kou, T., Asano, T.; *High Temp. Sci.* **24**, 1-19, 1987.
164. Wyers, G. P., Cordfunke, E. H. P., Ouweltjes, W.; *J. Chem. Thermodyn.* **21**, 1095-1100, 1989: Beyer, R. P., Bennington, O., Brown, R. R.; *J. Chem. Thermodyn.* **17**, 11-17, 1985: Kohli, R., Lacom, W.; *Thermochim. Acta* **84**, 391-395, 1985: Cordfunke, E. H. P., Ouweltjes, W., Van Vlaanderen, P.; *J. Chem. Thermodyn.* **19**, 1117-1120, 1987.
165. Vahlas, C., Chevalier, P. Y., Blanquet, E.; *CALPHAD* **13**, 273-293, 1989: Schlesinger, M. E.; *Chem. Rev.* **90**, 607-628, 1990.
166. Kale, G. M., Jacob, K. T.; *Metall. Trans.* **20B**, 687-691, 1989: Barsoum, M.; *J. Mater. Sci.* **25**, 4394-4400, 1990.
167. Chirico, R. D., Westrum, E. F. Jr.; *J. Chem. Thermodyn.* **12**, 71-85, 1980; **12**, 311-327, 1980; **13**, 519-525, 1981; **13**, 1087-1094, 1981: Chirico, R. D., Westrum, E. F. Jr., Gruber, J. B., Warmkessel, J.; *J. Chem. Thermodyn.* **11**, 835-850, 1979: Morss, L. R., Haar, C. M.; *J. Chem. Thermodyn.* **21**, 1079-1083, 1989.
168. Helgeson, H. C., Delaney, J. M., Nesbitt, H. W., Bird, D. K.; *Am. J. Sci.* **278A**, 1-220, 1978.
169. Hemingway, B. S., Barton, M. D., Robie, R. A., Haselton, H. T., Jr.; *Am. Mineralog.* **71**, 557-568, 1986.
170. Hildenbrand, D. L., Lau, K. H., Russell, T. D., Zubler, E. G., Struck, C. W.; *J. Electrochem. Soc.* **137**, 3275-3287, 1990.
171. Shaviv, R., Westrum, E. F., Jr., Gr nvold, F., St len, S., Inaba, A., Fujii, H., Chihara, H.; *J. Chem. Thermodyn.* **21**, 631-651, 1989.
172. Lvova, A. S., Feodosev, N. N.; *Zh. Neorg. Phys.* **9**, 2251, 1964.
173. Alcock, C. B., Li, B.; *J. Am. Ceram. Soc.* **73**, 1176-1180, 1990;Shaviv, R., Westrum, E. F. Jr., Yang, T. L., Alcock, C. B., Li, B.; *J. Chem. Thermodyn.* **22**, 1025-1034, 1990; Skolis, Yu. Ya., Khramtsova, L. A.; *Rus. J. Phys. Chem.* **64**, 1681-1683, 1990; Kovba, M. L., Skolis, Yu. Ya., Khramtsova, L.A.; *Rus. J. Phys. Chem.* **64**, 1684-1686, 1990; Hwang, N. M., Roth, R. S., Rawn, C. J.; *J. Am. Ceram. Soc.* **73**, 2531-2533, 1990; Tretyakov, Yu. D., Kaul, A. R., Makukin, N. V.; *J. Solid State Chem.* **17**, 183-189, 1976; Suzuki, R. O., Okada, S., Oishi, T., Ono, K.; *Mater. Trans. JIM* **31**, 1078-1084, 1990; Skolis, Yu. Ya., Kitsenko,

S. V.; *Rus. J. Phys. Chem.* **63**, 1132-1133, 1989; Morss, L. R., Sonnenberger, D. C., Thorn, R. J.; *Inorg. Chem.* **27**, 2106-2110, 1988; Atake, T; unpublished work; Matsui, T., Fujita, T., Naito, K., Takeshita, T.; *J. Solid State Chem.* **88**, 579-583, 1990; Skolis, Yu. Ya., Pashin, S. F., Kovba, M. L., Kitsenko, S. V.; *Rus. J. Phys. Chem.* **65**, 13-17, 1991; Pashin, S. F., Skolis, Yu. Ya.; *Rus. J. Phys. Chem.* **65**, 256-259, 1991.

174. Yokokawa, H. estimate; 1990-2020. Yokokawa,H, "Zirconia Engineering Ceramics: Old Challenges - New Ideas,"ed. Kisi, E., Trans Tech Pub. pp. 37-74, (1998).
175. Gallagher, S. A., Dworzak, W. R., J. Am. Ceram. Soc. 68, C206-C207 1985.
176. Jacob, K. T., Kale, G. M., Iyengar, G. N. K; J. Mater. Sci. 22, 4274-4280,1987.
177. Lvov, SN, Macdonald, DD., J. Power Sources 72, 136-145 1998.
178. Jacobson, NS., Opila, EJ., Myers, DL., Copland,EV., J. Chem. Thermodyn. 37, 1130-1137 2005.
179. Hildenbrand, DL., Lau, KH., J. Chem. Phys. 101, 6076-6079 1994.
180. Hildenbrand, DL., Lau, KH., J. Chem. Phys. 100, 8373-8376 1994.
181. Yokokawa, H. Estimation/evaluation on phospour containing compounds.
182. (a) Helean, KB., Navrotsky, A., J. Therm. anal. Calorim. 69, 751-771 2002. (b) Ushakov, SV., Helean, KB., Navrotsky, A., J. Mater. Res.16, 2623-2633 2001.
183. (a) LaPO4, GdPO4: Thiriet, C., Konings, RJM., Javorsky, P., Magnami, N., Wastin, F., J. Chem. Thermodyn. 37, 131-139 2005.(b) LaPO4 Popa, K., Sedmidubsky, D., Benes, O., Thiriet, C., Konings, RJM.,J. Chem. Thermodyn. 38, 825-829 2006.(c) EuPO4 SmPO4: Popa, K., Konnings, RJM., Thermochimica Acta 445, 49-52 2006. (d) LaPO4 : Gavrichev, KS., Ryumin, MA., Tyurin, AV., Gurevich, VM., Komissarova, LN., Thermochimica Acta 474, 47-51, 2008. (e) SmPO4: Gavrichev, KS., Gurevich, VM., Ryumin, MA., Tyurin, AV., Komissarova, LN., Geochemistry Internatinal 53(7), 607-616 2015.(f) EuPO4: Gavrichev, KS., Ryumin, MA., Tyurin, AV., Gurevich, VM., Komissarova, LN., Rus. J. Phys. Chem. A 83(6), 901-906 2009.(g) GdPO4: Gurevich, VM., Ryumin, MA., Tyurin, AV., Komissarova, LN., Geochmistry International 50 (8), 702-710 2012.(h) ErPO4:: Gavrichev, KS., Ryumin, MA., Tyuin, AV., Gurevich, VM., Khoroshilov, AV., Komissarova, LN., Thermochimica Acta 535, 1-7 2012.(i) TmPO4: Ryumin, MA., Gurevich, VM., Khoroshilov, AV., Tyurin, AV., Gavrichev, KS., Rus. J. Phys. Chem. A 91(12), 2310-2316 2017.(j)YbPO4: Gavrichev, KS., Ryumin, MA., Tyurin, AV., Gurevich,VM., Nikiforova, GE., Komissarova, LN., Inorganic Materials 49(7), 701-708 2013.(k) LuPO4: Gavrichev, KS., Smirnova, NN., Gurevich, VM., Danilov, VP., Tyurin, AV., Ryumin, MA., Komissarova, LN., Thermochimica Acta 448, 63-65

2006.(l) YPO4: Gavrichev, KS., Ryumin, MA., Tyurin, AV., Gurevich, VM., Komissarova, LN., Geochemistry International 48(9), 932-939 2010.(m) ScPO4: Gavrichev, KS., Ryumin, MA., Tyurin, AV., Gurevich, VM., Komissarova, LN., Geochemistry Internatinal 48(4), 390-397 2010.(n) TbPO4:Gavrichev, KS., Ryumin, MA., Khoroshilov, AV., Tyurin, AV., Efimov, NN., Gurevich, VM., Nikiforova, GE., Guskov, VN., Golushina, LN., Bryuhanova, KI., Kritskaya, AP., Thermochimica Acta, 641, 64-70 2016.(o)HoPO4: Tyurin, AV., Ryumin, MA., Khoroshilov, AV., Gurevich, VM., Gavrichev, KS., Thermochimica Acta 683, 178459 2020. (p) PrPO4: Gavrichev, KS., Gurevich, VM., Ryumin, MA., Tyurin, AV., Komissarova, LN., Geochemistry Internatinal 54(4),362-368 2016. (q) NdPO4: Popa, K., Jutier, F., Wastin, F., Konings, RJM., J. Chem. Thermodyn. 38, 1306-1311 2006.

184. Yokokawa, H, Estimation from ZrP2O7(ref 162). see also 181.

185. (a) Olafsen, A., Fjellvag, H., Stoelen, S., Atake, T., Kawaji, H., Matsui, K., J. Chem. Thermodyn. 31, 433-449 1999. (b) Sjastad, AO., Fjellvag, H., Helean, KB., Navrotsky, A., Thermochimica Acta 550, 76-82 2012. (c) Watanabe, Y., Miyasaki, S., Maruyama, T., Saito, Y., J. Mater. Sci. Letter 5, 135-136 1986. (d) Irmler, M., Koeppel, C., Pscheidt, H., Warkentin, E., Gmelin Handbook of Inorganic and Organometallic Chemistry 8th edition, Rare earth elements C12b Compounds with Carbon, Springer-Verlag, 1994.

186. Yokokawa, H., Sakai, N., Yamaji, K., Horita, T., Ishikawa, M., Solid Sate Ionics 113-115, 1-9 1998.

187. Yokokawa, H., Solid State Ionics 285, 126-135 2016.

188. Yokokawa, H., estimation of Cp.

189. (a) Luff, BB., Reed, RB., J. Chem. Eng. Data 24, 228-229 1979. (b) Luff, BB., Reed, RB., J. Chem. Eng. Data 24, 227-228 1979.

190. Gmati-Khaled, H., Khattech, I., J. Therm. Anal. Calorim. 118, 579-583 2014.

191. Cordfunke, EHP., Ouweltjes, W., J. Chem. Thermodyn. 25, 1011-1016 1993.

192. Cs4P2O7; quaoted in ref 190: Beglov BM. "Thermodynamic analysis of the reactions of formation of condensed lithium, rubidium, and cesium phosphates," Izv Akad Nauk SSSR. Neorg Mater. 13, 2236–2241 1977.

193. Hudon, P., Jung, IH., Metal. Mater. Trans. B, 46B, 494-522 2015.

194. (a) Modaressi, A., Kael, J.C., Malaman, B., Gerardin, R., Gleitzer, C., Mat. Res. Bull. 18, 101-109 1983. (b) Zhang, L., Schlesinger, M.E., Brow, R.K., J. Am. Ceram. Soc. 94, 1605-1610 2011. (c) Ong, S.P., Wang, L., Kang, B., Ceder, G., Chem. Mater. 20, 1798-1807 2008.(d1) Shi, Q., Zhang, L., Schlesinger, ME., Boerio-Goates, J., WoodField, BF., J. Chem. Thermodyn. 62, 35-42 2013.(d2) Shi, Q., Zhang, L., Schlesinger, ME., Boerio-Goates, J., Woodfield, BF., J. Chem. Thermodyn. 61, 51-57 2013. (d3) Shi, Q., Zhang, L., Schlesinger, ME.,

Boerio-Goates, J., Woodfield, BF., J. Chem. Thermodyn. 62, 86-91 2013. (e) Iyer, RG., Delacourt, C., Masquelier, C., Tarascon, JM., Navrosky, A., Electrochem. Solid State Lett. 9(2), A46-A48 2006. (f) Loos, S., Gruner, D., Abdel-Hafiez, M., Seidel, J., Huettl, R., Wolter, AUB., Bohmhammel, K., Merterns, F., J. Chem. Thermodyn. 85, 77-85 2015.(g) Shimizu, D., Nishimura, S., Barpanda, P., Yamada, A., Chem. Mater. 24, 2598-2603, 2012.

195. De Guire, M.R., Prasanna, T.R.S., Kalonji, G., O'Handley, R.C., J. Am. Ceram. Soc. 70(11), 831-837 1987.
196. Rahman, M., Hudon, P., Jung, I.H., Metal. Mater. Trans. B,44B, 837-851 2013.
197. Macdonald, D.D., Challingsworth, M.L., J. Electrochem. Soc.140(3), 606-609 1993.
198. Kishimoto, H., Horita, T., Yamaji, K., Brito, M.E., Xiong, Y.-P., Yokokawa,H., J. Electrochem. Soc. 157(6),B802-B813 2010.
199. Katayama, I., Makino, T., Iida, T., High Temper. Mater.Sci. 34(1-3), 127 1995.
200. Hildenbrand, D.L., Lau, K.H., J. Chem. Phys. 100, 8377-8380 1994.
201. Ebbinghaus, B.B., Combustion and Flame 93, 119-137 1993.
202. Gindorf, C., Hilpert, K., Singheiser, L., Proc. ECS, PV 2001-16, 793-802 2001.
203. Bolech, M, Janssen, FJJG, Booij, AS, Cordfunke, EHP, J. Chem. Thermodyn. 28, 1319-1324,1996. Bolech, M, Cordfunke, EHP, van Genderen, ACG, van der Laan, RR, Janssen, FJJG, van Milternburg, JC, Thermochimica Acta 284, 253-261 1996.
204. Risbud, AS, Helean, KB, Wilding MC, Lu, P, Navrotsky, A, J. Mater. Res. 16(10), 2780 2001.
205. Cordfunke, E.H.P., Groen, C.P., Huntelaar, M.E., Alexander, C.A., Ogden, J.S., J Chem. Thermodyn. 32, 839-845 2000.
206. Mathews, T., Krishnamurthy, D., Gnanasekaran, T., J. Nucl. Mater. 247, 280-284 1997.
207. Moosavi-Khoonsari, E., Jung, I.-H, Metal. Mater. Trans. B. 47B, 576-594 2016.
208. Yokokawa, H., estimation for Cp S for water contribution in hydrates.
209. Flotow, H.E., Osberne, D.W., Otto, K., Abraham, B.M., J. Chem. Phys. 38(11), 2620-2626 1963.
210. Yokokawa, H., Horita, T., Sakai, N., Dokiya, M., Kawada, T., Solid State Ionics 86-88, 1161-1165 1996.
211. Cheng, J., Navrotsky, A., J. Mater. Res. 18, 2501-2508 2003.
212. (a) Gavrichev, K.S., Ryumin, M.A., Tyurin, A.V., Gurevich, V.M., Inorganic Materials 48(8), 845-850 2012. (b) Dorogova, M., Navotsky, A., Boatner, L.A., J. Solid State Chem. 180, 847-851 2007.

213. Shugurov, S.M., Timoshkin, A.YU., Lopatin, S.I., Phosphorun, Sulfur and Silican 179, 2091-2098 2004
214. Shugurov, S.M., Lopatin, S.I., J. Chem. Thermodyn. 37, 715-719 2005.
215. Lopatin, S.I., Shugurov, S.M., Stolyarova, V.L., Turnina, Z.G., J. Chem. Thermodyn. 38, 1706-1710 2006.
216. Lopatin, S.I., Shugurov, S.M., Gunina, A.O., J. Phys. Chem. 113, 13469-13474 2009.
217. Emelyanova, K.A., Shugurov, S.M., Panin, A.I., Lopatin, S.I., J. Chem. Thermodyn. 101, 337-342 2016.
218. Yokokawa, H., Horita, T., Sakai, N., Kawada, T., Dokiya, M., Solid State Ionics 78, 203-210 1995.
219. (a) Konings R.J.M., Kovacs A, Handbook on the Physics and Chemistry of Rare Earths Vol. 33, 147-247 2003. (b) Kovacs A., Konings R.J.M., J. Phys. Chem. Ref. Data 33(1),377-404 2004.
220. Rycerz, L., Gaune-Escard, M., J. Chem. Eng. Data 49, 1078-1081 2004.
221. Rycerz, L., Gaune-Escard, M., Inorg. Chem. 46, 2299-2306 2007.
222. Konings, RJM., Hildenbrand, DL., J. Alloys Compunds. 271-273, 583-386 1998.
223. (a) Konings, RJM, Benes, O.,J. Phys. Chem. Ref. Data 39, 043102 2010.
(b) Konings, RJM, Benes, O., Kovacs, A., Manara, D., Sedmidubsky, D., Gorakhov, L., Iorish, VS., Yungman, V., Shenyavskaya, E., Osina, E., J. Phys. Chem. Ref. Data 43, 013101 2014.
224. Benes, O., Konings, RJM., Calphad 32, 121-128 2008.
225. (a) Benes, O., van der Meer, JPM., Konings, RJM., calphad 31, 209-216 2007. (b) Beilmann, M., Benes, O., Konings, RJM., Fanghanel, Th., J. Chem. Thermdyn. 43, 1515-1524 2011.
226. dos Santos, IA., Klimm, D., Baldochi, SL., Ranieri, IM., Thermochimica Acta 552, 137-141 2013.
227. Li, X., Wang, K., Xie, L., Fluid Phase Equilibria 449, 18-27 2017.
228. Ocadiz-Flores, JA., Capelli, E., Raison, PE., Konings, RJM., Smith, AL., J. Chem. Thermodyn. 121, 17-26 2018.
229. Yin, H., Zhang, P., An, X., Cheng, J., Li, X., Wu, S., Wu, X., Liu, W., Xie, L., J. Fluorine Chem. 209, 6-13 2018.
230. Das, G., Lencka, MM., Eslamimanesh, A., Wang, P., Anderko, A., Riman, RE., Navrotsky, A., J. Chem. Thermodyn. 131, 49-79 2019.
231. Yokokawa, H., Estimation. 2019.4.
232. Rard, JA., J. Solution Chem. 45, 1332-1376 2016.
233. Diakonov, II., Ragnarsdottr, KV., Tagirov, BR., Chem. Geology 151, 327-347 1998.
234. (a) Chirkst, DE., Lobacheva, OL., Berlinskii, IV., Rus. J. Phys. Chem. A 84, 2047-2050 2010. (b) Chirkst, DE, Lobacheva, OL., Berlinskii, IV., Dzhevaga, NV., Rus. J. Inorg. Chem. 57(4), 605-609 2012.

235. Suponitsky, Y., Laptev, VI., Rus. Chem. Bull. 46(2), 279-283 1997.
236. Shivaramaiah, R., Anderko, A., Riman, RE., Navrotsky, A., Am. Mineral. 101, 1129-1134 2016.
237. Kim, P., Anderko, A., Navrotsky, A., Riman, RE., Minerals 8, 106 2018.
238. Merli, L., Lambert, B., Fuger, J., J. Nucl. Mater. 247, 172-176 1997.
239. van der Meer, JPM., Konings, RJM., Sedmidubsky, D., van Genderen, ACG., Oonk, HAJ., J. Chem. Thermodyn. 38, 1260-1268 2006.
240. Prien, M., Seifert, HJ., J. Thermal Anal. 45, 349-358 1995.
241. Seifert, HJ., J. Thermal Anal. Calorim. 67, 789-826 2002;
242. Seifert, HJ., J. Thermal Anal. Calorim. 83, 479-505 2006.
243. (a) Gaune-Escard, M., Rycerz, L., Szczepaniak, W., Bogacz, A., J. Alloys Compnds. 204, 189-192 1994. (b) Gaune-Escard, M., Rycerz, L., Mon. Chem. 134, 777-786 2003.
244. Kapala, J., Rutlowska, I., calphad 28, 275-279 2004.
245. Butman, MF., Motalov, VB., Kudin, LS., Rycerz, L., Gaune-Escard, M., J. Chem. Eng. Data 53, 2346-2350 2008.
246. Lisek, I., Kapala, J., Miller, M., J. Alloys Compnds. 280, 77-84 1998. Lisek, I., Kapala, J., Miller, M., J. Alloys Compnds 278, 113-122 1998.
247. Rycerz, L., Gaune-Escard, M., J. Thermal Anal. Calorim. 68, 973-981 2002. Kapala, J., Salamon, B., calphad 43, 139-142 2013.
248. Hatem, G., Gaune-Escard, M., Thermochimica Acta 293, 137-142 1997.
249. Seifert HJ., Yuan, Y., J. Less-Common Metals 170, 135-143 1991.
250. Rycerz, L., Gaune-Escard, M., J. Alloys Compnds 56, 355-363 1999.
251. Ushakov, S.V., Navrotsky, A., Farmer, J. M., Boatner, L. A., J. Mater. Res.19(7), 2165-2175 2004.
252. Palumbo, M., Borzone, G., Delsante, S., Parodi, N., Cacciamani, G., Ferro, R., Battezzati, Baricco, M.,Intermetallics 12, 1367-1372 2004.
253. Rahou, Z., Mahdouk, J. Alloys Componds 648, 346-352 2015.
254. Subramanian, P. R., Smith, J. F., Metal. Trans. B, 16B, 577-584 1985.
255. Ghosh, G., J. Mater. Res. 9(3), 599-616 1994.
256. (a) Shimazu, M., Yamaji, K., Isobe, T., Ueno, A., Kishimoto, H., Katsumura, K., Yokokawa, H., Okada, K., Solid State Ionics 204-205, 120-128 2011. (b) Komissarova, L.N., Pokrovskii,B.I., Shaplygin,I.S. Inorg. Mater. (Engl. Transl.), 2 [2] 236-240 1966.
257. (a) Tanahashi, M., Furuta, N., Taniguchi, T., Yamauchi, C., ISIJ International 43(1), 7-13 2003. (b) Tsai, H.-T.T., Muan, A., J. Am. Ceram. Soc. 75, 1407 1992.
258. Schenck, R., Bathe, A., Keuth, H., and Suess, S., Z. Anorg. Chemie, 249, 88-99 1942. Phase Diagram for Ceramist Ag-Cr-O pp537-539.259. (a) Kaiser, A., Sommer, B., Woermann, E., J. Am. Ceram. Soc. 75(6), 1463-71 1992. (b) Kovba, M. L., Skolis, Yu.Ya., Rus. J. Phys. Chem.

64(6), 907-909 1990. (c) Kovba, M. L., Skolis, Yu.Ya., Popov, S.G., Rus. J. Phys. Chem. 64(1), 22-24 1990.

260. (a)Sakai, N., Kawada, T., Yokokawa, H., Dokiya, M., Kojima, I., J. Am. Ceram. Soc. 76(3), 609-616 1993. (b) Yokokawa, H., Sakai, N., Kawada, T., Dokiya, M., J. Electrochem. Soc. 138, 1018-1027 1991.
261. Meschter, P. J., Worrell, W. L., Metal. Trans. 8A, 503-509 1977.
262. O'Hare, PAG., Johnson, GK., Tasker, IR., Flotow, HE.,J. Chem. Thermodyn. 19,77-88 1987.
263. Oppermann, H., Ehrich, S., Henning, C., Zeit. Naturforsch. 52(3),305-310 1997.
264. Yokokawa, H., Sakai, N., Kawada, T., Dokiya, M., J. Electrochem. Soc. 138, 2719-2727 1991.
265. Yokokawa, H., Sakai, N., Kawada, T., Dokiya, M., Solid State Ionics 40/41, 398-401 1990.
266. Yokokawa,H., Horita, T., Sakai, N., Yamaji, K., Brito, ME., Xiong,Y-P., Kishimoto, H., Solid State Ionics 177, 1705-1714 2006.
267. Yokokawa, H. evaluation/estimation concerning SrO-GDC-YSZ interactions.
268. Stoelen, S., Groenvold, F., Brinks, H., Atake, T., Mori, H., J. Chem. Thermodynam.30, 365-377 1998.
269. Yokokawa, H., Sakai,N., Kawada, T., Dokiya,M. Denki Kagaku 58, 161-170 1990. (in Japanese)
270. (a) Pet'kov, VI., Asabina,EA., Markin, AV., Kir'yanov, KV., Thermochmica Acta, 403, 185-196, 2003. (b) Pet'kov, VI., Kir'yanov, KV., Orlova, AI., Kitaev, DB., Inorganic Materials 36(4) 387-391 2000. (c) Milne, SJ., West, AR., J. Solid State Chem. 57, 166-177 1985. (d) Tiets, F., AIMS Materials Science 4(6), 1305-1318 2017. (e) Pet'kov, VI., Asabina, EA., Markin, AV., Smirnova, NN., J. Chem. Eng. Data 55, 856-863 2010. (f) Yokokawa, H. Estimation from phase relations
271. Shock, EL., Sassani, DC., Willis, M., Sverjensky, DA., Geochimica Cosmochimia Acta 61(5),907-950 1997.
272. Accornero, M., Marini, L., Lelli, M., Applied Geochem. 25, 242-260 2010.
273. Marini, L., Accornero, M., Environ. Geol. 52, 1343-1363 2007. Marini, L., Accornero, M., Environ. Earth Sci.59, 1601-1606 2010.
274. (a) Cordfunke, EHP, Westrum, EF Jr., Thermochimica Acta 124, 285-296 1988. (b) Westrum, EF. Jr., Groenvold, F., J. Phys. Chem. Solids 23, 39-53 1962.
275. (a) Bolgar, AS., Muratov, VB., Blinder, AV., Kryklya, AI., Suodis, AP., J. Alloys Compnds. 201, 127-128 1993. (b) Premovic, M., Du, Y., Zhang, F., Sundman, B., Minic, D., Hu, B., Thermochimica Acta 657, 185-196 2017. (c) Hallemans, B., Wollants, P., Roos, JR., J. Phase Equilibr. 16(2), 137-145 1995. (d) Peng, Y., Du, Y., Zhang, L., Sga, C., Liu, S., Zheng,

F., Zhao, D., Yuan, X., Chen, L., calphad 35, 533-541 2011. (e) Bian, Y., Tang, K., Tranell, G., calphad 51, 206-210 2015.

276. Loiacono, GM., Jacco, JC., Mater. Letters 4(1), 27-29 1985.
277. Chiotti, P., J. Less Common Metals 80, 97-104 1981.
278. O'Hare, PAG., Jensen, KJ., Johnson, GK., J. Chem. Thermodyn. 18, 765-786 1986.
279. Coble, JW., Stephens, HP., McKinnon, IR., Westrum, EF. Jr., Inorganic chemistry 11(7), 1669-1674 1972.
280. Moriya, K., Matsuo, T., Suga, H., Thermochimica Acta 132, 133-140 1988.
281. Hartwig, P., Rabenau, A., Weppner, W., J. Less Common Metals 80, 81-90 1981.
282. Denielou L., Petltet, JP., Tequi, C., J. Chem. Eng. Data 29, 116-117 1984.
283. (a) Thomas, DF., Abdel-Hafiez, M., Gruber, T., Huettl, R., Seidel, J., Wolter, AUB., Bruechner, B., Kortus, J., Mertens, F., J. Chem. Thermodynan. 64, 205-225 2013. (b) Thomas, D., Zeilinger, M., Gruner, D., Huettl, R., Seidel, J., Wolter, AUB., Faessler, FF., Mertens, F., J. Chem. Thermodynm. 85, 178-190 2015. (c) Liang, SM, Taubert, F., Kozlov, A., Seidel, J., Merterns, F., Schmid-Fetzer, R., Intermetallics 81, 32-46 2017. (d) Taubert, F., Seidel, J., Huettl, R., Bobnar, M., Gumeniuk, R., Mertens, F., J. Chem. Thermodyn. 116, 323-329 2018.(e) Thomas, D., Bette, N., Taubert, F., Huettl, R., Seidel, J., Merterns, F., J. Chem. Thermodyn. 704, 398-405 2017.
284. (a) Li, D., Beutl, A., Flandorfer, H., Cupid, DM., J. Alloys Compnds., 701, 186-199 2017. (b) Beutl, A., Cupid, D., Flandorfer, H., J. Alloys Compnds., 695,1052-1060 2017. (c) Sangster, J., Pelton, AD., J. Phase Equilibria 14(4), 510-514 1993. (d) Sangster, J., Pelton, AD., J. Phase Equilibria 18(4), 390-393 1997. (e) Sangster, J., Pelton, AD., J. Phase Equilibria 18(4), 382-386 1997.
285. Li, D., Fuertauer, S., Flandorfer, H., Cupid, DM., CALPHAD 47, 181-195 2014.
286. (a) Lepple, M., Cupid, DM., Franke, P., Seifert, H., J. Phase Equil. Diff., 35, 650-657 2014. (b) Patat, S., Blunt, DP., Chippindale, AM., Dickens, PG., Solid State Ionics 46, 325-329 1991.(c) Lepple, M., Adam, R., Cupid, DM., Franke, P., Bergfeldt, T., Wadewitz, D., Rafaja, D., Seifert, HJ.,J. Mater. Sci. 48, 5818-5826 2013.
287. Li-Mn-O: (a) Zhang, W., Cupid, DM., Gotcu, P., Chang, K., Li, D., Du, Y., Seifert, HJ., Chem. Mater. 30, 2287-2298 2018. (b) Wang, M., Navrotsky, A., J. Solid State Chem. 178, 1230-1240 2005. (c) Wang, M., Navrotsky, A., J. Solid State Chem. 178, 1182-1189 2005. (d) Cupid, DM., Li, D., Geberet, C., Reif, A., Flandorfer, H., Seifert, J., J. Ceram. Soc. Japan 124(10), 1072-1082 2016.(e) Paulsen, JM., Dahn, JR., Chem. Mater. 11, 3065-3079 1999. (f) Luo, C., Martin, M., J. Mater. Sci. 42,

1955-1964 2007.

288. (a) Kawaji, H., Takematsu, M., Tojo, T., Atake, T., HIrano, A., Kanno, R., J. Thermal Analysis and Calorimetry 68, 833-839 2002. Kawaji, H., Oka,T., Tojo, T., Atake, T., Hirano, A., Kanno, R., Solid State Ionics 152-153, 195-198 2002.(b) Wang, M., Navrotsky, A., Solid State Ionics 166, 167-173 2004. (c) Gotcu-Freis, P., Cupid, DM., Rohde, M., Seifert, HJ., J. Chem. Thermodynam. 84, 118-127 2015.
289. Il'lna, EA., Raskovalov, AA., Electrochimica Acta 330, 135220, 2020.
290. van der Vis, MGM., Cordfunke, E., Konings, R., J. de Physique IV Colloque, 03(C3), C3-75-C3-82 1993.
291. Popa, K., Shvareva, T., Mazeina, L., Colineau, E., Wastin, F., Konings, RJM., Navrotsky, A., Am. Mineral. 93, 1356-1362 2008.
292. Hatada, N., Toyoura, K., Nose, Y., Uda, T., J. Chem. Thermodyn. 61, 147-153, 2013. Hatada, N., Nagai, T., Nose, Y., Uda, T., J. Phase Equilibria and Diffusion 34, 196-201 2013.
293. Forbes, TZ., Kurzman, JA., Seshadri, R., Navrotsky, A., J. Mater. Res. 26(10), 1188-1192 2011.
294. Tremaine, P., Xiao, C., J. Chem. Thermodyn. 31, 1307-1320 1999.
295. (a) Le, SN., Eng, HW., Navrotsky, A., J. Solid State Chem. 179, 3731-3738 2006. (b) Le, SN., Navrotsky, A., J. Solid State Chem. 181, 20-29 2008. (c) Iyer, RG., Delacourt, C., Masquelier, C., Tarascon, JM., Navrotsky, A., Electrochem. Soli-State Lett. 9(2), A46-A48 2006.
296. Carling, R., Westrum, EF., Jr., J. Chem. Thermodyn. 8, 269-276 1976.
297. Bordier, S., Chocard, A., Gosse, S., J. Nucl. Mater. 451, 120-129 2014. Olsen, T., Roest, E., Groenvold, F., Acta chemica Scandinavica A33, 251-256 1979.
298. Richter, KW., Ipser, H., J. Phase Equil. 15(2), 165-170 1994.
299. Saba, WG., Wallace, WE., Sadmo, H., Craig, RS., J. Chem. Phys. 35, 2148-2155 1961.
300. Smith, AL., Gueneau, C., Fleche, JL., Chatain, S., Benes, O., Konings, RJM., J. Chem. Thermodyn. 114, 93-115 2017.
301. (a) Shvareva, T., Fein, JB., Navrotsky, A., Ind. Eng. Chem. Res. 51 607-613 2012. (b) Navrotsky, A., Shvareva, T., Guo, X., Mineralogical Association of Canada Short Course 43, Chap 4. Winnipeg MB, May 2013.
302. Lukas, W., Gaune-Escard, M., J. Chem. Thermodyn. 14, 592-597 1982.
303. Deiseroth, HJ., Biehl, E., Rochnia, M., J. Alloys Compnds. 246, 80-90 1997.
304. Charaykova, MV., Krivovichev, VG., Depmeir, W., Geol. Ore Deposits, 52(8), 689-700 2010.
305. Smith, AL., Pignie, MC., van Eijck, L., Griveau, JL., Colineau, E., Konings, RJM., J. Chem. Thermodyn. 120, 205-216 2018.

306. Majzlan, J., Stevens, R., Boeria-Goates, J., Woodfield, BF., Navrotsky, A., Burns, PC., Crawford, MK., Amos, TG., Phys. Chem. Minerals 31, 518-531 2004.

307. (a) Kanke, Y., Navrotsky, A., J. Solid State Chem. 141, 424-436 1998. (b) Konings, RJM., van der Laan, RR., van Genderen, ACG., van Miltenburg, JC., Thermochimica Acta 313, 201-206 1998. (c) Mao, H., Sellby, M., Fabrichnaya, O., Calphad 32, 399-412 2008. (d) Fabrichnaya, O., Seifert, HJ., Calphad 34, 206-214 2010.

308. (a) Kopan, AR., Gorbachuk, MP., Lakiza, SM., Tishchenko, YS., Power Metall. Metal Ceramics,51(3-4), 209-216 2012.(b) Kopan, AR., Gorbachuk, MP., Lakiza, SM., Tishchenko, YS., Kirienko, SM., Power Metall. Metal Ceramics,52(5-6), 329-335 2013. (c) Fabrichnaya, O., Seifert, HJ., J. Alloys Compnds. 475, 86-95 2009. (d) Fabrichnaya, O., Savinykh, G., Zienert, T., Schreiber, G., Seifert, HJ., Int. J. Mater. Res. 103(12), 1469-1487 2012.

309. (a) Lakiza, S., Fabrichnaya, O., Wang, C., Zinkevich, M., Aldinger, F., J. Eur. Ceram. Soc. 26, 233-246 2006. (b) Fabrichnaya, O., Seifert, HJ., J. Phase Equil. Diffuison 32, 2-16 2011. c) Chaudhury, S., Parida, SC., Pillai, KT., Mudher, KDS., J. Solid State Chem. 180, 2393-2399 2007.

310. (a) van der Laan, RR., Konings, RJM., van Genderen, ACG., van Miltenburg, JC., Thermochimica Acta 329, 1-6 1999. (b) Saal, JE., Shin, DS., Stevenson, AJ., Messing, GL., Liu, ZK., J. Am. Ceram. Soc., 91(10), 3355-3361 2008. (c) Saal, JE., Shin, DS., Stevenson, AJ., Messing, GL., Liu, ZK., J. Am. Ceram. Soc., 93(12), 4158-4167 2010. (d) Fabrichnaya, O., Sefert, HJ., calphad 32, 142-151, 2008. (e) Fabrichnaya, O., Savinykh, G., Schreiber, G., Seifert, HJ., J. Eur. Ceram. Soc., 32, 3171-3185 2012.

311. (a) Schnelle, W., Fischer, R., Gmelin, E., J. Phys. D. Apl. Phys. 34, 846-851 2001. (b) Fabricgnaya, O., Zinkevich, M., Aldinger, F., Int. J. Mat. Res. 97(11), 1495-1501 2006. (c) Fabrichnaya, O., Lakiza, S., Wang, C., Zinkevich, M., Aldinger, M., J. Alloys Compnds. 453, 271-281 2008. (d) Fabrichnaya, O., Savinykh, G., Schreiber, G., J. Eur. Ceram. Soc. 33, 37-49 2013.(e) Cao, Z., Xie, W., Qiao, Z., Xing, X., J. Am. Ceram. Soc. 100, 365-377 2017.

312. (a) Yokokawa, H. 2020. 09. Estimation/Evaluation based on ref.307-311. (b) Wu, P., Pelton, AD., J. Alloys Compnds. 179, 259-287 1992.

313. Zinkevich, M., Geupel, S., Aldinger, F., Durygin, A., Saxena, SK., Yang, M., Liu, ZK., J. Phys Chem. Solid 67, 1901-1907 2006.

314. (a) Hisham, MWM., Benson, SW., J Phys. Chem. 90, 885-888 1986. (b) Burns, JB., Peterson, JR., Haire, RG., J. Alloys Compnds. 265, 146-152 1998. (c) Koch, CW., Broido, A., Cunningham, BB., J. Am. Chem. Soc. 74, 2349 1952. d) Koch, CW., Cunningham, BB., J. Am. Chem. Soc. 75, 796-797, 1953. (e) Koch, CW., Cunningham, BB., J. Am. Chem. Soc. 76, 1471-1474, 1954. (f) Koch, CW., Thesis: Thermodynamics of the tricholorides and oxychlorides of some of the lanthanide and actinide

elements," U. Calif. Radiation Laboratory, September 1953.

315. Yokokawa, H. Estimation based on rare earth oxyhalides.
316. Haschke, JM., Eick, HA., J. Am. Chem. Soc. 92(15), 4550-4553 1970.
317. Work, DE., Erick, HA., J. Phys. Chem. 74(16), 3130-3134 1970.
318. (a) Balak, GM., Skolis, YY., Zvezdina, IM., Levitskii, VA., Gerasimov, YI., Rus. J. phys. Chem. 59(9), 1985-1986 1985. (b) Skolis, YY., Pashina, SV., Rus. J. Phys. Chem. 75(11), 1774-1779 2001. (c) Petzel, T., Marx, V., Hormann, B., J. Alloys Compnds. 200, 27-31 1993.
319. (a) van Ende, MA., Jung, IH, J. Alloys Compnds. 548, 133-154 2013. (b) van Ende, MA., Jung, IH., Kim, YH., Kim, TS., Green Chem. 17, 2246-2262 2015. (c) Luis, F., Mate, B., Pique, C., Burriel, R., Bartolome, J., Buschow, KHJ., J. Mag. Mag. Mater. 101, 414-416 1991. (d) Spear, KE., Liao, PK., Bull. Alloy Phase Diagram 11(4), 321-324 1990.
320. Yokokawa, H. Estimation on heat capacities for RE-B-Fe systems.
321. (a) Capelli, E., Benes, O., Konings, RJM., J. Nucl. Mater. 501, 238-252 2018. (b) Vozarova, N., Smith, ALl., Colle, JY., Raison, PE., Bouexiere, D., Konings, RJM., Benes, O., J. Chem. Thermodym. 114, 71-82 2017.
322. Capelli, E., Benes, O., Konings, RJM., J. Nucl. Mater. 462, 43-53 2015.
323. (a)Capelli, E., Benes, O., Konings, RJM., J. Nucl. Mater.449, 111-121 2014. (b)Benes, O., Konings, RJM., J. Chem. Thermodym. 41, 1086-1095 2009.
324. (a)Jin, Z., Du, Y., calphad 16(4), 355-362 1992. (b)Li, Z., Wang, J., Li, B., Wang, S., Ali, W., Wang, S., Wang, X., Lu, X., Li, C., Wang, K., J. Eur. Ceram. Soc. 38, 323-332 2018. (c) Philippen, J., thesis "Fiber Crystal growth of cerium doped calcium scandate, strontium yttrium oxide, and tristrontium silicate,", Berlin Technical University, 2013.
325. (a) Kitayama, K., J. Solid State Chem. 151, 12-15 2000. (b) Yokokawa, H., estimation/evaluation on rare earth cobaltites, ferrite and cobaltite-ferrites.(2017); see Ref 154.
326. Yokokawa, H., Xiong, YP., Kishimoto, H., Yamaji, K., Brito, ME., Horita, T., ECS Tans. 28(11), 165-172 2010.
327. Zinkevich, M., Solak, N., Nitsche, H., Ahrens, M., Aldinger, F., J. Alloy Compnds. 438(1-2), 92-99 2007.
328. (a) Oishi, M., Yashiro, K., Hong, JO., Nigara, Y., Kawada, T., Mizusaki, J., Solid State Ionics 178, 307-312 2007.(b) Yokokawa, H., estimation based on La2CrNiO6. (c) Anderson, HU., Nasrallah, MM., Flandermeyer, BK., Agarwal, AK., J. Solid State Chem. 56, 325-334 1985.
329. Yokokawa, H 2011. estimation on RE-Ti-O based on Ref. 174.
330. Yokokawa, H 2003. Reevaluation based on refs. 173 and others.
331. Yokokawa, H.2005 estimation/evaluation on Li2CrO4, Na2CrO4 and Rb2CrO4.
332. Haas, JR., Shock, EL., Sassani, DC., Geochim. Cosmochim.Acta 59(21),

4329-4350 1995.

333. Sverjensky, DA., Shock, EL., Helgeson, HC., Geochim. Cosmochim. Acta 61 (7), 1359-1413 1997.
334. Sassani, D., Shock, EL., Geochim. CosmoChim. Acta 62(15), 2643-2671, 1998.
335. Schulte, MD., Shock, EL., Wood, RH., Geiochim. Cosmochim. Acta 65(21), 3919-3930, 2001.
336. Yokokawa, H., tentative treatment for heat capacity=0. for those aqueous species whose Cp is unknown.

Appendix2 Pourbaix Diagram in CHD version 2

A2.1 Basic Idea about how to handle Pourbaix Diagram in CHD version 2

As described in Appendix, the CHD program which was developed to construct the generalized chemical potential diagrams can be utilized to construct the Pourbaix diagrams which are constructed mainly for the low temperature equilibria associated with the aqueous solutions. In the First version of CHD, no special functions were prepared except for some description in Appendix.

1. On the occasion when the MALT for Windows started to include those data for aqueous solutions, new functions are prepared to assist users to construct the Pourbaix diagrams without detailed knowledge about the generalized chemical potential diagrams. This is because those users who want to construct the Pourbaix diagrams are not necessarily to be familiar with the high temperature materials chemistry which is essentially important knowledge to utilize the generalized chemical potential diagrams. On the other hand, the Pourbaix diagram has been well utilized and standardized in the formats on how to construct the Pourbaix diagrams. Thus, CHD version 2 provides the function of *automatic construction* of the Pourbaix diagrams by only selecting the target elements.

2. Even so, the customization should be made in the proper manner about the treatments of specifying conditions to construct the diagrams; namely, the display range of axes, the thermodynamic activities specified for the aqueous species, selections of compounds/species to be considered.

3. Furthermore, it is highly recommended to compare the electrochemical relations appearing in the Pourbaix diagrams with other electrochemical/chemical relations in the generalized schemes. Particularly, in the Pourbaix diagram for the two element system like the Fe-S-O-H-e- system, implicitly the iron(Fe) is selected as the target

element, and some relations associated with sulfur will be neglected. This indicates that those thermodynamic relations appearing in the Pourbaix diagram are just a part of those complicated relations in the multicomponent system and therefore there must be some cases where proper thermodynamic considerations cannot be made without such other relations neglected in the normal Pourbaix diagram. In such a case, it becomes essential to understand thermodynamic equilibria in different circumstances such as the aqueous, the hydrated and the dry systems.

Thus, CHD version 2 provides the followings:

1. Automatic construction based on the selected options.
2. Customization can be made on options for constructing diagrams.
3. Adoptions of the similar procedures and settings to construct the generalized chemical potential diagrams can lead to the construction of the generalized electrochemical potential diagrams.

A2-2 Automatic Construction of Pourbaix Diagrams

When one or two solute elements are selected in the aqueous solution, the Pourbaix diagram is automatically constructed. Only selection should be made on

1. Inclusion of the aqueous species on retrieval of the thermodynamic data in the MALT for Windows.
2. In the MALT for Windows, compounds should be searched by elements.
3. Select the menu of tools > CHD.
4. Obtained compound data are transferred and the construction of diagram is made automatically. Finally, the Pourbaix diagram will appear.

Automatic construction is made based on the following default settings:

1. Target states are the condensed phases as well as the aqueous species, allowing to show the equilibria between the aqueous species and the condensed phases.
2. When two solute elements are selected, the element having the higher NBS order can be selected as the targe element to display. Another element is treated to be transparent in the multicomponent diagram.
3. The display range of the coordinates are given prior to construction.
4. The equilibrium lines for evolving O2 or H2 are as One dissection. Originally this function of one dissection is to show the profile diagram along the dissected line. Here, however, the dissection line is displayed on

the original diagram without showing another profile diagram of presenting the activity profile of the aqueous species along the dissected line.

A2-3 Customization of constructing and displaying diagram

Selection of compounds or species is important to construct the diagram:

1. Predominance are diagram: When only the aqueous species with/without charge are included, so called predominance area diagram will be constructed. This diagram shows the dominant aqueous species as functions of *p*H and *E*/V. the whole area of the diagram is covered by those predominant species of the selected element which have polygon-type stable area. The border line between two different aqueous species corresponds to the electrochemical reaction. For example, the border line between FeO+ and Fe+2 indicates the following reaction:

   $$FeO^+ + 2H^+ + 2e^- = Fe^{+2} + H_2O \qquad (A2\text{-}1)$$

   Here those species of H+, e- and H2O indicating the species associated with the axes of the diagram and the solvent are involved. The stoichiometric coefficients of those species in the above reaction (A2-1) determines the slope of the border line. This is exactly the same as the normal construction conventions of the Pourbaix or related diagram.

2. The normal Pourbaix diagram can be constructed by choosing the aqueous species as well as the condensed phases.

3. Selections of elements becomes also important to draw the following diagrams:

   Selections of displaying polygon mode:

   The multi-solute system can be constructed as one of the generalized chemical potential diagrams. However, the conventional Pourbaix diagram for the multicomponent system is setup by focusing one element.

   Selection of elements in the profile diagram

   In the profile diagram, many profile lines can be shown corresponding to the existing aqueous species. Usually, the solvent related species can be neglected. If users have the focused element, those elements selecting the profile species can be selected.

Selection of thermodynamic activity of the aqueous species

A number of the diagrams can be constructed by changing the thermodynamic activities of the aqueous species. When once this activity value is adjusted, all aqueous species are set to have the same activity.

Selection of range of displaying diagram

The range of the horizontal and vertical axes can be changed. Furthermore, the axes variable itself can be changed.

Change display mode of polygons

Usually for selection of colors to be painted for the stability polygon, several choices are prepared:

Based on the stoichiometric numbers of compounds/species;

Based on the coordinates values;

Based on sequential use of preselected colors.

Furthermore, the brush style and the brightness of the selected color can be selected.

In the aqueous system, those selections can be made based on the state, namely the aqueous, the condensed or the gaseous species.

Selection of target elements for transparent display

Usually, the element having the higher NBS order is selected as the target element to show properly and species without this target element is shown in the transparent manner. This selection can be made among the non-solvent(that is solute) elements.

A2-4 Generalized electrochemical diagrams

For treatment of the aqueous solution, CHD prepares the following specifications associated with the aqueous solutions:

1. The coordinate values, *p*H, *p*E, *E*/V are prepared.

   $pH = -\log a(H+)$;

   $pE = -\log a(e-)$;

   $E/V = -(RT/F) \ln a(e-)$

   In the core part of the CHD algorithm, the charge is treated as pseudo

element. In the aqueous system, the thermodynamic conventions are adopted based on the H+; that is, the enthalpy, Gibbs energy, entropy, heat capacity are defined to be always zero. This leads to the natural adoption that the thermodynamic quantity associated with H+ species should be used as coordinate variable. This leads to the selection of (H+, e-, H2O) instead of (H, O, e-) as the system components. These coordinate variables also can be used as variables to determine the dissection value etc.

2. Other options/selections are the same as the normal generalized chemical potential diagrams. For example, the aqueous solution can be used as one solution or the respective species can be treated separately like in the predominance area diagram.

This means that there can be many approached to investigate the equilibria-related matter in the aqueous chemistry from the generalized electrochemical/chemical point of view. One typical point is the considerations concerning the nucleation of new phases in interfaces between condensed materials or between the condensed phase and the aqueous solution.

From the high temperature chemical point of view, it can be pointed out that some difficulties associated with the aqueous related chemistry is that the kinetic processes are hindered in many ways. In particular, the nucleation of solid substance at the interface between condensed materials seems to be hindered just because the reconstruction of ions to form new crystal structure will not be taken placed because of the kinetic barrier for nucleation. Here, however, the high temperature chemistry associated with the congruent or noncongruent decomposition (dissolution etc) provides some essential clue to resolve of the issue about how to apply the thermodynamic considerations to the low temperature chemistry.

For example, consider the Li-Mn-O system which is related to the battery positive electrode and its stability against the chemical environment: Here, we expect that the equilibria between solid materials are not achieved because of lack chances for ions to diffuse and reconstruct the crystal structure. Even when the cation cannot diffuse inside the crystals, the cations and anions can dissolve into the solvent simultaneously. This is so called the congruent dissolution of the condensed phase into the solution. This process is accompanied with only diffusion in the solution not in the solid state. Remember that the precipitation from the solutes in the solution can be treated as one of the equilibria between the solvent and solutes. This is the completely different equilibria from the first one for the congruent dissolution. As a result,

A2-5 Options for save and reproduction

Since one chd project can consist of several diagrams, it becomes convenient for users to save the selected options to construct the diagrams or the conditions of dissections as well as the used thermodynamic data.

Thus, New CHD provides the new functions of saving the thermodynamic data and calculational conditions and of reconstructing those diagrams using the stored thermodynamic data and the calculational conditions.

It is common to construct the different diagrams corresponding to the different conditions by using the same thermodynamic data. For such a case, a number of different selected options can be selected within the same chd project based on the same thermodynamic data.

New Features in gem 2.0

Modification for adopting the aqueous solution

Thermodynamic model for the aqueous solution

The aqueous solution consists of the solvent(H2O) and solutes. Gem treats this solution as the ideal dilute solution. The chemical potential of the aqueous species, for example Fe+2, is defined as

$$\mu(\mathrm{Fe+2}) = \mu^{\circ}(\mathrm{Fe+2}) + RT \ln c(\mathrm{Fe+2})$$

Here μ°(Fe+2) is the chemical potential value at the standard state and c(Fe+2) is the concentration of Fe+2. In the ideal solution, no other interactions between solvent and solute or among solutes are considered.

Specification of activity of the aqueous species in the Helmholtz mode

When Helmholtz energy is selected to be minimized to obtain the equilibrium state, the specification of partial pressure of the gaseous species can be applied. In a similar manner, specification of the activity of the aqueous solution can be setup when the aqueous species are available.