

## RICT-Cerm サーメット材料系データベース v.2.0

RICT-Cerm データベースはサーメット材料系の熱力学計算をするために用いることを目的に、CALPHAD(CALculation of PHAse Diagrams)法に基づいて構築された熱力学パラメータデータベースです。

### 1. 取り扱える元素成分

現在のところ取り扱える成分としては 以下の 21 元素です。

主成分元素 : Co Fe Ni Ti W および B C N

合金元素 : Al Cr Cu Hf Mg Mn Mo Nb Si Ta V Y Zr

取り扱える成分は今後順次増やして行く計画です。

本データベースには上記成分の酸化物, 燐化物, 硫化物のパラメータも多く収納しています。本データベースに含まれていない化合物(純物質)については他のデータベースを併用してください。

### 2. 二元系合金系

RICT-Cerm v.2.0 には 次ページに示している組み合わせの二元系および多くの三元系(一部四元系も)の熱力学パラメータが含まれており, これらから構成される多元系の相平衡を予測計算することができます。

### 3. 合金相の種類と構成

本データベースは 液相(LIQUID), 9 種の一次固溶体に加え, 54 種のホウ化物, 34 種の炭化物, 18 種の窒化物, 93 種の珪化物, 149 種の酸化物, 37 種の燐化物, 48 種の硫化物およびその他 196 種の合計 629 種の相を含んでいます。

以下にデータベースを構成している相の種類を示します。

#### 1) 液相と一次固溶体相の構成

液相, (Si)相(DIAMOND\_A4), 黒鉛(GRAPHITE)には正則溶体近似を用いています。その他の相は複副格子正則溶体近似を用いています。

なお, 純 P 相(RED\_P, WHITE\_P)および純 S 相(ALPHA\_S, BETA\_S)はそれぞれ燐化物相, 硫化物相の項に含めています。



相名 副格子と構成成分 (Va は空格子点)

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LIQUID	(Al, Al <sub>2</sub> S <sub>3</sub> , AlN, AlO <sub>3/2</sub> , B, C, Ca, CaO, CaS, Co, CoO, CoO <sub>3/2</sub> , CoS, Cr, CrO <sub>3/2</sub> , CrS, Cu, Cu <sub>2</sub> O, Cu <sub>2</sub> S, CuO, Fe, FeO, FeO <sub>3/2</sub> , FeS, Hf, Hf <sub>1/2</sub> O <sub>1</sub> , Mg, MgO, MgS, Mn, MnO, MnO <sub>3/2</sub> , MnS, Mo, Mo <sub>2</sub> S <sub>3</sub> , NoO <sub>2</sub> , MoO <sub>3</sub> , N, Nb, NbO <sub>1</sub> , NbO <sub>2</sub> , NbO <sub>5/2</sub> , Ni, NiO, NiS, O, P, P <sub>2</sub> O <sub>5</sub> , P <sub>4</sub> S <sub>3</sub> , P <sub>4</sub> S <sub>7</sub> , S, Si, SiO <sub>2</sub> , SiS <sub>2</sub> , Ta, Ta <sub>2/5</sub> O, Ti, TiO, TiO <sub>2</sub> , TiO <sub>3/2</sub> , V, VO, VO <sub>2</sub> , VO <sub>3/2</sub> , VO <sub>5/2</sub> , W, WO <sub>3</sub> , WS <sub>2</sub> , Y, YO <sub>2/3</sub> , Zr, Zr <sub>1/2</sub> O, Zr <sub>2</sub> S <sub>3</sub> , ZrS <sub>2</sub> ) <sub>1</sub>	
BCC_A2	(Al, Ca, Co, Cr, Cu, Fe, Hf, Mg, Mn, Mo, Nb, Ni, S, Si, Ta, Ti, V, Va, W, Y, Zr) <sub>1</sub> (B, C, N, O, Va) <sub>3</sub>	
BETA_RHOMBO_B	(B) <sub>93</sub> (B, C, Si) <sub>12</sub>	
CBCC_A12	(Al, Co, Cr, Cu, Fe, Mg, Mn, Mo, Nb, Ni, Si, Ta, Ti, V, Zr) <sub>1</sub> (C, N, Va) <sub>1</sub>	(αMn)
CUB_A13	(Al, Co, Cr, Cu, Fe, Hf, Mg, Mn, Mo, Nb, Ni, Si, Ta, Ti, V, Zr) <sub>1</sub> (C, N, Va) <sub>1</sub>	(βMn)
DIAMOND_A4	(Al, B, C, Si, Ti) <sub>1</sub>	(Si)
FCC_A1	(Al, Ca, Co, Cr, Cu, Fe, Hf, Mg, Mn, Mo, Nb, Ni, P, S, Si, Ta, Ti, V, W, Y, Zr) <sub>1</sub> (B, C, N, O, Va) <sub>1</sub> This is also NaCl-type M(C,N)	
GRAPHITE	(B, C) <sub>1</sub>	
HCP_A3	(Al, Ca, Co, Cr, Cu, Fe, Hf, Mg, Mn, Mo, Nb, Ni, S, Si, Ta, Ti, V, W, Y, Zr) <sub>1</sub> (B, C, N, O, Va) <sub>0.5</sub> This is also M <sub>2</sub> (C,N)	

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2) 規則相

相名 副格子と構成成分 (Va は空格子点)

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BCC_B2	(Al, Ca, Co, Cr, Cu, Fe, Hf, Mg, Mn, Mo, Nb, Ni, P, S, Si, Ta, Ti, V, Va, W, Y, Zr) <sub>0.5</sub> (Al, Ca, Co, Cr, Cu, Fe, Hf, Mg, Mn, Mo, Nb, Ni, P, S, Si, Ta, Ti, V, Va, W, Y, Zr) <sub>0.5</sub> (B, C, N, O, Va) <sub>3</sub>	
FCC_L12	(Al, Ca, Co, Cr, Cu, Fe, Hf, Mg, Mn, Mo, Nb, Ni, P, S, Si, Ta, Ti, V, W, Y, Zr) <sub>0.75</sub> (Al, Ca, Co, Cr, Cu, Fe, Hf, Mg, Mn, Mo, Nb, Ni, P, S, Si, Ta, Ti, V, W, Y, Zr) <sub>0.25</sub> (B, C, N, O, Va) <sub>1</sub>	
HCP_ORD	(Co, V) <sub>0.25</sub> (Co, V) <sub>0.25</sub> (Co, V) <sub>0.25</sub> (Co, V) <sub>0.25</sub> (Va) <sub>0.5</sub>	Co <sub>3</sub> V

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BCC\_B2 相は二副格子モデルの B2 規則相, FCC\_L12 相は二副格子モデルの L1<sub>2</sub> 規則相, HCP\_ORD 相は四副格子モデルの Co<sub>3</sub>V 規則相です. これらはスプリットモデルを用いた規則相で, 不規則部としてそれぞれ BCC\_A2 相, FCC\_A1 相, A3\_HCP 相を必要とします. 規則状態が現れないことが明らかな場合は計算から除外できますが, いずれも不規則部を除いた単独相として用いることはできません.

3) 硼化物, 炭化物, 窒化物, 珪化物

硼化物, 炭化物, 窒化物の順に並べています. なお, 硼炭化物, 炭窒化物のような複合化合物の場合はどちらか一方にのみ示しています.

硼化物相

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ALB12_ALPHA	ALBMO	ALCR2B2
ALCR3B4	CAB6_D21	CO3AL2B5
CO5TI3B2	CR5B3_D81	CRB4
FE10SI2B3	FE3NB3B4	FE5SI2B
FE5SIB2	FENBB_C22	M2B3
M2B_ORTH	M2B_TETR	M3B2_D5A
M3B4_D7B	M5B6	MB12_D2F
MB2_C32 [This is also Mo2B5]	MB_B27 [This is CoB,FeB,MnB,TiB and ZrB]	
MB_BF [This is CrB,NbB,NiB and VB]		MGB4
MGB7	MN2B_D1F	MNB4
MO2BC	MO3NI10B11	MOB4
MX2B2	MXB [This is CoMoB,CoWB,FeWB]	
NB2B3	NI3CR2B6	NI4B3_M
NI4B3_O	NI4SI2B	NI5ALB4
NI6SI2B	NI8ALB11	NICR3B6
SIB3	SIB6	SIB_N
TAB2_C32	T_M23B6	W2B5_D8H
WB4	WB_ALPHA	WB_BETA
YB4	YB6	YB66

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炭化物相

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AL4C3_D71	AL4SIC4	AL8SIC7
ALCCR2	B4C	CAC2_HT
CAC2_LT	CR2VC2	FE8SI2C
FECN_CHI	FEW3C	KAPPA_E21
KSI_CARBIDE [This is M3C carbide]		
M12C [This is Co6W6C/Ni6Mo6C]		M23C6
M3C2	M3X_D011 [This is also Cementite]	
M5C2	M6C	M7C3
MC_ETA	MC_SHP	MG2C3
MGC2	MW3C [This is CoW3C and NiW3C]	
SIC	TA4C3	TI3SIC2
Y15C19_H	Y15C19_R	Y2C3_H
Y2C3_R	YC2_C11A	YC_GAMMA

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窒化物相

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ALN_B4	BN_HP4	HF3N2
HF4N3	M3N2	M4N_LP1
MN6N4	MN6N5	
PI [This is Cr12.8(Fe,Ni)7.2N4]		SI3N4
TAN_EPS	TI2ALN	TI2N
TI3AL2N2	TI3ALN	TI3N2
TI4N3_ZETA	Z_PHASE	

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珪化物

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AL2CASI2	AL2MN2SI3_TAU1	AL2MNSI3_TAU10
AL3MN4SI2_TAU5	AL3MNSI2_TAU4	AL5MN6SI7_TAU2
ALFESI_ALPHA	ALFESI_BETA	ALFESI_DELTA
ALFESI_GAMMA	ALFESI_TAU1	ALFESI_TAU3
ALMNSI_TAU3	ALMNSI_TAU6	ALMNSI_TAU8
ALMNSI_TAU9	ALSIZR_TAU1	ALSIZR_TAU2
ALSIZR_TAU3	CASI2_C12	CASI_BF
CO2SI_ALPHA	CO2SI_BETA	CO3SI
COSI_B20	CR2NI2SI	CR3NI5SI2
CR3SI_A15	CRNBSI	CRSI2_C40
CU15SI4_EPSILON	CU19SI6_ETA	CU33SI7_DELTA
CU56SI11_GAMMA	CU5MN4SI	CU6NISI3
CUNISI_TAU2	FE2SI	FESI2_H
FE2SITI_L21	FESIZR_TAU1	FESIZR_TAU2
FESIZR_TAU3	FESIZR_TAU4	FESIZR_TAU5
FESIZR_TAU8	FESIZR_TAU9	M11SI8
M3SI2_D5A	M3SI_D03	M3SI_P
M5SI3_D88	M5SI3_D8L	M5X3_D8M
M6SI5	MG2SI	MN11SI19
MN6SI	MN9SI2	MNSI_X
MSI2_C1	MSI2_C11B	MSI2_C40
MSI2_C49	MSI2_OC48 [This is FeSi2_LT]	MSI_B27
MSI_B31	MX2_C54	MX_B20
NB5SI3_BETA	NI2SI_DELTA	NI2SI_THETA
NI3SI2_EPSILON	NI3SI_BETA2	NI3SI_BETA3
NI5SI2_GAMMA	NISITI_TAU1	NISITI_TAU2
NISITI_TAU3	NISITI_TAU4	NISITI_TAU5
TAVSI_TAU1	TAV_TAU2	Y3SI5_HT
Y3SI5_LT	YSI2_HT	YSI2_LT
Z5SI3_D88 [This is (Cr,Ti)5Si3(C,N,Va)x]		Z5SI4
Z6SI5	ZR3SI1	ZR5SI4_BETA
ZRSI_BF		

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4) 酸化物, 燐化物, 硫化物

酸化物相

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AL2CASI2	AL2MN2SI3_TAU1	AL2MNSI3_TAU10
AL18B4O33 [This is 9Al2O3.2B2O3]		AL2C1O1
AL2FE2O6 [This is Al2O3.Fe2O3]	AL2TIO5 [This is Aluminum Titanate]	
AL4B2O9 [This is 2Al2O3.B2O3]	AL4O4C	ALPHA_SPINEL
ANDALUSITE [This is Al2O3.SiO2 (High-pressure phase)]		
ANORTHITE [This is CaO.Al2O3.2SiO2]		B2O3
C13A6Z2 [This is 13CaO.6Al2O3.2ZrO2]	CA1AL12O19 [This is CaO.6Al2O3]	
CA1AL16MG2O27 [This is CaO.8Al2O3.2MgO]	CA1AL2O4 [This is CaO.Al2O3]	

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CA1AL407 [This is CaO.2Al2O3]  
 CA2AL28MG2O46 [This is 2CaO.14Al2O3.2MgO]  
 CA2FE2O5 [This is 2CaO.Fe2O3]  
 CA2SiO4\_ALPHA [This is Alpha-2CaO.SiO2]  
 CA2SiO4\_ALPHA\_PRIME [This is Alpha\_Prime-2CaO.SiO2]  
 CA3AL2O6 [This is 3CaO.Al2O3]  
 CA3AL4MGO10 [This is 3CaO.2Al2O3.MgO]  
 CA4FE17O29 [This is 4CaO.FeO.8Fe2O3]  
 CA4FE9O17 [This is 4CaO.FeO.4Fe2O3]  
 CA6ZR19O44 [This is 6CaO.19ZrO2 (Phi2)]  
 CA2SiO4\_ALPHA [This is Alpha-2CaO.SiO2]  
 CA2SiO4\_ALPHA\_PRIME [This is Alpha\_Prime-2CaO.SiO2]  
 CA3AL2O6 [This is 3CaO.Al2O3]  
 CA3AL4MGO10 [This is 3CaO.2Al2O3.MgO]  
 CA4FE17O29 [This is 4CaO.FeO.8Fe2O3]  
 CA4FE9O17 [This is 4CaO.FeO.4Fe2O3]  
 CA6ZR19O44 [This is 6CaO.19ZrO2 (Phi2)]  
 CACO3 CACR2O4\_A CACR2O4\_B  
 CAFE2O4 [This is CaO.Fe2O3] CAFE3O5 [This is CaO.FeO.Fe2O3]  
 CAFE4O7 [This is CaO.2Fe2O3] CAFE5O7 [This is CaO.3FeO.Fe2O3]  
 CAMN2O4 CAMNO3  
 CAZR4O9 [This is CaO.4ZrO2 (Phi1)] CAZRO3\_C [This is Cubic CaO.ZrO2]  
 CAZRO3\_O [This is Orthorhombic CaO.ZrO2]  
 CLINO\_PYROXENE [Clinoenstatite, Diopside, Pigeonite, Hedenbergite and Clinoferrosilite]  
 CO3O4 CORDIERITE [This is Mg2Al3(AlSi5)O18]  
 CORUNDUM [This is also Alpha-Al2O3, Hematite(Fe2O3) and Mn2O3]  
 CRISTOBALITE CUO CUPRITE\_C3  
 FE2S3O12 FE4NB2O9 FEC1O3  
 FEC5O5 FESIO3 [This is FeO.SiO2] FESO4  
 FLUORITE\_C1 [This is Gamma-ZrO2(Cubic)]  
 HALITE [This is also Lime(CaO), Wustite(FeO) and Periclase(MgO)]  
 HATRURITE [This is 3CaO.SiO2] HFSIO4  
 KYANITE [This is Al2O3.SiO2]  
 LARNITE [This is 2CaO.SiO2(metastable at 1atm)]  
 KYANITE [This is Al2O3.SiO2]  
 LARNITE [This is 2CaO.SiO2(metastable at 1atm)]  
 LOWCLINO\_PYROXENE [This is (Ca,Mg)MgSi2O6]  
 MELILITE [This is Gehlenite(2CaO.Al2O3.SiO2) and Akermanite(2CaO.MgO.2SiO2)]  
 MERWINITE [This is 3CaO.MgO.2SiO2] MN2O3  
 MN2YO5 MNYO3\_HEX MO4O11  
 MO8O23 MO9O26 MOO2  
 MOO3 MULLITE [This is 3Al2O3.2SiO2--2Al2O3.SiO2]  
 MWO4 NB2O5 NBO1  
 NBO2 NI6MNO8 NIMNO3  
 NIMOO4  
 OLIVINE [This is 2CaO.SiO2, Forsterite(CaO.MgO.SiO2) and Fayalite]  
 ORTHO\_PYROXENE [This is also Enstatite and Orthodiopside]

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PROTO_PYROXENE [This is also Protodiopside]		
PSEUDO_WOLLASTONITE [This is CaO.SiO <sub>2</sub> ]		
PT3O4	PTO2	QUARTZ
RANKINITE [This is 3CaO.2SiO <sub>2</sub> ]		RE2O7
REO2	REO3	
RHODONITE [This is MnO.SiO <sub>2</sub> ]		RUTILE_MO2
SAPPHIRINE		
SILLIMANITE [This is Al <sub>2</sub> O <sub>3</sub> .SiO <sub>2</sub> (High-pressure phase)]		
SPINEL [ This is also Magnetite(Fe <sub>3</sub> O <sub>4</sub> )]		TA2O5_ALPHA
TA2O5_BETA	TI10O19	TI20O39
TI2O3	TI3O2	TI3O5
TI4O7	TI5O9	TI6O11
TI7O13	TI8O15	TI9O17
TIOX	TIO_ALPHA	TRIDYMITTE
V2O5	V3O5_HT	V3O5_LT
V3O7	V4O7	
V52O64 [This is Delta-Prime]		V5O9
V6O11	V6O13	V7O13
V8O15	VO2_HT	VO_BETA
VO_GAMMA	W18O49	W20O58
W25O74	WO3_A	WO3_B
WO3_C	WOLLASTONITE [This is CaO.SiO <sub>2</sub> ]	
Y2CU2O5	Y2SI2O7_ALPHA	Y2SI2O7_BETA
Y2SI2O7_DELTA	Y2SI2O7_GAMMA	Y2SIO5
YAG [This is Y <sub>3</sub> (Al,Cr,Fe) <sub>5</sub> O <sub>12</sub> ]	YAM [This is Y <sub>4</sub> (Al,Si) <sub>2</sub> O <sub>9</sub> ]	
YAP [This is (Ca,Y)(Al,Cr,Fe) <sub>3</sub> O <sub>3</sub> ]		YCUO2
ZO2_MONO	ZO2_TETR	
ZRSIO4 [This is Tchernobylite]		ZRTI2O6
ZRTIO4_ALPHA	ZRTIO4_BETA	ZRW2O8

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燐化物相(純 P 相を含む)

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CO2P_C23	COP3_D02	CR12P7
CRP2	CRP4	CU2P7
CU3P_D021	CUP2	FENB2P
FENB4P	FEP2_C18	FEP4
FESI4P4	FEMP	M2P_C22
M3P_D0E	MN3P2	MNP4
MO3P	MOP_BH	MP_B31
NB3P	NB7P4	NBP1
NBP2	NI12P5_DELTA	NI12P5_GAMMA
NI5P2_HT	NI5P2_LT	RED_P
SIP	TI17P10	TI3P
TI4P3	TI5P3_D88	TIP2_C16
TIP_BI	WHITE_P	ZINCBLLENDE_B3

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硫化物相(純 S 相を含む)

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AL2CASI2	AL2MN2SI3_TAU1	AL2MNSI3_TAU10
AL2S3_S	ALS_S	ANILITE
CHALCOCITE_ALPHA	CHALCOCITE_BETA	CO3S4_H11
CO4S3_S	CO9S8_S	COVELLITE
CR1_03S	CR2S3_S1	CR2S3_S2
CR3S4_S	CR5S6_S	CR7S8_S
DIGENITE [This is Cu9S5]	DJURLEITE	
MARCASITE [This is Alpha-FeS2, OsS2]		MO2S3_S
MONOCLINIC [This is Beta-S]	MOS3_S	MS2_C6
MS2_C7	MS_B1 [This is MnS]	NI3S2_BETA
NI3S2_LT	NI3S4_ZETA	NI4S3_BETA2
NI7S6_GAMMAP	NIS_B13	
ORTHORHOMBIC_S [This is Alpha-S]		P2S3_S
P2S5_S	P4S3_ALPHA	P4S3_BETA
P4S5_S	P4S7_S	P4S9_S
PS_S	PYRITE [This is Beta-FeS2]	
PYRRHOTITE [This is Fe(1-x)S]		RE2S7
RES2	RES3	SIS_S
SIS2	TI2S	TI4C2S2
TI8S10	TI8S3	TI8S9
TIS3	ZR2S3 ALMNSI_TAU9	ALSIZR_TAU1
ALSIZR_TAU2		

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5) その他の化合物相

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AL10V	AL11CR2	AL11M4
AL11TI5	AL12M	AL12MG17
AL13CO4	AL13CR2	
AL13FE4 [This is Al3Fe]	AL14CA13	
AL15CO5 [Al <sub>15.1</sub> Co <sub>4.9</sub> ]	AL23V4	AL2CU_THETA
AL2CU3_DELTA	AL2CUMG_S	AL2FE
AL2TI	AL2W	AL2Z3
AL3CA8	AL3CO	AL3M_D022
AL3NB_D022	AL3NI2_D513	AL3NI5
AL3NI_D011	AL3X2	AL3X4
AL3Y_HT	AL3Y_LT	AL3Z_D023
AL4CA_D13	AL4CR	AL4M1
AL4MN	AL4ZR5	AL5CO2_D811
AL5FE2	AL5FE4 [This is ε in Al-Fe]	
AL5M1	AL62CU25FE13	AL63MO37
AL69TA39	AL6MN_D2H	AL77W23
AL7CU2FE	AL7TA5	AL7V

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AL7W3	AL8CR5_HT	AL8CR5_LT
AL8MN5_D810	AL8MO3	AL8V5
AL9CO2	AL9CR4_H	AL9CR4_L
AL9CU11_ZETA	ALCR2_C11B	ALCU3MN2
ALCU_EPSILON	ALCU_ETA	ALCU_GAMMA_D83
ALCU_GAMMA_H	ALFEZR_TAU1	ALFEZR_TAU2
ALFEZR_TAU3	ALM3_D019	ALMG_BETA
ALMG_EPSILON	ALMO_A2	ALTA
ALY2	ALZR2_B82	ALZR3_L12
B2_BCC	CA2M_C23	CACU
CHI_A12	CO10CU57TI33	CO11ZR2
CO3Y2	CO3Y4	CO5Y8
CO7HF	CO7Y6	COCRTI_TAU1
COCRTI_TAU2	COZR3	CR3MN5
CU2TI	CU2TIZR	CU2Y_HT
CU2Y_LT	CU3TI2	CU4TI_BETA
CU4TI3	CU4Y	CU51Z14
CU6Y	CU8M3	CUB_A15
CUFETI_TAU2	CUFETI_TAU3	CUFETI_TAU4
CUFETI_TAU5	CUMG2_CB	CUMTI_TAU1
CUNITI_TAU2	CUNITI_TAU4	CUNITI_TAU6
CUTI3	CUTI_B11	CUZ_B2
FCC_L10	FE2ZR_HEX	FEZR3
G_PHASE [This is Th6Mn23 prototype phase]		HFMN
HIGH_SIGMA	LAVES_C14	LAVES_C15
LAVES_C36	M10X7	M12Y_D2B
M17Y2	M2X_OI6	M3TI_TAU
M3X_D019	M3X_D024	M3Y
M5CA_D2D	M5Y_D2D	M5CA_D2D
M7X2	M7Y2	MG24Y5_A12
MG2NI	MN2ZR_C14	MN3TI
MN4TI	MNNI2	MNNI3
MNNI_ALPHA	MNNI_BETA	MNTA
MONI_DELTA	MU_PHASE	MX2_C16
MX3_A15	MY3_D011	MY_B27
MZ2_C11B	MZ2_C16	MZ2_E93
MZ_BF	NI11M9	NI21M8
NI2AL3Y_TAU6	NI2ALY2_TAU9	NI2TA_C11B
NI2Y3	NI3AL7Y2_TAU5	NI3AL9Y_TAU2
NI3ALY2_TAU11	NI3CA	NI3HF_ALPHA
NI3HF_BETA	NI3M_D0A	NI3V_D022
NI4X_D1A	NI4Y	NI6AL23Y4_TAU1
NI6AL2Y3_TAU10	NI7CA2	NI7HF3
NI8ALY3_TAU12	NI8M	NIAL2Y_TAU7
NIAL3Y_TAU4	NIAL4Y_TAU3	NIALY_TAU8
NIHF2_C16	NIHF_BETA	NITIZR_LAMBDA
NIV3_A15	NIW2	NIW_X

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(つづく)

(つづき)

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P_PHASE [This is Cr9Mo213Ni20]                                R_PHASE  
SIGMA                                         TA3FE2                                TIMN_ALPHA  
TIMN_BETA  
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以上

最終校正 2022 年 10 月 30 日

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