Supplementary Materials

Table. The experimental and calculated enthalpies of the formation of intermetallic compounds with the crystallographic information in the *RE*-Fe (*RE* = La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Lu, and Y) binary systems.

Compounds	Prototype	Space group	Enthalpies of formation (kJ/mol-atom)	Method
$Fe_{17}Ce_2$	Th_2Zn_{17} [39]	$R\bar{3}m$ [39]	6.634	First-principles calculation [141]
			1.4423	
			-1.6±2.8	First-principles calculation [140]
			2.5	
			0.394	Experiment [44]
			-1.4	Experiment [45]
			-1.529	Calphad calculation [18]
				Calphad calculation [47]
				Calphad calculation [29]
Fe_2Ce	$MgCu_2$ [39]	$Fd\bar{3}m$ [39]	16.057	First-principles calculation [141]
			2.98	
			-11.3	First-principles calculation [140]
			-4.866	
			-2.7	Experiment [45]
			-2.901	Calphad calculation [18]
				Calphad calculation [47]
				Calphad calculation [29]
$Fe_{17}Pr_2$	Th_2Zn_{17} [51]	$R\bar{3}m$ [51]	5.192	First-principles calculation [141]
			5.192	
			-0.426	First-principles calculation [140]
			-1.92	
			1.973	Calphad calculation [25]

			-0.2±3	Experiment [65]
			-3.2	Calphad calculation [18]
			1.09	Experiment [44]
				Ab into [44]
				Experiment [54]
$Fe_{17}Nd_2$	Th_2Zn_{17} [18]	$R\bar{3}m$ [18]	3.942	First-principles calculation [141]
			30.961	
			-0.593	First-principles calculation [140]
			0.53	
			-3±3.9	Calphad calculation [25]
			-3.8	Calphad calculation [18]
			-0.64±0.01	Experiment [44]
				Ab into [44]
				Experiment [54]
$Fe_{17}Nd_5$	—	$P6_3/mcm$ [18]	-0.61	Calphad calculation [25]
			0.523	Calphad calculation [18]
$Fe_{17}Sm_2$	Th_2Zn_{17} [69]	$R\bar{3}m$ [69]	1.923	First-principles calculation [141]
			28.557	
			-3.1±3.2	First-principles calculation [140]
			-3.13	
			1.578	Experiment [44]
			-0.355	Calphad calculation [26]
				Calphad calculation [18]
				Calphad calculation [82]
Fe_3Sm	$NbBe_3$ [69]	$R\bar{3}m$ [69]	0.57692	First-principles calculation [141]
			-4.80	
			-3.625	Calphad calculation [26]
			-3.55	Calphad calculation [18]
				Calphad calculation [82]

				First-principles calculation
			2.211	[141]
			2.115	First-principles calculation
Fe_2Sm	$MgCu_2$ [69]	$Fd\bar{3}m$ [69]	-4.47	[140]
			-5	Calphad calculation [26]
			-3.038	Calphad calculation [18]
				Calphad calculation [82]
			0.096	First-principles calculation
			-0.576	[141]
			-3.03±0.03	First-principles calculation
			-2.3	[140]
			-3.278	Experiment [54]
$Fe_{17}Gd_2$	Th_2Zn_{17} Th_2Ni_{17} [78]	$R\bar{3}m$/ $P6_3/mmc$ [78]	-2.505	Experiment [81]
			-4.1	Calphad calculation [26]
			-3.6	Calphad calculation [19]
			-4.246	Calphad calculation [86]
				Calphad calculation [85]
				Calphad calculation [84]
			-1.346	First-principles calculation
			118.7	[141]
			-6.503	First-principles calculation
			-5.918	[140]
$Fe_{23}Gd_6$	Th_6Mn_{23} [74]	$Fm\bar{3}m$ [74]	-9.0	Calphad calculation [26]
			-4.7	Calphad calculation [19]
			-7.71	Calphad calculation [86]
				Calphad calculation [85]
				Calphad calculation [84]
			-3.557	First-principles calculation
Fe_3Gd	$NbBe_3$ [74]	$R\bar{3}m$ [74]	-9.3	[141]
			-7.879	Experiment [81]

			-7.7	Calphad calculation [26]
			-9.63	Calphad calculation [19]
			-4.9	Calphad calculation [86]
			-9.527	Calphad calculation [85]
				Calphad calculation [84]
Fe_2Gd	$MgCu_2$ [74]	$Fd\bar{3}m$ [74]	-3.173	First-principles calculation [141]
			1.73	
			-1.8±3.4	First-principles calculation [140]
			-11.6	
			-3.5	Experiment [44]
			-9.428	Experiment [81]
			-8.833	Experiment [80]
			-11.18	Calphad calculation [26]
			-4.5	Calphad calculation [19]
			-12.181	Calphad calculation [86]
				Calphad calculation [85]
				Calphad calculation [84]
$Fe_{17}Tb_2$	Th_2Zn_{17} Th_2Ni_{17} [92]	$R\bar{3}m$/ $P6_3/mmc$ [92]	6.153	First-principles calculation [141]
			-0.384	
			-2.1±3.1	First-principles calculation [140]
			-3.3	
			-2.97	Experiment [102]
			-2.048	Experiment [54]
			-2.453	Calphad calculation [27]
			-2.528	Calphad calculation [104]
				Calphad calculation [19]
				This work (cal.)
$Fe_{23}Tb_6$	Th_6Mn_{23} [92]	$Fm\bar{3}m$ [92]	16.442	First-principles calculation [141]
			-3.173	
			-5.35	First-principles calculation

			-4.938	[140]
			-5.965	Calphad calculation [27]
			-5.284	Calphad calculation [104]
				Calphad calculation [19]
				This work (cal.)
Fe_3Tb	$PuNi_3$ [92]	$R\bar{3}m$ [92]	10.576	First-principles calculation [141]
			-5.192	
			-6.5	First-principles calculation [140]
			-6.339	
			-7.775	Calphad calculation [27]
			-6.757	Calphad calculation [104]
				Calphad calculation [19]
				This work (cal.)
Fe_2Tb	$MgCu_2$ [92]	$R\bar{3}m$ [92]	15.5769	First-principles calculation [141]
			-5.5±2.4	
			-7.81	Experiment [102]
			-8.271	Calphad calculation [27]
			-9.4	Calphad calculation [104]
			-9.005	Calphad calculation [19]
				This work (cal.)
$Fe_{17}Dy_2$	Th_2Ni_{17} [96]	$P6_3/mcm$ [96]	-1.249	First-principles calculation [141]
			25.384	
			-5.3±1.7	First-principles calculation [140]
			-4.6	
			-1.9	Experiment [102]
			-5.2	Experiment [54]
			-6.421	Experiment [44]
			-2.328	Calphad calculation [27]
			-2.636	Calphad calculation [104]
			-2.636	Calphad calculation [105]

			-4.988	Calphad calculation [83]
				Calphad calculation [19]
				This work (cal.)
$Fe_{23}Dy_6$	Th_6Mn_{23} [96]	$Fm\bar{3}m$ [96]	-4.326	First-principles calculation [141]
			19.423	
			-9.4	First-principles calculation [140]
			-12.649	
			-6.034	Calphad calculation [27]
			-6.034	Calphad calculation [104]
			-6.062	Calphad calculation [105]
			-8.786	Calphad calculation [83]
				Calphad calculation [19]
				This work (cal.)
Fe_3Dy	$PuNi_3$ [96]	$R\bar{3}m$ [96]	-6.827	First-principles calculation [141]
			-7.7	
			-10.3	Experiment [103]
			-12.528	Calphad calculation [27]
			-7.894	Calphad calculation [104]
			-7.475	Calphad calculation [105]
			-7.8	Calphad calculation [83]
			-10.319	Calphad calculation [19]
				This work (cal.)
Fe_2Dy	$MgCu_2$ [96]	$Fd\bar{3}m$ [96]	-7.5	First-principles calculation [141]
			10.57	
			-1.6±2.9	First-principles calculation [140]
			-11.1	
			-11.6	Experiment [102]
			-12.296	Experiment [103]
			-11.053	Calphad calculation [27]
			-9.766	Calphad calculation [104]

			-7.7	Calphad calculation [105]
			-9.766	Calphad calculation [83]
			-12.327	Calculation [44]
				Calphad calculation [19]
				This work (cal.)
$Fe_{17}Ho_2$	Th_2Ni_{17} [19]	$P6_3/mcm$ [19]	-1.538	First-principles calculation [141]
			-1.442	
			-6.7	First-principles calculation [140]
			-2.2	
			-2.4	Experiment [54]
			-2.36	Calphad calculation [91]
				Calphad calculation [19]
				Calphad calculation [28]
$Fe_{23}Ho_6$	Th_6Mn_{23} [19]	$Fm\bar{3}m$ [19]	-5.576	First-principles calculation [141]
			-5.769	
			-4.3	First-principles calculation [140]
			-6.13	
			-5.67	Calphad calculation [91]
				Calphad calculation [19]
				Calphad calculation [28]
Fe_3Ho	$NiPu_3$ [19]	$R\bar{3}m$ [19]	-8.269	First-principles calculation [141]
			-8.173	
			-5.3	First-principles calculation [140]
			-7.8	
			-7.32	Calphad calculation [91]
				Calphad calculation [19]
				Calphad calculation [28]
Fe_2Ho	$MgCu_2$ [19]	$Fd\bar{3}m$ [19]	-9.519	First-principles calculation [141]
			7.788	
			-2.6±3.3	First-principles calculation

			-6.98	[140]
			-10.0	Experiment [44]
			-10.62	Calphad calculation [91]
				Calphad calculation [19]
				Calphad calculation [28]
$Fe_{17}Er_2$	Th_2Ni_{17} [109]	$P6_3/mmc$ [109]	-1.923	First-principles calculation
			-1.826	[141]
			-6.6	First-principles calculation
			-2.447	[140]
			-9.85	Experiment [54]
			-5.43	Calphad calculation [19]
			--3.67	Calphad calculation [110]
			-3.255	Calphad calculation [111]
				Calphad calculation [112]
				This work (cal.)
$Fe_{23}Er_6$	Th_6Mn_{23} [109]	$Fm\bar{3}m$ [109]	-6.923	First-principles calculation
			5.384	[141]
			-6.139	First-principles calculation
			-11.1	[140]
			-11.0	Calphad calculation [19]
			-7.09	Calphad calculation [110]
			-7.216	Calphad calculation [111]
				Calphad calculation [112]
				This work (cal.)
Fe_3Er	$NiPu_3$ [109]	$R\bar{3}m$ [109]	-9.615	First-principles calculation
			-9.615	[141]
			-7.9	First-principles calculation
			-8.26	[140]
			-11.6	Experiment [103]
			-13.3	Calphad calculation [19]

			-8.56	Calphad calculation [110]
			-8.881	Calphad calculation [111]
				Calphad calculation [112]
				This work (cal.)
Fe_2Er	$MgCu_2$ [109]	$Fd\bar{3}m$ [109]	-11.538	First-principles calculation [141]
			5.48	
			-12.5	First-principles calculation [140]
			-1.9±3.0	
			-11.0	Experiment [103]
			-12.5	Experiment [44]
			-13.5	Calphad calculation [19]
			-12.05	Calphad calculation [110]
			-11.611	Calphad calculation [111]
				Calphad calculation [112]
				This work (cal.)
$Fe_{17}Tm_2$	Th_2Ni_{17} [89]	$P6_3/mcm$ [89]	-2.499	First-principles calculation [141]
			-2.307	
			-4.17±0.04	First-principles calculation [140]
			0.2	
			-2.478	Experiment [54]
			-3.54	Calphad calculation [90]
				Calphad calculation [19]
				Calphad calculation [28]
$Fe_{23}Tm_6$	Th_6Mn_{23} [89]	$Fm\bar{3}m$ [89]	-7.981	First-principles calculation [141]
			-8.365	
			-2.85	First-principles calculation [140]
			-6.482	
			-8.02	Calphad calculation [90]
				Calphad calculation [19]
				Calphad calculation [28]

			-11.057	First-principles calculation [141]
			-3.366	
Fe_3Tm	$NiPu_3$ [89]	$R\bar{3}m$ [89]	-8.35	Calphad calculation [90]
			-9.12	Calphad calculation [19]
				Calphad calculation [28]
			-13.461	First-principles calculation [141]
			-13.846	
			-2.2±2.8	First-principles calculation [140]
			-5.042	
Fe_2Tm	$MgCu_2$ [89]	$Fd\bar{3}m$ [89]	-11.233	Experiment [44]
			-11.63	Calphad calculation [90]
				Calphad calculation [19]
				Calphad calculation [28]
			-2.981	First-principles calculation [141]
			20.576	
			-2.97	First-principles calculation [140]
			-0.55	
$Fe_{17}Lu_2$	Th_2Ni_{17} [90]	$P6_3/mmc$ [90]	-5.4	Calphad calculation [19]
			-3.817	Calphad calculation [90]
				Experiment [54]
				This work (cal.)
			-9.807	First-principles calculation [141]
			10.096	
			-7.068	First-principles calculation [140]
			-4.48	
$Fe_{23}Lu_6$	Th_6Mn_{23} [90]	$Fm\bar{3}m$ [90]	-8.762	Calphad calculation [19]
				Calphad calculation [90]
				This work (cal.)
			-12.981	First-principles calculation [141]
Fe_3Lu	$NiPu_3$ [90]	$R\bar{3}m$ [90]	-8.475	

			-5.34	Calphad calculation [19]
			-10.615	Calphad calculation [90]
				This work (cal.)
Fe_2Lu	$MgCu_2$ [90]	$Fd\bar{3}m$ [90]	-16.346	First-principles calculation [141]
			-16.634	
			-3.6±3.1	First-principles calculation [140]
			-11.766	
			-6.02	Experiment [44]
			-11.957	Calphad calculation [19]
				Calphad calculation [90]
				This work (cal.)
$Fe_{17}Y_2$	Th_2Zn_{17} [133]	$R\bar{3}m$ [133]	-0.673	First-principles calculation [141]
			-0.673	
			-8.7	First-principles calculation [140]
			-6.38±0.31	
			-2.84	Experiment [54]
			-5.99	Experiment [123]
			-5.28	Calphad calculation [127]
			-4.36	Calphad calculation [131]
			-0.516	Calphad calculation [131]
			-2.287	Calphad calculation [132]
			-2.994	Calphad calculation [19]
				Calphad calculation [133]
				This work (cal.)
$Fe_{23}Y_6$	Th_6Mn_{23} [133]	$Fm\bar{3}m$ [133]	-4.038	First-principles calculation [141]
			-4.038	
			-8.09±0.49	First-principles calculation [140]
			-5.95	
			-12.05	Experiment [123]
			-12.97	Calphad calculation [127]

			-6.25	Calphad calculation [131]
			-0.862	Calphad calculation [131]
			-5.752	Calphad calculation [132]
			-5.061	Calphad calculation [19]
				Calphad calculation [133]
				This work (cal.)
Fe_3Y	$PuNi_3$ [133]	$R\bar{3}m$ [133]	-6.153	First-principles calculation [141]
			-8.97±0.54	Experiment [123]
			-7.24	Calphad calculation [127]
			-13.04	Calphad calculation [131]
			-13.31	Calphad calculation [131]
			-6.96	Calphad calculation [132]
			-1.75	Calphad calculation [19]
			-6.374	Calphad calculation [133]
			-6.417	This work (cal.)
Fe_2Y	$MgCu_2$ [133]	$Fd\bar{3}m$ [133]	-6.057	First-principles calculation [141]
			-6.057	First-principles calculation [140]
			-7.09±0.61	Experiment [123]
			-12.46	Calphad calculation [127]
			-9.99	Calphad calculation [131]
			-12.47	Calphad calculation [131]
			-6.3	Calphad calculation [132]
			-2.0	Calphad calculation [19]
			-6.412	Calphad calculation [133]
			-7.446	This work (cal.)