When topology meets geometry: topological motifs and uniformity of atomic sublattices in inorganic crystals

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Supplementary Information

Table S1. Topological types of boron substructures in inorganic borides.

Topological type	Occurrence			B/M ratio	Space group	Borides
bnn	235	99	58	0.5	*P6/mmm*	$M(1)M(2)_3B_2$ M(1) = REM, *d*-metals, An, Ca; M(2) = *d*-metals
			24		*C2/m*	
			4		*P-3*	
			11		*P-62m*	$NdRh_3B_2$; $(M_{0.5}Rh_{0.5})Rh_3B_2$ M = Ln, Y
			1		*Cmmm*	$TbCo_3B_2$
			1		*P6$_3$/mmc*	$Ca_{0.67}Pt_3B_2$
		65	38	0.2	*P6/mmm*	$M(1)M(2)_4B$ M(1) = REM*, U, Ca; M(2) = Fe, Co, Ni, Pt
			26			$(M(1)_{1-x}M(2)_x)(M(3)_{4-x}M(4)_x)B$ M(1), M(2) = REM; M(3), M(4) = Fe, Co, Ni
			1			$Eu_3Ni_7B_2$
		25	16	0.125	*P6/mmm*	$M(1)_3M(2)_{13}B_2$ M(1) = Ln, Y; M(2) = Co, Ni
			9			$M_3(Ni_{13-x}Co_x)B_2$ M = Nd, Y
		15	14	0.29	*P6/mmm*	$M_3Co_{11}B_4$ M = Ln, Y
			1		*P-62m*	$In_5Ir_9B_4$
		14		0.57	*P6/mmm*	$M_{0.5}Rh_3B_2$ M = Ln, Y
		11		0.33	*P6/mmm*	$M_2Co_7B_3$ M = Ln, Y
		4	3	0.25	*P6/mmm*	$M(1)_5M(2)_{19}B_6$ M(1) = Lu, Pr, Nd; M(2) = Co, Ni
			1			$NaPt_3B$
		1		0.15	*P6/mmm*	$Nd_5Co_{21}B_4$
		1		0.4	*Pbam*	$Li_2Rh_3B_2$
fcu	209	195	101	0.0625	*P4$_2$/mnm*	$M(1)_2(M(2)_xM(3)_yM(4)_z)_{14}B$ M(1) = Ln, Y; M(2), M(3), M(4) = *d*-metals, Al, Ga, Ge
			30			$M(1)_{2-x}M(2)_xM(3)_{14}B$ M(1), M(2) = REM, Zr, Hf, Th; M(3) = Fe, Co
			21			$M(1)_2M(2)_{14}B$ M(1) = REM, Th; M(2) = Fe, Co
			19			$M(1)_{2-x}M(2)_x(M(3)M(4)M(5))_{14}B$ M(1), M(2) = Ln, Ti, Zr, Hf; M(3), M(4), M(5) = *d*-metals, Al
			15			$M(1)_2Fe_{12}M(2)_2B$ M(1) = Ln, Y; M(2) = *d*-metals, Al, Ga
			8			$M_2(Fe_7Co_7)B$ M = REM

			1		*P1*	$Nd_2Fe_{14}B$
		4		0.125	*Fm-3m*	$M(1)_2M(2)_{6-x}M(3)_xB$ M = *d*-metals
		4	3	1	*Fm-3m*	MB M = Zr, Hf, Pu
			1		*F-43m*	TiB
		3		0.5	*Pnnm*	Pd_2B
					Fm-3m	Be_2B
					F-43m	AlBeB
		1		0.25	*P4/nmm*	Be_4B
		1		0.17	*R3m*	Li_4Ge_2B
		1		0.08	*I4$_1$/acd*	Ga_8Ir_4B
reo	106	100	35	0.26	*Fm-3m*	$M(1)_xM(2)_{23-x}B_6$ M(1) = *d*-, *p*-metals, Li, Mg, U; M(2) = *d*-metals
			32			$M(1)_2M(2)_{21}B_6$ M(1) = REM, *d*-, *p*-metals, Ca, U; M(2) = Co, Ni
			15			$M(1)_{0.8\text{-}2.72}M(2)_{19.96\text{-}22}B_6$ M(1) = *d*-metals, Ln, U; M(2) = Ni, Fe
			14			$M(1)_3M(2)_{20}B_6$ M(1) = *d*-metals, Al; M(2) = Co, Ni
			2			$MCo_{22}B_6$ M = In, Sb
			2			$Fe_{10.66}Nb_{0.84}B_3$; $Mn_{4.547}Co_{18.453}B_6$
		4		0.3	*Fm-3m*	$MNi_{6.7}B_2$ M = Al, Mg, Sn, Zn
		1		0.27	*Fm-3m*	$Cr_{7.9}Ir_{14.1}B_6$
		1		0.16	*R-3m*	$Sm_2Fe_{17}B_3$
pcu	93	60	47	0.25	*Pm-3m*	$M(1)M(2)_3B$ M(1) = REM, *p*-metals, Zr, Hf, U, Th; M(2) = *d*-metals
			11		*P4mm*	MPt_3B M = Ln, U
			2		*Pm-3m*	$Er(M_{3-x}Rh_x)B$ M = Pd, Pt
		25	14	0.5	*I4/mcm*	$M(1)_{2-x}M(2)_xB$ M = *d*-metals
			7			M(1)M(2)B M = *d*-metals
			4			M_2B M = Ta, Cr, Mo, W
		2		0.3	*Cmmm*	$Li_{1.1}Mg_{3.9}Rh_8B_4$; $Zn_5Rh_8B_4$
		2		0.2	*P4/mmm*	LaM_2Al_2B M = Ru, Os
		1		0.28	*P4/mmm*	$Al_3Ru_4B_2$
		1		0.27	*Pm-3m*	$YbRh_{2.67}B$
		1		0.25	*Fm-3m*	YPd_7B_2
		1		0.14	*I4/mcm*	Nb_5Ge_2B
sve	65	30		0.25	*P4/mbm*	$(M(1)_aM(2)_bM(3)_cM(4)_d)_8B_2$ M = *d*-metals, Mg *a*, *b*, *c*, *d* = 0–5.53

		22				$M(1)_2M(2)M(3)_5B_2$ M(1) = Mg, Sc, Ti, Nb; M(2) = *d*-metals, Ge, Ga, Al, Be; M(3) = Rh, Ir, Ru
		7				$M_2Fe(Rh_aRu_b)_5B_2$ M = Ti, Sc *a*, *b* = 1–4
		6				$M(1)_3M(2)_5B_2$ M(1) = Sc, Ti, Hf, Nb, Ta; M(2) = Ru, Co, Rh, Ir
fcu-11-Fdd2	32	29	15	0.67	*Fddd*	$M(1)M(2)_2B_2$ M(1) = REM, Ca, Sr; M(2) = Ru, Rh, Ir
			14		*F222*	$M(1)M(2)_2B_2$ M(1) = Ln, Th, La; M(2) = Ru, Os
		3	2	0.5	*Fdd2*	MIrB M = Cu, Pd
			1		*Fddd*	LiIrB
hcp	26	12	5	0.33	*Pnma*	$M(1)_{3-x}M(2)_xB$ M = Fe, Co, Ni, Rh, Ir
			4			M_3B M = Fe, Co, Ni, Pd
			2			$M(1)M(2)_2B$ M = Fe, Co, Ni
			1		*P2₁/c*	$TaCo_2B$
		7		0.08	*P6₃/mmc*	$M(1)_9M(2)_4B$ M(1) = Zr, Hf; M(2) = Mo, W, Re Os
		6	4	0.5	*Pnma*	M(1)M(2)B M(1) = Re, Mo, W; M(2) = Fe, Co
			1			Rh_2B
			1		*P6₃/mmc*	Pt_2B
		1		1	*P6₃/mmc*	RhB
11T618	23	20		0.46	*R-3m*	$M(1)M(2)_{12}B_6$ M(1) = AEM, REM; M(2) = Fe, Co, Ni
		2				$LaCo_6Fe_6B_6$; $YCo_{11.5}Fe_{0.5}B_6$
		1			*C2/m*	$La_{0.85}Ce_{0.15}Fe_{12}B_6$
nce	22	21	20	0.67	*I4/mmm*	$M(1)M(2)_2B_2$ M(1) = REM, Ba; M(2) = Fe, Co, Rh, Ir
			1			Co_4GdYB_4
		1		0.68		$Co_{1.92}TbB_2$
hex	15	9		0.125	*P6₃/mcm*	$M(1)_5M(2)_3B$ M(1) = REM, *d*-metals; M(2) = Ge, Sn, Pb
		2		0.5	*P-62m*	MFeB M = Nb, Ta
		2		0.18	*P-62m*	$Sn_5M_6B_2$ M = Rh, Ir
		1		1	*Cmcm*	RhB

		1	0.1	*P6$_3$/mmc*	Sn_4Rh_6B
10T1540	15	10	0.43	*P6$_3$mc*	$(M(1)_aM(2)_bM(3)_c)_7B_3$ M = *d*-metals *a*, *b*, *c* = 0–6.6
		3			M_7B_3 M = Tc, Ru, Rh
		2			MRh_6B_3 M = Fe, Co
6,7T1515	13	5	0.27	*P4/mbm*	$M_2Ru_{18}Ti_9B_8$ M = *d*-metals
		3			$Ti_8M_3Ru_{18}B_8$ M = Cr, Mn, Ni
		3			$(M(1)_aM(2)_bM(3)_c)_{29}B_8$ M = *d*-metals *a*, *b*, *c* = 0–18.95
		2			$Zn_{10}MRh_{18}B_8$ M = Fe, Ni
gra	11		0.2	*P6$_3$/mmc*	$M(1)_3M(2)_7B_2$ M(1) = Ln, Y, U; M(2) = Ni, Co
9,11^2,12T2	8		0.46	*Cmc2$_1$*	$MNi_{12}B_6$ M = REM, Th
10T21	7		0.33	*P6$_2$22*	MPt_2B M = REM
bct	5		0.33	*Cmcm*	$Re_{3-x}M_xB$ M = V, Cr, W; Tc_3B
svg	4		0.57	*Fmmm*	$M_2Rh_5B_4$ M = Ca, Sr, La, Eu
5,7T900	4		0.54	*Fmmm*	$M(1)_3M(2)_8B_6$ M(1) = Ca, Sr, Y, Eu; M(2) = Rh, Os
7T30	4	3	0.5	*Fddd*	$MnRe_3B_2$; $(Mo_{1.7}Ge_{0.3})B$; $(Re_{1.5}Cr_{0.5})B$
		1		*C222*	Cr_2B
kwh	4		0.2	*R-3m*	$Ca_3Ni_7B_2$; $Eu_3Pt_7B_2$; $(Mg_aNi_b)_{10}B_2$
ecf	3		0.43	*P6$_3$mc*	$Re_{7-x}M_xB_3$ M = Cr, W; Re_7B_3
bcu-x-13-P4$_2$/mnm	3		0.33	*P4$_2$/n*	$M_{3-x}Re_xB$ M = Fe, Co; Fe_3B
8^{2}T1742	3		0.33	*I4$_1$/amd*	$Lu_2Pd_{13.2}B_5$
			0.32		$Yb_2Pd_{13.6}B_5$
			0.3125		$Y_2Pd_{14}B_5$
lcy	3	2	0.2	*P4$_3$32*	Li_2M_3B M = Pt, Pd
		1		*P4$_1$32*	$(Pt_{0.67}Cu_{0.33})_3Cu_2B$
8,12T1	3		0.17	*P6$_3$/mmc*	$Hf_9M_3B_2$ M = Mo, W; $(Hf_{0.5}Zr_{0.5})_9Mo_3B_2$
dia	3	2	0.083	*Fd-3m*	Mg_8M_4B M = Pt, Rh
		1	0.2	*R-3m*	$Mg_{3.58}Ni_{6.42}B_2$
11T99	2		0.5	*Fddd*	Cr_2B; $(Re_{1.6}V_{0.4})B$
10T22	2		0.46	*R-3m*	$La_{0.85}Ce_{0.15}Fe_{12}B_6$; $YCo_{9.5}Fe_{2.5}B_6$
10,11,12^{2}T5	2		0.46	*Cmc2$_1$*	$MNi_{12}B_6$ M = Y, Pr
8,11T559	2		0.43	*P-62m*	$Ga_{2.7}Ir_9B_5$
			0.42		$Pt_9Cu_3B_5$
svi-x	2		0.33	*I4/mcm*	M_5GeB_2 M = Mo, Ta
11T106	2		0.33	*I-4*	Fe_3B; Fe_2NiB
4,5T428	2		0.29	*P6$_3$/mmc*	$M_2Co_5B_2$ M = Ce, Nd
7,10T481	2		0.25	*Pmma*	$Zn_5M_7B_3$ M = Rh, Ir
eca	2		0.2	*Pnma*	MPd_4B M = Sr, Ba
12T657	1		3	*P6$_3$/m*	PrB_3

ecu	1	1	*Cmcm*	$(Al_{0.1}Mo_{0.9})B$
8,10T2478	1	0.8	*P6$_3$/mmc*	Rh_5B_4
13T4	1	0.8	*I4$_1$/a*	Ir_5B_4
7,9,10T9	1	0.6	*Pmmm*	$ZnIr_4B_3$
9,11T2521	1	0.55	*I-43m*	$Mg_{10}Ir_{19}B_{16}$
6,8T1564	1	0.54	*Fmmm*	$La_3Ru_8B_6$
5^2,7T7	1	0.53	*Fmmm*	$Sr_5Rh_{14}B_{10}$
5^3,7T1	1	0.52	*Fmmm*	$Ca_7Rh_{20}B_{14}$
11,12,14T6	1	0.5	*Pmmn*	TaCoB
12T462	1	0.46	*R-3m*	$HoCo_{12}B_6$
12^2T2341	1	0.4375	*Ia-3d*	$AlPd_{15}B_7$
10,12T2862	1	0.43	*P6$_3$cm*	$Cu_{0.95}Pd_{6.05}B_3$
9,11^2T2	1	0.43	*P4/mbm*	$Li_{2.8}Ni_{16}B_8$
10,12T2861	1	0.43	*Pnma*	$Cu_{0.50}Pd_{6.51}B_3$
7,8^2T14	1	0.42	*Cmcm*	$Na_3Pt_9B_5$
fcu-11-C2/c	1	0.4	*C2/c*	Pd_5B_2
9,10T2661	1	0.4	*C2/c*	$La_2Os_2AlB_2$
5^3,6^3T3	1	0.39	*Pbam*	$Li_8Mg_4Rh_{19}B_{12}$
6,8T1563	1	0.33	*P-62c*	$Ga_3Pt_9B_4$
7^2T524	1	0.33	*C2/m*	$YbPt_5B_2$
5,7T489	1	0.29	*R-3m*	$Ce_2Ir_5B_2$
hcp-10-P6$_3$/m	1	0.27	*P6$_3$/m*	$Sn_4Ir_7B_3$
nin	1	0.25	*P-62m*	$LiPt_3B$
tck-8,8-Pnma	1	0.25	*Cmcm*	Zn_2Ir_2B
crs	1	0.2	*Fd-3m*	Al_2Re_3B
5,7T899	1	0.2	*P6$_3$/mmc*	$Ca_5Ni_{15}B_4$
4,5^2T80	1	0.2	*Imma*	$NdNi_4B$
tsi	1	0.2	*C2/m*	Ni_3Zn_2B
tck-7,8-Pbcm	1	0.1875	*Pmma*	$Zn_{7.4}Rh_{8.6}B_3$

*Hereafter REM = rare earth metals; AEM = alkaline earth metals

Table S2. Topological types of carbon substructures in inorganic carbides.

Topological type	Occurrence			C/M ratio	Space group	Carbides
fcu	181	106	48	1	*Fm-3m*	$(M(1)_aM(2)_bM(3)_c)C$ *a*, *b*, *c* = 0–0.9 M = *d*-metals, Al, Ce, U, Pu
			31			$M(1)M(2)C_2$ M = *d*-metals, An, Ce
			17			MC M = *d*-metals, An, Ce
			7			$M(1)M(2)M(3)_2C_4$ M(1), M(2) = *d*-metals, U; M(3) = Zr, Ta, Nb, W
			2			$(Ta_2V_3Zr_3C_8)_{0.5}$; $(Ta_{0.92}U_{1.08})C_2$
			1		*Fd-3m*	TiC
		24	13	0.0625	*P4₂/mnm*	$(M(1)_aM(2)_bM(3)_cM(4)_d)_{16}C$ *a*, *b*, *c*, *d* = 0–14 M = *d*-metals, Ln
			11			$M_2Fe_{14}C$ M = Ln, La
		21	8	0.5	*P4₂/mmc*	MCoC M = Ln, Y
			5		*R-3m*	M_2C M = REM
			3			$Y_{2-x}Sc_xC$
			3		*Pnnm*	$Ti_{0.11}V_{0.89}C_{0.5}$; $Mo_{1.5}W_{0.5}C$; Fe_2C
			1		*Fm-3m*	Be_2C
			1		*P2/m*	$Tb_4Co_2C_3$
		18	17	0.75	*C2/m*	$M(1)_2M(2)_2C_3$ M(1) = Ln, Y, W, U; M(2) = Cr, Mo, W, Re
			1		*Pnnm*	$Th_2Al_2C_3$
		6		0.034	*Fm-3m*	$M_6Mg_{23}C$ M = Ln, La
		4		2	*Fm-3m*	MC_2 M = Sr, Ba, Sc, U
		1		1.23	*Fm-3m*	$(Mo_{0.45}W_{0.36})C$
		1		0.33	*R-3c*	Ni_3C
pcu	147	144	132	0.25	*Pm-3m*	$M(1)M(2)_3C$ M(1) = *p*-, *d*-, *f*-metals, Mg, Ca; M(2) = *d*-metals, Ln, Mg
			5			$(M_aGa_b)Mn_3C$ M = Al, In, Zn *a*, *b* = 0.02–0.98
			2			$M(1)_{4-x}M(2)_xC$ M = Mn, Cr, Sn, Pt
			2		*P4/mmm*	$M(1)M(2)_3C$ M(1) = Ga, Sn; M(2) = Pt, Pd
			1			Mn_2Co_2C
			1		*I4/mcm*	Mn_3GeC
			1		*P-43m*	Fe_4C
		2		0.07	*I4/mcm*	$(La_aFe_bGa_c)_{14}C$ *a*, *b*, *c* = 1–10.1
		1		1	*Pm-3m*	LaC
hex	96	54	37	0.33	*P6₃/mmc*	$M(1)M(2)_2C$ M(1) = *p*-, *d*-metals; M(2) = *d*-metals

			7			$(M(1)_aM(2)_bM(3)_c)_3C$ M = *p*-, *d*-metals *a*, *b*, *c* = 0.066–2
			5			M(1)M(2)AlC M = Ti, V, Cr, Nb, Ta
			5			$(V_{1-x}Cr_x)_2GaC$
		19		0.125		$M(1)_3M(2)_5C$ M(1) = Ge, Sn, Al, Sb, Pb; M(2) = *d*-metals, Ln
		12	7	1	*P-6m2*	$W_{1-x}M_xC$ M = Al, Mo
			5			MC
		6	5	0.5	*P-3m1*	M_2C M = *d*-metals
			1		*P6₃/mmc*	Mo_2C
		3	2	0.25	*Cmcm*	M_3GeC M = Cr, V
			1		*P6₃/mmc*	Mo_2Ga_2C
		1		0.63	*P6₃/mmc*	$(TiV_{0.7}Cr_{0.05}NbTa)AlC_3$
		1		0.2	*C222₁*	$Mo_4Ce_4Al_7C_3$
crs	43	42	17	0.167	*Fd-3m*	$M(1)_3M(2)_3C$ M = *d*-metals
			12			$M(1)_2M(2)_4C$ M = *d*-metals
			8			$M(1)_3M(2)_{1.5}M(3)_{1.5}C$ M(1) = Ta, Nb; M(2), M(3) = *d*-metals
			3			$M(1)_2M(2)_2Ti_2C$ M = Ta, Co, Nb, Ni
			2			$M(1)Al_2M(2)_3C$ M(1) = Co, Ni; M(2) = Ti, Ta
		1		0.5		Ti_2C
reo	35	18	13	0.16	*R-3m*	$M(1)_2M(2)_{17}C_3$ M(1) = Ln, Y; M(2) = Fe, Mn
			5			$Sm_2Fe_{17-x}M_xC_3$ M = Co, Ga
		16	13	0.26	*Fm-3m*	$M(1)_{23-x}M(2)_xC_6$ M = *d*-metals
			2			$M_{23}C_6$ M = Cr, Mn
			1			$Cr_{16}Fe_5Mo_2C_6$
		1		0.75	*Pm-3m*	Nb_4C_3
hcp	32	13	11	0.75	*P6₃/mmc*	MAl_3C_3 M = REM, U
			2		*P6₃mc*	MAl_3C_3 M = Sc, U
		9	5	0.33	*Pnma*	$Fe_{3-x}M_xC$ M = Mn, Fe
			4			M_3C M = Fe, Co, Mn, Cr
		7	3	0.5	*Pbcn*	$M(1)_{2-x}M(2)_xC$ M = Cr, Mo, W, Mn
			2			M_2C M = V, W
			1			VCrC
			1		*P6₃/mmc*	Re_2C
		1		1	*P6₃/mmc*	$Hf_{0.5}Ta_{1.5}C_2$
		1		0.8	*P-3m1*	$(Zr_{0.72}Y_{0.28})Al_4C_4$
		1		0.67	*P-3m1*	Al_2MgC_2
10,12T215	22	20		1	*Pnma*	$M(1)M(2)C_2$

					M(1) = REM, U, Pu; M(2) = *d*-metals
		2	0.67	*Cmcm*	Cr_3C_2; Cr_2VC_2
tca	14	12	8	0.5	*P6₃/mmc*	$M(1)_3M(2)C_2$ M(1) = Ti, Zr, Ta; M(2) = Al, Zn, Ge, Sn, In, Ga
			3			$M_{3-x}Ti_xAlC_2$ M = Ta, Cr, Zr
			1			Mo_2TiAlC_2
		1		0.53		$(Ta_{0.25}Ti_{0.75})_3Al_{0.77}C_2$
		1		0.52		$(Ta_{0.38}Ti_{0.62})_3Al_{0.81}C_2$
cab	12	11	9	0.33	*Fm-3m*	$M(1)_{21}M(2)_8M(3)_7C_{12}$ M(1) = La, Ce, Pr; M(2) = Fe, Mn; M(3) = Sn, Bi, Sb
			2			$La_{21}M_8Ge_{7-x}Al_xC_{12}$ M = Fe, Mn
		1		0.34		$La_{21}Cr_{7.55}Al_{0.76}Ge_{6.24}C_{12}$
bct	12	10		0.0769	*I4/mmm*	$MFe_{11}TiC$ M = Ln, Y
		2		0.5	*Pmnn*	M_2C M = Co, Rh
8^2T414	11			0.67	*Pnma*	Ln_2ReC_2
kag	9	6		0.23	*P6₃/mmc*	$M(1)_6Al_3(Al_{2.5}M(2)_{1.5})C_3$ M(1) = Mo, W; M(2) = Fe, Co, Ni, Mn
		3				$Al_{11}Cu_3Mo_{12}C_6$; $W_9Al_3CoC_3$; $Ni_{10}W_3C_3$
10,13T588	9			0.125	*Cmca*	$M_2Ni_{22}C_3$ M = Ln, La
dia	9	6	5	0.083	*Fd-3m*	$M(1)_6M(2)_6C$ M = Fe, Co, Ni, Mo, W
			1		*Fd-3*	Fe_6W_6C
		2	1	0.25	*Fd-3*	Fe_2W_2C
			1		*Fd-3m*	$Nb_8Zn_4C_3$
		1		0.09	*Fd-3m*	Ni_5W_6C
13T1310	8			0.084	*Im-3m*	$M_{11}Ni_{60}C_6$ M = Ln, Y
nce	6	5		0.67	*I4/mmm*	MU_2C_2 M = Ir, Pt, Rh, Ru, Os
		1		0.68		$Th_2Ni_{0.96}C_2$
lcy	6	5		0.2	*P4₁32*	$M(1)_2M(2)_3C$ M(1) = Al, Re; M(2) = Mo, W, Nb, Ta
		1				Mo_3ReRuC
12,13T503	5			0.67	*P4₂/mnm*	$M(1)_2M(2)C_2$ M(1) = Pr, Nd, Ce; M(2) = Mo, W
10,12T2852	4	3		0.6	*P6₃/mmc*	$M(1)_4M(2)C_3$ M(1) = V, Nb, Ti; M(2) = Al, Ga
		1		1		MoC
10^2T1533	4			0.75	*C2/m*	$M_2Mo_2C_3$ M = Ln
10,12T2861	4	3		0.43	*Pnma*	M_7C_3 M = Mn, Fe, Cr

		1			$Mn_4Fe_3C_3$
fcu	4	2	0.4	*C2/c*	M_5C_2 M = Fe, Mn
		2			$Mn_{5-x}Fe_xC_2$
tcl	3	1	0.75	*R3mr*	Al_4C_3
		1		*R-3mr*	
		1		*R-3m*	
6,8T1565	3	2	0.31	*P6$_3$/mmc*	$W_{13-x}M_xC_4$ M = Co, Ni
		1	0.33		$Co_3W_9C_4$
tcj	2		1	*P6$_3$/mmc*	MC M = Mo, Re
bcu-x	2	1	1	*I-42d*	$FeUC_2$
		1	0.045	*Im-3m*	$U_6Co_{12}Ge_4C$
12^3T5	2		0.857	*R3m*	$(ZrC)_3Al_3(Al_{0.958}Ge_{0.042})C_3$; $Zr_3Al_4C_6$
10-layered packing/ chhhcchhhc	2	1	0.835	*P6$_3$/mmc*	$HfAlC_{1.67}$
		1	0.83	*P6$_3$mc*	$Zr_3Al_3C_5$
9^2,10^3T1	2	1	0.83	*P3$_1$12*	V_6C_5
		1		*P3$_1$*	
12^3T8	2		0.83	*R3m*	$(ZrC)_2Al_3(Al_{0.93}Ge_{0.07})C_3$; $Zr_2Al_4C_5$
8-layered packing/ chhhchhh	2		0.8	*P6$_3$mc*	$M_2Al_3C_4$ M = U, Zr
9,11T300	2		0.67	*Pnma*	Cr_3C_2; $(Cr_{2.55}W_{0.45})C_2$
10,12T2856	1		1	*P-6m2*	CrC
8,10,11T5	1		1	*P4/mbm*	$U_5Re_3C_8$
9,10,11T11	1		0.875	*P4$_3$32*	V_8C_7
9,10^2T7	1		0.83	*C2/m*	Nb_6C_5
6,7T1516	1		0.8	*P4/m*	UW_4C_4
11T106	1		0.8	*I4/m*	$ThAl_4C_4$
tce	1		0.8	*I4/m*	UCr_4C_4
9,10^2T8	1		0.75	*P2$_1$/c*	$Pr_2Mo_2C_3$
thp-x	1		0.75	*I-43d*	Sc_4C_3
10^2T3	1		0.67	*Pnma*	Y_2ReC_2
6,10,12T7	1		0.625	*R-3m*	Ti_8C_5
8,9^2T12	1		0.625	*R3m*	Ti_8C_5
11,12^3,13^3T1	1		0.56	*P3$_1$21*	$Fe_{10}Gd_{13}C_{13}$
8,9T1103	1		0.5	*P4/mbm*	$Y_5Al_3C_4$
cco	1		0.5	*Pbcn*	Mo_2C
chb	1		0.5	*Pna2$_1$*	Nb_2C
ecf	1		0.43	*P6$_3$mc*	Fe_7C_3
10^2,12T9	1		0.43	*P6$_3$mc*	Cr_7C_3
10^2,12T10	1		0.43	*Pbca*	Fe_7C_3
tcl	1		0.43	*P3*	$Ti_5Al_2C_3$
11^3,12T2	1		0.4	*P-1*	Fe_5C_2
14T2	1		0.33	*P6$_3$22*	Fe_3C
8,12T394	1		0.29	*C2/m*	$Mo_{12}Fe_{22}C_{10}$

6,7T1517	1	0.21	*Pbcm*	$Nd_8Co_{3.35}Al_{0.65}Ge_2C_3$
hxl	1	0.2	*P-1*	$Mo_4Ce_4Al_7C_3$
eca	1	0.04	*P6$_3$mc*	$Nd_{15}Ge_9C$

Table S3. Topological types of nitrogen substructures in inorganic nitrides.

Topological type	Occurrence			N/M ratio	Space group	Nitrides
fcu	224	118	46	1	*Fm-3m*	$M(1)M(2)N_2$ M = *d*-metals, Ln, An, Al, Mg, Sr
			36			MN M = *d*-metals, Ln, An, Al, Ga, In
			27			$M(1)_{1-x}M(2)_xN$ M = *d*-metals, Ln, An
			5			$(Ta_{4-x}M_x)N_4$ M = Li, Mg
			4			$M(1)_{2-x}M(2)_xN_2$ M = Ln, An, Mg, Sn
		6	5		*R-3m*	$M(1)M(2)N_2$ M(1) = Na, Sr; M(2) = *d*-metals, Ce
			1			UN
		2			*F-43m*	MN M = Fe, Co
		2			*Pmmn*	CrN; $(Cr_{0.95}Ti_{0.05})N$
		2			*Pnmm*	$Cr_{1-x}V_xN$
		1			*Pn-3m*	WN
		1			*I4/mmm*	MnN
		1			*C2/m*	$Li_2Ta_3N_5$
		8	6	0.5	*Pnma*	M(1)M(2)N M = AEM, *d*-metals, Li
			2			$SrLi_{1-x}Cu_xN$
		6	3		*Ia-3*	Li_3MN_2 M = Al, Ga, Sc
			2			$Li_{53.33}M_{10.67}N_{32}$ M = Ti, Ge
			1			$Li_{3.33}Ge_{0.67}N_2$
		5	4		*R-3m*	M_2N M = Ca, Sr, Ba
			1			$Ba_{1.04}Sr_{0.96}N$
		4	2		*P4₂/mnm*	$Ca_2Li_{2-x}Cu_xN_2$
			2			$Ca_2Li(Li_{0.18}Fe_{0.82})N_2$; Sr_2LiCoN_2
		3			*Pa-3*	Li_7MN_4 M = V, Nb, Ta
		3			*P4/nmm*	M(1)M(2)N M = *d*-metals, Ca, Ga
		3			*P-3m1*	$M_{0.5}N$ M = Ce, Nd, Pr
		3	2		*P4₂/mmc*	M(1)M(2)N M = Li, Ca, Sr, Ni
			1			$CaNi_{0.42}Li_{0.58}N$
		2			*P-43n*	Li_7MN_4 M = V, Mn
		2			*R-3mr*	M_2N M = Ca, Sr
		2			*Pmnn*	M_2N M = Co, Pd
		2			*Fm-3m*	LiMgN; $(Li_{7.2}Cr_{0.8})N_4$
		2			*P4bm*	NbCrN; $Ta_{0.8}Cr_{1.2}N$
		1			*F-43m*	LiZnN
		1			*P4₂/nmc*	Li_7VN_4
		1			*Ibam*	Li_3FeN_2
		1			*Pbcm*	$CuSr_{0.53}Ba_{0.47}N$
		1			*P2₁/c*	LiBeN
		1			*C2/c*	BaCuN
		6	5	0.67	*Ia-3*	M_3N_2 M = Be, Mg, Ca, Zn, Cd
			1		*Pmmn*	Li_5ReN_4
		5	2	1.33	*Fd-3m*	M_3N_4 M = Ge, Sn
			1		*Pm-3m*	W_3N_4
			1		*R-3m*	Th_3N_4
			1		*R-3mr*	Th_3N_4

		4		0.33	*P4/nmm*	BiM_2N M = La, Ce, Pr, Nd
		3		0.17	*I4/mmm*	$Ca_{4-x}M_xBi_2N$ M = La, Pr
		3		0.09	*R-3c*	$M(1)_5M(2)_6N$ M(1) = In, Ga; M(2) = Sr, Ba
		2		1.5	*P-3m1*	M_2N_3 M = Th, U
		2		1.33	*Fd-3m*	$MgSb_2N_4$; $MnTa_2N_4$
		2		1.25	*I4/m*	M_4N_5 M = Nb, Ta
		2		0.57	*P4₂/nmc*	Li_6MN_4 M = Mo, W
		2		0.25	*P2₁/m*	M_2GeGaN M = Sr, Ba
		1		1.32	*Fm-3m*	$Ti_{0.76}N$
		1		1.2	*Fm-3m*	$Ta_{0.83}N$
		1		1.14	*Fm-3m*	$((Zr_3Sc_4)N_8)_{0.5}$
		1		0.85	*R-3m*	$W_{7.08}N_6$
		1		0.6	*Ibca*	Li_4TaN_3
		1		0.53	*P4/ncc*	$Li_{15}Cr_2N_9$
		1		0.52	*Ibam*	$Li_3Fe_{0.86}N_2$
		1		0.036	*Fm-3m*	$Li_{16}Sr_6Ge_6N$
		1		0.0082	*F-43m*	$Li_{26}Na_{58}Ba_{38}N$
pcu	115	93	61	0.25	*Pm-3m*	$M(1)M(2)_3N$ M(1) = *p*-, *d*-metals; M(2) = *d*-metals, Ln, AEM
			28			$M(1)_{1-x}M(2)_xM(3)_3N$ M(1), M(2) = *p*-, *d*-metals, Gd; M(3) = Ti, Fe, Mn, Cr
			2			M_4N M = Mn, Fe
			2			$In_{0.4}Mn_{3.6}N$; $Cu_3Pd_{0.989}N$
		3			*I4/mcm*	$Cr_{3-x}Mn_xGeN$
		1			*P-42₁m*	Cr_3GeN
		4		0.67	*I4/mmm*	$M(1)M(2)_2N_2$ M(1) = Sb, Bi; M(2) = U, Th
		3	2	2	*Fm-3m*	MN_2 M = U, Np
			1		*R-3m*	WN_2
		3		0.33	*Pm-3m*	M_3N M = Cu, Na; $Cu_3Pd_{0.02}N$
		3	2	1	*P4/nmm*	MN M = La, Pr
			1		*P4/mmm*	$LaReN_2$
		1		0.5	*P4/mmm*	FeNiN
		1		0.4	*Pm-3m*	$Co_{2.5}N$
		1		0.34	*Pm-3m*	$(Li_{0.08}Cu_{0.02})(Li_{0.02}Cu_{2.79})N$
		1		0.28	*Fm-3m*	$Cu_3Au_{0.6}N$
		1		0.2	*Pmna*	$Sr_7Sn_3N_2$
hex	70	20	11	0.33	*P6/mmm*	$Li_2(Li_{1-x}M_x)N$ M = *d*-metals
			7			$Li_{3-x}M_xN$ M = Cu, Co, Ni
			2			M_3N M = Li, Na
		6			*P6₃/mmc*	$M(1)M(2)_2N$ M(1) = Al, Ga, In, Zn; M(2) = Ti, Cr, Zn
		2			*P6₃/mcm*	M_3N M = K, Ba
		1			*P-6m2*	Re_3N
		8	5	1	*P-6m2*	$M(1)_{1-x}M(2)_xN$ M = *d*-metals

			3			MN M = Nb, Ta, W
		2			*P6$_3$/mmc*	MN M = Nb, Ta
		1			*P-62m*	TaN
		1			*P-6*	TaN
		10	6	0.25	*Cmcm*	M(1)M(2)$_3$N M(1) = Al, Ga, Ge; M(2) = *d*-metals
			4		*P6$_3$/mmc*	MBa$_3$N M = Li, Na, Sb, Bi
		5		0.33–0.47	*P6/mmm*	$(Li_{1-x}M_x)Li_{1.14–1.98}N$ M = Cu, Ni
		4	3	0.375	*P-62m*	$Li_5(M_{1-x}Li_x)_3N_3$ M = Ni, Mn
			1			$Li_5Ni_3N_3$
		4	2	0.4	*Cmca*	$Ba_2Ni_3N_2$; $Ba_2(Ni_{0.57}Li_{0.43})Ni_2N_2$
			1		*P6/mmm*	$Li_{1.99}Co_{0.53}N$
			1		*Immm*	Li_4FeN_2
		2	1	0.5	*P-3m1*	$TaN_{0.5}$
			1		*P-6m2*	LiNiN
		2		0.34	*P6/mmm*	$Li_{2.94}N$; $Li_{2.92}N$
		2		0.125	*P6$_3$/mcm*	Al_3Hf_5N; Sn_3Zr_5N
hcp	55	15	7	1	*P6$_3$mc*	$Al_{1-x}Ga_xN$
			6			MN M = Al, Ga, In, Tl, Mo
			2			$GeZnN_2$; $(Ga_{0.3333}Ge_{0.3333}Zn_{0.3333})N$
		5	3		*Pna2$_1$*	$MGeN_2$ M = Zn, Mg, Mn
			2			$(ZnGeN_2)_{0.98}(GaN)_{0.04}$; $(ZnGeN_2)_{0.95}(GaN)_{0.1}$
		3			*P6$_3$/mmc*	MN M = Nb, Ta
		2			*Cmc2$_1$*	Mg_2SbN_3; $LiGe_2N_3$
		1			*Pmn2$_1$*	Zn_3MoN_4
		1			*P2$_1$*	$ZnGeN_2$
		5		0.67	*P-3m1*	M(1)M(2)$_2$N$_2$ M(1) = AEM, Zr, Ce; M(2) = Li, Mg, Be
		2			*P-3*	Li_2MN_2 M = U, Th
		2			*P2$_1$/c*	$LiCaMN_2$ M = Al, Ga
		2			*C2/m*	M_3N_2 M = Mg, Ca
		1			*P2$_1$/m*	$Li_3Ca_2V_{0.79}Nb_{0.21}N_4$
		1		0.5	*P6$_3$/mmc*	Re_2N
		1			*P6$_3$mc*	NaSnN
		1			*Pbna*	Mn_2N
		1			*P1*	Fe_2N
		1			*Pbcn*	Fe_2N
		1		0.75	*P6$_3$/mmc*	$Ca_2Mg_5GeN_6$
		1			*P6$_3$/m*	Sr_3CrN_3
		1			*P2$_1$/c*	Ca_3AlN_3
		2		0.6	*R-3*	$Li_6M_2Mn_2N_6$ M = Ca, Sr
		2	1	0.33	*P6$_3$/mmc*	Li_3N
			1		*Pnma*	Na_3N
		1		1.1	*P6$_3$mc*	$Mo_{0.93}N$
		1		0.91	*P31c*	$W_{1.1}N$
		1		0.83	*P6$_3$/mmc*	$Mg_3Al_3N_5$
		1		0.8	*P-3m1*	$Mg_3Al_2N_4$

crs	45	43	20	0.17	*Fd-3m*	$M(1)_4M(2)_2N$ M = *d*-metals
			12			$M(1)_3M(2)_3N$ M = *d*-metals
			7			$(M(1)_aM(2)_bM(3)_cM(4)_dM(5)_e)_6N$ M = *d*-metals, Al, Ge, Ga *a*, *b*, *c*, *d*, *e* = 0–3
			2			$Li_2(M_3N)_2Ga_4$ M = Ca, Sr
			2			$M(1)_{2.5}M(2)_{3.5}N$ M = Mn, Nb, Zr, V
		2	1	1	*Fd-3m*	$CsNbN_2$
			1		*I4₁*	$Cs_5NaW_4N_{10}$
lcy	44	29		0.2	*P4₁32*	$M(1)_{2-x}M(2)_xMo_3N$ M = *d*-metals
		8				$M(1)_2M(2)_3N$ M = *d*-metals, Ga Al
		5				$M(1)M(2)Mo_3N$ M = *d*-metals
		2				$(Fe_aPt_bMo_c)_5N$ *a*, *b*, *c* = 0.56–2.81
bct	27	24	14	0.077	*I4/mmm*	$M(1)M(2)_2Fe_{10}N$ M(1) = Ln, Y; M(2) = Mo, V
			9			$M(1)M(2)Fe_{11}N$ M(1) = REM; M(2) = Ti, Mo
			1			$NdFe_{10.44}Mo_{1.56}N$
		3	2	0.5	*P4₂/mnm*	$Mn_{2-x}Li_xN$
			1			Ti_2N
tca	25	9	4	1	*P6₃/mmc*	$M(1)M(2)N_2$ M = *d*-metals, Mg, Ba, Ce
			2			$W_{2-x}M_xN_2$ M = Li, Fe
			2			$Mn(Ta_aTi_b)_3N_4$ *a*, *b* = 0–3
			1			MoN
		4	2		*P6₃/mcm*	$Ta_{4-x}Li_xN_4$
			2			$M(1)_{3-x}M(2)_xN_3$ M(1) = Nb, Ta; M(2) = Mg, Mn
		2	1		*P-31c*	$FeWN_2$
			1			$(Fe_{0.81}Mo_{0.19})MoN_2$
		1			*P6₃mc*	$ZnMoN_2$
		2		1.2	*P6₃/mcm*	M_5N_6 M = Nb, Ta
		1		1.56	*P6₃/mmc*	$W_{2.56}N_4$
		1		1.24	*P6₃/mcm*	$Ta_{4.82}N_6$
		1		1.22	*P6₃/mmc*	$Mo_{0.82}N$
		1		1.18	*P6₃/mmc*	$Mo_{1.7}N_2$
		1		1.15	*P6₃/mmc*	$Fe_{0.74}WN_2$
		1		1.11	*P6₃/mmc*	$Mo_{1.8}N_2$
		1		0.87	*P6₃/mmc*	$W_{4.6}N_4$
reo	18	11	8	0.16	*R-3m*	$Ln_2M_{17}N_3$ M = Fe, Co
			3			$Ln_2(Fe_{17-x}Co_x)N_3$
		3	2	0.21	*Fm-3m*	$Na_{14}Ba_{14}MN_6$ M = Li, Ca
			1		*Fm-3c*	$LaFe_{10.8}Al_{2.2}N_3$
		2		0.2	*F-43m*	$(Na_{15-x}Li_x)Ba_{14}LiN_6$
		1		1.5	*Pm-3m*	$TaThN_3$
		1		0.17	*R-3m*	$Na_{15}Li_8Ba_{12}N_6$
10^2,11^2T1	9	4		1	*Pbca*	$M(1)_3M(2)N_4$ M(1) = Sr, Ba; M(2) = Mo, W, Cr
		3				$Sr_{3-x}Ba_xMN_4$ M = W, Mo
		1				Ca_2SrWN_4

		1				$Ba(Ba_{0.44}Ca_{0.56})CaWN_4$
11T106	9	5		0.8	*I4/m*	$M(1)Mg_2M(2)_2N_4$ M(1) = REM, Eu; M(2) = Al, Ga
		2				$Ba(Mg_{3.33}M_{0.67})N_4$ M = Nb, Ta
		1				$BaMg_3GeN_4$
		1				$(Sr_{0.985}Ce_{0.015})(Mg_{2.03}Al_{1.97})N_4$
nce	8	5	3	0.67	*I4/mmm*	M_2ZnN_2 M = REM
			1			Mn_3N_2
			1			$Mo(Mo_{0.5}Ta_{1.5})N_2$
		1			*F4/mmm*	Mn_3N_2
		2		0.18	*Pmmn*	$M_6Ge_5N_2$ M = Sr, Ba
mob	7	5		0.4	*I4₁/amd*	$M(1)Li_2(Li_{1-x}M(2)_x)_2N_2$ M(1) = Sr, Ca; M(2) = Cu, Fe
		1				Li_4SrN_2
		1				$(Li_{3.9}Ni_{0.1})SrN_2$
12,13T2334	6			0.8	*Pnna*	$M(1)_3M(2)_2N_4$ M(1) = Sr, Ba; M(2) = Al, Ga, Ge, Mg
hcp-10-$P6_3/m$	6			0.75	*P6₃/m*	$M(1)_3M(2)N_3$ M(1) = Sr, Ba; M(2) = Mn, Cr, Fe, Ga
12T2355	5			1.5	*Ia-3*	M_2N_3 M = Ln, Ta, Zr, U
tcd	5	4	3	1	*R3m*	M(1)M(2)N_2 M = Cr, Mo, W, Li
			1		*R-3m*	$CuTaN_2$
		1		1.5	*R3*	W_2N_3
7,12T29	5	4		1.2	*I4/mmm*	$La_3M_2N_6$ M = V, Nb, Ta, Cr
		1		1.21		$Ce_3Ta_{1.97}N_6$
tcj	5	1		1.33	*Pna2₁*	Zr_3N_4
		1			*Pnam*	Zr_3N_4
		1		1	*P6₃/mmc*	NbN
		1			*P6₃mc*	$MnWN_2$
		1		0.67	*P6₃/mmc*	Be_3N_2
bcu-x	5	2		0.045	*Im-3m*	$Na_{16}Ba_6N$; $Ag_{16}Ca_6N$
		2	1	0.67	*R-3c*	Ca_3N_2
			1		*Pbcn*	Zn_3N_2
		1		0.125	*I4/mmm*	$Fe_{16}N_2$
9,10^2,11T2	4			1	*Pbca*	$Ba_{3-x}M(1)_xM(2)N_4$ M(1) = Sr, Ca; M(2) = Mo, W
10^2,11,12T2	4			1	*C2/c*	$M(1)_2M(2)N_3$ M(1) = Sr, Ba; M(2) = Nb, V, Ta
9,10T2662	4	3		0.75	*Cmcm*	Ca_3MN_3 M = V, Cr, Mn
		1			*P2₁/m*	Ca_3VN_3
9,10T2652	4			0.71	*P6₃/mcm*	$M(1)_6M(2)N_5$ M(1) = Ca, Sr; M(2) = Ga, Fe, Mn
14T2	4	2		0.33	*P6₃22*	M_3N M = Fe, Ni
		1			*P6₃*	Fe_3N
		1			*P312*	Fe_3N
11T1587	3			1.5	*Ia-3*	M_2N_3 M = Ho, Lu, Np
10,12T215	3	2		1	*P2₁/m*	LiM_2ReN_4 M = Sr, Ba
		1			*Pnma*	UVN_2

8,12T48	3		1	*P4/nmm*	$M(1)M(2)N_2$ M(1) = Ba, Sr; M(2) = Ti, Zr, Hf
tcl	3	2	0.75	*R-3m*	Mg_3MN_3 M = Al, Ga
		1	0.6		$Li_2Ca_{2.78}Nb_{0.22}N_3$
11^2,12T10	3		0.67	*I4/m*	$MBe_{20}N_{14}$ M = Sr, Ba, Eu
svi-x	3		0.67	*I4/mcm*	MBe_2N_2 M = Ca, Sr, Ba
9T980	3		0.57	*P4/ncc*	$Ca_4Ba(MN_2)_2$ M = Cu, Co; $Ca_5(CoN_2)_2$
11,12T2	3	2	0.5	*P-31m*	M_2N M = Cr, Fe
		1		*P312*	Fe_2N
8,9T1103	3	2	0.5	*Pbam*	$(Ca_7N_4)Tl_{0.97}$; $(Ca_7N_4)In_{1.02}$
		1	0.48		$(Ca_7N_4)Ga_{1.34}$
7^2,8,9T5	3		0.42	*P4₂/n*	$Ba_{23}Na_{11}(MN_4)_4$ M = Nb, Ta; $Ba_{23}Na_{11}N_{12}((Ta_{0.28}V_{3.72})N_4)$
7,9T74	3		0.4	*P2₁/m*	$M_3Ge_2N_2$ M = Sr, Ba
chb	3		0.33	*Cmcm*	$M(1)_2M(2)N$ M(1) = Ca, Sr; M(2) = Au, In
fab	3		0.26	*Fm-3m*	$M(1)_{19}M(2)_8N_7$ M(1) = Ca, Sr; M(2) = In, Ag
lon	3		0.25	*P6₃/mmc*	$(Ba_{3-x}Sr_x)MN$ M = Bi, Sb
tsi	3	2	0.17	*I4₁/amd*	M_4In_2N M = Ca, Sr
		1	0.5		Ti_2N
11,12^2T4	2	1	1.67	*Cmcm*	Ta_3N_5
		1		*C2/m*	
hcp-10-R-3c	2	1	1.5	*R3c*	$LaWN_3$
		1		*I-1*	$LaReN_3$
11,12T2507	2		1.5	*P1*	$CeMN_3$ M = Mo, W
11T2	2		1.33	*I-43d*	M_3N_4 M = Zr, Hf
12T2171	2	1	1.29	*I-42d*	$Ca_{0.55}GeN_2$
		1	1		$CaGeN_2$
8,10T340	2		1	*Immm*	MCe_2N_3 M = Cr, Mn
6,10T202	2		1	*Immm*	MTh_2N_3 M = Cr, Mn
6,8T535	2		1	*Immm*	MU_2N_3 M = Cr, Mn
10,12T218	2	1	1	*Pmmn*	$CaTiN_2$
		1		*P2₁mn*	
12,14T1608	2		1	*Cmc2₁*	$NaGe_2N_3$; $(Ca_{0.8}Li_{0.2})(Al_{0.8}Ge_{1.2})N_3$
11^3,12T3	2		1	*C2/c*	La_2GaN_3; Sr_2TaN_3
9,10^3,11^3,13T1	2		1	*P2/n*	$LiBa_4M_2N_7$ M = Mo, W
6,7,8T23	2	1	0.96	*R-3c*	$Cs_{9.67}W_6N_{15}$
		1	0.94		$Cs_{9.98}Mo_6N_{15}$
9,10^2,15T1	2		0.83	*Pbcm*	$Ca_5(VN_4)N$; $Sr_5(NbN_4)N$
10,11,12T8	2		0.83	*C2/m*	$Ca_4Ge_3Mg_5N_{10}$; $Ca_2MgGa_3N_5$
12,13T1230	2		0.8	*C2/c*	$Ca_3M_2N_4$ M = Al, Ga
tci	2		0.75	*R-3*	$Ca_6Ge_2N_6$ M = Ca, Sr
11^2,12T11	2		0.75	*Pbcn*	$M_7(GeN_4)N_2$ M = Ca, Sr
10^2,11,12,13,14T1	2		0.75	*Cc*	Na_3MN_3 M = Mo, W
9,10^3T5	2		0.73	*C2/m*	$Sr_8(MN_3)_2(FeN_2)$ M = Mn, Fe
9,11T2523	2		0.67	*P4₂/mbc*	M_2GeN_2 M = Ca, Sr
11,12T2508	2		0.67	*Pnnm*	$Li_3Sr_2MN_4$ M = Nb, Ta

11,12T2063	2		0.67	*C2/c*	$Li_3Ba_2MN_4$ M = Nb, Ta
10^2T2411	2		0.6	*C2/c*	$M_2LiFe_2N_3$ M = Sr, Ba
svk	2	1	0.4	*Immm*	$Li_3Sr_3Ni_4N_4$
		1	0.2	*Cmmm*	$Ca_7Tl_3N_2$
7,10T482	2		0.33	*Immm*	$M_8Cu_3In_4N_5$ M = Sr, Ba
8,9,16^2T1	2		0.076	*I-42m*	$Ba_{39}Li_{80}N_9$; $Ba_{39}Li_{34.87}In_{45.13}N_9$
10^3,12T2	1		1.7	*P-6*	W_7N_{12}
10^4,12T2	1		1.67	*Pnma*	Ta_3N_5
10^2,12^2T6	1		1.67	*Pnma*	Ta_3N_5
tck-8,10-$P6_3$/mmc	1		1.5	*P6₃/mmc*	W_2N_3
9,10,11T12	1		1.5	*Pnma*	Nb_2N_3
11^2T2280	1		1.33	*P6₃/m*	Ge_3N_4
9,11^3T1	1		1.33	*P31c*	Ge_3N_4
11,12,13T5	1		1.33	*Pbnm*	Sn_3N_4
12,13T73	1		1.33	*P2₁/n*	Sn_3N_4
10,12^2T9	1		1.25	*Cmcm*	$NaTa_3N_5$
tcl-8,10-$P3_221$	1		1.19	*R-3m*	$Nb_{0.84}N$
tck	1		1.125	*P6₃/mcm*	$Nb_{3.72}Ta_{4.28}N_9$
kag	1		1	*P6/mmm*	TaN
bnn	1		1	*P-3m1*	MoN
6,9T412	1		1	*P-31m*	MoN
10^2,11^2T1	1		1	*P31c*	Ba_3MoN_4
9^5,10^6,11T1	1		1	*P31c*	Ba_3WN_4
10T4	1		1	*I4₁/amd*	$LiUN_2$
10,11T2644	1		1	*Fddd*	Ba_2CaWN_4
10,11,13T9	1		1	*Cmca*	Ba_2VN_3
10^2,11^2T3	1		1	*Pbca*	$Ba_2(Ba_{0.23}Ca_{0.77})MoN_4$
9,10,11^3,12 T1	1		1	*C2/c*	Sr_3MoN_4
10^3,11T1	1		1	*C2/c*	Ca_2VN_3
10^2,11^2,12^3 T1	1		1	*P-1*	$Sr_{10}(Mo_2N_6)(MoN_4)_2$
7,8,9T13	1		0.99	*R-3c*	$Rb_{9.15}W_6N_{15}$
8,10,12,13 T1	1		0.9	*Fm-3m*	$La_3Cr_{9.236}N_{11}$
9,10^9,11^4, 12^5T1	1		0.9	*P-1*	$Ba_{16}(NbN_4)_3(Nb_2N_7)$
10^3,11T2	1		0.875	*Pnnm*	$Sr_4LiAl_{11}N_{14}$
10^2,11^2T2	1		0.875	*C2/m*	$Sr_2MgAl_5N_7$
11^2,14T3	1		0.86	*C2/c*	$Sr_5Ge_2N_6$
8,9,10^2,11, 12T2	1		0.86	*P-1*	$Ba_{10}Ti_4N_{12}$
8^4,9^5,10^2, 11^3,12^4,13 T1	1		0.86	*P-1*	$Na_2K_{13}W_7N_{19}$
10,11^2,13^2 T1	1		0.83	*Pna2₁*	Eu_4MgTaN_5
10,11^2,12,	1		0.83	*C2/c*	$Ba_3Ga_3N_5$

14T1				
7,8,9T12	1	0.83	*C2/m*	$Ba_5(CrN_4)N$
9,10,11,12^2 T3	1	0.83	*P-1*	$Sr_3Ga_3N_5$
9,10,11^2,13 T2	1	0.83	*P-1*	$Al_3BeSr_2N_5$
8,9^4,10,11^2, 12T1	1	0.82	$P2_1/c$	$Sr_8(MnN_3)_2(MnN_3)$
11,12,13T6	1	0.8	$I4_1/acd$	$Ca_3Ga_2N_4$
10,11^3T3	1	0.8	$I4_1/a$	$CaLiAl_3N_4$
10,12^2T10	1	0.8	*Ibca*	Ca_4FeN_4
10^2,11^2,13^4 T1	1	0.8	$P2_12_12_1$	$Ca_3Al_2N_4$
10,11,12,13 T5	1	0.8	$P2_1/c$	Ca_4GeN_4
10,11,14,15 T1	1	0.8	$P2_1/c$	$Ca_3Al_2N_4$
9,11,12^2T2	1	0.8	$P2_1/c$	Sr_4GeN_4
10,11^3T4	1	0.8	*C2/m*	$CaBaLi_2Al_6N_8$
10,11,12,13 T4	1	0.8	*P-1*	Ca_4TiN_4
10^3,11^5T1	1	0.8	*P-1*	$SrLiAl_3N_4$
10^2,11^6T2	1	0.8	*P-1*	$Sr_{0.995}LiAl_3Eu_{0.005}N_4$
10,11^5,12^2 T1	1	0.8	*P-1*	$Sr_{0.595}Ca_{0.4}LiAl_3Eu_{0.005}N_4$
xak	1	0.75	*I4/mmm*	Nb_4N_3
11,12T911	1	0.75	*Pbca*	$Li_4Sr_2Cr_2N_6$
9,10,12^3,13 T1	1	0.75	*Pbca*	$Na_{11}Rb(WN_3)_4$
10,11,12,13 T6	1	0.75	*Pbcm*	Na_2KWN_3
9,10^5,11^2, 12^2,13,14T1	1	0.75	$P2_1/c$	$Na_5Rb(WN_3)_2$
9^2,10^6,12^4 T1	1	0.75	$P2_1/c$	$Na_5Cs(WN_3)_2$
10,11,12^4T1	1	0.74	*P3*	$Ca_{12}Mn_{19}N_{23}$
11^2,12T9	1	0.73	$P4_2/mnm$	$Ca_{11}N_8$
9,11T2471	1	0.67	*Cmca*	Sr_2GeN_2
9,11T300	1	0.67	*Pnma*	Fe_3N_2
9,10T225	1	0.67	*C2/m*	Ca_2FeN_2
11,12^3T3	1	0.67	*C2/m*	$LiSrGaN_2$
12^2T2342	1	0.67	*C2/m*	$Li_4Sr_3Ge_2N_6$
11^2,12^2,15 T2	1	0.67	*P-1*	Sr_2FeN_2
7,8,9^2,10^2, 11T1	1	0.61	*P-1*	$Sr_{17}Ge_2(GeN_3)_2(GeN_4)_2$
10,12T2852	1	0.6	$P6_3/mmc$	Ti_4AlN_3
12,13^2T8	1	0.6	*Cc*	Na_4ReN_3
10T1541	1	0.57	*P4/ncc*	$Sr_5(CoN_2)_2$
9,11T2522	1	0.57	*Cmca*	$Ca_5Ga_2N_4$
12^2,13T11	1	0.56	$P4_2mc$	$Sr_6(Cu_2N_3)(CuN_2)$

hxl	1	0.5	*P-3*	W_2N
dia	1	0.5	*I4$_1$/amd*	Mo_2N
11,12^{4}T1	1	0.5	*C2/c*	$Ba_8Ni_6N_7$
10,12T1513	1	0.43	*Cmmm*	$(Li_{0.78}Ni_{0.22})Li_4Sr_2N_3$
12^{3}T9	1	0.42	*P312*	$Fe_{24}N_{10}$
sve	1	0.4	*P4/mbm*	$CaLi_2(Li_{0.12}Mn_{1.88})N_2$
9,10T2663	1	0.4	*P4/nbm*	$Ge_4Sr_{11}N_6$
7^2,8,10T3	1	0.36	*Cc*	$Sr_8Ge_2(GeN_4)$
7^4,8,10T1	1	0.35	*P2/m*	$Ba_{14}Cu_2In_4N_7$
whb	1	0.33	*P4$_2$/nmc*	$LiBa_2N$
5,6^3,7^2,8^{2}T3	1	0.32	*C2/m*	$Ba_{19}In_9N_9$
tca	1	0.27	*R-3c*	$Na_7Ba_{14}CaN_6$
tcl-4,8-P3$_2$21	1	0.25	*R-3m*	$Sr_{0.86}Ba_{2.14}BiN$
7,8,9T14	1	0.19	*P-1*	$Na_{17}Ba_{14}CaN_6$
9^{2}T1978	1	0.17	*C2/m*	$Na_{21}Ba_{14}CaN_6$
ecf	1	0.16	*P6$_3$/mmc*	$Dy_2Fe_{17}N_3$
8,11T560	1	0.125	*A2/m*	$Nd_3Fe_{28.2}Ti_{0.8}N_4$

Table S4. Topological types of silicon substructures in inorganic silicides.

Topological type	Occurrence			Si/M ratio	Space group	Silicides
hcp	263	175	115	0.5	*Pnma*	M(1)M(2)Si M(1) = *d*-metals, Ln, AEM, U; M(2) = *d*-metals, AEM, Al
			11			$M(1)M(2)_{1-x}M(3)_xSi$ M(1) = Mn, Co, Ni; M(2), M(3) = Mn, Ti, Sc, Lu, V
			6			M_2Si M = *d*-metals, AEM, Eu
			2			$Sr_{1.25}Ca_{0.75}Si$; $Al_{0.45}Mg_{1.55}Si$
			1			$Co_2MnTiSi_2$
			21		*P6₃/mmc*	M(1)M(2)Si M(1) = Ln, *d*-metals, AEM, Be; M(2) = *d*-metals
			1			Ni_2Si
			6		*P6₃/mcm*	$Gd(Ti_{1-x}Mn_x)Si$
			3		*Pbnm*	MCuSi M = Ti, Zr, Hf
			2			M_2Si M = Ca, Ni
			2		*Pnam*	TiNiSi; HfWSi
			1			Co_2Si
			1		*P6₃mc*	YAuSi
			1		*P6₃22*	Ni_2Si
			1		*P-3m1*	Fe_2Si
			1		*Pbca*	PtSbSi
		60	23	0.6	*P6₃/mcm*	M_5Si_3 M = *d*-metals, Ln
			13			$M(1)_2M(2)_3Si_3$ M = *d*-metals
			7			$M(1)_{5-x}M(2)_xSi_3$ M = *d*-metals
			6			$M(1)M(2)_4Si_3$ M(1) = *d*-metals, Eu; M(2) = *d*-metals, Gd
			5			$M(1)_5M(2)_5Si_6$ M = *d*-metals
			3			$M(1)_7M(2)_3Si_6$ M(1) = V, Fe, Gd; M(2) = Ta, Mn, Pr
			2			$(Sc_{10-x}M_x)Si_6$ M = Fe, Y
			1		*Ccmm*	Mn_5Si_3
		14	11	0.67	*P-3m1*	MAl_2Si_2 M = Ln, AEM, Y
			1			Rh_3Si_2
			2		*P6₃/mmc*	M_3Si_2 M = Rh, Ir
		7	2	0.33	*P-3m1*	Li_2ZnSi
			1			Cu_3Si
			1		*P6₃mc*	$Li_{2.28}Mg_{0.72}Si$
			1		*P6₃/m*	$Al_{3.39}Li_{14.6}1Si_6$
			1		*Cmcm*	$Pt_8Sc_4Si_4$
			1		*Pnma*	Ni_3Si
		3		0.077	*P6₃/mmc*	M_4Hf_9Si M = Mo, Re
						$Hf_9(HfMo_3)Si$
		1		0.71	*P6₃/mmc*	$Rh_{1.4}Si$
		1		0.4	*Pnnm*	$DyMn_4Si_2$

		1		0.31	*P-3m1*	$Cu_{3.17}Si$
		1		0.18	*P6₃/mcm*	$Ca_{10}Pt_7Si_3$
fcu	170	93	47	0.5	*P4/nmm*	M(1)M(2)Si M(1) = Ln, AEM, *d*-metals, Na; M(2) = *d*-metals, Al, Mg
			22			$M(1)M(2)_{1-x}M(3)_xSi$ M(1) = REM, Mn; M(2), M(3) = *d*-metals
			11		*P2₁3*	M(1)M(2)Si M(1) = AEM, REM; M(2) = Ir, Pt, Pd, Rh
			4		*Fm-3m*	$(Mg_{2-x}Mn_x)Si$
			1			Mg_2Si
			3		*F-43m*	LiMSi M = Al, Ga
			2		*Pmmn*	MMnSi M = Pr, Nd
			1		*P-43m*	$Mg_{63}BiSi_{32}$
			1		*I4/mmm*	Pt_2Si
			1		*P4/nmm*	$GdLaMn_2Si_2$
		36	11	0.33	*Fm-3m*	$M(1)_2M(2)Si$ M(1) = *d*-metals, Li; M(2) = *d*-metals, Li, Mg
			3			$Fe_{3-x}M_xSi$ M = V, Cr, Ni
			2			M_3Si M = Mn, Fe
			2			$Fe_3M_3Si_2$ M = Mn, Co
			2			$Co_2(Cr_{0.2}Mn_{0.8})Si$; $Co_4(MnV)Si_2$
			9		*Pnma*	M_2LnSi M = Pd, Pt, Ni
			4		*Pmmn*	$M(1)_2M(2)Si$ M(1) = Li, Ni; M(2) = AEM
			2		*F-43m*	Co_2MnSi; Mn_2RuSi
			1		*P-43m*	$Li_{1.62}Mg_{1.38}Si$
		20	7	1	*P2₁3*	MSi M = *d*-metals
			7			$M(1)_{1-x}M(2)_xSi$ M = *d*-metals
			6			$M(1)M(2)Si_2$ M = *d*-metals
		8	3	0.25	*P2₁3*	$(Cr_{0.341}M_{0.061}Ni_{0.598})_4Si$ M = Fe, Cu, Pd
			2			$Fe_5Ni_3Si_2$; $Cr_3Ni_5Si_2$
			2			Mn_3MSi M = Co, Ir
			1		*C2/c*	Ca_2Ir_2Si
		3		0.2	*R-3m*	$M(1)_2M(2)_3Si$ M(1) = Mg, Er, Pr; M(2) = Ni, Rh
		2		0.42	*I4/m*	$Pt_{12}Si_5$
					P4/n	
		1		0.49	*Pm-3m*	$Mg_{64}BiSi_{32}$
		1		0.42	*F-43m*	$Li_{0.9}Mg_{1.49}Si$
		1		0.41	*F-43m*	$Li_{6.78}Al_{3.07}Si_4$
		1		0.4	*R-3m*	$BaMg_2Li_2Si_2$
		1		0.39	*F-43m*	$Li_{7.43}Al_{2.85}Si_4$
		1		0.36	*P-3*	$Ni_{18}Pd_7Si_9$
		1		0.035	*Fm-3m*	$Zr_6Zn_{22.915}Si$

		1		0.034	*Fm-3m*	$Ce_6Mg_{23}Si$
pcu	50	13		0.22	*Im-3m*	$Ln_3Ni_6Si_2$
		10	3	0.33	*Pm-3m*	M_3Si M = Ni, Nb, U
			2			$LiAg_2Si$; $(Fe_{0.5}Ni_{0.5})_3Si$
			2		*I4/mcm*	M_3Si M = Ir, U
			1		*P4/mbm*	Pt_3Si
			1		*Fmmm*	U_3Si
			1		*C2/m*	Pt_3Si
		5		0.18	*P4/nmm*	$LnNi_{10}Si_2$
		5		0.17	*P4/mmm*	MPt_5Si M = *p*-metals, Ag
		4		1	*Pm-3m*	MSi M = Co, Ru, Rh, Os
		3		0.25	*P4$_2$/mnm*	MAu_3Si M = Y, Gd
					P4/mbm	$Al_{3.75}Dy_3FeMg_{0.25}Si_2$
		3		0.125	*Imma*	$M(1)_3M(2)_5Si$ M(1) = Ce, La; M(2) = Pd, Pt
		2		0.053	*I4/mcm*	$M_6Fe_{13}Si$ M = Pr, Nd
		1		0.4	*C2/m*	$Rh_3Bi_2Si_2$
		1		0.26	*P4/mbm*	$Al_{3.5}FeMg_{0.5}Yb_{2.71}Si_2$
		1		0.18	*Pbam*	$Pt_7Sc_4Si_2$
		1		0.14	*I4/mcm*	La_5Ge_2Si
		1		0.11	*I4/mcm*	Tb_6Al_3Si
nin	45	43	27	0.5	*P-62m*	M(1)M(2)Si M = *d*-metals, Ln, Li
			2			M_2Si M = Pd, Pt
			2			$Pd_{2-x}Mn_xSi$
			2			$Ru(M_{0.5}Zr_{0.5})Si$ M = Nb, Ta
			10		*Ima2*	M(1)M(2)Si M = *d*-metals
		2		0.6	*Pbam*	M_5Si_3 M = Ru, Rh
bcu-x	42	40	27	0.33	*Pm-3n*	$M(1)_{3-x}M(2)_xSi$ M = *d*-metals
			5			M_3Si M = *d*-metals
			3			$M_3V_3Si_2$ M = Cr, Mo, Nb
			2			$V_{6-x}M_xSi_2$ M = Ni, Nb
			2		*P4$_2$/n*	Ti_3Si M = Ti, Ta
			1			$(Nb_{0.6}V_{0.4})_3Si$
		1		0.25	*C2cb*	Au_4Si
		1		0.0625	*Im-3m*	$Ce_4Rh_{12}Si$
hex	42	21	11	0.2	*P6$_3$/mmc*	$M(1)_2M(2)_3Si$ M(1) = *d*-metals, AEM, U; M(2) = *d*-metals, Mg
			9		*Cmmm*	MNi_4Si M = REM
			1			$NdNi_3CoSi$
		7	5	0.5	*P-6m2*	M(1)M(2)Si M(1) = AEM, An; M(2) = Li, Al, Au
			1			$Ce_2(Li_{0.39}Ni_{0.61})NiSi_2$
			1		*Pnma*	RhTbSi
		6		0.125	*P-62m*	$Ln_3Mn_3Ga_2Si$
		4		0.33	*P6$_3$/mmc*	$M(1)M(2)_2Si$ M(1) = Ca, Ti, Zn, Pt; M(2) = Li, Mg, Co, Ni

		2	0.27	*P6$_3$/mmc*	$Ho_3Ni_{12}Si_4$
				C2/c	$Sc_2Pt_9Si_3$
		1	0.09	*P6$_3$/mmc*	Ce_3Co_8Si
		1	0.083	*P6$_3$/mmc*	Al_9Mn_3Si
8,12T48	24		0.67	*P4/nmm*	$M(1)M(2)_2Si_2$ M(1) = REM, An; M(2) = Ir, Pt, Au
xau	24	22	21	0.32	*Fm-3m*	$M(1)_6M(2)_{16}Si_7$ M(1) = *d*-metals, Mg, U; M(2) = Fe, Co, Ni, Cu
			1			$(Mn_3Cr_3)Ni_{16}Si_7$
		1		0.33		$Ti_{18.72}Ni_{66.85}Si_{28}$
		1		0.3		$Mn_{8.3}Pd_{14.7}Si_7$
tsi	22	20	16	0.5	*I4$_1$md*	$M(1)M(2)Si$ M(1) = REM, Th; M(2) = Al, Ni, Pt
			4			$M(1)M(2)_{1-x}M(3)_xSi$ M(1) = Ce, La, Pt; M(2), M(3) = *d*-metals, Th
		1		0.55		$LaPt_{0.8}Si$
		1		0.53		$LaPt_{0.9}Si$
bnn	21	16	11	0.5	*P6/mmm*	$M(1)M(2)_3Si_2$ M(1) = REM; M(2) = Rh, Ru, Ir
			3		*P6$_3$/m*	MRu_3Si_2 M = Y, La, Th
			1			$Gd_{0.05}La_{0.95}Ru_3Si_2$
			1		*Cmcm*	Ag_2Si
		2		0.29	*P-62m*	$M_3Cu_4Si_2$ M = Zr, Hf
		2		0.13		$Ho_3Rh_9Sn_3Si_2$ M = Ho, Lu
		1		0.4	*Pbam*	$Sc_2Pt_3Si_2$
nce	15	7	6	0.5	*I4/mmm*	MScSi M = REM
			1		*I-1*	CeScSi
		4		0.67	*I4/mmm*	$M(1)M(2)_2Si_2$ M(1) = Sr, Ba, Er, Pu; M(2) = Al, Ni, Au
		3		0.4	*Immm*	$M_3Al_2Si_2$ M = AEM
		1		0.33	*Pnma*	$La_3Rh_3Si_2$
tcg-x	15	14		0.33	*Pnma*	$M(1)M(2)_2Si$ M(1) = REM; M(2) = Pt, Pd
		1		0.14		$Au_{5.6}Cu_{1.4}Si$
9T980	14	13		0.4	*I4/mcm*	$M(1)M(2)_9Si_4$ M(1) = REM; M(2) = Fe, Co, Ni
		1				$NdCo_8(Co_{0.5}Fe_{0.5})Si_4$
10T356	14	13		0.2	*I4$_1$/amd*	$M(1)M(2)_9Si_2$ M(1) = REM; M(2) = Co, Ni
		1				$Nd(Fe_{0.55}Co_{0.45})_9Si_2$
11T2	11	6		0.27	*I-43d*	$Li_{15-x}M_xSi_4$ M = Al, Mg, Zn
		2				$M_{15}Si_4$ M = Li, Cu
		2				$Li_{12}M_3Si_4$ M = Al, Mg
		1				$Li_{3.51}Mg_{0.24}Si$
9^2,12T3	10			0.42	*Fm-3m*	$M_3Pt_{23}Si_{11}$ M = Ln, U

bcu-x-13-P4_2/mnm	10	8	0.4	*P4_2/mnm*	M(1)M(2)$_4$Si$_2$ M(1) = REM, Zr; M(2) = Fe, Re
		2	0.33	*P4_2/n*	M_3Si M = Zr, Nb
crs	9	8	0.2	*Fd-3m*	M(1)$_3$M(2)$_2$Si M(1) = *d*-metals, Al; M(2) = Fe, Co, Ni
		1	0.23	*F-43m*	$Al_{13}Cr_4Si_4$
11^2,12T12	7	6	0.5	*Pnma*	MNi_5Si_3 M = REM, U
		1			$Y(Rh_{0.42}Ni_{0.58})Ni_4Si_3$
10,14T78	7		0.4	*Pnma*	M(1)$_4$M(2)Si$_2$ M(1) = Rh, Ir; M(2) = REM
tcm	6		0.44	*R-3m*	M(1)$_2$M(2)Al$_6$Si$_4$ M(1) = Gd, Tb, Dy; M(2) = Pt, Au
reo	6	4	0.26	*Fm-3m*	$M_3Pd_{20}Si_6$ M = Y, Ce, Lu, U
		1			$Ce_2Pd_{21}Si_6$
		1	0.19	*R-3m*	$Ce_2Ni_{14}Si_3$
lcy	5	3	1	*P2$_1$3*	MSi M = Cr, Mn, Ni
		2			$Cr_{1-x}M_xSi$ M = Mn, Ni
7,9,12T6	5		0.23	*I4/mmm*	$M_{11}In_6Si_4$ M = REM
10^{2}T4	4		0.5	*Pnma*	Ln_3NiSi_2
11^2,12T13	4		0.5	*P-6*	$Pt_9Sc_5Si_7$; $Al_4Cu_2Mg_8Si_7$; $Ba_2Yb_{0.88}Mg_{11.12}Si_7$; $Ba_{1.9}Ca_{2.4}Mg_{9.7}Si_7$
tcj	4	2	0.4	*Pbcm*	$M_3Rh_2Si_2$ M = Y, Ce
		2	0.39	*P321*	$Ni_{31}Si_{12}$; $Fe_{1.94}Ni_{5.81}Si_3$
12^{4}T6	4	2	0.24	*F-43m*	$Li_{21}Si_5$; $Li_{16.942}Zn_{0.025}Si_4$
		1	0.23		$Li_{17}Si_4$
		1		*F23*	$Li_{22}Si_5$
13T1310	3		0.54	*Im-3m*	M(1)$_4$M(2)$_7$Si$_6$ M(1) = Sc, U; M(2) = Tc, Re, Ir
ecu	3		0.5	*Cmcm*	MAlSi M = Y, Tm, Lu
feb	3		0.5	*Pnma*	LnCoSi
9,12^{2}T5	3		0.42	*Fm-3m*	$Ln_3Pt_{23}Si_{11}$
6,11^{2}T1	2		0.81	*Pnma*	$Ru_{3.71}Si_3$
			0.75		Ru_4Si_3
sve	2		0.67	*P4/mbm*	M_3Si_2 M = Nb, Mo
8,9T968	2		0.6	*I4/mcm*	$U_3Ga_2Si_3$
				I4	$U_3Al_2Si_3$
11,15T4	2		0.4	*Pnma*	Rh_4MSi_2 M = Y, Sc
tch	2		0.39	*P6$_3$/m*	$Ce_6Co_{1.63}Si_3$; $Ce_6Ni_{1.68}Si_3$
8,12T395	2		0.38	*P-62m*	$Al_9FeMg_3Si_5$; $Al_{8.64}FeMg_{3.36}Si_5$
12,13T2335	2		0.375	*C2/c*	$M_4Pd_4Si_3$ M = Ca, Sm
cco	2		0.33	*Pnma*	M_3Si M = Pd, Pt
10,14T410	2		0.29	*P6$_3$/mmc*	M(1)$_3$M(2)$_{11}$Si$_4$ M(1) = Sc, Tb; M(2) = Ni, Cu
10,11,12T9	2		0.24	*Cmcm*	$Li_{4.1}Si$
sqc7*	1		0.67	*I4/mmm*	$LuRu_2Si_2$
10,12T6	1		0.67	*Pnma*	$BaAl_2Si_2$

nbo	1	0.6	*P4$_2$/nnm*	$Li_3Ag_2Si_3$
10,12T2863	1	0.6	*P2$_1$/m*	Mn_5Si_3
ncb	1	0.57	*I-43m*	$Ca_3Ir_4Si_4$
10,11,12 T10	1	0.5	*P-62m*	$Ba_5Yb_{2.29}Mg_{16.71}Si_{12}$
10^2,11^2,12 T4	1	0.5	*P-6*	$Ba_6Mg_{18.16}Yb_{1.84}Si_{13}$
tck-8,10-P6$_3$/mmc	1	0.5	*P6$_3$*	CaAlSi
8,10^2T12	1	0.5	*P3*	CaAlSi
sxd	1	0.5	*Pnma*	NdFeSi
11,12^4T2	1	0.48	*Pm-3m*	$Mg_{64}BiSi_{31}$
8,10^4T1	1	0.48	*P6$_3$/m*	$La_{21}Ni_{10.35}Si_{15}$
xbo	1	0.45	*Pm-3m*	$Fe_{11}Si_5$
8,10^3T3	1	0.45	*P6$_3$/m*	$Pr_{15}Ni_7Si_{10}$
10^2T2412	1	0.44	*P6$_3$/m*	$Ce_5Ni_{1.85}Si_3$
tce	1	0.44	*I4/m*	$Nb_5Cu_4Si_4$
10,11,14T2	1	0.44	*Pnma*	$Ce_2Pt_7Si_4$
11,13T1	1	0.41	*Pnma*	$Ir_{3.84}CuSi_2$
4,5,8T43	1	0.38	*R-3m*	$Rh_9Y_4Si_5$
sqc1067	1	0.38	*P4/mmm*	$Mo_5Ru_8Si_5$
11^2T2	1	0.38	*Pnma*	$SrAu_{4.3}Si_2$
11,12T2509	1	0.375	*C2/c*	$Ce_4Rh_4Si_3$
eca	1	0.33	*P6$_3$/mmc*	Co_3Si
3,5,8T75	1	0.33	*P6$_3$/mmc*	YRh_2Si
mob	1	0.33	*I4$_1$/amd*	$CeIr_2Si$
11T106	1	0.33	*I-4*	Nb_3Si
chb	1	0.33	*Cmcm*	$CeRh_2Si$
11T770	1	0.33	*Pnma*	$Ce_3Rh_3Si_2$
9,11T300	1	0.33	*Pnma*	$Ca_3Ni_3Si_2$
8,10T2481	1	0.33	*C2/c*	$GdNi_8Si_3$
8,10T2479	1	0.31	*Pbcm*	$Pr_6Ni_7Si_4$
8,10T2480	1	0.3	*P4$_2$/nmc*	$Eu_2Ni_8Si_3$
bct-9-Cmce	1	0.29	*Cmca*	$Tm_5Sb_2Si_2$
13T1	1	0.25	*Pa-3*	$NaAu_3Si$
11^2T60	1	0.25	*Pnma*	$CuLi_7Si_2$
10,12T84	1	0.22	*Pnma*	Pd_9Si_2
12T495	1	0.2	*I4$_1$/amd*	$LaNi_9Si_2$
kag	1	0.1875	*P6$_3$/mmc*	$Er_2Fe_{14}Si_3$
sql	1	0.18	*C2/c*	$Al_{4.5}FeSi$
dia	1	0.14	*R32*	Li_4Pt_3Si
fcu-9-P4$_2$/n	1	0.1	*P4$_2$/n*	$Mg_{15}Ir_5Si_2$
bct	1	0.0625	*P4/nmm*	$Ce_2Pd_{14}Si$

*****The topology name of one of the nets from the EPINET database.