Supplemental information 3

The space-group, lattice parameters, relative energy and spin magnetic moment are shown in the following tables. These tables are classified by each combination of groups in the periodic table. For example, "I-XV" means that atom A and atom B are in group I and XV, respectively. T, H, and P represent the types of initial structures. The order of THP represents their stability. For example, "PTX" means the planar type initial structure is the most stable, the 1T type one is the second stable, and the 1H type one is much more unstable than the others. X represents a structure whose relative energy exceed 0.03 Hartree (≈ 0.82 eV) per the unit cell including 12 atoms. The space-groups of the obtained final structures for each initial states are also shown. The definitions of relative energies ΔE_1 and ΔE_2 are as follows: $\Delta E_1 = E_{\text{the second stable structure}} - E_{\text{the most stable structure}}$, and $\Delta E_2 = E_{\text{the third stable structure}} - E_{\text{the most stable structure}}$.

Table 1: List of I-I

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$LiLi_2$	HTX	$Cmmm(65)$	$Amm2(38)$	–	5.97	7.76	49.0	6.03	6.52	57.8	–	–	–	0.160	4.548	0.0	0.0	–
$LiCs_2$	HXX	–	$Amm2(38)$	–	–	–	–	12.59	12.52	46.3	–	–	–	0.865	1.607	–	0.0	–
RbK_2	TPX	$P\bar{3}m1(164)$	–	$P6/mmm(191)$	16.29	16.29	59.5	–	–	–	16.99	16.99	57.9	0.042	2.192	0.0	–	0.0
CsK_2	PTX	$P6/mmm(191)$	–	$P6/mmm(191)$	17.01	16.99	57.9	–	–	–	16.95	16.91	59.2	0.034	2.466	0.0	–	0.0
$CsRb_2$	PTX	$P6/mmm(191)$	–	$P6/mmm(191)$	17.64	17.65	59.0	–	–	–	17.85	17.84	58.6	0.012	2.173	0.0	–	0.0
$CsCs_2$	PTX	$P\bar{3}m1(164)$	–	$P6/mmm(191)$	18.62	18.63	58.2	–	–	–	18.82	18.97	58.7	0.027	2.081	0.0	–	0.0

Table 2: List of I-II

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$LiMg_2$	THX	$C2/m(12)$	$Amm2(38)$	–	6.15	6.61	56.9	6.60	6.17	57.5	–	–	–	0.152	3.972	0.0	0.0	–
$LiBa_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	12.24	8.58	44.8	–	–	–	1.109	6.245	–	0.0	–
KSr_2	HXX	–	$P1(1)$	–	–	–	–	14.90	12.22	34.9	–	–	–	4.308	4.310	–	0.0	–
KBa_2	HXX	–	$Amm2(38)$	–	–	–	–	14.40	14.44	34.8	–	–	–	1.099	1.172	–	0.0	–
$RbCa_2$	HXX	–	$P2_1/m(11)$	–	–	–	–	14.39	15.13	16.3	–	–	–	7.929	7.954	–	0.0	–
$RbSr_2$	HTP	$P6/mmm(191)$	$Amm2(38)$	$P6/mmm(191)$	15.62	15.61	60.1	16.32	16.39	30.0	15.95	15.95	58.0	0.754	0.786	0.0	0.0	0.0
$RbBa_2$	HXX	–	$Amm2(38)$	–	–	–	–	15.30	15.34	33.0	–	–	–	0.831	0.907	–	0.0	–
$CsCa_2$	TPX	$P6/mmm(191)$	–	$Cmmm(65)$	15.19	15.20	58.9	–	–	–	15.56	15.57	56.4	0.044	3.461	0.0	–	0.0
$CsSr_2$	TPX	$P6/mmm(191)$	–	$Cmmm(65)$	16.14	16.13	59.2	–	–	–	16.59	16.57	56.7	0.069	3.214	0.0	–	0.0

Table 3: List of I-XII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$LiCd_2$	HXX	–	$Cmmm(65)$	–	–	–	–	6.00	9.16	40.2	–	–	–	2.170	2.316	–	0.0	–
$LiHg_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.35	9.05	44.4	–	–	–	1.491	1.549	–	0.0	–

Table 4: List of I-XIII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$LiAl_2$	HTX	$P3m1(164)$	$P6m2(187)$	–	5.46	5.45	59.9	5.45	5.45	60.0	–	–	–	0.046	3.644	0.0	0.0	–
$LiIn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.58	9.07	43.7	–	–	–	1.741	2.532	–	0.0	–
$CsAl_2$	PTX	$Cmmm(65)$	–	$Cmme(67)$	15.07	15.07	36.6	–	–	–	14.58	14.59	37.7	0.159	6.625	0.0	–	0.0
$CsIn_2$	HTP	$C2/m(12)$	$P1(1)$	$Cmmm(65)$	15.03	15.01	41.2	13.63	12.06	43.9	15.17	15.15	40.9	0.504	0.543	0.0	0.0	0.0
$CsTl_2$	TPX	$C2/m(12)$	–	$P2_1/m(11)$	15.60	15.58	41.9	–	–	–	15.61	15.60	41.8	0.041	4.172	0.0	–	0.0

Table 5: List of I-XIV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$LiSn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.75	6.47	42.0	–	–	–	3.741	3.823	–	0.0	–
$NaSi_2$	TPX	$Cmmm(65)$	–	$Cmmm(65)$	12.29	12.29	36.3	–	–	–	11.82	11.81	38.2	0.281	6.475	0.0	–	0.0
$NaGe_2$	HXX	–	$Cmme(67)$	–	–	–	–	11.17	10.02	25.7	–	–	–	2.678	3.000	–	0.0	–
KSi_2	PXX	–	–	$P2/c(13)$	–	–	–	–	–	–	11.24	11.25	39.7	3.311	9.007	–	–	0.0
KSn_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	12.42	12.46	43.5	1.599	6.654	–	–	0.0
$RbGe_2$	PXX	–	–	$P2/c(13)$	–	–	–	–	–	–	12.98	11.83	30.7	0.890	6.183	–	–	0.0
$CsPb_2$	TPX	$P\bar{1}(2)$	–	$Cmmm(65)$	15.50	15.51	37.4	–	–	–	15.45	15.45	38.3	0.152	4.817	0.0	–	0.0

Table 6: List of I-XV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$LiBi_2$	HXX	–	$Pmma(51)$	–	–	–	–	10.80	8.20	39.4	–	–	–	1.327	1.585	–	0.0	–
NaN_2	THP	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$Cmmm(65)$	8.21	8.27	59.1	7.59	7.59	56.0	10.65	10.56	44.8	0.466	0.542	20.0	20.0	20.0
KN_2	TPX	$P\bar{3}m1(164)$	–	$P6/mmm(191)$	9.79	10.30	58.5	–	–	–	10.07	10.07	61.7	0.006	1.103	20.0	–	20.0
KBi_2	HXX	–	$P2/c(13)$	–	–	–	–	12.35	14.81	29.2	–	–	–	1.424	3.286	–	0.0	–
RbN_2	TPX	$P2/c(13)$	–	$P6/mmm(191)$	10.37	10.37	57.5	–	–	–	10.50	10.89	58.1	0.029	0.851	20.0	–	20.0
CsN_2	TPH	$P2/c(13)$	$Amm2(38)$	$Pmma(51)$	10.96	10.42	61.7	10.37	10.34	55.0	11.21	11.19	57.8	0.169	0.689	20.0	20.0	20.0
$CsBi_2$	TXX	$C2/m(12)$	–	–	15.08	15.10	35.0	–	–	–	–	–	–	1.192	4.126	0.0	–	–

Table 7: List of I-XVI

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
KS_2	TPX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	10.37	12.11	38.8	–	–	–	7.57	12.14	57.7	0.016	1.904	0.0	–	0.0
KSe_2	PTX	$C2/m(12)$	–	$P\bar{1}(2)$	12.40	12.43	41.7	–	–	–	12.07	10.58	41.8	0.400	1.789	0.0	–	0.0
RbS_2	TPX	$P\bar{1}(2)$	–	$C2(5)$	10.76	12.97	37.0	–	–	–	8.51	11.35	68.2	0.082	1.896	0.0	–	0.0
$RbSe_2$	PXX	–	–	$P2_1(4)$	–	–	–	–	–	–	10.60	13.06	36.9	0.841	2.222	–	–	0.0
$CsSe_2$	PTX	$C2/m(12)$	–	$P1(1)$	13.71	13.70	40.2	–	–	–	11.90	12.37	39.3	0.598	1.834	0.0	–	0.0
$CsTe_2$	TPX	$C2/m(12)$	–	$Cmmm(65)$	14.54	14.54	41.5	–	–	–	14.33	14.36	45.4	0.384	1.809	0.0	–	0.0

Table 8: List of I-XVII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$LiCl_2$	PXX	–	–	$P2/m(10)$	–	–	–	–	–	–	9.13	11.15	55.1	1.509	1.725	–	–	0.0
$NaCl_2$	PTX	$C2/m(12)$	–	$P1(1)$	8.40	10.16	51.8	–	–	–	12.18	10.56	43.9	0.731	0.955	4.0	–	2.0
$NaBr_2$	PXX	–	–	$P2/m(10)$	–	–	–	–	–	–	13.42	12.62	45.0	1.067	1.295	–	–	0.0
NaI_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	10.89	14.27	64.5	0.969	1.287	–	–	0.0
KF_2	THX	$P4mm(99)$	$P\bar{6}m2(187)$	–	7.36	10.45	44.6	8.83	8.81	56.8	–	–	–	0.434	1.186	4.0	4.0	–
KCl_2	THX	$P4/mmm(123)$	$P\bar{6}m2(187)$	–	8.54	12.06	45.0	10.13	10.20	57.7	–	–	–	0.294	1.368	4.0	4.0	–
KBr_2	PTX	$P4/mmm(123)$	–	$P2/m(10)$	9.94	9.94	53.0	–	–	–	12.65	12.78	57.8	0.683	1.014	4.0	–	0.0
KI_2	TPH	$P2/c(13)$	$Amm2(38)$	$P2/m(10)$	10.94	10.95	53.3	11.37	11.37	56.3	13.32	13.26	56.3	0.171	0.227	4.0	4.0	0.0
RbF_2	THX	$P4/mmm(123)$	$P\bar{6}m2(187)$	–	7.81	11.09	44.7	9.37	9.36	57.0	–	–	–	0.508	1.140	4.0	4.0	–
$RbCl_2$	THX	$P4/mmm(123)$	$P\bar{6}m2(187)$	–	8.99	12.73	45.1	10.82	10.87	56.7	–	–	–	0.349	1.122	4.0	4.0	–
$RbBr_2$	THX	$P4/mmm(123)$	$P\bar{6}m2(187)$	–	9.35	13.21	44.9	11.21	11.16	57.6	–	–	–	0.346	1.251	4.0	4.0	–
RbI_2	PTX	$P4/mmm(123)$	–	$P2/m(10)$	9.83	13.90	45.4	–	–	–	13.39	13.96	65.6	0.748	1.166	4.0	–	0.0
CsF_2	HPX	–	$Amm2(38)$	$Cmmm(65)$	–	–	–	10.12	10.13	55.1	11.40	9.82	53.9	0.512	1.732	–	4.0	4.0
$CsBr_2$	TXX	$P4/mmm(123)$	–	–	9.84	13.95	45.2	–	–	–	–	–	–	0.919	1.134	4.0	–	–
CsI_2	PTX	$P4/mmm(123)$	–	$P\bar{1}(2)$	10.42	14.74	44.9	–	–	–	13.76	15.04	61.7	0.796	1.746	4.0	–	0.0

Table 9: List of I-TM

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$LiSc_2$	PXX	–	–	$Pmma(51)$	–	–	–	–	–	–	7.23	7.23	52.5	3.306	3.363	–	–	0.0
$LiMn_2$	HXX	–	$P\bar{1}(2)$	–	–	–	–	7.75	10.43	29.6	–	–	–	2.707	5.736	–	32.3	–
$LiAg_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.83	5.84	59.9	–	–	–	3.253	3.264	–	0.0	–
$NaAu_2$	HXX	–	$Cmmm(65)$	–	–	–	–	5.81	9.01	38.3	–	–	–	1.783	1.787	–	0.0	–
KAg_2	HXX	–	$Aem2(39)$	–	–	–	–	13.20	12.24	20.9	–	–	–	2.265	2.295	–	0.0	–
RbY_2	HXX	–	$Cmm2(35)$	–	–	–	–	14.19	15.63	24.9	–	–	–	7.531	7.609	–	0.0	–
$RbAu_2$	PTX	$Cmmm(65)$	–	$Cmmm(65)$	13.37	13.42	46.9	–	–	–	13.40	13.44	46.8	0.003	4.908	0.0	–	0.0
$CsCr_2$	PTX	$Cmmm(65)$	–	$Cmmm(65)$	14.19	14.18	46.0	–	–	–	14.19	14.19	46.0	0.016	3.209	42.2	–	42.1
CsY_2	PTX	$C2/m(12)$	–	$Cmmm(65)$	15.79	15.78	43.4	–	–	–	15.56	15.55	45.8	0.040	4.966	14.0	–	13.4
$CsAg_2$	PTX	$Cmmm(65)$	–	$Cmmm(65)$	14.23	14.22	44.8	–	–	–	14.23	14.25	44.8	0.028	3.849	0.0	–	0.0
$CsAu_2$	PTX	$Cmmm(65)$	–	$Cmmm(65)$	13.95	13.95	45.0	–	–	–	13.95	13.96	45.0	0.002	4.896	0.0	–	0.0

Table 10: List of II-I

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BeK_2	PXX	–	–	$P1(2)$	–	–	–	–	–	–	9.21	8.57	62.5	2.140	4.508	–	–	0.0
$BeRb_2$	THX	$P\bar{3}m1(164)$	$Amm2(38)$	–	10.74	10.74	56.9	10.59	10.59	49.0	–	–	–	0.542	2.225	0.0	0.0	–
$BeCs_2$	THX	$P\bar{3}m1(164)$	$Amm2(38)$	–	10.99	10.99	59.2	11.24	11.25	50.2	–	–	–	0.787	2.815	0.0	0.0	–
CaK_2	HXX	–	$P2/m(10)$	–	–	–	–	8.35	13.97	33.5	–	–	–	4.431	4.483	–	0.0	–
$CaRb_2$	HXX	–	$Cmmm(65)$	–	–	–	–	13.13	8.80	41.5	–	–	–	3.612	3.733	–	0.0	–
SrK_2	HXX	–	$Cmmm(65)$	–	–	–	–	14.81	8.76	32.3	–	–	–	4.385	4.424	–	0.0	–
$SrCs_2$	HXX	–	$P2/m(10)$	–	–	–	–	9.91	15.60	36.5	–	–	–	3.320	3.326	–	0.0	–
BaK_2	HXX	–	$Cmmm(65)$	–	–	–	–	15.14	8.97	32.4	–	–	–	5.288	5.295	–	0.0	–
$BaRb_2$	HXX	–	$Cmmm(65)$	–	–	–	–	9.25	11.07	52.8	–	–	–	4.754	4.775	–	0.0	–
$BaCs_2$	HXX	–	$Amm2(38)$	–	–	–	–	15.57	15.52	35.9	–	–	–	1.937	2.001	–	0.0	–

Table 11: List of II-II

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$BeBe_2$	HTX	$Cmmm(65)$	$P\bar{6}m2(187)$	–	4.24	4.73	56.1	4.39	4.39	120.0	–	–	–	0.167	6.772	0.0	0.0	–
$BeMg_2$	THX	$P\bar{1}(2)$	$Amm2(38)$	–	6.15	7.68	52.1	6.11	6.31	60.8	–	–	–	0.494	6.478	0.0	0.0	–
$BeCa_2$	PTH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	8.62	8.62	58.8	7.77	7.76	59.9	8.32	8.33	60.2	0.020	0.231	0.0	0.0	0.0
$BeBa_2$	PTH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	10.03	10.03	57.0	8.97	8.96	58.2	9.87	9.85	58.8	0.007	0.278	0.0	0.0	0.0
$MgBa_2$	PTH	$C2/m(12)$	$Amm2(38)$	$P\bar{1}(2)$	11.05	8.90	51.5	8.84	8.86	59.6	12.04	11.07	44.4	0.101	0.322	0.0	0.0	0.0
$CaSr_2$	HXX	–	$Cmmm(65)$	–	–	–	–	8.12	11.93	42.7	–	–	–	5.908	6.058	–	0.0	–
$CaBa_2$	HXX	–	$Cmmm(65)$	–	–	–	–	8.41	13.79	34.9	–	–	–	5.809	6.597	–	0.0	–
$SrCa_2$	HXX	–	$Cmmm(65)$	–	–	–	–	7.90	13.16	34.6	–	–	–	6.178	6.180	–	0.0	–
$SrSr_2$	HXX	–	$Amm2(38)$	–	–	–	–	8.55	14.45	31.6	–	–	–	6.433	6.440	–	0.0	–
$SrBa_2$	HXX	–	$Cmmm(65)$	–	–	–	–	8.63	14.42	33.6	–	–	–	6.319	6.612	–	0.0	–
$BaCa_2$	HXX	–	$Amm2(38)$	–	–	–	–	13.20	13.23	34.5	–	–	–	1.951	1.981	–	0.0	–
$BaSr_2$	HXX	–	$Amm2(38)$	–	–	–	–	13.70	13.69	35.6	–	–	–	1.993	2.024	–	0.0	–
$BaBa_2$	HXX	–	$Amm2(38)$	–	–	–	–	14.13	14.12	34.9	–	–	–	2.303	2.377	–	0.0	–

Table 12: List of II-XII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$CaHg_2$	HPT	$C2/m(12)$	$Amm2(38)$	$P6/mmm(191)$	11.48	11.50	37.9	10.67	10.75	41.0	10.98	10.99	59.6	0.088	0.094	0.0	0.0	0.0
$SrCd_2$	HXX	–	$P2/c(13)$	–	–	–	–	8.32	11.91	43.6	–	–	–	1.436	2.675	–	0.0	–
$SrHg_2$	HXX	–	$Pmmn(59)$	–	–	–	–	9.48	12.86	41.3	–	–	–	1.553	1.834	–	0.0	–

Table 13: List of II-XIII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BeB_2	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	6.03	6.01	60.1	1.909	2.423	–	–	0.0
$BeAl_2$	HXX	–	$Pmm2(25)$	–	–	–	–	5.30	5.45	59.0	–	–	–	1.429	3.864	–	0.0	–
$BeIn_2$	HTX	$C2/m(12)$	$P1(1)$	–	6.90	7.89	50.3	6.92	5.95	61.2	–	–	–	0.494	6.038	0.0	0.0	–
$BeTl_2$	HTX	$P1(1)$	$P1(1)$	–	6.29	8.79	48.2	7.00	6.15	59.0	–	–	–	0.040	4.767	0.0	0.0	–
$MgIn_2$	HXX	–	$Pmmm(47)$	–	–	–	–	10.52	8.51	35.3	–	–	–	2.379	2.923	–	0.0	–
CaB_2	TPX	$Pmma(51)$	–	$Pmma(51)$	8.29	10.25	35.9	–	–	–	8.26	10.19	36.0	0.005	15.069	0.0	–	0.0
$CaTl_2$	HXX	–	$P2/c(13)$	–	–	–	–	8.22	12.19	36.0	–	–	–	2.239	2.264	–	0.0	–
SrB_2	PTX	$Cmmm(65)$	–	$Cmmm(65)$	10.86	10.88	34.3	–	–	–	10.88	10.87	34.2	0.005	12.283	0.0	–	0.0
$SrAl_2$	PXX	–	–	$P6mm(183)$	–	–	–	–	–	–	9.20	9.20	60.0	3.037	8.347	–	–	0.0
$SrIn_2$	HXX	–	$C2/m(12)$	–	–	–	–	12.52	11.36	24.8	–	–	–	3.379	4.365	–	0.0	–
$SrTl_2$	HXX	–	$Pmna(53)$	–	–	–	–	8.22	11.78	45.1	–	–	–	2.209	2.225	–	0.0	–
BaB_2	PXX	–	–	$Pmma(51)$	–	–	–	–	–	–	8.97	10.87	34.1	2.298	16.736	–	–	0.0
$BaAl_2$	PXX	–	–	$Cmm2(35)$	–	–	–	–	–	–	8.48	8.48	58.3	1.492	9.809	–	–	0.0

Table 14: List of II-XIV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$BeSi_2$	HTX	$C2/m(12)$	$Amm2(38)$	–	7.49	7.49	39.3	7.47	7.46	39.7	–	–	–	0.581	4.407	0.0	0.0	–
$BeGe_2$	HTX	$P\bar{3}m1(164)$	$Amm2(38)$	–	7.45	7.45	59.9	7.70	7.69	41.5	–	–	–	0.675	1.290	0.0	0.0	–
$BePb_2$	PTH	$P\bar{3}m1(164)$	$Amm2(38)$	$P\bar{3}m1(164)$	8.34	8.34	59.2	7.87	7.87	52.1	8.25	8.25	59.9	0.012	0.416	0.0	0.0	0.0
$MgSi_2$	HXX	–	$Pmma(51)$	–	–	–	–	9.92	7.60	38.3	–	–	–	1.732	2.165	–	0.0	–
$MgGe_2$	HXX	–	$Pmma(51)$	–	–	–	–	10.26	8.38	33.9	–	–	–	1.749	3.081	–	0.0	–
$MgSn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.89	9.95	37.1	–	–	–	1.742	2.456	–	0.0	–
$CaSi_2$	TPX	$C2/m(12)$	–	$Pmmn(59)$	11.52	11.52	39.0	–	–	–	11.42	11.42	39.4	0.030	5.564	0.0	–	0.0
$CaGe_2$	TPX	$C2/m(12)$	–	$Pmmn(59)$	11.48	11.48	40.7	–	–	–	11.27	11.27	41.4	0.007	4.591	0.0	–	0.0
$CaSn_2$	PTX	$C2/m(12)$	–	$Pmmn(59)$	11.94	11.94	44.0	–	–	–	11.99	12.00	43.6	0.053	4.749	0.0	–	0.0
SrC_2	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	8.26	10.52	50.3	2.001	34.056	–	–	0.0
$SrSi_2$	TPX	$C2/m(12)$	–	$P2/c(13)$	12.31	12.31	37.3	–	–	–	12.47	12.48	36.9	0.055	4.898	0.0	–	0.0
$SrGe_2$	TPX	$C2/m(12)$	–	$Cmmm(65)$	12.13	12.13	39.3	–	–	–	12.45	12.45	38.9	0.256	4.014	0.0	–	0.0
$SrSn_2$	TPX	$C2/m(12)$	–	$Cmmm(65)$	12.68	12.68	42.2	–	–	–	13.25	13.26	41.5	0.389	4.638	0.0	–	0.0
$SrPb_2$	TPX	$C2/m(12)$	–	$Cmmm(65)$	12.83	12.83	43.5	–	–	–	12.72	12.73	48.5	0.402	3.960	0.0	–	0.0
BaC_2	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	8.72	11.72	47.6	24.445	34.444	–	–	0.0
$BaSi_2$	PTX	$P2/c(13)$	–	$P2/c(13)$	12.20	12.21	37.3	–	–	–	12.25	12.29	37.3	0.017	5.115	0.0	–	0.0
$BaGe_2$	TPX	$P\bar{1}(2)$	–	$P2/c(13)$	12.23	12.08	38.8	–	–	–	12.26	12.47	39.0	0.066	4.080	0.0	–	0.0
$BaSn_2$	HXX	–	$Pc(7)$	–	–	–	–	8.68	9.40	75.0	–	–	–	1.507	1.720	–	0.0	–
$BaPb_2$	TPX	$C2/m(12)$	–	$Cmmm(65)$	13.51	13.52	42.2	–	–	–	13.58	13.58	44.3	0.021	4.013	0.0	–	0.0

Table 15: List of II-XV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BeP_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.79	6.79	60.0	–	–	–	1.270	1.864	–	0.0	–
$BeSb_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	7.71	7.71	59.2	–	–	–	1.290	1.822	–	0.0	–
$BeBi_2$	HPX	–	$P\bar{6}m2(187)$	$P1(1)$	–	–	–	7.90	7.89	59.7	8.65	8.01	47.7	0.342	1.070	–	0.0	0.0
CaN_2	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	6.97	7.94	55.9	2.686	21.815	–	–	0.0
$CaSb_2$	HXX	–	$Cmmm(65)$	–	–	–	–	9.52	11.96	36.0	–	–	–	1.402	4.121	–	0.0	–
$CaBi_2$	HXX	–	$Pmmm(47)$	–	–	–	–	12.04	9.66	36.2	–	–	–	1.884	1.930	–	0.0	–
SrN_2	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	8.47	7.45	56.0	1.588	21.284	–	–	0.9
SrP_2	TPX	$C2/m(12)$	–	$Cmmm(65)$	11.14	11.14	37.4	–	–	–	11.31	11.31	43.7	0.600	2.113	0.0	–	0.0
$SrSb_2$	HXX	–	$Cmmm(65)$	–	–	–	–	10.03	12.61	36.5	–	–	–	1.128	3.870	–	0.0	–
$SrBi_2$	HXX	–	$Pmma(51)$	–	–	–	–	10.24	12.70	35.8	–	–	–	1.319	1.366	–	0.0	–
BaN_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	9.18	9.23	60.7	–	–	–	19.750	19.780	–	3.8	–
BaP_2	TXX	$P\bar{1}(2)$	–	–	11.20	10.66	34.9	–	–	–	–	–	–	1.981	3.218	0.0	–	–
$BaSb_2$	HXX	–	$Cmmm(65)$	–	–	–	–	10.96	13.78	34.8	–	–	–	2.519	4.322	–	0.0	–
$BaBi_2$	HXX	–	$Pmma(51)$	–	–	–	–	13.57	11.01	34.7	–	–	–	1.568	3.780	–	0.0	–

Table 16: List of II-XVI

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BeO_2	HXX	–	$P1(1)$	–	–	–	–	5.58	5.74	60.2	–	–	–	1.771	1.878	–	2.0	–
BeS_2	PHX	–	$C2(5)$	$P1(1)$	–	–	–	7.15	7.16	78.3	8.85	6.88	51.6	0.065	3.706	–	0.0	0.0
$BeSe_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	10.46	6.44	52.1	2.049	3.159	–	–	0.0
$BeTe_2$	TPX	$P\bar{3}m1(164)$	–	$P\bar{1}(2)$	7.05	7.05	56.5	–	–	–	10.97	8.25	67.0	0.282	1.756	0.0	–	0.0
MgO_2	HPX	–	$P\bar{6}m2(187)$	$P2/c(13)$	–	–	–	6.61	6.63	59.7	7.91	5.99	47.3	0.056	4.414	–	0.0	0.0
CaO_2	PHX	–	$P\bar{6}m2(187)$	$P4/mmm(123)$	–	–	–	7.49	7.48	60.6	6.41	7.17	63.4	0.615	7.585	–	0.0	0.0
CaS_2	PHX	–	$P\bar{6}m2(187)$	$P4/mmm(123)$	–	–	–	9.02	9.01	58.4	8.58	7.66	63.3	0.388	7.064	–	0.0	0.0
$CaSe_2$	THX	$P4/mmm(123)$	$P\bar{6}m2(187)$	–	8.00	11.36	44.9	9.37	9.38	58.2	–	–	–	0.335	1.768	0.0	0.0	–
$CaTe_2$	THX	$C2/m(12)$	$P\bar{6}m2(187)$	–	11.55	9.01	49.8	9.86	9.90	59.2	–	–	–	0.410	2.140	0.0	0.0	–
SrS_2	PXX	–	–	$P4/mmm(123)$	–	–	–	–	–	–	8.10	11.48	45.0	0.837	7.807	–	–	0.0
$SrSe_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	9.99	9.99	57.9	–	–	–	2.071	5.736	–	0.0	–
BaS_2	PHX	–	$P\bar{6}m2(187)$	$P4/mmm(123)$	–	–	–	10.15	10.14	60.1	9.65	9.65	53.2	0.814	8.564	–	0.0	0.0
$BaSe_2$	PTX	$P4/mmm(123)$	–	$P4/mmm(123)$	8.90	12.61	45.0	–	–	–	8.91	12.62	45.0	0.022	0.868	0.0	–	0.0
$BaTe_2$	TPX	$P4/mmm(123)$	–	$P4/mmm(123)$	9.43	13.37	44.8	–	–	–	9.43	13.37	44.8	0.004	1.146	0.0	–	0.0

Table 17: List of II-XVII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$BeCl_2$	PHX	–	$P4m2(115)$	$Pccm(49)$	–	–	–	6.68	6.68	86.6	7.54	7.58	91.4	0.457	3.017	–	0.0	0.0
BeI_2	HXX	–	$C222(21)$	–	–	–	–	7.77	10.22	49.1	–	–	–	2.537	3.411	–	0.0	–
MgF_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	6.29	6.29	59.8	–	–	–	6.28	6.29	59.6	0.003	3.879	0.0	–	0.0
$MgCl_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.42	7.42	59.5	–	–	–	7.43	7.43	59.4	0.049	2.430	0.0	–	0.0
$MgBr_2$	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.81	7.82	59.5	–	–	–	7.81	7.82	59.5	0.005	2.072	0.0	–	0.0
MgI_2	THX	$P\bar{3}m1(164)$	$P\bar{3}m1(164)$	–	8.44	8.45	59.5	8.44	8.44	59.5	–	–	–	0.002	1.141	0.0	0.0	–
CaF_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.24	7.25	60.0	–	–	–	7.24	7.24	60.1	0.028	3.153	0.0	–	0.0
$CaCl_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	8.29	8.29	60.0	–	–	–	8.29	8.29	59.9	0.001	1.980	0.0	–	0.0
$CaBr_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	8.62	8.61	59.4	–	–	–	8.55	8.55	59.9	0.005	1.548	0.0	–	0.0
CaI_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.13	9.14	59.4	–	–	–	9.07	9.08	59.8	0.005	1.259	0.0	–	0.0
SrF_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.82	7.83	60.1	–	–	–	7.81	7.82	60.2	0.004	2.693	0.0	–	0.0
$SrCl_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	8.93	8.93	59.9	–	–	–	8.92	8.92	60.1	0.001	1.839	0.0	–	0.0
$SrBr_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.18	9.19	59.9	–	–	–	9.17	9.17	60.0	0.001	1.447	0.0	–	0.0
SrI_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.74	9.74	59.1	–	–	–	9.61	9.61	60.1	0.010	1.111	0.0	–	0.0
BaF_2	TPX	$P\bar{3}m1(164)$	–	$Pmmn(59)$	8.52	8.53	59.3	–	–	–	8.09	8.53	58.4	0.025	2.175	0.0	–	0.0
$BaCl_2$	TPX	$P\bar{3}m1(164)$	–	$Pmmn(59)$	9.70	9.73	59.5	–	–	–	9.55	9.31	59.0	0.213	1.705	0.0	–	0.0
$BaBr_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.03	10.02	59.4	–	–	–	9.92	9.91	59.9	0.009	1.318	0.0	–	0.0
BaI_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.50	10.51	59.1	–	–	–	10.35	10.34	59.8	0.012	0.973	0.0	–	0.0

Table 18: List of II-TM

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$BeSc_2$	HPX	–	$P4/mmm(123)$	$P\bar{1}(2)$	–	–	–	6.24	8.83	45.1	6.32	7.48	54.7	0.259	0.904	–	0.0	2.3
BeV_2	HXX	–	$Pbcm(57)$	–	–	–	–	5.68	7.25	38.3	–	–	–	2.015	3.622	–	0.0	–
$BeCr_2$	TXX	$Cm(8)$	–	–	6.78	6.78	24.9	–	–	–	–	–	–	1.808	15.575	1.8	–	–
$BeMn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	7.38	5.24	45.2	–	–	–	0.953	8.523	–	29.3	–
$BeZr_2$	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	6.05	8.11	41.6	1.302	2.180	–	–	0.0
$BeMo_2$	HPX	–	$P\bar{1}(2)$	$P\bar{1}(2)$	–	–	–	6.88	8.22	38.5	9.60	7.09	32.7	0.481	1.048	–	0.0	0.0
$BeRu_2$	TXX	$C2/m(12)$	–	–	8.70	7.49	30.6	–	–	–	–	–	–	1.128	9.799	0.0	–	–
$BeRh_2$	THX	$C2/m(12)$	$P\bar{6}m2(187)$	–	6.32	5.43	49.5	5.32	5.32	59.8	–	–	–	0.239	1.681	0.0	0.0	–
$BeAg_2$	THX	$P4/mmm(123)$	$Amm2(38)$	–	8.01	5.65	44.8	6.20	5.67	56.2	–	–	–	0.552	5.148	0.0	0.0	–
$BeHf_2$	HXX	–	$P4mm(99)$	–	–	–	–	7.98	5.64	45.0	–	–	–	1.142	1.145	–	0.0	–
$BeTa_2$	HXX	–	$P2_1/m(11)$	–	–	–	–	6.35	5.61	55.3	–	–	–	7.349	8.785	–	0.0	–
BeW_2	HXX	–	$P\bar{1}(2)$	–	–	–	–	7.34	8.14	37.4	–	–	–	1.613	1.652	–	0.0	–
$BeRe_2$	TXX	$C2/m(12)$	–	–	6.98	6.98	41.2	–	–	–	–	–	–	1.327	3.902	0.0	–	–
$BePt_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.51	5.52	60.0	–	–	–	1.509	11.273	–	0.0	–
$BeAu_2$	HTX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	6.13	6.10	54.9	6.08	6.09	55.7	–	–	–	0.104	0.949	0.0	0.0	–
$MgSc_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.73	9.54	44.8	–	–	–	3.061	9.615	–	0.0	–
$MgRh_2$	THX	$C2/m(12)$	$Amm2(38)$	–	9.63	9.64	33.2	9.07	9.07	33.3	–	–	–	0.102	1.958	3.6	0.0	–
$MgIr_2$	HXX	–	$Cm(8)$	–	–	–	–	9.92	9.91	28.9	–	–	–	5.421	6.766	–	0.0	–
$CaCr_2$	HXX	–	$Cmmm(65)$	–	–	–	–	6.42	10.52	34.3	–	–	–	3.709	3.723	–	36.4	–
$CaAg_2$	HXX	–	$P4/nmm(129)$	–	–	–	–	7.29	10.38	45.1	–	–	–	2.068	2.099	–	0.0	–
$CaIr_2$	HXX	–	$P1(1)$	–	–	–	–	10.09	8.92	30.6	–	–	–	7.678	7.791	–	0.0	–
$CaAu_2$	HXX	–	$Pmn2_1(31)$	–	–	–	–	7.61	8.88	54.2	–	–	–	1.218	1.219	–	0.0	–
$SrSc_2$	PXX	–	–	$P4mm(99)$	–	–	–	–	–	–	10.27	7.19	44.3	6.776	7.510	–	–	0.0
SrY_2	HXX	–	$P2/c(13)$	–	–	–	–	8.66	13.98	28.0	–	–	–	11.818	12.121	–	0.0	–
$SrPd_2$	HXX	–	$Pmma(51)$	–	–	–	–	8.94	6.47	43.0	–	–	–	5.686	7.687	–	0.0	–
$SrAg_2$	HXX	–	$P4/nmm(129)$	–	–	–	–	7.87	11.16	44.7	–	–	–	2.038	2.070	–	0.0	–
$SrAu_2$	TPH	$P6/mmm(191)$	$P\bar{6}m2(187)$	$Cmmm(65)$	10.80	10.84	60.1	8.49	8.59	60.0	11.38	11.38	53.5	0.060	0.644	0.0	0.0	0.0
$BaCr_2$	PTH	$Cmmm(65)$	$Pmmm(47)$	$Cmmm(65)$	12.36	12.35	51.8	10.35	12.66	34.6	12.37	12.37	51.7	0.012	0.318	40.8	38.5	40.8
BaY_2	TXX	$C2/m(12)$	–	–	14.17	14.16	30.4	–	–	–	–	–	–	4.497	11.981	0.0	–	–
$BaPd_2$	TPX	$C2/m(12)$	–	$Cmmm(65)$	11.56	11.56	46.8	–	–	–	11.61	11.62	48.4	0.173	1.447	0.0	–	0.0
$BaAg_2$	HXX	–	$Pmma(51)$	–	–	–	–	6.90	9.76	44.1	–	–	–	4.854	4.883	–	0.0	–
$BaAu_2$	HXX	–	$Pmn2_1(31)$	–	–	–	–	9.83	8.33	54.0	–	–	–	1.867	1.871	–	0.0	–

Table 19: List of XII-I

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$CdNa_2$	THX	$P1(2)$	$Amm2(38)$	–	9.91	10.42	37.9	10.08	10.08	38.0	–	–	–	0.815	1.987	0.0	0.0	–
CdK_2	HXX	–	$P4/mmm(123)$	–	–	–	–	8.43	11.95	44.6	–	–	–	1.278	2.679	–	0.0	–
$CdRb_2$	HXX	–	$P1(1)$	–	–	–	–	8.85	13.29	41.6	–	–	–	1.561	2.875	–	0.0	–
$HgLi_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.66	9.44	44.7	–	–	–	1.596	3.332	–	0.0	–
$HgCs_2$	TXX	$P\bar{3}m1(164)$	–	–	11.55	11.43	57.4	–	–	–	–	–	–	1.902	3.325	0.0	–	–

Table 20: List of XII-II

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$CdCa_2$	PTH	$C2/m(12)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	8.05	8.07	59.1	7.91	7.90	59.5	7.80	9.10	54.1	0.438	0.706	0.0	0.0	0.0
$CdBa_2$	HPT	$C2/m(12)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	10.64	10.61	56.1	9.24	9.19	58.5	10.29	10.26	60.1	0.497	0.549	0.0	0.0	0.0
$HgBe_2$	PHT	$P6/mmm(191)$	$P6/mmm(191)$	$P6/mmm(191)$	8.29	8.29	60.0	8.29	8.29	60.0	8.29	8.30	59.9	0.016	0.018	0.0	0.0	0.0
$HgCa_2$	THP	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	7.78	9.09	54.1	8.01	7.99	59.8	8.14	8.10	59.8	0.167	0.272	0.0	0.0	0.0
$HgSr_2$	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{1}(2)$	9.00	8.90	59.5	8.75	8.70	59.2	9.17	9.58	56.6	0.022	0.108	0.0	0.0	0.0
$HgBa_2$	PHX	–	$P\bar{6}m2(187)$	$C2/m(12)$	–	–	–	9.26	9.17	58.8	8.96	11.04	50.6	0.760	1.059	–	0.0	0.0

Table 21: List of XII-XII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P

Table 22: List of XII-XIII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$CdTl_2$	THX	$C2/m(12)$	$Amm2(38)$	–	9.39	9.40	41.4	9.32	9.26	40.5	–	–	–	0.451	2.846	0.0	0.0	–

Table 23: List of XII-XIV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$CdGe_2$	HXX	–	$Amm2$(38)	–	–	–	–	9.22	9.22	36.9	–	–	–	1.601	1.654	–	0.0	–
$CdSn_2$	HXX	–	$Amm2$(38)	–	–	–	–	9.63	9.78	37.6	–	–	–	1.492	2.923	–	0.0	–
$HgGe_2$	PXX	–	–	$P3m1$(156)	–	–	–	–	–	–	8.12	8.13	59.9	2.224	3.213	–	–	0.0
$HgSn_2$	HPX	–	$Amm2$(38)	Pm(6)	–	–	–	9.70	9.71	38.1	9.31	9.34	59.7	0.567	1.287	–	0.0	0.0

Table 24: List of XII-XV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CdP_2	TXX	$C2/m(12)$	–	–	11.38	11.29	34.1	–	–	–	–	–	–	0.824	2.323	0.0	–	–
$CdBi_2$	THX	$C2/m(12)$	$P\bar{6}m2(187)$	–	12.89	12.88	39.4	9.20	9.20	58.2	–	–	–	0.525	2.600	0.0	0.0	–
HgP_2	PTX	$P2/m(10)$	–	$P1(1)$	12.10	8.10	46.7	–	–	–	9.72	9.46	58.5	0.798	3.283	0.0	–	0.0
$HgBi_2$	TXX	$C2/m(12)$	–	–	13.27	13.23	38.3	–	–	–	–	–	–	2.268	3.304	0.0	–	–

Table 25: List of XII-XVI

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CdO_2	PXX	–	–	$P2/m(10)$	–	–	–	–	–	–	9.14	7.13	90.0	1.962	2.804	–	–	2.0
CdS_2	PHX	–	$Pc(7)$	$P1(1)$	–	–	–	9.47	9.49	54.0	9.68	8.44	55.2	0.408	5.042	–	0.0	0.0
$CdSe_2$	PHX	–	$C2(5)$	$Cm(8)$	–	–	–	11.60	8.63	47.4	9.39	9.40	54.1	0.364	4.240	–	0.0	0.0
HgO_2	PXX	–	–	$P2/m(10)$	–	–	–	–	–	–	9.53	7.97	59.4	2.593	4.809	–	–	0.0
$HgSe_2$	PHX	–	$C2/m(12)$	$P1(1)$	–	–	–	8.58	8.56	86.4	11.54	9.97	45.2	0.539	4.257	–	0.0	0.0

Table 26: List of XII-XVII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CdF_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.15	7.15	59.8	–	–	–	7.17	7.18	59.8	0.031	2.285	0.0	–	0.0
$CdCl_2$	HTP	$P\bar{3}m1(164)$	$P\bar{3}m1(164)$	$C222(21)$	7.91	7.91	58.7	7.83	7.83	59.7	8.08	8.08	79.4	0.006	0.771	0.0	0.0	0.0
$CdBr_2$	TXX	$P\bar{3}m1(164)$	–	–	8.21	8.21	58.9	–	–	–	–	–	–	0.874	1.427	0.0	–	–
HgF_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.45	7.46	59.4	–	–	–	7.45	7.45	59.6	0.001	1.882	0.0	–	0.0
$HgCl_2$	HTX	$P\bar{3}m1(164)$	$C2/m(12)$	–	8.21	8.22	57.2	9.88	8.34	53.0	–	–	–	0.350	1.827	0.0	0.0	–
$HgBr_2$	THX	$C2/m(12)$	$C2/m(12)$	–	8.49	9.57	54.9	8.43	8.41	68.4	–	–	–	0.079	0.926	0.0	0.0	–
HgI_2	HTX	$C2/m(12)$	$P\bar{4}m2(115)$	–	10.21	9.10	54.9	9.01	9.02	87.1	–	–	–	0.295	1.328	0.0	0.0	–

Table 27: List of XII-TM

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$CdCr_2$	HXX	–	$P2/c(13)$	–	–	–	–	7.69	10.38	34.0	–	–	–	2.805	3.215	–	36.1	–
CdY_2	PHT	$C2/m(12)$	$P4/mmm(123)$	$C2/m(12)$	9.02	9.89	46.7	9.81	6.93	45.0	10.05	7.29	56.9	0.040	0.730	0.0	0.0	1.5
$CdPd_2$	HTX	$C2/m(12)$	$Pmmm(47)$	–	10.32	10.33	31.8	10.31	8.33	34.1	–	–	–	0.203	3.136	0.0	0.0	–
$CdAg_2$	PXX	–	–	$P6/mmm(191)$	–	–	–	–	–	–	9.96	9.96	59.8	1.025	1.245	–	–	0.0
$CdAu_2$	HXX	–	$P2/c(13)$	–	–	–	–	8.60	7.54	41.5	–	–	–	1.506	1.517	–	0.0	–
$HgAg_2$	PTX	$P6/mmm(191)$	–	$P6/mmm(191)$	10.01	10.02	59.7	–	–	–	10.01	10.01	59.7	0.055	1.936	0.0	–	0.0
$HgPt_2$	PTX	$P6mm(183)$	–	$Pmmn(59)$	9.18	9.18	60.0	–	–	–	9.20	9.14	60.2	0.055	2.866	0.0	–	0.0

Table 28: List of XIII-I

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BK_2	THX	$P\bar{3}m1(164)$	$Amm2(38)$	–	10.11	10.12	57.7	9.22	9.21	52.3	–	–	–	0.565	2.933	11.1	3.4	–
BRb_2	TXX	$P\bar{3}m1(164)$	–	–	10.45	10.46	58.3	–	–	–	–	–	–	2.549	3.286	11.0	–	–
AlK_2	HTX	$C2/m(12)$	$Pmma(51)$	–	11.42	10.98	43.8	9.37	9.78	61.1	–	–	–	0.706	6.459	0.0	0.0	–
$AlRb_2$	THX	$C2/m(12)$	$Cmmm(65)$	–	11.40	11.84	44.1	10.18	13.18	40.0	–	–	–	0.424	5.631	0.0	0.0	–
$InLi_2$	HTX	$P4/mmm(123)$	$P4/mmm(123)$	–	6.32	9.04	45.6	9.15	6.45	45.0	–	–	–	0.051	4.573	0.0	0.0	–
$InNa_2$	THX	$Cmmm(65)$	$Pmma(51)$	–	8.86	11.40	38.1	8.85	11.33	37.7	–	–	–	0.056	3.600	0.0	0.0	–
InK_2	HTP	$C2/m(12)$	$Pmma(51)$	$P\bar{1}(2)$	11.36	10.25	48.2	10.39	9.49	57.2	10.57	10.48	51.1	0.234	0.567	0.0	0.0	0.0
$TlNa_2$	THX	$Pmmm(47)$	$Pmmm(47)$	–	8.95	11.56	37.8	8.91	11.53	37.9	–	–	–	0.024	3.001	0.0	0.0	–

Table 29: List of XIII-II

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BBe_2	TXX	$C2/m(12)$	–	–	4.04	5.97	59.4	–	–	–	–	–	–	1.451	1.965	0.0	–	–
BMg_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.45	7.43	55.6	–	–	–	7.20	7.24	55.8	0.003	1.172	0.0	–	0.0
BSr_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	16.42	15.21	16.1	3.136	4.685	–	–	0.0
BBa_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.32	9.29	58.0	–	–	–	9.19	9.25	59.1	0.012	1.120	4.2	–	4.2
$AlBe_2$	TXX	$C2/m(12)$	–	–	6.08	6.96	42.4	–	–	–	–	–	–	2.495	3.435	0.0	–	–
$AlCa_2$	HPX	–	$P4/mmm(123)$	$P\bar{1}(2)$	–	–	–	10.35	7.31	45.0	9.17	7.55	53.0	0.024	2.832	–	0.0	0.0
$AlSr_2$	HXX	–	$Pmmm(47)$	–	–	–	–	7.86	11.03	44.7	–	–	–	2.095	2.108	–	0.0	–
$AlBa_2$	HPX	–	$P4/mmm(123)$	$C2/m(12)$	–	–	–	11.80	8.34	45.0	9.58	10.87	47.6	0.688	2.324	–	0.0	0.0
$GaCa_2$	PTH	$P4/mmm(123)$	$P4/mmm(123)$	$P2_1/m(11)$	7.31	10.40	44.8	10.38	7.30	44.6	7.60	8.94	53.3	0.226	0.265	0.0	0.0	0.0
$InCa_2$	TXX	$P4/mmm(123)$	–	–	7.57	10.75	44.6	–	–	–	–	–	–	1.123	6.594	0.0	–	–
$InBa_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.51	12.04	45.1	–	–	–	2.067	2.487	–	0.0	–
$TlBe_2$	PTH	$P6/mmm(191)$	$P6/mmm(191)$	$P6/mmm(191)$	8.40	8.40	60.0	8.39	8.39	60.0	8.40	8.40	59.9	0.005	0.006	0.0	0.0	0.0
$TlCa_2$	HPX	–	$P4/mmm(123)$	$C2/m(12)$	–	–	–	7.66	10.85	45.0	9.88	8.16	51.4	0.389	1.984	–	0.0	0.0
$TlSr_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	8.58	10.54	51.4	1.108	1.465	–	–	0.0
$TlBa_2$	HPX	–	$P4/mmm(123)$	$P2_1/m(11)$	–	–	–	8.60	12.17	45.0	8.96	10.88	52.3	0.492	1.832	–	0.0	0.0

Table 30: List of XIII-XII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BCd_2	THX	$P1(2)$	$Pc(7)$	–	7.21	6.78	47.1	6.65	7.14	48.1	–	–	–	0.767	6.092	0.0	0.0	–
$AlCd_2$	THX	$P2/c(13)$	$P2/c(13)$	–	7.45	8.76	40.6	5.80	8.30	60.3	–	–	–	0.531	3.763	0.0	0.0	–
$AlHg_2$	THP	$P2_1/m(11)$	$Pc(7)$	$P\bar{1}(2)$	8.03	8.04	44.1	7.97	7.84	44.3	9.74	8.70	49.4	0.042	0.795	0.0	0.0	0.0

Table 31: List of XIII-XIII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BB_2	THX	$C2/m(12)$	$Amm2(38)$	–	5.12	5.68	33.6	5.37	4.94	35.3	–	–	–	0.713	1.914	0.0	0.0	–
BAl_2	HTX	$C2/m(12)$	$Amm2(38)$	–	6.48	6.65	59.2	6.66	6.34	45.2	–	–	–	0.492	2.832	0.0	0.0	–
AlB_2	THX	$P\bar{1}(2)$	$Pmn2_1(31)$	–	5.33	6.15	54.6	5.26	6.11	54.5	–	–	–	0.066	1.212	0.0	0.0	–
$AlAl_2$	THX	$P\bar{3}m1(164)$	$P4/mmm(123)$	–	5.51	5.51	62.7	5.48	5.48	87.5	–	–	–	0.676	6.286	0.0	0.0	–
$AlIn_2$	THX	$P1(1)$	$P1(1)$	–	6.16	7.74	50.9	7.37	6.28	53.4	–	–	–	0.041	5.934	0.0	0.0	–
$AlTl_2$	HXX	–	$Pm(6)$	–	–	–	–	7.10	7.12	55.6	–	–	–	1.199	2.662	–	0.0	–
$InAl_2$	PHX	–	$Amm2(38)$	$Cm(8)$	–	–	–	9.28	9.28	35.3	8.68	8.47	59.6	0.071	2.307	–	0.0	0.0
$InIn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.65	9.57	37.4	–	–	–	2.065	3.373	–	0.0	–
$InTl_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.94	6.95	59.9	–	–	–	3.251	4.456	–	0.0	–
$TlIn_2$	HPX	–	$Amm2(38)$	$Cm(8)$	–	–	–	6.97	6.64	58.4	6.74	7.77	64.0	0.448	4.086	–	0.0	0.0
$TlTl_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	7.10	7.09	58.7	–	–	–	2.866	3.135	–	0.0	–

Table 32: List of XIII-XIV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BSi_2	TPX	$P\bar{3}m1(164)$	–	$P2_1/m(11)$	6.43	6.42	60.0	–	–	–	7.80	7.16	89.9	0.443	1.111	0.0	–	0.0
BGe_2	TXX	$P\bar{3}m1(164)$	–	–	6.71	6.71	60.0	–	–	–	–	–	–	0.916	1.964	0.0	–	–
BSn_2	TXX	$P\bar{3}m1(164)$	–	–	7.36	7.36	60.0	–	–	–	–	–	–	1.261	2.480	0.0	–	–
AlC_2	HTP	$P\bar{1}(2)$	$P1(1)$	$Cmme(67)$	6.99	6.75	39.5	6.26	5.90	41.9	8.45	8.45	40.0	0.144	0.327	0.0	0.0	0.0
$AlSi_2$	HTX	$P\bar{1}(2)$	$Pc(7)$	–	7.44	7.78	56.2	7.02	7.35	54.3	–	–	–	0.623	4.540	0.0	0.0	–
$AlGe_2$	HTX	$C2/m(12)$	$Pc(7)$	–	8.95	8.97	36.6	8.00	8.07	46.4	–	–	–	0.389	5.203	0.0	0.0	–
$AlSn_2$	HXX	–	$Amm2(38)$	–	–	–	–	8.68	8.68	45.5	–	–	–	1.491	5.250	–	0.0	–
$AlPb_2$	HXX	–	$Amm2(38)$	–	–	–	–	8.86	8.86	46.7	–	–	–	1.361	2.072	–	0.0	–
$GaSn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.90	9.94	36.7	–	–	–	3.145	5.782	–	0.2	–

Table 33: List of XIII-XV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BP_2	TXX	$C2/m(12)$	–	–	7.19	7.19	52.4	–	–	–	–	–	–	3.719	4.235	0.0	–	–
BSb_2	HXX	–	$Cm(8)$	–	–	–	–	7.20	8.84	51.6	–	–	–	1.994	2.447	–	0.0	–
BBi_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	8.53	8.92	57.6	0.982	1.241	–	–	0.0
AlN_2	PXX	–	–	$P2(3)$	–	–	–	–	–	–	8.22	10.27	37.9	0.943	3.355	–	–	0.0
AlP_2	TXX	$P\bar{1}(2)$	–	–	7.62	7.84	41.5	–	–	–	–	–	–	1.290	1.807	0.0	–	–
$AlSb_2$	HTP	$P\bar{1}(2)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	10.18	8.75	44.0	8.25	8.26	59.2	10.29	8.07	50.1	0.176	0.251	0.0	0.0	0.0
$AlBi_2$	TXX	$P\bar{1}(2)$	–	–	9.06	8.59	43.3	–	–	–	–	–	–	1.782	1.864	0.0	–	–
TlN_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	11.28	9.45	61.4	17.897	18.774	–	–	0.0

Table 34: List of XIII-XVI

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BSe_2	HTX	$P1(1)$	$Cm(8)$	–	8.00	6.40	49.8	6.32	6.18	77.4	–	–	–	0.665	5.197	0.0	0.0	–
AlO_2	TXX	$P\bar{3}m1(164)$	–	–	5.71	5.71	64.4	–	–	–	–	–	–	2.061	2.775	4.0	–	–
AlS_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	6.71	8.14	56.4	1.041	1.615	–	–	0.0
$AlSe_2$	TXX	$C2/m(12)$	–	–	7.29	7.29	49.9	–	–	–	–	–	–	2.444	2.936	0.0	–	–
InO_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	6.67	6.69	65.5	–	–	–	7.17	6.69	57.8	0.154	1.285	4.0	–	4.0
InS_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	8.90	8.91	60.3	1.836	2.242	–	–	0.0
$InTe_2$	HTP	$C2/m(12)$	$C222(21)$	$P2_1/m(11)$	8.51	8.50	47.8	8.53	8.53	46.2	9.24	9.24	68.7	0.058	0.390	0.0	0.0	0.0
TlS_2	PXX	–	–	$P2(3)$	–	–	–	–	–	–	7.82	8.95	94.4	5.582	5.834	–	–	0.0

Table 35: List of XIII-XVII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BF_2	TXX	$P1(2)$	–	–	6.80	8.63	68.0	–	–	–	–	–	–	1.761	4.861	0.0	–	–
BCl_2	HXX	–	$P1(1)$	–	–	–	–	8.10	7.03	79.3	–	–	–	5.713	5.724	–	0.0	–
BBr_2	TXX	$P1(1)$	–	–	9.54	7.93	73.5	–	–	–	–	–	–	3.011	3.019	0.0	–	–
AlF_2	HTX	$C2/m(12)$	$P1(1)$	–	6.76	5.18	59.3	6.79	5.75	65.4	–	–	–	0.168	2.742	0.0	0.0	–
$AlBr_2$	HXX	–	$P2(3)$	–	–	–	–	11.39	7.31	65.4	–	–	–	0.908	2.623	–	0.0	–
$TlBr_2$	HPT	$P2/m(10)$	$P2(3)$	$P\bar{1}(2)$	9.39	8.65	62.1	11.31	11.75	41.1	8.42	13.59	55.8	0.204	0.207	0.0	0.0	0.0
TlI_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{1}(2)$	9.18	9.17	57.7	–	–	–	10.73	11.54	71.8	0.527	1.204	0.0	–	0.0

Table 36: List of XIII-TM

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
BTi_2	PTX	$P\bar{3}m1(164)$	–	$P1(1)$	6.16	6.17	60.1	–	–	–	7.35	7.10	36.3	0.451	3.307	0.0	–	0.0
BCr_2	HPX	–	$P2/m(10)$	$P2_1/m(11)$	–	–	–	5.02	6.08	49.1	6.24	6.26	53.9	0.558	2.198	–	0.0	0.0
BMn_2	TXX	$P2_1/m(11)$	–	–	6.30	6.31	60.1	–	–	–	–	–	–	1.940	5.815	27.5	–	–
BNi_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	5.27	5.27	59.6	5.12	5.12	59.6	–	–	–	0.413	4.629	0.0	0.0	–
BY_2	TXX	$P\bar{3}m1(164)$	–	–	7.71	7.70	59.8	–	–	–	–	–	–	1.297	3.219	0.0	–	–
BNb_2	TXX	$P\bar{3}m1(164)$	–	–	6.32	6.31	59.9	–	–	–	–	–	–	4.132	13.651	0.0	–	–
BRu_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.57	5.58	60.0	–	–	–	1.003	1.062	–	0.0	–
BRh_2	TPH	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	5.51	5.51	60.0	5.47	5.47	60.0	5.51	5.51	60.0	0.015	0.267	0.0	0.0	0.0
BPd_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	5.87	5.87	60.0	5.73	5.73	59.9	–	–	–	0.724	3.647	0.0	0.0	–
BAg_2	TXX	$Pmma(51)$	–	–	5.42	6.23	54.3	–	–	–	–	–	–	5.683	7.225	0.0	–	–
BHf_2	HTX	$P\bar{3}m1(164)$	$Cm(8)$	–	6.59	6.59	60.0	6.32	6.33	53.9	–	–	–	0.060	2.799	0.0	0.0	–
BTa_2	TXX	$P\bar{3}m1(164)$	–	–	6.25	6.25	60.0	–	–	–	–	–	–	1.487	4.771	0.0	–	–
BW_2	HTX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	6.16	6.16	60.0	5.77	5.77	59.9	–	–	–	0.647	4.847	0.0	0.0	–
BRe_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.66	5.66	60.0	–	–	–	4.914	7.263	–	0.0	–
BOs_2	HTX	$P2_1/m(11)$	$Pmm2(25)$	–	5.50	5.41	59.4	5.48	5.42	59.6	–	–	–	0.517	11.452	0.0	0.0	–
BIr_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	5.43	5.43	60.0	5.46	5.46	60.0	–	–	–	0.226	13.691	0.0	0.0	–
BPt_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	5.71	5.72	60.0	5.68	5.69	60.0	–	–	–	0.524	2.810	0.0	0.0	–
BAu_2	PXX	–	–	$P4/mbm(127)$	–	–	–	–	–	–	11.00	8.09	47.1	1.297	1.488	–	–	0.0
$AlSc_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.77	6.20	45.0	–	–	–	1.330	1.376	–	0.0	–
$AlCr_2$	TXX	$P2/c(13)$	–	–	7.23	7.98	39.4	–	–	–	–	–	–	4.443	11.654	0.0	–	–
AlY_2	HXX	–	$P4/mmm(123)$	–	–	–	–	9.56	6.76	45.1	–	–	–	0.888	4.155	–	0.0	–
$AlZr_2$	HXX	–	$Pbcm(57)$	–	–	–	–	8.90	7.23	35.7	–	–	–	1.093	2.313	–	0.0	–
$AlMo_2$	PHX	–	$P2/c(13)$	$P\bar{1}(2)$	–	–	–	7.39	10.20	30.8	7.46	7.73	41.3	0.309	0.821	–	0.0	0.0
$AlRu_2$	HXX	–	$C2/m(12)$	–	–	–	–	7.72	6.69	43.7	–	–	–	7.612	8.751	–	0.0	–
$AlRh_2$	PHX	–	$P4/mmm(123)$	$C2/m(12)$	–	–	–	7.78	5.50	45.0	6.78	7.81	43.0	0.265	1.125	–	0.0	0.0
$AlPd_2$	THX	$C2/m(12)$	$P\bar{6}m2(187)$	–	6.96	5.63	53.2	5.88	5.88	59.9	–	–	–	0.287	1.642	0.0	0.0	–
$AlAg_2$	THX	$C2/m(12)$	$P4/mmm(123)$	–	7.19	8.24	43.0	5.82	8.36	44.1	–	–	–	0.366	3.429	0.0	0.0	–
$AlHf_2$	TXX	$C2/m(12)$	–	–	7.70	7.69	45.9	–	–	–	–	–	–	2.870	4.085	0.0	–	–
AlW_2	THP	$P2_1/c(14)$	$P2/c(13)$	$P2/c(13)$	9.17	7.79	30.9	8.03	7.39	40.6	10.11	7.34	31.2	0.293	0.613	0.0	0.0	0.0
$AlIr_2$	HXX	–	$C2/m(12)$	–	–	–	–	7.81	6.82	42.6	–	–	–	1.127	6.685	–	0.0	–
$AlPt_2$	THX	$P4/mmm(123)$	$P\bar{6}m2(187)$	–	8.00	5.65	44.7	5.81	5.82	60.1	–	–	–	0.212	6.625	0.0	0.0	–
$AlAu_2$	THX	$C2/m(12)$	$P4/mmm(123)$	–	8.03	6.92	43.7	5.85	8.32	46.1	–	–	–	0.701	2.688	0.0	0.0	–
$GaTi_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	6.10	8.18	63.1	3.154	3.531	–	–	0.0
$GaCr_2$	TXX	$P4/mmm(123)$	–	–	6.04	8.64	43.3	–	–	–	–	–	–	0.958	5.749	33.7	–	–
$GaMn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	5.78	8.35	41.9	–	–	–	3.209	4.275	–	31.7	–
GaY_2	PHX	–	$P4/mmm(123)$	$C2/m(12)$	–	–	–	7.03	9.96	44.9	8.50	9.40	46.9	0.142	2.547	–	0.0	0.0
$InSc_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.65	9.46	45.0	–	–	–	3.680	6.339	–	0.0	–
$InTi_2$	TXX	$C2/m(12)$	–	–	10.64	10.63	31.5	–	–	–	–	–	–	1.117	5.256	0.0	–	–
InV_2	TXX	$C2/m(12)$	–	–	10.66	10.65	31.1	–	–	–	–	–	–	3.078	3.226	0.0	–	–
$InCr_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.11	8.63	45.1	–	–	–	1.595	2.770	–	35.6	–
$InMn_2$	PXX	–	–	$P6/mmm(191)$	–	–	–	–	–	–	9.24	9.20	59.8	2.572	2.657	–	–	22.2
InY_2	HXX	–	$P4/mmm(123)$	–	–	–	–	6.81	9.62	45.1	–	–	–	2.618	3.690	–	0.0	–
$InPd_2$	PXX	–	–	$P\bar{3}m1(164)$	–	–	–	–	–	–	8.97	9.04	59.4	3.730	4.080	–	–	0.0
$InOs_2$	PXX	–	–	$P6/mmm(191)$	–	–	–	–	–	–	8.97	8.96	60.0	7.610	8.673	–	–	0.0
$InAu_2$	TPX	$P6/mmm(191)$	–	$P6/mmm(191)$	9.88	9.87	60.1	–	–	–	9.90	9.87	60.1	0.001	1.107	0.0	–	0.0
$TlCr_2$	HXX	–	$P\bar{1}(2)$	–	–	–	–	11.10	7.66	33.2	–	–	–	5.563	5.653	–	26.6	–

Table 37: List of XIV-I

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CK_2	TXX	$P\bar{3}m1(164)$	–	–	9.26	9.28	58.4	–	–	–	–	–	–	1.062	2.497	8.0	–	–
CRb_2	TXX	$P\bar{3}m1(164)$	–	–	9.55	9.56	58.4	–	–	–	–	–	–	0.985	2.050	8.1	–	–
CCs_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.98	9.99	58.0	–	–	–	9.78	9.77	59.7	0.035	0.996	8.1	–	8.1
$SiNa_2$	PTX	$C2/m(12)$	–	$P\bar{1}(2)$	9.31	9.86	43.7	–	–	–	10.15	9.47	42.4	0.679	1.723	0.0	–	0.0
SiK_2	HXX	–	$Amm2(38)$	–	–	–	–	9.75	10.41	46.2	–	–	–	3.611	3.632	–	0.0	–
$SiRb_2$	HXX	–	$Amm2(38)$	–	–	–	–	10.13	10.81	46.4	–	–	–	3.591	5.384	–	0.0	–
$SiCs_2$	PTX	$P\bar{3}m1(164)$	–	$P2_1/m(11)$	11.81	11.79	58.3	–	–	–	11.48	11.52	59.8	0.013	1.126	8.0	–	8.0
GeK_2	HXX	–	$Amm2(38)$	–	–	–	–	10.57	9.90	46.0	–	–	–	2.766	3.054	–	0.0	–
$GeRb_2$	HXX	–	$Amm2(38)$	–	–	–	–	10.96	10.28	46.3	–	–	–	2.719	4.539	–	0.0	–
$GeCs_2$	PTH	$P\bar{3}m1(164)$	$Amm2(38)$	$P\bar{3}m1(164)$	11.87	11.83	58.2	11.13	11.12	48.6	11.60	11.60	59.4	0.015	0.776	8.0	5.3	8.0
SnK_2	HXX	–	$Amm2(38)$	–	–	–	–	10.55	11.48	45.0	–	–	–	2.288	2.307	–	0.0	–
$SnRb_2$	HXX	–	$Amm2(38)$	–	–	–	–	10.89	11.68	45.6	–	–	–	2.089	2.099	–	0.0	–
$SnCs_2$	HXX	–	$Cmmm(65)$	–	–	–	–	10.34	13.50	39.4	–	–	–	2.435	2.463	–	0.0	–
$PbRb_2$	HXX	–	$Amm2(38)$	–	–	–	–	10.96	11.95	46.2	–	–	–	1.818	3.099	–	0.0	–
$PbCs_2$	HXX	–	$Cmmm(65)$	–	–	–	–	10.34	13.60	40.1	–	–	–	2.093	3.761	–	0.0	–

Table 38: List of XIV-II

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CBe_2	PTX	$P\bar{3}m1(164)$	–	$Pmmn(59)$	5.95	5.95	60.0	–	–	–	5.68	5.95	58.4	0.101	5.950	0.0	–	0.0
CMg_2	TXX	$P\bar{3}m1(164)$	–	–	7.16	7.16	59.6	–	–	–	–	–	–	2.292	3.812	0.0	–	–
CCa_2	TXX	$P\bar{3}m1(164)$	–	–	7.94	7.94	58.9	–	–	–	–	–	–	1.278	3.176	0.0	–	–
CBa_2	TXX	$P\bar{3}m1(164)$	–	–	8.49	8.49	59.8	–	–	–	–	–	–	1.533	2.727	0.0	–	–
$SiBe_2$	TXX	$Cmme(67)$	–	–	7.70	7.03	29.8	–	–	–	–	–	–	2.089	5.750	0.0	–	–
$SiCa_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.44	9.44	59.8	–	–	–	9.41	9.41	60.1	0.000	2.665	0.0	–	0.0
$SiSr_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.90	9.90	59.6	–	–	–	9.84	9.84	60.0	0.003	2.382	0.0	–	0.0
$SiBa_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.28	10.27	59.0	–	–	–	10.14	10.14	60.1	0.013	1.590	0.0	–	0.0
$GeBe_2$	HPT	$P6mm(183)$	$Pmn2_1(31)$	$Pmmn(59)$	7.51	7.53	60.0	6.45	6.45	47.0	7.59	7.34	58.9	0.620	0.717	0.0	0.0	0.0
$GeMg_2$	PTX	$P\bar{3}m1(164)$	–	$Pmmn(59)$	8.89	8.90	59.6	–	–	–	9.01	8.04	55.4	0.432	1.688	0.0	–	0.0
$GeCa_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.50	9.50	59.6	–	–	–	9.43	9.44	60.1	0.005	2.573	0.0	–	0.0
$GeSr_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.92	9.92	59.6	–	–	–	9.86	9.87	59.9	0.003	2.266	0.0	–	0.0
$GeBa_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.28	10.28	59.2	–	–	–	10.16	10.16	60.2	0.010	1.539	0.0	–	0.0
$SnBe_2$	HXX	–	$Pma2(28)$	–	–	–	–	7.19	8.34	30.2	–	–	–	4.465	4.815	–	0.0	–
$SnCa_2$	TPH	$P\bar{3}m1(164)$	$P4/mmm(123)$	$P\bar{3}m1(164)$	10.12	10.12	60.0	7.62	10.79	44.8	10.11	10.11	60.0	0.018	0.590	0.0	0.0	0.0
$SnSr_2$	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.51	10.53	60.0	–	–	–	10.49	10.54	60.1	0.070	2.162	0.0	–	0.0
$SnBa_2$	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.86	10.91	59.6	–	–	–	10.95	10.84	59.7	0.029	1.678	0.0	–	0.0
$PbBe_2$	PTX	$P6mm(183)$	–	$P6mm(183)$	8.03	8.03	60.0	–	–	–	8.03	8.03	60.0	0.000	6.908	0.0	–	0.0
$PbCa_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.26	10.26	59.7	–	–	–	10.22	10.21	60.0	0.006	2.093	0.0	–	0.0
$PbSr_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.69	10.68	59.7	–	–	–	10.64	10.63	59.9	0.004	1.946	0.0	–	0.0
$PbBa_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	11.06	11.04	59.4	–	–	–	10.96	10.94	59.7	0.007	1.629	0.0	–	0.0

Table 39: List of XIV-XII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CCd_2	THX	$P2_1/m(11)$	$Pmn2_1(31)$	–	7.22	6.86	58.1	6.80	6.80	52.1	–	–	–	0.346	2.386	0.0	0.0	–
$GeCd_2$	HTX	$P\bar{3}m1(164)$	$Amm2(38)$	–	9.08	9.08	59.8	8.87	8.84	38.0	–	–	–	0.761	0.863	0.0	0.0	–
$SnHg_2$	HXX	–	$P2/m(10)$	–	–	–	–	10.65	13.41	26.7	–	–	–	2.336	3.721	–	0.0	–

Table 40: List of XIV-XIII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CB_2	TPX	$P1(2)$	–	$P1(1)$	5.21	5.53	36.1	–	–	–	5.28	6.63	83.9	0.085	3.588	0.0	–	0.0
CTl_2	TXX	$P3m1(156)$	–	–	7.80	7.80	59.6	–	–	–	–	–	–	1.855	2.813	0.0	–	–
SiB_2	HTP	$Cm(8)$	$C2(5)$	$P\bar{1}(2)$	7.35	7.35	48.3	6.88	6.87	43.4	5.96	7.86	60.7	0.471	0.528	0.0	0.0	0.0
$SiAl_2$	HXX	–	$Pmn2_1(31)$	–	–	–	–	7.52	7.52	41.7	–	–	–	2.678	4.125	–	0.0	–
$GeAl_2$	HXX	–	$Amm2(38)$	–	–	–	–	8.11	8.10	39.7	–	–	–	1.794	2.666	–	0.0	–
$GeIn_2$	HXX	–	$Pm(6)$	–	–	–	–	8.81	8.97	40.7	–	–	–	0.867	0.879	–	0.0	–
$GeTl_2$	HXX	–	$Pm(6)$	–	–	–	–	8.49	7.08	51.7	–	–	–	1.926	1.934	–	0.0	–
$SnAl_2$	PXX	–	–	$P1(1)$	–	–	–	–	–	–	6.54	6.69	55.2	3.860	5.502	–	–	0.0
$SnIn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.54	9.31	39.1	–	–	–	1.481	1.499	–	0.0	–
$PbIn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.90	9.90	38.4	–	–	–	1.235	1.498	–	0.0	–
$PbTl_2$	HXX	–	$P2/m(10)$	–	–	–	–	12.44	9.42	33.2	–	–	–	2.366	3.528	–	0.0	–

Table 41: List of XIV-XIV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CC_2	HXX	–	$Cm(8)$	–	–	–	–	4.27	4.94	30.1	–	–	–	4.542	4.575	–	0.0	–
CSi_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	7.72	8.38	74.2	1.633	1.697	–	–	0.0
CGe_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	6.25	6.26	60.0	6.19	6.19	60.0	–	–	–	0.382	1.232	0.0	0.0	–
CPb_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	7.28	7.29	59.9	7.15	7.16	59.8	–	–	–	0.592	3.316	0.0	0.0	–
$SiGe_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	7.45	7.45	60.0	–	–	–	0.902	1.448	–	0.0	–
$SiSn_2$	HPX	–	$P\bar{6}m2(187)$	$P\bar{1}(2)$	–	–	–	8.03	8.04	59.5	8.18	8.04	61.6	0.724	0.855	–	0.0	0.0
$SiPb_2$	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$C2/m(12)$	8.80	8.80	58.1	8.38	8.38	57.9	8.09	9.08	55.7	0.653	0.740	0.0	0.0	0.0
GeC_2	PXX	–	–	$P\bar{4}2_1m(113)$	–	–	–	–	–	–	6.49	6.48	90.0	2.928	5.387	–	–	0.0
$GeGe_2$	HPX	–	$P\bar{6}m2(187)$	$P1(1)$	–	–	–	7.72	7.73	60.0	8.18	6.15	69.2	0.126	1.722	–	0.0	0.0
$GeSn_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	8.21	8.23	60.0	–	–	–	0.915	1.077	–	0.0	–
$SnPb_2$	PHX	–	$P\bar{6}m2(187)$	$P\bar{1}(2)$	–	–	–	9.08	9.09	59.6	8.45	10.32	49.2	0.438	1.695	–	0.0	0.0
$PbGe_2$	TXX	$P\bar{1}(2)$	–	–	11.49	8.02	39.4	–	–	–	–	–	–	0.906	3.153	0.0	–	–

Table 42: List of XIV-XV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CP_2	HXX	–	$P1(1)$	–	–	–	–	5.87	5.85	60.9	–	–	–	1.045	5.705	–	0.0	–
CBi_2	HXX	–	$Cm(8)$	–	–	–	–	7.08	6.99	75.4	–	–	–	3.044	7.253	–	0.0	–
SiP_2	PHX	–	$Cm(8)$	$P2/c(13)$	–	–	–	7.60	7.60	51.1	7.44	8.45	41.2	0.713	3.531	–	0.0	0.0
PbN_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	8.61	8.11	80.3	17.363	17.365	–	–	0.0

Table 43: List of XIV-XVI

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CS_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	11.20	10.63	100.3	2.451	2.971	–	–	0.0
SiO_2	THP	$P\bar{3}m1(164)$	$P\bar{3}m1(164)$	$Amm2(38)$	5.41	5.41	60.0	5.41	5.41	60.0	8.79	4.95	92.6	0.010	0.562	0.0	0.0	0.0
SiS_2	THX	$P\bar{3}m1(164)$	$P\bar{4}m2(115)$	–	6.62	6.62	60.0	9.57	6.78	45.1	–	–	–	0.016	2.884	0.0	0.0	–
GeO_2	THX	$P\bar{3}m1(164)$	$P\bar{3}m1(164)$	–	5.81	5.81	60.0	5.81	5.81	60.0	–	–	–	0.005	2.317	0.0	0.0	–
$GeSe_2$	HTX	$P\bar{3}m1(164)$	$C222(21)$	–	7.28	7.28	59.7	7.47	7.47	78.8	–	–	–	0.394	1.030	0.0	0.0	–
$GeTe_2$	TPX	$P\bar{3}m1(164)$	–	$P\bar{1}(2)$	7.84	7.84	59.0	–	–	–	9.44	9.40	69.4	0.284	0.953	0.0	–	0.0
SnO_2	PXX	–	–	$P\bar{3}m1(164)$	–	–	–	–	–	–	6.18	6.19	60.1	2.221	2.222	–	–	0.0
SnS_2	TXX	$P\bar{3}m1(164)$	–	–	7.46	7.46	60.0	–	–	–	–	–	–	1.498	3.010	0.0	–	–
PbO_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	6.88	6.88	60.0	–	–	–	6.88	6.88	59.9	0.006	4.286	0.0	–	0.0
PbS_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	8.63	8.17	84.5	2.214	2.219	–	–	0.0
$PbSe_2$	PXX	–	–	$P1(1)$	–	–	–	–	–	–	10.24	8.22	73.1	1.315	3.941	–	–	0.0

Table 44: List of XIV-XVII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CBr_2	PTH	$P1(1)$	$Pmn2_1(31)$	$Pc(7)$	8.51	8.37	66.6	8.16	8.17	72.3	10.68	10.70	103.8	0.047	0.084	0.0	0.0	0.0
$SiCl_2$	TPH	$P\bar{1}(2)$	$Amm2(38)$	$P\bar{1}(2)$	7.11	9.49	72.3	8.64	8.69	86.9	8.82	9.42	93.9	0.153	0.713	0.0	0.0	0.0
$SiBr_2$	TPX	$P\bar{1}(2)$	–	$P1(1)$	9.79	7.24	65.0	–	–	–	8.55	9.41	88.0	0.336	1.155	0.0	–	0.0
SiI_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{1}(2)$	8.37	8.37	60.4	–	–	–	10.77	8.54	91.5	0.482	0.976	0.0	–	0.0
$GeCl_2$	TPX	$P\bar{3}m1(164)$	–	$P1(1)$	7.86	7.86	60.6	–	–	–	8.29	8.29	79.8	0.279	0.979	0.0	–	0.0
$GeBr_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	8.10	8.10	60.6	–	–	–	8.16	7.06	90.0	0.045	1.381	0.0	–	0.0
$SnCl_2$	TPX	$P2_1/m(11)$	–	$P2_1/m(11)$	8.91	8.91	57.2	–	–	–	8.91	8.94	57.1	0.024	1.262	0.0	–	0.0
$SnBr_2$	TPX	$P\bar{3}m1(164)$	–	$P\bar{1}(2)$	8.77	8.77	59.9	–	–	–	8.88	8.41	75.8	0.806	1.045	0.0	–	0.0
SnI_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.18	9.18	59.7	–	–	–	9.14	9.12	59.8	0.004	0.937	0.0	–	0.0
PbF_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	8.05	8.06	59.8	–	–	–	8.06	8.07	59.6	0.013	1.893	0.0	–	0.0
$PbCl_2$	TPX	$P\bar{3}m1(164)$	–	$Pmmn(59)$	8.81	8.81	59.9	–	–	–	8.99	8.70	58.2	0.336	1.116	0.0	–	0.0
$PbBr_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	8.95	8.94	60.2	–	–	–	8.94	8.94	59.9	0.004	0.939	0.0	–	0.0
PbI_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.33	9.33	59.4	–	–	–	9.26	9.26	60.0	0.002	0.862	0.0	–	0.0

Table 45: List of XIV-TM

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CTi_2	TXX	$P\bar{3}m1(164)$	–	–	6.10	6.11	60.0	–	–	–	–	–	–	4.952	12.161	7.7	–	–
CV_2	TXX	$P\bar{3}m1(164)$	–	–	5.76	5.77	60.0	–	–	–	–	–	–	3.652	4.154	0.0	–	–
CCr_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	5.62	5.65	59.8	5.27	5.26	59.8	–	–	–	0.352	7.427	0.0	0.0	–
CNi_2	TXX	$P\bar{3}m1(164)$	–	–	5.80	5.80	59.7	–	–	–	–	–	–	2.230	2.701	0.0	–	–
CY_2	THX	$P\bar{3}m1(164)$	$P\bar{3}m1(164)$	–	7.10	7.11	60.1	7.10	7.11	60.1	–	–	–	0.003	5.500	0.0	0.0	–
CNb_2	TXX	$P\bar{3}m1(164)$	–	–	6.25	6.26	60.0	–	–	–	–	–	–	3.403	8.561	0.0	–	–
CMo_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.73	5.71	59.6	–	–	–	0.933	6.554	–	0.0	–
CTc_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	6.57	5.77	48.7	1.882	2.940	–	–	0.0
CRu_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.55	5.56	59.5	–	–	–	1.540	3.671	–	0.0	–
CPd_2	TXX	$P\bar{3}m1(164)$	–	–	6.24	6.24	59.9	–	–	–	–	–	–	1.217	1.591	0.0	–	–
CAg_2	HTX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	6.42	6.43	59.6	6.13	6.11	59.7	–	–	–	0.322	0.848	0.0	0.0	–
CHf_2	TXX	$P\bar{3}m1(164)$	–	–	6.42	6.43	60.1	–	–	–	–	–	–	6.411	8.695	0.0	–	–
CTa_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{1}(2)$	6.16	6.16	59.9	–	–	–	7.15	5.86	54.3	0.107	3.898	0.0	–	0.0
CW_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.72	5.71	59.8	–	–	–	1.818	3.061	–	0.0	–
CRe_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.58	5.57	60.0	–	–	–	1.894	5.864	–	0.0	–
CPt_2	HXX	–	$Cm(8)$	–	–	–	–	5.73	5.37	74.5	–	–	–	1.432	2.786	–	0.0	–
$SiTi_2$	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	7.96	8.13	37.9	1.712	3.520	–	–	0.0
$SiCr_2$	HXX	–	$Cmmm(65)$	–	–	–	–	4.84	6.22	49.9	–	–	–	2.504	5.007	–	0.0	–
$SiZr_2$	HPT	$C2/m(12)$	$Cmmm(65)$	$P\bar{1}(2)$	7.94	8.03	59.0	5.96	7.48	51.1	6.72	7.11	64.7	0.030	0.736	0.0	0.0	0.0
$SiPd_2$	HTP	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	7.11	7.08	48.2	6.11	6.11	59.7	7.15	7.20	59.7	0.083	0.668	0.0	0.0	0.0
$SiPt_2$	THX	$C2/m(12)$	$P\bar{6}m2(187)$	–	6.46	6.49	52.7	5.96	6.44	57.4	–	–	–	0.390	1.688	0.0	0.0	–
$GeCr_2$	THX	$P2_1/m(11)$	$P4/mmm(123)$	–	7.43	7.87	58.0	5.95	8.44	44.8	–	–	–	0.593	2.554	31.9	32.5	–
$GePd_2$	PTH	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	7.57	7.59	45.3	6.11	6.11	59.9	5.78	7.27	66.1	0.230	0.630	0.0	0.0	0.0
$GePt_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.95	5.97	60.1	–	–	–	0.991	2.490	–	0.0	–
$GeAu_2$	THX	$P2_1/m(11)$	$Pmn2_1(31)$	–	7.84	7.85	42.0	7.78	7.78	42.5	–	–	–	0.120	1.981	0.0	0.0	–
SnV_2	HXX	–	$P\bar{1}(2)$	–	–	–	–	5.42	9.17	39.5	–	–	–	11.665	12.496	–	0.0	–
$SnCr_2$	HTX	$P2_1/m(11)$	$C2/m(12)$	–	8.19	8.23	45.0	7.40	8.58	44.3	–	–	–	0.589	1.785	34.3	33.5	–
SnY_2	PXX	–	–	$Cmme(67)$	–	–	–	–	–	–	8.74	5.79	70.5	2.673	3.095	–	–	0.7
$PbSc_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	8.07	6.17	67.4	2.664	6.488	–	–	0.0

Table 46: List of XV-I

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
NLi_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	6.31	6.33	59.6	–	–	–	6.28	6.31	60.0	0.001	1.793	4.0	–	4.0
NNa_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.55	7.57	59.3	–	–	–	7.53	7.54	59.5	0.044	1.432	4.0	–	4.0
NK_2	TXX	$P\bar{3}m1(164)$	–	–	8.68	8.68	58.5	–	–	–	–	–	–	0.972	3.156	4.0	–	–
NRb_2	TXX	$P\bar{3}m1(164)$	–	–	9.12	9.12	57.1	–	–	–	–	–	–	0.850	1.934	4.1	–	–
NCs_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.48	9.47	56.1	–	–	–	9.40	9.14	58.2	0.029	1.020	4.1	–	4.0
PLi_2	TXX	$C2/m(12)$	–	–	8.24	8.01	42.9	–	–	–	–	–	–	1.238	3.853	0.0	–	–
PNa_2	TXX	$C2/m(12)$	–	–	9.39	9.01	43.0	–	–	–	–	–	–	0.865	2.517	0.0	–	–
PK_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.24	10.24	58.2	–	–	–	10.09	10.08	59.5	0.031	1.049	4.0	–	4.0
PRb_2	TPX	$P\bar{3}m1(164)$	–	$Pmmn(59)$	10.75	10.76	58.1	–	–	–	10.20	10.44	60.0	0.295	0.931	4.0	–	4.0
PCs_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	11.24	11.25	58.4	–	–	–	11.05	11.06	59.4	0.013	0.944	4.0	–	4.0
$AsRb_2$	HXX	–	$Cmmm(65)$	–	–	–	–	9.67	12.74	36.5	–	–	–	2.480	2.557	–	0.0	–
$AsCs_2$	TPX	$P\bar{3}m1(164)$	–	$Cm(8)$	11.37	11.31	59.6	–	–	–	11.44	11.32	58.7	0.116	0.844	4.0	–	4.0
$SbLi_2$	THX	$P\bar{1}(2)$	$Amm2(38)$	–	9.10	9.50	41.1	9.25	9.22	41.5	–	–	–	0.694	2.421	0.0	0.0	–
SbK_2	HPX	–	$Pm(6)$	$P\bar{3}m1(164)$	–	–	–	10.75	11.36	43.9	11.21	11.14	58.3	0.737	0.960	–	0.0	4.0
$SbRb_2$	HXX	–	$Amm2(38)$	–	–	–	–	10.78	11.48	45.7	–	–	–	1.195	2.554	–	0.0	–
$SbCs_2$	HXX	–	$Amm2(38)$	–	–	–	–	11.27	11.95	44.4	–	–	–	1.231	1.308	–	0.0	–
$BiLi_2$	THX	$P\bar{1}(2)$	$Amm2(38)$	–	10.13	9.04	39.2	9.50	9.45	41.8	–	–	–	0.802	2.355	0.0	0.0	–
BiK_2	HXX	–	$Pmmm(47)$	–	–	–	–	9.43	9.69	58.6	–	–	–	1.483	2.678	–	0.0	–
$BiRb_2$	HXX	–	$Pmmm(47)$	–	–	–	–	9.89	12.97	39.9	–	–	–	1.454	2.790	–	0.0	–
$BiCs_2$	HXX	–	$Pm(6)$	–	–	–	–	11.35	12.72	42.6	–	–	–	1.364	2.997	–	0.0	–

Table 47: List of XV-II

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
NBe_2	TPX	$C2/m(12)$	–	$P\bar{1}(2)$	4.94	4.95	64.7	–	–	–	7.86	7.35	40.1	0.427	2.340	0.0	–	0.0
NCa_2	TXX	$P\bar{3}m1(164)$	–	–	7.22	7.22	60.0	–	–	–	–	–	–	2.863	3.023	0.0	–	–
NSr_2	TXX	$P\bar{3}m1(164)$	–	–	7.71	7.71	60.0	–	–	–	–	–	–	2.541	4.094	0.0	–	–
PBe_2	PXX	–	–	$P3m1(156)$	–	–	–	–	–	–	3.99	6.92	90.0	2.887	4.350	–	–	0.0
PCa_2	PTX	$P\bar{3}m1(164)$	–	$C2/m(12)$	8.42	8.42	59.9	–	–	–	8.45	8.47	59.9	0.082	1.612	0.0	–	0.0
PSr_2	PTX	$P\bar{3}m1(164)$	–	$P2_1/m(11)$	8.94	8.94	59.4	–	–	–	8.93	8.92	59.7	0.005	1.668	0.0	–	0.0
PBa_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.32	9.31	59.4	–	–	–	9.26	12.25	40.9	0.103	1.678	0.0	–	2.6
$AsCa_2$	PTX	$P\bar{3}m1(164)$	–	$Cm(8)$	8.66	8.68	59.8	–	–	–	8.71	8.73	59.6	0.154	1.572	0.0	–	0.0
$AsSr_2$	PTX	$P\bar{3}m1(164)$	–	$P2_1/m(11)$	9.11	9.12	60.0	–	–	–	9.13	9.21	59.6	0.033	1.587	0.0	–	1.8
$AsBa_2$	TPX	$P\bar{3}m1(164)$	–	$P2_1/m(11)$	9.46	9.52	60.2	–	–	–	9.67	9.56	59.2	0.018	1.636	0.0	–	0.1
$SbCa_2$	PTX	$C2/m(12)$	–	$C2/m(12)$	9.29	9.28	60.5	–	–	–	9.38	9.31	59.7	0.075	1.341	0.0	–	1.4
$SbSr_2$	PTX	$C2/m(12)$	–	$C2/m(12)$	9.82	9.78	60.4	–	–	–	9.78	9.90	59.3	0.004	1.210	0.0	–	0.0
$SbBa_2$	TXX	$P\bar{3}m1(164)$	–	–	10.03	10.07	59.9	–	–	–	–	–	–	1.313	6.828	0.0	–	–
$BiBe_2$	PTX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	5.67	7.92	66.9	–	–	–	5.31	8.06	53.2	0.032	10.589	0.0	–	0.0
$BiCa_2$	TPX	$C2/m(12)$	–	$C2/m(12)$	9.52	9.42	59.6	–	–	–	9.41	9.44	60.7	0.001	1.141	0.0	–	0.0
$BiSr_2$	TPX	$C2/m(12)$	–	$P\bar{1}(2)$	10.03	9.93	59.8	–	–	–	9.92	10.01	59.9	0.009	1.115	0.0	–	0.0
$BiBa_2$	TPX	$P\bar{3}m1(164)$	–	$P2_1/m(11)$	10.20	10.20	59.7	–	–	–	10.36	10.18	60.7	0.022	1.152	0.0	–	0.0

Table 48: List of XV-XII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
PCd_2	HPX	–	$Aem2$(39)	$C2/m$(12)	–	–	–	7.24	7.25	63.0	8.33	11.24	55.2	0.111	1.459	–	0.0	0.0
$SbCd_2$	PXX	–	–	$P2/c$(13)	–	–	–	–	–	–	11.86	9.43	39.4	1.297	3.037	–	–	0.0
$BiHg_2$	HXX	–	$Amm2$(38)	–	–	–	–	10.97	10.95	33.0	–	–	–	0.957	1.721	–	0.0	–

Table 49: List of XV-XIII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
NAl_2	HXX	–	$Pmn2_1(31)$	–	–	–	–	5.34	5.34	65.7	–	–	–	3.125	4.334	–	0.0	–
PAl_2	PHX	–	$P1(1)$	$P2/c(13)$	–	–	–	7.23	6.55	60.2	7.55	6.17	72.3	0.725	0.921	–	0.0	0.0
PTl_2	TPH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{1}(2)$	8.73	8.73	59.5	8.33	8.33	59.3	9.18	7.67	76.7	0.359	0.726	0.0	0.0	0.0
$SbIn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.02	9.00	43.2	–	–	–	0.937	3.263	–	0.0	–
$SbTl_2$	HPX	–	$Amm2(38)$	$P2/c(13)$	–	–	–	9.69	9.65	41.1	9.76	7.23	68.4	0.209	1.189	–	0.0	0.0
$BiAl_2$	PHT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P6/mmm(191)$	8.84	8.84	59.7	8.63	8.60	58.5	10.25	10.25	62.2	0.564	0.719	0.0	0.0	0.0
$BiIn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.32	9.28	42.6	–	–	–	1.375	2.254	–	0.0	–
$BiTl_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.88	9.86	41.5	–	–	–	1.495	1.525	–	0.0	–

Table 50: List of XV-XIV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
NC_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	5.22	5.51	86.1	5.134	10.406	–	–	0.0
NSi_2	HTP	$Pc(7)$	$Cm(8)$	$P1(1)$	5.53	5.65	60.7	5.63	5.62	59.9	8.28	7.51	59.9	0.007	0.722	0.0	0.0	0.0
NPb_2	HTP	$P\bar{3}m1(164)$	$Cm(8)$	$P2_1/m(11)$	6.97	6.97	59.6	6.82	7.08	61.1	8.87	8.87	47.5	0.027	0.306	0.0	0.0	0.0
PSi_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	8.81	8.81	49.0	1.687	4.190	–	–	0.0
PGe_2	PHT	$P2_1/m(11)$	$P\bar{6}m2(187)$	$Cm(8)$	6.75	6.75	59.4	7.03	7.40	58.4	8.92	8.89	52.0	0.002	0.320	0.0	0.0	0.0
PSn_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	7.39	7.39	59.6	7.52	7.52	59.9	–	–	–	0.222	1.592	0.0	0.0	–
PPb_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	7.71	7.72	59.6	7.93	7.92	59.4	–	–	–	0.271	1.080	0.0	0.0	–
$AsSn_2$	PTH	$P\bar{3}m1(164)$	$P3m1(156)$	$P\bar{1}(2)$	7.43	7.39	59.4	7.89	7.88	59.2	7.95	9.70	54.5	0.071	0.233	0.0	0.0	0.0
$BiSi_2$	PTX	$P\bar{1}(2)$	–	$P2_1/m(11)$	10.50	13.65	30.6	–	–	–	9.28	9.28	50.1	0.606	6.198	0.0	–	0.0
$BiGe_2$	PXX	–	–	$Pc(7)$	–	–	–	–	–	–	10.82	7.27	47.6	1.002	2.791	–	–	0.0
$BiPb_2$	THP	$P\bar{1}(2)$	$Pmn2_1(31)$	$P1(1)$	11.60	12.02	33.3	9.73	9.74	53.9	10.41	9.97	50.7	0.090	0.223	0.0	0.0	0.0

Table 51: List of XV-XV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
NBi_2	HTP	$P1(1)$	$Pc(7)$	$P1(1)$	7.90	6.84	53.8	6.58	7.43	59.5	11.59	10.80	32.0	0.405	0.811	0.0	0.0	0.0
PP_2	HPX	–	$P1(1)$	$P1(1)$	–	–	–	6.57	6.49	60.8	7.52	7.88	61.4	0.183	2.348	–	0.0	0.0
$SbBi_2$	PTX	$P1(1)$	–	$P1(1)$	9.16	9.21	41.9	–	–	–	9.81	9.91	67.2	0.195	2.661	0.0	–	0.0
BiP_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	9.70	7.16	67.1	1.029	10.019	–	–	0.0
$BiBi_2$	TPX	$P\bar{1}(2)$	–	$P1(1)$	8.12	12.03	72.0	–	–	–	8.98	12.04	56.4	0.133	2.147	0.0	–	0.0

Table 52: List of XV-XVI

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
PS_2	TXX	$P\bar{3}m1(164)$	–	–	6.59	6.59	60.0	–	–	–	–	–	–	1.396	1.559	0.0	–	–
PSe_2	TXX	$P\bar{3}m1(164)$	–	–	6.99	6.99	60.0	–	–	–	–	–	–	0.943	2.920	0.0	–	–
PTe_2	TXX	$P\bar{3}m1(164)$	–	–	7.50	7.51	59.8	–	–	–	–	–	–	1.708	1.971	0.0	–	–
AsS_2	TPX	$P\bar{3}m1(164)$	–	$P1(1)$	7.00	7.01	59.5	–	–	–	6.59	10.23	67.7	0.402	3.003	0.0	–	0.0
$AsSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.33	7.34	59.3	–	–	–	–	–	–	1.864	1.925	0.0	–	–
$AsTe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.81	7.78	58.8	–	–	–	–	–	–	1.290	1.502	0.0	–	–
SbS_2	TPX	$P\bar{3}m1(164)$	–	$P1(1)$	7.58	7.58	59.7	–	–	–	12.71	6.94	63.5	0.467	2.805	0.0	–	0.0
$SbSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.84	7.84	59.6	–	–	–	–	–	–	0.925	2.376	0.0	–	–
$SbTe_2$	TXX	$P\bar{3}m1(164)$	–	–	8.33	8.32	58.5	–	–	–	–	–	–	1.259	1.772	0.0	–	–
BiO_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	7.52	6.43	59.3	0.895	3.859	–	–	0.0
BiS_2	PTX	$P\bar{3}m1(164)$	–	$P2_1/m(11)$	7.87	7.86	59.6	–	–	–	9.95	8.55	63.7	0.397	2.636	0.0	–	0.0
$BiSe_2$	PXX	–	–	$Cm(8)$	–	–	–	–	–	–	8.04	9.24	64.0	0.884	2.750	–	–	0.0
$BiTe_2$	THX	$P\bar{3}m1(164)$	$P1(1)$	–	8.59	8.59	56.1	9.56	10.21	51.3	–	–	–	0.370	0.993	0.0	0.0	–

Table 53: List of XV-XVII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
PCl_2	THX	$P1(2)$	$Pc(7)$	–	8.05	10.81	55.7	9.58	7.78	60.3	–	–	–	0.248	3.548	0.0	0.0	–
PI_2	HXX	–	$P2/m(10)$	–	–	–	–	9.55	9.95	51.9	–	–	–	2.502	2.885	–	0.0	–
$SbBr_2$	HXX	–	$Pm(6)$	–	–	–	–	8.58	8.89	55.8	–	–	–	2.203	2.925	–	0.0	–
SbI_2	HXX	–	$Pm(6)$	–	–	–	–	9.45	9.00	56.4	–	–	–	1.739	2.914	–	0.0	–
$BiCl_2$	HXX	–	$Pm(6)$	–	–	–	–	8.48	7.95	64.7	–	–	–	1.887	2.316	–	0.0	–
$BiBr_2$	HXX	–	$Pm(6)$	–	–	–	–	8.66	9.05	54.8	–	–	–	1.745	2.808	–	0.0	–
BiI_2	HXX	–	$Pm(6)$	–	–	–	–	9.05	8.79	62.4	–	–	–	0.896	1.507	–	0.0	–

Table 54: List of XV-TM

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
NTi_2	TXX	$P\bar{3}m1(164)$	–	–	5.93	5.95	60.1	–	–	–	–	–	–	3.872	9.483	4.7	–	–
NV_2	TXX	$P\bar{3}m1(164)$	–	–	5.75	5.76	60.0	–	–	–	–	–	–	1.010	1.398	0.0	–	–
NCr_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	5.67	5.67	60.7	5.25	5.22	59.6	–	–	–	0.144	3.984	7.2	0.0	–
NNi_2	TPX	$P\bar{3}m1(164)$	–	$Cmmm(65)$	5.64	5.65	59.5	–	–	–	9.50	9.50	33.3	0.040	0.850	0.0	–	0.0
NY_2	THX	$P\bar{3}m1(164)$	$P\bar{3}m1(164)$	–	6.89	6.90	60.1	6.89	6.89	60.0	–	–	–	0.002	7.381	0.0	0.0	–
NZr_2	TXX	$P\bar{3}m1(164)$	–	–	6.46	6.48	60.1	–	–	–	–	–	–	3.576	9.888	0.0	–	–
NNb_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	6.29	6.29	60.1	5.86	5.84	59.9	–	–	–	0.283	4.541	0.0	0.0	–
NPd_2	PXX	–	–	$P2/c(13)$	–	–	–	–	–	–	9.92	10.99	28.8	2.012	2.055	–	–	0.0
NHf_2	TXX	$P\bar{3}m1(164)$	–	–	6.34	6.36	60.1	–	–	–	–	–	–	3.563	4.401	0.0	–	–
NTa_2	HTX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	6.16	6.17	60.0	5.79	5.78	59.9	–	–	–	0.657	2.060	0.0	0.0	–
NOs_2	HXX	–	$Pmc2_1(26)$	–	–	–	–	5.43	7.21	41.2	–	–	–	2.289	3.111	–	0.0	–
NIr_2	HXX	–	$Pmn2_1(31)$	–	–	–	–	5.28	5.44	59.1	–	–	–	1.975	4.578	–	0.0	–
NPt_2	HXX	–	$Pmn2_1(31)$	–	–	–	–	5.85	5.39	57.2	–	–	–	1.617	2.099	–	0.0	–
PSc_2	PTX	$P2_1/m(11)$	–	$P2_1/m(11)$	7.57	7.30	61.2	–	–	–	7.55	7.30	61.2	0.000	2.459	0.0	–	0.0
PTi_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	7.28	6.79	62.1	0.856	3.023	–	–	0.0
PV_2	TXX	$P2_1/m(11)$	–	–	6.91	6.13	63.4	–	–	–	–	–	–	3.931	5.400	0.0	–	–
PCr_2	TPX	$P2_1/m(11)$	–	$Pmmn(59)$	7.17	7.04	60.5	–	–	–	6.76	7.40	56.7	0.187	2.486	27.8	–	27.4
PMn_2	TXX	$P2_1/m(11)$	–	–	6.78	6.77	57.9	–	–	–	–	–	–	2.465	6.119	23.4	–	–
PFe_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	7.94	7.94	60.0	5.69	5.67	59.9	–	–	–	0.202	1.151	18.0	11.8	–
PCo_2	TXX	$P2_1/m(11)$	–	–	6.46	6.46	47.9	–	–	–	–	–	–	2.829	4.078	7.8	–	–
PNi_2	PTX	$P2_1/m(11)$	–	$P2_1/m(11)$	6.63	6.63	58.5	–	–	–	7.00	6.53	57.0	0.214	2.323	0.0	–	0.0
PY_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.63	7.63	60.0	–	–	–	7.64	7.63	60.0	0.037	2.802	0.0	–	0.0
PNb_2	TXX	$P2_1/m(11)$	–	–	6.68	7.58	63.8	–	–	–	–	–	–	2.057	4.823	0.0	–	–
PMo_2	TXX	$P2_1/m(11)$	–	–	7.24	7.24	49.2	–	–	–	–	–	–	3.085	3.334	0.0	–	–
PTc_2	TXX	$P2_1/m(11)$	–	–	7.10	5.63	66.6	–	–	–	–	–	–	3.599	7.906	0.0	–	–
PRu_2	TXX	$P2_1/m(11)$	–	–	7.02	7.02	47.1	–	–	–	–	–	–	1.103	4.425	0.0	–	–
PRh_2	PTX	$P2_1/m(11)$	–	$Pmmn(59)$	7.21	6.95	58.7	–	–	–	9.06	7.11	38.3	0.760	1.307	0.0	–	0.0
PPd_2	PTX	$P2_1/m(11)$	–	$P\bar{1}(2)$	7.19	7.19	60.5	–	–	–	7.29	7.27	56.1	0.089	1.098	0.0	–	0.0
PAg_2	HPX	–	$P2/c(13)$	$Cm(8)$	–	–	–	7.99	7.19	43.5	7.91	8.54	61.8	0.677	1.887	–	0.0	0.0
PHf_2	PTX	$P2_1/m(11)$	–	$P2_1/m(11)$	7.69	7.70	52.4	–	–	–	7.83	6.91	63.8	0.077	1.660	0.0	–	0.0
PPt_2	HTP	$P2_1/m(11)$	$Pmn2_1(31)$	$Pc(7)$	6.86	6.86	49.2	6.44	6.44	53.1	9.12	9.79	43.4	0.060	0.541	0.0	0.0	0.0
$AsSc_2$	TPX	$P2_1/m(11)$	–	$P2_1/m(11)$	7.89	7.47	61.3	–	–	–	7.97	7.52	61.6	0.008	2.161	0.0	–	0.0
$AsTi_2$	HXX	–	$P2/c(13)$	–	–	–	–	6.16	8.05	48.4	–	–	–	5.888	8.074	–	1.9	–
AsV_2	TXX	$P2_1/m(11)$	–	–	6.21	6.96	62.8	–	–	–	–	–	–	7.718	8.634	0.0	–	–
$AsCr_2$	TXX	$P\bar{1}(2)$	–	–	7.05	7.27	60.7	–	–	–	–	–	–	2.208	4.659	15.9	–	–
$AsZr_2$	TPX	$P2_1/m(11)$	–	$P2_1/m(11)$	8.17	8.22	51.8	–	–	–	7.26	8.15	63.3	0.078	2.960	0.0	–	0.0
$AsPd_2$	HTP	$C2/m(12)$	$Pmn2_1(31)$	$P\bar{3}m1(164)$	8.55	8.54	40.6	7.31	6.09	65.1	8.60	8.60	59.4	0.242	0.782	0.0	0.0	0.0
$AsHf_2$	PTX	$P2_1/m(11)$	–	$P2_1/m(11)$	6.99	8.10	64.3	–	–	–	8.14	8.16	50.3	0.155	2.724	0.0	–	0.0
SbV_2	HXX	–	$Pmn2_1(31)$	–	–	–	–	7.55	7.53	47.0	–	–	–	4.077	4.090	–	0.0	–
$SbPd_2$	HXX	–	$Pmn2_1(31)$	–	–	–	–	7.79	7.78	48.3	–	–	–	0.833	1.455	–	0.0	–
$BiSc_2$	TXX	$P\bar{1}(2)$	–	–	8.76	8.31	62.9	–	–	–	–	–	–	1.271	3.748	1.8	–	–
BiV_2	HXX	–	$Pm(6)$	–	–	–	–	7.64	9.06	31.0	–	–	–	13.294	13.298	–	0.0	–
BiY_2	TPX	$P2_1/m(11)$	–	$Cm(8)$	9.36	8.46	63.0	–	–	–	9.48	8.47	55.8	0.565	1.703	0.0	–	1.7
$BiRe_2$	HXX	–	$Aem2(39)$	–	–	–	–	10.43	10.45	23.7	–	–	–	5.278	16.490	–	0.0	–

Table 55: List of XVI-I

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
OLi_2	TXX	$P\bar{3}m1(164)$	–	–	6.19	6.21	60.0	–	–	–	–	–	–	1.274	3.622	0.0	–	–
ONa_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{1}(2)$	7.52	7.53	59.4	–	–	–	9.67	9.07	41.9	0.756	2.577	0.0	–	0.0
OK_2	TPX	$P\bar{3}m1(164)$	–	$Pmmn(59)$	8.26	8.27	59.3	–	–	–	8.17	14.38	29.1	0.294	1.823	0.0	–	0.0
ORb_2	TXX	$P\bar{3}m1(164)$	–	–	8.36	8.36	59.7	–	–	–	–	–	–	1.533	1.866	0.0	–	–
OCs_2	PTX	$C2/m(12)$	–	$P\bar{3}m1(164)$	9.81	9.81	50.4	–	–	–	8.54	8.53	59.4	0.733	1.339	0.0	–	0.0
SLi_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.89	7.87	59.8	–	–	–	7.86	7.86	59.9	0.025	2.651	0.0	–	0.0
SNa_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.01	9.02	59.5	–	–	–	9.02	9.03	59.6	0.033	2.464	0.0	–	0.0
SK_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.17	10.17	57.5	–	–	–	9.92	9.91	59.6	0.063	1.948	0.0	–	0.0
SRb_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.37	10.37	59.1	–	–	–	10.21	10.23	60.1	0.019	1.635	0.0	–	0.0
SCs_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.67	10.69	58.8	–	–	–	10.51	10.52	59.8	0.020	1.312	0.0	–	0.0
$SeLi_2$	TPX	$P\bar{3}m1(164)$	–	$P2_1/m(11)$	8.32	8.31	59.8	–	–	–	8.33	8.31	59.8	0.043	2.199	0.0	–	0.0
$SeNa_2$	TXX	$P\bar{3}m1(164)$	–	–	9.39	9.40	59.6	–	–	–	–	–	–	2.205	2.205	0.0	–	–
SeK_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.65	10.65	57.2	–	–	–	10.35	10.34	59.7	0.075	1.818	0.0	–	0.0
$SeRb_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.88	10.87	58.8	–	–	–	10.72	10.71	59.6	0.015	1.665	0.0	–	0.0
$SeCs_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	11.22	11.19	58.8	–	–	–	11.06	11.04	59.8	0.018	1.302	0.0	–	0.0
$TeLi_2$	PTX	$P\bar{3}m1(164)$	–	$P2_1/m(11)$	9.17	9.17	59.3	–	–	–	9.11	9.13	59.5	0.038	1.715	0.0	–	0.0
$TeNa_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.19	10.20	59.5	–	–	–	10.21	10.21	59.4	0.005	2.006	0.0	–	0.0
TeK_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	11.31	11.33	58.6	–	–	–	11.19	11.20	59.7	0.013	1.709	0.0	–	0.0
$TeRb_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	11.86	11.88	58.1	–	–	–	11.64	11.67	59.6	0.032	1.515	0.0	–	0.0
$TeCs_2$	TXX	$P\bar{3}m1(164)$	–	–	12.04	12.14	59.4	–	–	–	–	–	–	1.228	2.144	0.0	–	–

Table 56: List of XVI-II

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
OBe_2	TXX	$P2_1/m(11)$	–	–	5.17	4.95	58.5	–	–	–	–	–	–	1.114	3.420	0.0	–	–
OMg_2	PTX	$P\bar{3}m1(164)$	–	$Cmmm(65)$	6.14	6.14	59.2	–	–	–	11.46	11.46	29.6	0.770	1.747	0.0	–	0.0
OCa_2	PXX	–	–	$P2/c(13)$	–	–	–	–	–	–	13.93	12.08	24.9	1.945	2.182	–	–	0.0
OSr_2	PXX	–	–	$Pccm(49)$	–	–	–	–	–	–	13.71	12.22	27.0	1.619	2.157	–	–	0.0
OBa_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	9.20	9.19	59.2	2.125	2.135	–	–	0.0
SBe_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	6.83	5.30	90.0	2.333	4.987	–	–	0.0
SCa_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	7.82	7.81	60.0	7.73	7.73	59.8	–	–	–	0.798	2.382	0.4	0.0	–
SSr_2	TXX	$P\bar{3}m1(164)$	–	–	8.35	8.35	59.7	–	–	–	–	–	–	0.977	2.337	0.0	–	–
SBa_2	TXX	$P\bar{3}m1(164)$	–	–	8.84	8.84	59.6	–	–	–	–	–	–	1.845	2.529	0.0	–	–
$SeBe_2$	PXX	–	–	$P1(1)$	–	–	–	–	–	–	5.42	7.01	69.5	1.058	1.540	–	–	0.0
$SeCa_2$	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	8.06	8.06	60.0	8.00	7.99	59.8	–	–	–	0.534	1.206	0.0	0.0	–
$SeSr_2$	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	8.59	8.58	59.5	8.53	8.53	59.4	–	–	–	0.726	2.660	0.0	0.0	–
$SeBa_2$	TXX	$P\bar{3}m1(164)$	–	–	9.11	9.10	59.5	–	–	–	–	–	–	1.546	1.697	0.0	–	–
$TeCa_2$	THX	$P2_1/m(11)$	$P\bar{6}m2(187)$	–	8.45	9.16	62.8	8.41	8.37	59.7	–	–	–	0.767	0.919	0.0	0.0	–
$TeSr_2$	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	8.91	8.95	60.3	8.94	8.88	59.3	–	–	–	0.500	2.067	0.0	0.0	–

Table 57: List of XVI-XII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$TeCd_2$	PXX	–	–	$P2(3)$	–	–	–	–	–	–	10.08	12.42	49.0	1.789	1.844	–	–	0.0

Table 58: List of XVI-XIII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
OAl_2	HXX	–	$Pmn2_1(31)$	–	–	–	–	5.09	5.53	57.2	–	–	–	2.374	2.973	–	0.0	–
OIn_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	6.64	6.63	60.2	6.60	6.58	60.2	–	–	–	0.488	2.401	0.0	0.0	–
OTl_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	7.40	7.39	58.7	7.17	7.16	59.4	–	–	–	0.417	1.002	0.0	0.0	–
SAl_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	8.09	7.99	54.2	2.727	2.786	–	–	0.0
STl_2	TPH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	8.54	8.54	59.0	8.33	8.33	59.4	8.62	8.54	58.5	0.008	0.169	0.0	0.0	0.0
$SeIn_2$	HTX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	8.13	8.11	60.6	7.98	7.97	60.6	–	–	–	0.285	2.427	0.0	0.0	–
$SeTl_2$	PTH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	9.00	9.00	58.8	8.70	8.70	58.1	8.99	8.98	58.6	0.005	0.055	0.0	0.0	0.0
TeB_2	PXX	–	–	$P2/c(13)$	–	–	–	–	–	–	6.22	8.93	79.7	17.621	18.239	–	–	0.0
$TeTl_2$	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	9.79	9.80	58.4	9.28	9.32	58.4	9.76	9.77	58.2	0.032	0.034	0.0	0.0	0.0

Table 59: List of XVI-XIV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
OSi_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	6.67	7.90	67.9	1.102	2.497	–	–	0.0
OPb_2	TXX	$C222(21)$	–	–	7.28	6.85	57.6	–	–	–	–	–	–	1.078	4.459	0.0	–	–
SGe_2	HTP	$P1(1)$	$P1(1)$	$P1(1)$	6.73	6.89	60.9	6.72	6.90	60.6	7.33	8.51	78.8	0.002	0.771	0.0	0.0	0.0
SSn_2	TPH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P1(1)$	7.14	7.16	59.7	7.02	7.02	59.1	8.69	8.33	85.7	0.037	0.309	0.0	0.0	0.0
SPb_2	PHT	$P\bar{3}m1(164)$	$Pmmn(59)$	$P2_1/m(11)$	7.45	7.44	59.7	7.54	6.88	56.4	10.21	10.26	43.9	0.289	0.527	0.0	0.0	0.0
$SeSn_2$	PTX	$P2_1/m(11)$	–	$P1(1)$	7.46	7.46	59.0	–	–	–	8.39	9.21	80.6	0.327	0.868	0.0	–	0.0
$SePb_2$	PHT	$P2_1/m(11)$	$Pmmn(59)$	$P2_1/m(11)$	7.94	7.94	57.5	7.02	7.77	55.9	10.61	10.61	43.2	0.379	0.517	0.0	0.0	0.0
$TePb_2$	PHX	–	$Pc(7)$	$P\bar{1}(2)$	–	–	–	9.27	13.39	42.8	10.57	10.84	48.5	0.103	1.349	–	0.0	0.0

Table 60: List of XVI-XV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
SBi_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	9.73	10.66	56.2	1.536	1.745	–	–	0.0
$SeSb_2$	PTX	$P\bar{1}(2)$	–	$P1(1)$	7.56	7.90	59.6	–	–	–	11.69	10.10	42.7	0.546	2.176	0.0	–	0.0
$SeBi_2$	PXX	–	–	$P1(1)$	–	–	–	–	–	–	11.73	8.77	58.6	1.572	1.751	–	–	0.0

Table 61: List of XVI-XVI

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
SS_2	HXX	–	$Pc(7)$	–	–	–	–	8.20	11.18	43.5	–	–	–	2.451	2.703	–	0.0	–
SSe_2	HPX	–	$Pc(7)$	$P1(1)$	–	–	–	8.81	11.67	41.4	8.54	8.91	76.9	0.744	2.519	–	0.0	0.0
SeS_2	PTX	$P\bar{3}m1(164)$	–	$P1(1)$	7.14	7.14	60.3	–	–	–	9.50	8.02	80.9	0.729	4.000	0.0	–	0.0
$SeSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.47	7.47	60.3	–	–	–	–	–	–	0.859	2.830	0.0	–	–
TeS_2	TXX	$P\bar{3}m1(164)$	–	–	7.71	7.71	59.8	–	–	–	–	–	–	2.292	2.634	0.0	–	–
$TeSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.97	7.97	59.8	–	–	–	–	–	–	0.931	2.325	0.0	–	–
$TeTe_2$	TXX	$P\bar{3}m1(164)$	–	–	8.57	8.57	59.3	–	–	–	–	–	–	1.102	1.829	0.0	–	–

Table 62: List of XVI-XVII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
SCl_2	HTP	$P\bar{1}(2)$	$P1(1)$	$P2/c(13)$	7.47	8.27	78.4	7.16	9.40	96.0	9.96	10.57	96.2	0.379	0.641	0.0	0.0	0.0
SBr_2	THP	$P2_1/c(14)$	$Pm(6)$	$P1(1)$	8.48	8.48	73.3	7.93	8.36	65.1	11.15	11.13	72.1	0.222	0.350	0.0	0.0	0.0
SI_2	HPT	$P1(1)$	$Amm2(38)$	$P\bar{1}(2)$	7.91	9.57	75.7	7.96	9.56	64.8	9.98	12.93	55.3	0.019	0.038	0.0	0.0	0.0
$SeBr_2$	HXX	–	$P1(1)$	–	–	–	–	8.07	7.30	76.7	–	–	–	0.853	0.872	–	0.0	–
SeI_2	HTX	$P\bar{1}(2)$	$Cmmm(65)$	–	7.92	10.24	76.2	9.54	7.92	65.7	–	–	–	0.078	0.890	0.0	0.0	–

Table 63: List of XVI-TM

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
OSc_2	TXX	$P\bar{3}m1(164)$	–	–	6.38	6.39	60.0	–	–	–	–	–	–	0.915	3.979	4.8	–	–
OTi_2	HTX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	5.96	5.98	59.9	5.60	5.60	59.9	–	–	–	0.164	1.350	0.0	0.0	–
OV_2	HTP	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P2/c(13)$	5.32	5.30	59.9	5.32	5.31	59.1	10.12	8.59	28.5	0.555	0.671	0.0	0.0	0.0
OCr_2	HTP	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P2/c(13)$	5.74	5.73	59.9	5.08	5.08	59.8	10.96	10.98	28.8	0.403	0.650	29.1	0.0	31.9
OFe_2	PHT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$Cmmm(65)$	5.37	5.37	59.8	5.33	5.32	59.8	10.08	10.07	30.6	0.083	0.553	26.4	25.4	24.2
OY_2	PXX	–	–	$Pccm(49)$	–	–	–	–	–	–	11.90	10.49	27.8	0.988	0.991	–	–	0.0
OZr_2	THX	$P2_1/m(11)$	$P\bar{6}m2(187)$	–	6.46	6.45	57.9	6.13	6.13	60.0	–	–	–	0.613	1.683	0.0	0.0	–
ONb_2	HTX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	5.84	5.85	57.8	5.83	5.83	58.3	–	–	–	0.242	1.484	0.0	0.0	–
OMo_2	TXX	$P2_1/m(11)$	–	–	6.79	6.55	50.1	–	–	–	–	–	–	1.871	7.775	0.0	–	–
ORu_2	HPX	–	$P1(1)$	$Pc(7)$	–	–	–	5.02	5.38	56.6	9.62	9.32	30.4	0.143	0.846	–	0.0	0.0
OHf_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	5.03	8.57	91.0	2.913	3.990	–	–	0.0
OTa_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	7.81	7.79	59.9	0.937	1.474	–	–	0.0
OW_2	PHX	–	$Pmn2_1(31)$	$P1(1)$	–	–	–	5.19	5.19	62.2	8.22	5.88	57.5	0.128	2.842	–	0.0	0.0
OPt_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	7.29	7.30	98.4	1.894	1.908	–	–	0.0
OAu_2	THP	$P2_1/m(11)$	$Pmn2_1(31)$	$P2/c(13)$	6.46	6.46	54.4	6.45	6.46	54.6	6.26	10.81	73.5	0.035	0.733	0.0	0.0	0.0
SSc_2	TPH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P3m1(156)$	7.04	7.03	60.0	6.79	6.79	60.0	6.95	6.98	60.2	0.224	0.717	0.0	0.0	0.0
STi_2	PTX	$P2_1/m(11)$	–	$P2_1/m(11)$	6.56	7.28	63.1	–	–	–	6.57	7.29	63.1	0.014	3.411	0.0	–	0.0
SV_2	PTX	$P2_1/m(11)$	–	$P2_1/m(11)$	6.89	6.89	53.0	–	–	–	6.89	6.89	53.1	0.008	5.997	0.0	–	0.0
SY_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{1}(2)$	7.49	7.49	59.9	–	–	–	8.89	7.20	54.2	0.273	1.130	0.0	–	0.0
SZr_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	7.97	7.04	63.8	1.250	2.169	–	–	0.0
SNb_2	TXX	$P\bar{1}(2)$	–	–	7.56	7.30	50.3	–	–	–	–	–	–	1.868	3.667	0.0	–	–
STc_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	4.62	6.99	64.7	4.769	11.245	–	–	0.0
SAu_2	TXX	$P42_12(90)$	–	–	8.04	11.46	44.3	–	–	–	–	–	–	1.498	2.257	0.0	–	–
$SeSc_2$	TPH	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	8.11	8.12	52.2	6.98	6.97	60.0	8.12	8.12	52.1	0.003	0.776	0.0	0.0	0.0
SeV_2	TXX	$P\bar{1}(2)$	–	–	6.59	6.77	60.4	–	–	–	–	–	–	9.914	10.090	0.0	–	–
SeY_2	HTP	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	7.66	7.65	60.0	7.39	7.38	59.9	7.53	8.63	64.1	0.058	0.150	0.0	0.0	0.0
$SeZr_2$	PTX	$P2_1/m(11)$	–	$P2_1/m(11)$	8.16	8.15	52.1	–	–	–	7.17	8.16	63.9	0.023	3.252	0.0	–	0.0
$TeSc_2$	TPX	$P\bar{1}(2)$	–	$P2_1/m(11)$	7.64	8.55	63.8	–	–	–	8.62	7.54	63.9	0.150	2.466	0.5	–	0.0

Table 64: List of XVII-I

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
FLi_2	PHX	–	$Pmmn(59)$	$Cmmm(65)$	–	–	–	4.92	4.92	73.3	11.48	11.46	27.6	0.134	1.185	–	0.0	0.0
FNa_2	PTH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$Cmmm(65)$	7.04	7.03	59.0	6.84	6.85	59.1	13.89	13.93	26.9	0.347	0.787	0.0	0.0	0.0
FK_2	PTH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$Cmmm(65)$	8.42	8.42	56.0	8.30	8.30	55.6	16.17	16.20	27.0	0.070	0.574	0.0	0.0	0.0
FRb_2	PTH	$P\bar{3}m1(164)$	$C2/m(12)$	$Cmmm(65)$	8.94	8.93	55.9	10.25	10.22	46.2	17.12	17.14	27.1	0.007	0.138	0.0	0.0	0.0
ClK_2	TPH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	9.24	9.26	57.9	9.08	9.10	57.3	10.37	10.65	89.6	0.130	0.236	0.0	0.0	0.0
$ClRb_2$	THP	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P1(1)$	9.82	9.83	58.0	9.69	9.71	56.6	11.98	11.99	91.3	0.278	0.393	0.0	0.0	0.0
$ClCs_2$	TPH	$P\bar{3}m1(164)$	$Amm2(38)$	$P1(1)$	10.58	10.58	56.8	10.64	10.65	54.1	11.64	10.89	78.7	0.183	0.436	0.0	0.0	0.0
$BrLi_2$	TPH	$C2/m(12)$	$Pc(7)$	$P2_1/m(11)$	7.43	7.77	57.0	6.71	6.66	72.0	8.01	7.42	89.9	0.103	0.215	0.0	0.0	0.0
BrK_2	THP	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	9.59	9.57	58.4	9.58	9.55	56.4	11.19	11.15	90.5	0.245	0.281	0.0	0.0	0.0
$BrRb_2$	THP	$P\bar{3}m1(164)$	$Amm2(38)$	$P2_1/m(11)$	10.19	10.17	58.1	10.14	10.12	56.1	11.31	11.73	90.6	0.241	0.304	0.0	0.0	0.0
$BrCs_2$	THP	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{4}m2(115)$	10.65	10.61	59.4	10.61	10.59	57.1	13.20	13.24	90.0	0.309	0.629	0.0	0.0	0.0
IK_2	TPH	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P\bar{1}(2)$	9.84	9.86	59.0	10.00	9.98	56.2	11.61	12.07	90.0	0.041	0.189	0.0	0.0	0.0
IRb_2	HPX	–	$Amm2(38)$	$P1(1)$	–	–	–	10.57	10.55	55.9	13.18	12.60	89.9	0.072	0.937	–	0.0	0.0
ICs_2	THP	$P\bar{3}m1(164)$	$Amm2(38)$	$P1(1)$	10.99	10.96	58.9	11.22	11.18	55.7	12.27	12.09	74.1	0.245	0.271	0.0	0.0	0.0

Table 65: List of XVII-II

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
FSr_2	HTX	$P1(1)$	$P1(1)$	–	8.16	9.88	54.2	8.63	8.62	60.6	–	–	–	0.101	1.923	0.0	0.0	–
$ClCa_2$	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	7.63	7.62	59.7	7.59	7.59	59.7	–	–	–	0.303	1.497	0.0	0.0	–
$ClSr_2$	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	8.25	8.24	59.6	8.33	8.33	57.7	–	–	–	0.343	2.532	0.0	0.0	–
$ClBa_2$	TPH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$Pmna(53)$	8.71	8.71	59.9	8.57	8.57	59.8	12.62	7.36	90.0	0.026	0.085	0.0	0.0	0.9
$BrCa_2$	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	7.79	7.79	59.7	7.77	7.77	60.0	–	–	–	0.200	2.747	0.0	0.0	–
$BrSr_2$	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	8.38	8.38	59.6	8.30	8.30	59.7	–	–	–	0.198	1.454	0.0	0.0	–
$BrBa_2$	HTX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	8.85	8.85	59.8	8.72	8.72	59.7	–	–	–	0.055	3.475	0.0	0.0	–
ISr_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	8.54	8.55	59.8	8.57	8.57	59.0	–	–	–	0.115	1.645	0.0	0.0	–

Table 66: List of XVII-XII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
FCd_2	THX	$P\bar{3}m1$(164)	$P\bar{6}m2$(187)	–	6.19	6.19	58.3	6.26	6.25	56.7	–	–	–	0.085	1.061	0.0	0.0	–

Table 67: List of XVII-XIII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
FIn_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	6.56	6.56	60.2	6.54	6.54	60.1	–	–	–	0.072	1.818	0.0	0.0	–
FTl_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	7.19	7.19	58.3	7.08	7.07	59.0	–	–	–	0.183	2.788	0.0	0.0	–
$ClIn_2$	THP	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P1(1)$	7.02	7.02	60.6	6.97	6.98	60.4	10.11	7.62	85.3	0.043	0.467	0.0	0.0	0.0
$ClTl_2$	THX	$P\bar{3}m1(164)$	$Amm2(38)$	–	7.71	7.69	57.7	7.69	7.67	55.8	–	–	–	0.235	2.120	0.0	0.0	–
$BrAl_2$	PXX	–	–	$P2(3)$	–	–	–	–	–	–	6.99	7.56	83.1	5.015	5.034	–	–	0.0
$BrTl_2$	PTH	$P\bar{3}m1(164)$	$Amm2(38)$	$P\bar{1}(2)$	7.88	7.87	58.6	8.04	8.06	54.7	9.87	8.39	83.2	0.056	0.449	0.0	0.0	0.0

Table 68: List of XVII-XIV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$ClSn_2$	PHX	–	$Amm2(38)$	$P1(1)$	–	–	–	6.81	6.81	59.8	8.91	9.05	65.3	0.211	1.219	–	0.0	0.0
$ClPb_2$	PXX	–	–	$P1(1)$	–	–	–	–	–	–	6.71	13.42	46.4	1.535	1.646	–	–	0.0
$BrGe_2$	PXX	–	–	$P1(1)$	–	–	–	–	–	–	7.85	7.74	73.6	1.999	2.060	–	–	0.0
$BrSn_2$	PTX	$P2_1/m(11)$	–	$Pm(6)$	6.19	6.18	71.5	–	–	–	9.74	7.25	67.7	0.121	1.408	0.0	–	0.0
$BrPb_2$	PXX	–	–	$P1(1)$	–	–	–	–	–	–	10.47	9.88	38.8	1.434	2.317	–	–	0.0

Table 69: List of XVII-XV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
IN_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	9.18	9.72	78.0	21.899	22.768	–	–	0.0

Table 70: List of XVII-XVI

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$BrSe_2$	PHX	–	$P1(1)$	$P1(1)$	–	–	–	8.53	6.62	56.6	8.08	8.51	109.5	0.617	2.111	–	0.0	0.0
IS_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	11.21	9.66	71.1	4.600	5.349	–	–	1.9
ISe_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	9.35	12.58	70.5	4.298	4.658	–	–	0.0

Table 71: List of XVII-XVII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$ClCl_2$	PHX	–	$P1(1)$	$P2/c(13)$	–	–	–	10.28	6.52	94.6	10.76	10.84	98.2	0.715	2.022	–	0.0	0.0
$ClBr_2$	PHX	–	$P1(1)$	$P2/c(13)$	–	–	–	8.78	7.23	80.9	10.62	10.63	94.8	0.159	2.528	–	0.0	0.0
BrF_2	HTP	$P2/m(10)$	$P\bar{1}(2)$	$P\bar{1}(2)$	8.04	5.93	90.6	8.79	5.94	62.1	7.31	8.37	74.4	0.070	0.577	0.0	0.0	0.0
$BrCl_2$	PHT	$P\bar{1}(2)$	$P\bar{1}(2)$	$P1(1)$	8.01	8.38	80.5	8.06	8.01	70.2	11.19	11.29	102.7	0.218	0.228	0.0	0.0	0.0
$BrBr_2$	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	11.50	10.75	95.9	1.125	1.130	–	–	0.0
BrI_2	PXX	–	–	$Pc(7)$	–	–	–	–	–	–	13.24	11.46	66.2	1.177	3.073	–	–	0.0
ICl_2	THP	$P\bar{1}(2)$	$P1(1)$	$P\bar{1}(2)$	9.36	8.62	80.0	7.93	8.97	75.1	13.63	8.65	81.4	0.112	0.159	0.0	0.0	0.0
IBr_2	TPH	$P\bar{1}(2)$	$P1(1)$	$P1(1)$	9.08	9.40	76.7	8.93	9.22	78.3	10.74	10.83	87.9	0.019	0.075	0.0	0.0	0.0
II_2	PHT	$P\bar{1}(2)$	$P\bar{1}(2)$	$P2/m(10)$	9.69	9.61	84.7	9.73	9.58	62.4	11.74	13.03	94.1	0.444	0.501	0.0	0.0	0.0

Table 72: List of XVII-TM

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
FTa_2	PXX	–	–	$P1(2)$	–	–	–	–	–	–	5.99	5.71	62.9	10.357	10.429	–	–	0.0
FAu_2	PTH	$Pmmn(59)$	$Pmmn(59)$	$P2/m(10)$	4.95	4.95	72.4	5.86	4.96	53.7	13.06	5.77	72.8	0.662	0.666	0.0	0.0	0.0
$ClSc_2$	PXX	–	–	$P1(1)$	–	–	–	–	–	–	6.41	6.73	73.6	5.835	6.699	–	–	0.0
ClY_2	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P2_12_12(18)$	7.08	7.08	60.1	7.05	7.04	60.1	8.72	8.72	81.4	0.622	0.748	0.0	0.0	0.0
$BrSc_2$	PXX	–	–	$P1(1)$	–	–	–	–	–	–	6.24	6.51	79.3	6.190	7.243	–	–	0.0
$BrTi_2$	TXX	$Pmma(51)$	–	–	7.80	5.55	45.2	–	–	–	–	–	–	14.720	20.222	0.0	–	–
$BrHf_2$	THP	$P2_1/m(11)$	$Pm(6)$	$Pm(6)$	6.60	6.70	59.5	6.59	6.58	60.3	8.66	5.58	49.6	0.551	0.623	0.0	0.0	0.0
$BrRe_2$	PXX	–	–	$Cm(8)$	–	–	–	–	–	–	5.65	5.65	60.0	4.136	47.650	–	–	0.0

Table 73: List of TM-I

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
CrK_2	HXX	–	$P2_1/m(11)$	–	–	–	–	8.68	10.18	53.9	–	–	–	1.711	3.942	–	20.3	–
$CrCs_2$	THX	$P\bar{3}m1(164)$	$Amm2(38)$	–	11.35	11.40	58.3	11.95	11.92	48.4	–	–	–	0.599	2.505	22.1	21.2	–
$RhLi_2$	PTH	$P4/mmm(123)$	$P4/mmm(123)$	$C2/m(12)$	5.54	7.85	45.2	5.54	7.84	45.1	6.85	5.78	49.1	0.133	0.149	0.0	0.0	0.0
PdK_2	HPT	$P\bar{3}m1(164)$	$Pmmm(47)$	$P\bar{3}m1(164)$	10.58	10.59	57.8	8.38	11.28	41.7	10.26	10.28	59.7	0.480	0.512	0.0	0.0	0.0
$PdRb_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	10.86	10.89	58.4	–	–	–	10.62	10.64	60.2	0.019	1.091	0.0	–	0.0
$PdCs_2$	TXX	$P\bar{3}m1(164)$	–	–	10.85	10.91	59.8	–	–	–	–	–	–	0.882	2.308	0.0	–	–
AgK_2	THX	$C2/m(12)$	$Amm2(38)$	–	10.05	10.04	56.1	10.08	10.29	50.5	–	–	–	0.348	2.338	0.0	0.0	–
$AgCs_2$	TPH	$P\bar{3}m1(164)$	$Amm2(38)$	$Cm(8)$	11.02	11.02	60.0	10.98	10.94	54.6	15.91	15.99	38.2	0.267	0.523	0.0	0.0	0.0
$ReCs_2$	TXX	$C2/m(12)$	–	–	10.91	11.87	45.3	–	–	–	–	–	–	10.951	11.154	6.0	–	–
$OsCs_2$	HXX	–	$P2/c(13)$	–	–	–	–	12.42	9.66	40.3	–	–	–	5.639	5.702	–	8.2	–
PtK_2	TPX	$P\bar{3}m1(164)$	–	$Pmmn(59)$	10.23	10.22	59.1	–	–	–	9.82	10.05	59.2	0.380	1.658	0.0	–	0.0
$PtRb_2$	TPX	$P\bar{3}m1(164)$	–	$Pmmn(59)$	10.62	10.61	58.8	–	–	–	10.24	10.23	60.6	0.306	1.460	0.0	–	0.0
$PtCs_2$	THX	$P\bar{3}m1(164)$	$P\bar{3}m1(164)$	–	10.67	10.67	60.0	10.67	10.67	60.0	–	–	–	0.038	0.939	0.0	0.0	–
$AuNa_2$	THX	$P2_1/m(11)$	$Cmmm(65)$	–	9.75	7.58	48.7	7.50	10.43	42.6	–	–	–	0.527	3.404	0.0	0.0	–
AuK_2	PTH	$P\bar{3}m1(164)$	$Amm2(38)$	$P\bar{1}(2)$	9.75	9.76	59.6	10.01	10.08	50.6	9.73	11.17	51.1	0.142	0.621	0.0	0.0	0.0
$AuRb_2$	THP	$P\bar{3}m1(164)$	$Amm2(38)$	$P2_1/m(11)$	10.14	10.17	60.1	10.04	10.00	55.1	13.99	13.98	40.8	0.437	0.491	0.0	0.0	0.0
$AuCs_2$	THP	$P\bar{3}m1(164)$	$Amm2(38)$	$P\bar{1}(2)$	10.73	10.72	59.6	10.62	10.69	55.1	14.80	15.03	37.9	0.621	0.654	0.0	0.0	0.0

Table 74: List of TM-II

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$ScCa_2$	HTX	$P4/mmm(123)$	$P4/mmm(123)$	–	7.35	10.44	44.6	7.32	10.32	45.2	–	–	–	0.003	9.863	0.0	0.0	–
$TiBe_2$	THP	$P4/mmm(123)$	$P4/mmm(123)$	$P1(1)$	5.26	7.31	43.8	7.30	5.26	43.9	6.65	5.28	53.9	0.027	0.467	0.0	0.0	0.0
$TiMg_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	6.14	8.75	44.4	6.04	8.60	44.5	–	–	–	0.025	10.966	0.0	0.0	–
$TiCa_2$	HTX	$Pmma(51)$	$P4/mmm(123)$	–	10.20	7.09	45.9	10.33	7.30	44.9	–	–	–	0.530	11.273	8.6	9.6	–
VBe_2	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	4.80	6.81	44.4	6.81	4.81	44.8	–	–	–	0.003	9.537	0.0	0.0	–
VSr_2	TXX	$C2/m(12)$	–	–	7.76	10.28	48.5	–	–	–	–	–	–	2.329	2.557	1.4	–	–
$CrMg_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	6.26	9.01	43.8	6.25	8.95	44.1	–	–	–	0.060	5.738	14.8	14.8	–
$CrCa_2$	THX	$P2_1/m(11)$	$P4/mmm(123)$	–	7.62	8.88	54.4	7.42	10.52	44.9	–	–	–	0.640	8.018	16.0	17.7	–
$CrSr_2$	PHX	–	$P4/mmm(123)$	$P\bar{1}(2)$	–	–	–	7.97	11.30	44.9	10.01	8.10	52.3	0.577	1.952	–	19.1	17.3
$CrBa_2$	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	8.70	9.16	58.2	1.423	2.977	–	–	0.0
$MnBe_2$	HTX	$P4/mmm(123)$	$Cmmm(65)$	–	5.15	7.25	45.2	4.60	7.51	35.3	–	–	–	0.801	7.736	7.7	0.0	–
$MnCa_2$	TPH	$P2_1/m(11)$	$P4/mmm(123)$	$P\bar{1}(2)$	7.55	8.78	54.5	7.37	10.46	44.7	7.99	9.55	50.0	0.441	0.589	14.7	17.2	14.8
$FeBe_2$	HTX	$P4/mmm(123)$	$P4/mmm(123)$	–	7.37	5.21	45.0	7.29	5.15	45.0	–	–	–	0.475	9.512	0.0	5.0	–
$NiBe_2$	THX	$P\bar{3}m1(164)$	$P4/mmm(123)$	–	7.41	6.38	29.8	5.12	7.26	44.9	–	–	–	0.315	6.864	0.0	0.0	–
$ZrBe_2$	PXX	–	–	$P4/nmm(129)$	–	–	–	–	–	–	5.07	7.18	45.0	6.083	6.270	–	–	0.0
$ZrMg_2$	TXX	$P4/mmm(123)$	–	–	6.58	9.37	42.1	–	–	–	–	–	–	1.262	14.651	0.0	–	–
$ZrCa_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	7.16	10.14	45.0	10.16	7.18	44.9	–	–	–	0.017	13.243	0.0	0.0	–
$NbBe_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	7.84	5.43	43.8	5.43	7.85	43.7	–	–	–	0.001	4.217	0.0	0.0	–
$NbCa_2$	THX	$P2_1/m(11)$	$Pmma(51)$	–	6.86	10.30	48.0	6.92	10.11	46.5	–	–	–	0.468	14.491	0.0	0.0	–
$MoBe_2$	HTX	$Cmmm(65)$	$Pmm2(25)$	–	5.16	8.03	38.9	8.81	8.21	21.2	–	–	–	0.355	6.371	0.0	0.0	–
$TcBe_2$	HTX	$P\bar{1}(2)$	$Pmma(51)$	–	7.50	6.57	33.5	7.99	6.00	41.4	–	–	–	0.715	3.892	0.0	0.0	–
$RuBe_2$	HXX	–	$Pmma(51)$	–	–	–	–	5.71	8.08	45.0	–	–	–	1.933	5.762	–	0.0	–
$RuCa_2$	TXX	$P2_1/m(11)$	–	–	8.83	7.22	52.3	–	–	–	–	–	–	1.040	1.344	0.0	–	–
$RhBe_2$	PXX	–	–	$P4/nmm(129)$	–	–	–	–	–	–	4.58	4.58	90.0	1.291	2.630	–	–	0.0
$PdCa_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	8.53	8.54	59.8	–	–	–	8.51	8.52	60.0	0.006	1.685	0.0	–	0.0
$PdSr_2$	TXX	$P\bar{3}m1(164)$	–	–	9.14	9.14	59.2	–	–	–	–	–	–	2.115	4.412	0.0	–	–
$AgCa_2$	THX	$P\bar{3}m1(164)$	$Amm2(38)$	–	8.98	8.97	59.5	7.78	7.80	60.9	–	–	–	0.101	1.069	0.0	0.0	–
$AgSr_2$	TXX	$P\bar{3}m1(164)$	–	–	9.53	9.53	59.8	–	–	–	–	–	–	0.860	4.582	0.0	–	–
$AgBa_2$	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	9.97	9.96	59.7	–	–	–	9.87	10.08	58.9	0.019	1.129	0.0	–	0.0
$HfBe_2$	PHX	–	$P4/mmm(123)$	$Cmm2(35)$	–	–	–	8.00	5.79	43.7	6.93	7.58	46.5	0.718	3.790	–	0.0	0.0
$HfCa_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	9.97	7.05	45.0	7.08	9.99	44.8	–	–	–	0.011	13.950	0.0	0.0	–
$TaBe_2$	THX	$Pmm2(25)$	$P4/mmm(123)$	–	8.54	9.17	21.4	5.47	7.80	44.5	–	–	–	0.199	5.207	0.0	0.0	–
WBe_2	THX	$Pm(6)$	$Cmmm(65)$	–	7.49	8.17	23.4	5.20	8.09	38.9	–	–	–	0.512	3.976	0.0	0.0	–
WSr_2	HPT	$P2_1/m(11)$	$P\bar{1}(2)$	$P2_1/m(11)$	8.17	7.80	58.5	7.99	9.00	53.0	8.23	7.87	58.2	0.192	0.208	0.0	0.0	0.0
$OsBe_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	5.72	8.07	44.9	–	–	–	2.085	7.582	–	0.0	–
$OsMg_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.01	6.25	44.6	–	–	–	1.045	12.251	–	0.0	–
$OsBa_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	10.04	9.05	47.4	1.409	3.666	–	–	2.5
$IrBe_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	5.65	8.00	45.0	–	–	–	3.811	6.232	–	0.0	–
$IrMg_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	9.00	6.35	44.8	–	–	–	3.230	10.834	–	0.0	–
$IrCa_2$	PHX	–	$P4/mmm(123)$	$P2_1/m(11)$	–	–	–	6.95	9.83	45.0	8.85	7.32	52.8	0.250	2.053	–	0.0	0.0
$IrSr_2$	HTX	$P\bar{3}m1(164)$	$P4/mmm(123)$	–	8.93	8.95	59.5	7.46	10.57	44.9	–	–	–	0.362	1.981	0.0	0.0	–
$IrBa_2$	TXX	$P\bar{3}m1(164)$	–	–	9.28	9.29	59.5	–	–	–	–	–	–	0.965	2.130	0.0	–	–
$PtBe_2$	HXX	–	$Cmmm(65)$	–	–	–	–	6.41	8.39	40.2	–	–	–	2.567	2.855	–	0.0	–
$PtSr_2$	TXX	$P\bar{3}m1(164)$	–	–	9.07	9.07	59.5	–	–	–	–	–	–	2.234	5.942	0.0	–	–
$AuBe_2$	PXX	–	–	$P6/mmm(191)$	–	–	–	–	–	–	8.17	8.16	60.0	2.167	5.488	–	–	0.0
$AuCa_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	8.88	8.88	59.2	–	–	–	8.79	8.78	59.9	0.007	0.922	0.0	–	0.0
$AuSr_2$	TXX	$P\bar{3}m1(164)$	–	–	9.34	9.35	59.4	–	–	–	–	–	–	1.124	1.688	0.0	–	–

Table 75: List of TM-XII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$ScHg_2$	THX	$P4/mmm(123)$	$P\bar{6}m2(187)$	–	6.60	9.37	44.8	7.03	6.76	58.3	–	–	–	0.457	3.630	0.0	0.0	–
VCd_2	HTX	$Cmmm(65)$	$Cmmm(65)$	–	6.93	9.05	39.6	8.64	5.99	43.7	–	–	–	0.725	8.211	0.0	0.0	–
$MnCd_2$	TXX	$Cmmm(65)$	–	–	6.34	9.15	40.1	–	–	–	–	–	–	0.878	5.182	15.5	–	–
$NiHg_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.51	5.99	43.8	–	–	–	3.814	3.885	–	0.0	–
$RhHg_2$	TXX	$P4/mmm(123)$	–	–	6.61	9.22	43.2	–	–	–	–	–	–	1.278	6.618	0.0	–	–
$PdHg_2$	HTX	$C2/m(12)$	$Pmmm(47)$	–	8.86	8.87	40.0	9.71	7.61	37.8	–	–	–	0.741	2.403	0.0	0.0	–
$PtCd_2$	HXX	–	$Pmmm(47)$	–	–	–	–	9.56	7.53	37.9	–	–	–	2.899	2.922	–	0.0	–
$PtHg_2$	HTX	$P\bar{3}m1(164)$	$Amm2(38)$	–	8.73	8.72	59.8	8.89	8.87	38.3	–	–	–	0.655	1.251	0.0	0.0	–
$AuHg_2$	HTX	$P\bar{3}m1(164)$	$Amm2(38)$	–	9.44	9.43	58.5	9.11	9.09	36.8	–	–	–	0.323	0.914	0.0	0.0	–

Table 76: List of TM-XIII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$ScIn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.75	9.55	45.2	–	–	–	5.359	5.523	–	0.0	–
TiB_2	PXX	–	–	$P2/c(13)$	–	–	–	–	–	–	8.32	8.29	42.5	1.852	1.853	–	–	0.0
$TiAl_2$	HTX	$Pmma(51)$	$P4/mmm(123)$	–	9.02	6.93	39.8	8.08	5.57	43.5	–	–	–	0.695	8.486	0.0	0.0	–
$TiIn_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	6.24	8.81	45.0	9.05	6.39	45.2	–	–	–	0.062	8.034	0.0	0.0	–
$TiTl_2$	HTX	$P4/mmm(123)$	$Cmmm(65)$	–	6.71	9.49	44.8	9.77	7.01	43.5	–	–	–	0.061	6.409	0.0	0.0	–
VB_2	HPX	–	$Cmmm(65)$	$Cmmm(65)$	–	–	–	6.29	7.98	37.9	8.18	8.18	42.6	0.806	2.263	–	0.0	4.0
VAl_2	HTX	$Pmmm(47)$	$Pmmm(47)$	–	6.68	8.71	39.9	8.70	6.68	39.9	–	–	–	0.002	8.146	0.0	0.0	–
$CrAl_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	6.35	8.44	41.2	5.94	8.41	45.0	–	–	–	0.061	5.287	0.0	0.0	–
$CrGa_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	5.95	8.45	44.8	5.97	8.46	44.7	–	–	–	0.039	5.490	10.4	10.3	–
MnB_2	PXX	–	–	$Cmmm(65)$	–	–	–	–	–	–	7.88	7.88	44.5	1.841	4.105	–	–	11.0
$MnAl_2$	HXX	–	$Pmma(51)$	–	–	–	–	6.66	8.60	39.0	–	–	–	0.941	5.969	–	10.9	–
$MnIn_2$	HTX	$P4/mmm(123)$	$P4/mmm(123)$	–	6.36	9.06	45.4	9.07	6.39	45.3	–	–	–	0.000	4.674	15.2	15.2	–
FeB_2	TXX	$C2/m(12)$	–	–	5.59	5.97	36.8	–	–	–	–	–	–	4.107	4.694	0.0	–	–
$FeAl_2$	HTX	$P4/mmm(123)$	$P4/mmm(123)$	–	5.68	8.05	45.0	5.68	8.05	45.0	–	–	–	0.092	7.347	0.0	1.8	–
CoB_2	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	6.68	6.69	53.2	1.582	1.617	–	–	0.0
$CoAl_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	5.72	7.87	43.2	5.43	7.82	45.7	–	–	–	0.020	6.863	0.0	0.0	–
$NiAl_2$	THX	$Pmma(51)$	$Pmma(51)$	–	6.20	8.15	40.1	5.64	8.05	45.1	–	–	–	0.007	4.662	0.0	0.0	–
$NiIn_2$	HXX	–	$Pmmm(47)$	–	–	–	–	9.15	6.93	39.5	–	–	–	2.741	4.089	–	0.0	–
YB_2	TPX	$Cmmm(65)$	–	$Cmmm(65)$	9.96	9.96	37.0	–	–	–	9.95	9.95	37.0	0.002	9.924	0.0	–	0.0
ZrB_2	PHT	$P2/c(13)$	$P2/c(13)$	$P2/c(13)$	8.79	8.74	41.0	8.78	8.74	41.1	8.80	8.76	41.0	0.003	0.004	0.0	0.0	0.0
$ZrIn_2$	HPT	$P4/mmm(123)$	$Pmma(51)$	$P4/mmm(123)$	6.32	8.90	45.2	7.29	9.78	42.0	6.58	9.34	44.9	0.014	0.372	0.0	0.0	0.0
$ZrTl_2$	THX	$P4/mmm(123)$	$Pmma(51)$	–	9.89	7.07	43.7	10.12	7.58	41.4	–	–	–	0.755	9.882	0.0	0.0	–
$NbAl_2$	HTX	$Pmmm(47)$	$Pmmm(47)$	–	9.41	7.43	37.8	7.44	9.41	37.8	–	–	–	0.004	8.037	0.0	0.0	–
$NbGa_2$	THX	$Pmmm(47)$	$Pmmm(47)$	–	7.41	9.47	38.3	7.46	9.50	38.1	–	–	–	0.109	10.646	0.0	0.0	–
$MoIn_2$	HXX	–	$P\bar{1}(2)$	–	–	–	–	6.42	9.25	38.8	–	–	–	9.001	9.719	–	0.0	–
$MoTl_2$	HXX	–	$Amm2(38)$	–	–	–	–	8.14	9.52	27.5	–	–	–	12.878	12.901	–	0.0	–
$RuAl_2$	HTX	$P4/nmm(129)$	$P4/nmm(129)$	–	8.44	5.97	45.0	8.41	5.95	45.0	–	–	–	0.178	8.136	0.0	0.0	–
RhB_2	TPX	$Pmmn(59)$	–	$Cmmm(65)$	7.53	7.53	48.0	–	–	–	7.97	7.97	44.7	0.399	8.642	0.0	–	0.0
$RhGa_2$	THX	$C2/m(12)$	$Amm2(38)$	–	7.96	7.94	42.9	7.56	7.50	45.0	–	–	–	0.346	4.161	0.0	0.0	–
$RhIn_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.43	6.38	58.1	–	–	–	1.550	1.883	–	0.0	–
PdB_2	PTH	$Cmmm(65)$	$Cmmm(65)$	$Cmmm(65)$	8.13	8.13	44.4	8.13	8.13	44.4	8.13	8.13	44.4	0.013	0.016	0.0	0.0	0.0
$PdAl_2$	HXX	–	$C2/m(12)$	–	–	–	–	7.11	5.87	50.2	–	–	–	3.293	3.299	–	0.0	–
$PdIn_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.36	6.35	60.1	–	–	–	1.708	1.943	–	0.0	–
$PdTl_2$	HTP	$P\bar{3}m1(164)$	$Amm2(38)$	$C2/m(12)$	8.85	8.83	56.7	8.37	8.29	44.7	9.41	9.42	44.6	0.489	0.506	0.0	0.0	0.0
AgB_2	HTP	$Cmmm(65)$	$P1(1)$	$Cmmm(65)$	8.90	8.90	40.6	8.41	7.22	31.9	8.88	8.89	40.6	0.222	0.245	0.0	0.0	0.0
$AgAl_2$	TPH	$P\bar{3}m1(164)$	$Amm2(38)$	$P6/mmm(191)$	9.05	9.05	60.0	8.48	8.48	36.2	9.11	9.11	60.0	0.025	0.098	0.0	0.0	0.0
$AgIn_2$	HXX	–	$C2/m(12)$	–	–	–	–	8.95	7.89	42.5	–	–	–	2.390	3.107	–	0.0	–
$AgTl_2$	HXX	–	$P2/m(10)$	–	–	–	–	10.80	7.64	37.6	–	–	–	0.855	3.872	–	0.0	–
HfB_2	PTX	$P2/c(13)$	–	$P2/c(13)$	8.80	8.82	40.6	–	–	–	8.82	8.81	40.6	0.008	2.755	0.0	–	0.0
$HfTl_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	9.49	6.71	44.9	6.72	9.51	44.9	–	–	–	0.018	9.804	0.0	0.0	–
$TaIn_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	6.69	6.07	45.2	2.749	2.836	–	–	0.0
WB_2	HXX	–	$Pmma(51)$	–	–	–	–	6.08	7.90	39.7	–	–	–	2.009	2.281	–	0.0	–
WAl_2	THX	$Pmmm(47)$	$Pmmm(47)$	–	9.22	7.38	36.8	7.90	7.90	40.9	–	–	–	0.033	10.429	0.0	0.0	–
ReB_2	THP	$P2/c(13)$	$Pmma(51)$	$Cmmm(65)$	7.83	6.85	44.1	5.75	5.83	59.6	8.26	8.26	42.0	0.213	0.278	0.0	0.0	4.3
OsB_2	PXX	–	–	$P2/c(13)$	–	–	–	–	–	–	7.99	7.79	40.5	1.783	5.686	–	–	0.0
IrB_2	TPX	$Pmmn(59)$	–	$Pmmn(59)$	7.61	7.61	47.7	–	–	–	7.61	7.61	47.7	0.002	6.441	0.0	–	0.0
$IrAl_2$	THX	$P2_1/m(11)$	$Pmmm(47)$	–	8.48	6.52	49.5	8.80	6.84	39.0	–	–	–	0.307	2.068	0.0	0.0	–
$IrIn_2$	HPT	$P\bar{3}m1(164)$	$Amm2(38)$	$P\bar{3}m1(164)$	8.28	8.27	60.2	8.14	8.15	43.4	8.18	8.18	60.5	0.330	0.337	0.0	0.0	0.0
$IrTl_2$	HPT	$P\bar{3}m1(164)$	$Pm(6)$	$P\bar{3}m1(164)$	8.66	8.63	59.2	8.32	8.40	44.5	8.57	8.55	60.0	0.682	0.691	0.0	0.0	0.0
PtB_2	TPX	$Cmmm(65)$	–	$Cmmm(65)$	8.01	8.01	45.8	–	–	–	8.01	8.01	45.8	0.008	10.620	0.0	–	0.0
$PtAl_2$	HXX	–	$C2/m(12)$	–	–	–	–	7.62	6.51	46.1	–	–	–	2.256	2.423	–	0.0	–
$PtGa_2$	HTX	$P\bar{3}m1(164)$	$Amm2(38)$	–	8.10	8.10	59.8	7.80	7.78	41.5	–	–	–	0.189	2.943	0.0	0.0	–
$PtIn_2$	HTX	$P\bar{3}m1(164)$	$Amm2(38)$	–	8.56	8.53	60.2	8.10	8.10	42.5	–	–	–	0.408	3.977	0.0	0.0	–
$PtTl_2$	PHT	$P\bar{3}m1(164)$	$Amm2(38)$	$P2_1/m(11)$	8.73	8.72	58.9	8.37	8.39	43.6	8.63	8.37	58.9	0.035	0.093	0.0	0.0	0.0
AuB_2	TPH	$P2/c(13)$	$P2/c(13)$	$P2/c(13)$	8.66	8.40	42.2	8.42	8.67	42.2	8.65	8.40	42.3	0.004	0.005	0.0	0.0	0.0
$AuAl_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	8.87	8.88	59.9	–	–	–	8.88	8.88	60.0	0.008	0.908	0.0	–	0.0
$AuGa_2$	THX	$C2/m(12)$	$Amm2(38)$	–	8.84	8.84	35.9	8.86	8.82	35.7	–	–	–	0.157	0.838	0.0	0.0	–
$AuIn_2$	THX	$P\bar{3}m1(164)$	$Pmm2(25)$	–	7.33	7.31	61.8	7.13	7.03	51.4	–	–	–	0.403	1.982	0.0	0.0	–

Table 77: List of TM-XIV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
ScC_2	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	6.80	8.20	52.8	1.291	6.761	–	–	0.0
$ScGe_2$	HXX	–	$Cmmm(65)$	–	–	–	–	7.97	10.15	38.2	–	–	–	2.631	2.774	–	0.0	–
$ScSn_2$	PHX	–	$Pmmm(47)$	$Pmmm(47)$	–	–	–	10.92	8.91	35.2	10.98	8.93	35.0	0.109	4.083	–	0.0	0.0
$ScPb_2$	PHT	$Pmmm(47)$	$Pmma(51)$	$Pmmn(59)$	10.98	8.71	37.3	10.97	8.67	37.5	10.56	7.36	45.2	0.502	0.573	0.0	0.0	0.0
TiC_2	PXX	–	–	$Cm(8)$	–	–	–	–	–	–	7.09	7.08	47.9	3.522	5.376	–	–	0.0
$TiGe_2$	THX	$Pmmm(47)$	$Pmmm(47)$	–	9.73	8.02	34.4	8.02	9.72	34.5	–	–	–	0.003	1.876	0.0	0.0	–
$TiSn_2$	THX	$Pmmm(47)$	$Pmmm(47)$	–	8.37	10.36	35.7	8.37	10.33	35.8	–	–	–	0.013	9.388	0.0	0.0	–
VGe_2	PTH	$Pmmm(47)$	$Pmmm(47)$	$Pmmm(47)$	9.32	7.61	35.5	9.25	7.60	35.8	9.46	7.79	34.4	0.548	0.549	0.0	0.0	2.7
VSn_2	HXX	–	$P\bar{1}(2)$	–	–	–	–	8.31	6.11	45.9	–	–	–	7.157	10.323	–	1.1	–
VPb_2	PHX	–	$P4/mmm(123)$	$C2/m(12)$	–	–	–	6.92	9.80	44.9	8.97	6.97	48.7	0.758	4.917	–	12.5	0.5
CrC_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	6.61	7.26	47.4	1.637	5.024	–	–	7.6
$CrGe_2$	PXX	–	–	$Pmma(51)$	–	–	–	–	–	–	6.68	6.68	50.7	0.941	1.385	–	–	8.8
$CrSn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.80	6.45	42.3	–	–	–	4.969	7.754	–	14.5	–
$CrPb_2$	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	6.65	8.87	67.5	0.910	1.161	–	–	18.2
$MnSi_2$	HTX	$Pmmm(47)$	$Pmmm(47)$	–	7.44	9.01	34.0	9.01	7.45	34.0	–	–	–	0.017	2.663	11.0	11.1	–
$MnSn_2$	HXX	–	$Pmmm(47)$	–	–	–	–	9.98	7.95	36.9	–	–	–	3.872	7.001	–	15.3	–
$MnPb_2$	PHX	–	$P4/mmm(123)$	$P4/mmm(123)$	–	–	–	7.17	10.13	43.5	7.18	7.84	62.6	0.124	3.399	–	15.7	15.9
$FeGe_2$	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	6.08	7.02	47.5	1.728	1.741	–	–	7.6
$FeSn_2$	THX	$Pmmm(47)$	$Pmmm(47)$	–	6.41	8.64	42.0	8.64	6.42	42.0	–	–	–	0.018	8.822	9.7	9.7	–
CoC_2	TXX	$C2/m(12)$	–	–	5.89	5.61	44.4	–	–	–	–	–	–	2.261	3.502	0.0	–	–
$CoSi_2$	HXX	–	$Pbcm(57)$	–	–	–	–	8.55	7.06	34.0	–	–	–	1.204	1.329	–	0.0	–
$NiSn_2$	HTP	$P2_1/m(11)$	$Pmmm(47)$	$P\bar{1}(2)$	8.32	6.49	49.8	7.04	7.04	49.5	6.70	8.17	52.9	0.383	0.556	0.0	0.0	0.0
YC_2	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	8.76	7.27	53.1	3.385	6.174	–	–	0.0
YSi_2	HXX	–	$Pmma(51)$	–	–	–	–	10.27	7.92	39.4	–	–	–	3.207	3.681	–	0.0	–
YGe_2	PTX	$C2/m(12)$	–	$P2/c(13)$	10.75	10.75	42.9	–	–	–	10.61	10.31	43.3	0.387	4.699	0.0	–	0.0
YSn_2	HXX	–	$Pmmm(47)$	–	–	–	–	9.40	11.44	34.7	–	–	–	3.455	5.582	–	0.0	–
YPb_2	PTH	$Pmmm(47)$	$Pmmm(47)$	$P2/c(13)$	11.67	9.46	35.7	9.48	11.69	35.6	11.57	10.45	31.2	0.012	0.023	0.0	0.0	0.0
ZrC_2	PTX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	7.66	8.50	44.5	–	–	–	7.03	7.33	51.5	0.479	5.712	0.0	–	0.0
$ZrSi_2$	HXX	–	$Pmma(51)$	–	–	–	–	9.67	7.38	40.2	–	–	–	2.408	7.072	–	0.0	–
$ZrGe_2$	HPX	–	$Pmmm(47)$	$P2(3)$	–	–	–	8.50	10.32	34.5	9.13	8.88	40.2	0.736	4.903	–	0.0	0.0
$ZrSn_2$	PTH	$Pmmm(47)$	$Pmmm(47)$	$P\bar{1}(2)$	8.90	10.88	35.0	9.42	9.42	38.7	8.07	9.15	40.0	0.061	0.091	0.0	0.0	0.0
$ZrPb_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	6.49	7.75	51.3	0.916	0.927	–	–	0.0
NbC_2	PXX	–	–	$P2/c(13)$	–	–	–	–	–	–	6.49	6.65	46.5	3.852	11.023	–	–	0.0
$MoSi_2$	PXX	–	–	$P1(1)$	–	–	–	–	–	–	7.58	6.86	38.4	1.556	1.700	–	–	0.0
TcC_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	7.13	7.91	41.1	5.542	6.515	–	–	0.0
$TcSi_2$	THX	$C2/m(12)$	$Amm2(38)$	–	8.59	8.59	40.4	7.47	7.49	51.3	–	–	–	0.278	0.964	0.0	0.0	–
RuC_2	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	7.23	8.98	36.9	3.319	7.440	–	–	0.0
$PdPb_2$	PTH	$P\bar{1}(2)$	$Pmm2(25)$	$P\bar{1}(2)$	8.63	7.22	52.8	7.09	7.11	55.3	7.37	7.41	53.1	0.027	0.619	0.0	0.0	0.0
$AgSi_2$	HXX	–	$P2/c(13)$	–	–	–	–	9.06	9.98	29.1	–	–	–	1.521	3.989	–	0.0	–
$AgGe_2$	PHX	–	$P\bar{1}(2)$	$P1(1)$	–	–	–	9.05	9.47	35.7	6.07	6.72	75.7	0.406	2.470	–	0.0	0.0
$AgPb_2$	TXX	$C2/m(12)$	–	–	8.87	9.45	43.8	–	–	–	–	–	–	1.367	1.829	0.0	–	–
HfC_2	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	7.56	6.48	54.2	4.052	8.259	–	–	0.0
$HfSi_2$	PHX	–	$Pmma(51)$	$Pmma(51)$	–	–	–	7.33	9.57	40.0	9.57	7.33	39.9	0.002	6.863	–	0.0	0.0
$HfGe_2$	PXX	–	–	$Pmma(51)$	–	–	–	–	–	–	7.57	9.82	39.6	0.955	0.956	–	–	0.0
$HfPb_2$	PXX	–	–	$Pmmm(47)$	–	–	–	–	–	–	9.16	11.20	34.3	0.916	3.420	–	–	0.0
TaC_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	6.84	7.07	49.0	4.651	10.043	–	–	0.0
WSn_2	HXX	–	$P\bar{1}(2)$	–	–	–	–	6.14	9.01	40.7	–	–	–	5.683	15.239	–	0.0	–
$ReSi_2$	TXX	$C2/m(12)$	–	–	8.56	8.56	40.3	–	–	–	–	–	–	0.861	1.573	0.0	–	–
$OsSi_2$	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	6.82	5.82	64.7	2.880	3.261	–	–	0.0
$OsPb_2$	HXX	–	$Pm(6)$	–	–	–	–	7.65	6.39	51.9	–	–	–	4.336	4.336	–	0.0	–
$IrSi_2$	HTX	$P\bar{1}(2)$	$Pc(7)$	–	8.20	7.97	51.6	8.00	6.78	42.8	–	–	–	0.639	1.006	0.0	0.0	–
$IrGe_2$	HXX	–	$Aem2(39)$	–	–	–	–	7.04	7.04	47.0	–	–	–	1.108	1.459	–	0.0	–
$IrPb_2$	TPX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	7.34	7.05	61.7	–	–	–	7.37	7.06	60.9	0.051	0.971	0.0	–	0.0
$PtSi_2$	HXX	–	$Pmc2_1(26)$	–	–	–	–	7.68	9.04	31.8	–	–	–	1.233	1.760	–	0.0	–
$PtPb_2$	TPH	$P2_1/m(11)$	$P\bar{6}(174)$	$P2_1/m(11)$	7.39	8.04	57.0	7.24	7.22	60.0	7.38	8.03	57.0	0.005	0.141	0.0	0.0	0.0
$AuSi_2$	HXX	–	$Pmma(51)$	–	–	–	–	9.64	8.43	31.2	–	–	–	1.789	3.293	–	0.0	–
$AuGe_2$	HXX	–	$Amm2(38)$	–	–	–	–	8.91	8.89	36.1	–	–	–	0.908	0.962	–	0.0	–
$AuSn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.49	8.83	42.3	–	–	–	2.861	2.870	–	0.0	–

(Continued on next page)

Table 77: List of TM-XIV

(Continued from previous page)

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$AuPb_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	7.20	10.40	43.9	–	–	–	0.933	0.981	–	0.0	–

Table 78: List of TM-XV

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
ScN_2	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	7.35	7.36	49.7	1.883	14.128	–	–	0.0
$ScBi_2$	THP	$Pmmm(47)$	$P4/mmm(123)$	$Pmmm(47)$	11.21	8.36	40.9	8.35	11.21	41.0	8.38	8.50	59.7	0.028	0.076	0.0	0.0	0.0
TiN_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.50	6.52	60.3	–	–	–	1.634	7.641	–	0.0	–
$TiBi_2$	PTX	$P\bar{1}(2)$	–	$C2/m(12)$	7.59	8.85	39.9	–	–	–	6.56	7.85	51.3	0.501	2.761	0.0	–	0.0
VN_2	PHX	–	$Cm(8)$	$P\bar{1}(2)$	–	–	–	6.08	6.10	59.8	6.49	5.78	58.2	0.561	3.376	–	0.0	0.0
VP_2	PHX	–	$P\bar{6}m2(187)$	$P1(1)$	–	–	–	7.25	7.25	60.0	7.26	6.71	45.4	0.214	1.818	–	1.3	0.0
VAs_2	HTX	$C2/m(12)$	$P\bar{6}m2(187)$	–	8.60	8.63	42.2	7.50	7.48	59.8	–	–	–	0.205	1.563	5.1	4.0	–
VSb_2	PTH	$C2/m(12)$	$Amm2(38)$	$C2/m(12)$	9.16	9.17	43.4	8.88	8.90	43.6	9.19	9.18	43.1	0.058	0.300	8.3	10.3	8.4
VBi_2	PTH	$C2/m(12)$	$Amm2(38)$	$C2/m(12)$	9.46	9.46	42.2	9.12	9.13	44.1	9.48	9.46	42.0	0.004	0.007	9.9	10.4	10.0
CrP_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	6.88	6.79	42.4	0.835	1.359	–	–	1.8
$CrSb_2$	PXX	–	–	$Pmmm(47)$	–	–	–	–	–	–	6.31	9.98	49.5	0.975	1.011	–	–	13.6
$CrBi_2$	HPT	$C2/m(12)$	$Amm2(38)$	$C2/m(12)$	9.44	9.44	42.1	9.27	9.30	42.3	9.44	9.46	42.0	0.055	0.058	14.2	14.6	14.2
MnP_2	PHT	$C2/m(12)$	$P\bar{6}m2(187)$	$C2/m(12)$	8.01	8.01	42.7	7.33	7.36	58.7	6.80	6.61	59.0	0.219	0.766	10.0	12.0	0.0
FeP_2	PTH	$C2/m(12)$	$Amm2(38)$	$P\bar{1}(2)$	7.74	7.75	42.3	7.31	7.34	50.7	7.38	7.68	50.5	0.161	0.538	6.3	8.1	1.9
$FeAs_2$	THX	$C2/m(12)$	$Amm2(38)$	–	8.04	8.10	43.2	7.62	7.64	50.7	–	–	–	0.444	7.230	7.7	9.2	–
$FeBi_2$	PXX	–	–	$P1(1)$	–	–	–	–	–	–	7.01	8.44	50.6	2.146	2.272	–	–	8.0
$CoSb_2$	HXX	–	$Pmm2(25)$	–	–	–	–	6.95	6.94	55.2	–	–	–	1.237	9.025	–	0.6	–
NiP_2	HPT	$P\bar{1}(2)$	$Pc(7)$	$C2/m(12)$	7.54	7.82	40.9	7.62	7.67	40.8	7.87	7.87	47.2	0.405	0.553	0.0	0.0	0.0
$NiAs_2$	HTX	$C2/m(12)$	$Amm2(38)$	–	8.09	7.79	43.3	7.94	7.94	41.8	–	–	–	0.030	2.912	0.0	0.0	–
$NiBi_2$	HXX	–	$Amm2(38)$	–	–	–	–	8.51	6.89	50.3	–	–	–	1.937	1.956	–	0.0	–
YN_2	PXX	–	–	$P4/mmm(123)$	–	–	–	–	–	–	7.32	7.31	53.3	1.584	13.358	–	–	0.0
YP_2	HPX	–	$P4/mmm(123)$	$P1(1)$	–	–	–	10.63	7.74	43.2	8.52	7.76	63.5	0.602	1.434	–	0.0	0.0
YAs_2	HXX	–	$P4/mmm(123)$	–	–	–	–	7.85	11.13	42.7	–	–	–	2.041	2.109	–	0.0	–
YBi_2	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	8.65	11.78	41.7	8.63	11.77	41.9	–	–	–	0.003	2.813	0.0	0.0	–
ZrN_2	HPX	–	$P\bar{6}m2(187)$	$P1(1)$	–	–	–	7.01	7.04	60.2	6.67	6.05	69.1	0.260	7.170	–	0.0	0.0
ZrP_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	8.14	8.13	59.8	–	–	–	1.562	9.368	–	0.0	–
$ZrBi_2$	PXX	–	–	$Cmmm(65)$	–	–	–	–	–	–	8.00	6.69	54.5	1.087	4.002	–	–	0.0
NbP_2	THX	$P\bar{1}(2)$	$P\bar{6}m2(187)$	–	7.57	7.86	44.9	7.80	7.80	57.8	–	–	–	0.163	1.567	0.0	0.0	–
$NbBi_2$	TPX	$C2/m(12)$	–	$P\bar{1}(2)$	7.07	7.08	54.3	–	–	–	8.09	8.85	44.5	0.312	4.848	0.0	–	0.0
MoN_2	TXX	$P\bar{1}(2)$	–	–	6.49	6.50	55.7	–	–	–	–	–	–	1.347	2.470	0.0	–	–
MoP_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	6.14	6.91	63.6	1.389	3.230	–	–	0.0
$MoSb_2$	HTX	$C2/m(12)$	$P\bar{6}m2(187)$	–	9.19	9.19	42.4	7.84	7.94	59.2	–	–	–	0.638	7.676	0.0	0.0	–
$MoBi_2$	TXX	$P\bar{1}(2)$	–	–	6.70	7.90	51.7	–	–	–	–	–	–	0.960	1.056	0.0	–	–
TcN_2	PTH	$P1(1)$	$P\bar{6}m2(187)$	$Pc(7)$	6.34	6.09	59.0	5.74	5.75	60.1	6.98	6.22	59.9	0.406	0.515	0.0	0.3	0.0
TcP_2	HXX	–	$Amm2(38)$	–	–	–	–	7.28	7.28	52.2	–	–	–	1.228	1.912	–	0.0	–
$TcSb_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.65	6.65	60.0	–	–	–	3.596	11.384	–	0.0	–
$TcBi_2$	PHX	–	$P\bar{6}m2(187)$	$P\bar{1}(2)$	–	–	–	6.89	6.88	60.1	7.30	8.47	46.4	0.659	4.313	–	0.0	0.0
RuN_2	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	6.80	7.22	76.4	4.664	5.141	–	–	0.0
RuP_2	PHT	$P2_1/m(11)$	$Pmn2_1(31)$	$Pmmn(59)$	7.89	7.89	43.4	7.58	7.59	45.9	5.88	8.04	68.5	0.004	0.305	0.0	0.0	0.0
$RuSb_2$	TXX	$P\bar{1}(2)$	–	–	7.19	7.32	59.7	–	–	–	–	–	–	0.833	11.598	0.0	–	–
RhP_2	THP	$P\bar{1}(2)$	$Pc(7)$	$P1(1)$	7.66	8.15	50.3	7.93	7.92	40.0	7.29	7.83	51.8	0.007	0.413	0.0	0.0	0.0
$RhAs_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	7.00	7.05	58.4	1.109	1.242	–	–	0.0
$RhBi_2$	TPX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	8.80	7.19	52.5	–	–	–	7.22	8.79	52.3	0.006	1.307	0.0	–	0.0
PdP_2	HTX	$Pc(7)$	$Pc(7)$	–	9.07	9.08	42.3	8.49	8.52	38.4	–	–	–	0.395	1.051	0.0	0.0	–
$PdAs_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.09	8.78	37.4	–	–	–	2.195	7.320	–	0.0	–
$PdSb_2$	THX	$C2/m(12)$	$Amm2(38)$	–	8.93	8.93	54.1	8.87	8.87	42.2	–	–	–	0.077	5.364	0.0	0.0	–
AgP_2	TPX	$P2/m(10)$	–	$P\bar{1}(2)$	11.30	8.95	37.0	–	–	–	11.25	6.60	52.2	0.402	1.672	0.0	–	0.0
$AgSb_2$	THX	$P\bar{1}(2)$	$Pc(7)$	–	9.50	13.53	38.5	9.52	9.55	40.5	–	–	–	0.095	4.273	0.0	0.0	–
$AgBi_2$	THX	$P\bar{1}(2)$	$Amm2(38)$	–	13.84	9.79	39.2	9.49	9.48	42.9	–	–	–	0.078	0.890	0.0	0.0	–
HfN_2	HXX	–	$Pmn2_1(31)$	–	–	–	–	6.81	6.88	59.9	–	–	–	1.434	6.335	–	0.0	–
HfP_2	THX	$P\bar{1}(2)$	$P\bar{6}m2(187)$	–	8.16	7.93	48.6	8.03	8.02	59.5	–	–	–	0.106	1.575	0.0	0.0	–
$HfBi_2$	TXX	$Cmmm(65)$	–	–	8.41	6.60	50.4	–	–	–	–	–	–	2.365	4.070	0.0	–	–
TaN_2	TXX	$P\bar{3}m1(164)$	–	–	6.32	6.32	60.0	–	–	–	–	–	–	1.284	5.132	3.7	–	–
TaP_2	TXX	$P\bar{1}(2)$	–	–	7.30	7.71	50.3	–	–	–	–	–	–	1.257	11.721	0.0	–	–
$TaAs_2$	TPX	$P2_1/m(11)$	–	$P2_1/m(11)$	7.58	7.59	51.6	–	–	–	7.68	6.65	63.8	0.173	1.714	0.0	–	0.0
$TaBi_2$	TPX	$C2/m(12)$	–	$P2_1/m(11)$	7.10	7.11	53.7	–	–	–	8.00	8.00	47.9	0.322	5.303	0.0	–	0.0
WN_2	TXX	$P3(143)$	–	–	6.22	6.22	60.1	–	–	–	–	–	–	2.445	3.081	0.0	–	–
WP_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	7.13	6.50	62.8	1.196	3.803	–	–	0.0

(Continued on next page)

Table 78: List of TM-XV

(Continued from previous page)

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
WAs_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	7.39	7.43	60.2	–	–	–	2.084	10.262	–	0.0	–
WSb_2	TPX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	7.99	7.13	46.8	–	–	–	7.40	6.81	63.7	0.049	4.571	0.0	–	0.0
ReN_2	THX	$P1(1)$	$P\bar{6}m2(187)$	–	6.36	6.10	57.8	5.76	5.77	60.1	–	–	–	0.018	1.863	0.0	0.0	–
$ReBi_2$	TPX	$P2_1/m(11)$	–	$P\bar{1}(2)$	7.38	7.37	54.4	–	–	–	7.37	7.32	54.2	0.382	1.551	0.0	–	0.0
OsN_2	THX	$P1(1)$	$P\bar{6}m2(187)$	–	6.17	6.49	58.1	5.65	5.64	59.8	–	–	–	0.049	0.888	0.0	0.0	–
$OsSb_2$	TPX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	7.32	7.18	59.6	–	–	–	7.21	7.18	61.1	0.007	1.738	0.0	–	0.0
$OsBi_2$	PTH	$P\bar{1}(2)$	$Pmm2(25)$	$P\bar{1}(2)$	7.32	7.31	61.0	7.32	7.32	52.2	7.42	7.32	59.6	0.001	0.655	0.0	0.0	0.0
IrN_2	TPX	$C2/m(12)$	–	$C2/m(12)$	6.08	6.12	59.9	–	–	–	6.12	6.09	59.9	0.001	1.903	0.0	–	0.0
IrP_2	TPX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	7.53	8.02	51.0	–	–	–	8.03	7.53	51.1	0.010	0.974	0.0	–	0.0
$IrSb_2$	TXX	$P2_1/m(11)$	–	–	7.25	8.03	56.3	–	–	–	–	–	–	0.937	1.265	0.0	–	–
PtP_2	TPH	$C2/m(12)$	$Pm(6)$	$C2/m(12)$	7.99	7.99	53.2	7.78	7.73	51.1	7.98	7.98	53.4	0.007	0.282	0.0	0.0	0.0
$PtAs_2$	TPH	$C2/m(12)$	$Amm2(38)$	$C2/m(12)$	8.31	8.31	53.4	8.32	8.32	40.4	8.31	8.31	53.4	0.052	0.125	0.0	0.0	0.0
$PtBi_2$	HTP	$P\bar{3}m1(164)$	$Amm2(38)$	$P\bar{3}m1(164)$	8.76	8.68	58.8	7.10	8.60	52.6	8.70	8.64	59.6	0.545	0.554	0.0	0.0	0.0
AuP_2	TPX	$P2/m(10)$	–	$C2/m(12)$	11.09	7.68	46.9	–	–	–	9.01	9.00	50.4	0.664	1.583	0.0	–	0.0
$AuSb_2$	HTX	$P\bar{3}m1(164)$	$Pc(7)$	–	8.60	8.57	59.3	9.04	9.05	44.3	–	–	–	0.171	1.440	0.0	0.0	–
$AuBi_2$	HPT	$P\bar{3}m1(164)$	$Amm2(38)$	$P1(1)$	8.89	8.88	57.7	9.23	9.23	45.5	9.27	8.77	46.1	0.112	0.325	0.0	0.0	0.0

Table 79: List of TM-XVI

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
ScO_2	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	5.77	7.32	55.5	2.577	3.186	–	–	0.0
ScS_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	9.53	8.94	46.3	1.311	1.457	–	–	0.0
$ScSe_2$	TXX	$P\bar{1}(2)$	–	–	7.56	8.62	56.9	–	–	–	–	–	–	0.967	2.324	0.0	–	–
$ScTe_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{1}(2)$	7.92	7.54	58.5	–	–	–	9.18	8.25	56.4	0.464	2.029	0.0	–	0.0
TiS_2	TXX	$P\bar{3}m1(164)$	–	–	6.80	6.79	60.0	–	–	–	–	–	–	1.138	1.607	0.0	–	–
$TiSe_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.01	6.99	59.8	–	–	–	7.00	6.99	60.0	0.001	1.296	0.0	–	0.0
$TiTe_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.51	7.50	59.8	–	–	–	7.53	7.52	59.5	0.046	1.148	0.0	–	0.0
VO_2	TPX	$P2_1/m(11)$	–	$P2/c(13)$	5.77	5.77	60.6	–	–	–	7.19	7.26	43.1	0.555	1.228	4.0	–	4.0
VS_2	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	6.35	6.34	59.9	6.34	6.34	60.0	6.34	6.34	60.0	0.327	0.329	1.9	3.7	1.9
VSe_2	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	6.61	6.61	59.9	6.64	6.63	59.9	6.61	6.60	60.0	0.333	0.335	2.3	3.9	2.3
VTe_2	PTH	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	7.42	7.45	57.1	7.26	7.25	59.9	7.49	7.50	56.0	0.062	0.215	5.3	4.0	5.5
CrO_2	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	5.74	5.73	60.0	5.23	5.23	60.0	5.73	5.73	60.0	0.416	0.437	8.0	0.0	8.0
CrS_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.08	6.08	59.9	–	–	–	1.347	1.351	–	0.0	–
$CrSe_2$	TPH	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	6.86	6.81	59.5	6.76	6.75	59.8	6.81	6.87	59.4	0.016	0.811	8.6	8.0	8.6
MnO_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	5.75	5.75	60.0	–	–	–	5.75	5.74	60.0	0.014	4.768	12.0	–	12.0
MnS_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	6.70	6.71	60.1	–	–	–	6.70	6.71	60.1	0.003	1.757	11.8	–	11.8
$MnSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.02	7.03	60.0	–	–	–	–	–	–	1.765	2.984	11.5	–	–
FeO_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	5.58	5.58	60.0	–	–	–	5.59	5.58	60.0	0.005	3.965	8.0	–	8.0
FeS_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	6.37	6.40	60.2	6.31	6.30	60.0	–	–	–	0.666	1.421	7.1	5.9	–
$FeSe_2$	PTH	$C2/m(12)$	$P\bar{6}m2(187)$	$Cm(8)$	6.60	6.60	59.7	6.60	6.58	59.7	6.63	6.71	59.3	0.037	0.674	3.9	8.0	2.0
CoO_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	5.65	5.64	59.7	–	–	–	5.65	5.64	59.7	0.010	5.514	3.3	–	3.3
CoS_2	TPX	$P\bar{1}(2)$	–	$P2/c(13)$	6.67	6.63	53.8	–	–	–	7.57	7.06	43.4	0.041	1.218	0.0	–	0.0
$CoSe_2$	TPX	$P\bar{1}(2)$	–	$P2_1/m(11)$	7.00	7.04	53.3	–	–	–	6.68	6.82	59.7	0.153	1.557	0.0	–	0.0
NiO_2	THX	$P\bar{3}m1(164)$	$P\bar{3}m1(164)$	–	5.67	5.67	59.7	5.69	5.67	59.8	–	–	–	0.002	2.454	0.0	0.0	–
NiS_2	TXX	$P\bar{3}m1(164)$	–	–	6.72	6.72	59.7	–	–	–	–	–	–	1.559	1.922	0.0	–	–
$NiSe_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.16	7.18	58.9	–	–	–	7.16	7.16	59.1	0.016	1.992	0.0	–	0.0
YO_2	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	6.76	6.19	74.2	3.184	3.324	–	–	0.0
YS_2	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	9.29	7.83	49.2	3.022	3.234	–	–	0.0
YSe_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	9.82	7.90	53.8	1.937	1.979	–	–	0.0
ZrO_2	HXX	–	$Pmmn(59)$	–	–	–	–	5.19	6.59	50.6	–	–	–	1.087	1.287	–	0.0	–
ZrS_2	TXX	$P\bar{3}m1(164)$	–	–	7.38	7.38	59.9	–	–	–	–	–	–	0.872	2.041	0.0	–	–
$ZrSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.58	7.58	60.0	–	–	–	–	–	–	1.099	1.565	0.0	–	–
$ZrTe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.95	7.94	59.9	–	–	–	–	–	–	1.091	1.342	0.0	–	–
NbO_2	THX	$C2/m(12)$	$P\bar{6}m2(187)$	–	6.21	6.18	60.2	6.01	5.96	60.4	–	–	–	0.651	1.777	0.0	0.0	–
NbS_2	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$C2/m(12)$	6.77	6.77	60.0	6.72	6.73	59.7	6.13	7.70	55.4	0.379	0.410	0.0	0.0	0.0
$NbSe_2$	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$C2/m(12)$	6.96	6.96	59.9	6.95	6.94	60.0	6.35	6.85	74.3	0.171	0.417	0.0	0.0	0.0
$NbTe_2$	HTX	$P2_1/m(11)$	$P\bar{6}m2(187)$	–	7.52	7.51	54.3	7.40	7.40	60.0	–	–	–	0.124	1.416	0.0	0.0	–
MoO_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.69	5.68	60.0	–	–	–	2.347	2.376	–	0.0	–
MoS_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.39	6.39	60.0	–	–	–	2.625	3.668	–	0.0	–
$MoSe_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.65	6.65	60.1	–	–	–	1.444	1.489	–	0.0	–
$MoTe_2$	THP	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	7.29	7.28	57.3	7.16	7.16	60.1	7.31	7.31	57.0	0.006	0.064	0.0	0.0	0.0
TcO_2	TPX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	5.77	5.70	59.9	–	–	–	5.70	5.77	60.0	0.022	3.508	0.0	–	0.0
TcS_2	PTX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	6.60	6.54	58.6	–	–	–	6.43	6.60	60.2	0.000	1.813	0.0	–	0.0
$TcSe_2$	TPX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	6.67	6.86	60.3	–	–	–	6.67	6.80	61.2	0.004	1.746	0.0	–	0.0
$TcTe_2$	TPX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	7.31	7.27	58.5	–	–	–	7.32	7.29	58.2	0.013	1.768	0.0	–	0.0
RuO_2	TPX	$P2_1/m(11)$	–	$P2_1/m(11)$	6.19	5.77	57.7	–	–	–	5.78	6.19	57.6	0.066	3.979	0.0	–	0.0
RuS_2	TPX	$P2_1/m(11)$	–	$C2/m(12)$	6.94	6.60	58.3	–	–	–	6.91	6.57	58.3	0.210	3.164	0.0	–	0.0
$RuSe_2$	TXX	$P2_1/m(11)$	–	–	7.22	6.86	58.2	–	–	–	–	–	–	2.201	2.763	0.0	–	–
$RuTe_2$	PTX	$P2_1/m(11)$	–	$P2_1/m(11)$	7.30	7.69	58.3	–	–	–	7.33	7.72	57.9	0.017	1.365	0.0	–	0.0
RhO_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	6.17	6.16	59.9	–	–	–	6.16	6.17	60.0	0.026	4.539	0.0	–	0.0
RhS_2	PTX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	7.13	7.06	54.0	–	–	–	7.13	7.06	54.0	0.000	2.867	0.0	–	0.0
$RhSe_2$	TXX	$P\bar{1}(2)$	–	–	7.46	7.39	53.3	–	–	–	–	–	–	2.124	2.438	0.0	–	–
$RhTe_2$	TXX	$P\bar{1}(2)$	–	–	7.97	7.92	52.7	–	–	–	–	–	–	1.716	3.389	0.0	–	–
PdO_2	HTP	$P\bar{3}m1(164)$	$P\bar{3}m1(164)$	$P\bar{3}m1(164)$	6.20	6.19	59.8	6.18	6.18	60.1	6.18	6.18	59.9	0.004	0.009	0.0	0.0	0.0
PdS_2	TXX	$P\bar{3}m1(164)$	–	–	7.14	7.14	60.0	–	–	–	–	–	–	0.888	2.958	0.0	–	–
$PdSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.51	7.51	59.8	–	–	–	–	–	–	2.841	4.700	0.0	–	–
$PdTe_2$	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	8.08	8.08	59.8	–	–	–	6.98	8.06	90.0	0.025	2.028	0.0	–	0.0
AgO_2	PXX	–	–	$Cmme(67)$	–	–	–	–	–	–	10.94	8.10	38.4	3.783	7.092	–	–	0.0

(Continued on next page)

Table 79: List of TM-XVI

(Continued from previous page)

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
AgS_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	9.42	12.17	37.6	2.184	4.385	–	–	0.0
$AgSe_2$	PXX	–	–	$Cmme(67)$	–	–	–	–	–	–	10.39	13.02	35.2	2.171	3.360	–	–	0.0
HfO_2	HXX	–	$Pmmn(59)$	–	–	–	–	5.09	6.52	50.2	–	–	–	1.359	1.371	–	0.0	–
HfS_2	TXX	$P\bar{3}m1(164)$	–	–	7.30	7.29	59.8	–	–	–	–	–	–	1.150	2.406	0.0	–	–
$HfSe_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.49	7.48	60.0	–	–	–	7.49	7.48	60.0	0.001	1.854	0.0	–	0.0
$HfTe_2$	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.91	7.91	60.0	–	–	–	7.90	7.90	60.0	0.005	1.351	0.0	–	0.0
TaO_2	TPH	$C2/m(12)$	$P\bar{6}m2(187)$	$Pmmn(59)$	6.14	6.13	60.0	5.95	5.92	60.4	6.01	6.00	60.2	0.239	0.595	0.0	0.0	0.0
TaS_2	HTP	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$C2/m(12)$	6.76	6.76	60.1	6.68	6.68	60.0	6.57	7.69	50.1	0.242	0.728	0.0	0.0	0.0
$TaSe_2$	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	7.00	7.00	59.8	6.94	6.94	60.0	6.99	7.00	59.9	0.282	0.284	0.0	0.0	0.0
$TaTe_2$	PTH	$P2_1/m(11)$	$P\bar{6}m2(187)$	$C2/m(12)$	7.50	7.50	54.7	7.44	7.43	59.9	6.88	8.65	55.4	0.111	0.115	0.0	0.0	0.0
WO_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.70	5.70	60.0	–	–	–	2.620	2.722	–	0.0	–
WS_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.40	6.40	60.0	–	–	–	2.345	4.115	–	0.0	–
WSe_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.66	6.66	59.9	–	–	–	1.257	1.281	–	0.0	–
WTe_2	TPH	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	7.05	7.27	61.0	7.18	7.18	60.0	7.27	7.04	61.0	0.004	0.473	0.0	0.0	0.0
ReO_2	TPX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	5.70	5.78	60.1	–	–	–	5.78	5.74	59.3	0.013	3.965	0.0	–	0.0
ReS_2	PTX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	6.60	6.54	58.7	–	–	–	6.44	6.60	60.2	0.004	2.516	0.0	–	0.0
$ReSe_2$	TPX	$C2/m(12)$	–	$P\bar{1}(2)$	6.86	6.67	60.3	–	–	–	6.86	6.68	60.2	0.093	2.313	0.0	–	0.0
$ReTe_2$	TPX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	7.13	7.31	60.4	–	–	–	7.30	7.26	58.6	0.007	1.876	0.0	–	0.0
OsS_2	TPX	$P2_1/m(11)$	–	$P2_1/m(11)$	6.63	7.11	57.6	–	–	–	7.11	6.62	57.6	0.005	3.611	0.0	–	0.0
$OsSe_2$	TPX	$P2_1/m(11)$	–	$P2_1/m(11)$	6.87	7.37	57.6	–	–	–	7.37	6.87	57.6	0.005	3.117	0.0	–	0.0
$OsTe_2$	TPX	$P2_1/m(11)$	–	$C2/m(12)$	7.80	7.32	57.8	–	–	–	7.79	7.32	57.6	0.221	3.032	0.0	–	0.0
IrO_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	6.35	6.37	55.1	–	–	–	6.29	6.29	60.4	0.059	2.606	0.0	–	0.0
IrS_2	TXX	$P\bar{1}(2)$	–	–	7.16	7.23	53.7	–	–	–	–	–	–	2.809	3.443	0.0	–	–
$IrSe_2$	TXX	$P\bar{1}(2)$	–	–	7.46	7.54	53.3	–	–	–	–	–	–	2.084	3.579	0.0	–	–
$IrTe_2$	TXX	$P\bar{1}(2)$	–	–	7.96	8.03	53.1	–	–	–	–	–	–	2.618	2.666	0.0	–	–
PtO_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	6.30	6.30	60.1	–	–	–	6.31	6.31	60.0	0.002	4.501	0.0	–	0.0
PtS_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.20	7.20	60.0	–	–	–	7.20	7.20	60.0	0.007	2.936	0.0	–	0.0
$PtSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.53	7.53	60.1	–	–	–	–	–	–	3.643	5.429	0.0	–	–
$PtTe_2$	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	8.06	8.06	60.0	–	–	–	8.07	8.07	59.9	0.033	3.900	0.0	–	0.0
AuO_2	PTH	$C2/m(12)$	$C2/m(12)$	$P2/m(10)$	6.93	6.93	53.9	6.14	7.79	66.7	6.91	6.91	54.5	0.278	0.371	3.3	4.0	0.0
AuS_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	10.41	7.81	62.5	1.049	1.253	–	–	0.0
$AuSe_2$	HPT	$P\bar{3}m1(164)$	$Pmm2(25)$	$C2/m(12)$	7.62	7.61	60.0	7.83	11.25	44.2	9.54	9.89	66.3	0.426	0.545	0.0	0.0	0.0
$AuTe_2$	TPX	$P\bar{3}m1(164)$	–	$P2_1/m(11)$	8.11	8.10	59.9	–	–	–	10.47	10.47	61.3	0.024	0.917	0.0	–	0.0

Table 80: List of TM-XVII

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
ScF_2	PHX	–	$P\bar{6}m2(187)$	$P1(2)$	–	–	–	6.28	6.29	60.0	6.30	6.83	63.1	0.652	0.827	–	4.0	0.0
$ScCl_2$	HTX	$C2/m(12)$	$P\bar{6}m2(187)$	–	7.28	7.28	59.7	7.11	7.11	59.9	–	–	–	0.085	2.970	0.7	3.7	–
$ScBr_2$	HTX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	7.61	7.61	59.4	7.43	7.42	59.9	–	–	–	0.156	2.274	0.0	3.8	–
ScI_2	THX	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	8.16	8.16	59.9	8.00	7.99	59.9	–	–	–	0.125	0.956	0.0	3.7	–
TiF_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.70	5.69	60.0	–	–	–	2.451	2.491	–	0.0	–
$TiCl_2$	HPX	–	$P\bar{6}m2(187)$	$P2_1/m(11)$	–	–	–	6.55	6.55	59.9	6.51	6.71	60.9	0.179	1.369	–	0.0	0.0
$TiBr_2$	HTP	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	7.36	7.64	58.7	6.94	6.93	60.0	9.56	6.77	69.3	0.670	0.720	7.8	0.0	0.0
VF_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	6.43	6.45	60.0	–	–	–	6.42	6.44	60.1	0.014	2.829	12.0	–	12.0
VCl_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.21	7.21	59.8	–	–	–	7.19	7.19	60.0	0.001	1.961	12.0	–	12.0
VBr_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.58	7.58	60.0	–	–	–	7.58	7.57	60.0	0.007	1.825	12.0	–	12.0
VI_2	TXX	$P\bar{3}m1(164)$	–	–	8.17	8.18	59.9	–	–	–	–	–	–	1.407	3.176	12.0	–	–
$CrBr_2$	THX	$C2/m(12)$	$Cmmm(65)$	–	8.07	8.07	53.5	8.02	8.02	53.5	–	–	–	0.554	2.069	16.0	16.0	–
CrI_2	HTX	$C2/m(12)$	$C2/m(12)$	–	8.68	8.68	53.8	8.57	8.57	54.6	–	–	–	0.001	3.470	16.0	16.0	–
MnF_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	6.73	6.73	59.8	–	–	–	6.73	6.73	59.8	0.004	2.553	20.0	–	20.0
$MnCl_2$	TXX	$P\bar{3}m1(164)$	–	–	7.45	7.46	59.8	–	–	–	–	–	–	0.942	1.647	20.0	–	–
$MnBr_2$	TXX	$P\bar{3}m1(164)$	–	–	7.79	7.80	59.8	–	–	–	–	–	–	0.941	1.621	20.0	–	–
FeF_2	TPH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	6.35	6.39	59.6	5.85	5.86	59.7	6.33	6.34	59.6	0.001	0.566	16.0	16.0	16.0
CoF_2	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	6.30	6.30	59.3	–	–	–	6.32	6.30	59.4	0.032	2.104	12.0	–	12.0
$CoBr_2$	TXX	$P\bar{3}m1(164)$	–	–	7.47	7.48	59.6	–	–	–	–	–	–	1.436	2.428	11.9	–	–
$NiBr_2$	TXX	$P\bar{3}m1(164)$	–	–	7.40	7.39	59.6	–	–	–	–	–	–	1.535	1.574	8.0	–	–
NiI_2	TXX	$P\bar{3}m1(164)$	–	–	7.96	7.95	59.6	–	–	–	–	–	–	2.497	3.016	7.8	–	–
YF_2	HPX	–	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	–	–	–	6.85	6.85	60.0	7.86	7.88	60.1	0.756	0.865	–	4.0	3.6
YCl_2	HPX	–	$P\bar{6}m2(187)$	$P3m1(156)$	–	–	–	7.53	7.52	59.8	7.60	7.62	60.0	0.685	0.867	–	3.9	0.0
YBr_2	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$C2/m(12)$	7.91	7.90	58.4	7.77	7.77	59.6	7.87	7.86	60.4	0.601	0.698	0.0	3.9	0.9
YI_2	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$C2/m(12)$	8.39	8.39	58.9	8.25	8.25	59.6	8.33	8.34	60.3	0.339	0.412	0.0	3.7	0.8
ZrF_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.23	6.23	60.0	–	–	–	0.876	0.892	–	0.0	–
$ZrCl_2$	HTP	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	7.11	6.71	61.8	6.84	6.84	60.1	7.11	7.11	56.3	0.436	0.440	0.0	0.0	0.0
$ZrBr_2$	HTP	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	7.01	7.40	61.6	7.13	7.13	60.1	7.40	7.40	56.6	0.024	0.028	0.0	0.0	0.0
ZrI_2	TPH	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	7.57	7.88	61.3	7.69	7.69	60.0	7.88	7.57	61.3	0.035	0.337	0.0	0.0	0.0
NbF_2	HXX	–	$P\bar{1}(2)$	–	–	–	–	6.58	6.46	52.4	–	–	–	2.240	4.478	–	0.8	–
$NbCl_2$	HXX	–	$Pmm2(25)$	–	–	–	–	6.74	6.60	60.6	–	–	–	3.274	3.278	–	0.0	–
$NbBr_2$	HXX	–	$Pmm2(25)$	–	–	–	–	7.09	7.09	57.9	–	–	–	2.904	2.906	–	0.0	–
NbI_2	HXX	–	$Pmm2(25)$	–	–	–	–	7.65	7.65	57.4	–	–	–	1.714	1.715	–	0.0	–
MoF_2	HXX	–	$P2/m(10)$	–	–	–	–	7.42	5.75	52.0	–	–	–	6.516	6.522	–	0.0	–
$MoCl_2$	PTH	$C2/m(12)$	$Cmmm(65)$	$P2_1/c(14)$	8.81	8.81	49.2	8.21	8.21	52.9	7.99	8.00	64.2	0.039	0.176	16.0	16.0	16.0
$MoBr_2$	THP	$C2/m(12)$	$Cmmm(65)$	$C2/m(12)$	8.92	8.92	50.9	8.32	8.31	54.8	14.76	7.59	74.9	0.198	0.629	16.0	16.0	16.0
MoI_2	THX	$C2/m(12)$	$Cmmm(65)$	–	9.33	9.33	51.8	8.96	8.97	54.0	–	–	–	0.269	2.477	15.9	16.0	–
TcF_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	6.92	6.66	60.7	0.992	2.717	–	–	16.0
TcI_2	TXX	$P\bar{3}m1(164)$	–	–	8.19	8.19	57.3	–	–	–	–	–	–	2.457	3.271	4.0	–	–
RuF_2	PTX	$P\bar{1}(2)$	–	$Cm(8)$	7.14	6.99	51.8	–	–	–	6.59	6.17	60.9	0.793	0.962	15.9	–	12.0
$RuCl_2$	TXX	$P\bar{3}m1(164)$	–	–	7.24	7.24	59.9	–	–	–	–	–	–	3.699	4.041	0.0	–	–
$RuBr_2$	TXX	$P\bar{3}m1(164)$	–	–	7.63	7.63	59.9	–	–	–	–	–	–	1.206	4.004	0.0	–	–
RhF_2	PXX	–	–	$Cmmm(65)$	–	–	–	–	–	–	15.14	15.34	22.8	2.132	4.657	–	–	4.0
RhI_2	THX	$P\bar{3}m1(164)$	$P\bar{3}m1(164)$	–	8.07	8.07	60.0	8.08	8.08	59.9	–	–	–	0.004	2.418	3.5	3.5	–
PdF_2	PTH	$P\bar{3}m1(164)$	$C2/m(12)$	$P2_1/c(14)$	6.83	6.84	59.9	6.54	7.64	48.8	6.98	6.98	72.0	0.177	0.237	8.0	3.9	0.0
$PdCl_2$	HTX	$P\bar{3}m1(164)$	$Cmmm(65)$	–	7.48	7.48	59.9	8.56	8.54	47.4	–	–	–	0.753	3.561	8.0	0.0	–
$PdBr_2$	PHT	$P\bar{3}m1(164)$	$Cmmm(65)$	$P\bar{1}(2)$	7.84	7.84	59.8	8.63	8.63	49.7	15.26	6.63	60.1	0.020	0.475	7.9	0.0	0.0
PdI_2	THP	$C2/m(12)$	$Cmmm(65)$	$P\bar{1}(2)$	10.07	10.07	45.5	8.96	8.96	51.8	14.21	7.29	75.9	0.153	0.225	0.0	0.0	0.0
AgF_2	HTX	$C2/m(12)$	$P\bar{1}(2)$	–	7.74	7.75	50.8	11.61	11.31	34.2	–	–	–	0.309	1.359	3.7	0.0	–
$AgCl_2$	THP	$C2/m(12)$	$Cmmm(65)$	$Cmmm(65)$	8.35	8.34	52.2	8.09	8.09	54.0	12.12	12.12	36.2	0.354	0.505	3.0	2.8	0.0
AgI_2	THP	$C2/m(12)$	$C2/m(12)$	$P2/m(10)$	9.23	9.23	50.7	9.35	9.35	50.1	10.18	14.09	66.1	0.005	0.026	0.0	0.0	0.0
HfF_2	HTP	$P2_1/m(11)$	$P\bar{6}m2(187)$	$Pm(6)$	6.99	6.98	50.7	6.08	6.08	59.9	5.97	7.04	64.7	0.463	0.726	0.0	0.0	0.0
$HfCl_2$	HTP	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	6.57	6.98	61.8	6.69	6.69	60.2	6.98	6.98	56.1	0.536	0.536	0.0	0.0	0.0
$HfBr_2$	TPH	$P2_1/m(11)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	6.88	7.28	61.8	6.99	6.99	60.1	7.28	7.28	56.4	0.001	0.039	0.0	0.0	0.0
HfI_2	PTH	$C2/m(12)$	$P\bar{6}m2(187)$	$P2_1/m(11)$	7.59	7.84	59.7	7.56	7.56	59.8	7.76	7.75	57.3	0.231	0.516	0.0	0.0	0.0
TaF_2	HXX	–	$Pmmn(59)$	–	–	–	–	6.09	6.11	52.2	–	–	–	4.641	8.674	–	0.0	–
TaI_2	HTX	$P\bar{1}(2)$	$Cm(8)$	–	7.63	7.43	61.3	7.81	7.79	60.1	–	–	–	0.119	5.416	0.0	0.0	–
WCl_2	HXX	–	$P2/m(10)$	–	–	–	–	8.60	7.59	46.7	–	–	–	10.252	10.470	–	0.0	–

(Continued on next page)

Table 80: List of TM-XVII

(Continued from previous page)

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
WBr_2	HTP	$C2/m(12)$	$Cmmm(65)$	$C2/m(12)$	9.46	9.46	47.9	8.60	8.57	53.1	7.67	14.49	74.5	0.039	0.356	15.9	15.9	15.9
WI_2	HXX	–	$P\bar{1}(2)$	–	–	–	–	11.12	10.24	35.6	–	–	–	7.959	9.436	–	0.0	–
OsF_2	HXX	–	$P2/c(13)$	–	–	–	–	5.58	6.86	48.1	–	–	–	2.329	12.030	–	0.0	–
$OsBr_2$	HTX	$P\bar{3}m1(164)$	$Cm(8)$	–	7.70	7.70	60.0	7.15	7.16	55.5	–	–	–	0.714	5.472	0.0	0.0	–
OsI_2	TXX	$P\bar{3}m1(164)$	–	–	8.13	8.13	60.1	–	–	–	–	–	–	2.659	5.434	0.0	–	–
IrF_2	HTP	$Pmma(51)$	$Pmmm(47)$	$Pbcm(57)$	6.24	6.23	62.0	8.41	6.40	39.9	9.04	7.26	36.1	0.084	0.743	0.0	0.0	0.0
$IrBr_2$	HXX	–	$Cmmm(65)$	–	–	–	–	7.41	9.03	52.7	–	–	–	1.219	1.663	–	0.0	–
IrI_2	TXX	$P\bar{3}m1(164)$	–	–	8.10	8.10	59.8	–	–	–	–	–	–	1.852	2.785	0.0	–	–
PtF_2	HXX	–	$Pmmm(47)$	–	–	–	–	8.83	6.67	39.2	–	–	–	0.865	3.365	–	2.4	–
$PtCl_2$	PTH	$P1(1)$	$Cmmm(65)$	$Pmna(53)$	10.87	10.48	36.1	8.74	8.63	47.1	7.80	7.82	68.6	0.189	0.364	0.0	0.0	0.0
PtI_2	THX	$C2/m(12)$	$Cmmm(65)$	–	10.27	10.31	44.7	9.81	9.74	47.3	–	–	–	0.019	2.617	0.0	0.0	–
$AuCl_2$	THP	$C2/m(12)$	$Cmmm(65)$	$P2/m(10)$	9.06	9.08	47.6	8.19	8.16	53.3	14.73	7.34	64.9	0.056	0.313	3.2	3.1	0.0
$AuBr_2$	THX	$C2/m(12)$	$Cmmm(65)$	–	9.13	9.14	49.1	8.48	8.48	53.4	–	–	–	0.020	0.853	0.0	0.0	–
AuI_2	THX	$C2/m(12)$	$Cmmm(65)$	–	9.66	9.68	48.9	9.12	9.12	52.3	–	–	–	0.111	0.875	0.0	0.0	–

Table 81: List of TM-TM

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
$ScSc_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.56	9.28	45.0	–	–	–	5.445	12.533	–	0.0	–
$ScCr_2$	HXX	–	$Cmmm(65)$	–	–	–	–	6.02	9.89	34.7	–	–	–	5.287	8.769	–	32.2	–
$ScTc_2$	HXX	–	$P2/c(13)$	–	–	–	–	7.27	10.03	35.5	–	–	–	2.727	8.818	–	0.0	–
$ScAg_2$	HTX	$P4/mmm(123)$	$P4/mmm(123)$	–	6.11	8.71	44.6	6.10	8.67	44.7	–	–	–	0.005	6.321	0.0	0.0	–
$ScPt_2$	HTX	$Cmme(67)$	$P4/mmm(123)$	–	8.24	10.28	29.8	5.91	8.33	45.1	–	–	–	0.742	6.458	0.0	0.0	–
$ScAu_2$	HTX	$C2/m(12)$	$P4/mmm(123)$	–	8.12	6.79	51.1	6.47	9.14	44.9	–	–	–	0.019	4.427	0.0	0.0	–
$TiHf_2$	PHX	–	$P4/mmm(123)$	$P\bar{1}(2)$	–	–	–	6.01	8.51	45.0	5.48	7.03	49.3	0.179	6.492	–	0.0	0.0
VSc_2	PXX	–	–	$P4/mmm(123)$	–	–	–	–	–	–	6.36	9.05	44.6	0.966	1.508	–	–	0.0
VTi_2	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	5.89	8.37	44.3	5.88	8.31	44.9	–	–	–	0.228	4.235	0.0	0.0	–
VV_2	HXX	–	$Cmmm(65)$	–	–	–	–	8.01	5.10	35.3	–	–	–	6.097	19.320	–	0.0	–
VMn_2	HTX	$P4/mmm(123)$	$P4/mmm(123)$	–	5.79	8.22	44.9	5.77	8.22	44.6	–	–	–	0.023	16.527	21.1	21.1	–
VY_2	PTH	$P4/mmm(123)$	$Pmmm(47)$	$P2_1/m(11)$	9.96	7.04	44.8	6.99	9.84	44.7	7.04	7.03	62.2	0.366	0.558	9.8	6.2	0.0
VZr_2	TPH	$P4/mmm(123)$	$P4/mmm(123)$	$P4/mmm(123)$	6.31	8.91	45.0	6.30	8.91	45.1	6.31	8.94	44.9	0.001	0.004	0.0	0.0	0.0
$CrSc_2$	PHT	$P4/mmm(123)$	$P4/mmm(123)$	$P\bar{1}(2)$	6.42	9.09	45.0	6.42	9.09	44.9	7.40	6.70	52.5	0.209	0.213	7.0	7.0	0.0
$CrMn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.00	5.65	44.9	–	–	–	11.904	16.133	–	23.7	–
CrY_2	HTP	$C2/m(12)$	$P4/mmm(123)$	$P2_1/c(14)$	8.81	6.98	53.0	6.86	9.72	44.9	10.19	7.21	44.0	0.498	0.712	7.6	6.1	7.8
$CrZr_2$	PHT	$P4/mmm(123)$	$P4/mmm(123)$	$P4/mmm(123)$	8.68	6.38	45.3	6.29	8.64	46.4	9.15	6.28	43.3	0.094	0.119	0.0	0.0	0.0
$CrRu_2$	HXX	–	$C2/m(12)$	–	–	–	–	6.88	7.84	41.6	–	–	–	1.187	5.058	–	0.0	–
$CrHf_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.24	8.82	45.0	–	–	–	2.721	5.543	–	0.0	–
$MnSc_2$	PHT	$P\bar{1}(2)$	$P4/mmm(123)$	$P2_1/m(11)$	6.56	8.25	53.2	6.30	8.92	44.9	6.81	8.28	52.2	0.107	0.154	5.8	0.0	5.1
$MnCr_2$	HXX	–	$Pccm(49)$	–	–	–	–	5.00	7.11	45.0	–	–	–	16.040	17.407	–	8.2	–
$MnMn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	5.56	7.87	45.0	–	–	–	9.663	13.770	–	27.3	–
$MnZr_2$	THP	$P4/mmm(123)$	$P4/mmm(123)$	$P\bar{1}(2)$	6.23	8.86	44.6	6.24	8.80	45.1	6.83	6.35	58.3	0.015	0.188	0.0	0.0	0.0
$MnOs_2$	HXX	–	$Pmma(51)$	–	–	–	–	7.02	8.72	36.5	–	–	–	5.890	6.289	–	5.9	–
$MnAu_2$	HTX	$P\bar{3}m1(164)$	$P4/mmm(123)$	–	5.96	5.96	59.3	6.68	6.68	52.5	–	–	–	0.711	3.227	17.2	18.0	–
$FeSc_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	6.20	8.77	45.1	6.20	8.79	44.9	–	–	–	0.002	1.286	0.0	0.0	–
$FeZr_2$	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	8.22	6.70	50.2	1.057	1.825	–	–	0.0
$FeTc_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	5.31	7.92	59.9	3.152	7.289	–	–	0.0
$FePd_2$	HTX	$Cmmm(65)$	$P\bar{6}m2(187)$	–	5.54	8.18	41.8	5.48	5.48	59.9	–	–	–	0.217	1.393	15.4	15.7	–
$CoZr_2$	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	7.79	6.52	52.6	2.502	2.631	–	–	0.0
$CoHf_2$	TPX	$C2/m(12)$	–	$C2/m(12)$	6.43	7.81	51.7	–	–	–	7.82	6.45	51.7	0.000	2.055	0.0	–	0.0
$CoIr_2$	HTX	$C2/m(12)$	$Amm2(38)$	–	8.38	8.39	35.6	8.23	8.24	35.8	–	–	–	0.363	0.833	5.0	6.3	–
$NiSc_2$	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	7.47	7.51	59.4	6.82	6.85	59.7	7.46	7.49	59.6	0.008	0.030	0.0	0.0	0.0
NiY_2	TPX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	8.04	8.08	59.7	–	–	–	8.07	8.09	59.3	0.002	0.841	0.0	–	0.0
$NiHf_2$	PTX	$C2/m(12)$	–	$C2/m(12)$	6.43	8.31	54.4	–	–	–	8.32	6.42	54.6	0.023	1.233	0.0	–	0.0
$NiIr_2$	HPT	$C2/m(12)$	$Amm2(38)$	$Pmmn(59)$	8.49	8.49	34.7	8.41	8.44	34.6	8.69	8.69	53.7	0.275	0.300	0.0	0.0	2.6
YY_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	10.21	11.25	34.0	3.582	4.649	–	–	0.0
YZr_2	HTX	$Cmme(67)$	$Cmme(67)$	–	11.03	9.78	27.6	9.77	11.02	27.6	–	–	–	0.007	2.366	0.0	0.0	–
$ZrTi_2$	HXX	–	$P2/c(13)$	–	–	–	–	5.76	9.53	35.4	–	–	–	2.361	6.522	–	0.0	–
$ZrCr_2$	HXX	–	$Cmmm(65)$	–	–	–	–	6.06	9.42	39.0	–	–	–	7.350	13.581	–	29.3	–
$ZrNb_2$	HTX	$P\bar{1}(2)$	$P2/c(13)$	–	10.55	8.26	31.9	11.36	8.50	28.5	–	–	–	0.765	14.293	0.0	0.0	–
$ZrPd_2$	TPH	$P4/mmm(123)$	$P4/mmm(123)$	$P4/mmm(123)$	8.79	6.31	42.6	6.19	8.63	43.9	6.97	6.98	50.3	0.238	0.516	0.0	0.0	0.0
$ZrHf_2$	HPX	–	$C2/m(12)$	$Cm(8)$	–	–	–	8.59	9.71	40.1	9.25	7.52	51.6	0.404	3.838	–	0.0	0.0
$ZrAu_2$	HTX	$P4/mmm(123)$	$P4/mmm(123)$	–	8.64	6.12	45.1	8.63	6.11	45.0	–	–	–	0.009	7.649	0.0	0.0	–
NbV_2	PXX	–	–	$P1(1)$	–	–	–	–	–	–	6.48	6.49	49.9	0.861	1.278	–	–	0.0
$NbNb_2$	HTX	$P2/c(13)$	$P2/c(13)$	–	8.44	8.19	38.4	8.44	8.19	38.4	–	–	–	0.005	3.812	0.0	0.0	–
$NbRu_2$	TXX	$P2_1/m(11)$	–	–	9.02	7.79	30.2	–	–	–	–	–	–	2.016	2.038	0.0	–	–
$MoMn_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	6.15	8.72	43.9	6.07	8.59	45.0	–	–	–	0.406	12.003	26.2	26.1	–
MoY_2	PHX	–	$Pmmm(47)$	$P\bar{1}(2)$	–	–	–	6.81	9.50	44.0	8.88	7.07	53.3	0.460	0.934	–	0.0	0.0
$TcTi_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.64	6.11	45.0	–	–	–	2.445	2.569	–	0.0	–
TcV_2	PXX	–	–	$P2/c(13)$	–	–	–	–	–	–	9.01	7.21	35.2	2.589	2.619	–	–	0.0
$TcMn_2$	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	8.44	5.97	44.9	8.32	5.82	45.4	–	–	–	0.042	11.865	29.7	12.6	–
TcY_2	HXX	–	$P4/mmm(123)$	–	–	–	–	9.74	6.89	45.0	–	–	–	1.260	1.275	–	0.0	–
$TcTa_2$	THX	$C2/m(12)$	$P2/c(13)$	–	8.15	8.89	35.1	7.50	9.08	38.3	–	–	–	0.488	0.844	0.0	0.0	–
$RuSc_2$	HPX	–	$P4/mmm(123)$	$P4/mmm(123)$	–	–	–	6.40	9.05	45.0	7.17	7.16	53.1	0.053	1.564	–	0.0	0.0
$RuTi_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	5.93	8.40	44.6	–	–	–	0.919	1.873	–	0.0	–
RuV_2	THX	$C2/m(12)$	$C2/m(12)$	–	7.53	8.24	34.8	6.46	7.59	46.1	–	–	–	0.353	1.832	0.0	0.0	–
$RuMn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.41	5.93	44.4	–	–	–	2.015	11.563	–	33.2	–

(Continued on next page)

Table 81: List of TM-TM

(Continued from previous page)

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
RuY_2	HPX	–	$P4/mmm(123)$	$C2/m(12)$	–	–	–	6.79	9.60	45.0	8.98	7.56	50.4	0.414	1.389	–	0.0	0.0
$RuTc_2$	TXX	$C2/m(12)$	–	–	8.15	9.42	30.0	–	–	–	–	–	–	4.418	5.983	0.0	–	–
$RuRu_2$	HXX	–	$P2/c(13)$	–	–	–	–	8.06	6.89	38.8	–	–	–	1.030	5.235	–	0.0	–
$RuPd_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.51	5.51	59.8	–	–	–	6.269	7.276	–	0.0	–
$RuTa_2$	HTX	$C2/m(12)$	$C2/m(12)$	–	8.83	8.10	35.0	6.93	8.12	45.8	–	–	–	0.412	7.279	0.0	0.0	–
$RuOs_2$	TXX	$P2_1/m(11)$	–	–	8.36	8.36	37.6	–	–	–	–	–	–	2.801	5.282	0.0	–	–
$RhSc_2$	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	7.09	8.58	51.0	0.904	2.281	–	–	0.0
RhY_2	PTX	$P\bar{3}m1(164)$	–	$P2_1/m(11)$	8.22	8.23	59.9	–	–	–	10.37	8.57	33.8	0.349	2.516	0.0	–	0.0
$RhAg_2$	HXX	–	$Pmmm(47)$	–	–	–	–	8.14	5.75	43.3	–	–	–	8.602	8.637	–	0.0	–
$RhAu_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	7.96	5.61	44.3	–	–	–	5.785	5.794	–	0.0	–
$PdSc_2$	HPT	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	7.99	7.97	59.6	6.91	6.93	60.1	7.97	7.95	60.0	0.376	0.382	0.0	0.0	0.0
$PdZr_2$	HXX	–	$C2/m(12)$	–	–	–	–	8.73	7.47	45.6	–	–	–	0.831	4.247	–	0.0	–
$PdRu_2$	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	8.34	8.33	36.9	3.878	3.891	–	–	0.0
$PdAg_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	5.83	8.37	43.3	–	–	–	6.189	6.315	–	0.0	–
$PdIr_2$	PHX	–	$Amm2(38)$	$Pmmn(59)$	–	–	–	9.21	9.21	32.4	8.73	8.72	55.8	0.795	1.191	–	0.0	0.0
$PdPt_2$	TPX	$C2/m(12)$	–	$Pmmn(59)$	9.36	9.36	33.0	–	–	–	9.04	9.03	57.0	0.607	0.845	0.0	–	0.0
$PdAu_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.72	5.71	59.6	–	–	–	5.169	5.185	–	0.0	–
$AgSc_2$	TPH	$C2/m(12)$	$P4/mmm(123)$	$C2/m(12)$	9.29	6.62	57.6	6.51	9.21	45.0	9.30	6.64	57.5	0.003	0.219	0.0	0.0	0.0
$AgMn_2$	THX	$C2/m(12)$	$P1(1)$	–	8.19	5.68	57.8	7.79	8.67	39.0	–	–	–	0.126	6.400	33.0	34.4	–
AgY_2	PXX	–	–	$P\bar{1}(2)$	–	–	–	–	–	–	7.85	10.58	33.5	1.843	2.438	–	–	0.0
$AgPd_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	10.12	5.58	46.0	1.479	3.669	–	–	0.0
$AgHf_2$	HXX	–	$P1(1)$	–	–	–	–	6.06	10.15	34.5	–	–	–	2.380	7.840	–	0.0	–
HfV_2	THX	$Cmme(67)$	$Cmme(67)$	–	10.52	9.63	23.2	9.62	10.50	23.3	–	–	–	0.008	14.503	0.0	0.0	–
HfY_2	THX	$P4/mmm(123)$	$P4/mmm(123)$	–	10.14	7.15	44.6	9.39	6.75	45.8	–	–	–	0.502	5.011	0.0	2.5	–
$HfAu_2$	THX	$C2/m(12)$	$P\bar{6}m2(187)$	–	7.35	6.29	50.1	6.18	6.19	60.1	–	–	–	0.297	7.760	0.0	0.0	–
TaY_2	HXX	–	$P4/mmm(123)$	–	–	–	–	6.98	9.88	44.9	–	–	–	0.849	4.248	–	0.0	–
WNb_2	HXX	–	$P\bar{1}(2)$	–	–	–	–	6.80	8.14	41.9	–	–	–	1.420	1.877	–	0.0	–
WTa_2	HPT	$C2/m(12)$	$P\bar{1}(2)$	$P1(1)$	9.13	8.16	32.9	8.94	7.45	38.0	6.10	8.07	59.2	0.614	0.738	0.0	0.0	0.0
$ReSc_2$	PHT	$P4/mmm(123)$	$P4/mmm(123)$	$P4/mmm(123)$	6.49	9.16	45.0	6.48	9.17	45.0	6.48	9.17	45.0	0.001	0.001	0.0	0.0	0.0
$ReTi_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.12	8.66	45.0	–	–	–	2.452	3.638	–	0.0	–
$OsSc_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	9.06	6.40	45.0	–	–	–	1.942	5.550	–	0.0	–
$OsTi_2$	HPX	–	$P4/mmm(123)$	$P4/mmm(123)$	–	–	–	5.96	8.44	44.7	6.66	5.97	63.4	0.005	2.918	–	0.0	0.0
OsV_2	HXX	–	$P2/c(13)$	–	–	–	–	9.15	7.17	36.0	–	–	–	1.739	6.933	–	0.0	–
$OsMn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.30	5.87	45.0	–	–	–	1.335	12.451	–	32.3	–
$OsZr_2$	TPH	$P\bar{1}(2)$	$P\bar{6}m2(187)$	$P\bar{1}(2)$	8.12	8.43	49.5	7.09	7.13	61.1	9.30	8.10	43.7	0.125	0.816	0.0	0.0	0.0
$OsNb_2$	HTX	$C2/m(12)$	$Pmmm(47)$	–	7.99	8.64	46.1	9.59	7.60	37.6	–	–	–	0.293	2.822	0.0	0.0	–
$OsHf_2$	TPX	$P\bar{1}(2)$	–	$P\bar{1}(2)$	7.95	8.40	50.1	–	–	–	7.87	8.40	50.4	0.007	0.966	0.0	–	0.0
$IrSc_2$	PTX	$P\bar{3}m1(164)$	–	$P\bar{3}m1(164)$	7.97	7.96	59.7	–	–	–	7.93	7.93	60.0	0.002	1.432	0.0	–	0.0
$IrTi_2$	HXX	–	$P2/m(10)$	–	–	–	–	8.77	6.56	40.4	–	–	–	2.498	2.506	–	6.4	–
IrY_2	PTX	$P\bar{3}m1(164)$	–	$C2/m(12)$	8.37	8.37	59.6	–	–	–	7.75	9.08	50.1	0.156	2.223	0.0	–	0.0
$IrZr_2$	HTP	$P\bar{3}m1(164)$	$P4/mmm(123)$	$P\bar{3}m1(164)$	8.28	8.25	60.0	8.47	5.99	45.0	8.28	8.26	59.9	0.648	0.649	0.0	0.0	0.0
$IrHf_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	6.66	8.17	52.1	1.216	1.762	–	–	0.0
$IrOs_2$	HXX	–	$P2/c(13)$	–	–	–	–	8.11	6.97	39.2	–	–	–	7.871	9.036	–	0.0	–
$PtSc_2$	PTH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	8.13	8.11	59.0	7.26	7.28	60.1	8.02	8.07	59.7	0.019	0.447	0.0	0.0	0.0
$PtTi_2$	HXX	–	$Pmmm(47)$	–	–	–	–	9.50	7.72	35.7	–	–	–	2.145	2.147	–	0.0	–
PtV_2	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	7.51	6.20	45.1	3.050	5.944	–	–	0.0
PtY_2	TPH	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	8.43	8.45	60.0	7.69	7.75	59.7	8.42	8.46	60.1	0.002	0.602	0.0	0.0	0.0
$PtZr_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	8.68	6.52	55.6	1.498	3.438	–	–	0.0
$PtNb_2$	PHX	–	$P\bar{1}(2)$	$Cmmm(65)$	–	–	–	9.95	8.57	34.2	9.67	7.29	41.3	0.740	2.650	–	0.0	0.0
$PtRu_2$	THP	$C2/m(12)$	$Amm2(38)$	$Pmmn(59)$	9.42	9.42	33.1	9.04	9.04	33.5	8.86	8.86	50.4	0.224	0.255	5.8	0.0	0.0
$PtRh_2$	TXX	$C2/m(12)$	–	–	9.23	9.23	33.5	–	–	–	–	–	–	1.102	3.120	0.0	–	–
$PtHf_2$	TXX	$C2/m(12)$	–	–	6.43	8.63	56.0	–	–	–	–	–	–	1.333	2.460	0.0	–	–
$PtIr_2$	HTX	$C2/m(12)$	$Amm2(38)$	–	9.25	9.25	33.1	9.09	9.10	33.2	–	–	–	0.235	1.098	0.0	0.0	–
$PtAu_2$	HXX	–	$C2/m(12)$	–	–	–	–	7.88	6.77	44.4	–	–	–	3.958	3.996	–	0.0	–
$AuSc_2$	HTP	$C2/m(12)$	$P\bar{6}m2(187)$	$P\bar{3}m1(164)$	8.70	8.65	55.4	6.98	6.98	60.0	8.68	8.60	56.4	0.216	0.241	0.0	0.0	0.0
$AuCr_2$	HXX	–	$C2/m(12)$	–	–	–	–	8.58	7.43	42.8	–	–	–	3.104	3.114	–	36.8	–
$AuMn_2$	TXX	$P\bar{1}(2)$	–	–	8.41	7.57	39.5	–	–	–	–	–	–	4.828	5.453	33.6	–	–

(Continued on next page)

Table 81: List of TM-TM

(Continued from previous page)

species	Initial structure indices	space group			lattice parameters									relative energy		spin moment [μ_B/unit cell]		
		T	H	P	T			H			P			ΔE_1	ΔE_2			
					a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	a [Å]	b [Å]	γ [deg]	[eV]	[eV]	T	H	P
AuY_2	HPT	$C2/m(12)$	$P\bar{6}m2(187)$	$C2/m(12)$	9.06	9.01	55.0	7.58	7.60	60.2	9.01	8.97	55.0	0.274	0.282	0.0	0.0	0.0
$AuPd_2$	THX	$C2/m(12)$	$Amm2(38)$	–	9.68	9.67	32.9	9.40	9.42	33.5	–	–	–	0.742	2.001	0.0	0.0	–
$AuAg_2$	PTH	$P6/mmm(191)$	$Amm2(38)$	$P6/mmm(191)$	9.75	9.75	59.9	9.14	9.10	35.8	9.75	9.75	59.9	0.028	0.460	0.0	0.0	0.0
$AuIr_2$	PTX	$Pmmn(59)$	–	$Pmmn(59)$	8.35	8.87	57.9	–	–	–	8.38	8.37	63.9	0.161	2.445	0.0	–	0.0