Supplemental information 1

The space-group, lattice parameters, relative energy and spin magnetic moment are shown in the following tables. These tables are classified by the space-groups: $P\bar{3}m1(164)$, $P2_1/m(11)$, $P4mmm(123)$, $C2/m(12)$, $P\bar{6}m2(187)$, $Amm2(38)$, $Cmmm(65)$, Memory structures, Planar structures, Distorted planar structures.

T, H, and P represent the types of initial structures. X means the structure is not in the group "three stable structures" mentioned in the paper. 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. In other words, X means 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 $P\bar{3}m1(164)$

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	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	5.46	5.45	59.9	5.45	5.45	60.0	–	–	–	0.046	3.644	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
$BeGe_2$	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	–
$BeRb_2$	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	–
$BeTe_2$	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
$BeCs_2$	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	–
$BeBa_2$	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
$BeAu_2$	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	–
$BePb_2$	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
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
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
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	–
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
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	–
BGe_2	TXX	$P\bar{3}m1(164)$	–	–	6.71	6.71	60.0	–	–	–	–	–	–	0.916	1.964	0.0	–	–
BRb_2	TXX	$P\bar{3}m1(164)$	–	–	10.45	10.46	58.3	–	–	–	–	–	–	2.549	3.286	11.0	–	–
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	–	–
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	–
BSn_2	TXX	$P\bar{3}m1(164)$	–	–	7.36	7.36	60.0	–	–	–	–	–	–	1.261	2.480	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
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	–
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	–
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	–	–
CK_2	TXX	$P\bar{3}m1(164)$	–	–	9.26	9.28	58.4	–	–	–	–	–	–	1.062	2.497	8.0	–	–
CCa_2	TXX	$P\bar{3}m1(164)$	–	–	7.94	7.94	58.9	–	–	–	–	–	–	1.278	3.176	0.0	–	–
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	–	–
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	–
CRb_2	TXX	$P\bar{3}m1(164)$	–	–	9.55	9.56	58.4	–	–	–	–	–	–	0.985	2.050	8.1	–	–
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	–	–
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	–
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
CBa_2	TXX	$P\bar{3}m1(164)$	–	–	8.49	8.49	59.8	–	–	–	–	–	–	1.533	2.727	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
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	–
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	–	–
NCa_2	TXX	$P\bar{3}m1(164)$	–	–	7.22	7.22	60.0	–	–	–	–	–	–	2.863	3.023	0.0	–	–
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
NRb_2	TXX	$P\bar{3}m1(164)$	–	–	9.12	9.12	57.1	–	–	–	–	–	–	0.850	1.934	4.1	–	–
NSr_2	TXX	$P\bar{3}m1(164)$	–	–	7.71	7.71	60.0	–	–	–	–	–	–	2.541	4.094	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	–	–

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Table 1: List of $P\bar{3}m1(164)$

(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
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	–
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
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	–
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
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
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
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
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
ORb_2	TXX	$P\bar{3}m1(164)$	–	–	8.36	8.36	59.7	–	–	–	–	–	–	1.533	1.866	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	–
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	–
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
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	–
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
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	–
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	–
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
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	–
AlO_2	TXX	$P\bar{3}m1(164)$	–	–	5.71	5.71	64.4	–	–	–	–	–	–	2.061	2.775	4.0	–	–
$AlAl_2$	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	–
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	–
$SiCa_2$	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
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
$SiCs_2$	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
$SiBa_2$	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
$SiPb_2$	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
PS_2	TXX	$P\bar{3}m1(164)$	–	–	6.59	6.59	60.0	–	–	–	–	–	–	1.396	1.559	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
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
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	–
PSe_2	TXX	$P\bar{3}m1(164)$	–	–	6.99	6.99	60.0	–	–	–	–	–	–	0.943	2.920	0.0	–	–
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
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
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
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	–
PTe_2	TXX	$P\bar{3}m1(164)$	–	–	7.50	7.51	59.8	–	–	–	–	–	–	1.708	1.971	0.0	–	–
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
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
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
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	–
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

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Table 1: List of $P\bar{3}m1(164)$

(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
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	–
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
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
SSr_2	TXX	$P\bar{3}m1(164)$	–	–	8.35	8.35	59.7	–	–	–	–	–	–	0.977	2.337	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
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
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
SBa_2	TXX	$P\bar{3}m1(164)$	–	–	8.84	8.84	59.6	–	–	–	–	–	–	1.845	2.529	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
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
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
$ClCa_2$	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	–
$ClRb_2$	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
$ClSr_2$	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	–
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
$ClIn_2$	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
$ClCs_2$	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
$ClBa_2$	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
$ClTl_2$	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	–
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
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
$ScBr_2$	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	–
$ScTe_2$	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
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	–
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
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
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
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
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
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	–	–
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
$CrSe_2$	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
$CrCs_2$	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	–
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
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
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
$MnCl_2$	TXX	$P\bar{3}m1(164)$	–	–	7.45	7.46	59.8	–	–	–	–	–	–	0.942	1.647	20.0	–	–
$MnSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.02	7.03	60.0	–	–	–	–	–	–	1.765	2.984	11.5	–	–
$MnBr_2$	TXX	$P\bar{3}m1(164)$	–	–	7.79	7.80	59.8	–	–	–	–	–	–	0.941	1.621	20.0	–	–
$MnAu_2$	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	–
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
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
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	–
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
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	–	–
$NiBe_2$	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	–
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	–	–
$NiSc_2$	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
$NiSe_2$	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

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Table 1: List of $P\bar{3}m1(164)$

(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
$NiBr_2$	TXX	$P\bar{3}m1(164)$	–	–	7.40	7.39	59.6	–	–	–	–	–	–	1.535	1.574	8.0	–	–
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
NiI_2	TXX	$P\bar{3}m1(164)$	–	–	7.96	7.95	59.6	–	–	–	–	–	–	2.497	3.016	7.8	–	–
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	–
$GeMg_2$	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
$GeCl_2$	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
$GeCa_2$	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
$GeSe_2$	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	–
$GeBr_2$	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
$GeSr_2$	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
$GeCd_2$	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	–
$GeTe_2$	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
$GeCs_2$	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
$GeBa_2$	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
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
$AsCa_2$	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
$AsSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.33	7.34	59.3	–	–	–	–	–	–	1.864	1.925	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
$AsPd_2$	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
$AsSn_2$	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
$AsTe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.81	7.78	58.8	–	–	–	–	–	–	1.290	1.502	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
$AsBa_2$	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
$SeLi_2$	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	–	–
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
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
$SeCa_2$	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	–
$SeSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.47	7.47	60.3	–	–	–	–	–	–	0.859	2.830	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
$SeSr_2$	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	–
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
$SeIn_2$	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	–
$SeCs_2$	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
$SeBa_2$	TXX	$P\bar{3}m1(164)$	–	–	9.11	9.10	59.5	–	–	–	–	–	–	1.546	1.697	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
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
$BrCa_2$	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	–
$BrRb_2$	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
$BrSr_2$	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	–
$BrCs_2$	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
$BrBa_2$	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	–
$BrTl_2$	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
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
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
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
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
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	–	–
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
TcI_2	TXX	$P\bar{3}m1(164)$	–	–	8.19	8.19	57.3	–	–	–	–	–	–	2.457	3.271	4.0	–	–

(Continued on next page)

Table 1: List of $P\bar{3}m1(164)$

(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
$RuCl_2$	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	–	–
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
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
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	–
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
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
PdS_2	TXX	$P\bar{3}m1(164)$	–	–	7.14	7.14	60.0	–	–	–	–	–	–	0.888	2.958	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	–
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
$PdCa_2$	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
$PdSc_2$	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
$PdSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.51	7.51	59.8	–	–	–	–	–	–	2.841	4.700	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
$PdRb_2$	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
$PdSr_2$	TXX	$P\bar{3}m1(164)$	–	–	9.14	9.14	59.2	–	–	–	–	–	–	2.115	4.412	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
$PdCs_2$	TXX	$P\bar{3}m1(164)$	–	–	10.85	10.91	59.8	–	–	–	–	–	–	0.882	2.308	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
$AgAl_2$	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
$AgCa_2$	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	–	–
$AgCs_2$	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
$AgBa_2$	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
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	–	–
$CdBa_2$	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
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
$InPd_2$	PXX	–	–	$P\bar{3}m1(164)$	–	–	–	–	–	–	8.97	9.04	59.4	3.730	4.080	–	–	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	–	–
$SnCa_2$	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
$SnBr_2$	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
$SnSr_2$	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
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
$SnBa_2$	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
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
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
$SbSe_2$	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	–	–
$SbBa_2$	TXX	$P\bar{3}m1(164)$	–	–	10.03	10.07	59.9	–	–	–	–	–	–	1.313	6.828	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
TeS_2	TXX	$P\bar{3}m1(164)$	–	–	7.71	7.71	59.8	–	–	–	–	–	–	2.292	2.634	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
$TeSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.97	7.97	59.8	–	–	–	–	–	–	0.931	2.325	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
$TeSr_2$	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	–
$TeTe_2$	TXX	$P\bar{3}m1(164)$	–	–	8.57	8.57	59.3	–	–	–	–	–	–	1.102	1.829	0.0	–	–
$TeCs_2$	TXX	$P\bar{3}m1(164)$	–	–	12.04	12.14	59.4	–	–	–	–	–	–	1.228	2.144	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
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	–
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
$CsCs_2$	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
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

(Continued on next page)

Table 1: List of $P\bar{3}m1(164)$

(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
$BaBr_2$	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
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
TaN_2	TXX	$P\bar{3}m1(164)$	–	–	6.32	6.32	60.0	–	–	–	–	–	–	1.284	5.132	3.7	–	–
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
$OsBr_2$	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	–	–
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
$IrSc_2$	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
$IrSr_2$	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	–
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
$IrIn_2$	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
IrI_2	TXX	$P\bar{3}m1(164)$	–	–	8.10	8.10	59.8	–	–	–	–	–	–	1.852	2.785	0.0	–	–
$IrBa_2$	TXX	$P\bar{3}m1(164)$	–	–	9.28	9.29	59.5	–	–	–	–	–	–	0.965	2.130	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
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
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
$PtSc_2$	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
$PtGa_2$	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	–
$PtSe_2$	TXX	$P\bar{3}m1(164)$	–	–	7.53	7.53	60.1	–	–	–	–	–	–	3.643	5.429	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
$PtSr_2$	TXX	$P\bar{3}m1(164)$	–	–	9.07	9.07	59.5	–	–	–	–	–	–	2.234	5.942	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
$PtIn_2$	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	–
$PtTe_2$	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
$PtCs_2$	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	–
$PtHg_2$	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	–
$PtTl_2$	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
$PtBi_2$	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
$AuAl_2$	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
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
$AuCa_2$	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
$AuSc_2$	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
$AuSe_2$	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
$AuRb_2$	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
$AuSr_2$	TXX	$P\bar{3}m1(164)$	–	–	9.34	9.35	59.4	–	–	–	–	–	–	1.124	1.688	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	–
$AuSb_2$	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	–
$AuTe_2$	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
$AuCs_2$	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
$AuHg_2$	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	–
$AuBi_2$	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
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	–
$HgCa_2$	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
$HgCs_2$	TXX	$P\bar{3}m1(164)$	–	–	11.55	11.43	57.4	–	–	–	–	–	–	1.902	3.325	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
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
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
$PbCa_2$	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

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Table 1: List of $P\bar{3}m1(164)$

(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
$PbBr_2$	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
$PbSr_2$	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
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
$PbBa_2$	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
$BiAl_2$	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
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
$BiTe_2$	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	–
$BiBa_2$	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 2: List of $P2_1/m(11)$

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
$BeZr_2$	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	6.05	8.11	41.6	1.302	2.180	–	–	0.0
$BeTa_2$	HXX	–	$P2_1/m(11)$	–	–	–	–	6.35	5.61	55.3	–	–	–	7.349	8.785	–	0.0	–
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
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	–	–
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
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	–
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	–
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
OBe_2	TXX	$P2_1/m(11)$	–	–	5.17	4.95	58.5	–	–	–	–	–	–	1.114	3.420	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	–
OMo_2	TXX	$P2_1/m(11)$	–	–	6.79	6.55	50.1	–	–	–	–	–	–	1.871	7.775	0.0	–	–
OBa_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	9.20	9.19	59.2	2.125	2.135	–	–	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
$AlSb_2$	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
$AlHg_2$	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
$SiPd_2$	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
$SiCs_2$	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
PSi_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	8.81	8.81	49.0	1.687	4.190	–	–	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	–	–
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
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
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
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
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
SBe_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	6.83	5.30	90.0	2.333	4.987	–	–	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
SZr_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	7.97	7.04	63.8	1.250	2.169	–	–	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
SBi_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	9.73	10.66	56.2	1.536	1.745	–	–	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
$TiCl_2$	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
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
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
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
CrK_2	HXX	–	$P2_1/m(11)$	–	–	–	–	8.68	10.18	53.9	–	–	–	1.711	3.942	–	20.3	–
$CrCa_2$	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	–
$CrSe_2$	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
$CrBa_2$	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	8.70	9.16	58.2	1.423	2.977	–	–	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
$MnSc_2$	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
$CoSe_2$	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
$CoZr_2$	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	7.79	6.52	52.6	2.502	2.631	–	–	0.0

(Continued on next page)

Table 2: List of $P2_1/m(11)$

(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
$NiSn_2$	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
$GaCa_2$	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
$GeCr_2$	THX	$P2_1/m(11)$	–	–	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
$GeAu_2$	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	–
$AsSc_2$	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
AsV_2	TXX	$P2_1/m(11)$	–	–	6.21	6.96	62.8	–	–	–	–	–	–	7.718	8.634	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
$AsZr_2$	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
$AsBa_2$	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
$AsHf_2$	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
$SeLi_2$	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
$SeSc_2$	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
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
$SeSn_2$	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
$BrLi_2$	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
$BrSn_2$	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
$BrHf_2$	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
$RbCa_2$	HXX	–	$P2_1/m(11)$	–	–	–	–	14.39	15.13	16.3	–	–	–	7.929	7.954	–	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
$NbCa_2$	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	–
$NbRu_2$	TXX	$P2_1/m(11)$	–	–	9.02	7.79	30.2	–	–	–	–	–	–	2.016	2.038	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	–
MoP_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	6.14	6.91	63.6	1.389	3.230	–	–	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
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
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
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
$RuCa_2$	TXX	$P2_1/m(11)$	–	–	8.83	7.22	52.3	–	–	–	–	–	–	1.040	1.344	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
$RuOs_2$	TXX	$P2_1/m(11)$	–	–	8.36	8.36	37.6	–	–	–	–	–	–	2.801	5.282	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
$CdCa_2$	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
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
$SnCl_2$	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
$SnCr_2$	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	–
$TeLi_2$	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
$TeCa_2$	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	–
$TeSc_2$	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
$TeTl_2$	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
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
$CsTl_2$	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
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
$TaAs_2$	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
$TaTe_2$	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
$TaBi_2$	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

(Continued on next page)

Table 2: List of $P2_1/m(11)$

(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
WP_2	PXX	–	–	$P2_1/m(11)$	–	–	–	–	–	–	7.13	6.50	62.8	1.196	3.803	–	–	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
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
$ReBi_2$	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
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
$IrAl_2$	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	–
$IrCa_2$	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
$IrSb_2$	TXX	$P2_1/m(11)$	–	–	7.25	8.03	56.3	–	–	–	–	–	–	0.937	1.265	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
$PtPb_2$	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
$AuNa_2$	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	–
$AuRb_2$	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
$AuTe_2$	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
$HgCa_2$	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
$TlBa_2$	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
$BiSi_2$	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
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
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
$BiBa_2$	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 3: List of $P4mmm(123)$

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
$LiIn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.58	9.07	43.7	–	–	–	1.741	2.532	–	0.0	–
$LiSn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.75	6.47	42.0	–	–	–	3.741	3.823	–	0.0	–
$LiBa_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	12.24	8.58	44.8	–	–	–	1.109	6.245	–	0.0	–
$LiHg_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.35	9.05	44.4	–	–	–	1.491	1.549	–	0.0	–
$BeSc_2$	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
$BeMn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	7.38	5.24	45.2	–	–	–	0.953	8.523	–	29.3	–
$BeAg_2$	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	–
$MgSc_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.73	9.54	44.8	–	–	–	3.061	9.615	–	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	–
$AlCa_2$	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
$AlSc_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.77	6.20	45.0	–	–	–	1.330	1.376	–	0.0	–
AlY_2	HXX	–	$P4/mmm(123)$	–	–	–	–	9.56	6.76	45.1	–	–	–	0.888	4.155	–	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
$AlAg_2$	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	–
$AlBa_2$	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
$AlPt_2$	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	–
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
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	–
$ScCa_2$	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	–
$ScSc_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.56	9.28	45.0	–	–	–	5.445	12.533	–	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	–
$ScIn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.75	9.55	45.2	–	–	–	5.359	5.523	–	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	–
$ScHg_2$	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	–
$ScBi_2$	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
$TiBe_2$	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	–
$TiAl_2$	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	–
$TiCa_2$	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	–
$TiIn_2$	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	–
$TiHf_2$	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
$TiTl_2$	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	–
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	–
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	–
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
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
$CrMg_2$	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	–
$CrAl_2$	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	–
$CrCa_2$	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	–
$CrSc_2$	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	–
$CrGa_2$	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	–
$CrSr_2$	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
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
$CrSn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.80	6.45	42.3	–	–	–	4.969	7.754	–	14.5	–
$CrHf_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.24	8.82	45.0	–	–	–	2.721	5.543	–	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

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Table 3: List of $P4mmm(123)$

(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
$MnSc_2$	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
$MnMn_2$	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
$MnIn_2$	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	–
$MnAu_2$	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	–
$MnPb_2$	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
$FeBe_2$	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	–
$FeAl_2$	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	–
$FeSc_2$	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	–
$CoAl_2$	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	–
$NiBe_2$	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	–
$NiHg_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.51	5.99	43.8	–	–	–	3.814	3.885	–	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
$GaCr_2$	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
$GeCr_2$	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	–
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
SrS_2	PXX	–	–	$P4/mmm(123)$	–	–	–	–	–	–	8.10	11.48	45.0	0.837	7.807	–	–	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	–
$ZrMg_2$	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	–
$ZrPd_2$	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
$ZrIn_2$	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
$ZrAu_2$	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	–
$ZrTl_2$	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	–
$NbBe_2$	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	–
$MoMn_2$	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	–
$TcTi_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.64	6.11	45.0	–	–	–	2.445	2.569	–	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	–
$RuSc_2$	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	–
$RuMn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.41	5.93	44.4	–	–	–	2.015	11.563	–	33.2	–
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
$RhLi_2$	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
$RhAu_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	7.96	5.61	44.3	–	–	–	5.785	5.794	–	0.0	–
$RhHg_2$	TXX	$P4/mmm(123)$	–	–	6.61	9.22	43.2	–	–	–	–	–	–	1.278	6.618	0.0	–	–
$PdAg_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	5.83	8.37	43.3	–	–	–	6.189	6.315	–	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
CdK_2	HXX	–	$P4/mmm(123)$	–	–	–	–	8.43	11.95	44.6	–	–	–	1.278	2.679	–	0.0	–
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
$InLi_2$	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	–
$InCa_2$	TXX	$P4/mmm(123)$	–	–	7.57	10.75	44.6	–	–	–	–	–	–	1.123	6.594	0.0	–	–
$InSc_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.65	9.46	45.0	–	–	–	3.680	6.339	–	0.0	–
$InCr_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.11	8.63	45.1	–	–	–	1.595	2.770	–	35.6	–
InY_2	HXX	–	$P4/mmm(123)$	–	–	–	–	6.81	9.62	45.1	–	–	–	2.618	3.690	–	0.0	–
$InBa_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.51	12.04	45.1	–	–	–	2.067	2.487	–	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
$CsBr_2$	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

(Continued on next page)

Table 3: List of $P4mmm(123)$

(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
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
$HfBe_2$	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	–
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	–
$HfTl_2$	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	–
$TaBe_2$	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	–
TaY_2	HXX	–	$P4/mmm(123)$	–	–	–	–	6.98	9.88	44.9	–	–	–	0.849	4.248	–	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	–
$OsBe_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	5.72	8.07	44.9	–	–	–	2.085	7.582	–	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
$OsMn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	8.30	5.87	45.0	–	–	–	1.335	12.451	–	32.3	–
$IrBe_2$	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	–
$IrZr_2$	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
$AuSn_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.49	8.83	42.3	–	–	–	2.861	2.870	–	0.0	–
$AuPb_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	7.20	10.40	43.9	–	–	–	0.933	0.981	–	0.0	–
$HgLi_2$	HXX	–	$P4/mmm(123)$	–	–	–	–	6.66	9.44	44.7	–	–	–	1.596	3.332	–	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
$TlBa_2$	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 4: List of $C2/m(12)$

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	–
$BeSi_2$	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	–
$BeSe_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	10.46	6.44	52.1	2.049	3.159	–	–	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	–
$BeIn_2$	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	–
$BeRe_2$	TXX	$C2/m(12)$	–	–	6.98	6.98	41.2	–	–	–	–	–	–	1.327	3.902	0.0	–	–
BBe_2	TXX	$C2/m(12)$	–	–	4.04	5.97	59.4	–	–	–	–	–	–	1.451	1.965	0.0	–	–
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	–
BP_2	TXX	$C2/m(12)$	–	–	7.19	7.19	52.4	–	–	–	–	–	–	3.719	4.235	0.0	–	–
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
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
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
$NaCl_2$	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
$MgRh_2$	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	–
$MgBa_2$	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
$AlBe_2$	TXX	$C2/m(12)$	–	–	6.08	6.96	42.4	–	–	–	–	–	–	2.495	3.435	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	–
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	–
$AlGe_2$	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	–
$AlSe_2$	TXX	$C2/m(12)$	–	–	7.29	7.29	49.9	–	–	–	–	–	–	2.444	2.936	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	–
$AlRu_2$	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	–
$AlBa_2$	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
$AlHf_2$	TXX	$C2/m(12)$	–	–	7.70	7.69	45.9	–	–	–	–	–	–	2.870	4.085	0.0	–	–
$AlIr_2$	HXX	–	$C2/m(12)$	–	–	–	–	7.81	6.82	42.6	–	–	–	1.127	6.685	–	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	–
$SiNa_2$	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
$SiZr_2$	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
$SiPt_2$	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	–
$SiPb_2$	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
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	–	–
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
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
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
$CaSi_2$	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
$CaTe_2$	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	–
$CaHg_2$	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
ScN_2	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	7.35	7.36	49.7	1.883	14.128	–	–	0.0
ScO_2	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	5.77	7.32	55.5	2.577	3.186	–	–	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	–
$ScAu_2$	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	–
$TiBi_2$	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
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	–
VSr_2	TXX	$C2/m(12)$	–	–	7.76	10.28	48.5	–	–	–	–	–	–	2.329	2.557	1.4	–	–
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
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
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
$CrBr_2$	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	–
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

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Table 4: List of $C2/m(12)$

(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
$CrRu_2$	HXX	–	$C2/m(12)$	–	–	–	–	6.88	7.84	41.6	–	–	–	1.187	5.058	–	0.0	–
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	–
$CrBi_2$	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
FeB_2	TXX	$C2/m(12)$	–	–	5.59	5.97	36.8	–	–	–	–	–	–	4.107	4.694	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	–
$FeSe_2$	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
$FeTc_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	5.31	7.92	59.9	3.152	7.289	–	–	0.0
CoC_2	TXX	$C2/m(12)$	–	–	5.89	5.61	44.4	–	–	–	–	–	–	2.261	3.502	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	–
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	–
$NiHf_2$	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
$GaTi_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	6.10	8.18	63.1	3.154	3.531	–	–	0.0
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
$AsPd_2$	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
$BrLi_2$	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
$SrSi_2$	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
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
$SrGe_2$	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
$SrIn_2$	HXX	–	$C2/m(12)$	–	–	–	–	12.52	11.36	24.8	–	–	–	3.379	4.365	–	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
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
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
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
$ZrHf_2$	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
$ZrPb_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	6.49	7.75	51.3	0.916	0.927	–	–	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
$NbBi_2$	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
$MoCl_2$	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
$MoSb_2$	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	–
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	–
$TcSi_2$	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	–
$TcTa_2$	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	–
RuC_2	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	7.23	8.98	36.9	3.319	7.440	–	–	0.0
RuN_2	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	6.80	7.22	76.4	4.664	5.141	–	–	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
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	–
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	–	–
$RuTa_2$	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	–
$RhLi_2$	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
$RhGa_2$	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	–
$RhAs_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	7.00	7.05	58.4	1.109	1.242	–	–	0.0
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
$PdAl_2$	HXX	–	$C2/m(12)$	–	–	–	–	7.11	5.87	50.2	–	–	–	3.293	3.299	–	0.0	–
$PdZr_2$	HXX	–	$C2/m(12)$	–	–	–	–	8.73	7.47	45.6	–	–	–	0.831	4.247	–	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	–

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Table 4: List of $C2/m(12)$

(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
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
$PdPt_2$	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
$PdHg_2$	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	–
$PdTl_2$	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
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
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	–
$AgSc_2$	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	–
$AgPd_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	10.12	5.58	46.0	1.479	3.669	–	–	0.0
$AgIn_2$	HXX	–	$C2/m(12)$	–	–	–	–	8.95	7.89	42.5	–	–	–	2.390	3.107	–	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
$AgPb_2$	TXX	$C2/m(12)$	–	–	8.87	9.45	43.8	–	–	–	–	–	–	1.367	1.829	0.0	–	–
CdP_2	TXX	$C2/m(12)$	–	–	11.38	11.29	34.1	–	–	–	–	–	–	0.824	2.323	0.0	–	–
$CdCa_2$	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
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	–
$CdBa_2$	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
$CdTl_2$	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	–
$CdBi_2$	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	–
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
$InTi_2$	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	–	–
$InTe_2$	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
$SnCr_2$	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	–
$SbCa_2$	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
$CsSe_2$	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
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
$CsIn_2$	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
$CsTe_2$	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
$CsTl_2$	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
$CsBi_2$	TXX	$C2/m(12)$	–	–	15.08	15.10	35.0	–	–	–	–	–	–	1.192	4.126	0.0	–	–
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
$BaPb_2$	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
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
$HfAu_2$	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	–
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
$TaIn_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	6.69	6.07	45.2	2.749	2.836	–	–	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
$TaBi_2$	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
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
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
$ReSi_2$	TXX	$C2/m(12)$	–	–	8.56	8.56	40.3	–	–	–	–	–	–	0.861	1.573	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
$ReCs_2$	TXX	$C2/m(12)$	–	–	10.91	11.87	45.3	–	–	–	–	–	–	10.951	11.154	6.0	–	–
$OsNb_2$	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	–
$OsTe_2$	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
$OsBa_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	10.04	9.05	47.4	1.409	3.666	–	–	2.5
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
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
$IrHf_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	6.66	8.17	52.1	1.216	1.762	–	–	0.0
$PtAl_2$	HXX	–	$C2/m(12)$	–	–	–	–	7.62	6.51	46.1	–	–	–	2.256	2.423	–	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
PtV_2	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	7.51	6.20	45.1	3.050	5.944	–	–	0.0

(Continued on next page)

Table 4: List of $C2/m(12)$

(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
$PtAs_2$	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
$PtZr_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	8.68	6.52	55.6	1.498	3.438	–	–	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	–	–
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	–
$PtHf_2$	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	–
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
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
$AuCl_2$	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
$AuSc_2$	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	–
$AuGa_2$	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	–
$AuSe_2$	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
$AuBr_2$	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	–
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	–
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	–
$HgCl_2$	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	–
$HgSe_2$	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
$HgBr_2$	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	–
$HgBa_2$	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
$HgBi_2$	TXX	$C2/m(12)$	–	–	13.27	13.23	38.3	–	–	–	–	–	–	2.268	3.304	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
$PbSc_2$	PXX	–	–	$C2/m(12)$	–	–	–	–	–	–	8.07	6.17	67.4	2.664	6.488	–	–	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

Table 5: List of $P\bar{6}m2(187)$

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	$P\bar{3}m1(164)$	$P\bar{6}m2(187)$	–	5.46	5.45	59.9	5.45	5.45	60.0	–	–	–	0.046	3.644	0.0	0.0	–
$LiAg_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.83	5.84	59.9	–	–	–	3.253	3.264	–	0.0	–
$BeBe_2$	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	–
BeP_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.79	6.79	60.0	–	–	–	1.270	1.864	–	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
$BeRh_2$	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	–
$BeSb_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	7.71	7.71	59.2	–	–	–	1.290	1.822	–	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
$BePt_2$	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	–
$BeBi_2$	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
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	–
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	–
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	–
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	–
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	–
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	–
CMo_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.73	5.71	59.6	–	–	–	0.933	6.554	–	0.0	–
CRu_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.55	5.56	59.5	–	–	–	1.540	3.671	–	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	–
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	–
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	–
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	–
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	–
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	–
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
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	–
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	–
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
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	–
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	–
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
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
$AlPd_2$	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	–
$AlSb_2$	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
$AlPt_2$	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	–
$SiGe_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	7.45	7.45	60.0	–	–	–	0.902	1.448	–	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
$SiSn_2$	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
$SiPt_2$	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	–
$SiPb_2$	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
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	–
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	–
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

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Table 5: List of $P\bar{6}m2(187)$

(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
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	–
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	–
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
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
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
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
$ClCa_2$	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	–
$ClRb_2$	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
$ClSr_2$	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	–
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
$ClIn_2$	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
$ClBa_2$	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
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	–
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	–
ScF_2	PHX	–	$P\bar{6}m2(187)$	$P\bar{1}(2)$	–	–	–	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	–
$ScHg_2$	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	–
TiN_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.50	6.52	60.3	–	–	–	1.634	7.641	–	0.0	–
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
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
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
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	–
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
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
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
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
$FePd_2$	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	–
$NiSc_2$	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
$GeGe_2$	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
$GePd_2$	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
$GeSn_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	8.21	8.23	60.0	–	–	–	0.915	1.077	–	0.0	–
$GePt_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.95	5.97	60.1	–	–	–	0.991	2.490	–	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	–
$SeSc_2$	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
$SeSr_2$	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	–
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
$SeIn_2$	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
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
$BrCa_2$	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	–
$BrCs_2$	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
$BrBa_2$	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	–
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	–

(Continued on next page)

Table 5: List of $P\bar{6}m2(187)$

(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
$RbCl_2$	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	–
$SrSe_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	9.99	9.99	57.9	–	–	–	2.071	5.736	–	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
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
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
ZrF_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.23	6.23	60.0	–	–	–	0.876	0.892	–	0.0	–
ZrP_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	8.14	8.13	59.8	–	–	–	1.562	9.368	–	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
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	–
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	–
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	–
$MoSb_2$	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	–
$MoTe_2$	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
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
$TcSb_2$	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
$RuPd_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.51	5.51	59.8	–	–	–	6.269	7.276	–	0.0	–
$RhIn_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.43	6.38	58.1	–	–	–	1.550	1.883	–	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
$PdIn_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.36	6.35	60.1	–	–	–	1.708	1.943	–	0.0	–
$PdAu_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	5.72	5.71	59.6	–	–	–	5.169	5.185	–	0.0	–
$CdCa_2$	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
$CdBi_2$	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	–
$InTl_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	6.94	6.95	59.9	–	–	–	3.251	4.456	–	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
$TeCa_2$	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	–
$TeTl_2$	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
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
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	–
BaN_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	9.18	9.23	60.7	–	–	–	19.750	19.780	–	3.8	–
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
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
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	–
$HfCl_2$	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
$HfAu_2$	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	–
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	–
WAs_2	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	7.39	7.43	60.2	–	–	–	2.084	10.262	–	0.0	–

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Table 5: List of $P\bar{6}m2(187)$

(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
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
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	–
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	–
$OsZr_2$	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
$PtSc_2$	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
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
$AuSc_2$	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
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
$HgCa_2$	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
$TlTl_2$	HXX	–	$P\bar{6}m2(187)$	–	–	–	–	7.10	7.09	58.7	–	–	–	2.866	3.135	–	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

Table 6: List of $Amm2(38)$

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	–
$LiMg_2$	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	–
$LiCs_2$	HXX	–	$Amm2(38)$	–	–	–	–	12.59	12.52	46.3	–	–	–	0.865	1.607	–	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	–
$BeSi_2$	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	–
$BeRb_2$	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	–
$BeAg_2$	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	–
$BeCs_2$	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	–
$BePb_2$	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
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	–
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	–
$MgRh_2$	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	–
$MgSn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.89	9.95	37.1	–	–	–	1.742	2.456	–	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
$AlSn_2$	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	–
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
$SiCl_2$	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
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	–
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
$ClSn_2$	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
$ClCs_2$	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
$ClTl_2$	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	–
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
KBa_2	HXX	–	$Amm2(38)$	–	–	–	–	14.40	14.44	34.8	–	–	–	1.099	1.172	–	0.0	–
$CaHg_2$	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
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
$CrCs_2$	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	–
$CrBi_2$	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
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	–
$CoIr_2$	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	–
$NiAs_2$	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	–
$NiIr_2$	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
$NiBi_2$	HXX	–	$Amm2(38)$	–	–	–	–	8.51	6.89	50.3	–	–	–	1.937	1.956	–	0.0	–
$GaSn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.90	9.94	36.7	–	–	–	3.145	5.782	–	0.2	–
$GeAl_2$	HXX	–	$Amm2(38)$	–	–	–	–	8.11	8.10	39.7	–	–	–	1.794	2.666	–	0.0	–
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	–
$GeCd_2$	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	–
$GeCs_2$	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
$BrRb_2$	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
$BrTl_2$	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
$RbSr_2$	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	–
$SrSr_2$	HXX	–	$Amm2(38)$	–	–	–	–	8.55	14.45	31.6	–	–	–	6.433	6.440	–	0.0	–
$MoTl_2$	HXX	–	$Amm2(38)$	–	–	–	–	8.14	9.52	27.5	–	–	–	12.878	12.901	–	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	–
TcP_2	HXX	–	$Amm2(38)$	–	–	–	–	7.28	7.28	52.2	–	–	–	1.228	1.912	–	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	–
$PdAs_2$	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	–
$PdIr_2$	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

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Table 6: List of $Amm2(38)$

(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
$PdTl_2$	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
$AgAl_2$	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
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	–
$AgCa_2$	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	–
$AgCs_2$	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
$AgBi_2$	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	–
$CdGe_2$	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	–
$CdTl_2$	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	–
$InAl_2$	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	–
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	–
$SnIn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.54	9.31	39.1	–	–	–	1.481	1.499	–	0.0	–
$SbLi_2$	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	–
$SbRb_2$	HXX	–	$Amm2(38)$	–	–	–	–	10.78	11.48	45.7	–	–	–	1.195	2.554	–	0.0	–
$SbIn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.02	9.00	43.2	–	–	–	0.937	3.263	–	0.0	–
$SbCs_2$	HXX	–	$Amm2(38)$	–	–	–	–	11.27	11.95	44.4	–	–	–	1.231	1.308	–	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
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
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
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
$BaCa_2$	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	–
$BaCs_2$	HXX	–	$Amm2(38)$	–	–	–	–	15.57	15.52	35.9	–	–	–	1.937	2.001	–	0.0	–
$BaBa_2$	HXX	–	$Amm2(38)$	–	–	–	–	14.13	14.12	34.9	–	–	–	2.303	2.377	–	0.0	–
$OsMg_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.01	6.25	44.6	–	–	–	1.045	12.251	–	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
$PtGa_2$	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	–
$PtAs_2$	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
$PtRu_2$	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
$PtIn_2$	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	–
$PtIr_2$	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	–
$PtHg_2$	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	–
$PtTl_2$	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
$PtBi_2$	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
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
$AuGa_2$	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	–
$AuGe_2$	HXX	–	$Amm2(38)$	–	–	–	–	8.91	8.89	36.1	–	–	–	0.908	0.962	–	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
$AuPd_2$	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
$AuCs_2$	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
$AuHg_2$	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	–
$AuBi_2$	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
$HgSn_2$	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
$TlIn_2$	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
$PbRb_2$	HXX	–	$Amm2(38)$	–	–	–	–	10.96	11.95	46.2	–	–	–	1.818	3.099	–	0.0	–
$PbIn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.90	9.90	38.4	–	–	–	1.235	1.498	–	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	–
$BiIn_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.32	9.28	42.6	–	–	–	1.375	2.254	–	0.0	–
$BiHg_2$	HXX	–	$Amm2(38)$	–	–	–	–	10.97	10.95	33.0	–	–	–	0.957	1.721	–	0.0	–
$BiTl_2$	HXX	–	$Amm2(38)$	–	–	–	–	9.88	9.86	41.5	–	–	–	1.495	1.525	–	0.0	–

Table 7: List of $Cmmm(65)$

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	–
$LiCd_2$	HXX	–	$Cmmm(65)$	–	–	–	–	6.00	9.16	40.2	–	–	–	2.170	2.316	–	0.0	–
$BeBe_2$	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	–
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
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
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
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
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
$NaSi_2$	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
$NaAu_2$	HXX	–	$Cmmm(65)$	–	–	–	–	5.81	9.01	38.3	–	–	–	1.783	1.787	–	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	–
$SiCr_2$	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
$CaCr_2$	HXX	–	$Cmmm(65)$	–	–	–	–	6.42	10.52	34.3	–	–	–	3.709	3.723	–	36.4	–
$CaRb_2$	HXX	–	$Cmmm(65)$	–	–	–	–	13.13	8.80	41.5	–	–	–	3.612	3.733	–	0.0	–
$CaSr_2$	HXX	–	$Cmmm(65)$	–	–	–	–	8.12	11.93	42.7	–	–	–	5.908	6.058	–	0.0	–
$CaSb_2$	HXX	–	$Cmmm(65)$	–	–	–	–	9.52	11.96	36.0	–	–	–	1.402	4.121	–	0.0	–
$CaBa_2$	HXX	–	$Cmmm(65)$	–	–	–	–	8.41	13.79	34.9	–	–	–	5.809	6.597	–	0.0	–
$ScCr_2$	HXX	–	$Cmmm(65)$	–	–	–	–	6.02	9.89	34.7	–	–	–	5.287	8.769	–	32.2	–
$ScGe_2$	HXX	–	$Cmmm(65)$	–	–	–	–	7.97	10.15	38.2	–	–	–	2.631	2.774	–	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
VV_2	HXX	–	$Cmmm(65)$	–	–	–	–	8.01	5.10	35.3	–	–	–	6.097	19.320	–	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	–
$CrBr_2$	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	–
$MnBe_2$	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	–
MnB_2	PXX	–	–	$Cmmm(65)$	–	–	–	–	–	–	7.88	7.88	44.5	1.841	4.105	–	–	11.0
$FePd_2$	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	–
$AsRb_2$	HXX	–	$Cmmm(65)$	–	–	–	–	9.67	12.74	36.5	–	–	–	2.480	2.557	–	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	–
$RbAu_2$	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
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
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
SrK_2	HXX	–	$Cmmm(65)$	–	–	–	–	14.81	8.76	32.3	–	–	–	4.385	4.424	–	0.0	–
$SrCa_2$	HXX	–	$Cmmm(65)$	–	–	–	–	7.90	13.16	34.6	–	–	–	6.178	6.180	–	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
$SrSb_2$	HXX	–	$Cmmm(65)$	–	–	–	–	10.03	12.61	36.5	–	–	–	1.128	3.870	–	0.0	–
$SrBa_2$	HXX	–	$Cmmm(65)$	–	–	–	–	8.63	14.42	33.6	–	–	–	6.319	6.612	–	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
$SrPb_2$	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
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
$ZrCr_2$	HXX	–	$Cmmm(65)$	–	–	–	–	6.06	9.42	39.0	–	–	–	7.350	13.581	–	29.3	–
$ZrBi_2$	PXX	–	–	$Cmmm(65)$	–	–	–	–	–	–	8.00	6.69	54.5	1.087	4.002	–	–	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	–
$MoCl_2$	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	–
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
RhF_2	PXX	–	–	$Cmmm(65)$	–	–	–	–	–	–	15.14	15.34	22.8	2.132	4.657	–	–	4.0
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
$PdCl_2$	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

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Table 7: List of $Cmmm(65)$

(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
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
$AgCl_2$	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
$InNa_2$	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	–
$SnCs_2$	HXX	–	$Cmmm(65)$	–	–	–	–	10.34	13.50	39.4	–	–	–	2.435	2.463	–	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
$CsAl_2$	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
$CsCa_2$	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
$CsCr_2$	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
$CsSr_2$	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
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
$CsIn_2$	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
$CsTe_2$	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
$CsAu_2$	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
$CsPb_2$	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
BaK_2	HXX	–	$Cmmm(65)$	–	–	–	–	15.14	8.97	32.4	–	–	–	5.288	5.295	–	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
$BaRb_2$	HXX	–	$Cmmm(65)$	–	–	–	–	9.25	11.07	52.8	–	–	–	4.754	4.775	–	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
$BaSb_2$	HXX	–	$Cmmm(65)$	–	–	–	–	10.96	13.78	34.8	–	–	–	2.519	4.322	–	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
$HfBi_2$	TXX	$Cmmm(65)$	–	–	8.41	6.60	50.4	–	–	–	–	–	–	2.365	4.070	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	–
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
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
$IrBr_2$	HXX	–	$Cmmm(65)$	–	–	–	–	7.41	9.03	52.7	–	–	–	1.219	1.663	–	0.0	–
$PtBe_2$	HXX	–	$Cmmm(65)$	–	–	–	–	6.41	8.39	40.2	–	–	–	2.567	2.855	–	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
$PtCl_2$	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
$PtNb_2$	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
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	–
$AuNa_2$	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	–
$AuCl_2$	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	–
$PbCs_2$	HXX	–	$Cmmm(65)$	–	–	–	–	10.34	13.60	40.1	–	–	–	2.093	3.761	–	0.0	–

Table 8: List of Memory structures

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
CoB_2	PXX	–	–	$Pmmn(59)$	–	–	–	–	–	–	6.68	6.69	53.2	1.582	1.617	–	–	0.0
$SrAl_2$	PXX	–	–	$P6mm(183)$	–	–	–	–	–	–	9.20	9.20	60.0	3.037	8.347	–	–	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
$PdIr_2$	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
$CsAl_2$	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
$AuIr_2$	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
$HgPt_2$	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
$PbBe_2$	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

Table 9: List of Planar structures

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
$CdAg_2$	PXX	–	–	$P6/mmm(191)$	–	–	–	–	–	–	9.96	9.96	59.8	1.025	1.245	–	–	0.0
$InOs_2$	PXX	–	–	$P6/mmm(191)$	–	–	–	–	–	–	8.97	8.96	60.0	7.610	8.673	–	–	0.0
$AuBe_2$	PXX	–	–	$P6/mmm(191)$	–	–	–	–	–	–	8.17	8.16	60.0	2.167	5.488	–	–	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
$HgBe_2$	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
$HgAg_2$	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
$TlBe_2$	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

Table 10: List of Distorted planar structures

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
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
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
MnB_2	PXX	–	–	$Cmmm$(65)	–	–	–	–	–	–	7.88	7.88	44.5	1.841	4.105	–	–	11.0
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
$RbSr_2$	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
$SrAu_2$	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
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
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
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
$AgAl_2$	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
$InMn_2$	PXX	–	–	$P6/mmm$(191)	–	–	–	–	–	–	9.24	9.20	59.8	2.572	2.657	–	–	22.2
$InAu_2$	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
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
$CsCa_2$	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
$CsIn_2$	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
$CsTe_2$	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
$CsCs_2$	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
$BaCr_2$	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
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
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
$BiAl_2$	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