

SUPPLEMENTARY INFORMATION

The calculated elastic constants and structural parameters for 240 M_2AX phases are given in Tables IX to XVIII. The tables are split according to the different M elements and contain the a , c , d_{MX} , and d_{MA} structural parameters as well as the five elastic constants and three elastic moduli. For the 17 phases that were found to be unstable (see discussion in Section 2.4) only the hexagonal lattice parameters of the lowest energy stationary point are given.

M ₂ AX phase	<i>a</i>	<i>c</i>	d _{MX}	d _{MA}	C ₁₁	C ₁₂	C ₁₃	C ₃₃	C ₄₄	B	G	E
Sc ₂ AlC	3.297	15.04	1.242	2.517	175	59	33	191	44	88	57	140
Sc ₂ AlN	3.217	14.53	1.231	2.401	213	60	48	228	72	107	77	187
Sc ₂ SiC	3.301	13.95	1.242	2.247	203	62	48	234	74	106	76	184
Sc ₂ SiN	3.219	13.50	1.231	2.143	231	65	74	266	96	128	89	218
Sc ₂ PC	3.365	12.77	1.250	1.944	190	95	71	233	88	121	70	175
Sc ₂ PN	3.403	11.89	1.236	1.737	197	89	95	277	106	137	80	200
Sc ₂ SC	3.451	11.95	1.225	1.763	247	69	59	267	89	126	91	221
Sc ₂ SN	3.368	11.79	1.192	1.755	261	75	78	284	109	141	101	244
Sc ₂ GaC	3.306	14.70	1.240	2.433	174	64	37	179	40	89	53	133
Sc ₂ GaN	3.232	14.11	1.230	2.298	214	60	57	214	70	110	75	183
Sc ₂ GeC	3.324	14.06	1.235	2.279	200	61	48	216	68	103	72	175
Sc ₂ GeN	3.244	13.63	1.218	2.190	229	63	67	242	84	122	84	204
Sc ₂ AsC	3.380	13.26	1.229	2.086	186	83	66	218	76	113	66	165
Sc ₂ AsN	3.376	12.55	1.216	1.921	152	104	106	239	92	131	57	148
Sc ₂ CdC	3.324	15.63	1.230	2.678	152	57	27	130	12	73	36	92
Sc ₂ CdN	3.248	15.12	1.217	2.563	173	76	37	174	15	92	40	106
Sc ₂ InC	3.355	15.36	1.226	2.614	175	59	33	173	41	86	54	135
Sc ₂ InN	3.279	14.90	1.202	2.524	204	60	47	199	59	102	68	167
Sc ₂ SnC	3.380	14.87	1.211	2.507	190	58	42	181	55	93	63	154
Sc ₂ SnN	3.306	14.48	1.184	2.437	217	60	53	220	68	110	75	184
Sc ₂ TlC	3.375	15.31	1.221	2.607	180	54	30	166	37	84	55	135
Sc ₂ TlN	3.304	14.86	1.193	2.523	205	62	48	192	54	102	65	162
Sc ₂ PbC	3.411	15.10	1.198	2.577	186	57	35	160	46	87	58	142
Sc ₂ PbN	3.342	14.68	1.166	2.504	212	61	45	186	53	101	67	165

TABLE IX: Calculated lattice parameters (in Å), elastic constants, and moduli (in GPa) of the Sc₂AX phases.

M_2AX phase	a	c	d_{MX}	d_{MA}	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	B	G	E
Ti ₂ AlC	3.071	13.73	1.147	2.286	302	62	61	269	109	138	113	267
Ti ₂ AlN	2.999	13.63	1.165	2.243	309	66	91	280	125	155	118	281
Ti ₂ SiC	3.057	12.85	1.179	2.034	300	81	110	314	140	169	119	288
Ti ₂ SiN	2.990	12.83	1.188	2.019	284	108	125	359	149	183	115	285
Ti ₂ PC	3.191	11.50	1.166	1.710	252	123	148	343	168	187	109	273
Ti ₂ PN	3.161	11.34	1.122	1.712	329	113	133	384	174	200	135	331
Ti ₂ SC	3.208	11.27	1.118	1.700	331	98	97	348	157	177	134	321
Ti ₂ SN	3.202	11.06	1.051	1.715	321	89	118	341	135	181	121	297
Ti ₂ GaC	3.083	13.43	1.143	2.215	303	66	63	263	101	139	109	260
Ti ₂ GaN	3.016	13.33	1.154	2.178	298	78	100	276	118	159	109	265
Ti ₂ GeC	3.093	13.01	1.157	2.097	278	75	96	283	118	152	106	257
Ti ₂ GeN	3.042	12.94	1.154	2.081	254	113	118	298	122	167	94	236
Ti ₂ AsC	3.195	12.12	1.138	1.892	225	147	123	286	142	169	87	224
Ti ₂ AsN	3.201	11.72	1.086	1.844	290	109	125	326	148	181	114	281
Ti ₂ CdC	3.106	14.54	1.127	2.509	253	71	47	203	31	116	67	168
Ti ₂ CdN	3.082	14.15	1.088	2.450	270	83	58	235	68	130	84	208
Ti ₂ InC	3.148	14.20	1.110	2.440	282	65	55	240	86	128	98	234
Ti ₂ InN	3.095	14.05	1.111	2.401	229	56	106	248	92	138	83	208
Ti ₂ SnC	3.180	13.79	1.111	2.335	260	78	70	254	93	135	93	226
Ti ₂ SnN	3.180	13.46	1.045	2.320	238	86	81	254	79	136	79	198
Ti ₂ TlC	3.177	14.22	1.098	2.457	278	71	51	226	74	125	91	219
Ti ₂ TlN	3.167	13.85	1.044	2.418	246	78	69	237	74	129	81	200
Ti ₂ PbC	3.231	14.01	1.080	2.423	235	90	53	211	66	119	73	182
Ti ₂ PbN	3.239	13.65	0.998	2.415	235	92	56	211	56	121	68	173

TABLE X: Calculated lattice parameters (in Å), elastic constants, and moduli (in GPa) of the Ti₂AX phases.

M ₂ AX phase	<i>a</i>	<i>c</i>	d _{MX}	d _{MA}	C ₁₁	C ₁₂	C ₁₃	C ₃₃	C ₄₄	B	G	E
V ₂ AlC	2.914	13.11	1.119	2.159	339	71	111	310	147	175	132	316
V ₂ AlN	2.877	13.13	1.122	2.160	325	60	127	341	140	180	128	310
V ₂ SiC	2.965	11.96	1.114	1.877	309	117	180	325	189	211	126	315
V ₂ SiN	2.944	12.02	1.083	1.922	286	142	171	344	148	209	102	263
V ₂ PC	3.079	10.90	1.070	1.654	376	113	168	386	204	227	154	376
V ₂ PN	3.046	11.03	1.038	1.720	350	135	176	384	153	229	122	312
V ₂ SC	3.124	10.76	1.012	1.679	335	101	147	330	125	199	114	286
V ₂ SN*	3.177	10.50	0.909	1.715								
V ₂ GaC	2.942	12.85	1.098	2.114	334	81	111	299	138	175	125	302
V ₂ GaN	2.933	12.73	1.072	2.110	281	71	142	293	128	174	105	263
V ₂ GeC	3.016	12.18	1.070	1.976	289	122	134	279	142	182	105	263
V ₂ GeN	3.007	12.10	1.035	1.989	274	146	153	292	121	194	87	226
V ₂ AsC	3.113	11.42	1.040	1.816	330	124	137	320	161	197	124	307
V ₂ AsN	3.084	11.52	1.011	1.868	307	145	145	345	108	203	94	245
V ₂ CdC	2.995	13.85	1.048	2.414	228	0	104	205	77	120	84	203
V ₂ CdN	2.974	13.74	1.028	2.408	308	81	99	249	82	158	95	236
V ₂ InC	3.030	13.59	1.053	2.345	306	85	93	271	103	158	104	256
V ₂ InN	3.041	13.33	1.001	2.332	244	91	112	264	89	154	80	204
V ₂ SnC	3.133	12.92	0.980	2.251	224	75	100	247	80	138	75	189
V ₂ SnN	3.138	12.74	0.924	2.261	176	133	102	257	52	143	43	117
V ₂ TlC	3.115	13.44	0.981	2.379	195	41	93	225	70	119	69	173
V ₂ TlN	3.159	12.98	0.884	2.362	219	164	68	225	66	140	56	148
V ₂ PbC	3.204	13.14	0.920	2.364	232	104	61	195	53	123	63	161
V ₂ PbN	3.206	12.98	0.867	2.378	211	148	46	200	17	122	39	105

TABLE XI: Calculated lattice parameters (in Å), elastic constants, and moduli (in GPa) of the V₂AX phases.

* V₂SN was found to be unstable (*cf.* Section 2.4). For this structure we only report the lattice parameters of the lowest energy stationary point with hexagonal symmetry.

M ₂ AX phase	<i>a</i>	<i>c</i>	d _{MX}	d _{MA}	C ₁₁	C ₁₂	C ₁₃	C ₃₃	C ₄₄	B	G	E
Cr ₂ AlC	2.848	12.68	1.074	2.096	365	84	102	369	140	186	138	332
Cr ₂ AlN	2.835	12.73	1.063	2.119	279	66	150	368	84	184	92	237
Cr ₂ SiC	2.878	11.89	1.068	1.905	307	129	167	400	81	215	87	229
Cr ₂ SiN	2.880	11.85	1.028	1.935	249	165	190	410	42	222	49	138
Cr ₂ PC	3.002	10.88	1.027	1.693	295	141	197	353	139	224	98	257
Cr ₂ PN	2.995	10.94	1.037	1.697	294	109	172	400	119	210	101	262
Cr ₂ SC	3.111	10.47	0.949	1.668	324	127	136	287	81	192	88	229
Cr ₂ SN*	3.131	10.40	0.932	1.667								
Cr ₂ GaC	2.875	12.50	1.060	2.066	312	81	139	325	128	185	114	283
Cr ₂ GaN	2.910	12.29	0.995	2.077	198	94	151	309	94	166	68	180
Cr ₂ GeC	2.942	12.02	1.024	1.979	308	147	140	333	74	200	81	213
Cr ₂ GeN	2.972	11.79	0.966	1.981	231	168	146	336	62	191	53	147
Cr ₂ AsC	3.042	11.38	0.984	1.861	227	104	203	275	87	195	62	168
Cr ₂ AsN	3.070	11.15	0.897	1.889	285	194	140	334	63	206	63	171
Cr ₂ CdC	2.927	13.58	1.008	2.386	311	83	97	247	74	158	92	230
Cr ₂ CdN	3.004	13.20	0.924	2.375	262	98	72	238	58	139	74	189
Cr ₂ InC	3.026	13.05	0.963	2.299	189	70	95	244	70	127	64	163
Cr ₂ InN	3.062	12.72	0.891	2.289	245	149	88	262	72	156	67	175
Cr ₂ SnC	3.102	12.54	0.926	2.208	245	142	94	252	57	156	60	160
Cr ₂ SnN	3.087	12.45	0.890	2.221	247	164	89	285	37	163	52	141
Cr ₂ TlC	3.093	13.16	0.931	2.359	243	114	22	213	52	113	70	173
Cr ₂ TlN	3.107	12.80	0.868	2.331	257	157	69	207	60	146	62	163
Cr ₂ PbC	3.161	12.85	0.889	2.324	239	122	75	171	36	133	51	136
Cr ₂ PbN	3.153	12.78	0.849	2.345	239	147	46	144	10	122	39	105

TABLE XII: Calculated lattice parameters (in Å), elastic constants, and moduli (in GPa) of the Cr₂AX phases.

* Cr₂SN was found to be unstable (*cf.* Section 2.4). For this structure we only report the lattice parameters of the lowest energy stationary point with hexagonal symmetry.

M ₂ AX phase	<i>a</i>	<i>c</i>	d _{MX}	d _{MA}	C ₁₁	C ₁₂	C ₁₃	C ₃₃	C ₄₄	B	G	E
Mo ₂ AlC	3.038	13.48	1.207	2.162	333	97	144	327	137	196	119	296
Mo ₂ AlN*	2.862	14.66	1.412	2.253								
Mo ₂ SiC	3.119	12.39	1.159	1.938	311	149	192	338	124	225	94	248
Mo ₂ SiN*	3.008	12.94	1.297	1.937								
Mo ₂ PC	3.200	11.62	1.113	1.793	262	148	218	329	105	225	71	193
Mo ₂ PN	3.324	10.94	0.965	1.771	303	223	163	329	79	226	65	179
Mo ₂ SC*	3.366	11.00	0.941	1.809								
Mo ₂ SN	3.340	10.96	0.955	1.785	301	196	145	267	19	204	44	122
Mo ₂ GaC	3.084	13.16	1.168	2.121	294	98	160	289	127	190	101	257
Mo ₂ GaN	2.878	14.51	1.399	2.229	249	225	172	377	66	224	49	137
Mo ₂ GeC	3.149	12.64	1.131	2.028	299	151	170	325	97	212	83	219
Mo ₂ GeN*	3.229	12.13	1.029	2.003								
Mo ₂ AsC	3.225	12.17	1.082	1.959	247	140	200	306	60	209	52	144
Mo ₂ AsN	3.342	11.47	0.950	1.917	309	176	144	329	74	208	75	201
Mo ₂ CdC	3.089	14.37	1.142	2.450	287	80	116	256	77	162	86	218
Mo ₂ CdN	2.919	15.36	1.343	2.498	216	165	151	300	94	185	60	163
Mo ₂ InC	3.140	14.01	1.126	2.375	270	94	127	286	85	169	83	215
Mo ₂ InN*	3.235	13.40	1.010	2.340								
Mo ₂ SnC	3.203	13.52	1.095	2.285	262	149	133	301	43	184	56	152
Mo ₂ SnN*	3.270	13.08	1.002	2.268								
Mo ₂ TlC	3.191	14.02	1.085	2.418	241	105	126	230	65	158	63	167
Mo ₂ TlN	3.321	13.30	0.929	2.395	226	124	77	213	55	136	58	153
Mo ₂ PbC	3.241	13.84	1.068	2.392	231	136	115	225	10	158	35	97
Mo ₂ PbN	3.340	13.23	0.944	2.364	221	89	106	228	35	141	52	138

TABLE XIII: Calculated lattice parameters (in Å), elastic constants, and moduli (in GPa) of the Mo₂AX phases.

* Mo₂AlN, Mo₂SiN, Mo₂SC, Mo₂GeN, Mo₂InN and Mo₂SnN were found to be unstable (*cf.* Section 2.4). For these structures we only report the lattice parameters of the lowest energy stationary point with hexagonal symmetry.

M ₂ AX phase	<i>a</i>	<i>c</i>	d _{MX}	d _{MA}	C ₁₁	C ₁₂	C ₁₃	C ₃₃	C ₄₄	B	G	E
Nb ₂ AlC	3.125	13.91	1.238	2.239	310	90	118	289	139	173	116	285
Nb ₂ AlN	3.009	14.38	1.349	2.247	309	136	132	331	144	194	112	281
Nb ₂ SiC	3.233	12.38	1.197	1.899	303	131	169	333	183	209	122	305
Nb ₂ SiN	3.242	12.15	1.146	1.891	279	167	177	316	170	213	103	265
Nb ₂ PC	3.303	11.61	1.158	1.745	369	113	171	385	187	226	145	358
Nb ₂ PN	3.294	11.53	1.119	1.763	296	129	192	352	142	219	102	266
Nb ₂ SC	3.312	11.65	1.110	1.803	309	106	159	310	118	197	101	258
Nb ₂ SN	3.145	12.29	1.294	1.779	317	130	197	328	144	223	106	273
Nb ₂ GaC	3.153	13.59	1.214	2.183	309	80	138	262	126	177	108	270
Nb ₂ GaN	3.007	14.32	1.355	2.226	312	139	135	340	136	198	109	275
Nb ₂ GeC	3.259	12.60	1.166	1.985	287	126	160	266	159	192	106	268
Nb ₂ GeN	3.269	12.35	1.118	1.969	266	167	161	290	147	200	91	236
Nb ₂ AsC	3.339	12.00	1.129	1.870	327	108	155	347	162	204	126	312
Nb ₂ AsN	3.322	11.97	1.091	1.901	274	134	176	325	115	205	86	226
Nb ₂ CdC	3.175	14.65	1.183	2.479	281	89	90	232	81	148	87	217
Nb ₂ CdN	3.176	14.40	1.142	2.457	271	90	104	230	73	152	79	202
Nb ₂ InC	3.196	14.47	1.188	2.430	291	76	108	267	102	159	99	247
Nb ₂ InN	3.215	14.13	1.131	2.401	236	87	133	244	94	158	77	197
Nb ₂ SnC	3.273	13.85	1.141	2.321	252	96	129	244	99	162	81	209
Nb ₂ SnN	3.282	13.60	1.088	2.311	211	136	131	256	75	164	56	151
Nb ₂ TlC	3.235	14.47	1.157	2.460	270	88	95	240	72	149	80	204
Nb ₂ TlN	3.313	13.75	1.044	2.394	105	21	148	164	78	112	43	115
Nb ₂ PbC	3.313	14.10	1.110	2.414	228	76	116	210	74	142	69	177
Nb ₂ PbN	3.386	13.51	0.993	2.384	150	143	87	220	40	128	30	84

TABLE XIV: Calculated lattice parameters (in Å), elastic constants, and moduli (in GPa) of the Nb₂AX phases.

M_2AX phase	a	c	d_{MX}	d_{MA}	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	B	G	E
Zr ₂ AlC	3.333	14.59	1.269	2.380	261	63	63	224	87	125	92	221
Zr ₂ AlN	3.266	14.40	1.282	2.319	264	77	89	235	105	141	94	231
Zr ₂ SiC	3.331	13.61	1.297	2.106	261	83	105	264	116	152	97	240
Zr ₂ SiN	3.278	13.49	1.290	2.081	224	111	136	272	128	165	85	217
Zr ₂ PC	3.467	12.25	1.282	1.779	290	99	110	343	142	174	116	285
Zr ₂ PN	3.427	12.08	1.233	1.786	290	114	126	332	152	183	115	284
Zr ₂ SC	3.435	12.25	1.233	1.830	288	94	104	312	135	165	113	275
Zr ₂ SN	3.418	12.02	1.178	1.827	274	99	124	299	124	171	101	252
Zr ₂ GaC	3.343	14.25	1.267	2.295	264	69	69	216	81	128	88	214
Zr ₂ GaN	3.283	14.04	1.272	2.238	262	89	93	237	102	145	90	224
Zr ₂ GeC	3.346	13.82	1.281	2.173	249	80	102	248	99	146	87	218
Zr ₂ GeN	3.304	13.64	1.266	2.144	222	107	126	247	110	156	78	200
Zr ₂ AsC	3.484	12.67	1.263	1.905	220	114	124	280	131	161	87	221
Zr ₂ AsN	3.460	12.41	1.210	1.893	268	103	119	315	138	171	106	263
Zr ₂ CdC	3.345	15.36	1.255	2.585	203	84	50	173	21	105	46	121
Zr ₂ CdN	3.331	14.87	1.214	2.503	231	74	69	205	59	121	70	175
Zr ₂ InC	3.376	15.09	1.241	2.531	251	62	58	215	73	119	84	204
Zr ₂ InN	3.307	14.98	1.258	2.487	241	71	89	223	85	134	81	202
Zr ₂ SnC	3.384	14.73	1.255	2.428	225	62	90	224	88	129	80	199
Zr ₂ SnN	3.321	14.71	1.260	2.418	216	93	102	238	83	140	70	181
Zr ₂ TlC	3.392	15.12	1.232	2.547	246	65	57	206	62	117	78	191
Zr ₂ TlN	3.332	14.98	1.240	2.504	217	71	95	204	75	129	69	176
Zr ₂ PbC	3.418	14.95	1.229	2.510	219	70	67	206	68	117	71	177
Zr ₂ PbN	3.357	14.95	1.234	2.502	204	84	90	208	63	127	61	157

TABLE XV: Calculated lattice parameters (in Å), elastic constants, and moduli (in GPa) of the Zr₂AX phases.

M ₂ AX phase	<i>a</i>	<i>c</i>	d _{MX}	d _{MA}	C ₁₁	C ₁₂	C ₁₃	C ₃₃	C ₄₄	B	G	E
Hf ₂ AlC	3.278	14.39	1.248	2.349	291	66	69	256	101	138	105	252
Hf ₂ AlN	3.198	14.28	1.275	2.296	300	80	98	265	120	158	109	266
Hf ₂ SiC	3.277	13.42	1.274	2.082	285	84	117	297	128	167	108	266
Hf ₂ SiN	3.217	13.34	1.277	2.057	256	110	149	307	142	182	99	250
Hf ₂ PC	3.422	12.04	1.255	1.755	317	95	126	368	158	188	129	315
Hf ₂ PN	3.376	11.89	1.215	1.758	317	115	137	374	167	198	128	316
Hf ₂ SC	3.383	12.06	1.205	1.811	320	91	114	334	148	179	126	305
Hf ₂ SN	3.347	11.92	1.172	1.809	277	115	148	297	130	186	97	249
Hf ₂ GaC	3.289	14.04	1.244	2.266	295	71	72	247	92	141	101	244
Hf ₂ GaN	3.217	13.91	1.263	2.215	295	88	105	258	112	160	102	253
Hf ₂ GeC	3.298	13.61	1.255	2.147	269	77	109	264	107	155	96	238
Hf ₂ GeN	3.250	13.44	1.249	2.111	246	111	137	271	121	170	87	223
Hf ₂ AsC	3.441	12.46	1.233	1.880	261	106	135	302	143	175	103	257
Hf ₂ AsN	3.413	12.21	1.190	1.863	287	107	129	340	150	183	114	284
Hf ₂ CdC	3.293	15.15	1.237	2.551	254	74	53	201	40	119	69	174
Hf ₂ CdN	3.270	14.69	1.204	2.468	259	74	84	224	68	136	79	198
Hf ₂ InC	3.327	14.87	1.218	2.499	281	66	61	242	82	131	95	230
Hf ₂ InN	3.245	14.87	1.250	2.467	274	74	98	237	93	147	91	227
Hf ₂ SnC	3.341	14.52	1.227	2.402	240	62	103	236	92	139	84	210
Hf ₂ SnN	3.265	14.59	1.248	2.399	241	91	114	247	85	152	76	196
Hf ₂ TlC	3.346	14.87	1.207	2.510	273	70	63	227	69	129	86	212
Hf ₂ TlN	3.269	14.88	1.235	2.484	250	74	104	221	77	142	78	197
Hf ₂ PbC	3.379	14.71	1.196	2.483	241	77	70	222	69	126	77	191
Hf ₂ PbN	3.305	14.80	1.219	2.482	213	78	107	199	61	134	60	157

TABLE XVI: Calculated lattice parameters (in Å), elastic constants, and moduli (in GPa) of the Hf₂AX phases.

M_2AX phase	a	c	d_{MX}	d_{MA}	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	B	G	E
Ta ₂ AlC	3.102	13.95	1.256	2.231	334	114	130	322	148	193	122	303
Ta ₂ AlN	2.984	14.49	1.382	2.241	335	175	144	355	154	217	115	293
Ta ₂ SiC	3.234	12.32	1.193	1.888	312	147	191	348	200	226	126	318
Ta ₂ SiN	3.242	12.09	1.157	1.866	293	183	188	367	172	230	106	275
Ta ₂ PC	3.304	11.56	1.150	1.740	384	126	185	422	198	243	151	375
Ta ₂ PN	3.157	12.24	1.320	1.741	356	158	221	383	173	255	122	315
Ta ₂ SC	3.305	11.67	1.102	1.815	314	110	172	319	104	206	95	247
Ta ₂ SN	3.102	12.55	1.343	1.793	357	176	197	354	145	246	109	285
Ta ₂ GaC	3.133	13.62	1.229	2.176	335	106	137	315	137	194	118	294
Ta ₂ GaN	2.982	14.45	1.387	2.226	333	187	150	364	141	223	107	277
Ta ₂ GeC	3.265	12.49	1.159	1.964	300	141	169	299	172	206	113	286
Ta ₂ GeN	3.275	12.22	1.124	1.932	271	182	180	327	152	217	92	241
Ta ₂ AsC	3.344	11.93	1.117	1.865	343	118	170	374	167	219	129	324
Ta ₂ AsN	3.332	11.89	1.091	1.882	269	146	189	354	94	216	74	200
Ta ₂ CdC	3.150	14.69	1.202	2.470	312	118	101	253	94	168	94	238
Ta ₂ CdN	3.137	14.55	1.184	2.453	282	89	129	252	71	168	79	205
Ta ₂ InC	3.176	14.50	1.201	2.423	313	84	121	298	108	175	106	265
Ta ₂ InN	3.182	14.26	1.164	2.400	237	93	157	263	91	172	73	191
Ta ₂ SnC	3.273	13.76	1.136	2.304	262	110	143	270	98	176	81	211
Ta ₂ SnN	3.281	13.53	1.093	2.290	201	158	149	270	64	176	44	122
Ta ₂ TlC	3.216	14.48	1.168	2.452	288	98	114	254	78	165	84	214
Ta ₂ TlN	3.340	13.50	1.023	2.353	126	74	149	228	76	136	43	116
Ta ₂ PbC	3.317	13.97	1.100	2.393	192	45	133	212	73	135	63	163
Ta ₂ PbN	3.392	13.44	0.997	2.362	144	154	91	213	15	130	16	46

TABLE XVII: Calculated lattice parameters (in Å), elastic constants and moduli (in GPa) of the Ta₂AX phases.

M ₂ AX phase	<i>a</i>	<i>c</i>	d _{MX}	d _{MA}	C ₁₁	C ₁₂	C ₁₃	C ₃₃	C ₄₄	B	G	E
W ₂ AlC	3.013	13.68	1.243	2.176	309	92	191	358	136	214	110	280
W ₂ AlN*	2.841	14.92	1.461	2.269								
W ₂ SiC	3.150	12.22	1.148	1.906	329	162	230	358	130	251	95	253
W ₂ SiN*	2.892	13.92	1.444	2.036								
W ₂ PC	3.272	11.27	1.059	1.758	226	216	239	342	92	242	45	126
W ₂ PN	3.367	10.80	0.951	1.750	303	232	162	354	71	230	62	171
W ₂ SC*	3.387	11.07	0.921	1.847								
W ₂ SN*	3.168	11.91	1.123	1.854								
W ₂ GaC	3.087	13.15	1.174	2.115	301	112	194	298	129	211	97	252
W ₂ GaN*	2.849	14.86	1.460	2.254								
W ₂ GeC	3.180	12.44	1.119	1.990	313	171	198	349	97	234	80	216
W ₂ GeN*	3.264	11.91	1.025	1.953								
W ₂ AsC	3.298	11.80	1.030	1.920	215	220	210	331	65	227	34	96
W ₂ AsN	3.391	11.31	0.930	1.896	309	180	148	347	61	213	70	189
W ₂ CdC	3.050	14.63	1.189	2.468	304	74	143	282	85	179	93	236
W ₂ CdN	2.868	15.83	1.436	2.521	373	210	129	347	103	226	99	259
W ₂ InC	3.141	14.02	1.131	2.375	278	120	145	304	76	187	76	201
W ₂ InN*	3.264	13.26	0.996	2.319								
W ₂ SnC	3.205	13.54	1.100	2.284	266	165	154	322	6	200	38	107
W ₂ SnN*	3.292	12.96	1.002	2.238								
W ₂ TlC	3.192	14.01	1.091	2.412	235	124	143	253	61	171	57	153
W ₂ TlN	3.349	13.18	0.921	2.375	237	149	76	232	51	145	56	149
W ₂ PbC*	3.250	13.81	1.065	2.388								
W ₂ PbN	3.391	13.07	0.917	2.351	211	120	61	217	28	125	47	124

TABLE XVIII: Calculated lattice parameters (in Å), elastic constants and moduli (in GPa) of the W₂AX phases.

* W₂AlN, W₂SiN, W₂SC, W₂SN, W₂GaN, W₂GeN, W₂InN, W₂SnN and W₂PbC were found to be unstable (*cf.* Section 2.4). For these structures we only report the lattice parameters of the lowest energy stationary point with hexagonal symmetry.