Electronic supplementary information

Theoretical study of ternary silver fluorides $AgMF_4$ (M = Cu, Ni, Co) formation at pressures up to 20 GPa

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S1. Estimated phase-transition pressures for the substrates

The calculations were performed for the pressures up to 20 GPa, thus we considered the known phase transitions (PTs) for AgF_2[1] (sequence $Pbca \rightarrow Pca2_1$ (~8 GPa) → $Pbcn$ (~14 GPa)), AgF[2] (NaCl-type → CsCl-type (1-3 GPa)), CoF_2[3,4] (rutile → $Pnnm$ (~4 GPa) → $Pbca/Pa\overline{3}$ (~8 GPa) → $I4/mmm$ (~12 GPa)), NiF_2[4] (rutile → $Pnnm$ (~4 GPa) → $I4/mmm$ (~10 GPa)) and CuF_2[5] ($P2_1/c \rightarrow Pbca$ (~9 GPa)).

Our results are presented on the **Figure S3** and in the **Table S1**. All of the abovementioned PTs were confirmed using a chosen theoretical approach, resulting in PT pressure differences smaller than 1.0 GPa (the only exception is nearly 2 GPa shift for 3rd PT of CoF_2). We indicate also that the so-called in literature "distorted fluorite" HP polymorph of NiF_2 (assumed $I4/mmm$) would have too high enthalpy. Instead, we propose formation of orthorhombic distorted PdF_2 type structure (*Pbca* symmetry), which is consistent with CoF_2 and CuF_2 sequences of pressure-induced PTs.

S2. Supplementary Figures

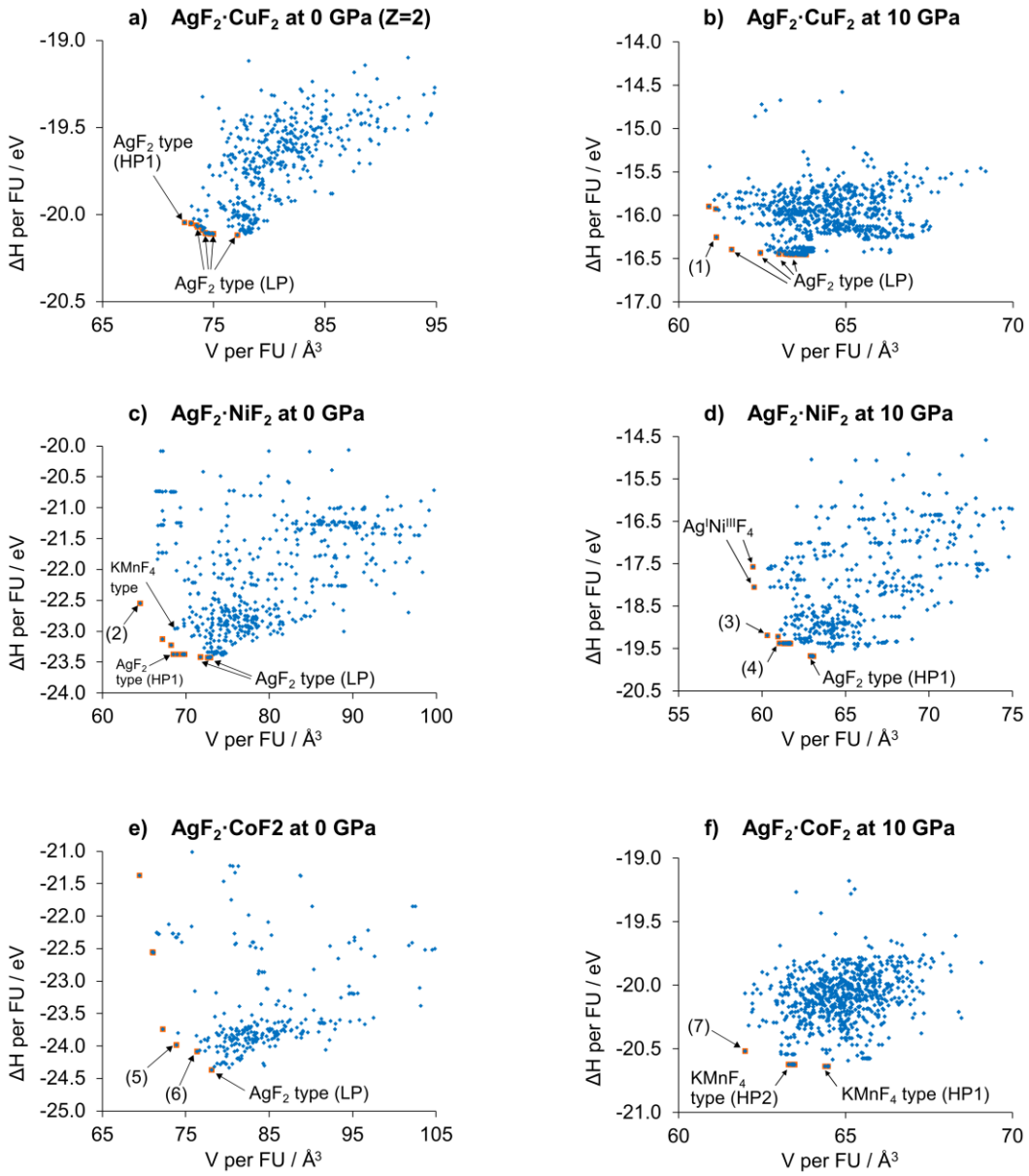

Figure S1. Performed XtalOpt quests for the lowest-enthalpy structures for the $AgCuF_4$, $AgNiF_4$ and $AgCoF_4$ stoichiometries for Z=4 at 10 GPa (with the exception for $AgF_2{\cdot}CuF_2$ systems, studied with Z=2). All structures energies are marked with blue diamonds, while structures with simultaneously the lowest enthalpy & volume are marked with orange squares (they are candidate for higher pressures phases). Brief description of structures not mentioned in the main article: (1) $Ag^{II}Cu^{II}F_4$ structure with linked pure layers (of AgF_2 and CuF_2); (2) $Ag^{II}Ni^{II}F_4$ with infinite flat chains $[AgF_{4/2}]$ and $[NiF_{4/2}]$; (3) $Ag^{II}Ni^{II}F_4$ flat layers consisting of both Ag(II) and Ni; (4) $Ag^{II}Ni^{II}F_4$ buckle layers consisting of both Ag and Ni; (5) $Ag^{II}Co^{II}F_4$ polymorph of distorted $KBrF_4$ type; (6) $AgCoF_4$ polymorph with mixed valences Ag(I,II) and Co(II,III) of distorted rutile type; (7) $Ag^{I}Co^{III}F_4$ with infinite chains of $[CoF_{2/1}F_{4/2}]$ and Ag(I). All indicated AgF_2 type structures feature $Ag^{II}M^{II}F_4$ valences, while all KMnF4 feature $Ag^{I}M^{III}F_4$ valences.

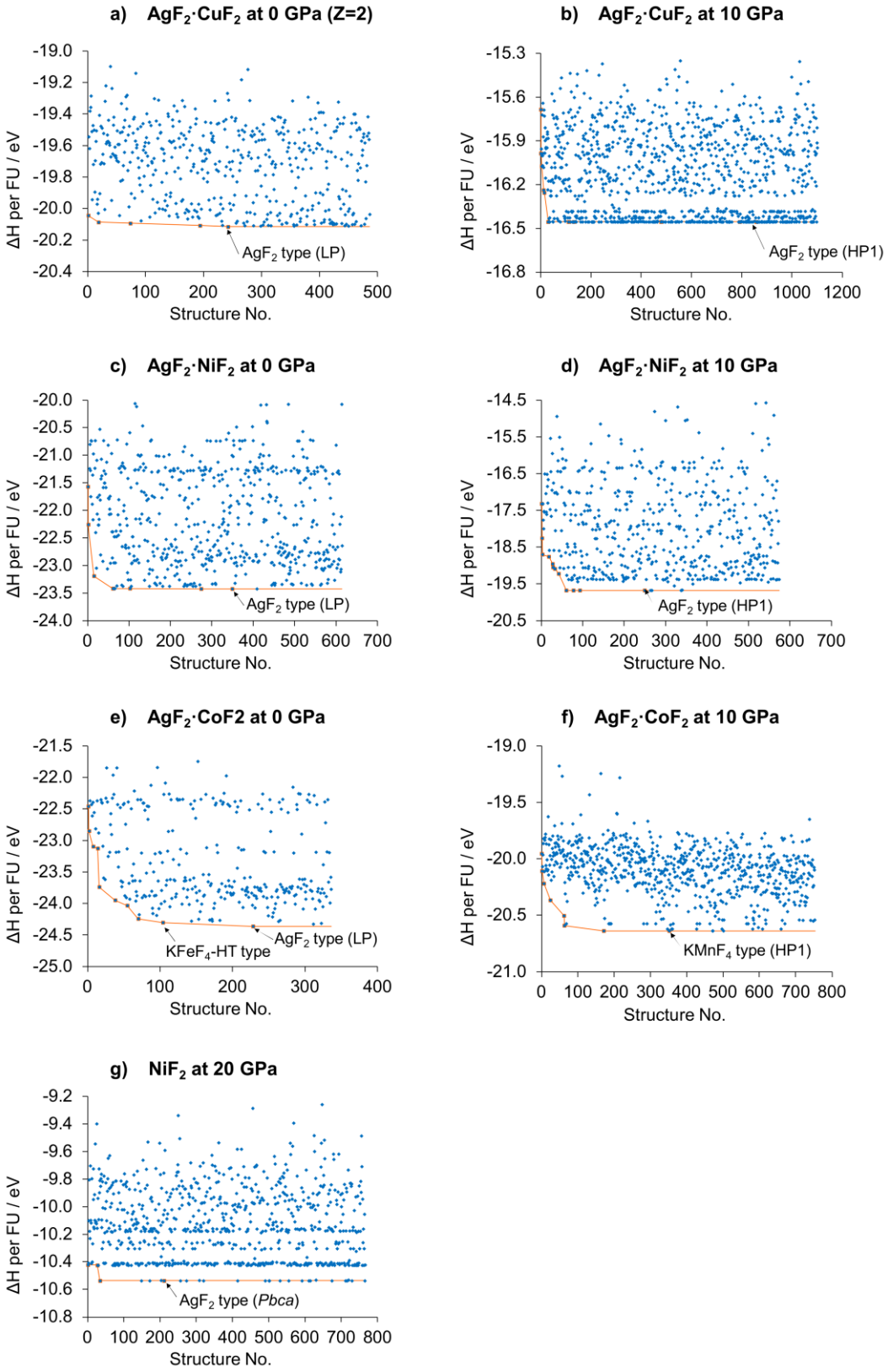

Figure S2. Performed EA quests for the lowest-enthalpy structures for the $AgCuF_4$, $AgNiF_4$, $AgCoF_4$ and NiF_2 stoichiometries for Z=4 (with the exception for $AgF_2{\cdot}CuF_2$ systems, studied with Z=2). All structures energies are marked with blue diamonds, while structures with simultaneously the lowest enthalpy & volume are marked with orange squares and are connected with orange lines. During the search for $AgCuF_4$ at 10 GPa **(b)** many AgF_2 type polymorphs were found of nearly equal energy, so finally application of the lowest-energy antiferromagnetic model was crucial and lead to HP1 polymorph. In the search **(e)** obtained polymorphs' energies were higher than for manually found $KFeF_4$-LT polymorph (LP). For each composition and pressure the total number (including duplicates, not shown on the plots above) of obtained structures is: (a) 500, (b) 1200, (c) 1000, (d) 1000, (e) 500, (f) 800, and (g) 1000. The number of unique structures obtained is (a) 486, (b) 1102, (c) 614, (d) 574, (e) 336, (f) 753, and (g) 765 structures, for each system respectively.

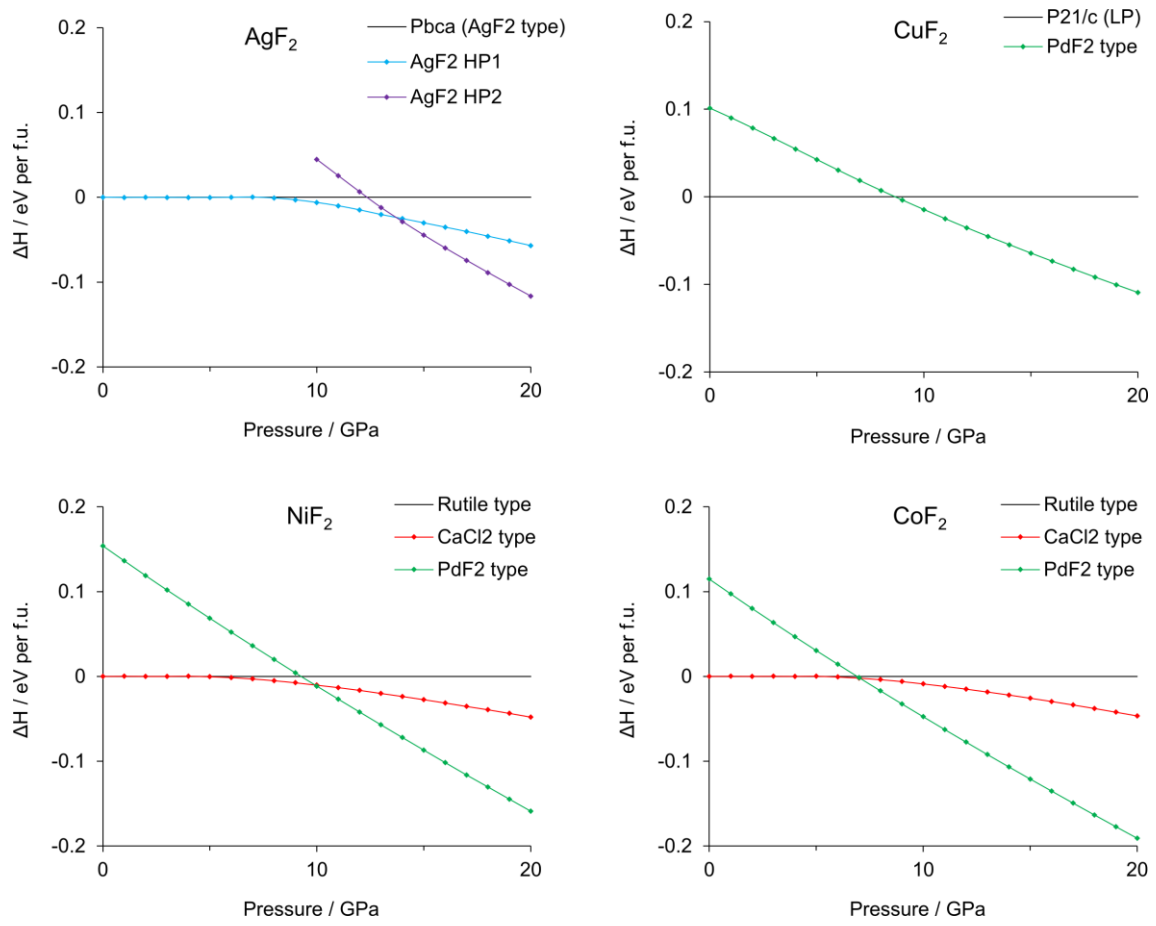

Figure S3. Enthalpy versus pressure diagrams for parent binary fluorides.

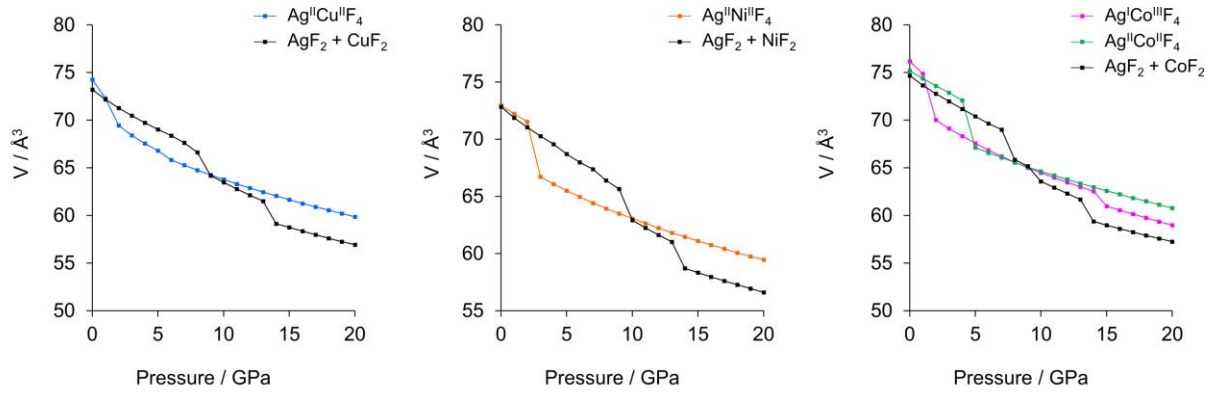

Figure S4. Pressure versus volume plots for the lowest-enthalpy polymorphs of $AgCuF_4$, $AgNiF_4$ and $AgCoF_4$ with respect to the considered substrates.

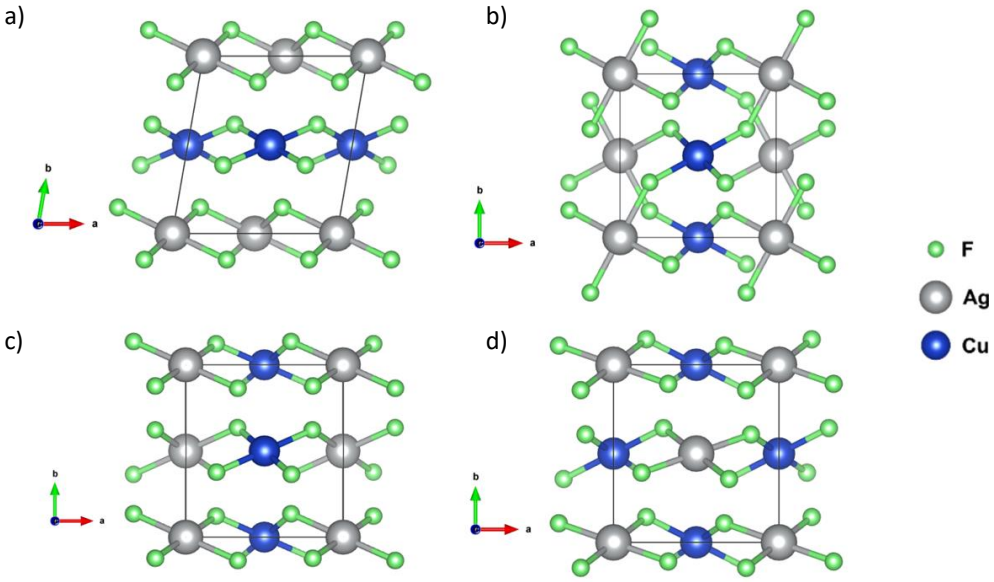

Figure S5. Structures of $AgCuF_4$ originating from various substitutions within AgF_2 type structure enabled by its orthorhombic symmetry, after sequential geometry optimization runs: (a) $\perp\vec{b}$ separate layers polymorph, (b) $\perp\vec{a}$ (HP1 polytype), (c) $\perp\vec{a}$ mixed-layers polymorph, and (d) $\perp\vec{c}$ mixed-layers polymorph.

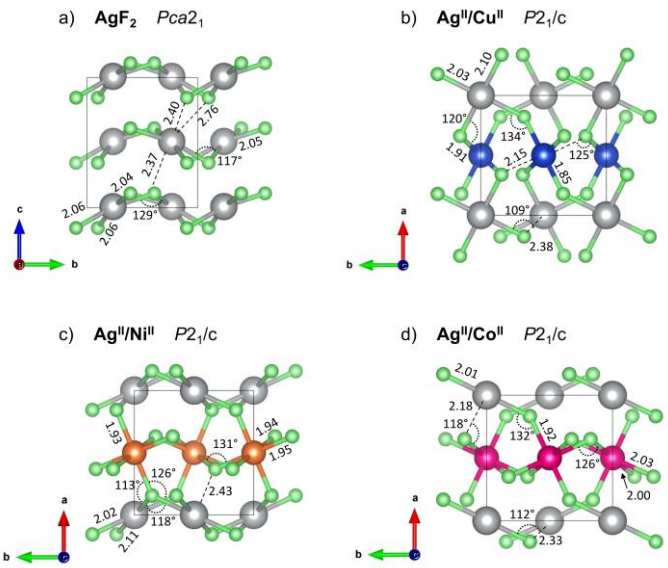

Figure S6. Crystal structures of (a) parent AgF_2, and the lowest-energy predicted (b) $AgCuF_4$, and (c) $AgNiF_4$, and metastable (d) $Ag^{II}Co^{II}F_4$ at 10 GPa (HP1 structure of each). The threshold for Ag-F bond drawing is 2.15 Å in all cases. This view is rotated by 90° along c (in AgF_2 case) or a (in the other cases) with respect to the **Figure 3**.

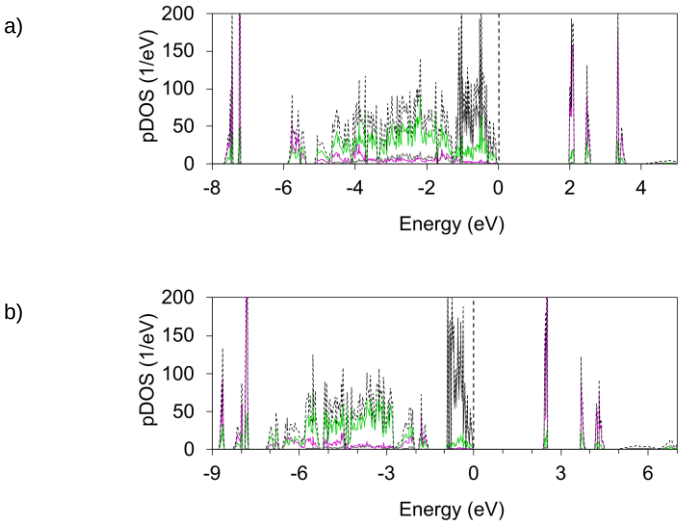

Figure S7. Orbital-projected electronic density of states (pDOS) of $Ag^{I}Co^{III}F_4$ at 0 GPa, calculated on DFT+U (a) HSE06 level (b). Dashed lines indicate total DOS, while silver states are drawn in grey, fluorine in green, and cobalt in magenta.

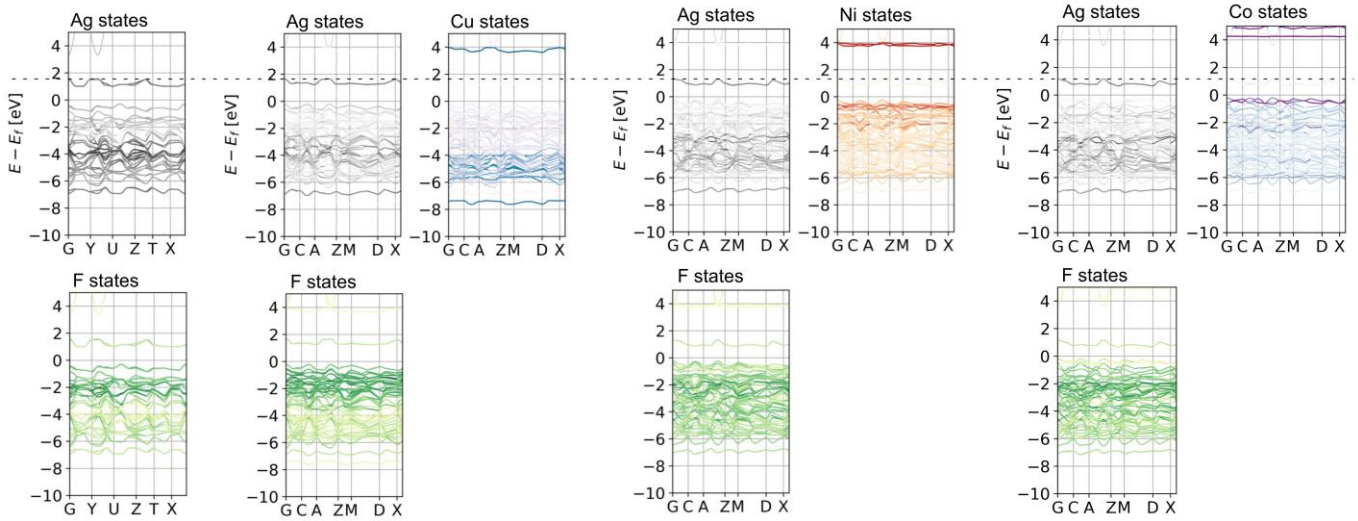

Figure S8. Atom-projected electronic band structures of the lowest-energy polymorphs of AgF_2, $AgCuF_4$, $AgNiF_4$ and $Ag^{II}Co^{II}F_4$ (from left to right, respectively) at 0 GPa. Colour intensities relate to atomic contribution to a given band. Dotted line marks the maximum energy of Ag(II) upper Hubbard band, showing the increasing contribution of M^{2+} in valence bands.

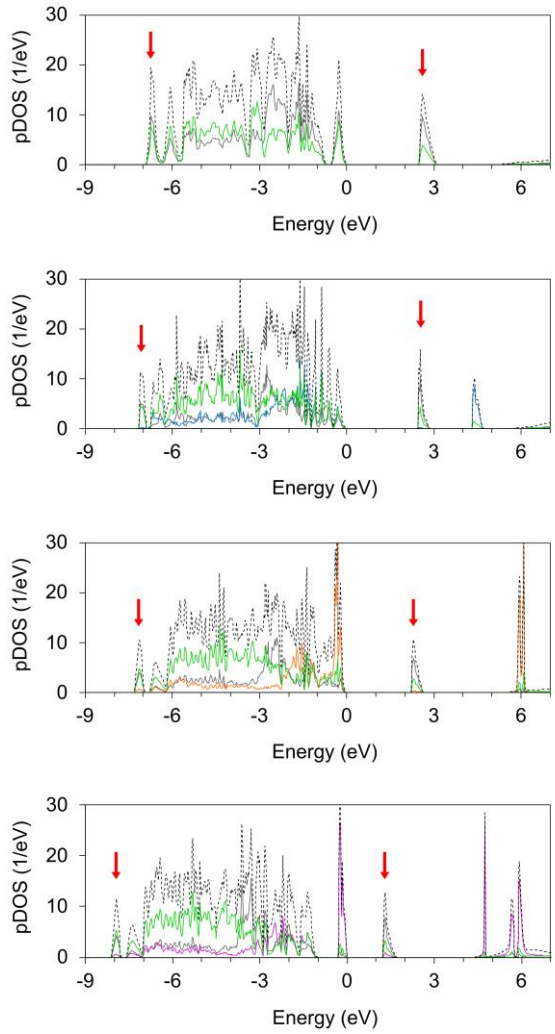

Figure S9. Orbital projected electronic density of states (pDOS) of presented here systems, calculated on HSE06 level. From the top to bottom: parent AgF_2 and considered $Ag^{II}M^{II}F_4$ (M = Cu, Ni, Co) compounds. Red arrows indicate lower and upper Hubbard (LHB and UHB) bands of Ag^{2+}. Dashed lines indicate total DOS, while silver states are drawn in grey, fluorine in green, copper in blue, nickel in orange and cobalt in magenta.

S3. Supplementary Tables

Table S1. Phase transition pressures obtained from DFT+U calculations for parent binary fluorides compared with experimental data.

Substrates phase transitions < 20 GPa

AgF_2			
PT	Calc.	Exp.	Ref.
I	7.3	7.8	[1]
II	13.7	14.2	[1]

CoF_2			
PT	Calc.	Exp.	Ref.
I	4.0	3.6	[3]
II	7.0	8	[3]
III	9.9	12	[3]

NiF_2			
PT	Calc.	Exp.	Ref.
I	4.4	4-5	[4]
II	9.9	10	[4]

CuF_2			
PT	Calc.	Exp.	Ref.
I	8.6	9	[5]

*all data given in GPa

Table S2. Comparison of DFT+U and hybrid HSE06 energies of formation and volume for presented ternary fluorides and parent phases of binary fluorides. ΔE_f denotes formation energy with respect to binary fluorides with d-metals at +II oxidation state.

Structures at 0 GPa			DFT+U			HSE06			
System	Structure type	Symmetry	ΔE_f / kJ/mol	V / Å^3	V_{prod}/V_{substr}	ΔE_f / kJ/mol	V / Å^3	V_{prod}/V_{substr}	E_{gap} / eV
$Ag^{II}Co^{II}F_4$	AgF_2 type (LP)	$P2_1/c$	5.7	75.18	100.7%	6.7	77.32	100.1%	1.240
			*-20.2			*-5.6			
$Ag^{I}Co^{III}F_4$	$KFeF_4$ type	Pnma	-4.2	76.19	102.0%	-25.1	77.32	103.0%	2.445
			*-30.1			*-37.4			
$AgNiF_4$	AgF_2 type (LP)	$P2_1/c$	8.6	72.98	100.2%	12.0	73.38	99.8%	2.238
$AgCuF_4$	AgF_2 type (LP)	$P2_1/c$	6.7	74.25	101.4%	6.1	75.78	101.3%	2.501
AgF_2	LP	Pbca	-	40.48	-	-	41.06	-	2.510
CuF_2	CuF_2 type	$P2_1/c$	-	32.74	-		33.77		4.556
NiF_2	Rutile type	P4/mmm	-	32.37	-		32.46		5.538
CoF_2	Rutile type	P4/mmm	-	34.19	-		34.03		4.360

*with respect to the AgF + CoF_3 reaction

Structures at 10 GPa			DFT+U			HSE06			
System	Structure type	Symmetry	ΔH_f / kJ/mol	V / Å^3	V_{prod}/V_{substr}	ΔH_f / kJ/mol	V / Å^3	V_{prod}/V_{substr}	E_{gap} / eV
$Ag^{II}Co^{II}F_4$	AgF_2 type (HP1)	$P2_1/c$	3.2	64.63	101.6%	5.9	65.02	101.9%	1.275
$Ag^{I}Co^{III}F_4$	$KMnF_4$ type (HP1)	$P2_1/m$	-12.6	64.49	101.4%	-26.4	65.39	103.0%	2.142
$AgNiF_4$	AgF_2 type (HP1)	$P2_1/c$	-3.9	63.07	100.2%	-2.1	63.57	100.2%	1.690
$AgCuF_4$	AgF_2 type (HP1)	$P2_1/c$	-1.9	63.78	100.5%	-3.5	64.94	100.4%	2.433
AgF_2	HP1	$Pca2_1$	-	35.19	-	-	35.62	-	2.493
CuF_2	AgF_2 type	Pbca	-	28.28	-	-	29.06	-	5.542
NiF_2	AgF_2 type	Pbca	-	27.73	-	-	27.83	-	5.431
CoF_2	AgF_2 type	Pbca	-	28.40	-	-	28.16	-	4.376

Table S3. Electronic band gaps dependency on pressure elevation for the lowest-enthalpy structures of AgF_2, $AgCuF_4$, $AgNiF_4$, and $AgCoF_4$ calculated on DFT+U level.

p / GPa	AgF_2		$AgCuF_4$			$AgNiF_4$			$Ag^{II}Co^{II}F_4$			$Ag^{I}Co^{III}F_4$		
	E_{gap} / eV	Structure	E_{gap} / eV	ΔH_f / kJ/mol	Structure	E_{gap} / eV	ΔH_f / kJ/mol	Structure	E_{gap} / eV	ΔH_f / kJ/mol	Structure	E_{gap} / eV	ΔH_f / kJ/mol	Structure
0	1.334	LP	1.463	6.72	LP	1.091	8.61	LP	0.899	5.66	LP	2.020	-4.25	LP
1	1.302	LP	1.437	7.43	LP	1.094	8.73	LP	0.867	5.98	LP	1.965	-3.34	LP
2	1.307	LP	1.444	6.93	LP	1.079	8.94	LP	0.851	6.43	LP	2.057	-3.73	HP1
3	1.293	LP	1.429	5.83	LP	0.587	8.45	HP1	0.834	6.95	LP	1.991	-5.34	HP1
4	1.277	LP	1.433	4.53	LP	0.589	6.32	HP1	0.836	7.42	HP1	1.961	-7.05	HP1
5	1.281	LP	1.417	3.24	LP	0.590	4.28	HP1	0.812	7.65	HP1	1.911	-8.82	HP1
6	1.266	LP	1.538	1.70	HP1	0.591	2.33	HP1	0.798	5.67	HP1	1.898	-10.49	HP1
7	1.269	LP	1.530	0.24	HP1	0.593	0.49	HP1	0.792	3.82	HP1	1.847	-12.15	HP1
8	1.275	HP1	1.532	-1.11	HP1	0.615	-1.20	HP1	0.772	3.41	HP1	1.833	-12.44	HP1
9	1.282	HP1	1.519	-1.90	HP1	0.596	-2.70	HP1	0.774	3.23	HP1	1.800	-12.59	HP1
10	1.311	HP1	1.522	-1.85	HP1	0.618	-3.90	HP1	0.753	3.24	HP1	1.786	-12.62	HP1
11	1.337	HP1	1.507	-1.69	HP1	0.620	-3.82	HP1	0.756	3.86	HP1	1.753	-12.09	HP1
12	1.341	HP1	1.511	-1.38	HP1	0.620	-3.61	HP1	0.735	4.57	HP1	1.738	-11.47	HP1
13	1.364	HP1	1.495	-0.93	HP1	0.622	-3.25	HP1	0.737	5.46	HP1	1.723	-10.76	HP1
14	1.347	HP2	1.497	0.00	HP1	0.603	-2.41	HP1	0.717	6.82	HP1	1.690	-9.64	HP1
15	1.330	HP2	1.501	1.74	HP1	0.624	-0.79	HP1	0.718	8.96	HP1	2.069	-7.80	HP2
16	1.314	HP2	1.484	3.49	HP1	0.625	0.87	HP1	0.719	11.12	HP1	2.053	-6.59	HP2
17	1.318	HP2	1.505	5.25	HP1	0.606	2.55	HP1	0.699	13.29	HP1	2.058	-5.42	HP2
18	1.301	HP2	1.509	7.01	HP1	0.627	4.23	HP1	0.700	15.44	HP1	2.022	-4.29	HP2
19	1.285	HP2	1.493	8.77	HP1	0.608	5.92	HP1	0.680	17.58	HP1	2.025	-3.19	HP2
20	1.288	HP2	1.495	10.49	HP1	0.629	7.62	HP1	0.681	19.72	HP1	2.009	-2.12	HP2

S4. Γ-point vibration frequencies

Γ-point vibration frequencies (in cm^{-1}) calculated at DFT+U level of theory, in each case 3 acoustic modes are omitted.

AgCuF4 LP at 0 GPa (P2_1/c)
1 f = 526
2 f = 499
3 f = 490
4 f = 461
5 f = 455
6 f = 444
7 f = 375
8 f = 361
9 f = 350
10 f = 339
11 f = 327
12 f = 316
13 f = 302
14 f = 272
15 f = 263
16 f = 235
17 f = 233
18 f = 231
19 f = 212
20 f = 206
21 f = 200
22 f = 190
23 f = 185
24 f = 169
25 f = 165
26 f = 156
27 f = 140
28 f = 120
29 f = 112
30 f = 104
31 f = 73
32 f = 70
33 f = 58

AgCuF4 HP1 at 10 GPa (P2_1/c)
1 f = 572
2 f = 565
3 f = 529
4 f = 520
5 f = 499
6 f = 455
7 f = 453
8 f = 409
9 f = 406
10 f = 378
11 f = 372
12 f = 355
13 f = 352
14 f = 313
15 f = 300
16 f = 296
17 f = 259
18 f = 246
19 f = 232
20 f = 225
21 f = 214
22 f = 212
23 f = 199
24 f = 196
25 f = 192
26 f = 172
27 f = 156
28 f = 129
29 f = 127
30 f = 126
31 f = 125
32 f = 102
33 f = 69

AgNiF4 LP at 0 GPa (P2_1/c)
1 f = 512
2 f = 512
3 f = 488
4 f = 453
5 f = 407
6 f = 405
7 f = 398
8 f = 358
9 f = 356
10 f = 341
11 f = 318
12 f = 314
13 f = 313
14 f = 308
15 f = 263
16 f = 252
17 f = 249
18 f = 238
19 f = 226
20 f = 207
21 f = 202
22 f = 174
23 f = 172
24 f = 166
25 f = 165
26 f = 159
27 f = 150
28 f = 136
29 f = 129
30 f = 123
31 f = 83
32 f = 75
33 f = 64

AgNiF4 HP1 at 10 GPa (P2_1/c)
1 f = 533
2 f = 531
3 f = 508
4 f = 493
5 f = 472
6 f = 453
7 f = 452
8 f = 445
9 f = 435
10 f = 395

11 f = 380
12 f = 364
13 f = 357
14 f = 326
15 f = 314
16 f = 294
17 f = 286
18 f = 252
19 f = 241
20 f = 240
21 f = 238
22 f = 220
23 f = 217
24 f = 204
25 f = 204
26 f = 172
27 f = 151
28 f = 142
29 f = 141
30 f = 138
31 f = 129
32 f = 91
33 f = 86

Ag(II)Co(II)F4 LP at 0 GPa (P2_1/c)
1 f = 496
2 f = 495
3 f = 480
4 f = 430
5 f = 393
6 f = 393
7 f = 369
8 f = 355
9 f = 350
10 f = 329
11 f = 313
12 f = 309
13 f = 295
14 f = 287
15 f = 258
16 f = 245
17 f = 236
18 f = 230
19 f = 219
20 f = 181
21 f = 181
22 f = 164
23 f = 163
24 f = 161
25 f = 161
26 f = 150
27 f = 147
28 f = 131
29 f = 128
30 f = 125
31 f = 80
32 f = 74
33 f = 66

Ag(II)Co(II)F4 HP1 at 10 GPa (P2_1/c)
1 f = 557
2 f = 553
3 f = 497
4 f = 484
5 f = 457
6 f = 421
7 f = 407
8 f = 404
9 f = 395
10 f = 381
11 f = 375
12 f = 355
13 f = 351
14 f = 323
15 f = 288
16 f = 277
17 f = 253
18 f = 246
19 f = 244
20 f = 237
21 f = 232
22 f = 209
23 f = 209
24 f = 197
25 f = 184
26 f = 166
27 f = 164
28 f = 142
29 f = 141
30 f = 122
31 f = 106
32 f = 104
33 f = 58

Ag(I)Co(III)F4 LP at 0 GPa (Pnma)
1 f = 614
2 f = 564
3 f = 564
4 f = 549
5 f = 547
6 f = 546
7 f = 545
8 f = 544
9 f = 535
10 f = 530
11 f = 529
12 f = 521
13 f = 520
14 f = 513
15 f = 498
16 f = 498
17 f = 491
18 f = 491
19 f = 487
20 f = 483
21 f = 473
22 f = 470
23 f = 469
24 f = 468
25 f = 426
26 f = 426
27 f = 419
28 f = 418
29 f = 412

30 f = 389
31 f = 388
32 f = 385
33 f = 379
34 f = 378
35 f = 376
36 f = 372
37 f = 356
38 f = 355
39 f = 340
40 f = 340
41 f = 311
42 f = 297
43 f = 297
44 f = 296
45 f = 288
46 f = 288
47 f = 288
48 f = 280
49 f = 269
50 f = 269
51 f = 267
52 f = 265
53 f = 257
54 f = 257
55 f = 255
56 f = 253
57 f = 251
58 f = 250
59 f = 243
60 f = 243
61 f = 241
62 f = 238
63 f = 238
64 f = 235
65 f = 235
66 f = 232
67 f = 223
68 f = 222
69 f = 213
70 f = 210
71 f = 209
72 f = 204
73 f = 204
74 f = 203
75 f = 201
76 f = 200
77 f = 199
78 f = 198
79 f = 196
80 f = 195
81 f = 191
82 f = 187
83 f = 187
84 f = 186
85 f = 185
86 f = 183
87 f = 183
88 f = 181
89 f = 181
90 f = 179
91 f = 175
92 f = 174
93 f = 171
94 f = 170
95 f = 168
96 f = 166
97 f = 166
98 f = 163
99 f = 141
100 f = 139
101 f = 138
102 f = 138
103 f = 124
104 f = 122
105 f = 121
106 f = 116
107 f = 111
108 f = 109
109 f = 103
110 f = 99
111 f = 99
112 f = 98
113 f = 95
114 f = 95
115 f = 94
116 f = 92
117 f = 88
118 f = 88
119 f = 88
120 f = 87
121 f = 86
122 f = 79
123 f = 79
124 f = 78
125 f = 77
126 f = 75
127 f = 72
128 f = 70
129 f = 70
130 f = 69
131 f = 68
132 f = 63
133 f = 63
134 f = 62
135 f = 57
136 f = 46
137 f = 45
138 f = 42
139 f = 41
140 f = 30
141 f = 27

Ag(I)Co(III)F4 HP1 at 10 GPa (P2_1/m)
1 f = 634
2 f = 619
3 f = 601
4 f = 587
5 f = 582
6 f = 565
7 f = 564
8 f = 543
9 f = 518
10 f = 512

11 f = 504
12 f = 500
13 f = 464
14 f = 464
15 f = 450
16 f = 446
17 f = 399
18 f = 387
19 f = 379
20 f = 378
21 f = 350
22 f = 348
23 f = 332
24 f = 332
25 f = 318
26 f = 299
27 f = 288
28 f = 287
29 f = 283
30 f = 272
31 f = 265
32 f = 253
33 f = 249
34 f = 245
35 f = 244
36 f = 244
37 f = 242
38 f = 240
39 f = 235
40 f = 231
41 f = 211
42 f = 208
43 f = 205
44 f = 197
45 f = 194
46 f = 191
47 f = 178
48 f = 178
49 f = 173
50 f = 155
51 f = 147
52 f = 143
53 f = 132
54 f = 130
55 f = 130
56 f = 127
57 f = 119
58 f = 116
59 f = 112
60 f = 109
61 f = 99
62 f = 99
63 f = 96
64 f = 91
65 f = 79
66 f = 78
67 f = 73
68 f = 72
69 f = 11

Ag(I)Co(III)F4 HP2 at 20 GPa HP2 (C2/c)
1 f = 728
2 f = 647
3 f = 634
4 f = 623
5 f = 619
6 f = 616
7 f = 602
8 f = 563
9 f = 562
10 f = 562
11 f = 560
12 f = 548
13 f = 498
14 f = 498
15 f = 488
16 f = 480
17 f = 458
18 f = 447
19 f = 438
20 f = 436
21 f = 386
22 f = 384
23 f = 350
24 f = 348
25 f = 347
26 f = 345
27 f = 342
28 f = 325
29 f = 321
30 f = 318
31 f = 314
32 f = 305
33 f = 274
34 f = 269
35 f = 266
36 f = 256
37 f = 253
38 f = 248
39 f = 246
40 f = 233
41 f = 230
42 f = 229
43 f = 228
44 f = 211
45 f = 210
46 f = 198
47 f = 197
48 f = 187
49 f = 184
50 f = 183
51 f = 175
52 f = 174
53 f = 171
54 f = 158
55 f = 158
56 f = 152
57 f = 127
58 f = 117
59 f = 111
60 f = 111
61 f = 109
62 f = 105
63 f = 102

64 f = 100
65 f = 88
66 f = 76
67 f = 69
68 f = 61
69 f = 55

S5. Crystal structures in POSCAR format

AgCuF4 LP at 0 GPa (P2_1/c)
1.00000000000000
5.3901036487284317 0.7313930884644128 0.0000000000000000
0.7999934734740585 5.8918165998868357 0.0000000000000000
0.0000000000000000 0.0000000000000000 4.7638498089899999
Ag Cu F
2 2 8
Direct
-0.0000000000000000 -0.0000000000000000 -0.0000000000000000
0.5000000000000000 -0.0000000000000000 0.5000000000000000
-0.0000000000000000 0.5000000000000000 0.5000000000000000
0.5000000000000000 0.5000000000000000 -0.0000000000000000
0.3610222200924554 0.8549158998614186 0.1646245680338823
0.6389777799075446 0.1450840701385790 0.8353754559661197
0.1389777799075446 0.1450840701385790 0.6646245910338806
0.8610222630924554 0.8549158998614186 0.3353754559661197
0.7865728171829347 0.3876784498046880 0.2457279423781989
0.2134271828170653 0.6123215501953191 0.7542721046218013
0.7134272258170653 0.6123215501953191 0.7457279423781991
0.2865728171829346 0.3876784498046880 0.2542720816218031

AgCuF4 HP1 at 10 GPa (P2_1/c)
1.00000000000000
4.9274005811963182 0.0000000000000000 -0.0515194211623682
0.0000000000000000 5.1535447840790782 0.0000000000000000
-0.0654618047501239 0.0000000000000000 5.0237402810958489
Ag Cu F
2 2 8
Direct
0.0000000000000000 -0.0000000000000000 -0.0000000000000000
0.0000000000000000 0.5000000000000000 0.5000000000000000
0.5000000000000000 0.5000000000000000 -0.0000000000000000
0.5000000000000000 -0.0000000000000000 0.5000000000000000
0.3389463792717425 0.8347599318493771 0.1960332912334153
0.6610536207282576 0.1652400381506133 0.8039667327665866
0.1779727376733418 0.1555907884328188 0.5930914897534010
0.8220273053266582 0.8444091815671787 0.4069085572465994
0.6610536207282576 0.3347599718493946 0.3039667327665866
0.3389463792717425 0.6652400281506196 0.6960333142334137
0.8220273053266582 0.6555907784328180 0.9069085572465994
0.1779727376733418 0.3444092215671749 0.0930914667534026

AgNiF4 LP at 0 GPa (P2_1/c)

1.0

5.6236634254	0.0000000000	0.0000000000
0.0000000000	4.8052668571	0.0000000000
-1.6601559382	0.0000000000	5.4010045697

Ag Ni F

2 2 8

Direct

0.000000000	0.000000000	0.000000000
0.000000010	0.500000000	0.500000021
0.500000000	0.500000000	0.000000000
0.500000021	-0.000000000	0.500000021
0.631682708	0.291337303	0.316754088
0.368317340	0.708662772	0.683245975
0.827889647	0.830939754	0.599213142
0.172110334	0.169060234	0.400786943
0.368316524	0.791337526	0.183244983
0.631683475	0.208662449	0.816755058
0.172111236	0.330939109	0.900784888
0.827888830	0.669060842	0.099215164

AgNiF4 HP1 at 10 GPa (P2_1/c)

1.00000000000000

5.0886782073707630	0.0000000000000000	0.1368241482182605
0.0000000000000000	4.8499977824595426	0.0000000000000000
-0.8194022892055097	0.0000000000000000	5.0886650244517631

Ag Ni F

2 2 8

Direct

0.5000000100000008	0.0000000000000000	0.5000000000000000
0.5000000000000000	0.5000000000000000	0.0000000000000000
-0.0000000000000000	0.0000000000000000	-0.0000000000000000
0.9999999990000035	0.5000000000000000	0.5000000000000000
0.8690903136360084	0.1781934389142069	0.2948350645973958
0.1309096353639909	0.8218065730857941	0.7051649114026022
0.1309096403639878	0.6781934269142059	0.2051649344026005
0.8690903276360096	0.3218065730857941	0.7948350875973942
0.3441785184272516	0.3509922888094633	0.6260187667631506
0.6558214965727461	0.6490076871905347	0.3739812102368510
0.6558215105727473	0.8509922638094648	0.8739812322368529
0.3441785114272546	0.1490077231905305	0.1260187787631515

Ag(II)Co(II)F4 LP at 0 GPa (P2_1/c)
1.00000000000000
5.6487181814348668 0.0000000000000000 0.8705559842994591
0.0000000000000000 4.7966123818777637 0.0000000000000000
0.8335073341660164 0.0000000000000000 5.6775525026755611
Ag Co F
2 2 8
Direct
0.0000000079369471 0.9999999948358820 0.0000000122691972
0.0000000070824271 0.4999999937418309 0.5000000147838151
0.5000000078270190 0.4999999940541215 0.0000000151427599
0.5000000088426475 0.9999999944523950 0.5000000132403599
0.3646845072837090 0.7090677643434778 0.3187136694565240
0.6353155106426589 0.2909322259645061 0.6812863543366817
0.1713874856880992 0.1760145372191981 0.6083881821922573
0.8286125251250894 0.8239854571578935 0.3916118382755302
0.6353162529146947 0.2090675199736202 0.1812853857767081
0.3646837610545115 0.7909324710898554 0.8187146334764420
0.8286116307139949 0.6760151514236366 0.8916097905991763
0.1713883808882088 0.3239848357435638 0.1083902324505387

Ag(II)Co(II)F4 HP1 at 10 GPa (P2_1/c)
1.00000000000000
5.0113510437132049 0.0000000000000000 -0.0120514716588119
0.0000000000000000 5.1217300185273924 0.0000000000000000
-0.0030819420495324 0.0000000000000000 5.0359640778897736
Ag Co F
2 2 8
Direct
0.0000000079369471 0.9999999948358820 0.0000000122691972
0.0000000070824271 0.4999999937418309 0.5000000147838151
0.5000000078270190 0.4999999940541215 0.0000000151427599
0.5000000088426475 0.9999999944523950 0.5000000132403599
0.3520378802523892 0.6758580122448016 0.3217449400954530
0.6479621376739787 0.3241419780631823 0.6782550836977527
0.1670019561746445 0.1576663222419242 0.4020726368552900
0.8329980546385439 0.8423336721351674 0.5979273836124974
0.6479628799460145 0.1758577678749439 0.1782541151377791
0.3520371340231916 0.8241422231885317 0.8217459041153711
0.8329971602274494 0.6576669364463626 0.0979253359361436
0.1670028513747541 0.3423330507208378 0.9020746871135714

Ag(I)Co(III)F4 LP at 0 GPa (Pnma)

1.00000000000000

11.0229778442210424 0.0000000000000000 0.0000000000000000

0.0000000000000000 7.3311291705040329 0.0000000000000000

0.0000000000000000 -0.0000000000000000 7.5425856227456265

Ag Co F

8 8 32

Direct

0.9683188982466118 0.2500000000000000 0.1255183651661389

0.0316810847533832 0.7500000160000013 0.8744816728338642

0.9837239260802026 0.2500000000000000 0.6228451327222728

0.0162760599197891 0.7500000160000013 0.3771549282777215

0.5316811017533882 0.7500000160000013 0.6255183571661382

0.4683188982466118 0.2500000000000000 0.3744816428338617

0.5162760739197974 0.7500000160000013 0.1228450867222762

0.4837239260802098 0.2500000000000000 0.8771548982777262

0.7467105127796945 0.4990345616993822 0.3738868254660963

0.7532894872203055 0.9990345616993822 0.8738868864660977

0.7532894872203055 0.5009654383006178 0.8738868864660977

0.7467105127796945 0.0009654253006132 0.3738868254660963

0.2532895072203000 0.9990345616993822 0.6261131435339048

0.2467105127797016 0.4990345616993822 0.1261131665339031

0.2467105127797016 0.0009654253006132 0.1261131665339031

0.2532895072203000 0.5009654383006178 0.6261131435339048

0.7539609126181328 0.0535814051346022 0.1238451037124495

0.2460390493818711 0.9464186048653986 0.8761549272875495

0.7460390873818672 0.9464186048653986 0.6238451037124495

0.2539608926181312 0.0535814051346022 0.3761548962875505

0.2460390493818711 0.5535814261346075 0.8761549272875495

0.7539609126181328 0.4464185738653925 0.1238451037124495

0.2539608926181312 0.4464185738653925 0.3761548962875505

0.7460390873818672 0.5535814261346075 0.6238451037124495

0.1963206150647456 0.2500000000000000 0.0795629127220840

0.8036793849352544 0.7500000160000013 0.9204370722779112

0.3036793649352528 0.7500000160000013 0.5795628977220864

0.6963206150647456 0.2500000000000000 0.4204370722779112

0.2938130443724235 0.7500000160000013 0.1739096856442099

0.7061869556275694 0.2500000000000000 0.8260903443557925

0.2061869556275765 0.2500000000000000 0.6739096856442099

0.7938130443724306 0.7500000160000013 0.3260903143557901

0.4070914288000720 0.0605024491404656 0.1132071308650861

0.5929085711999279 0.9394975318595364 0.8867929071349100

0.0929085711999280 0.9394975318595364 0.6132071228650925

0.9070913908000761 0.0605024491404656 0.3867928771349146

0.5929085711999279 0.5605025001404662 0.8867929071349100

0.4070914288000720 0.4394975628595353 0.1132071308650861

0.9070913908000761 0.4394975628595353 0.3867928771349146

0.0929085711999280 0.5605025001404662 0.6132071228650925

0.0859978345849887 0.9426344231570277 0.1375159744150148

0.9140022044150110 0.0573655528429703 0.8624839795849886

0.4140021654150113 0.0573655528429703 0.6375159894150124

0.5859977955849890 0.9426344231570277 0.3624840105849875

0.9140022044150110 0.4426343921570288 0.8624839795849886

0.0859978345849887 0.5573655448429696 0.1375159744150148

0.5859977955849890 0.5573655448429696 0.3624840105849875

0.4140021654150113 0.4426343921570288 0.6375159894150124

Ag(I)Co(III)F4 HP1 at 10 GPa (P2_1/m)
1.00000000000000
5.1645581604201301 -0.0000000000000000 -0.0000000000000000
-0.0000000000000000 7.1288208007760936 -0.0000000000000000
-0.2681686183553522 -0.0000000000000000 7.0060921224724524
Ag Co F
4 4 16
Direct
0.5012381913199817 0.7500003415348069 0.1765428341331357
0.4987584773613909 0.2499994627704109 0.8234548225013257
0.5381112012013892 0.7499996533152838 0.6908786788800290
0.4618853107046126 0.2500005035353399 0.3091227344654247
-0.0000080995564997 -0.0000008442355662 0.4999975127345845
-0.0000136385151722 0.4999966396965198 0.0000037605234955
-0.0000053607764640 0.5000003312156946 0.4999980065919969
-0.0000158398237898 0.0000035478031278 0.0000043805271134
0.8618168068943673 0.7499999387999645 0.9640632722255620
0.1381785410167011 0.2499997827395836 0.0359365976662595
0.0792269506274666 0.7500002627852215 0.5860037788829671
0.9207721279647567 0.2499998008160619 0.4139949585530782
0.8640631688274300 0.0550811181571014 0.7465654681665583
0.3048455422020692 0.9313245384715036 0.9115906634229285
0.3172011439669050 0.4282452760175758 0.5771973510137838
0.8640608187847351 0.4449219082362519 0.7465646471760112
0.6951527704141568 0.4313202880577797 0.0884028473736006
0.1359367482347910 0.5550776190818745 0.2534349664641848
0.1359326286795765 0.9449190249828796 0.2534343815857265
0.6827992686805414 0.9282422440873904 0.4228086446263350
0.6828011167966012 0.5717550420208358 0.4228025545828132
0.3048465151447165 0.5686799473612165 0.9115951781725444
0.3172010542296453 0.0717584667452880 0.5771919250978584
0.6951523036200709 0.0686742860038426 0.0884073746326691

Ag(I)Co(III)F4 HP2 at 20 GPa (C2/c)
1.00000000000000
11.0812628404247011 0.0000000000000000 -0.0059732377468867
0.0000000000000000 4.4484920880475007 0.0000000000000000
-1.5545900041669392 0.0000000000000000 4.7871892623391794
Ag Co F
4 4 16
Direct
-0.0000000000000000 0.9854499414981792 -0.0000000000000000
0.5000000000000000 0.4854499414981792 -0.0000000000000000
0.0000000049999969 0.6930680766525872 0.5000000189999980
0.5000000260000022 0.1930680386525841 0.5000000189999980
0.7499826645943405 0.0891191538441723 0.2499874905508578
0.2499826645943404 0.5891191278441701 0.2499874905508578
0.7500173424056565 0.5891191278441701 0.7500125234491434
0.2500173524056575 0.0891191538441723 0.7500125234491434
0.9046789962279855 0.4494612861620155 0.7950579031525441
0.4046789542279891 0.9494613381620199 0.7950579031525441
0.9046364545787734 0.2288860483661350 0.2951229472303552
0.4046364965787698 0.7288860743661372 0.2951229472303552
0.0953635414212262 0.2288860483661350 0.7048770657696495
0.5953635514212271 0.7288860743661372 0.7048770657696495
0.0953210617720122 0.4494612861620155 0.2049421348474519
0.5953210977720151 0.9494613381620199 0.2049421348474519
0.6901823796910656 0.4408622789629895 0.3802029965247833
0.1901823796910656 0.9408622789629895 0.3802029965247833
0.6901711840959881 0.2374122220893062 0.8801913918524845
0.1901711530959890 0.7374122220893062 0.8801913918524845
0.8098288629040051 0.7374122220893062 0.1198086101475157
0.3098288409040105 0.2374122220893062 0.1198086101475157
0.8098176273089386 0.9408622789629895 0.6197970174752178
0.3098176273089385 0.4408622789629895 0.6197970174752178

```
NiF2 orthorhombic PdF2-type at 20 GPa (Pbca)
  1.00000000000000
    4.7184679081789511   -0.0000000000000000    0.0000000000000000
    0.0000000000000000    4.7140006131837016    0.0000000000000000
    0.0000000000000000    0.0000000000000000    4.7425333960465874
   Ni   F
    4    8
Direct
 -0.0000000000000000 -0.0000000000000000 -0.0000000000000000
  0.5000000000000000 -0.0000000000000000  0.5000000000000000
  0.0000000000000000  0.5000000000000000  0.5000000000000000
  0.5000000000000000  0.5000000000000000 -0.0000000000000000
  0.3483211307683596  0.3482448345408198  0.3468214467687561
  0.6516788462316349  0.6517551424591748  0.6531785302312455
  0.1516788692316403  0.6517551424591748  0.8468214697687545
  0.8483211537683651  0.3482448345408198  0.1531785532312439
  0.6516788462316349  0.8482448575408252  0.1531785532312439
  0.3483211307683596  0.1517551654591802  0.8468214697687545
  0.8483211537683651  0.1517551654591802  0.6531785302312455
  0.1516788692316403  0.8482448575408252  0.3468214467687561
```

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