

# AFLOW V 3.1.111

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*          aflow - STEFANO CURTAROLO Duke University 2003-2017
*          High-Throughput ab-initio Computing Project
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## PROTOTYPES LIB1

| STR#              | Symmetry | Name     | TYPE | PROTO   | SG   | conc          |
|-------------------|----------|----------|------|---------|------|---------------|
| -----             |          |          |      |         |      |               |
| FCC               |          |          |      |         |      |               |
| A1,FCC,1,2        | fcc/cF4  | Fm-3m    | A1   | Cu      | #225 |               |
| A2,BCC,58,59      | bcc/cI2  | Im-3m    | A2   | W       | #229 |               |
| A3,HCP,115,117    | hcp/hcp2 | P6_3/mmc | A3   | Mg      | #194 |               |
| A4,DIA,301,302    | cF8      | Fd-3m    | A4   | C (DIA) | #227 | books         |
| A5,betaSn,305,306 | tI4      | I41/amd  | A5   | betaSn  | #141 | Navy Database |
| A6,In,303,304     | tI2      | I4/mmm   | A6   | Indium  | #139 | Navy Database |
| A7,As,307,308     | hR6      | R-3m     | A7   | alphaAs | #166 | Kolmogorov    |
| A8                |          |          |      |         |      |               |
| A9                |          |          |      |         |      |               |
| A10,Hg,349,350    | hR1      | R-3m     | A10  | alphaHg | #166 | ICSD          |

## PROTOTYPES BINARY

| STR#          | Pearson | Symmetry  | Name               | TYPE      | PROTO | SG   | notes                                |
|---------------|---------|-----------|--------------------|-----------|-------|------|--------------------------------------|
| -----         |         |           |                    |           |       |      |                                      |
| FCC           |         |           |                    |           |       |      |                                      |
| 1,2           | fcc/cF4 | Fm-3m     | A1                 | Cu        |       | #225 | G(pic1N1)                            |
| 1.cub,2.cub   | fcc/cF4 | Fm-3m     | A1                 | Cu        |       | #225 | G(pic1N1)                            |
| 3             | tP2     | P4/mmm    | L1_0               | AuCu      |       | #123 | AB along [001] G(pic1N2,1)           |
| 4             | hR2     | R-3m      | L1_1               | CuPt      |       | #166 | AB along [111] G(pic1N2,2)           |
| 5,6           | tI6     | I4/mmm    | beta1/2            | AB2       |       | #139 | AB2 along [100]z G(pic1N3,2,"        |
| 7,8           | oI6     | Immm      | -                  | MoPt2     |       | #71  | AB2 along [011] G(pic1N3,1)          |
| 9,10          | hP3     | P-3m1     | alpha1/2           | AB2       |       | #164 | AB2 along [111]z G(pic1N3,3,"        |
| 11,12         | oS8     | Cmmm      | "L1_3"(unofficial) | AB3       |       | #65  | "(A.5B.5)B along [111]" M(CdPt3,PdPt |
| 13,15         | tP4     | P4/mmm    | Z1/3               | AB3       |       | #123 | AB3 along [001]z M(PtTc3) G(         |
| 14            | tP4     | P4/nmm    | Z2                 | A2B2      |       | #129 | A2B2 along [001]z G(pic1N4,3,"       |
| 16,18         | mS8     | C2/m      | ?                  | AB3       |       | #12  | AB3 along [113] G(pic1N4,12)         |
| 17            | mS8     | C2/m      | W2                 | A2B2      |       | #12  | A2B2 along [311]z G(pic1N4,7)        |
| 19,21         | oP4     | Pmmm      | Y1/3               | AB3       |       | #47  | AB3 along [011]z G(pic1N4,9)         |
| 20            | oP4     | Pmmm      | Y2                 | A2B2      |       | #47  | A2B2 along [011]z M(AgZr) G(pi       |
| 22,24         | tI8     | I4/mmm    | DO_22              | Al3Ti     |       | #139 | AB3 along [201] G(pic1N4,11)         |
| 23            | tI8     | I41/amd   | CH "40"            | NbP       |       | #141 | A2B2 along [201] G(pic1N4,6,N        |
| 25,26         | cP4     | Pm3(bar)m | L1_2               | AuCu3     |       | #221 | "(A.5B.5)B along [001]" G(pic1N4,1)  |
| 27,29         | hR4     | R-3m      | V1/3               | AB3       |       | #166 | AB3 along [111]z G(pic1N4,10)        |
| 28            | hR4     | R-3m      | V2                 | A2B2      |       | #166 | A2B2 along [111]z G(pic1N4,5)        |
| BCC           |         |           |                    |           |       |      |                                      |
| 58,59         | bcc/cI2 | Im-3m     | A2                 | W         |       | #229 |                                      |
| 58.cub,59.cub | bcc/cI2 | Im-3m     | A2                 | W         |       | #229 |                                      |
| 60            | oS4     | Cmmm      | D^19_2h            | gamma-IrV |       | #65  | AB along [101]                       |
| 61            | cP2     | Pm-3m     | B2                 | CsCl      |       | #221 | AB along [001]                       |
| 62,63         | hP3     | P-3m1     | ?                  | AB2       |       | #164 | AB2 along [211]                      |
| 64,65         | oF12    | Fmmm      | ?                  | AB2       |       | #69  | AB2 along [011] WARNI FIX NpPd       |
| 66,67         | tI6     | I4/mmm    | C11_b              | MoSi2     |       | #139 | AB2 along [001] WARNI FIX NpPd       |
| 68,69         | hR4     | R-3m      | ?                  | AB3       |       | #166 | UNDEF                                |
| 70,72         | oS8     | Cmmm      | ?                  | AB3       |       | #65  | UNDEF                                |

|                  |          |           |                          |            |      |                          |                                 |
|------------------|----------|-----------|--------------------------|------------|------|--------------------------|---------------------------------|
| 71               | oS8      | Cmma      | ?                        | A2B2       | #67  | UNDEF                    |                                 |
| 73,75            | mP4      | P2/m      | ?                        | AB3        | #10  | UNDEF                    |                                 |
| 74               | mP4      | P21/m     | ?                        | A2B2       | #11  | UNDEF                    |                                 |
| 76,78            | tP4      | P4/mmm    | ?                        | AB3        | #123 | AB3 along [001]z         |                                 |
| 77               | tP4      | P4/nmm    | B11                      | gamma-CuTi | #129 | A2B2 along [001]z        |                                 |
| 79,81            | oI8      | Immm      | ?                        | AB3        | #71  | UNDEF                    | M(MoTi3, Mo3Ti, Nb3Tc, MoTi3, M |
| 80               | oI8      | Imma      | ?                        | A2B2       | #74  | UNDEF                    | M(MoTi)                         |
| 82,83            | tP4      | P4/mmm    | L6_0                     | CuTi3      | #123 |                          |                                 |
| 84,86            | cF16     | Fm-3m     | D0_3                     | AlFe3/BiF3 | #225 |                          |                                 |
| 85               | cF16     | Fd-3m     | B32                      | NaTl       | #227 |                          |                                 |
| HCP              |          |           |                          |            |      |                          |                                 |
| 115,117          | hcp/hcp2 | P6_3/mmc  | A3                       | Mg         | #194 |                          |                                 |
| 116              | hP2      | P_6m2     | B_h                      | WC         | #187 |                          |                                 |
| 118,121          | oP4      | Pmm2      | ?                        | AB3        | #25  | UNDEF                    |                                 |
| 119              | oP4      | Pmmn      | -                        | CuTe       | #59  |                          |                                 |
| 120              | oP4      | Pmma      | B19                      | AuCd       | #51  |                          |                                 |
| 123              | oI8      | C2/m      | ?                        | A2B2       | #12  | UNDEF                    |                                 |
| 122,124          | oI8      | Imm2      | ?                        | AB3        | #44  | UNDEF                    |                                 |
| 125,127          | hP4      | P-6m2     | ?                        | AB3        | #187 | UNDEF                    |                                 |
| 126              | hP4      | P-3m1     | ?                        | A2B2       | #164 | UNDEF                    | M(RhRu)                         |
| 128,132          | mS12     | Cm        | ?                        | AB5        | #8   | UNDEF                    |                                 |
| 129,134          | mS12     | C2/m      | ?                        | A4B2       | #12  | BiHf2-134                | #12 Hf-Paper                    |
| 130,137          | mS12     | C2/m      | ?                        | A4B2       | #12  |                          |                                 |
| 131,135          | mS12     | C2/m      | ?                        | A4B2       | #12  |                          |                                 |
| 133,140          | mS12     | Cm        | ?                        | A2B4       | #8   | UNDEF                    |                                 |
| 136              | mS12     | Cm        | ?                        | A3B3       | #8   | UNDEF                    |                                 |
| 138,139          | mS12     | Cm        | ?                        | A3B3       | #8   | UNDEF                    |                                 |
| 141,145          | oS12     | Amm2      | ?                        | AB5        | #38  |                          |                                 |
| 142,147          | oS12     | Cmcm      | ?                        | A4B2       | #63  | M(RhRu2)                 |                                 |
| 143,150          | oS12     | Cmcm      | ?                        | A4B2       | #63  | mistaken for C49, beware |                                 |
| *144,148         | oS12     | Cmcm      | ?                        | A4B2       | #63  | NOT RUN                  |                                 |
| *146,153         | oS12     | Amm2      | ?                        | A2B4       | #38  | NOT RUN                  |                                 |
| *149,151         | oS12     | Amm2      | ?                        | A3B3       | #38  | NOT RUN                  |                                 |
| *152,157         | oS12     | Amm2      | ?                        | A3B3       | #38  | NOT RUN                  |                                 |
| *154,160         | hP6      | P-62m     | ?                        | AB5        | #189 | NOT RUN                  |                                 |
| *155,158         | hP6      | P-62m     | ?                        | A2B4       | #189 | NOT RUN                  |                                 |
| *156,159         | hP6      | Cmcm      | ?                        | A2B4       | #63  | NOT RUN                  |                                 |
| *161,167         | hR6      | R32       | ?                        | AB5        | #155 | NOT RUN                  |                                 |
| *162,165         | hR6      | R32       | ?                        | A2B4       | #155 | NOT RUN                  |                                 |
| *163,166         | hR6      | C2/c      | ?                        | A2B4       | #15  | NOT RUN                  |                                 |
| *164             | hR6      | C2        | ?                        | A3B3       | #5   | NOT RUN                  |                                 |
| *168,169         | hP6      | P-6m2     | ?                        | AB5        | #187 | NOT RUN                  |                                 |
| *170,175         | hP6      | P-6m2     | ?                        | A2B4       | #187 | NOT RUN                  |                                 |
| *172             | mS8      | P-6m2     | ?                        | A3B3       | #187 | NOT RUN                  |                                 |
| *171,176         | hP6      | P-3m1     | ?                        | A2B4       | #164 | NOT RUN                  |                                 |
| *173,177         | hP6      | P63/mmc   | ?                        | A2B4       | #194 | NOT RUN                  |                                 |
| *174             | hP6      | P3m1      | ?                        | A3B3       | #156 | NOT RUN                  |                                 |
| LAVES AND OMEGAS |          |           |                          |            |      |                          |                                 |
| 178,179          | hP12     | P6_3/mm   | C14                      | MgZn2      | #194 | A4B8 Hex Laves Str       |                                 |
| 180,181          | oP16     | Pnma      | D0_11                    | Fe3C       | #62  |                          |                                 |
| 182,183          | cF24     | Fd-3m     | C15                      | Cu2Mg      | #227 | Cub Laves Phase          |                                 |
| 184,185          | cP8      | Pm3(bar)n | A15                      | Cr3Si      | #223 |                          |                                 |
| 186,187          | hP8      | P6_3/mmc  | D0_19                    | Ni3Sn      | #194 |                          |                                 |
| 188,189          | oS12     | Cmcm      | C49                      | ZrSi2      | #63  |                          |                                 |
| 190,191          | hP3      | P3m1      | omega phase with Z=1/4 ! |            | #164 |                          |                                 |
| 192,193          | oS8      | Cmcm      | B33B_f                   | CrB        | #63  |                          |                                 |
| 194              | oS8      | Cmcm      |                          | ITl ITl    | #63  | Pauling                  |                                 |
| 195              | cP8      | P2_13     | B20                      | FeSi       | #198 | Pauling                  |                                 |
| 196,197          | tP4      | P4/nmm 02 |                          | CdTi       | #129 | Pauling                  |                                 |
| 198              | oP24     | Pbcm      |                          | InTh       | #57  | Pauling                  |                                 |
| 199              | tI16     | I4/mcm    | B37                      | SeTl       | #140 | Pauling                  |                                 |
| 201              | cF8      | Fm-3m     | B1                       | NaCl       | #225 |                          |                                 |
| 202,203          | tI10     | I4/mmm    | D1_3                     | BaAl4      | #139 | NEW                      |                                 |
| 204,205          | hP6      | P6/mmm    | D2_d                     | CaCu5      | #191 |                          |                                 |

|                |       |             |          |                  |      |                                |
|----------------|-------|-------------|----------|------------------|------|--------------------------------|
| 206,207        | tI26  | I4/mmm      | D2_b     | ThMn12           | #139 |                                |
| 208,209        | hP9   | P-62m       | C22      | Fe2P             | #189 |                                |
| 210,211        | oP12  | Pnma        | C37      | Co2Si            | #62  | AL1851.cif                     |
| 212,213        | hR19  |             |          | Th2Zn17          | #166 |                                |
| 214,215        | cI28  | I-43d       | D7_3     | Th3P4            | #220 |                                |
| 216,217        | hP3   | P6/mmm      | C32      | AlB2             | #191 |                                |
| 218            | cF8   | F-43m       | B3       | ZnS              | #216 |                                |
| 219            | hP4   | P63/mc      | B4       | ZnS              | #186 |                                |
| 220,221        | hP4   | P63/mmc     | B8_1     | NiAs             | #194 |                                |
| 222,223        | hP16  | P63/mcm     | D8_8     | Mn5Si3           | #193 | 128601.cif                     |
| 224,225        | hP38  | P63/mmc     |          | Th2Ni17          | #194 |                                |
| 226,227        | cP8   | Pm-3n       | A15      | Cr3Si            | #223 |                                |
| 228,229        | tP6   | P4/nmm      | C38      | Cu2Sb            | #129 |                                |
| 230,231        | tI12  |             | C16      | CuAl2            | #140 |                                |
| 232,233        | tI6   | I4/mmm      | C11_b    | MoSi2            | #139 |                                |
| 234,235        | tI12  | I4/mcm      | C16      | Al2Cu            | #140 | 130617.cif                     |
| 236,237        | hP142 | P63/mmc     |          | Cd58Y13          | #194 | ICSD_102087                    |
| ****NO 236,237 |       | cI184       | Im-3     | Cd6Y (Y12Cd68)   | #204 | 130045.cif                     |
| ****NO 238,239 |       | hp24        | P-6m2    | Co3V             | #187 | 130340.cif                     |
| 238,239        | hp24  | P63/mmc     | Pu3Al    |                  | #194 | Pauling FILE = Co3V            |
| ***240,241     |       | P42/mnm     | D8_b     | CrFe             | #136 | 130307.cif ???? HARD           |
| 242,243        | oP24  | Pmnm02      |          | NbPd3            | #59  | 130379.cif                     |
| 244,245        |       | P63/mmc     | DO_24    | Ni3Ti            | #194 | AL5957.cif                     |
| 246,247        | hP6   | P63/mmc     |          | CaIn2            | #194 | AL5296.cif                     |
| 248,249        | tI12  | I41/amd     | C_c      | ThSi2            | #141 | AL2272.cif                     |
| ***250,251     | tI6   | I4/mmm      | C11_a    | CaC2             | #139 | AL1909.cif UNRUNNABLE          |
| 252,253        | cF24  | F-43m       | C15_b    | AuBe5            | #216 | AL3669.cif                     |
| 254,255        | tI32  | I4/mcm      |          | W5Si3            | #140 | AL2650.cif                     |
|                | hP5   | P63/mmc     | D5_2     | La2O3            | #194 | 130882.cif FRAC OCCUP          |
| 256            | oP8   | Pnma        | B27      | BFe              | #62  | AL1744.cif                     |
| 257,258        | oP6   | Pnmm        | C18      | FeS2             | #58  | marcasite AL1657.cif           |
| 259,260        | hR5   | R-3m        | C33      | Bi2Te3           | #166 | 120146.cif                     |
| 261,262        | cF96  | Fd-3m       |          | Ti2Ni            | #227 |                                |
| 263,264        | tI14  | I4/mmm      |          | Ti3Cu4           | #139 | 120654.cif                     |
| 265,266        | tP10  |             |          | Ti2Cu3           | #129 | IMPOSSIBLE                     |
| 267,268        | oP6   | Pnmm        | C18      | FeS2             | #52  | marcasite AL1657.cif           |
| 269,270        | hP3   | P-3m1       | C6       | CdI2             | #164 | AL4899.cif                     |
| 271,272        | oS16  | Cmcm        |          | Cd3Y             | #63  | 18260.cif                      |
| 273,274        | hP6   | P63/mmc     | B8_2     | Ni2In            | #194 | 28249.cif                      |
| 273p,274p      | hP5   | P-6m2       | Fe1.5Ge1 | partial of Ni2In | #187 | Pauling S525640                |
| 275,276        | hP6   | P63/m       |          | Ni2Si            | #176 | AL5234.cif                     |
| 277,278        | oP8   | Pmnm01      | DO_a     | betaCu3Ti        | #59  | AL1729.cif                     |
| 279,280        | tI16  | I4/mmm      | DO_23    | Al3Zr            | #139 | Navy Database                  |
| 281,282        | cP12  | Pa-3        | C2       | FeS2             | #205 | chris pyrite                   |
| 283,284        | oI12  | Imma        |          | GdSi2(1.4)       | #74  | chris z=(0.0362,0.2138,0.6250) |
| 285,286        | tI10  | I4/m        | D1_a     | MoNi4            | #87  | Navy Database                  |
| 287,288        | tI6   | I4/mmm      |          | CuZr2            | #139 | Pauling file                   |
| 289,290        | cP4   | Pm-3m       | DO_9     | alphaReO3        | #221 | Navy Database                  |
| 291,292        | tP4   | P4/nmm      | B10      | Pb0/PbS          | #129 | Navy Database                  |
| 301,302        | cF8   | Fd-3m       | A4       | C (DIA)          | #227 | books                          |
| 303,304        | tI2   | I4/mmm      | A6       | Indium           | #139 | Navy Database                  |
| 305,306        | tI4   | I41/amd     | A5       | betaSn           | #141 | Navy Database                  |
| 307,308        | hR6   | R-3m        | A7       | alphaAs          | #166 | Kolmo                          |
| 309,310        | cF32  | Fm-3m       |          | CuPt7            | #225 | (Ca7Ge) Gus Navy Database      |
| 311,312        | tI18  | I4/mmm      |          | NbNi8            | #139 | (Pt8Ti) Gus Navy Database      |
| 313,314        | tI18  | I4/mmm      |          | V4Zn5            | #139 | Navy Database                  |
| 315,316        | hP24  | P6_3/mmc    | C36      | MgNi2            | #194 | Navy Database                  |
| 317,318        | oS8   | Cmca        | A11      | alphaGa          | #64  | Navy Database                  |
| 319,320        | cI58  | I(-4)3m     | A12      | alphaMn          | #217 | Navy Database                  |
| 321,322        | cP20  | P4_132      | A13      | betaMn           | #213 | Navy Database                  |
| 323,324        | hP3   | P3_21-D_3^6 | A8       | gammaSe          | #152 | Navy Database                  |
| 325,326        | hP4   | P63/mmc     | A9       | graphite         | #194 | Navy Database                  |
| 327,328        | tI2   | I4/mmm      | Aa       | alphaPa          | #139 | Navy Database                  |
| 329,330        | tP30  | P4_2/mnm    | Ab       | betaU            | #136 | Navy Database/Pauling          |
| 331,332        | oP8   | I4/mmm      | Ac       | alphaNp          | #62  | Navy Database/Pauling          |

|            |       |                 |                     |                |      |                                     |
|------------|-------|-----------------|---------------------|----------------|------|-------------------------------------|
| 333,334    | tP4   | P4/nmm          | Ad                  | betaNp         | #129 | Navy Database/Pauling               |
| 335,336    | hP1   | P6/mmm          | Af hex              | HgSn_{6-10}    | #191 | Navy Database                       |
| 337,338    | todo  | Ag T-50 boron   |                     |                |      |                                     |
| 339,340    | todo  | Ah simple cubic |                     |                |      |                                     |
| 341,342    | todo  | Ai betaPo       |                     |                |      |                                     |
| 343,344    | todo  | Ak alphaSe      |                     |                |      |                                     |
| 345,346    | todo  | Al betaSe       |                     |                |      |                                     |
| 347,348    | todo  | A3' alphaLa     |                     |                |      |                                     |
| 349,350    | hR1   | R-3m            | A10                 | alphaHg        | #166 | ICSD A10.A/B                        |
| 351,352    | todo  | A14 In2         |                     |                |      |                                     |
| 353,354    | todo  | A16 alphaS      |                     |                |      |                                     |
| 355,356    | todo  | A17 black P     |                     |                |      |                                     |
| 357,358    | todo  | A20 alphaU      |                     |                |      |                                     |
| 359,360    | hP18  | P63/mcm         |                     | Ga4Ti5         | #193 | Pauling                             |
| 361,362    | tP20  | P42/mnm         |                     | Al2Zr3         | #136 | Pauling                             |
| 363,364    | hP7   | P6/mmm          |                     | Al3Zr4         | #191 | Pauling                             |
| 365,366    | oF40  | F2dd            |                     | Al3Zr2         | #43  | Pauling                             |
| 367,368    | cF112 | Fm-3c           |                     | NaZn13         | #226 | Pauling                             |
| 369,370    | cP7   | Pm-3m           |                     | CaB6           | #221 | Pauling                             |
| 371,372    | hP5   | P-3m1           | D5_19               | Al3Ni2         | #164 | Navy Database                       |
| 373,374    | cI40  | I-43m           | Ga4Ni(Ga3.62Ni0.97) |                | #217 | Navy Database (vacancies I23, #197) |
| 375,376    | oS16  | Cmmm            |                     | Ga3Pt5         | #65  | Navy Database                       |
| 377,378    | mS44  | C12/m1          |                     | Ga9Ni13        | #12  | Pauling                             |
| 379,380    | cI112 | Ia(-3)d         |                     | Ga4Ni3         | #230 | Navy Database                       |
| 381,382    | tI24  | I4_1/amd        |                     | Ga2Hf          | #141 | Navy Database                       |
| 383,384    | cF116 | Fm-m            |                     | C6Mn23         | #225 | ICSD                                |
| 385,386    | oP44  | Pnma            |                     | Cu8Hf3         | #62  | ICSD                                |
| 387,388    | oS68  | Cmca            |                     | Ni10Zr7        | #64  | ICSD_240191                         |
| 389,390    | tP3   | P4/mmm          |                     | Hg2Pt          | #123 | ICSD_104339                         |
| 391,392    | oP20  | Pnma            |                     | B4Mg           | #62  | Pauling                             |
| 393,394    | oI64  | Imma            |                     | B7Mg           | #74  | Pauling                             |
| 395,396    | oP16  | Pbam            |                     | Ge3Rh5         | #55  | Pauling                             |
| 397,398    | tP14  | P4/mbm          |                     | In4Ti3         | #127 | Pauling                             |
| 399,400    | tP34  | P4/nmm.O2       | V8Sb9               | V7.49Sb9       | #129 | Pauling                             |
| 401,402    | tI160 | I-42d           |                     | Li3B14         | #122 | Pauling/Kolmogorov                  |
| 403,404    | tP20  | Pa/mbm          |                     | LiB3           | #127 | Pauling/Kolmogorov                  |
| 405,406    | hR4   | R-3m            |                     | LiB-MS1        | #166 | Pauling                             |
| 407,408    | hP8   | P63/mmc         |                     | LiB-MS2        | #194 | Pauling                             |
| 411,412    | cI58  | I-43m           |                     | Re24Ti5        | #217 | Pauling                             |
| 413,414    | mS36  | C12/m1          |                     | Ni7Zr2         | #12  | Pauling                             |
| 415,416    | tI40  | I4/m            |                     | Pt11Zr9        | #87  | Pauling                             |
| 417,418    | oP20  | Pnma            |                     | Au4Zr          | #62  | Pauling                             |
| 419,420    | oI142 | Immm            |                     | Hf540s17       | #71  | Pauling                             |
| 421,422    | hP9   | P6_222          | C40                 | CrSi2          | #180 | Pauling                             |
| 423.424.t0 | hP68  | P6/m            |                     | Ag51Gd14.o3.t0 | #175 | Pauling                             |
| 423.424.t1 | hP68  | P6/m            |                     | Ag51Gd14.o3.t1 | #175 | Pauling                             |
| 423.424.t2 | hP68  | P6/m            |                     | Ag51Gd14.o3.t2 | #175 | Pauling                             |
| 423.424.t3 | hP68  | P6/m            |                     | Ag51Gd14.o2.t3 | #175 | Pauling                             |
| 423.424.t4 | hP68  | P6/m            |                     | Ag51Gd14.o2.t4 | #175 | Pauling                             |
| 423.424.t5 | hP68  | P6/m            |                     | Ag51Gd14.o2.t5 | #175 | Pauling                             |
| 423.424.t6 | hP68  | P6/m            |                     | Ag51Gd14.o2.t6 | #175 | Pauling                             |
| 423.424.t7 | hP68  | P6/m            |                     | Ag51Gd14.o1.t7 | #175 | Pauling                             |
| 423.424.t8 | hP68  | P6/m            |                     | Ag51Gd14.o1.t8 | #175 | Pauling                             |
| 423.424.t9 | hP68  | P6/m            |                     | Ag51Gd14.o1.t9 | #175 | Pauling                             |
| 425,426    | cF184 | Fd-3m           |                     | Zn22Zr         | #227 | Pauling                             |
| 427,428    | oP24  | Pnmm            |                     | As2Ti          | #58  | Pauling                             |
| 429,430    | tI84  | I4/mmm          |                     | Ge10Ho11       | #139 | Pauling                             |
| 431,432    | hP48  | P6_122          |                     | Ir3Zr5         | #178 | Pauling                             |
| 433,434    | oP6   | Pnmm            |                     | CaCl2          | #58  | Pauling                             |
| 435,436    | cP5   | P-43m           |                     | CFe4           | #215 | Pauling                             |
| 437,438    | mS28  | C12/c1          |                     | C2Mn5          | #15  | Pauling                             |
| 439,440    | oP40  | Pnma            |                     | C3Mn7          | #62  | Pauling                             |
| 441,442    | hP20  | P6_3mc          |                     | Fe3Th7         | #186 | Pauling                             |
| 443,444    | hR24  | R-3cr           |                     | F3Fe           | #167 | Pauling                             |

|         |        |          |            |             |        |                                       |
|---------|--------|----------|------------|-------------|--------|---------------------------------------|
| 445,446 | hR24   | P321     |            | F3Fe        | #150   | Pauling                               |
| 447,448 | mP4    | P12_1/m1 |            | NiTi        | #11    | Pauling                               |
| 449,450 | cP6    | Pn-3m    | C3         | Ag20        | #224   | ICSD_281041 Cuprite                   |
| 451,452 | hP9    | P-3      | Bb         | etaAg2Zn    | #147   | Navy Database                         |
| 453,454 | mS16   | C2/m     | DO_15      | AlCl3       | #12    | ICSD_39566                            |
| 455,456 | hR8    | R32      | DO_14      | AlF3        | #155   | ICSD_30274                            |
| 457,458 | hR10   | R-3c     | D5_1       | alphaAl203  | #167   | ICSD_75479 Corundum                   |
| 459,460 | cI26   | Im-3     |            | Al12W       | #204   | ICSD_58207                            |
| 461,462 | oP12   | P212121  |            | Ag2Se       | #19    | ICSD_15213 Naumannite                 |
| 463,464 | hR26   | R-3      |            | AlPd        | #148   | ICSD_58112                            |
| 465,466 | cP16   | Pa-3     | SC16       | AlSb        | #205   | ICSD_41994                            |
| 467,468 | cI52   | I-43m    | gammaBrass | Cu5Zn8      | #217   | Pauling                               |
| 469,470 | hR36   | R-3m h   |            | BaPb3       | #166   | Pauling                               |
| 471,472 | hP8    | Cmcm     |            | Hf3Sc*-h321 | #63    | Hf-Paper                              |
| 473,474 | hP6    | P-62m    |            | Hf5Sc-h51   | #189   | Hf-Paper                              |
| 475,476 | mS12   | C2/m     |            | BiHf2-134   | #12    | Hf-Paper                              |
| 477,478 | tP6    | P4/mmm   |            | Hf5Pb-f63   | #123   | Hf-Paper                              |
| 479,480 | oS12   | Cmmm     |            | HfPd5       | #65    | Hf-Paper                              |
| 481,482 | hR276  | R-3ch    |            | Re25Zr21    | #167.2 | Pauling                               |
| 483,484 | tP6    | P4/mmm   | B11_3      |             | #123   | Mike Mehl bcc_AAABBB^[001]            |
| 485,486 | tP6    | P4mm     | B11_3'     |             | #99    | Mike Mehl bcc_AABBBAB^[001]           |
| 487,488 | tP6    | P4/mmm   | Z3         |             | #123   | Mike Mehl fcc_AAABBB^[001]            |
| 489,490 | tP6    | P4mm     | Z3'        |             | #99    | Mike Mehl fcc_AABBBAB^[001]           |
| 491,492 | oP102  | Pmn2_1   | Al13Co4    |             | #31    | Pauling - Grin J_Al_Comp_206_243_1994 |
| 493,494 | ms102  | C1m1     | Al12.13Co4 | eta         | #8     | Pauling - Hurd Acta Cryst 15 441 1962 |
| 495,496 | hP28   | P6_3/mmc | Al5Co2     | D8_11       | #194   | Pauling                               |
| 497,498 | mp22   | P12_1/c1 | Al9Co2     |             | #14    | Pauling                               |
| 499,500 | tP10   | P-42_1c  |            | Pd4Se       | #114   | Pauling                               |
| 501,502 | cF1192 | Fd(-3)m  |            | NaCd2       | #227   | Samson, Nature 195, 259 (1962)        |
| 503,504 | hP10   | P6_3/m   |            | Er3Ru2      | #176   | Pauling                               |
| 505,506 | oP40   | Pnma     |            | Pt3Sr7      | #62    | Pauling                               |
| 507,508 | cF120  | Fm-3m    |            | Ir4Sc11     | #225   | Pauling                               |
| 509,510 | oP276  | Pnna     |            | Ru25Y44     | #52    | Pauling                               |
| 511,512 | cP252  | P4_132   |            | RuZn6       | #213   | Pauling                               |
| 513,514 | mP4    | P21/m    | B19'       | NbRu-Beta'' | #11    | Eur.Phys.J.B 72 575(2009)             |
| 515,516 | cF96   | Fd-3m    |            | delta(CdNi) | #227.2 | Pauling                               |
| 517,518 | hP3    | P-3m1    |            | Cd2Ce       | #164   | Pauling                               |
| 519,520 | hP3    | P6/mmm   |            | Hg2U        | #191   | Pauling                               |
| 521,522 | hP9    | P-62m    |            | InMg2       | #189   | Pauling                               |
| 523,524 | oS16   | Cmcm     |            | Cd3Er       | #63    | Pauling                               |
| 525,526 | hP8    | P6_3/mmc |            | CdMg3       | #194   | Pauling                               |
| 527,528 | hP24   | P6_3/mmc |            | CeNi3       | #194   | Pauling                               |
| 529,530 | oP32   | Pnma     |            | CoSc3       | #62    | Pauling                               |
| 531,532 | tP4    | P4/mmm   |            | Pb3Sr       | #123   | Pauling                               |
| 533,534 | hR36   | R-3mh    |            | PuNi3       | #166   | Pauling                               |
| 535,536 | oP16   | Pnma     |            | YZn3        | #62    | Pauling                               |
| 537,538 | hR4    | R-3m     |            | Co2Y2*      | #166   | hcp-paper definition                  |
| 539,540 | mS12   | C2/m     |            | Sc2Zr*      | #12    | hcp-paper definition                  |
| 541,542 | oI8    | Immm     |            | Mo3Ti*-81   | #71    | hcp-paper/monster                     |
| 543,544 | oI8    | Imma     |            | MoTi*-80    | #74    | hcp-paper/monster                     |
| 545,546 | hR3    | P-3m1    |            | ReTi2*-81   | #164   | hcp-paper                             |
| 547,548 | tI6    | I4/mmm   |            | Hf2Tl*-6    | #139   | hf-paper                              |
| 549,550 | oF12   | Fmmm     |            | Be2Zn*-65   | #69    | hcp-paper                             |
| 551,552 | oI8    | Imm2     |            | Re3Ru*-124  | #44    | hcp-paper                             |
| 553,554 | hP24   | P63cm    | DO_21      | Cu2.82P     | #185   | Pauling                               |
| 555,556 | oP108  | Pnma     |            | Mg2Au       | #62    | Pauling                               |
| 557,558 | cF16   | Fm-3m    |            | BiF3        | #225   | Pearson's crystal data                |
| 559,560 | cI58   | I-43m    |            | Al12Mg17    | #217   | Pauling                               |
| 561,562 | oS160  | Cmcm     |            | MgAu3-x     | #63    | Pauling                               |
| 563,564 | oS64   | Cmcm     |            | MgAu3+x     | #63    | Pauling                               |
| 565,566 | oF48   | Fddd     |            | Mg2Cu       | #70    | Pauling                               |
| 567,568 | hP18   | P-62c    |            | Mg2Ga       | #190   | Pauling                               |
| 569,570 | Pbam   | Pbam     |            | MgGa2       | #55    | Pauling                               |
| 571,572 | oI28   | Ibam     |            | Mg5Ga2      | #72    | Pauling                               |
| 573,574 | tI28   | I4/mmm   |            | Mg2Ga5      | #139   | Pauling                               |

|  |         |           |                          |           |      |   |
|--|---------|-----------|--------------------------|-----------|------|---|
| 575,576  | tI32    | I41/a     |                          | MgGa      | #88  | Pauling                                     |
| 577,578  | hR72/24 | R32       |                          | Mg3Hg     | #155 | Pauling                                     |
| 579,580  | hR48/16 | R-3m      |                          | Mg3In     | #166 | Pauling                                     |
| 581,582  | cF408   | F-43m     |                          | Mg44Rh7   | #216 | Pauling                                     |
| 583,584  | cF12    | Fm-3m     |                          | CaF2      | #225 | Pauling                                     |
| 585,586  | hP8     | P63/mmc   | DO_18                    | Al3Ir     | #194 | Pauling                                     |
| 587,588  | cP116   | Fm-3m     |                          | Mn23Th6   | #225 | Pauling                                     |
| 589,590  | cP39    | Pm-3      |                          | Mg2Zn11   | #200 | Pauling                                     |
| 591,592  | mS110   | C2/m      |                          | Mg4Zn7    | #12  | Pauling                                     |
| 593,594  | cP20    | P4_132    |                          | Mg3Ru2    | #213 | Pauling                                     |
| 595,596  | oS12    | Cmcm      |                          | Au2V      | #63  | Pauling                                     |
| 597,598  | hP94    | P63/mmc   |                          | Sr9Mg38   | #194 | Pauling                                     |
| 600.ABCDE  | tP30    | P4_2/mnm  | sigma                    | CrFe      | #136 | Pauling                                     |
| 600.XXXXX where X can be A,B (a total of 32 poscars) |         |           |                          |           |      |   |
| 611,612  | cP140   | Pm-3      |                          | Rh13Sc57  | #200 | Pauling                                     |
| 613,614  | hR13    | Imm2      |                          | Fe7W6     | #166 | Pauling                                     |
| 615,616  | oP24    | Pbca      |                          | AuSn2     | #61  | Pauling                                     |
| 617,618  | mS12    | C2./m     |                          | Bi2Pd     | #12  | Pauling                                     |
| 619,620  | mS28    | C2./m     |                          | Bi2Pd5    | #12  | Pauling                                     |
| 621,622  | oP16    | Pnma      |                          | Bi3Ni     | #62  | Pauling                                     |
| 623,624  | oP32    | Pnma      |                          | Bi3Y5     | #62  | Pauling                                     |
| 625,626  | cI120   | Ia-3d     |                          | Bi4Rh     | #230 | Pauling                                     |
| 627,628  | hR48    | R-3m      |                          | BiMn3     | #166 | Pauling                                     |
| 629,630  | oP16    | Pmma      |                          | BiPd3     | #51  | Pauling                                     |
| 631,632  | tI12    | I4/mmm    |                          | BiTi2     | #139 | Pauling                                     |
| 633,634  | mP12    | P2_{1}./c |                          | CoSb2     | #14  | Pauling                                     |
| 635,636  | hR78    | R3m       |                          | Cu7Hg6    | #160 | Pearson (Gamma-Brass Cu5Zn8 Modified)       |
| 637,638  | oI12    | Imma      |                          | Hg2K      | #74  | Pauling                                     |
| 639,640  | cI52    | I-43m     |                          | Ir2Zn11   | #217 | Pauling files (Gamma-Brass Cu5Zn8 Modified) |
| 641,642  | tI32    | I-4       | DO_e                     | Ni3P      | #82  | Pauling                                     |
| 643.AB/BA  | aP32    | P-1       |                          | KP15      | #2   | Pauling                                     |
| 644.AB/BA  | tI116   | I4_1/a    |                          | Pu28Zr    | #88  | Pauling                                     |
| 645.AB/BA  | cF52    | Fm-3m     |                          | Bi2U      | #225 | Pauling                                     |
| 646.AB/BA  | oS68    | Cmcm      |                          | TiZn16    | #63  | Pauling                                     |
| 647.AB/BA  | tI140   | I4/mcm    |                          | Rh2Y3     | #140 | Pauling                                     |
| 648.AB/BA  | tP32    | P4/ncc    |                          | Rh3Pu5    | #130 | Pauling                                     |
| 649.AB/BA  | tI32    | I-42m     |                          | alpha-SV3 | #121 | Pauling                                     |
| 650.AB   | oP12    | Pmma      |                          | IrTa      | #51  | Pauling                                     |
| 651.AB/BA  | oP36    | Pnma      |                          | Ge4Sm5    | #62  | Pauling                                     |
| 652.AB/BA  | oP12    | Pnma      |                          | Cl2Pb     | #62  | Pauling                                     |
| 653.AB/BA  | mP16    | P12_1     |                          | NbPt3     | #11  | Pauling                                     |
| 654.AB/BA  | cI10    | Im-3m     |                          | Hg4Pt     | #229 | Pauling                                     |
| 655.AB/BA  | hR14    | R-3       |                          | Pd4Pu3    | #148 | Pauling                                     |
| 656.AB/BA  | hR15    | R-3       |                          | Er3Ni2    | #148 | Pauling                                     |
| 657.AB/BA  | oI6     | Immm      |                          | Pd2Ti     | #71  | Pauling                                     |
| 658.AB/BA  | tP8     | P4/mmm    |                          | Pd5Ti3    | #123 | Pauling                                     |
| 659.AB/BA  | oS20    | Cmcm      |                          | Pd3Ti2    | #63  | Pauling                                     |
| 660.AB/BA  | tP14    | P4/mbm    |                          | Hg5Mn2    | #127 | Pauling                                     |
| 661.AB/BA  | oS32    | Cmcm      |                          | Pu3Pd5    | #63  | Pauling                                     |
| 662.AB/BA  | oS12    | Cmmm      |                          | Ga2Zr     | #65  | G. Ghosh and M.Asta, Acta Mat. 53, 322      |
| 663.AB/BA  | mP30    | P21/c     |                          | FeP4_mP30 | #14  | Pauling                                     |
| 664.AB/BA  | mS40    | C2/C      |                          | FeP4_mS40 | #15  | Pauling                                     |
| 665.AB/BA  | tP16    | P4/2mmm   |                          | In3Ir     | #136 | Pauling                                     |
| 666.AB/BA  | mS44    | C2/m      |                          | Fe6Ge5    | #12  | Pauling                                     |
| 667.AB/BA  | mS42    | C2/m      |                          | Fe3Ga4    | #12  | Pauling                                     |
| 668.AB/BA  | oS28    | Cmcm      |                          | Al6Mn     | #63  | Pauling                                     |
| 669.AB   | oP8     | Pnma      |                          | AsFe      | #62  | Pauling                                     |
| 670.AB/BA  | hP6     | P6/mmm    | B35                      | CoSn      | #191 | Pauling                                     |
| 671.AB/BA  | cI32    | Im-3      | DO_2                     | As3Co     | #204 | Pauling                                     |
| 672.AB/BA  | cI32    | Im-3m     |                          |           | #229 | Mike - 16 atom scell fcc, A15B1             |
| 673.AB/BA  | cP16    | Pm-3m     |                          |           | #221 | Mike - 16 atom scell bcc, A15B1             |
| 674.A/B  | hP3     | P6/mmm    |                          |           | #191 | Mike - omega phase (C32) in pure form       |
| 675.A/B  | cP8     | Pm-3n     |                          |           | #223 | Mike - A15 phase in pure form               |
| 676.AB/BA  | hP22    | P6/mmc    | Fe6.5Ge4-ideal (Fe14Ge8) |           | #194 | Pauling                                     |
| 676p.AB/BA   | oS42    | Amm2      | Fe6.5Ge4-part (Fe13Ge8)  |           | #38  | Pauling                                     |

|                      |      |          |          |             |        |                      |                          |
|----------------------|------|----------|----------|-------------|--------|----------------------|--------------------------|
| 677.AB/BA            | hR26 | R3m      |          | Al8Cr5      | #160.2 | ICSD_606753          |                          |
| 678.AB/BA            | tI24 | I4mm     |          | Co5Ge7      | #107   | ICSD_43386           |                          |
| 679.AB/BA            | cP5  | Pm-3m    | E2_1     |             | #221   | NAVY                 |                          |
| 680.AB/BA            | tP12 | P4/mmm   |          | beta-NW2    | #123   | NAVY (Hagg, sort of) |                          |
| 681.AB/BA            | hR3  | R3m      |          | alpha-MoS2  | #160   | NAVY                 |                          |
| 682.AB/BA            | hR13 | R-3m     | D8_5r    |             | #166   | NAVY                 |                          |
| 683.AB/BA            | cI50 | Im-3m    |          | Na13Cl12v7  | #229   | NAVY                 |                          |
| 684.A/B              | cP8  | P2_13    |          | alpha-N2    | #198   | NAVY                 |                          |
| 685.A/B              | cP8  | Pa-3     |          | alpha-N2p   | #205   | NAVY                 |                          |
| 686.A/B              | hP4  | P6_3/mmc |          | beta-N2     | #194   | NAVY                 |                          |
| 687.A/B              | hR16 | R-3c     |          | epsilon-N2  | #167   | NAVY                 |                          |
| 688.A/B              | tP4  | P4_2/mnm |          | gamma-N2    | #136   | NAVY                 |                          |
| 689.AB/BA            | hP6  | P6_3/mmc |          | WN2_194af   | #194   | NAVY                 |                          |
| 690.AB/BA            | mP12 | P2_1/c   |          | Ag2Te       | #14    | NAVY                 |                          |
| 691.AB/BA            | cF12 | Fm-3m    | C1       |             | #225   | NAVY                 |                          |
| 692.AB/BA            | hR3  | R-3m     | C19      |             | #166   | NAVY                 |                          |
| 693.AB/BA            | tP6  | P4_2/mnm | C4       |             | #136   | NAVY                 |                          |
| 694.AB/BA            | hP6  | P6_3/mmc | C7       |             | #194   | NAVY                 |                          |
| 695.AB/BA            | hP3  | P-6m2    |          | WN2_187fg   | #187   | NAVY                 |                          |
| 696.AB/BA            | hP6  | P6_3/mmc |          | WN2_194de   | #194   | NAVY                 |                          |
| 697.AB/BA            | tP10 | P4_2/mmc |          | Hagg_N4W6   | #131   | NAVY                 |                          |
| 698.AB/BA            | oP16 | Pnma     |          | MoO3        | #62    | NAVY                 |                          |
| 699.AB/BA            | hP12 | P6/mmm   |          | O3W         | #191   | NAVY                 |                          |
| 700.AB/BA            | oP16 | Pnma     |          | P3Tc        | #62    | NAVY                 |                          |
| 701.AB/BA            | hP5  | P-3m1    |          | WN4_164ad   | #164   | NAVY                 |                          |
| 702.AB/BA            | hP20 | P6_3/mmc |          | B4W         | #194   | NAVY                 |                          |
| 703.AB/BA            | oP40 | Pbca     |          | P4Re        | #61    | NAVY                 |                          |
| 704.AB/BA            | hP14 | P6_3/mmc | B8_1v2   |             | #194   | NAVY                 |                          |
| 705.AB/BA            | oS28 | Cmca     | B8_1v2p  |             | #64    | NAVY                 |                          |
| 706.AB/BA            | oS14 | Cmmm     |          | Na4Cl3v1    | #65    | NAVY                 |                          |
| 707.AB/BA            | cP7  | P-43m    |          | C4W3        | #215   | NAVY                 |                          |
| 708.AB/BA            | cP7  | Pm-3m    |          | S3U4        | #221   | NAVY                 |                          |
| 709.AB/BA            | mS14 | C2/m     |          | O5Nb2       | #12    | NAVY                 |                          |
| 710.AB/BA            | hP13 | P-3m1    | B8_1v3   |             | #164   | NAVY                 |                          |
| 711.AB/BA            | cF52 | Fm-3m    |          | Na7Cl6_v3   | #225   | NAVY                 |                          |
| 712.AB/BA            | cF60 | Fm-3m    |          | Na7Cl8v1    | #225   | NAVY                 |                          |
| 713.AB/BA            | hP15 | P-3m1    | B8_1v1   |             | #164   | NAVY                 |                          |
| 714.AB/BA            | hP15 | P-6m2    | B8_1v1p  |             | #187   | NAVY                 |                          |
| 715.AB/BA            | tP2  | P4/mmm   |          | Na1Cl1v2    | #123   | NAVY                 |                          |
| 716.AB/BA            | tP6  | P4/mmm   |          | Na3Cl3v2    | #123   | NAVY                 |                          |
| 717.AB/BA            | hP14 | P3m1     | B8_1v2pp |             | #156   | NAVY                 |                          |
| 718.AB/BA            | hR6  | R3m      | B3v2     |             | #160   | NAVY                 |                          |
| 719.AB/BA            | cF56 | F-43m    |          | Na7Cl7v2    | #216   | NAVY                 |                          |
| 720.AB/BA            | cF8  | Fm-3m    | B1       |             | #225   | NAVY                 |                          |
| 721.AB/BA            | hP6  | P-62m    |          | NTa         | #189   | NAVY                 |                          |
| 722.AB/BA            | cP6  | Pm-3m    |          | NbO         | #221   | NAVY                 |                          |
| 723.AB/BA            | hP16 | P6_3mc   |          | NbS         | #186   | NAVY                 |                          |
| 724.AB/BA            | tP3  | P4/mmm   |          | Hagg_NW2    | #123   | NAVY                 |                          |
| 725.AB/BA            | tI12 | I4_1/amd |          | Mo2N        | #141   | NAVY                 |                          |
| 726.AB/BA            | hP9  | P-31m    |          | NV2         | #162   | NAVY                 |                          |
| 727.AB/BA            | hP9  | P-3m1    |          | NW2_Pearson | #164   | NAVY                 |                          |
| 728.A/B              | cP8  | Pm-3n    | beta-W   |             | #223   | NAVY                 |                          |
| 729.AB/BA            | oP76 | Pnma     |          | Ge8Mn11     | #62    | Pauling              |                          |
| 730.AB/BA            | hP48 | P-3c1    |          | NaTe3       | #165   | ICSD_61355           |                          |
| 731.AB/BA            | oP48 | Pbcn     |          | NaTe        | #60    | ICSD_61382           |                          |
| 732.AB/BA            | mP40 | P121/c1  |          | Sb3Sr2      | #60    | ICSD_32033           |                          |
| 733.AB/BA            | mS16 | C12/m1   |          | SrAs3       | #12    | ICSD_41831           |                          |
| 734.AB/BA            | tI12 | I4/mmm   |          | La2Sb       | #139   | ICSD_10442           |                          |
| 735.AB/BA            | oP32 | Pnma     |          | Ga5Tm3      | #62    | ICSD_104009          |                          |
| **** BORIDES PROJECT |      |          |          |             |        |                      |                          |
| 1000.AB/BA           | cP7  | Pm-3m    |          | B6Si1       | #221   | ICSD_20240           | binary_boride_ICSD_frequ |
| 1001.AB/BA           | cF52 | Fm-3m    |          | B12Y1       | #225   | ICSD_23860           | binary_boride_ICSD_frequ |
| 1002.AB/BA           | tP20 | P4/mbm   |          | B4La1       | #127   | ICSD_2360            | binary_boride_ICSD_frequ |
| 1003.AB/BA           | hP3  | P6/mmm   |          | B2Nb1       | #191   | ICSD_30328           | binary_boride_ICSD_frequ |
| 1004.AB/BA           | hP3  | P6/mmm   |          | B2Pu1       | #191   | ICSD_43660           | binary_boride_ICSD_frequ |

|            |       |            |        |      |                          |                          |
|------------|-------|------------|--------|------|--------------------------|--------------------------|
| 1005.AB/BA | tI12  | I4/mcm     | B1Mo2  | #140 | ICSD_24278               | binary_boride_ICSD_frequ |
| 1006.AB/BA | oS8   | Cmcm       | B1Ni1  | #63  | ICSD_26937               | binary_boride_ICSD_frequ |
| 1007.AB/BA | hP3   | P6/mmm     | B2Mg1  | #191 | ICSD_26675               | binary_boride_ICSD_frequ |
| 1008.AB    | cF8   | F-43m      | As1B1  | #216 | ICSD_43871               | binary_boride_ICSD_frequ |
| 1009.AB/BA | oI14  | Immm       | B4Cr3  | #71  | ICSD_33704               | binary_boride_ICSD_frequ |
| 1010.AB    | cF8   | Fm-3m      | B1Pu1  | #225 | ICSD_43661               | binary_boride_ICSD_frequ |
| 1011.AB/BA | tP10  | P4/mbm     | B2V3   | #127 | ICSD_88317               | binary_boride_ICSD_frequ |
| 1012.AB/BA | oP8   | Pnma       | B1Ti1  | #62  | ICSD_24701               | binary_boride_ICSD_frequ |
| 1013.AB/BA | hP20  | P6_{3}/mcc | B3Ru7  | #186 | ICSD_44343               | binary_boride_ICSD_frequ |
| 1014.AB/BA | oS20  | Cmcm       | B3V2   | #63  | ICSD_79258               | binary_boride_ICSD_frequ |
| 1015.AB/BA | cF116 | Fm-3m      | B6Fe23 | #225 | ICSD_54786               | binary_boride_ICSD_frequ |
| 1016.AB/BA | hP3   | P6/mmm     | Ag1B2  | #191 | ICSD_43821               | binary_boride_ICSD_frequ |
| 1017.AB/BA | oP8   | Pnma       | B1Co1  | #62  | ICSD_612863              | binary_boride_ICSD_frequ |
| 1018.AB/BA | tI12  | I4/mcm     | B1Co2  | #140 | ICSD_42531               | binary_boride_ICSD_frequ |
| 1019.AB/BA | oP16  | Pnma       | B1Co3  | #62  | ICSD_44339               | binary_boride_ICSD_frequ |
| 1020.AB/BA | tI16  | I4_{1}/amd | B1Mo1  | #141 | ICSD_24280               | binary_boride_ICSD_frequ |
| 1021.AB/BA | oS16  | Cmcm       | B1Re3  | #63  | ICSD_43662               | binary_boride_ICSD_frequ |
| 1022.AB    | hP2   | P-6m2      | B1Tc1  | #187 | ICSD_168895              | binary_boride_ICSD_frequ |
| 1023.AB/BA | hP6   | P6_{3}/mmc | B2Re1  | #194 | ICSD_23871               | binary_boride_ICSD_frequ |
| 1024.AB/BA | oP6   | Pnmm       | B2Ru1  | #59  | ICSD_31871               | binary_boride_ICSD_frequ |
| 1025.AB/BA | hP10  | P6_{3}/mmc | B3Ru2  | #194 | ICSD_23715               | binary_boride_ICSD_frequ |
| 1026.AB/BA | oP10  | Pnmm       | B4Cr1  | #58  | ICSD_186851              | binary_boride_ICSD_frequ |
| 1027.AB/BA | oI10  | C2/m       | B4Mn1  | #12  | ICSD_15079               | binary_boride_ICSD_frequ |
| 1028.AB/BA | hR7   | R-3m       | B5W2   | #166 | ICSD_20326               | binary_boride_ICSD_frequ |
| 1029.AB/BA | cF48  | F-43m      | B1Li1  | #216 | ICSD_164841              | binary_boride_ICSD_frequ |
| 1030.AB/BA | hR12  | R3m        | B1Li1  | #160 | ICSD_164842              | binary_boride_ICSD_frequ |
| 1031.AB/BA | cF48  | F-43m      | B1Li1  | #216 | ICSD_164843              | binary_boride_ICSD_frequ |
| 1032.AB/BA | tI24  | I-4m2      | B1Li1  | #119 | ICSD_164844              | binary_boride_ICSD_frequ |
| 1033.AB/BA | tI24  | I-4m2      | B1Li1  | #119 | ICSD_164845              | binary_boride_ICSD_frequ |
| 1034.AB/BA | tI26  | I4/mmm     | B12Sc1 | #139 | ICSD_615424              | binary_boride_ICSD_frequ |
| 1035.AB/BA | hR15  | R-3m       | B12Si3 | #166 | ICSD_615435              | binary_boride_ICSD_frequ |
| 1036.AB/BA | cF12  | Fm-3m      | B1Be2  | #225 | ICSD_20384               | binary_boride_ICSD_frequ |
| 1037.AB/BA | oP16  | Pnma       | B1Co3  | #62  | ICSD_603543              | binary_boride_ICSD_frequ |
| 1038.AB/BA | oP16  | Pnma       | B1Co3  | #62  | ICSD_612862              | binary_boride_ICSD_frequ |
| 1039.AB/BA | oF48  | Fddd       | B1Cr2  | #70  | ICSD_188474              | binary_boride_ICSD_frequ |
| 1040.AB/BA | tP3   | I4/mcm     | B1Fe2  | #140 | ICSD_160789              | binary_boride_ICSD_frequ |
| 1041.AB/BA | tI12  | I-42m      | B1Fe2  | #121 | ICSD_16809               | binary_boride_ICSD_frequ |
| 1042.AB/BA | hP8   | P6_{3}22   | B1Fe3  | #182 | ICSD_184958              | binary_boride_ICSD_frequ |
| 1043.AB/BA | oP8   | Pnma       | B1Li1  | #62  | ICSD_153291              | binary_boride_ICSD_frequ |
| 1044.AB/BA | oP16  | Pnma       | B1Ni3  | #62  | ICSD_24306               | binary_boride_ICSD_frequ |
| 1045.AB/BA | oP6   | Pnmm       | B1Pd2  | #58  | ICSD_10487               | binary_boride_ICSD_frequ |
| 1046.AB/BA | oP16  | Pnma       | B1Pd3  | #62  | ICSD_43514               | binary_boride_ICSD_frequ |
| 1047.AB/BA | hP4   | P6_{3}/mmc | B1Pt1  | #194 | ICSD_24363               | binary_boride_ICSD_frequ |
| 1048.AB/BA | hP4   | P6_{3}/mmc | B1Pt1  | #194 | ICSD_615210              | binary_boride_ICSD_frequ |
| 1049.AB/BA | hP6   | P6_{3}/mmc | B1Pt2  | #194 | ICSD_615207              | binary_boride_ICSD_frequ |
| 1050.AB/BA | oS8   | Cmcm       | B1Rh1  | #63  | ICSD_150732              | binary_boride_ICSD_frequ |
| 1051.AB/BA | oP12  | Pnma       | B1Rh2  | #62  | ICSD_24699               | binary_boride_ICSD_frequ |
| 1052.AB/BA | hP4   | P6_{3}/mmc | B1Tc1  | #194 | ICSD_168897              | binary_boride_ICSD_frequ |
| 1053.AB/BA | hP4   | P6_{3}/mmc | B1Tc1  | #194 | ICSD_168898              | binary_boride_ICSD_frequ |
| 1054.AB    | cP2   | Pm-3m      | B1Tc1  | #221 | ICSD_168900              | binary_boride_ICSD_frequ |
| 1055.AB/BA | tI12  | I4/mcm     | B1Ti2  | #140 | ICSD_189385              | binary_boride_ICSD_frequ |
| 1056.AB/BA | oS46  | Cmmm       | B20Na3 | #65  | ICSD_407159              | binary_boride_ICSD_frequ |
| 1057.AB/BA | oP12  | Pnma       | B2Fe1  | #62  | ICSD_425310              | binary_boride_ICSD_frequ |
| 1058.AB/BA | hR4   | R-3m       | B2Li2  | #166 | Kolmogorov-Curtarolo LiB | binary_boride_ICSD_frequ |
| 1059.AB/BA | hP8   | P6_{3}/mmc | B2Li2  | #194 | Kolmogorov-Curtarolo LiB | binary_boride_ICSD_frequ |
| 1060.AB/BA | mS28  | C2/c       | B2Pd5  | #15  | ICSD_43513               | binary_boride_ICSD_frequ |
| 1061.AB/BA | cF24  | Fd-3m      | B2Sc1  | #227 | ICSD_106903              | binary_boride_ICSD_frequ |
| 1062.AB/BA | oS6   | P6/mmm     | B2Tm1  | #191 | ICSD_44598               | binary_boride_ICSD_frequ |
| 1063.AB/BA | hP12  | P6_{3}/mmc | B2W1   | #194 | ICSD_23716               | binary_boride_ICSD_frequ |
| 1064.AB/BA | tI32  | I4/mcm     | B3Cr5  | #140 | ICSD_41932               | binary_boride_ICSD_frequ |
| 1065.AB/BA | hR8   | R-3m       | B3Mo1  | #166 | ICSD_167734              | binary_boride_ICSD_frequ |
| 1066.AB/BA | oP28  | Pnma       | B3Ni4  | #62  | ICSD_24307               | binary_boride_ICSD_frequ |
| 1067.AB/BA | mS28  | C2/c       | B3Ni4  | #15  | ICSD_24308               | binary_boride_ICSD_frequ |
| 1068.AB/BA | hP8   | P6_{3}/mmc | B3Re1  | #194 | ICSD_24361               | binary_boride_ICSD_frequ |
| 1069.AB/BA | oS20  | P6_{3}/mmc | B3Ru2  | #194 | ICSD_108082              | binary_boride_ICSD_frequ |



|            |      |            |  |        |      |             |                          |
|------------|------|------------|--|--------|------|-------------|--------------------------|
| 1070.AB/BA | oI64 | Imma       |  | B3Si1  | #74  | ICSD_412621 | binary_boride_ICSD_frequ |
| 1071.AB/BA | oI14 | Immm       |  | B4Mn3  | #71  | ICSD_44446  | binary_boride_ICSD_frequ |
| 1072.AB/BA | tP16 | P4_{2}/mmc |  | B4Mn4  | #131 | ICSD_74985  | binary_boride_ICSD_frequ |
| 1073.AB/BA | hP10 | P6_{3}/mmc |  | B4Mo1  | #194 | ICSD_167735 | binary_boride_ICSD_frequ |
| 1074.AB/BA | hP20 | P6_{3}/mmc |  | B4Mo1  | #194 | ICSD_182095 | binary_boride_ICSD_frequ |
| 1075.AB/BA | hR6  | R-3m       |  | B4Mo2  | #166 | ICSD_39554  | binary_boride_ICSD_frequ |
| 1076.AB/BA | hP18 | P6_{3}/mmc |  | B4Rh5  | #194 | ICSD_86395  | binary_boride_ICSD_frequ |
| 1077.AB/BA | hP20 | P6_{3}/mmc |  | B4W1   | #194 | ICSD_43193  | binary_boride_ICSD_frequ |
| 1078.AB/BA | tP20 | P4/mbm     |  | B4W1   | #127 | ICSD_615683 | binary_boride_ICSD_frequ |
| 1079.AB/BA | mP28 | P2_{1}/c   |  | B5Gd2  | #14  | ICSD_62067  | binary_boride_ICSD_frequ |
| 1080.AB/BA | hP14 | P6_{3}/mmc |  | B5Mo2  | #194 | ICSD_167733 | binary_boride_ICSD_frequ |
| 1081.AB/BA | mS14 | C2/m       |  | B5W2   | #12  | ICSD_20326  | binary_boride_ICSD_frequ |
| 1082.AB/BA | hP14 | P6_{3}/mmc |  | B5W2   | #194 | ICSD_615696 | binary_boride_ICSD_frequ |
| 1083.AB/BA | oS22 | Cmmm       |  | B6Ta5  | #65  | ICSD_68538  | binary_boride_ICSD_frequ |
| 1084.AB/BA | oP38 | Pbam       |  | B8Ru11 | #55  | ICSD_43663  | binary_boride_ICSD_frequ |
| 1085.AB/BA | hP20 | P6_{3}cm   |  | B9Li1  | #185 | ICSD_164625 | binary_boride_ICSD_frequ |

\*\*\*\* CARBIDE PROJECT

|            |         |            |     |         |      |               |                           |
|------------|---------|------------|-----|---------|------|---------------|---------------------------|
| 001.AA     | fcc/cF4 | Fm-3m      | A1  | Cu      | #225 | from gndstate |                           |
| 001.BB     | fcc/cF4 | Fm-3m      | A1  | Cu      | #225 | from gndstate |                           |
| 058.AA     | bcc/cI2 | Im-3m      | A2  | W       | #229 | from gndstate |                           |
| 058.BB     | bcc/cI2 | Im-3m      | A2  | W       | #229 | from gndstate |                           |
| 115.AA     | hcp/hcp | P6_3/mmc   | A3  | Mg      | #194 | from gndstate |                           |
| 115.BB     | hcp/hcp | P6_3/mmc   | A3  | Mg      | #194 | from gndstate |                           |
| 201.AB     | cF8     | Fm-3m      | B1  | NaCl    | #225 | from gndstate |                           |
| 061.AB     | cP2     | Pm-3m      | B2  | CsCl    | #221 | from gndstate |                           |
| 218.AB     | cF8     | F-43m      | B3  | ZnS     | #216 | from gndstate |                           |
| 219.AB     | hP4     | P63/mc     | B4  | ZnS     | #186 | from gndstate |                           |
| 116.AB     | hP2     | P_6m2      | B_h | WC      | #187 | from gndstate |                           |
| 301.AA     | cF8     | Fd-3m      | A4  | C (DIA) | #227 | BOOK          |                           |
| 301.BB     | cF8     | Fd-3m      | A4  | C (DIA) | #227 | BOOK          |                           |
| 325.AA     | hP4     | P63/mmc    | A9  | C (GRA) | #194 | BOOK          |                           |
| 325.BB     | hP4     | P63/mmc    | A9  | C (GRA) | #194 | BOOK          |                           |
| 1200.AB    | cF8     | Fm-3m      |     | C1Ti1   | #225 | ICSD_1546     | binary_carbide_ICSD_frequ |
| 1201.AB    | cF8     | F-43m      |     | C1Si1   | #216 | ICSD_24217    | binary_carbide_ICSD_frequ |
| 1202.AB/BA | tI6     | I4/mmm     |     | C2U1    | #139 | ICSD_14330    | binary_carbide_ICSD_frequ |
| 1203.AB/BA | cI40    | I-43d      |     | C3Pr2   | #220 | ICSD_2444     | binary_carbide_ICSD_frequ |
| 1204.AB    | hP2     | P-6m2      |     | C1W1    | #187 | ICSD_15406    | binary_carbide_ICSD_frequ |
| 1205.AB    | cP2     | Pm-3m      |     | C1Sc1   | #221 | ICSD_181048   | binary_carbide_ICSD_frequ |
| 1206.AB/BA | hR3     | R-3m       |     | C1Y2    | #166 | ICSD_22283    | binary_carbide_ICSD_frequ |
| 1207.AB/BA | tP70    | P4/mnc     |     | C4Sc3   | #128 | ICSD_71145    | binary_carbide_ICSD_frequ |
| 1208.AB/BA | tP68    | P-42_{1}c  |     | C19Er15 | #114 | ICSD_76817    | binary_carbide_ICSD_frequ |
| 1209.AB/BA | oP16    | Pnma       |     | C1Fe3   | #62  | ICSD_16593    | binary_carbide_ICSD_frequ |
| 1210.AB/BA | hP3     | P-3m1      |     | C1Nb2   | #164 | ICSD_43670    | binary_carbide_ICSD_frequ |
| 1211.AB/BA | mS12    | C2/c       |     | C2Ca1   | #15  | ICSD_54184    | binary_carbide_ICSD_frequ |
| 1212.AB/BA | cP12    | Pa-3       |     | C2Th1   | #205 | ICSD_77470    | binary_carbide_ICSD_frequ |
| 1213.AB/BA | oP18    | Pbam       |     | C5Y4    | #55  | ICSD_84869    | binary_carbide_ICSD_frequ |
| 1214.AB/BA | cI132   | Im-3       |     | C6OK6   | #204 | ICSD_66879    | binary_carbide_ICSD_frequ |
| 1215.AB/BA | cF116   | Fm-3m      |     | C6Cr23  | #225 | ICSD_62667    | binary_carbide_ICSD_frequ |
| 1216.AB/BA | mP22    | P2_{1}/c   |     | C7Ho4   | #14  | ICSD_83381    | binary_carbide_ICSD_frequ |
| 1217.AB/BA | cF12    | Fm-3m      |     | Be2C1   | #225 | ICSD_41567    | binary_carbide_ICSD_frequ |
| 1218.AB/BA | oP6     | Pnmm       |     | C1Fe2   | #58  | ICSD_76826    | binary_carbide_ICSD_frequ |
| 1219.AB/BA | hP4     | P6_{3}/mmc |     | C10s1   | #194 | ICSD_168278   | binary_carbide_ICSD_frequ |
| 1220.AB/BA | oP12    | Pbcn       |     | C1V2    | #60  | ICSD_9965     | binary_carbide_ICSD_frequ |
| 1221.AB/BA | mS28    | C2/c       |     | C2Fe5   | #15  | ICSD_43194    | binary_carbide_ICSD_frequ |
| 1222.AB/BA | hP3     | P-6m2      |     | C20s1   | #187 | ICSD_168279   | binary_carbide_ICSD_frequ |
| 1223.AB/BA | hP6     | P6_{3}/mmc |     | C20s1   | #194 | ICSD_168280   | binary_carbide_ICSD_frequ |
| 1224.AB/BA | oP16    | Pnma       |     | C2Rb2   | #62  | ICSD_51529    | binary_carbide_ICSD_frequ |
| 1225.AB/BA | cI132   | Im-3       |     | C60Sr6  | #204 | ICSD_75356    | binary_carbide_ICSD_frequ |
| 1226.AB/BA | hR7     | R3m        |     | A14C3   | #160 | ICSD_14397    | binary_carbide_ICSD_frequ |
| 1227.AB/BA | cP7     | P-43m      |     | As4C3   | #215 | ICSD_163831   | binary_carbide_ICSD_frequ |
| 1228.AB/BA | hR15    | R-3m       |     | B13C2   | #166 | ICSD_446      | binary_carbide_ICSD_frequ |
| 1229.AB/BA | tI24    | I-4m2      |     | B1C5    | #119 | ICSD_166553   | binary_carbide_ICSD_frequ |
| 1230.AB/BA | oI12    | Imm2       |     | B1C5    | #44  | ICSD_166554   | binary_carbide_ICSD_frequ |

|            |       |            |         |      |             |                              |
|------------|-------|------------|---------|------|-------------|------------------------------|
| 1231.AB/BA | hP6   | P3m1       | B1C5    | #156 | ICSD_166555 | binary_carbide_ICSD_freq     |
| 1232.AB/BA | aP12  | P-1        | B1C5    | #2   | ICSD_166556 | binary_carbide_ICSD_freq     |
| 1233.AB/BA | tP8   | P-4m2      | B1C7    | #115 | ICSD_181952 | binary_carbide_ICSD_freq     |
| 1234.AB/BA | hP8   | P3m1       | B1C7    | #156 | ICSD_181953 | binary_carbide_ICSD_freq     |
| 1235.AB/BA | cP8   | P-43m      | B1C7    | #215 | ICSD_181954 | binary_carbide_ICSD_freq     |
| 1236.AB/BA | oP8   | Pmm2       | B1C7    | #25  | ICSD_181955 | binary_carbide_ICSD_freq     |
| 1237.AB/BA | hR8   | R3m        | B1C7    | #160 | ICSD_181956 | binary_carbide_ICSD_freq     |
| 1238.AB/BA | hR15  | R-3m       | B4C1    | #166 | ICSD_29093  | binary_carbide_ICSD_freq     |
| 1239.AB/BA | oP24  | Pnma       | Ba1C2   | #62  | ICSD_168408 | binary_carbide_ICSD_freq     |
| 1240.AB/BA | hR3   | R-3m       | Ba1C2   | #166 | ICSD_186576 | binary_carbide_ICSD_freq     |
| 1241.AB/BA | cP126 | Pm-3n      | Ba3C60  | #223 | ICSD_70063  | binary_carbide_ICSD_freq     |
| 1242.AB/BA | cI132 | Im-3       | C10Cs1  | #204 | ICSD_657337 | binary_carbide_ICSD_freq     |
| 1243.AB/BA | tP68  | P-42_{1}c  | C19Sc15 | #114 | ICSD_42631  | binary_carbide_ICSD_freq     |
| 1244.AB/BA | oP16  | Pnma       | C1Cr3   | #62  | ICSD_603557 | binary_carbide_ICSD_freq     |
| 1245.AB/BA | hP3   | P6/mmm     | C1Fe2   | #191 | ICSD_162103 | binary_carbide_ICSD_freq     |
| 1246.AB/BA | oP12  | Pnma       | C1Fe2   | #62  | ICSD_187138 | binary_carbide_ICSD_freq     |
| 1247.AB/BA | tI32  | I-4        | C1Fe3   | #82  | ICSD_187142 | binary_carbide_ICSD_freq     |
| 1248.AB/BA | hP8   | P6_{3}22   | C1Fe3   | #182 | ICSD_42542  | binary_carbide_ICSD_freq     |
| 1249.AB/BA | oP16  | Pnma       | C1Fe3   | #62  | ICSD_43522  | binary_carbide_ICSD_freq     |
| 1250.AB/BA | mP10  | P2_{1}/m   | C1Fe4   | #11  | ICSD_187143 | binary_carbide_ICSD_freq     |
| 1251.AB/BA | tI10  | I4/m       | C1Fe4   | #87  | ICSD_187144 | binary_carbide_ICSD_freq     |
| 1252.AB/BA | cP5   | P-43m      | C1Fe4   | #215 | ICSD_44729  | binary_carbide_ICSD_freq     |
| 1253.AB/BA | oP16  | Pnma       | C1Mn3   | #62  | ICSD_603556 | binary_carbide_ICSD_freq     |
| 1254.AB/BA | cF112 | Fd-3m      | C1Mn6   | #227 | ICSD_187037 | binary_carbide_ICSD_freq     |
| 1255.AB/BA | hP12  | P6_{3}/mmc | C1Mo1   | #194 | ICSD_44987  | binary_carbide_ICSD_freq     |
| 1256.AB/BA | hP8   | P6_{3}/mmc | C1Mo1   | #194 | ICSD_618298 | binary_carbide_ICSD_freq     |
| 1257.AB/BA | hP3   | P-6m2      | C1Mo2   | #187 | ICSD_43669  | binary_carbide_ICSD_freq     |
| 1258.AB    | hP4   | P6_{3}mc   | C1Nb1   | #186 | ICSD_189092 | binary_carbide_ICSD_freq     |
| 1259.AB/BA | hP4   | P6_{3}/mmc | C1Nb1   | #194 | ICSD_189093 | binary_carbide_ICSD_freq     |
| 1260.AB/BA | oP12  | Pnma       | C1Nb2   | #62  | ICSD_31973  | binary_carbide_ICSD_freq     |
| 1261.AB/BA | oP12  | Pmma       | C1Nb2   | #51  | ICSD_653912 | binary_carbide_ICSD_freq     |
| 1262.AB/BA | hR8   | R-3c       | C1Ni3   | #167 | ICSD_17005  | binary_carbide_ICSD_freq     |
| 1263.AB/BA | cP8   | P2_{1}3    | C10s1   | #198 | ICSD_168277 | binary_carbide_ICSD_freq     |
| 1264.AB/BA | hP8   | P6_{3}/mmc | C1Re1   | #194 | ICSD_618702 | binary_carbide_ICSD_freq     |
| 1265.AB/BA | hP6   | P6_{3}/mmc | C1Re2   | #194 | ICSD_180376 | binary_carbide_ICSD_freq     |
| 1266.AB/BA | hR4   | R-3m       | C1Ru1   | #166 | ICSD_188285 | binary_carbide_ICSD_freq     |
| 1267.AB/BA | hP3   | P-3m1      | C1Sc2   | #164 | ICSD_280743 | binary_carbide_ICSD_freq     |
| 1268.AB    | hP10  | P3m1       | C1Si1   | #156 | ICSD_107204 | binary_carbide_ICSD_frequenc |
| 1269.AB    | hP12  | P6_{3}mc   | C1Si1   | #186 | ICSD_15325  | binary_carbide_ICSD_frequen  |
| 1270.AB    | hR16  | R3m        | C1Si1   | #160 | ICSD_18136  | binary_carbide_ICSD_freq     |
| 1271.AB    | hR10  | R3m        | C1Si1   | #160 | ICSD_24168  | binary_carbide_ICSD_freq     |
| 1272.AB    | hP8   | P6_{3}mc   | C1Si1   | #186 | ICSD_24170  | binary_carbide_ICSD_freq     |
| 1273.AB    | hP4   | P6_{3}mc   | C1Si1   | #186 | ICSD_24261  | binary_carbide_ICSD_freq     |
| 1274.AB    | hP16  | P6_{3}mc   | C1Si1   | #186 | ICSD_24630  | binary_carbide_ICSD_freq     |
| 1275.AB    | hR18  | R3m        | C1Si1   | #160 | ICSD_24631  | binary_carbide_ICSD_freq     |
| 1276.AB    | hP38  | P3m1       | C1Si1   | #156 | ICSD_27635  | binary_carbide_ICSD_freq     |
| 1277.AB    | hP28  | P3m1       | C1Si1   | #156 | ICSD_28303  | binary_carbide_ICSD_freq     |
| 1278.AB    | hP20  | P3m1       | C1Si1   | #156 | ICSD_38150  | binary_carbide_ICSD_freq     |
| 1279.AB    | hR14  | R3m        | C1Si1   | #160 | ICSD_42513  | binary_carbide_ICSD_freq     |
| 1280.AB    | hP32  | P6_{3}mc   | C1Si1   | #186 | ICSD_42858  | binary_carbide_ICSD_freq     |
| 1281.AB    | hP36  | P3m1       | C1Si1   | #156 | ICSD_42859  | binary_carbide_ICSD_freq     |
| 1282.AB    | hP42  | P3m1       | C1Si1   | #156 | ICSD_43827  | binary_carbide_ICSD_freq     |
| 1283.AB/BA | cF48  | Fd-3m      | C1Ti2   | #227 | ICSD_77473  | binary_carbide_ICSD_freq     |
| 1284.AB/BA | hP9   | P-31m      | C1W2    | #162 | ICSD_162419 | binary_carbide_ICSD_freq     |
| 1285.AB/BA | oP12  | Pbcn       | C1W2    | #60  | ICSD_43017  | binary_carbide_ICSD_freq     |
| 1286.AB/BA | mP12  | P2_{1}/c   | C2Ca1   | #14  | ICSD_24074  | binary_carbide_ICSD_freq     |
| 1287.AB/BA | cP12  | Pn-3m      | C2Ca1   | #224 | ICSD_31092  | binary_carbide_ICSD_freq     |
| 1288.AB/BA | mS12  | C2/m       | C2Ca1   | #12  | ICSD_54185  | binary_carbide_ICSD_freq     |
| 1289.AB/BA | aP12  | P-1        | C2Ca1   | #2   | ICSD_66663  | binary_carbide_ICSD_freq     |
| 1290.AB/BA | oP20  | Pnma       | C2Cr3   | #62  | ICSD_15086  | binary_carbide_ICSD_freq     |
| 1291.AB/BA | oS20  | Cmcm       | C2Cr3   | #63  | ICSD_57009  | binary_carbide_ICSD_freq     |
| 1292.AB/BA | oP20  | Pnma       | C2Cr3   | #62  | ICSD_653958 | binary_carbide_ICSD_freq     |
| 1293.AB/BA | oP16  | Pnma       | C2Cs2   | #62  | ICSD_51531  | binary_carbide_ICSD_freq     |
| 1294.AB/BA | hP12  | P-62m      | C2Cs2   | #189 | ICSD_51533  | binary_carbide_ICSD_freq     |
| 1295.AB/BA | mS12  | C2/c       | C2Eu1   | #15  | ICSD_380495 | binary_carbide_ICSD_freq     |

|            |       |            |        |      |             |                          |
|------------|-------|------------|--------|------|-------------|--------------------------|
| 1296.AB/BA | mS28  | C2/c       | C2Fe5  | #15  | ICSD_423888 | binary_carbide_ICSD_freq |
| 1297.AB/BA | mS28  | C2/c       | C2Fe5  | #15  | ICSD_89328  | binary_carbide_ICSD_freq |
| 1298.AB/BA | mS12  | C2/m       | C2Ir1  | #12  | ICSD_181488 | binary_carbide_ICSD_freq |
| 1299.AB/BA | tI12  | I4/mcm     | C2Ir1  | #140 | ICSD_181489 | binary_carbide_ICSD_freq |
| 1300.AB/BA | tI6   | I4/mmm     | C2Ir1  | #139 | ICSD_181490 | binary_carbide_ICSD_freq |
| 1301.AB/BA | tI32  | I4_{1}/acd | C2K2   | #142 | ICSD_36142  | binary_carbide_ICSD_freq |
| 1302.AB/BA | tI64  | I4_{1}/acd | C2K2   | #142 | ICSD_89528  | binary_carbide_ICSD_freq |
| 1303.AB/BA | oI8   | Immm       | C2Li2  | #71  | ICSD_25705  | binary_carbide_ICSD_freq |
| 1304.AB/BA | tP6   | P4_{2}/mmm | C2Mg1  | #136 | ICSD_88057  | binary_carbide_ICSD_freq |
| 1305.AB/BA | mS28  | C2/c       | C2Mn5  | #15  | ICSD_618246 | binary_carbide_ICSD_freq |
| 1306.AB/BA | mS28  | C2/c       | C2Mn5  | #15  | ICSD_69535  | binary_carbide_ICSD_freq |
| 1307.AB/BA | cP12  | P4_{3}32   | C2Na1  | #212 | ICSD_186177 | binary_carbide_ICSD_freq |
| 1308.AB/BA | tI32  | I4_{1}/acd | C2Na2  | #142 | ICSD_28066  | binary_carbide_ICSD_freq |
| 1309.AB/BA | oI8   | Immm       | C2Na2  | #71  | ICSD_95835  | binary_carbide_ICSD_freq |
| 1310.AB/BA | hP6   | P6_{3}/mmc | C2Re1  | #194 | ICSD_184660 | binary_carbide_ICSD_freq |
| 1311.AB/BA | tI6   | I4/mmm     | C2Re1  | #139 | ICSD_184661 | binary_carbide_ICSD_freq |
| 1312.AB/BA | tP3   | P4/mmm     | C2Re1  | #123 | ICSD_184664 | binary_carbide_ICSD_freq |
| 1313.AB/BA | tP6   | P4_{2}/mmc | C2Si1  | #131 | ICSD_187721 | binary_carbide_ICSD_freq |
| 1314.AB/BA | mS12  | C2/c       | C2Th1  | #15  | ICSD_26568  | binary_carbide_ICSD_freq |
| 1315.AB/BA | tP6   | P4_{2}/mmc | C2Th1  | #131 | ICSD_77469  | binary_carbide_ICSD_freq |
| 1316.AB/BA | hP20  | P6_{3}mc   | C3Fe7  | #186 | ICSD_76830  | binary_carbide_ICSD_freq |
| 1317.AB/BA | oP16  | Pnma       | C3Ir1  | #62  | ICSD_181492 | binary_carbide_ICSD_freq |
| 1318.AB/BA | oP16  | Pbam       | C3Ir5  | #55  | ICSD_181485 | binary_carbide_ICSD_freq |
| 1319.AB/BA | oP10  | Pnnm       | C3Mg2  | #58  | ICSD_71941  | binary_carbide_ICSD_freq |
| 1320.AB/BA | cP7   | Pm-3m      | C3Nb4  | #221 | ICSD_42758  | binary_carbide_ICSD_freq |
| 1321.AB/BA | tP20  | P-4c2      | C3Os2  | #116 | ICSD_168275 | binary_carbide_ICSD_freq |
| 1322.AB/BA | oP40  | Pbcn       | C3Os2  | #60  | ICSD_168276 | binary_carbide_ICSD_freq |
| 1323.AB/BA | cI28  | I-43d      | C3Sc4  | #220 | ICSD_42760  | binary_carbide_ICSD_freq |
| 1324.AB/BA | mP10  | P2_{1}/c   | C4Ir1  | #14  | ICSD_181493 | binary_carbide_ICSD_freq |
| 1325.AB/BA | oF20  | Ccce       | C4Ir1  | #68  | ICSD_181496 | binary_carbide_ICSD_freq |
| 1326.AB/BA | tP5   | P4/nbm     | C4Ir1  | #125 | ICSD_181497 | binary_carbide_ICSD_freq |
| 1327.AB/BA | oS40  | P6_{3}/mmc | C4Ir1  | #194 | ICSD_181498 | binary_carbide_ICSD_freq |
| 1328.AB/BA | tP36  | P-4c2      | C5Ir4  | #116 | ICSD_181486 | binary_carbide_ICSD_freq |
| 1329.AB/BA | mS22  | C2/m       | C5Nb6  | #12  | ICSD_20695  | binary_carbide_ICSD_freq |
| 1330.AB/BA | hR13  | R-3m       | C5Ti8  | #166 | ICSD_20822  | binary_carbide_ICSD_freq |
| 1331.AB/BA | hP33  | P3_{1}12   | C5V6   | #151 | ICSD_71098  | binary_carbide_ICSD_freq |
| 1332.AB/BA | cP126 | Pm-3       | C6OSr3 | #200 | ICSD_75354  | binary_carbide_ICSD_freq |
| 1333.AB/BA | hP14  | P6_{3}/mmc | C6Eu1  | #194 | ICSD_169041 | binary_carbide_ICSD_freq |
| 1334.AB/BA | hP14  | P6_{3}/mmc | C6Yb1  | #194 | ICSD_601565 | binary_carbide_ICSD_freq |
| 1335.AB/BA | mP44  | P2_{1}/c   | C7Ho4  | #14  | ICSD_74817  | binary_carbide_ICSD_freq |
| 1336.AB/BA | cI40  | Im-3m      | C7Ir3  | #229 | ICSD_181491 | binary_carbide_ICSD_freq |
| 1337.AB/BA | cP60  | P4_{3}32   | C7V8   | #212 | ICSD_22177  | binary_carbide_ICSD_freq |
| 1338.AB/BA | cP60  | P4_{3}32   | C7V8   | #212 | ICSD_43259  | binary_carbide_ICSD_freq |
| 1339.AB/BA | hP9   | P6/mmm     | C8Cs1  | #191 | ICSD_74641  | binary_carbide_ICSD_freq |
| 1340.AB/BA | oF72  | Fddd       | C8K1   | #70  | ICSD_70020  | binary_carbide_ICSD_freq |
| 1341.AB/BA | oF72  | Fddd       | C8Rb1  | #70  | ICSD_200563 | binary_carbide_ICSD_freq |

\*\*\* TERNARIES

|                                   |      |         |                            |                             |             |                            |
|-----------------------------------|------|---------|----------------------------|-----------------------------|-------------|----------------------------|
| T0001.A2BC/AB2C/ABC2              |      | cF16    | Fm(-3)m                    | AlCu2Mn-Heusler             | #225        | Navy [Wyckoff A^C, 3 prot  |
| T0001[-tet[+,-]*%].A2BC/AB2C/ABC2 |      | cF16    | Fm(-3)m                    | AlCu2Mn-Heusler-tet*%       | #225        | Navy [Wyckoff A^C, 3 prot  |
| T0002.A2BC/AB2C/ABC2              |      | cF16    | F-43m                      | Cu1Li2Sn1-antiHeusler       | #216        | ICSD_15130 [Wyckoff A^C, . |
| T0002[-tet[+,-]*%].A2BC/AB2C/ABC2 |      | cF16    | F-43m                      | Cu1Li2Sn1-antiHeusler-tet*% | #216        | ICSD_15130 [Wyckoff A^C, . |
| T0001.{ABC}                       |      | cF16    | Fm(-3)m                    | AlCu2Mn-Heusler             | #225        | Navy [Wyckoff A^C, 3 prot  |
| T0001[-tet[+,-]*%].{ABC}          |      | cF16    | Fm(-3)m                    | AlCu2Mn-Heusler-tet*%       | #225        | Navy [Wyckoff A^C, 3 prot  |
| T0002.{ABC}                       |      | cF16    | F-43m                      | Cu1Li2Sn1-antiHeusler       | #216        | ICSD_15130 [Wyckoff A^C, . |
| T0002[-tet[+,-]*%].{ABC}          |      | cF16    | F-43m                      | Cu1Li2Sn1-antiHeusler-tet*% | #216        | ICSD_15130 [Wyckoff A^C, . |
| T0003.{ABC}                       |      | cF12    | F-43m                      | AgAsMg-halfHeusler          | C1b #216    | ICSD_43819                 |
| T0003[-tet[+,-]*%].{ABC}          |      | cF12    | F-43m                      | AgAsMg-halfHeusler-tet*%    | C1b #216    | ICSD_43819 TET distorted   |
| T0004.{ABC}                       | oP12 | Pnma    | Co1Ge1Mn1_ICSD_52968       | #62                         | ICSD_52968  |                            |
| T0005.{ABC}                       | hP6  | P63/mmc | Co1Ge1Mn1_ICSD_623495      | #194                        | ICSD_623495 |                            |
| T0006.{ABC}                       | hP12 | P63/mmc | Co3Ge1Mn2_ICSD_52972       | #194                        | ICSD_52972  |                            |
| T0007.{ABC}                       | oP12 | Pnma    | Cl1La1Se1_ICSD_425686      | #62                         | ICSD_425686 |                            |
| T0008.{ABC}                       | oP12 | Pnma    | Cd1Na1P1 Co2Si1_ICSD_44858 | #62                         | ICSD_44858  |                            |
| T0009.{ABC}                       | cP5  | Pm-3m   | perovskite                 | #221                        |             |                            |

|             |      |        |           |      |      |             |
|-------------|------|--------|-----------|------|------|-------------|
| T0010.{ABC} | cF24 | F-43m  | Cu4MgSn   | C15b | #216 | ICSD_108141 |
| T0011.{ABC} | tI10 | I4/mmm | As2Ce1Pd2 |      | #139 | ICSD_604354 |

\*\*\* TERNARY SQS

|                   |      |      |  |         |     |         |
|-------------------|------|------|--|---------|-----|---------|
| TS001.ABC/BCA/CBA | oS64 | Cmma |  | SQS_L12 | #67 | SQS_L12 |
|-------------------|------|------|--|---------|-----|---------|

\*\*\* TERNARY FCC

|                     |     |        |                |      |       |
|---------------------|-----|--------|----------------|------|-------|
| TFCC001.ABC         | hP3 | P3m1   | ternary_fcc_1  | #156 | 3cell |
| TFCC002.ABC         | oI6 | Imm2   | ternary_fcc_2  | #44  | 3cell |
| TFCC003.ABC         | tI6 | I4mm   | ternary_fcc_3  | #107 | 3cell |
| TFCC004.ABC/BCA/CAB | hR4 | R3m    | ternary_fcc_4  | #160 | 4cell |
| TFCC005.ABC/BCA/CAB | oP4 | Pmm2   | ternary_fcc_5  | #25  | 4cell |
| TFCC006.ABC/BCA/CAB | mS8 | Cm     | ternary_fcc_6  | #8   | 4cell |
| TFCC007.ABC/BCA/CAB | tP4 | P4mm   | ternary_fcc_7  | #99  | 4cell |
| TFCC008.ABC/BCA/CAB | tI8 | I-4m2  | ternary_fcc_8  | #119 | 4cell |
| TFCC009.ABC/BCA/CAB | hR4 | R-3m   | ternary_fcc_9  | #166 | 4cell |
| TFCC010.ABC/BCA/CAB | oP4 | Pmmm   | ternary_fcc_10 | #47  | 4cell |
| TFCC011.ABC/BCA/CAB | mS8 | C2/m   | ternary_fcc_11 | #12  | 4cell |
| TFCC012.ABC/BCA/CAB | tP4 | P4/mmm | ternary_fcc_12 | #123 | 4cell |
| TFCC013.ABC/BCA/CAB | tI8 | I4/mmm | ternary_fcc_13 | #139 | 4cell |
| TFCC014.ABC/BCA/CAB | mP4 | P2/m   | ternary_fcc_14 | #10  | 4cell |
| TFCC015.ABC/BCA/CAB | oS8 | Cmmm   | ternary_fcc_15 | #65  | 4cell |
| TFCC016.ABC/BCA/CAB | tP4 | P4/mmm | ternary_fcc_16 | #123 | 4cell |

\*\*\* TERNARY BCC

|                     |      |        |                |      |                                    |
|---------------------|------|--------|----------------|------|------------------------------------|
| TBCC001.ABC         | oF12 | Fmm2   | ternary_bcc_1  | #42  | 3cell                              |
| TBCC002.ABC         | hP3  | P3m1   | ternary_bcc_2  | #156 | 3cell                              |
| TBCC003.ABC         | tI6  | I4mm   | ternary_bcc_3  | #107 | 3cell                              |
| TBCC004.ABC/BCA/CAB | oS8  | Cmm2   | ternary_bcc_4  | #35  | 4cell                              |
| TBCC005.ABC/BCA/CAB | mP4  | Pm     | ternary_bcc_5  | #6   | 4cell                              |
| TBCC006.ABC/BCA/CAB | tP4  | P4mm   | ternary_bcc_6  | #99  | 4cell                              |
| TBCC007.ABC/BCA/CAB | oI8  | Imm2   | ternary_bcc_7  | #44  | 4cell                              |
| TBCC008.ABC/BCA/CAB | cF16 | F-43m  | ternary_bcc_8  | #216 | 4cell same as T0002 (anti-Heusler) |
| TBCC009.ABC/BCA/CAB | oS8  | Cmmm   | ternary_bcc_9  | #65  | 4cell                              |
| TBCC010.ABC/BCA/CAB | mP4  | P2/m   | ternary_bcc_10 | #10  | 4cell                              |
| TBCC011.ABC/BCA/CAB | tP4  | P4/mmm | ternary_bcc_11 | #123 | 4cell                              |
| TBCC012.ABC/BCA/CAB | oI8  | Cmmm   | ternary_bcc_12 | #65  | 4cell                              |
| TBCC013.ABC/BCA/CAB | cF16 | Fm-3m  | ternary_bcc_13 | #225 | 4cell same as T0001 (Heusler)      |
| TBCC014.ABC/BCA/CAB | mS8  | C2/m   | ternary_bcc_14 | #12  | 4cell                              |
| TBCC015.ABC/BCA/CAB | oP4  | Pmmm   | ternary_bcc_15 | #47  | 4cell                              |
| TBCC016.ABC/BCA/CAB | tP4  | P4/mmm | ternary_bcc_16 | #123 | 4cell                              |

\*\*\* QUATERNARY

|              |      |         |                      |      |  |
|--------------|------|---------|----------------------|------|--|
| Q0001.{ABCD} | cF40 | Fm(-3)m | Al1F6K2Na1_ICSD_6027 | #225 | ICSD_6027 Elpasolite [Wyckoff all dist |
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