Supporting Information for

**Chemical Trends in the Thermodynamic Stability and Bandgaps of 980 Halide Double Perovskites: A High-Throughput First-Principles Study**

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**Table S1**. The 112 thermodynamically stable double-perovskites and 27 double-perovskites which had been reported to be stable in literature and are actually unstable after considering more competing compounds. The decomposition paths that determine their energies above convex hull *Ehull* are also listed.

|  |  |  |  |
| --- | --- | --- | --- |
| Compound | Decomposition Path | *Ehull* | Stability |
| Cs2AgAlF6 | 0.333333\*Ag2F+0.166667\*Cs2AgF4+0.5\*Cs3Al2F9+0.166667\*CsAgF3 | -0.00868 | stable |
| Cs2AgBiBr6 | 0.75\*AgBr+0.25\*Cs2AgBr3+0.5\*Cs3Bi2Br9 | -0.01436 | stable |
| Cs2AgBiCl6 | 1.0\*AgCl+0.333333\*Cs3Bi2Cl9+0.333333\*Cs3BiCl6 | -0.02753 | stable |
| Cs2AgBiF6 | 0.333333\*Ag2F+0.166667\*Cs2AgF4+0.5\*Cs3Bi2F9+0.166667\*CsAgF3 | -0.04612 | stable |
| Cs2AgGaF6 | 0.333333\*Ag2F+0.166667\*Cs2AgF4+0.5\*Cs3Ga2F9+0.166667\*CsAgF3 | -0.01637 | stable |
| Cs2AgInCl6 | 0.5\*AgCl+0.5\*Cs3In2Cl9+0.5\*CsAgCl2 | -0.00553 | stable |
| Cs2AgInF6 | 0.333333\*Ag2F+0.166667\*Cs2AgF4+0.5\*Cs3In2F9+0.166667\*CsAgF3 | -0.03674 | stable |
| Cs2AgSbCl6 | 0.5\*AgCl+0.5\*Cs3Sb2Cl9+0.5\*CsAgCl2 | -0.00352 | stable |
| Cs2AgScCl6 | 0.5\*AgCl+0.5\*Cs3Sc2Cl9+0.5\*CsAgCl2 | -0.00356 | stable |
| Cs2AgScF6 | 0.333333\*Ag2F+0.444444\*Cs3Sc2F9+0.111111\*Cs3ScF6+0.333333\*CsAgF3 | -0.02532 | stable |
| Cs2AgYCl6 | 1.0\*AgCl+1.0\*Cs2YCl5 | -0.00913 | stable |
| Cs2AgYF6 | 0.333333\*Ag2F+0.166667\*Cs2AgF4+0.5\*Cs3Y2F9+0.166667\*CsAgF3 | -0.03559 | stable |
| Cs2CsAlF6 | 0.5\*Cs3Al2F9+1.5\*CsF | -0.03912 | stable |
| Cs2CsBiF6 | 0.5\*Cs3Bi2F9+1.5\*CsF | -0.04456 | stable |
| Cs2CsGaF6 | 0.5\*Cs3Ga2F9+1.5\*CsF | -0.03851 | stable |
| Cs2CsInF6 | 0.5\*Cs3In2F9+1.5\*CsF | -0.04597 | stable |
| Cs2CsYF6 | 1.0\*Cs3YF6 | -0.03406 | stable |
| Cs2KAlF6 | 0.5\*Cs3Al2F9+0.5\*CsF+1.0\*KF | -0.06486 | stable |
| Cs2KBiBr6 | 0.5\*Cs3Bi2Br9+0.5\*CsBr+1.0\*KBr | -0.0004 | stable |
| Cs2KBiCl6 | 0.5\*Cs3BiCl6+0.5\*CsK2BiCl6 | -0.00368 | stable |
| Cs2KBiF6 | 0.25\*Cs3Bi2F9+1.25\*CsF+0.5\*K2BiF5 | -0.06259 | stable |
| Cs2KGaF6 | 0.5\*Cs3Ga2F9+0.5\*CsF+1.0\*KF | -0.06695 | stable |
| Cs2KInCl6 | 0.5\*Cs3In2Cl9+0.5\*CsCl+1.0\*KCl | -0.00797 | stable |
| Cs2KInF6 | 0.333333\*Cs3In2F9+1.0\*CsF+0.333333\*K3InF6 | -0.07112 | stable |
| Cs2KScCl6 | 0.333333\*Cs3Sc2Cl9+0.333333\*Cs3ScCl6+1.0\*KCl | -0.0089 | stable |
| Cs2KScF6 | 0.666667\*Cs3ScF6+0.666666\*KF+0.333333\*KScF4 | -0.046 | stable |
| Cs2KYBr6 | 0.5\*Cs3Y2Br9+0.5\*CsBr+1.0\*KBr | -0.00108 | stable |
| Cs2KYCl6 | 1.0\*Cs2YCl5+1.0\*KCl | -0.00727 | stable |
| Cs2KYF6 | 2.0\*CsF+1.0\*KYF4 | -0.04967 | stable |
| Cs2LiBiBr6 | 0.5\*Cs3Bi2Br9+0.5\*CsBr+1.0\*LiBr | -0.0047 | stable |
| Cs2LiBiCl6 | 0.333333\*Cs3Bi2Cl9+0.333333\*Cs3BiCl6+1.0\*LiCl | -0.00552 | stable |
| Cs2LiBiF6 | 0.5\*Cs3Bi2F9+0.5\*CsLiF2+0.5\*LiF | -0.02017 | stable |
| Cs2LiInF6 | 0.5\*Cs3In2F9+0.5\*CsLiF2+0.5\*LiF | -0.00218 | stable |
| Cs2LiYBr6 | 0.5\*Cs3Y2Br9+0.5\*CsBr+1.0\*LiBr | -0.00369 | stable |
| Cs2LiYCl6 | 1.0\*Cs2YCl5+1.0\*LiCl | -0.00142 | stable |
| Cs2LiYF6 | 0.666667\*Cs3YF6+0.666666\*LiF+0.333333\*LiYF4 | -0.00705 | stable |
| Cs2NaBiBr6 | 0.5\*Cs3Bi2Br9+0.5\*CsBr+1.0\*NaBr | -0.01378 | stable |
| Cs2NaBiCl6 | 0.333333\*Cs3Bi2Cl9+0.333333\*Cs3BiCl6+1.0\*NaCl | -0.02039 | stable |
| Cs2NaBiF6 | 0.5\*Cs3Bi2F9+0.5\*CsF+1.0\*NaF | -0.07337 | stable |
| Cs2NaInCl6 | 0.5\*Cs3In2Cl9+0.5\*CsCl+1.0\*NaCl | -0.01278 | stable |
| Cs2NaInF6 | 0.5\*Cs3In2F9+0.5\*CsF+1.0\*NaF | -0.06608 | stable |
| Cs2NaScBr6 | 0.5\*Cs3Sc2Br9+0.5\*CsBr+1.0\*NaBr | -0.00052 | stable |
| Cs2NaScCl6 | 0.333333\*Cs3Sc2Cl9+0.333333\*Cs3ScCl6+1.0\*NaCl | -0.01641 | stable |
| Cs2NaScF6 | 0.666667\*Cs3ScF6+0.333333\*Na3ScF6 | -0.03096 | stable |
| Cs2NaYBr6 | 0.5\*Cs3Y2Br9+0.5\*CsBr+1.0\*NaBr | -0.01477 | stable |
| Cs2NaYCl6 | 1.0\*Cs2YCl5+1.0\*NaCl | -0.01868 | stable |
| Cs2NaYF6 | 0.666667\*Cs3YF6+0.666666\*NaF+0.333333\*NaYF4 | -0.0632 | stable |
| Cs2RbAlF6 | 0.5\*Cs3Al2F9+0.5\*CsF+1.0\*RbF | -0.05893 | stable |
| Cs2RbBiF6 | 0.5\*Cs3Bi2F9+0.5\*CsF+1.0\*RbF | -0.06618 | stable |
| Cs2RbGaF6 | 0.5\*Cs3Ga2F9+0.5\*CsF+1.0\*RbF | -0.05903 | stable |
| Cs2RbInF6 | 0.5\*Cs3In2F9+0.5\*CsF+1.0\*RbF | -0.06799 | stable |
| Cs2RbScF6 | 0.666667\*Cs3ScF6+0.333333\*Rb3ScF6 | -0.01487 | stable |
| Cs2RbYF6 | 0.333333\*Cs3Y2F9+0.333333\*Cs3YF6+1.0\*RbF | -0.05995 | stable |
| K2AgAlF6 | 1.0\*AgF+1.0\*K2AlF5 | -0.00355 | stable |
| K2AgBiCl6 | 1.0\*AgCl+0.5\*K3Bi2Cl9+0.5\*KCl | -0.01599 | stable |
| K2AgGaF6 | 0.333333\*Ag2F+0.166667\*K2AgF4+0.5\*K3Ga2F9+0.166667\*KAgF3 | -0.02165 | stable |
| K2KGaF6 | 0.5\*K3Ga2F9+1.5\*KF | -0.03861 | stable |
| K2KScF6 | 2.0\*KF+1.0\*KScF4 | -0.0108 | stable |
| K2LiBiCl6 | 0.5\*K3Bi2Cl9+0.5\*KCl+1.0\*LiCl | -0.00728 | stable |
| K2LiGaF6 | 0.5\*K3Ga2F9+0.5\*KF+1.0\*LiF | -0.05104 | stable |
| K2LiInF6 | 0.25\*K3InF6+0.25\*K5In3F14+1.0\*LiF | -0.00069 | stable |
| K2LiScCl6 | 0.5\*K3Sc2Cl9+0.5\*KCl+1.0\*LiCl | -0.00286 | stable |
| K2LiScF6 | 1.0\*KF+1.0\*KScF4+1.0\*LiF | -0.03343 | stable |
| K2NaAlF6 | 1.0\*K2AlF5+1.0\*NaF | -0.05016 | stable |
| K2NaBiCl6 | 0.5\*K3Bi2Cl9+0.5\*KCl+1.0\*NaCl | -0.00585 | stable |
| K2NaGaF6 | 0.5\*K3Ga2F9+0.5\*KF+1.0\*NaF | -0.07348 | stable |
| K2NaInF6 | 0.666667\*K3InF6+0.333333\*Na3InF6 | -0.01359 | stable |
| K2NaScCl6 | 0.5\*K3Sc2Cl9+0.5\*KCl+1.0\*NaCl | -0.00203 | stable |
| K2NaScF6 | 1.0\*KF+1.0\*KScF4+1.0\*NaF | -0.04946 | stable |
| Rb2AgAlF6 | 0.333333\*Ag2F+0.5\*Rb3Al2F9+0.333333\*RbAgF3+0.166667\*RbF | -0.02662 | stable |
| Rb2AgBiCl6 | 0.75\*AgCl+0.25\*Rb2AgCl3+0.5\*Rb3Bi2Cl9 | -0.0279 | stable |
| Rb2AgGaF6 | 0.333333\*Ag2F+0.5\*Rb3Ga2F9+0.333333\*RbAgF3+0.166667\*RbF | -0.02702 | stable |
| Rb2AgInCl6 | 0.75\*AgCl+0.25\*Rb2AgCl3+0.5\*Rb3In2Cl9 | -0.0043 | stable |
| Rb2AgInF6 | 0.333333\*Ag2F+0.5\*Rb3In2F9+0.333333\*RbAgF3+0.166667\*RbF | -0.03558 | stable |
| Rb2AgSbCl6 | 0.75\*AgCl+0.25\*Rb2AgCl3+0.5\*Rb3Sb2Cl9 | -0.01098 | stable |
| Rb2AgScCl6 | 0.75\*AgCl+0.25\*Rb2AgCl3+0.5\*Rb3Sc2Cl9 | -0.00288 | stable |
| Rb2AgScF6 | 0.333333\*Ag2F+0.555556\*Rb3ScF6+0.333333\*RbAgF3+0.444445\*ScF3 | -0.02149 | stable |
| Rb2AgYF6 | 0.333333\*Ag2F+0.333333\*RbAgF3+1.666667\*RbF+1.0\*YF3 | -0.02322 | stable |
| Rb2CsAlF6 | 0.333333\*Cs3Al2F9+0.333333\*RbAlF4+1.666667\*RbF | -0.00881 | stable |
| Rb2CsGaF6 | 0.333333\*Cs3Ga2F9+0.333333\*GaF3+2.0\*RbF | -0.03053 | stable |
| Rb2CsInF6 | 0.333333\*Cs3In2F9+0.111111\*Rb2In3F11+1.777778\*RbF | -0.00175 | stable |
| Rb2KAlF6 | 0.5\*K2AlF5+0.5\*RbAlF4+1.5\*RbF | -0.06882 | stable |
| Rb2KBiF6 | 0.5\*K2BiF5+0.166667\*RbBi3F10+1.833334\*RbF | -0.01813 | stable |
| Rb2KScCl6 | 0.333333\*K3Sc2Cl9+2.0\*RbCl+0.333333\*ScCl3 | -0.02151 | stable |
| Rb2LiAlF6 | 1.0\*LiF+1.0\*RbAlF4+1.0\*RbF | -0.03322 | stable |
| Rb2LiBiCl6 | 1.0\*BiCl3+1.0\*LiCl+2.0\*RbCl | -0.0654 | stable |
| Rb2LiInCl6 | 0.666667\*InCl3+0.333333\*Li3InCl6+2.0\*RbCl | -0.07406 | stable |
| Rb2LiInF6 | 1.0\*LiF+0.333333\*Rb2In3F11+1.333333\*RbF | -0.05913 | stable |
| Rb2LiSbCl6 | 1.0\*LiCl+2.0\*RbCl+1.0\*SbCl3 | -0.02154 | stable |
| Rb2LiScCl6 | 1.0\*LiCl+2.0\*RbCl+1.0\*ScCl3 | -0.04396 | stable |
| Rb2LiScF6 | 1.0\*LiF+0.666667\*Rb3ScF6+0.333333\*ScF3 | -0.01352 | stable |
| Rb2LiScI6 | 1.0\*LiI+2.0\*RbI+1.0\*ScI3 | -0.00077 | stable |
| Rb2LiYBr6 | 1.0\*LiBr+2.0\*RbBr+1.0\*YBr3 | -0.0113 | stable |
| Rb2LiYF6 | 1.0\*LiYF4+2.0\*RbF | -0.01558 | stable |
| Rb2NaAlF6 | 0.333333\*Na3AlF6+0.666667\*RbAlF4+1.333333\*RbF | -0.07996 | stable |
| Rb2NaBiCl6 | 1.0\*BiCl3+1.0\*NaCl+2.0\*RbCl | -0.07028 | stable |
| Rb2NaBiF6 | 1.0\*NaF+0.333333\*RbBi3F10+1.666667\*RbF | -0.05651 | stable |
| Rb2NaGaF6 | 0.4\*GaF3+0.2\*Na5Ga3F14+2.0\*RbF | -0.13379 | stable |
| Rb2NaInCl6 | 0.666667\*InCl3+0.333333\*Na3InCl6+2.0\*RbCl | -0.06904 | stable |
| Rb2NaInF6 | 0.333333\*Na3InF6+0.222222\*Rb2In3F11+1.555555\*RbF | -0.08904 | stable |
| Rb2NaSbCl6 | 1.0\*NaCl+2.0\*RbCl+1.0\*SbCl3 | -0.02631 | stable |
| Rb2NaSbF6 | 0.5\*Na2SbF5+1.75\*RbF+0.25\*RbSb2F7 | -0.02467 | stable |
| Rb2NaScCl6 | 1.0\*NaScCl4+2.0\*RbCl | -0.05033 | stable |
| Rb2NaScF6 | 0.333333\*Na3ScF6+0.666667\*Rb3ScF6 | -0.03811 | stable |
| Rb2NaScI6 | 1.0\*NaI+2.0\*RbI+1.0\*ScI3 | -0.00442 | stable |
| Rb2NaYBr6 | 1.0\*NaBr+2.0\*RbBr+1.0\*YBr3 | -0.01399 | stable |
| Rb2NaYCl6 | 1.0\*NaCl+0.6\*Rb3YCl6+0.2\*RbY2Cl7 | -0.00076 | stable |
| Rb2NaYF6 | 1.0\*NaYF4+2.0\*RbF | -0.04509 | stable |
| Rb2RbAlF6 | 0.5\*Rb3Al2F9+1.5\*RbF | -0.04354 | stable |
| Rb2RbGaF6 | 0.5\*Rb3Ga2F9+1.5\*RbF | -0.03885 | stable |
| Rb2RbInF6 | 0.5\*Rb3In2F9+1.5\*RbF | -0.04189 | stable |
| Rb2RbYF6 | 3.0\*RbF+1.0\*YF3 | -0.02783 | stable |
| Cs2NaSbF6 | 1.0\*Cs2SbF5+1.0\*NaF | 0.03228 | unstable/reported stable |
| Cs2NaSbCl6 | 0.5\*Cs3Sb2Cl9+0.5\*CsCl+1.0\*NaCl | 0.00143 | unstable/reported stable |
| Cs2NaSbBr6 | 0.5\*Cs3Sb2Br9+0.5\*CsBr+1.0\*NaBr | 0.01321 | unstable/reported stable |
| Cs2NaSbI6 | 0.5\*Cs3Sb2I9+0.5\*CsI+1.0\*NaI | 0.02996 | unstable/reported stable |
| Cs2NaBiI6 | 0.5\*Cs3Bi2I9+0.5\*CsI+1.0\*NaI | 0.00966 | unstable/reported stable |
| Cs2KSbF6 | 1.0\*Cs2SbF5+1.0\*KF | 0.02365 | unstable/reported stable |
| Cs2KSbCl6 | 0.5\*Cs3Sb2Cl9+0.5\*CsCl+1.0\*KCl | 0.01225 | unstable/reported stable |
| Cs2KSbBr6 | 0.5\*Cs3Sb2Br9+0.5\*CsBr+1.0\*KBr | 0.02631 | unstable/reported stable |
| Cs2RbSbF6 | 1.0\*Cs2SbF5+1.0\*RbF | 0.03498 | unstable/reported stable |
| Cs2RbSbCl6 | 0.5\*Cs3Sb2Cl9+0.5\*CsCl+1.0\*RbCl | 0.02468 | unstable/reported stable |
| Cs2RbSbBr6 | 0.5\*Cs3Sb2Br9+0.5\*CsBr+1.0\*RbBr | 0.03769 | unstable/reported stable |
| Cs2RbBiCl6 | 0.333333\*Cs3Bi2Cl9+0.333333\*Cs3BiCl6+1.0\*RbCl | 0.00356 | unstable/reported stable |
| Cs2RbBiBr6 | 0.5\*Cs3Bi2Br9+0.5\*CsBr+1.0\*RbBr | 0.0111 | unstable/reported stable |
| Cs2CuSbF6 | 0.714286\*Cs2SbF5+0.071429\*Cs4Cu3F10+0.285714\*CsSbF6+0.785714\*Cu | 0.18852 | unstable/reported stable |
| Cs2CuSbCl6 | 0.5\*Cs3Sb2Cl9+0.5\*CsCu2Cl3 | 0.0729 | unstable/reported stable |
| Cs2CuSbBr6 | 0.5\*Cs3Sb2Br9+0.5\*CsCu2Br3 | 0.07451 | unstable/reported stable |
| Cs2CuBiF6 | 0.111111\*BiF3+0.444444\*Cs3Bi2F9+0.166667\*Cs4Cu3F10+0.5\*Cu | 0.0858 | unstable/reported stable |
| Cs2CuBiCl6 | 0.5\*Cs3Bi2Cl9+0.5\*CsCu2Cl3 | 0.04644 | unstable/reported stable |
| Cs2CuBiBr6 | 0.5\*Cs3Bi2Br9+0.5\*CsCu2Br3 | 0.05251 | unstable/reported stable |
| Cs2AgSbF6 | 1.0\*Ag+0.5\*Cs2SbF5+0.5\*CsF+0.5\*CsSbF6 | 0.08711 | unstable/reported stable |
| Cs2AgSbBr6 | 0.75\*AgBr+0.25\*Cs2AgBr3+0.5\*Cs3Sb2Br9 | 0.00764 | unstable/reported stable |
| Cs2AgSbI6 | 0.75\*AgI+0.25\*Cs2AgI3+0.5\*Cs3Sb2I9 | 0.02779 | unstable/reported stable |
| Cs2AgBiI6 | 0.75\*AgI+0.25\*Cs2AgI3+0.5\*Cs3Bi2I9 | 0.01258 | unstable/reported stable |
| Cs2AgInBr6 | 0.75\*AgBr+0.25\*Cs2AgBr3+0.5\*Cs3In2Br9 | 0.01076 | unstable/reported stable |
| Rb2AgInBr6 | 0.5\*Rb2AgBr3+0.5\*AgBr+1\*RbInBr4 | 0.0306 | unstable/reported stable |
| Rb2CuInCl6 | 0.5\*Cu+0.5\*Rb3In2Cl9+0.5\*RbCuCl3 | 0.0631 | unstable/reported stable |
| Rb2CuInBr6 | 0.5\*Rb3In2Br9+0.5\*RbCu2Br3 | 0.07345 | unstable/reported stable |

**Table S2.** The double-perovskites which are slightly unstable with positive *Ehull* in the range 0-0.1 eV/atom. The decomposition paths that determine their energies above convex hull *Ehull* are also listed.

|  |  |  |  |
| --- | --- | --- | --- |
| Compound | Decomposition Path | *Ehull* | Stability |
| Rb2KGaF6 | 1.0\*KRb2GaF6 | 0.00029 | unstable |
| K2AgScF6 | 0.333333\*Ag2F+0.333333\*K2AgF4+0.333333\*KF+1.0\*KScF4 | 0.00126 | unstable |
| Cs2NaSbCl6 | 0.5\*Cs3Sb2Cl9+0.5\*CsCl+1.0\*NaCl | 0.00143 | unstable |
| K2LiAlF6 | 1.0\*K2LiAlF6 | 0.00161 | unstable |
| Cs2NaYI6 | 0.5\*Cs3Y2I9+0.5\*CsI+1.0\*NaI | 0.0026 | unstable |
| Rb2LiSbF6 | 1.0\*LiF+1.5\*RbF+0.5\*RbSb2F7 | 0.00285 | unstable |
| Cs2RbInCl6 | 0.5\*Cs3In2Cl9+0.5\*CsCl+1.0\*RbCl | 0.00317 | unstable |
| Rb2LiInBr6 | 1.0\*InBr3+1.0\*LiBr+2.0\*RbBr | 0.00347 | unstable |
| Cs2RbBiCl6 | 0.333333\*Cs3Bi2Cl9+0.333333\*Cs3BiCl6+1.0\*RbCl | 0.00356 | unstable |
| Cs2RbScCl6 | 0.333333\*Cs3Sc2Cl9+0.333333\*Cs3ScCl6+1.0\*RbCl | 0.00394 | unstable |
| K2AgScCl6 | 1.0\*AgCl+0.5\*K3Sc2Cl9+0.5\*KCl | 0.00432 | unstable |
| Cs2NaInBr6 | 0.5\*Cs3In2Br9+0.5\*CsBr+1.0\*NaBr | 0.00434 | unstable |
| Rb2LiYCl6 | 1.0\*LiCl+0.6\*Rb3YCl6+0.2\*RbY2Cl7 | 0.00492 | unstable |
| Cs2AgYBr6 | 0.75\*AgBr+0.25\*Cs2AgBr3+0.5\*Cs3Y2Br9 | 0.00546 | unstable |
| Cs2RbYCl6 | 1.0\*Cs2YCl5+1.0\*RbCl | 0.00647 | unstable |
| Rb2RbSbF6 | 2.5\*RbF+0.5\*RbSb2F7 | 0.00702 | unstable |
| Rb2NaScBr6 | 1.0\*NaBr+0.5\*Rb3Sc2Br9+0.5\*RbBr | 0.00755 | unstable |
| Cs2AgSbBr6 | 0.75\*AgBr+0.25\*Cs2AgBr3+0.5\*Cs3Sb2Br9 | 0.00764 | unstable |
| Rb2KSbCl6 | 0.5\*K2SbCl5+2.0\*RbCl+0.5\*SbCl3 | 0.00772 | unstable |
| Rb2AgYCl6 | 1.0\*AgCl+0.6\*Rb3YCl6+0.2\*RbY2Cl7 | 0.0078 | unstable |
| Rb2KYBr6 | 1.0\*KBr+2.0\*RbBr+1.0\*YBr3 | 0.0083 | unstable |
| Cs2NaGaF6 | 1.0\*Cs2NaGaF6 | 0.00879 | unstable |
| Rb2AgBiBr6 | 1.0\*AgBr+0.333333\*Rb3Bi2Br9+0.333333\*Rb3BiBr6 | 0.0088 | unstable |
| Cs2NaBiI6 | 0.5\*Cs3Bi2I9+0.5\*CsI+1.0\*NaI | 0.00966 | unstable |
| Cs2KScBr6 | 0.5\*Cs3Sc2Br9+0.5\*CsBr+1.0\*KBr | 0.00997 | unstable |
| Cs2LiYI6 | 0.5\*Cs3Y2I9+0.5\*CsI+1.0\*LiI | 0.01006 | unstable |
| Rb2KSbF6 | 0.5\*K2SbF5+1.75\*RbF+0.25\*RbSb2F7 | 0.0104 | unstable |
| Cs2AgInBr6 | 0.75\*AgBr+0.25\*Cs2AgBr3+0.5\*Cs3In2Br9 | 0.01076 | unstable |
| Cs2RbBiBr6 | 0.5\*Cs3Bi2Br9+0.5\*CsBr+1.0\*RbBr | 0.0111 | unstable |
| Cs2NaScI6 | 0.5\*Cs3Sc2I9+0.5\*CsI+1.0\*NaI | 0.01156 | unstable |
| Cs2RbYBr6 | 0.5\*Cs3Y2Br9+0.5\*CsBr+1.0\*RbBr | 0.01171 | unstable |
| Rb2KScF6 | 1.0\*KRb2ScF6 | 0.01194 | unstable |
| Cs2KInBr6 | 0.5\*Cs3In2Br9+0.5\*CsBr+1.0\*KBr | 0.01213 | unstable |
| Rb2LiScBr6 | 1.0\*LiBr+0.5\*Rb3Sc2Br9+0.5\*RbBr | 0.01214 | unstable |
| Rb2AgYBr6 | 0.75\*AgBr+0.25\*Rb2AgBr3+0.5\*Rb3Y2Br9 | 0.01217 | unstable |
| Cs2KSbCl6 | 0.5\*Cs3Sb2Cl9+0.5\*CsCl+1.0\*KCl | 0.01225 | unstable |
| Cs2CsScF6 | 1.0\*Cs3ScF6 | 0.01231 | unstable |
| Cs2AgBiI6 | 0.75\*AgI+0.25\*Cs2AgI3+0.5\*Cs3Bi2I9 | 0.01258 | unstable |
| Cs2LiScCl6 | 1.0\*Cs2LiScCl6 | 0.01298 | unstable |
| K2RbAlF6 | 1.0\*K2AlF5+1.0\*RbF | 0.01304 | unstable |
| Cs2NaSbBr6 | 0.5\*Cs3Sb2Br9+0.5\*CsBr+1.0\*NaBr | 0.01321 | unstable |
| Cs2LiInCl6 | 1.0\*Cs2LiInCl6 | 0.01357 | unstable |
| Cs2LiScBr6 | 0.5\*Cs3Sc2Br9+0.5\*CsBr+1.0\*LiBr | 0.01376 | unstable |
| K2AgInCl6 | 1.0\*AgCl+0.333333\*K3In2Cl9+0.333333\*K3InCl6 | 0.01403 | unstable |
| K2LiScBr6 | 0.5\*K3Sc2Br9+0.5\*KBr+1.0\*LiBr | 0.01439 | unstable |
| Rb2LiGaF6 | 1.0\*Rb2LiGaF6 | 0.01439 | unstable |
| Cs2LiBiI6 | 0.5\*Cs3Bi2I9+0.5\*CsI+1.0\*LiI | 0.01513 | unstable |
| Rb2RbBiCl6 | 0.5\*Rb3Bi2Cl9+1.5\*RbCl | 0.01534 | unstable |
| Rb2AgInBr6 | 0.5\*Rb2AgBr3+0.5\*AgBr+1\*RbInBr4 | 0.0306 | unstable |
| Rb2CsBiF6 | 0.333333\*Cs3Bi2F9+0.111111\*RbBi3F10+1.888889\*RbF | 0.01577 | unstable |
| Cs2NaAlF6 | 1.0\*Cs2NaAlF6 | 0.01611 | unstable |
| Rb2NaBiBr6 | 1.0\*NaBr+0.333333\*Rb3Bi2Br9+0.333333\*Rb3BiBr6 | 0.0162 | unstable |
| K2AgSbBr6 | 1.0\*AgBr+0.5\*K3Sb2Br9+0.5\*KBr | 0.01631 | unstable |
| Rb2KInF6 | 1.0\*KRb2InF6 | 0.01633 | unstable |
| Rb2CsYF6 | 0.333333\*Cs3Y2F9+2.0\*RbF+0.333333\*YF3 | 0.01639 | unstable |
| Rb2KScI6 | 0.333333\*K3Sc2I9+2.0\*RbI+0.333333\*ScI3 | 0.01721 | unstable |
| K2NaScBr6 | 0.333333\*K3Sc2Br9+1.0\*KBr+0.333333\*Na3ScBr6 | 0.01722 | unstable |
| Cs2KYI6 | 0.5\*Cs3Y2I9+0.5\*CsI+1.0\*KI | 0.01786 | unstable |
| Rb2LiBiBr6 | 1.0\*LiBr+0.333333\*Rb3Bi2Br9+0.333333\*Rb3BiBr6 | 0.01799 | unstable |
| Cs2AgScBr6 | 0.75\*AgBr+0.25\*Cs2AgBr3+0.5\*Cs3Sc2Br9 | 0.01841 | unstable |
| Cs2LiSbCl6 | 0.5\*Cs3Sb2Cl9+0.5\*CsLiCl2+0.5\*LiCl | 0.01846 | unstable |
| K2AgBiBr6 | 1.0\*AgBr+1.0\*BiBr3+2.0\*KBr | 0.01876 | unstable |
| K2LiInCl6 | 0.333333\*K3In2Cl9+0.333333\*K3InCl6+1.0\*LiCl | 0.01884 | unstable |
| Na2LiGaF6 | 1.0\*LiF+0.333333\*Na5Ga3F14+0.333333\*NaF | 0.01917 | unstable |
| Cs2LiInBr6 | 0.5\*Cs3In2Br9+0.5\*CsBr+1.0\*LiBr | 0.01932 | unstable |
| Rb2AgSbBr6 | 0.75\*AgBr+0.25\*Rb2AgBr3+0.5\*Rb3Sb2Br9 | 0.02064 | unstable |
| Rb2RbScF6 | 1.0\*Rb3ScF6 | 0.02068 | unstable |
| Cs2LiScI6 | 0.5\*Cs3Sc2I9+0.5\*CsI+1.0\*LiI | 0.02121 | unstable |
| Cs2CsInCl6 | 0.5\*Cs3In2Cl9+1.5\*CsCl | 0.02128 | unstable |
| Cs2RbScBr6 | 0.5\*Cs3Sc2Br9+0.5\*CsBr+1.0\*RbBr | 0.02197 | unstable |
| K2KBiCl6 | 0.5\*K3Bi2Cl9+1.5\*KCl | 0.02197 | unstable |
| Rb2AgScBr6 | 0.75\*AgBr+0.25\*Rb2AgBr3+0.5\*Rb3Sc2Br9 | 0.02206 | unstable |
| Cs2RbInBr6 | 0.5\*Cs3In2Br9+0.5\*CsBr+1.0\*RbBr | 0.02222 | unstable |
| Cs2LiSbBr6 | 0.5\*Cs3Sb2Br9+0.5\*CsBr+1.0\*LiBr | 0.0226 | unstable |
| Cs2KSbF6 | 1.0\*Cs2SbF5+1.0\*KF | 0.02365 | unstable |
| K2LiYBr6 | 2.0\*KBr+1.0\*LiBr+1.0\*YBr3 | 0.02371 | unstable |
| Cs2KScI6 | 0.5\*Cs3Sc2I9+0.5\*CsI+1.0\*KI | 0.0245 | unstable |
| Cs2RbSbCl6 | 0.5\*Cs3Sb2Cl9+0.5\*CsCl+1.0\*RbCl | 0.02468 | unstable |
| Rb2NaYI6 | 1.0\*NaI+2.0\*RbI+1.0\*YI3 | 0.02469 | unstable |
| K2LiBiBr6 | 1.0\*BiBr3+2.0\*KBr+1.0\*LiBr | 0.02495 | unstable |
| Cs2KBiI6 | 0.5\*Cs3Bi2I9+0.5\*CsI+1.0\*KI | 0.02501 | unstable |
| K2AgSbCl6 | 1.0\*AgCl+1.0\*K2SbCl5 | 0.02581 | unstable |
| K2LiYCl6 | 1.0\*K2YCl5+1.0\*LiCl | 0.02619 | unstable |
| Cs2KSbBr6 | 0.5\*Cs3Sb2Br9+0.5\*CsBr+1.0\*KBr | 0.02631 | unstable |
| K2NaYBr6 | 2.0\*KBr+1.0\*NaBr+1.0\*YBr3 | 0.02652 | unstable |
| Rb2RbScCl6 | 0.5\*Rb3Sc2Cl9+1.5\*RbCl | 0.02686 | unstable |
| Rb2LiYI6 | 1.0\*LiI+2.0\*RbI+1.0\*YI3 | 0.02695 | unstable |
| K2AgScBr6 | 1.0\*AgBr+0.5\*K3Sc2Br9+0.5\*KBr | 0.02721 | unstable |
| Cs2LiScF6 | 0.333333\*Cs3Sc2F9+0.333333\*Cs3ScF6+1.0\*LiF | 0.02739 | unstable |
| K2AgInF6 | 0.333333\*Ag2F+0.333333\*K5In3F14+0.333333\*KAgF3 | 0.02747 | unstable |
| Cs2CsBiBr6 | 0.5\*Cs3Bi2Br9+1.5\*CsBr | 0.02754 | unstable |
| Cs2CsYCl6 | 1.0\*Cs2YCl5+1.0\*CsCl | 0.02758 | unstable |
| K2LiSbBr6 | 0.5\*K3Sb2Br9+0.5\*KBr+1.0\*LiBr | 0.02759 | unstable |
| Rb2RbInCl6 | 0.5\*Rb3In2Cl9+1.5\*RbCl | 0.02774 | unstable |
| Cs2AgSbI6 | 0.75\*AgI+0.25\*Cs2AgI3+0.5\*Cs3Sb2I9 | 0.02779 | unstable |
| K2NaYCl6 | 1.0\*K2YCl5+1.0\*NaCl | 0.02792 | unstable |
| K2NaBiBr6 | 1.0\*BiBr3+2.0\*KBr+1.0\*NaBr | 0.02796 | unstable |
| Rb2KScBr6 | 1.0\*KBr+0.5\*Rb3Sc2Br9+0.5\*RbBr | 0.02834 | unstable |
| K2NaInCl6 | 0.666667\*K3InCl6+0.333333\*Na3InCl6 | 0.02904 | unstable |
| Cs2CsScCl6 | 1.0\*Cs3ScCl6 | 0.02905 | unstable |
| K2KScCl6 | 0.5\*K3Sc2Cl9+1.5\*KCl | 0.02908 | unstable |
| Cs2RbYI6 | 0.5\*Cs3Y2I9+0.5\*CsI+1.0\*RbI | 0.02964 | unstable |
| Cs2AgYI6 | 0.75\*AgI+0.25\*Cs2AgI3+0.5\*Cs3Y2I9 | 0.02983 | unstable |
| Cs2NaSbI6 | 0.5\*Cs3Sb2I9+0.5\*CsI+1.0\*NaI | 0.02996 | unstable |
| Rb2KYF6 | 1.0\*KRb2YF6 | 0.03065 | unstable |
| K2NaBiF6 | 1.0\*K2BiF5+1.0\*NaF | 0.03076 | unstable |
| Cs2CsYBr6 | 0.5\*Cs3Y2Br9+1.5\*CsBr | 0.03085 | unstable |
| K2NaSbBr6 | 0.5\*K3Sb2Br9+0.5\*KBr+1.0\*NaBr | 0.03131 | unstable |
| Rb2KYCl6 | 0.333333\*K3YCl6+0.666667\*Rb3YCl6 | 0.0314 | unstable |
| Rb2NaSbBr6 | 1.0\*NaBr+0.5\*Rb3Sb2Br9+0.5\*RbBr | 0.03143 | unstable |
| K2RbGaF6 | 0.25\*K3Ga2F9+0.75\*KF+0.5\*KRb2GaF6 | 0.03164 | unstable |
| Rb2AgBiI6 | 0.75\*AgI+0.25\*Rb2AgI3+0.5\*Rb3Bi2I9 | 0.03191 | unstable |
| Cs2NaSbF6 | 1.0\*Cs2SbF5+1.0\*NaF | 0.03228 | unstable |
| K2NaYF6 | 1.0\*K2YF5+1.0\*NaF | 0.03244 | unstable |
| Rb2LiSbBr6 | 1.0\*LiBr+0.5\*Rb3Sb2Br9+0.5\*RbBr | 0.03292 | unstable |
| Cs2KAlCl6 | 1.0\*CsAlCl4+1.0\*CsCl+1.0\*KCl | 0.03301 | unstable |
| Rb2CuBiCl6 | 0.5\*Cu+0.5\*Rb3Bi2Cl9+0.5\*RbCuCl3 | 0.03389 | unstable |
| K2CuBiCl6 | 0.75\*CuCl+0.25\*K2CuCl3+0.5\*K3Bi2Cl9 | 0.03404 | unstable |
| Rb2NaBiI6 | 1.0\*NaI+0.5\*Rb3Bi2I9+0.5\*RbI | 0.03408 | unstable |
| Na2LiAlF6 | 0.333333\*Na3AlF6+0.333333\*Na3Li3Al2F12 | 0.03413 | unstable |
| Rb2RbYBr6 | 0.5\*Rb3Y2Br9+1.5\*RbBr | 0.03415 | unstable |
| K2LiScI6 | 0.5\*K3Sc2I9+0.5\*KI+1.0\*LiI | 0.03443 | unstable |
| Rb2LiBiI6 | 1.0\*LiI+0.5\*Rb3Bi2I9+0.5\*RbI | 0.03484 | unstable |
| K2NaScI6 | 0.5\*K3Sc2I9+0.5\*KI+1.0\*NaI | 0.03486 | unstable |
| Cs2RbSbF6 | 1.0\*Cs2SbF5+1.0\*RbF | 0.03498 | unstable |
| Rb2KInBr6 | 1.0\*KInBr4+2.0\*RbBr | 0.0352 | unstable |
| Cs2LiSbI6 | 0.5\*Cs3Sb2I9+0.5\*CsI+1.0\*LiI | 0.03543 | unstable |
| Cs2RbBiI6 | 0.5\*Cs3Bi2I9+0.5\*CsI+1.0\*RbI | 0.0355 | unstable |
| Cs2RbScI6 | 0.5\*Cs3Sc2I9+0.5\*CsI+1.0\*RbI | 0.0356 | unstable |
| Rb2NaAlCl6 | 1.0\*NaCl+1.0\*RbAlCl4+1.0\*RbCl | 0.0359 | unstable |
| Cs2NaAlCl6 | 1.0\*CsAlCl4+1.0\*CsCl+1.0\*NaCl | 0.0362 | unstable |
| K2AgYCl6 | 1.0\*AgCl+1.0\*K2YCl5 | 0.03648 | unstable |
| Rb2KBiBr6 | 1.0\*KBr+0.333333\*Rb3Bi2Br9+0.333333\*Rb3BiBr6 | 0.03698 | unstable |
| K2KInF6 | 1.0\*K3InF6 | 0.0374 | unstable |
| Cs2CsInBr6 | 0.5\*Cs3In2Br9+1.5\*CsBr | 0.03766 | unstable |
| Cs2AgScI6 | 0.75\*AgI+0.25\*Cs2AgI3+0.5\*Cs3Sc2I9 | 0.03767 | unstable |
| Cs2RbSbBr6 | 0.5\*Cs3Sb2Br9+0.5\*CsBr+1.0\*RbBr | 0.03769 | unstable |
| Rb2RbSbCl6 | 0.5\*Rb3Sb2Cl9+1.5\*RbCl | 0.03786 | unstable |
| Rb2CsInCl6 | 0.333333\*Cs3In2Cl9+0.333333\*InCl3+2.0\*RbCl | 0.03802 | unstable |
| K2LiSbCl6 | 1.0\*K2SbCl5+1.0\*LiCl | 0.03912 | unstable |
| Cs2CsBiCl6 | 1.0\*Cs3BiCl6 | 0.03917 | unstable |
| K2AgYBr6 | 1.0\*AgBr+2.0\*KBr+1.0\*YBr3 | 0.03973 | unstable |
| K2RbBiCl6 | 0.5\*K3Bi2Cl9+0.5\*KCl+1.0\*RbCl | 0.0403 | unstable |
| Cs2CsScBr6 | 0.5\*Cs3Sc2Br9+1.5\*CsBr | 0.04052 | unstable |
| Na2NaGaF6 | 0.333333\*Na5Ga3F14+1.333333\*NaF | 0.04093 | unstable |
| K2NaSbCl6 | 1.0\*K2SbCl5+1.0\*NaCl | 0.04124 | unstable |
| Cs2RbAlCl6 | 1.0\*CsAlCl4+1.0\*CsCl+1.0\*RbCl | 0.04225 | unstable |
| Cs2KAlI6 | 1.0\*AlI3+2.0\*CsI+1.0\*KI | 0.04297 | unstable |
| Cs2CsSbCl6 | 0.5\*Cs3Sb2Cl9+1.5\*CsCl | 0.04339 | unstable |
| Rb2AgScI6 | 0.75\*AgI+0.25\*Rb2AgI3+0.5\*Rb3Sc2I9 | 0.04347 | unstable |
| Rb2CsBiCl6 | 0.333333\*BiCl3+0.333333\*Cs3Bi2Cl9+2.0\*RbCl | 0.04353 | unstable |
| K2KScBr6 | 0.5\*K3Sc2Br9+1.5\*KBr | 0.04369 | unstable |
| Rb2AgSbI6 | 0.75\*AgI+0.25\*Rb2AgI3+0.5\*Rb3Sb2I9 | 0.044 | unstable |
| Rb2RbScBr6 | 0.5\*Rb3Sc2Br9+1.5\*RbBr | 0.04424 | unstable |
| Cs2NaInI6 | 1.0\*CsI+1.0\*CsInI4+1.0\*NaI | 0.04471 | unstable |
| Rb2RbInBr6 | 0.5\*Rb3In2Br9+1.5\*RbBr | 0.04474 | unstable |
| K2LiBiF6 | 1.0\*K2BiF5+1.0\*LiF | 0.0452 | unstable |
| Rb2KYI6 | 1.0\*KI+2.0\*RbI+1.0\*YI3 | 0.04545 | unstable |
| Cs2KSbI6 | 0.5\*Cs3Sb2I9+0.5\*CsI+1.0\*KI | 0.04562 | unstable |
| Cs2CsYI6 | 0.5\*Cs3Y2I9+1.5\*CsI | 0.04615 | unstable |
| Cs2CuBiCl6 | 0.5\*Cs3Bi2Cl9+0.5\*CsCu2Cl3 | 0.04644 | unstable |
| K2LiYF6 | 1.0\*K2YF5+1.0\*LiF | 0.04677 | unstable |
| Cs2CsBiI6 | 0.5\*Cs3Bi2I9+1.5\*CsI | 0.04941 | unstable |
| Rb2KAlCl6 | 1.0\*KCl+1.0\*RbAlCl4+1.0\*RbCl | 0.04941 | unstable |
| Rb2AgYI6 | 1.0\*Rb2AgI3+1.0\*YI3 | 0.04965 | unstable |
| Rb2CuSbCl6 | 0.5\*Cu+0.5\*Rb3Sb2Cl9+0.5\*RbCuCl3 | 0.05032 | unstable |
| K2RbScCl6 | 0.5\*K3Sc2Cl9+0.5\*KCl+1.0\*RbCl | 0.05042 | unstable |
| Cs2RbAlI6 | 1.0\*AlI3+2.0\*CsI+1.0\*RbI | 0.05117 | unstable |
| Cs2CsScI6 | 0.5\*Cs3Sc2I9+1.5\*CsI | 0.0513 | unstable |
| Cs2LiAlI6 | 1.0\*AlI3+2.0\*CsI+1.0\*LiI | 0.05158 | unstable |
| K2NaAlCl6 | 1.0\*KAlCl4+1.0\*KCl+1.0\*NaCl | 0.05172 | unstable |
| Rb2NaSbI6 | 1.0\*NaI+0.5\*Rb3Sb2I9+0.5\*RbI | 0.05196 | unstable |
| Cs2KGaCl6 | 1.0\*CsCl+1.0\*CsGaCl4+1.0\*KCl | 0.05197 | unstable |
| Rb2LiSbI6 | 1.0\*LiI+0.5\*Rb3Sb2I9+0.5\*RbI | 0.05212 | unstable |
| Rb2AgAlCl6 | 0.5\*AgCl+0.5\*Rb2AgCl3+1.0\*RbAlCl4 | 0.05246 | unstable |
| Rb2LiAlCl6 | 1.0\*LiCl+1.0\*RbAlCl4+1.0\*RbCl | 0.05247 | unstable |
| Cs2CuBiBr6 | 0.5\*Cs3Bi2Br9+0.5\*CsCu2Br3 | 0.05251 | unstable |
| K2CsGaF6 | 0.333333\*Cs3Ga2F9+1.666667\*KF+0.333333\*KGaF4 | 0.05253 | unstable |
| Rb2KSbBr6 | 1.0\*KBr+0.5\*Rb3Sb2Br9+0.5\*RbBr | 0.05262 | unstable |
| K2AgScI6 | 1.0\*AgI+0.5\*K3Sc2I9+0.5\*KI | 0.05296 | unstable |
| Cs2NaGaCl6 | 1.0\*CsCl+1.0\*CsGaCl4+1.0\*NaCl | 0.05315 | unstable |
| Cs2AgInI6 | 0.5\*AgI+0.5\*Cs2AgI3+1.0\*CsInI4 | 0.05316 | unstable |
| K2KBiBr6 | 1.0\*BiBr3+3.0\*KBr | 0.05344 | unstable |
| K2AgInBr6 | 1.0\*AgBr+1.0\*KBr+1.0\*KInBr4 | 0.05362 | unstable |
| Cs2CsSbBr6 | 0.5\*Cs3Sb2Br9+1.5\*CsBr | 0.05394 | unstable |
| Rb2CsScCl6 | 0.333333\*Cs3Sc2Cl9+2.0\*RbCl+0.333333\*ScCl3 | 0.05417 | unstable |
| Cs2LiInI6 | 1.0\*CsI+1.0\*CsInI4+1.0\*LiI | 0.05437 | unstable |
| Rb2KBiI6 | 1.0\*KI+0.5\*Rb3Bi2I9+0.5\*RbI | 0.05442 | unstable |
| K2KYBr6 | 3.0\*KBr+1.0\*YBr3 | 0.05451 | unstable |
| K2RbScF6 | 1.0\*KF+0.5\*KRb2ScF6+0.5\*KScF4 | 0.05498 | unstable |
| Rb2RbScI6 | 0.5\*Rb3Sc2I9+1.5\*RbI | 0.05518 | unstable |
| Cs2NaAlBr6 | 1.0\*CsAlBr4+1.0\*CsBr+1.0\*NaBr | 0.05544 | unstable |
| Cs2NaAlI6 | 2.0\*CsI+1.0\*NaAlI4 | 0.05567 | unstable |
| Cs2KInI6 | 1.0\*CsI+1.0\*CsInI4+1.0\*KI | 0.05596 | unstable |
| Cs2RbSbI6 | 0.5\*Cs3Sb2I9+0.5\*CsI+1.0\*RbI | 0.056 | unstable |
| Rb2NaGaCl6 | 1.0\*NaCl+1.0\*RbCl+1.0\*RbGaCl4 | 0.056 | unstable |
| K2NaInBr6 | 1.0\*KBr+1.0\*KInBr4+1.0\*NaBr | 0.05601 | unstable |
| Cs2CsSbF6 | 1.0\*Cs2SbF5+1.0\*CsF | 0.0564 | unstable |
| K2CsAlF6 | 0.333333\*Cs3Al2F9+0.333333\*K2AlF5+1.333333\*KF | 0.05659 | unstable |
| K2LiInBr6 | 1.0\*KBr+1.0\*KInBr4+1.0\*LiBr | 0.0568 | unstable |
| Cs2KAlBr6 | 1.0\*CsAlBr4+1.0\*CsBr+1.0\*KBr | 0.05702 | unstable |
| Rb2RbYCl6 | 1.0\*Rb3YCl6 | 0.05719 | unstable |
| K2KSbBr6 | 0.5\*K3Sb2Br9+1.5\*KBr | 0.05769 | unstable |
| Rb2CsScF6 | 0.333333\*Cs3ScF6+0.666667\*Rb3ScF6 | 0.05786 | unstable |
| K2NaSbF6 | 1.0\*K2SbF5+1.0\*NaF | 0.05789 | unstable |
| K2LiAlCl6 | 1.0\*KAlCl4+1.0\*KCl+1.0\*LiCl | 0.05808 | unstable |
| K2KScI6 | 0.5\*K3Sc2I9+1.5\*KI | 0.05842 | unstable |
| K2AgBiI6 | 1.0\*AgI+1.0\*BiI3+2.0\*KI | 0.0589 | unstable |
| Rb2RbYI6 | 3.0\*RbI+1.0\*YI3 | 0.05933 | unstable |
| Cs2CsAlCl6 | 1.0\*CsAlCl4+2.0\*CsCl | 0.05956 | unstable |
| Rb2RbBiBr6 | 1.0\*Rb3BiBr6 | 0.05967 | unstable |
| Cs2LiGaF6 | 1.0\*Cs2LiGaF6 | 0.05968 | unstable |
| K2AgAlCl6 | 1.0\*AgCl+1.0\*KAlCl4+1.0\*KCl | 0.06057 | unstable |
| Rb2AgGaCl6 | 0.5\*AgCl+0.5\*Rb2AgCl3+1.0\*RbGaCl4 | 0.06117 | unstable |
| Cs2RbGaCl6 | 1.0\*CsCl+1.0\*CsGaCl4+1.0\*RbCl | 0.0613 | unstable |
| Na2NaAlF6 | 1.0\*Na3AlF6 | 0.06135 | unstable |
| Cs2AgAlCl6 | 1.0\*CsAgCl2+1.0\*CsAlCl4 | 0.06144 | unstable |
| K2LiYI6 | 2.0\*KI+1.0\*LiI+1.0\*YI3 | 0.06167 | unstable |
| Rb2NaAlBr6 | 1.0\*NaBr+1.0\*RbAlBr4+1.0\*RbBr | 0.06169 | unstable |
| K2RbInCl6 | 0.333333\*K3In2Cl9+0.333333\*K3InCl6+1.0\*RbCl | 0.06183 | unstable |
| K2LiBiI6 | 1.0\*BiI3+2.0\*KI+1.0\*LiI | 0.06187 | unstable |
| K2CuSbBr6 | 0.75\*CuBr+0.25\*K2CuBr3+0.5\*K3Sb2Br9 | 0.0619 | unstable |
| K2NaYI6 | 2.0\*KI+1.0\*NaI+1.0\*YI3 | 0.06301 | unstable |
| Rb2CuInCl6 | 0.5\*Cu+0.5\*Rb3In2Cl9+0.5\*RbCuCl3 | 0.0631 | unstable |
| Cs2CsAlI6 | 1.0\*AlI3+3.0\*CsI | 0.06327 | unstable |
| K2KBiF6 | 1.0\*K2BiF5+1.0\*KF | 0.06334 | unstable |
| Cs2AgAlI6 | 1.0\*AlI3+1.0\*Cs2AgI3 | 0.06363 | unstable |
| Rb2CuBiBr6 | 0.5\*Rb3Bi2Br9+0.5\*RbCu2Br3 | 0.06395 | unstable |
| K2NaBiI6 | 1.0\*BiI3+2.0\*KI+1.0\*NaI | 0.06431 | unstable |
| K2AgBiF6 | 1.0\*AgF+1.0\*K2BiF5 | 0.06448 | unstable |
| K2CuScCl6 | 0.75\*CuCl+0.25\*K2CuCl3+0.5\*K3Sc2Cl9 | 0.06455 | unstable |
| K2KInCl6 | 1.0\*K3InCl6 | 0.06486 | unstable |
| K2AgSbI6 | 1.0\*AgI+2.0\*KI+1.0\*SbI3 | 0.06509 | unstable |
| Rb2RbAlCl6 | 1.0\*RbAlCl4+2.0\*RbCl | 0.06515 | unstable |
| K2KYCl6 | 1.0\*K3YCl6 | 0.06533 | unstable |
| Cs2RbInI6 | 1.0\*CsI+1.0\*CsInI4+1.0\*RbI | 0.06535 | unstable |
| Cs2RbAlBr6 | 1.0\*CsAlBr4+1.0\*CsBr+1.0\*RbBr | 0.06572 | unstable |
| K2CuInCl6 | 1.0\*CuCl+0.333333\*K3In2Cl9+0.333333\*K3InCl6 | 0.06621 | unstable |
| Cs2NaGaI6 | 2.0\*CsI+1.0\*GaI3+1.0\*NaI | 0.06626 | unstable |
| Rb2RbBiI6 | 0.5\*Rb3Bi2I9+1.5\*RbI | 0.06672 | unstable |
| Rb2RbSbBr6 | 0.5\*Rb3Sb2Br9+1.5\*RbBr | 0.06692 | unstable |
| K2CuBiBr6 | 1.0\*BiBr3+1.0\*K2CuBr3 | 0.06715 | unstable |
| Cs2AgGaCl6 | 1.0\*CsAgCl2+1.0\*CsGaCl4 | 0.0679 | unstable |
| Cs2CsSbI6 | 0.5\*Cs3Sb2I9+1.5\*CsI | 0.06971 | unstable |
| Rb2AgSbF6 | 1.0\*Ag+1.25\*RbF+0.25\*RbSb2F7+0.5\*RbSbF6 | 0.06983 | unstable |
| K2KSbCl6 | 1.0\*K2SbCl5+1.0\*KCl | 0.06997 | unstable |
| Cs2LiAlCl6 | 1.0\*CsAlCl4+1.0\*CsLiCl2 | 0.07011 | unstable |
| Rb2CsYBr6 | 0.333333\*Cs3Y2Br9+2.0\*RbBr+0.333333\*YBr3 | 0.07029 | unstable |
| Rb2KGaCl6 | 1.0\*KCl+1.0\*RbCl+1.0\*RbGaCl4 | 0.07042 | unstable |
| Rb2LiGaCl6 | 1.0\*LiCl+1.0\*RbCl+1.0\*RbGaCl4 | 0.07048 | unstable |
| K2KYF6 | 1.0\*K3YF6 | 0.07099 | unstable |
| Rb2CuScCl6 | 0.5\*Cu+0.5\*Rb3Sc2Cl9+0.5\*RbCuCl3 | 0.07222 | unstable |
| Cs2AgGaI6 | 1.0\*Cs2AgI3+1.0\*GaI3 | 0.07246 | unstable |
| K2RbYBr6 | 2.0\*KBr+1.0\*RbBr+1.0\*YBr3 | 0.0725 | unstable |
| K2AgGaCl6 | 1.0\*AgCl+1.0\*KCl+1.0\*KGaCl4 | 0.0728 | unstable |
| K2CuSbCl6 | 1.0\*CuCl+1.0\*K2SbCl5 | 0.07288 | unstable |
| Cs2CuSbCl6 | 0.5\*Cs3Sb2Cl9+0.5\*CsCu2Cl3 | 0.0729 | unstable |
| Rb2KSbI6 | 1.0\*KI+0.5\*Rb3Sb2I9+0.5\*RbI | 0.07291 | unstable |
| K2LiSbF6 | 1.0\*K2SbF5+1.0\*LiF | 0.07303 | unstable |
| Rb2CsInBr6 | 0.333333\*Cs3In2Br9+0.333333\*InBr3+2.0\*RbBr | 0.07308 | unstable |
| K2LiSbI6 | 2.0\*KI+1.0\*LiI+1.0\*SbI3 | 0.07327 | unstable |
| Rb2LiAlBr6 | 1.0\*LiBr+1.0\*RbAlBr4+1.0\*RbBr | 0.07337 | unstable |
| Rb2CuInBr6 | 0.5\*Rb3In2Br9+0.5\*RbCu2Br3 | 0.07345 | unstable |
| K2RbScI6 | 0.5\*K3Sc2I9+0.5\*KI+1.0\*RbI | 0.0737 | unstable |
| Cs2CuSbBr6 | 0.5\*Cs3Sb2Br9+0.5\*CsCu2Br3 | 0.07451 | unstable |
| Rb2LiAlI6 | 1.0\*AlI3+1.0\*LiI+2.0\*RbI | 0.07486 | unstable |
| Rb2KAlBr6 | 1.0\*KBr+1.0\*RbAlBr4+1.0\*RbBr | 0.07488 | unstable |
| Cs2NaGaBr6 | 1.0\*CsBr+1.0\*CsGaBr4+1.0\*NaBr | 0.07522 | unstable |
| K2NaGaCl6 | 1.0\*KCl+1.0\*KGaCl4+1.0\*NaCl | 0.07594 | unstable |
| K2KAlCl6 | 1.0\*KAlCl4+2.0\*KCl | 0.07623 | unstable |
| Rb2NaInI6 | 1.0\*NaI+1.0\*RbI+1.0\*RbInI4 | 0.07628 | unstable |
| K2NaSbI6 | 2.0\*KI+1.0\*NaI+1.0\*SbI3 | 0.0766 | unstable |
| K2AgInI6 | 1.0\*AgI+1.0\*InI3+2.0\*KI | 0.07701 | unstable |
| Rb2CuSbBr6 | 0.5\*Rb3Sb2Br9+0.5\*RbCu2Br3 | 0.07702 | unstable |
| Cs2CuYCl6 | 0.5\*Cs3Y2Cl9+0.5\*CsCu2Cl3 | 0.07703 | unstable |
| Rb2CsSbCl6 | 0.333333\*Cs3Sb2Cl9+2.0\*RbCl+0.333333\*SbCl3 | 0.0772 | unstable |
| K2AgYF6 | 0.333333\*Ag2F+0.666667\*K2YF5+0.333333\*KAgF3+0.333333\*KYF4 | 0.07734 | unstable |
| Cs2LiAlBr6 | 1.0\*CsAlBr4+1.0\*CsBr+1.0\*LiBr | 0.07742 | unstable |
| Rb2CsSbF6 | 0.428571\*Cs2SbF5+0.142857\*CsRb2Sb4F15+1.714286\*RbF | 0.07788 | unstable |
| Rb2AgAlBr6 | 0.5\*AgBr+0.5\*Rb2AgBr3+1.0\*RbAlBr4 | 0.07789 | unstable |
| Cs2CsGaCl6 | 2.0\*CsCl+1.0\*CsGaCl4 | 0.07791 | unstable |
| Cs2CsInI6 | 2.0\*CsI+1.0\*CsInI4 | 0.07805 | unstable |
| Rb2AgInI6 | 0.5\*AgI+0.5\*Rb2AgI3+1.0\*RbInI4 | 0.07827 | unstable |
| Cs2AgAlBr6 | 0.5\*AgBr+0.5\*Cs2AgBr3+1.0\*CsAlBr4 | 0.07838 | unstable |
| Cs2CuInCl6 | 0.5\*Cs3In2Cl9+0.5\*CsCu2Cl3 | 0.07839 | unstable |
| Rb2CuYCl6 | 0.5\*Cu+0.4\*Rb3YCl6+0.5\*RbCuCl3+0.3\*RbY2Cl7 | 0.0785 | unstable |
| Cs2KGaBr6 | 1.0\*CsBr+1.0\*CsGaBr4+1.0\*KBr | 0.0787 | unstable |
| K2KInBr6 | 2.0\*KBr+1.0\*KInBr4 | 0.07901 | unstable |
| Cs2CuBiI6 | 0.5\*Cs3Bi2I9+0.166667\*Cs3Cu2I5+0.666666\*CuI | 0.07902 | unstable |
| Na2LiScF6 | 0.333333\*Na3Li3Sc2F12+0.333333\*Na3ScF6 | 0.07908 | unstable |
| Rb2KAlI6 | 1.0\*AlI3+1.0\*KI+2.0\*RbI | 0.07926 | unstable |
| Rb2CsBiBr6 | 0.333333\*Cs3Bi2Br9+0.333333\*Rb3BiBr6+1.0\*RbBr | 0.07927 | unstable |
| Cs2LiAlF6 | 1.0\*Cs2LiAlF6 | 0.07945 | unstable |
| Cs2CuInBr6 | 0.5\*Cs3In2Br9+0.5\*CsCu2Br3 | 0.07963 | unstable |
| Rb2CsScI6 | 0.333333\*Cs3Sc2I9+2.0\*RbI+0.333333\*ScI3 | 0.07977 | unstable |
| Cs2CsAlBr6 | 1.0\*CsAlBr4+2.0\*CsBr | 0.08057 | unstable |
| K2RbScBr6 | 0.166667\*K3Sc2Br9+1.5\*KBr+0.333333\*Rb3Sc2Br9 | 0.08082 | unstable |
| Rb2LiInI6 | 1.0\*LiI+1.0\*RbI+1.0\*RbInI4 | 0.08085 | unstable |
| K2LiGaCl6 | 1.0\*KCl+1.0\*KGaCl4+1.0\*LiCl | 0.08091 | unstable |
| K2RbInF6 | 0.5\*K3InF6+0.5\*KRb2InF6 | 0.08097 | unstable |
| K2CsScF6 | 0.333333\*Cs3ScF6+1.333333\*KF+0.666667\*KScF4 | 0.08141 | unstable |
| Rb2CsScBr6 | 0.333333\*Cs3Sc2Br9+0.166667\*Rb3Sc2Br9+1.5\*RbBr | 0.08158 | unstable |
| Rb2CuYBr6 | 0.5\*Rb3Y2Br9+0.5\*RbCu2Br3 | 0.08195 | unstable |
| Rb2CuInF6 | 0.5\*Cu+0.5\*Rb3In2F9+0.5\*RbCuF3 | 0.08252 | unstable |
| Rb2CsYCl6 | 0.5\*Cs2YCl5+0.5\*Rb3YCl6+0.5\*RbCl | 0.08268 | unstable |
| K2AgYI6 | 1.0\*AgI+2.0\*KI+1.0\*YI3 | 0.08311 | unstable |
| K2LiInI6 | 2.0\*KI+1.0\*LiInI4 | 0.08338 | unstable |
| Cs2LiGaI6 | 2.0\*CsI+1.0\*LiGaI4 | 0.08341 | unstable |
| Rb2AgAlI6 | 1.0\*AlI3+1.0\*Rb2AgI3 | 0.08346 | unstable |
| Cs2RbGaI6 | 2.0\*CsI+1.0\*GaI3+1.0\*RbI | 0.0838 | unstable |
| Rb2NaGaBr6 | 1.0\*NaBr+1.0\*RbBr+1.0\*RbGaBr4 | 0.08381 | unstable |
| Cs2AgGaBr6 | 0.5\*AgBr+0.5\*Cs2AgBr3+1.0\*CsGaBr4 | 0.08435 | unstable |
| Cs2LiGaCl6 | 1.0\*CsGaCl4+1.0\*CsLiCl2 | 0.08436 | unstable |
| K2CuScBr6 | 0.75\*CuBr+0.25\*K2CuBr3+0.5\*K3Sc2Br9 | 0.08439 | unstable |
| Rb2NaAlI6 | 1.0\*NaAlI4+2.0\*RbI | 0.08507 | unstable |
| Rb2RbSbI6 | 0.5\*Rb3Sb2I9+1.5\*RbI | 0.0854 | unstable |
| Rb2AgGaBr6 | 0.5\*AgBr+0.5\*Rb2AgBr3+1.0\*RbGaBr4 | 0.0855 | unstable |
| Cs2CuBiF6 | 0.111111\*BiF3+0.444444\*Cs3Bi2F9+0.166667\*Cs4Cu3F10+0.5\*Cu | 0.0858 | unstable |
| Rb2RbGaCl6 | 2.0\*RbCl+1.0\*RbGaCl4 | 0.08585 | unstable |
| Cs2CuYBr6 | 0.5\*Cs3Y2Br9+0.5\*CsCu2Br3 | 0.08612 | unstable |
| K2NaAlBr6 | 1.0\*KAlBr4+1.0\*KBr+1.0\*NaBr | 0.08662 | unstable |
| K2RbBiBr6 | 0.333333\*BiBr3+2.0\*KBr+0.333333\*Rb3Bi2Br9 | 0.08702 | unstable |
| Cs2AgSbF6 | 1.0\*Ag+0.5\*Cs2SbF5+0.5\*CsF+0.5\*CsSbF6 | 0.08711 | unstable |
| Cs2RbGaBr6 | 1.0\*CsBr+1.0\*CsGaBr4+1.0\*RbBr | 0.0874 | unstable |
| K2KYI6 | 3.0\*KI+1.0\*YI3 | 0.08747 | unstable |
| K2RbBiF6 | 1.0\*K2BiF5+1.0\*RbF | 0.08756 | unstable |
| K2KBiI6 | 1.0\*BiI3+3.0\*KI | 0.08796 | unstable |
| Rb2CsYI6 | 0.333333\*Cs3Y2I9+2.0\*RbI+0.333333\*YI3 | 0.0881 | unstable |
| Rb2RbAlBr6 | 1.0\*RbAlBr4+2.0\*RbBr | 0.08828 | unstable |
| K2RbSbCl6 | 1.0\*K2SbCl5+1.0\*RbCl | 0.08879 | unstable |
| Cs2LiSbF6 | 1.0\*Cs2SbF5+1.0\*LiF | 0.08911 | unstable |
| Cs2CuScCl6 | 0.5\*Cs3Sc2Cl9+0.5\*CsCu2Cl3 | 0.08997 | unstable |
| Rb2RbAlI6 | 1.0\*AlI3+3.0\*RbI | 0.09025 | unstable |
| K2KSbF6 | 1.0\*K2SbF5+1.0\*KF | 0.09116 | unstable |
| K2LiAlBr6 | 1.0\*KAlBr4+1.0\*KBr+1.0\*LiBr | 0.09131 | unstable |
| Rb2CuScBr6 | 0.5\*Rb3Sc2Br9+0.5\*RbCu2Br3 | 0.09165 | unstable |
| Rb2CsBiI6 | 0.333333\*Cs3Bi2I9+0.166667\*Rb3Bi2I9+1.5\*RbI | 0.09191 | unstable |
| Rb2CuBiI6 | 1.0\*CuI+0.5\*Rb3Bi2I9+0.5\*RbI | 0.09197 | unstable |
| K2CsInF6 | 0.166667\*Cs3In2F9+0.5\*CsF+0.666667\*K3InF6 | 0.09255 | unstable |
| Rb2LiGaBr6 | 1.0\*LiBr+1.0\*RbBr+1.0\*RbGaBr4 | 0.09309 | unstable |
| Rb2AgGaI6 | 1.0\*GaI3+1.0\*Rb2AgI3 | 0.0931 | unstable |
| Rb2KInI6 | 1.0\*KI+1.0\*RbI+1.0\*RbInI4 | 0.09324 | unstable |
| Cs2CuSbI6 | 0.166667\*Cs3Cu2I5+0.5\*Cs3Sb2I9+0.666666\*CuI | 0.09332 | unstable |
| K2RbYCl6 | 0.666667\*K3YCl6+0.333333\*Rb3YCl6 | 0.09372 | unstable |
| Cs2LiGaBr6 | 1.0\*CsBr+1.0\*CsGaBr4+1.0\*LiBr | 0.0944 | unstable |
| K2RbInBr6 | 1.0\*KBr+1.0\*KInBr4+1.0\*RbBr | 0.095 | unstable |
| Cs2CsGaI6 | 3.0\*CsI+1.0\*GaI3 | 0.09541 | unstable |
| K2NaInI6 | 2.0\*KI+1.0\*NaInI4 | 0.09648 | unstable |
| K2AgAlBr6 | 1.0\*AgBr+1.0\*KAlBr4+1.0\*KBr | 0.09663 | unstable |
| Rb2NaGaI6 | 1.0\*GaI3+1.0\*NaI+2.0\*RbI | 0.09684 | unstable |
| K2CuGaF6 | 0.5\*Cu+0.5\*K3Ga2F9+0.5\*KCuF3 | 0.097 | unstable |
| K2CuYCl6 | 1.0\*CuCl+1.0\*K2YCl5 | 0.09716 | unstable |
| Rb2KGaBr6 | 1.0\*KBr+1.0\*RbBr+1.0\*RbGaBr4 | 0.09819 | unstable |
| Rb2CsSbBr6 | 0.333333\*Cs3Sb2Br9+0.166667\*Rb3Sb2Br9+1.5\*RbBr | 0.09869 | unstable |
| Na2LiInF6 | 0.333333\*Na3InF6+0.333333\*Na3Li3In2F12 | 0.09895 | unstable |
| K2CuYBr6 | 1.0\*K2CuBr3+1.0\*YBr3 | 0.09981 | unstable |
| K2KInI6 | 1.0\*InI3+3.0\*KI | 0.09987 | unstable |