|  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | Material ID | Formula | Crystal System | Space Group Symbol | Space Group Number | Sites | Formation Energy | Volume | Density |
| 1 | mp-580931 | MgZn5 | Monoclinic | C2/m | 12 | 24 | -0.037 | 392.276 | 5.949 |
| 2 | mp-2313 | MgIn | Tetragonal | P4/mmm | 123 | 2 | -0.076 | 45.277 | 5.102 |
| 3 | mp-1249 | MgF2 | Tetragonal | P4\_2/mnm | 136 | 6 | -3.824 | 64.918 | 3.187 |
| 4 | mp-23710 | MgH2 | Tetragonal | P4\_2/mnm | 136 | 6 | -0.283 | 59.973 | 1.458 |
| 5 | mp-29771 | MgC2 | Tetragonal | P4\_2/mnm | 136 | 6 | 0.44 | 77.842 | 2.062 |
| 6 | mp-1061691 | MgNi2 | Tetragonal | I4/mmm | 139 | 3 | -0.032 | 38.464 | 6.117 |
| 7 | mp-11464 | MgHg2 | Tetragonal | I4/mmm | 139 | 3 | -0.109 | 65.439 | 10.797 |
| 8 | mp-12742 | MgPd3 | Tetragonal | I4/mmm | 139 | 8 | -0.489 | 121.994 | 9.353 |
| 9 | mp-13497 | Er2Mg | Tetragonal | I4/mmm | 139 | 3 | -0.018 | 84.751 | 7.031 |
| 10 | mp-13498 | Tb2Mg | Tetragonal | I4/mmm | 139 | 3 | -0.028 | 88.019 | 6.455 |
| 11 | mp-384 | MgP4 | Monoclinic | P2\_1/c | 14 | 10 | -0.298 | 196.771 | 2.501 |
| 12 | mp-1102064 | MgAl2 | Tetragonal | I4\_1/amd | 141 | 12 | 0.03 | 221.373 | 2.348 |
| 13 | mp-23205 | MgI2 | Trigonal | P-3m1 | 164 | 3 | -1.304 | 108.329 | 4.263 |
| 14 | mp-30034 | MgBr2 | Trigonal | P-3m1 | 164 | 3 | -1.854 | 82.498 | 3.706 |
| 15 | mp-570259 | MgCl2 | Trigonal | P-3m1 | 164 | 3 | -2.255 | 68.518 | 2.307 |
| 16 | mp-1061635 | MgNb2 | Trigonal | R-3m | 166 | 3 | 0.3 | 57.457 | 6.073 |
| 17 | mp-1061732 | MgZr2 | Trigonal | R-3m | 166 | 3 | 0.041 | 70.395 | 4.877 |
| 18 | mp-23210 | MgCl2 | Trigonal | R-3m | 166 | 3 | -2.255 | 69.504 | 2.275 |
| 19 | mp-1018040 | MgSe | Hexagonal | P6\_3mc | 186 | 4 | -1.474 | 105.2 | 3.26 |
| 20 | mp-1039 | MgTe | Hexagonal | P6\_3mc | 186 | 4 | -1.072 | 135.719 | 3.717 |
| 21 | mp-549706 | MgO | Hexagonal | P6\_3mc | 186 | 4 | -2.92 | 47.216 | 2.835 |
| 22 | mp-1009129 | MgO | Hexagonal | P-6m2 | 187 | 2 | -2.701 | 20.032 | 3.341 |
| 23 | mp-763 | MgB2 | Hexagonal | P6/mmm | 191 | 3 | -0.176 | 28.603 | 2.666 |
| 24 | mp-1124 | MgZn2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.131 | 192.827 | 5.343 |
| 25 | mp-11883 | MgIr2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.293 | 194.788 | 13.938 |
| 26 | mp-2675 | MgNi2 | Hexagonal | P6\_3/mmc | 194 | 24 | -0.21 | 306.11 | 6.149 |
| 27 | mp-30491 | MgCd3 | Hexagonal | P6\_3/mmc | 194 | 8 | -0.034 | 168.544 | 7.124 |
| 28 | mp-30651 | MgGa2 | Hexagonal | P6\_3/mmc | 194 | 6 | -0.115 | 110.225 | 4.934 |
| 29 | mp-864931 | MgCo2 | Hexagonal | P6\_3/mmc | 194 | 12 | 0.018 | 157.306 | 6.003 |
| 30 | mp-12651 | MgPt | Cubic | P2\_13 | 198 | 8 | -0.696 | 128.196 | 11.367 |
| 31 | mp-1103590 | MgSe2 | Cubic | Pa-3 | 205 | 12 | -1.133 | 269.586 | 4.49 |
| 32 | mp-1746 | MgF2 | Cubic | Pa-3 | 205 | 12 | -3.758 | 125.928 | 3.286 |
| 33 | mp-2589 | MgO2 | Cubic | Pa-3 | 205 | 12 | -2.011 | 112.582 | 3.322 |
| 34 | mp-2604 | MgTe2 | Cubic | Pa-3 | 205 | 12 | -0.849 | 356.016 | 5.215 |
| 35 | mp-1062 | CeMg | Cubic | Pm-3m | 221 | 2 | 0.069 | 56.567 | 4.827 |
| 36 | mp-1063661 | MgNi3 | Cubic | Pm-3m | 221 | 4 | -0.064 | 48.335 | 6.884 |
| 37 | mp-1104 | LaMg | Cubic | Pm-3m | 221 | 2 | -0.095 | 62.927 | 4.307 |
| 38 | mp-11498 | MgTl | Cubic | Pm-3m | 221 | 2 | -0.017 | 48.141 | 7.888 |
| 39 | mp-1172 | MgRh | Cubic | Pm-3m | 221 | 2 | -0.45 | 29.414 | 7.182 |
| 40 | mp-1174 | MgSc | Cubic | Pm-3m | 221 | 2 | -0.025 | 46.518 | 2.472 |
| 41 | mp-1199 | HoMg | Cubic | Pm-3m | 221 | 2 | -0.051 | 53.7 | 5.852 |
| 42 | mp-1327 | NdMg | Cubic | Pm-3m | 221 | 2 | -0.094 | 58.931 | 4.749 |
| 43 | mp-1408 | MgHg | Cubic | Pm-3m | 221 | 2 | -0.197 | 40.959 | 9.118 |
| 44 | mp-1505 | TmMg | Cubic | Pm-3m | 221 | 2 | -0.075 | 52.607 | 6.1 |
| 45 | mp-1548 | PrMg | Cubic | Pm-3m | 221 | 2 | -0.09 | 60.166 | 4.56 |
| 46 | mp-1635 | TbMg | Cubic | Pm-3m | 221 | 2 | -0.069 | 54.823 | 5.55 |
| 47 | mp-20566 | MgIn3 | Cubic | Pm-3m | 221 | 4 | 0 | 96.6 | 6.339 |
| 48 | mp-2077 | DyMg | Cubic | Pm-3m | 221 | 2 | -0.059 | 54.134 | 5.73 |
| 49 | mp-2195 | LuMg | Cubic | Pm-3m | 221 | 2 | -0.031 | 51.293 | 6.451 |
| 50 | mp-2228 | ErMg | Cubic | Pm-3m | 221 | 2 | -0.052 | 53.18 | 5.982 |
| 51 | mp-2558 | SmMg | Cubic | Pm-3m | 221 | 2 | -0.085 | 57.184 | 5.072 |
| 52 | mp-2564 | SrMg | Cubic | Pm-3m | 221 | 2 | -0.021 | 73.577 | 2.526 |
| 53 | mp-2636 | GdMg | Cubic | Pm-3m | 221 | 2 | -0.079 | 56.21 | 5.363 |
| 54 | mp-2696 | MgAg | Cubic | Pm-3m | 221 | 2 | -0.23 | 36.066 | 6.086 |
| 55 | mp-30351 | MgAg3 | Cubic | Pm-3m | 221 | 4 | -0.136 | 69.852 | 8.271 |
| 56 | mp-437 | MgAu | Cubic | Pm-3m | 221 | 2 | -0.592 | 35.079 | 10.474 |
| 57 | mp-506 | MgPd | Cubic | Pm-3m | 221 | 2 | -0.727 | 31.416 | 6.91 |
| 58 | mp-615 | YMg | Cubic | Pm-3m | 221 | 2 | -0.074 | 55.244 | 3.403 |
| 59 | mp-7753 | MgPd3 | Cubic | Pm-3m | 221 | 4 | -0.477 | 60.978 | 9.356 |
| 60 | mp-10760 | MgSe | Cubic | Fm-3m | 225 | 2 | -1.464 | 40.86 | 4.197 |
| 61 | mp-1265 | MgO | Cubic | Fm-3m | 225 | 2 | -3.038 | 18.443 | 3.629 |
| 62 | mp-1315 | MgS | Cubic | Fm-3m | 225 | 2 | -1.662 | 35.331 | 2.649 |
| 63 | mp-21152 | Pu2Mg | Cubic | Fm-3m | 225 | 3 | 0.692 | 97.577 | 8.718 |
| 64 | mp-855 | MgBe13 | Cubic | Fm-3c | 226 | 28 | 0.001 | 257.356 | 1.826 |
| 65 | mp-1038 | MgCu2 | Cubic | Fd-3m | 227 | 6 | -0.124 | 84.373 | 5.959 |
| 66 | mp-1077016 | MgIn2 | Cubic | Fd-3m | 227 | 6 | 0.139 | 163.139 | 5.17 |
| 67 | mp-542488 | MgCo | Cubic | Fd-3m | 227 | 24 | 0.028 | 365.889 | 4.533 |
| 68 | mp-569051 | MgH2 | Orthorhombic | Pca2\_1 | 29 | 12 | -0.239 | 107.08 | 1.633 |
| 69 | mp-11307 | MgCd | Orthorhombic | Pmma | 51 | 4 | -0.095 | 83.611 | 5.43 |
| 70 | mp-567539 | MgGa2 | Orthorhombic | Pbam | 55 | 24 | -0.103 | 443.073 | 4.91 |
| 71 | mp-1072956 | MgF2 | Orthorhombic | Pnnm | 58 | 6 | -3.822 | 67.997 | 3.043 |
| 72 | mp-23711 | MgH2 | Orthorhombic | Pbcn | 60 | 12 | -0.281 | 118.246 | 1.479 |
| 73 | mp-568441 | MgH2 | Orthorhombic | Pbca | 61 | 24 | -0.237 | 214.007 | 1.634 |
| 74 | mp-12741 | MgPd2 | Orthorhombic | Pnma | 62 | 12 | -0.597 | 183.744 | 8.573 |
| 75 | mp-23712 | MgH2 | Orthorhombic | Pnma | 62 | 12 | -0.201 | 98.965 | 1.767 |
| 76 | mp-365 | MgB4 | Orthorhombic | Pnma | 62 | 20 | -0.173 | 177.513 | 2.528 |
| 77 | mp-30408 | MgAu3 | Orthorhombic | Cmcm | 63 | 32 | -0.398 | 552.409 | 14.794 |
| 78 | mp-567626 | MgZn2 | Orthorhombic | Cmcm | 63 | 6 | 0.015 | 106.198 | 4.851 |
| 79 | mp-683946 | MgIr | Orthorhombic | Cmce | 64 | 152 | -0.361 | 2561.028 | 10.67 |
| 80 | mp-978275 | MgB7 | Orthorhombic | Imma | 74 | 32 | -0.158 | 251.905 | 2.636 |
| 81 | mp-1078930 | MgN8 | Tetragonal | I4/m | 87 | 9 | 1.222 | 172.49 | 1.313 |
| 82 | mp-574266 | MgGa | Tetragonal | I4\_1/a | 88 | 32 | -0.133 | 605.629 | 4.125 |
| 83 | mp-7623 | MgAs4 | Tetragonal | P4\_12\_12 | 92 | 20 | -0.305 | 469.74 | 4.581 |
| 84 | mp-12693 | Mg2Rh | Tetragonal | I4/mmm | 139 | 3 | -0.402 | 50.851 | 4.948 |
| 85 | mp-27668 | Mg2Ga5 | Tetragonal | I4/mmm | 139 | 14 | -0.116 | 259.549 | 5.083 |
| 86 | mp-13208 | Mg2Pt | Tetragonal | I4/mcm | 140 | 6 | -0.688 | 111.903 | 7.232 |
| 87 | mp-2137 | Mg2Ni | Hexagonal | P6\_222 | 180 | 18 | -0.153 | 300.366 | 3.559 |
| 88 | mp-31326 | Mg2In | Hexagonal | P-62m | 189 | 9 | -0.051 | 202.52 | 4.02 |
| 89 | mp-567244 | Mg2Tl | Hexagonal | P-62m | 189 | 9 | -0.001 | 207.811 | 6.065 |
| 90 | mp-30650 | Mg2Ga | Hexagonal | P-62c | 190 | 18 | -0.117 | 353.791 | 3.332 |
| 91 | mp-1095697 | LaMg2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.078 | 338.948 | 3.675 |
| 92 | mp-1101792 | EuMg2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.086 | 352.363 | 3.781 |
| 93 | mp-1102767 | CeMg2 | Hexagonal | P6\_3/mmc | 194 | 12 | 0.047 | 366.433 | 3.421 |
| 94 | mp-11497 | TbMg2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.046 | 310.617 | 4.438 |
| 95 | mp-11499 | YMg2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.052 | 312.009 | 2.927 |
| 96 | mp-13499 | HoMg2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.033 | 305.202 | 4.647 |
| 97 | mp-1935 | BaMg2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.052 | 404.629 | 3.052 |
| 98 | mp-2214 | TmMg2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.061 | 299.918 | 4.818 |
| 99 | mp-2432 | CaMg2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.086 | 337.903 | 1.743 |
| 100 | mp-2572 | SrMg2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.09 | 375.214 | 2.412 |
| 101 | mp-30602 | DyMg2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.038 | 307.721 | 4.557 |
| 102 | mp-30607 | ErMg2 | Hexagonal | P6\_3/mmc | 194 | 12 | -0.033 | 302.354 | 4.742 |
| 103 | mp-570571 | ThMg2 | Hexagonal | P6\_3/mmc | 194 | 24 | 0.041 | 623.484 | 5.98 |
| 104 | mp-30784 | Mg2Zn11 | Cubic | Pm-3 | 200 | 39 | -0.062 | 595.185 | 6.429 |
| 105 | mp-1367 | Mg2Si | Cubic | Fm-3m | 225 | 3 | -0.109 | 63.699 | 1.999 |
| 106 | mp-20724 | Mg2Pb | Cubic | Fm-3m | 225 | 3 | -0.036 | 79.588 | 5.337 |
| 107 | mp-2343 | Mg2Sn | Cubic | Fm-3m | 225 | 3 | -0.167 | 77.239 | 3.597 |
| 108 | mp-408 | Mg2Ge | Cubic | Fm-3m | 225 | 3 | -0.344 | 64.576 | 3.118 |
| 109 | mp-18316 | Mg2Pd | Cubic | Fd-3m | 227 | 24 | -0.508 | 434.248 | 4.743 |
| 110 | mp-1909 | LaMg2 | Cubic | Fd-3m | 227 | 6 | -0.104 | 169.418 | 3.676 |
| 111 | mp-21049 | GdMg2 | Cubic | Fd-3m | 227 | 6 | -0.096 | 159.395 | 4.289 |
| 112 | mp-21419 | CeMg2 | Cubic | Fd-3m | 227 | 6 | -0.005 | 160.413 | 3.907 |
| 113 | mp-2389 | NdMg2 | Cubic | Fd-3m | 227 | 6 | -0.081 | 162.656 | 3.938 |
| 114 | mp-250 | Mg2Ge | Cubic | Fd-3m | 227 | 6 | 0.139 | 130.613 | 3.083 |
| 115 | mp-30775 | PrMg2 | Cubic | Fd-3m | 227 | 6 | -0.083 | 164.673 | 3.822 |
| 116 | mp-529 | SmMg2 | Cubic | Fd-3m | 227 | 6 | -0.067 | 159.45 | 4.144 |
| 117 | mp-570543 | Mg2Sn | Cubic | Fd-3m | 227 | 6 | 0.053 | 145.457 | 3.82 |
| 118 | mp-570657 | Mg2Si | Cubic | Fd-3m | 227 | 6 | 0.474 | 123.417 | 2.064 |
| 119 | mp-745 | ThMg2 | Cubic | Fd-3m | 227 | 6 | 0.028 | 156.422 | 5.959 |
| 120 | mp-28793 | Mg2C3 | Orthorhombic | Pnnm | 58 | 10 | 0.184 | 127.68 | 2.202 |
| 121 | mp-1102915 | Mg2Pb | Orthorhombic | Pnma | 62 | 12 | 0.028 | 295.797 | 5.744 |
| 122 | mp-11250 | Mg2Au | Orthorhombic | Pnma | 62 | 12 | -0.481 | 228.519 | 7.138 |
| 123 | mp-30719 | Mg2Hg | Orthorhombic | Pnma | 62 | 12 | -0.173 | 250.213 | 6.615 |
| 124 | mp-1077234 | Mg2Ru | Orthorhombic | Cmcm | 63 | 6 | 0.141 | 123.306 | 4.031 |
| 125 | mp-2481 | Mg2Cu | Orthorhombic | Fddd | 70 | 12 | -0.087 | 211.918 | 3.515 |
| 126 | mp-1101861 | Mg2Ni | Monoclinic | Cc | 9 | 12 | 0.072 | 226.189 | 3.151 |
| 127 | mp-1079919 | Mg3Mn | Monoclinic | P2\_1/m | 11 | 8 | 0.416 | 188.302 | 2.255 |
| 128 | mp-569103 | Mg3Hg | Trigonal | R32 | 155 | 24 | -0.105 | 516.143 | 5.28 |
| 129 | mp-2646 | Mg3Sb2 | Trigonal | P-3m1 | 164 | 5 | -0.421 | 131.179 | 4.006 |
| 130 | mp-569018 | Mg3Bi2 | Trigonal | P-3m1 | 164 | 5 | -0.179 | 140.255 | 5.812 |
| 131 | mp-1557 | Mg3Au | Trigonal | P-3c1 | 165 | 24 | -0.392 | 465.404 | 5.778 |
| 132 | mp-697180 | Mg3In | Trigonal | R-3m | 166 | 16 | -0.074 | 354.115 | 3.521 |
| 133 | mp-642855 | Mg3Ge | Hexagonal | P6\_3/m | 176 | 8 | -0.116 | 178.03 | 2.715 |
| 134 | mp-643067 | Mg3Sn | Hexagonal | P6\_3/m | 176 | 24 | -0.089 | 548.386 | 3.481 |
| 135 | mp-17783 | Mg3Au | Hexagonal | P6\_3cm | 185 | 24 | -0.393 | 474.947 | 5.661 |
| 136 | mp-18707 | Mg3Pt | Hexagonal | P6\_3cm | 185 | 24 | -0.562 | 449.888 | 5.935 |
| 137 | mp-18712 | Mg3Pd | Hexagonal | P6\_3cm | 185 | 24 | -0.399 | 459.865 | 3.885 |
| 138 | mp-542429 | Mg3Rh | Hexagonal | P6\_3cm | 185 | 24 | -0.33 | 441.708 | 3.966 |
| 139 | mp-568419 | Mg3Ir | Hexagonal | P6\_3cm | 185 | 24 | -0.321 | 436.996 | 6.045 |
| 140 | mp-1078964 | Mg3Au | Hexagonal | P6\_3/mmc | 194 | 8 | -0.376 | 159.672 | 5.613 |
| 141 | mp-1079072 | Mg3In | Hexagonal | P6\_3/mmc | 194 | 8 | -0.073 | 176.431 | 3.534 |
| 142 | mp-1079229 | Mg3Pd | Hexagonal | P6\_3/mmc | 194 | 8 | -0.376 | 154.505 | 3.855 |
| 143 | mp-11251 | Mg3Au | Hexagonal | P6\_3/mmc | 194 | 8 | -0.177 | 176.938 | 5.066 |
| 144 | mp-30490 | Mg3Cd | Hexagonal | P6\_3/mmc | 194 | 8 | -0.051 | 170.053 | 3.619 |
| 145 | mp-30739 | Mg3Ir | Hexagonal | P6\_3/mmc | 194 | 8 | -0.307 | 146.235 | 6.021 |
| 146 | mp-569265 | Mg3Pt | Hexagonal | P6\_3/mmc | 194 | 8 | -0.543 | 151.114 | 5.89 |
| 147 | mp-731 | Mg3Hg | Hexagonal | P6\_3/mmc | 194 | 8 | -0.115 | 173.221 | 5.244 |
| 148 | mp-1559 | Mg3N2 | Cubic | Ia-3 | 206 | 40 | -0.942 | 489.827 | 2.737 |
| 149 | mp-1990 | Mg3As2 | Cubic | Ia-3 | 206 | 40 | -0.788 | 944.615 | 3.133 |
| 150 | mp-2514 | Mg3P2 | Cubic | Ia-3 | 206 | 40 | -0.648 | 866.292 | 2.068 |
| 151 | mp-625 | Mg3Ru2 | Cubic | P4\_132 | 213 | 20 | -0.125 | 329.274 | 5.548 |
| 152 | mp-569125 | Mg3In | Cubic | Pm-3m | 221 | 4 | -0.058 | 88.551 | 3.52 |
| 153 | mp-7844 | Mg3As2 | Cubic | Pn-3m | 224 | 10 | -0.622 | 240.59 | 3.075 |
| 154 | mp-8085 | Mg3P2 | Cubic | Pn-3m | 224 | 10 | -0.461 | 218.649 | 2.048 |
| 155 | mp-1546 | DyMg3 | Cubic | Fm-3m | 225 | 4 | -0.049 | 96.219 | 4.063 |
| 156 | mp-1787 | NdMg3 | Cubic | Fm-3m | 225 | 4 | -0.102 | 100.859 | 3.575 |
| 157 | mp-1798 | CeMg3 | Cubic | Fm-3m | 225 | 4 | -0.055 | 100.275 | 3.528 |
| 158 | mp-20534 | GdMg3 | Cubic | Fm-3m | 225 | 4 | -0.067 | 98.352 | 3.886 |
| 159 | mp-2306 | LaMg3 | Cubic | Fm-3m | 225 | 8 | -0.11 | 208.894 | 3.368 |
| 160 | mp-30779 | SmMg3 | Cubic | Fm-3m | 225 | 4 | -0.083 | 99.263 | 3.735 |
| 161 | mp-428 | PrMg3 | Cubic | Fm-3m | 225 | 4 | -0.1 | 101.933 | 3.483 |
| 162 | mp-7381 | TbMg3 | Cubic | Fm-3m | 225 | 4 | -0.056 | 96.838 | 3.976 |
| 163 | mp-1180365 | Mg3Cr | Orthorhombic | Pnma | 62 | 16 | 0.363 | 354.663 | 2.339 |
| 164 | mp-2047263 | Mg4Zn7 | Monoclinic | C2/m | 12 | 55 | -0.146 | 894.017 | 5.155 |
| 165 | mp-567526 | SrMg4 | Hexagonal | P6\_3/mmc | 194 | 90 | -0.026 | 2646.81 | 2.087 |
| 166 | mp-568306 | Mg5Si6 | Monoclinic | C2/m | 12 | 11 | 0.079 | 197.514 | 2.438 |
| 167 | mp-11465 | Mg5Hg3 | Hexagonal | P6\_3/mcm | 193 | 16 | -0.197 | 344.003 | 6.983 |
| 168 | mp-1198512 | EuMg5 | Hexagonal | P6\_3/mmc | 194 | 36 | 0.027 | 1038.723 | 2.623 |
| 169 | mp-2406 | Mg5Pd2 | Hexagonal | P6\_3/mmc | 194 | 28 | -0.451 | 527.361 | 4.211 |
| 170 | mp-30778 | Mg5Rh2 | Hexagonal | P6\_3/mmc | 194 | 28 | -0.361 | 504.728 | 4.308 |
| 171 | mp-1770 | Mg5Ga2 | Orthorhombic | Ibam | 72 | 14 | -0.107 | 281.309 | 3.081 |
| 172 | mp-22570 | Mg5In2 | Orthorhombic | Ibam | 72 | 14 | -0.049 | 319.138 | 3.654 |
| 173 | mp-570849 | Mg5Tl2 | Orthorhombic | Ibam | 72 | 14 | -0.006 | 319.778 | 5.507 |
| 174 | mp-1078138 | Mg6V | Cubic | Fm-3m | 225 | 7 | 0.271 | 162.676 | 2.009 |
| 175 | mp-1078548 | Mg7Ti | Cubic | Fm-3m | 225 | 8 | 0.112 | 175.006 | 2.069 |
| 176 | mp-31503 | Mg9Sn5 | Trigonal | R3 | 146 | 28 | -0.156 | 669.012 | 4.032 |
| 177 | mp-542854 | Mg9Si5 | Hexagonal | P6\_3/m | 176 | 28 | -0.064 | 541.951 | 2.201 |
| 178 | mp-1103919 | CeMg12 | Tetragonal | I4/mmm | 139 | 13 | -0.035 | 310.046 | 2.313 |
| 179 | mp-30772 | NdMg12 | Tetragonal | I4/mmm | 139 | 13 | -0.006 | 308.636 | 2.345 |
| 180 | mp-30776 | PrMg12 | Tetragonal | I4/mmm | 139 | 13 | -0.01 | 309.693 | 2.319 |
| 181 | mp-16860 | Mg13Ir3 | Trigonal | R-3c | 167 | 32 | -0.232 | 619.351 | 4.786 |
| 182 | mp-30407 | Mg13Au41 | Hexagonal | P6\_3/mcm | 193 | 108 | -0.386 | 1933.798 | 14.412 |
| 183 | mp-1194114 | Mg13Al16 | Cubic | I-43m | 217 | 29 | 0.033 | 566.238 | 2.193 |
| 184 | mp-12766 | Mg13Al14 | Cubic | Im-3m | 229 | 27 | 0.079 | 530.186 | 2.173 |
| 185 | mp-1813 | Ba2Mg17 | Trigonal | R-3m | 166 | 19 | -0.03 | 503.248 | 2.27 |
| 186 | mp-1116 | Sr2Mg17 | Hexagonal | P6\_3/mmc | 194 | 38 | -0.04 | 974.354 | 2.006 |
| 187 | mp-30752 | La2Mg17 | Hexagonal | P6\_3/mmc | 194 | 38 | -0.034 | 934.911 | 2.455 |
| 188 | mp-680564 | Ce2Mg17 | Hexagonal | P6\_3/mmc | 194 | 38 | -0.005 | 936.589 | 2.459 |
| 189 | mp-2151 | Mg17Al12 | Cubic | I-43m | 217 | 29 | -0.009 | 568.369 | 2.153 |
| 190 | mp-570025 | Mg21Zn25 | Trigonal | R-3c | 167 | 92 | -0.115 | 1634.633 | 4.359 |
| 191 | mp-17659 | Mg23Al30 | Trigonal | R-3 | 148 | 53 | -0.01 | 1023.462 | 2.22 |
| 192 | mp-30782 | Sr6Mg23 | Cubic | Fm-3m | 225 | 29 | -0.07 | 820.691 | 2.195 |
| 193 | mp-568512 | Ba6Mg23 | Cubic | Fm-3m | 225 | 29 | -0.05 | 876.896 | 2.619 |
| 194 | mp-570442 | Th6Mg23 | Cubic | Fm-3m | 225 | 29 | 0.029 | 727.665 | 4.453 |
| 195 | mp-1192487 | Ho5Mg24 | Cubic | I-43m | 217 | 29 | -0.008 | 701.012 | 3.335 |
| 196 | mp-1192763 | Tb5Mg24 | Cubic | I-43m | 217 | 29 | -0.017 | 709.049 | 3.227 |
| 197 | mp-1192842 | Lu5Mg24 | Cubic | I-43m | 217 | 29 | 0.004 | 687.326 | 3.523 |
| 198 | mp-1988 | Y5Mg24 | Cubic | I-43m | 217 | 29 | -0.022 | 709.32 | 2.406 |
| 199 | mp-1993 | Tm5Mg24 | Cubic | I-43m | 217 | 29 | -0.033 | 693.978 | 3.417 |
| 200 | mp-2218 | Er5Mg24 | Cubic | I-43m | 217 | 29 | -0.01 | 696.524 | 3.384 |
| 201 | mp-672670 | Dy5Mg24 | Cubic | I-43m | 217 | 29 | -0.012 | 704.75 | 3.289 |
| 202 | mp-31499 | Mg29Ir4 | Cubic | F-43m | 216 | 99 | -0.164 | 1965.366 | 3.735 |
| 203 | mp-30783 | Sr9Mg38 | Hexagonal | P6\_3/mmc | 194 | 94 | -0.06 | 2673.121 | 2.127 |
| 204 | mp-568106 | Mg41Al67 | Cubic | Pm-3m | 221 | 108 | 0.04 | 2023.085 | 2.302 |
| 205 | mp-1197847 | Pr5Mg41 | Tetragonal | I4/m | 87 | 46 | -0.033 | 1137.414 | 2.483 |
| 206 | mp-1199923 | Nd5Mg41 | Tetragonal | I4/m | 87 | 46 | -0.029 | 1128.557 | 2.527 |
| 207 | mp-1201293 | Sm5Mg41 | Tetragonal | I4/m | 87 | 46 | -0.019 | 1113.688 | 2.607 |
| 208 | mp-680586 | Ce5Mg41 | Tetragonal | I4/m | 87 | 46 | -0.028 | 1147.209 | 2.456 |
| 209 | mp-569273 | Mg44Ir7 | Cubic | F-43m | 216 | 102 | -0.187 | 1984.746 | 4.041 |
| 210 | mp-570153 | Mg44Rh7 | Cubic | F-43m | 216 | 102 | -0.197 | 2052.797 | 2.896 |
| 211 | mp-678 | Mg54Ag17 | Orthorhombic | Immm | 71 | 71 | -0.11 | 1482.248 | 3.525 |
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| 1 | mp-1023506 | Mg15Al | Hexagonal | P-6m2 | 187 | 16 | 0.04 | 351.543 | 1.85 |
| 2 | mp-1094685 | Mg16Al13 | Monoclinic | Cm | 8 | 29 | -0.006 | 577.888 | 2.125 |
| 3 | mp-1094700 | Mg18Al11 | Monoclinic | Cm | 8 | 29 | 0.003 | 591.169 | 2.063 |
| 4 | mp-1210739 | Mg2Al3 | Tetragonal | I4\_1/amd | 141 | 20 | 0.106 | 399.051 | 2.156 |
| 5 | mp-978271 | Mg3Al | Cubic | Pm-3m | 221 | 4 | 0.022 | 82.188 | 2.018 |
| 6 | mp-1016271 | Mg7Al | Hexagonal | P-6m2 | 187 | 8 | 0.041 | 172.075 | 1.902 |
| 7 | mp-1039141 | MgAl | Tetragonal | P4/mmm | 123 | 2 | 0.014 | 37.591 | 2.266 |
| 8 | mp-1038916 | MgAl3 | Tetragonal | I4/mmm | 139 | 4 | 0.016 | 68.958 | 2.534 |
| 9 | mp-1094177 | La2Mg | Monoclinic | C2/m | 12 | 6 | -0.033 | 198.74 | 5.049 |
| 10 | mp-1094855 | La3Mg | Cubic | Pm-3m | 221 | 4 | -0.007 | 135.725 | 5.396 |
| 11 | mp-1222990 | La4Mg | Tetragonal | I4/mmm | 139 | 5 | -0.018 | 173.192 | 5.56 |
| 12 | mp-1094178 | La5Mg | Monoclinic | Cm | 8 | 6 | 0.013 | 209.867 | 5.688 |
| 13 | mp-1211590 | La5Mg41 | Tetragonal | I4/m | 87 | 46 | -0.042 | 1146.082 | 2.45 |
| 14 | mp-1104815 | LaMg12 | Tetragonal | I4/mmm | 139 | 13 | -0.02 | 312.567 | 2.287 |
| 15 | mp-1023560 | LaMg15 | Hexagonal | P-6m2 | 187 | 16 | 0.045 | 390.121 | 2.143 |
| 16 | mp-1094186 | LaMg5 | Monoclinic | Cm | 8 | 6 | 0.037 | 155.797 | 2.776 |
| 17 | mp-1016316 | LaMg7 | Hexagonal | P-6m2 | 187 | 8 | 0.046 | 206.27 | 2.488 |