Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

# Supplementary Information (SI) for Prediction of ultraviolet optical materials in the $K_2O$-$B_2O_3$ system

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# Supplementary Discussion

**Impact of temperature and pressure on phase stability.**

As demonstrated by many precious studies, temperature has been found to play an important role in stabilizing structures that are metastable at 0 K. For instance, *oP*112-1-$KB_5O_8$ is stable at 0 K [1], while o*P*112-2-$KB_5O_8$ is a metastable phase at 0 K. Previous experimental research has shown that o*P*112-2-$KB_5O_8$ can be synthesized at 760 °C, indicating its stability as a high-temperature phase [1]. Thus, for the newly predicted structures, particularly those that are metastable, synthesizing at elevated temperature presents a promising approach to realizing them in practice.

To clarify the impact of pressure on the stability of these structures, we have further calculated the thermodynamic convex hull at 3 GPa (Fig. S1). The metastable structures observed at 0 GPa, namely *mP*28-2-$K_3BO_3$, *mC*72-$KB_3O_5$, *oP*112-2-$KB_5O_8$, become thermodynamically stable at 3 GPa, suggesting that pressure enhances the stability of these structures. Notably, *mC*72-$KB_3O_5$ has been successfully synthesized at 3 GPa and 600 °C in experiments and is recognized as a high-pressure phase in the literature [2-3], underscoring the reliability of our results. Therefore, considering the effects of temperature and pressure on phase stability, it is plausible that metastable phases in the $K_2O$-$B_2O_3$ system could be synthesized experimentally.

**Nonlinear optical response.**

The general expression for the nonlinear optical susceptibility depends on the frequency of E(ω). The second-order susceptibility tensor $\chi^{(2)}_{ijk}$ (-2ω; ω, ω) is commonly represented as $\chi^{(2)}_{ijk}$(ω). Since that *hR*21-$K_3BO_3$ belongs to the 3m point group, the non-zero components of the susceptibility tensor are: $\chi^{(2)}_{112}$(ω), $\chi^{(2)}_{131}$(ω), $\chi^{(2)}_{211}$(ω), $\chi^{(2)}_{222}$(ω), $\chi^{(2)}_{223}$(ω), $\chi^{(2)}_{311}$(ω), $\chi^{(2)}_{322}$(ω), and $\chi^{(2)}_{333}$(ω) (1, 2, and 3 refer to the *x*, *y* and *z* axes, respectively). Figs. S5a and S5b illustrate the real and imaginary parts of these eight second-order susceptibility components [4-5]. The trends of $\chi^{(2)}_{113}$ (ω), $\chi^{(2)}_{311}$ (ω), $\chi^{(2)}_{322}$ (ω), and $\chi^{(2)}_{223}$ (ω) are nearly coincident, while $\chi^{(2)}_{112}$ (ω) and $\chi^{(2)}_{211}$ (ω) exhibit identical trends. Therefore, we have analyzed the intraband and interband contributions to $\chi^{(2)}_{222}(\omega)$, $\chi^{(2)}_{333}(\omega)$, $\chi^{(2)}_{223}(\omega)$and $\chi^{(2)}_{112}(\omega)$ (Figs. S5c-f). Among these, $\chi^{(2)}_{222}(\omega)$ and $\chi^{(2)}_{112}(\omega)$ have equal magnitudes but opposite signs, and they are the principal components of SHG.

Within the energy range of 0 to 2.3 eV, the real part changes slowly, and the imaginary part is zero, indicating that $\chi^{(2)}_{ijk}(\omega)$ is purely dispersive. Importantly, the 2ω terms dominate in the low energy regions, while high energy states exhibit mixed ω and 2ω terms. This distinction between ω and 2ω patterns highlights the relatively strong birefringence nature of *hR*21-$K_3BO_3$.

In addition, comparing the total contribution with the intraband and interband contributions, we find that the overall value of the second harmonic generation is very small due to the cancellation of intraband and interband components, which have values of opposite signs. Therefore, 2ω terms start contributing at an energy of Eg/2, while the ω terms begin contributing at energy above Eg. Consequently, any anisotropy in the linear optical properties is more significantly enhanced in the nonlinear spectra.

## Supplementary Figures

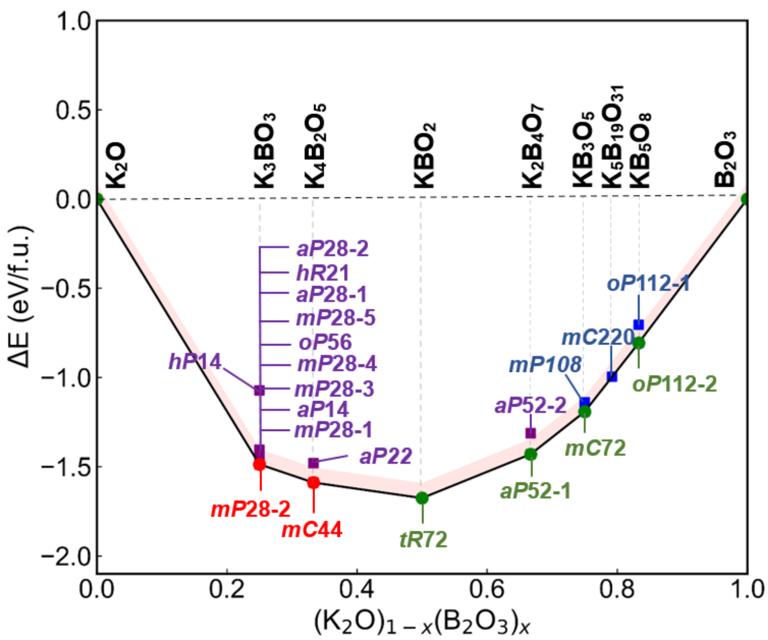
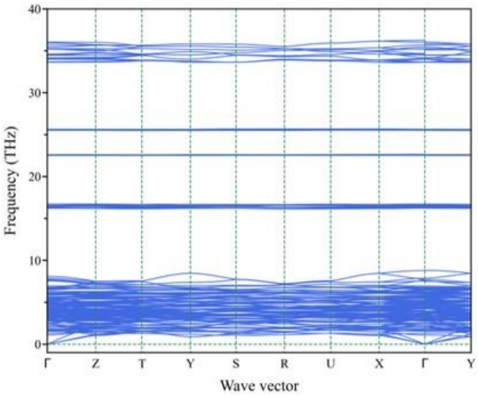
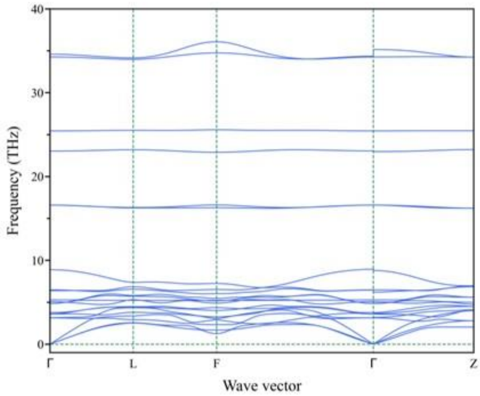



Figure S1. Thermodynamic convex hull of the $K_2O$-$B_2O_3$ system at 0 K and 3 GPa. Thermodynamically stable structures are denoted by red and green dots. Metastable structures are represented by purple and blue squares.

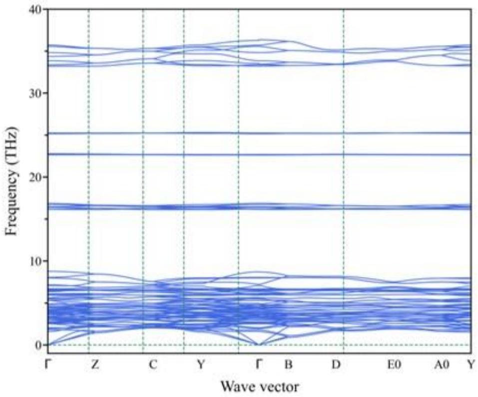
Phonon dispersion curves of $oP56$-$K_3BO_3$



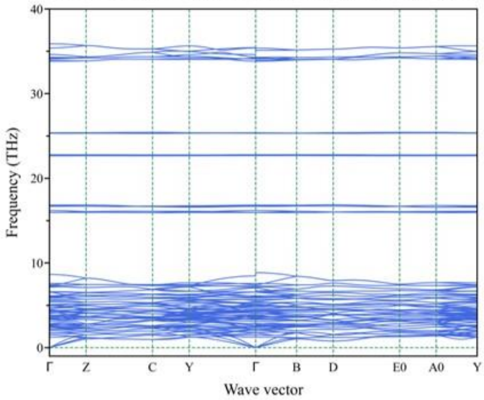

Phonon dispersion curves of $hR21$-$K_3BO_3$



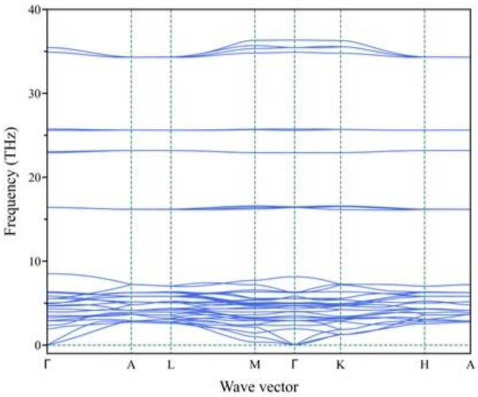

Phonon dispersion curves of $mP28$-1-$K_3BO_3$



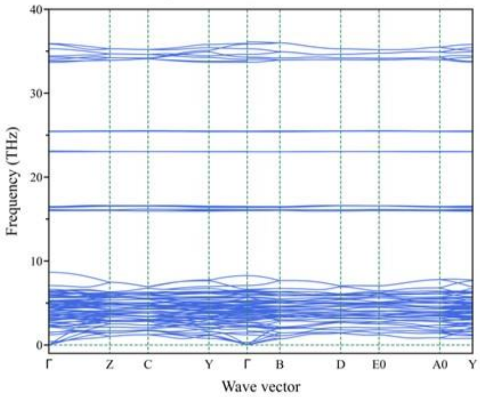

Phonon dispersion curves of $mP28$-2-$K_3BO_3$



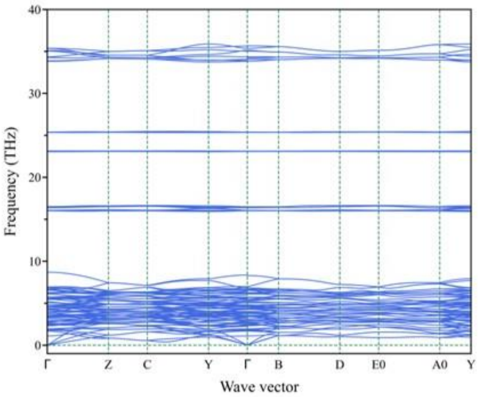

Phonon dispersion curves of $hP14$-$K_3BO_3$



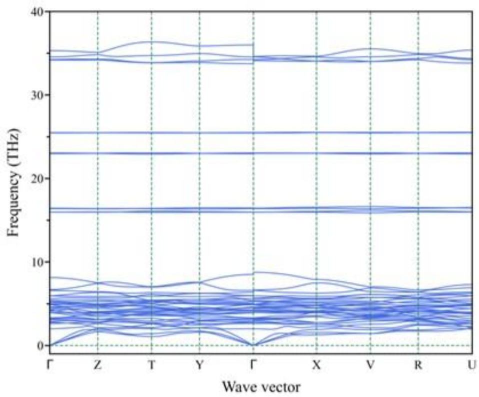

Phonon dispersion curves of $mP28$-3-$K_3BO_3$




Phonon dispersion curves of $mP28$-4-$K_3BO_3$




Phonon dispersion curves of $aP14$-$K_3BO_3$



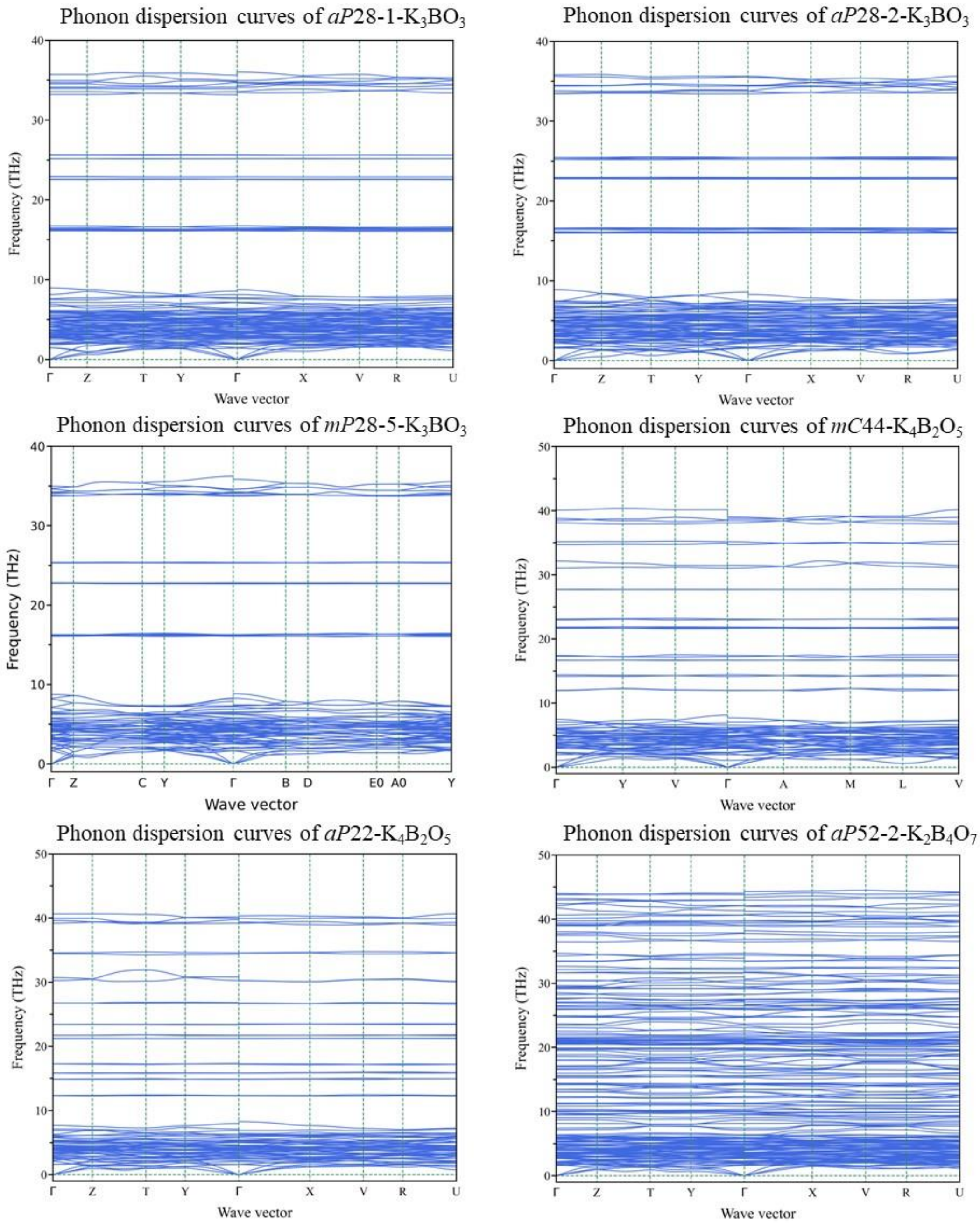



Figure S2. The phonon dispersion curves of fourteen predicted structures.

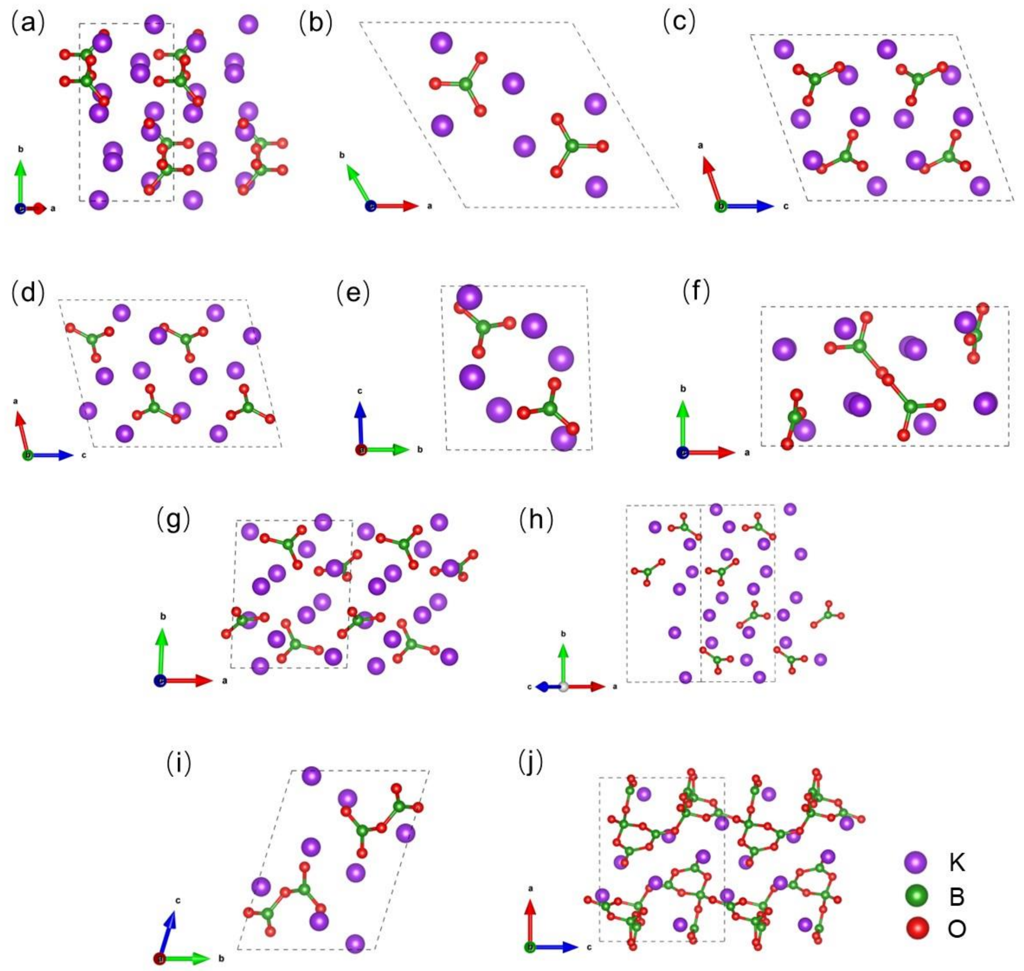
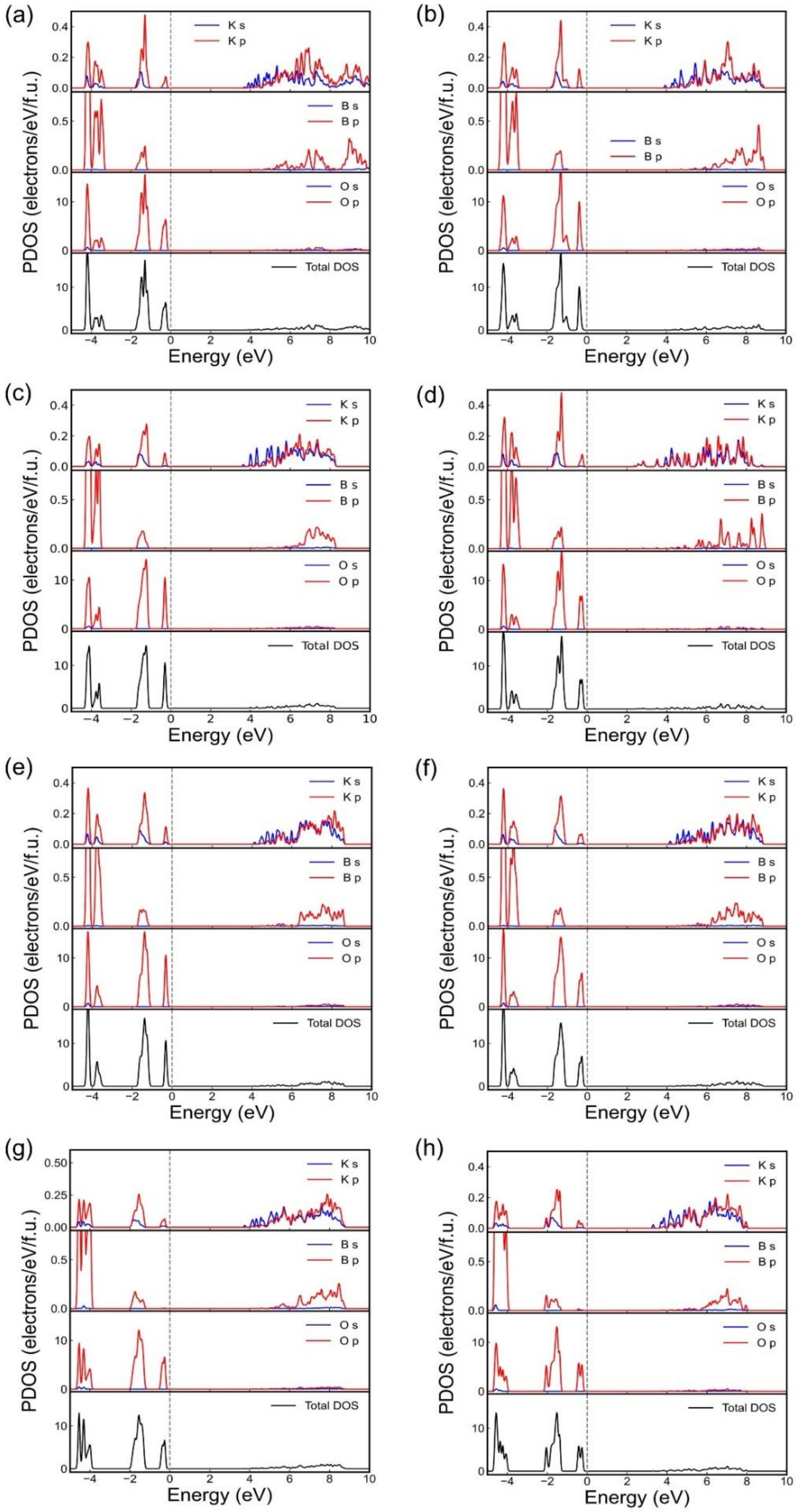



Figure S3. Crystal structures. (a) *mP*28-2-$K_3BO_3$, (b) *hP*14-$K_3BO_3$, (c) *mP*28-3-$K_3BO_3$, (d) *mP*28-4-$K_3BO_3$, (e) *aP*14-$K_3BO_3$, (f) *aP*28-1-$K_3BO_3$, (g) *aP*28-2-$K_3BO_3$, (h) *mP*28-5-$K_3BO_3$, (i) *aP*22-$K_4B_2O_5$, (j) *aP*52-2-$K_2B_4O_7$.



(a)
(b)
(c)
(d)
(e)
(f)
(g)
(h)
K s
K p
B s
B p
O s
O p
Total DOS
PDOS (electrons/eV/f.u.)
Energy (eV)

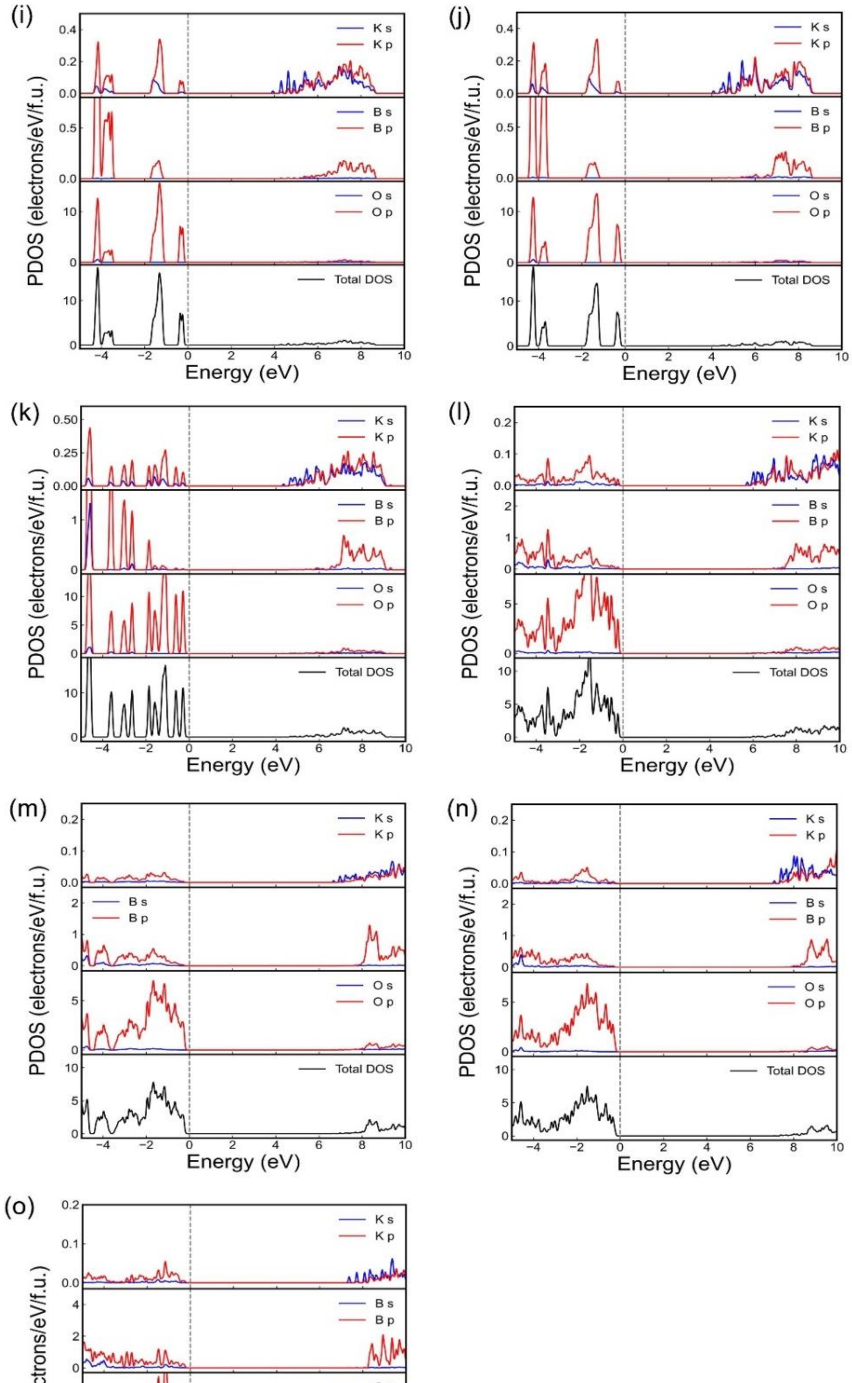



Figure S4. Projected density of states. (a) *hR*21-$K_3BO_3$, (b) *mP*28-1-$K_3BO_3$, (c) *mP*28-2-$K_3BO_3$, (d) *hP*14-$K_3BO_3$, (e) *mP*28-3-$K_3BO_3$, (f) *mP*28-4-$K_3BO_3$, (g) *aP*14-$K_3BO_3$, (h) *aP*28-1-$K_3BO_3$, (i) *aP*28-2-$K_3BO_3$, (j) *mP*28-5-$K_3BO_3$, (k) *aP*22-$K_4B_2O_5$, (l) *aP*52-2-$K_2B_4O_7$, (m) *mP*108-$KB_3O_5$, (n) *mC*72-$KB_3O_5$, (o) *oP*112-2-$KB_5O_8$.

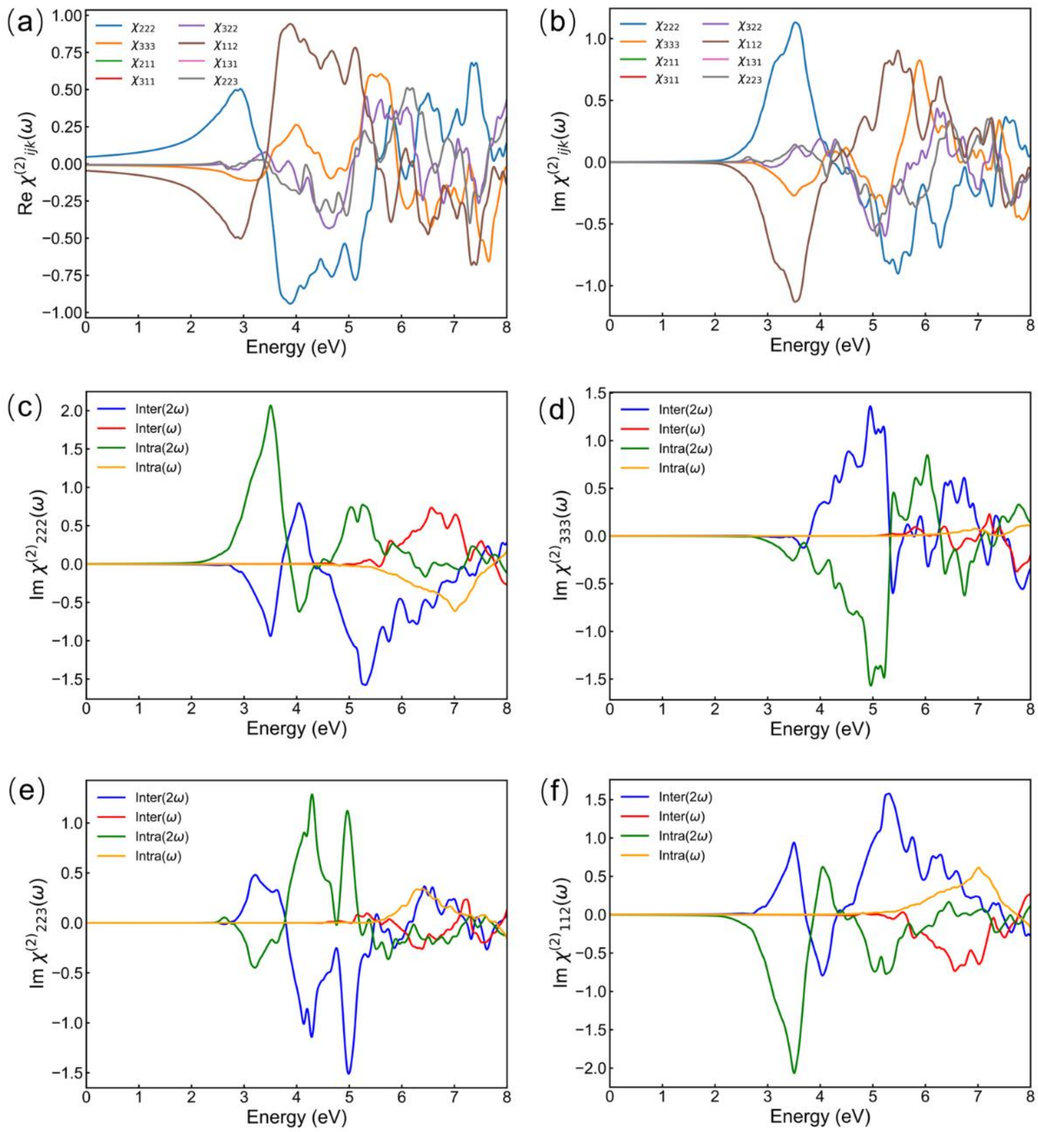



Figure S5. Calculated (a) real and (b) imaginary parts of $\chi_{ijk}^{(2)}(\omega)$. Calculated (c) Im $\chi_{222}^{(2)}(\omega)$, (d) Im $\chi_{333}^{(2)}(\omega)$, (e) Im $\chi_{223}^{(2)}(\omega)$, (f) Im $\chi_{112}^{(2)}(\omega)$ spectra along with the intraband and interband contributions. All Im $\chi_{ijk}^{(2)}(\omega)$ are given in units of $10^{-7}$ esu.

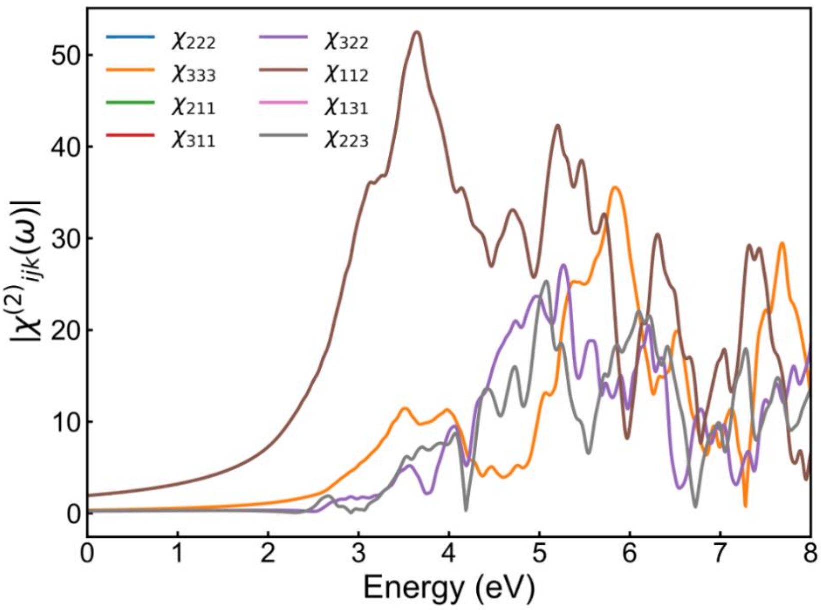



Figure S6. Calculated absolute values of $\chi^{(2)}_{ijk}(\omega)$. All $|\chi^{(2)}_{ijk}(\omega)|$ are expressed in units of pm/V.

# Supplementary Tables

Table S1. Crystal structural information and bond valence sum (BVS) for predicted structures.

| Phase | Pearson symbol | Space group & cell (Å) | Atom | Wyckoff position | x(a) | y(b) | z(c) | ΔE (eV/f.u.) | BVS |
|---|---|---|---|---|---|---|---|---|---|
| | | | K1 | 8*i* | 0.2530 | 0.2628 | 0.2498 | | 0.864 |
| | | | K2 | 4*g* | 0.3432 | 0.4816 | 0.0000 | | 0.998 |
| | | | K3 | 4*h* | 0.4792 | 0.1619 | 0.5000 | | 0.974 |
| | | *Pbam* | K4 | 4*f* | 0.5000 | 0.0000 | 0.1849 | | 1.006 |
| | | a=10.1355, | K5 | 4*e* | 0.5000 | 0.5000 | 0.3157 | | 1.060 |
| **$K_3BO_3$** | ***oP*56** | b=10.2473, | B1 | 4*h* | 0.2483 | 0.4660 | 0.5000 | -1.4804 | 2.733 |
| | | c=9.6536, | B2 | 4*g* | 0.4558 | 0.7486 | 0.0000 | | 2.736 |
| | | α=β=γ=90° | O1 | 8*i* | 0.3037 | 0.0101 | 0.3730 | | 1.774 |
| | | | O2 | 4*h* | 0.3491 | 0.3727 | 0.5000 | | 2.013 |
| | | | O3 | 4*g* | 0.1312 | 0.3542 | 0.0000 | | 2.018 |
| | | | O4 | 8*i* | 0.5031 | 0.3063 | 0.1268 | | 1.778 |
| | | *R*3*m* | K1 | 9*b* | 0.8799 | 0.1201 | 0.5327 | | 0.945 |
| **$K_3BO_3$** | ***hR*21** | a=b=10.7671, c=3.935, | B1 | 3*a* | 0.0000 | 0.0000 | 0.0364 | -1.4800 | 2.733 |
| | | α=β=90°, γ=120° | O1 | 9*b* | 0.0754 | 0.1507 | 0.0373 | | 1.856 |
| | | | K1 | 4*e* | 0.2996 | 0.4982 | 0.1082 | | 1.021 |
| | | $P2_1/c$ | K2 | 4*e* | 0.2970 | 0.4989 | 0.5914 | | 0.947 |
| | | a=6.1891, b=7.0517, | K3 | 4*e* | 0.1372 | 0.6643 | 0.8177 | | 0.902 |
| **$K_3BO_3$** | ***mP*28-1** | c=12.2249, α=γ=90°, | B1 | 4*e* | 0.2909 | 0.2333 | 0.3945 | -1.4768 | 2.718 |
| | | β=111.69° | O1 | 4*e* | 0.5070 | 0.7536 | 0.5048 | | 2.057 |
| | | | O2 | 4*e* | 0.0716 | 0.2254 | 0.4055 | | 1.765 |
| | | | O3 | 4*e* | 0.3063 | 0.2799 | 0.7823 | | 1.762 |
| | | | K1 | 4*e* | 0.8607 | 0.1090 | 0.5600 | | 0.744 |
| | | $P2_1/c$ | K2 | 4*e* | 0.7995 | 0.5047 | 0.5470 | | 1.016 |
| | | a=6.3963, b=9.1951, | K3 | 4*e* | 0.4518 | 0.7801 | 0.2984 | | 1.026 |
| **$K_3BO_3$** | ***mP*28-2** | c=10.3901, α=γ=90°, | B1 | 4*e* | 0.2638 | 0.3235 | 0.8446 | -1.4592 | 2.726 |
| | | β=127.28° | O1 | 4*e* | 0.6990 | 0.5621 | 0.2293 | | 1.785 |
| | | | O2 | 4*e* | 0.4415 | 0.2063 | 0.9105 | | 2.060 |
| | | | O3 | 4*e* | 0.9447 | 0.8254 | 0.6441 | | 1.667 |
| | | $P6_3/m$ | K1 | 6*h* | 0.6696 | 0.1110 | 0.7500 | | 0.939 |
| **$K_3BO_3$** | ***hP*14** | a=b=9.8507, c=4.0335, | B1 | 2*d* | 0.3333 | 0.6667 | 0.7500 | -1.4464 | 2.748 |
| | | α=β=90°, γ=120° | O1 | 6*h* | 0.3304 | 0.5227 | 0.7500 | | 1.855 |
| | | | K1 | 4*e* | 0.4939 | 0.7925 | 0.6044 | | 0.996 |
| | | | K2 | 4*e* | 0.7565 | 0.8874 | 0.9068 | | 0.796 |
| | | $P2_1/c$ | K3 | 4*e* | 0.0875 | 0.5506 | 0.8608 | | 0.794 |
| **$K_3BO_3$** | ***mP*28-3** | a=9.0306, b=5.3518, | B1 | 4*e* | 0.2673 | 0.9140 | 0.7595 | | 2.731 |
| | | c=10.5727, α=γ=90°, | O1 | 4*e* | 0.3977 | 0.7692 | 0.8296 | -1.4449 | 1.751 |
| | | β=109.03° | O2 | 4*e* | 0.1942 | 0.8773 | 0.6214 | | 1.891 |
| | | | O3 | 4*e* | 0.2085 | 0.4000 | 0.3245 | | 1.817 |
| | | | K1 | 4*e* | 0.2555 | 0.6200 | 0.4845 | | 0.831 |
| | | $P2_1/c$ | K2 | 4*e* | 0.0194 | 0.2749 | 0.8524 | | 0.949 |
| | | a=8.6535, b=5.3321, | K3 | 4*e* | 0.4111 | 0.4697 | 0.8188 | | 0.924 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **$K_3BO_3$** | ***mP*28-4** | c=10.7458, | B1 | 4*e* | 0.2330 | 0.1194 | 0.6277 | -1.4381 | 2.729 |
| | | α=90°, β=103.47°, | O1 | 4*e* | 0.2847 | 0.9494 | 0.7293 | | 1.703 |
| | | γ=90° | O2 | 4*e* | 0.1052 | 0.2826 | 0.6259 | | 1.676 |
| | | | O3 | 4*e* | 0.3102 | 0.3757 | 0.0263 | | 1.941 |
| | | | K1 | 2*i* | 0.2960 | 0.3695 | 0.2434 | | 0.818 |
| | | $P\bar{1}$ | K2 | 2*i* | 0.2415 | 0.8082 | 0.0680 | | 1.004 |
| | | a=5.4682, b=6.3878, | K3 | 2*i* | 0.2104 | 0.8074 | 0.5565 | | 0.910 |
| **$K_3BO_3$** | ***aP*14** | c=7.1551, α=99.06°, | B1 | 2*i* | 0.2467 | 0.2801 | 0.7486 | -1.4320 | 2.731 |
| | | β=99.27°, γ=101.20° | O1 | 2*i* | 0.7768 | 0.8719 | 0.1295 | | 1.646 |
| | | | O2 | 2*i* | 0.1370 | 0.4615 | 0.7742 | | 1.757 |
| | | | O3 | 2*i* | 0.3791 | 0.2469 | 0.5972 | | 1.807 |
| | | | K1 | 2*i* | 0.6977 | 0.9459 | 0.9035 | | 1.051 |
| | | | K2 | 2*i* | 0.6935 | 0.4846 | 0.3767 | | 1.082 |
| | | | K3 | 2*i* | 0.7106 | 0.9919 | 0.3983 | | 0.869 |
| | | | K4 | 2*i* | 0.6921 | 0.4491 | 0.9098 | | 0.791 |
| | | | K5 | 2*i* | 0.8874 | 0.2013 | 0.1743 | | 0.925 |
| | | $P\bar{1}$ | K6 | 2*i* | 0.8426 | 0.3391 | 0.6609 | | 0.770 |
| | | a=6.3446, b=7.2240, | B1 | 2*i* | 0.7172 | 0.7313 | 0.6033 | | 2.712 |
| **$K_3BO_3$** | ***aP*28-1** | c=11.2510, α=94.22°, | B2 | 2*i* | 0.2056 | 0.2617 | 0.8651 | -1.4239 | 2.737 |
| | | β=104.94°, γ=93.75° | O1 | 2*i* | 0.4746 | 0.2466 | 0.4877 | | 2.014 |
| | | | O2 | 2*i* | 0.7039 | 0.6850 | 0.7207 | | 1.960 |
| | | | O3 | 2*i* | 0.0142 | 0.1957 | 0.8955 | | 1.673 |
| | | | O4 | 2*i* | 0.3669 | 0.1403 | 0.8577 | | 1.778 |
| | | | O5 | 2*i* | 0.9224 | 0.7746 | 0.5751 | | 1.649 |
| | | | O6 | 2*i* | 0.2349 | 0.4491 | 0.8431 | | 2.023 |
| | | | K1 | 2*i* | 0.6344 | 0.3588 | 0.4291 | | 0.762 |
| | | | K2 | 2*i* | 0.8804 | 0.0757 | 0.8432 | | 0.825 |
| | | | K3 | 2*i* | 0.7664 | 0.4468 | 0.0154 | | 0.982 |
| | | | K4 | 2*i* | 0.7468 | 0.9873 | 0.4633 | | 1.051 |
| | | | K5 | 2*i* | 0.8612 | 0.6765 | 0.6976 | | 0.904 |
| | | $P\bar{1}$ | K6 | 2*i* | 0.6156 | 0.8049 | 0.1546 | | 0.940 |
| | | a=6.7031, b=8.5088, | B1 | 2*i* | 0.5490 | 0.1612 | 0.1744 | | 2.720 |
| **$K_3BO_3$** | ***aP*28-2** | c=8.8861, | B2 | 2*i* | 0.9194 | 0.6771 | 0.3548 | -1.4206 | 2.723 |
| | | α=87.80°, β=88.11°, | O1 | 2*i* | 0.5404 | 0.6992 | 0.8863 | | 1.925 |
| | | γ=87.64° | O2 | 2*i* | 0.4354 | 0.0639 | 0.2719 | | 1.881 |
| | | | O3 | 2*i* | 0.9719 | 0.6187 | 0.2127 | | 1.764 |
| | | | O4 | 2*i* | 0.9483 | 0.2305 | 0.5704 | | 1.915 |
| | | | O5 | 2*i* | 0.7521 | 0.1204 | 0.1423 | | 1.503 |
| | | | O6 | 2*i* | 0.7261 | 0.6565 | 0.4178 | | 1.919 |
| | | | K1 | 4*e* | 0.4953 | 0.2791 | 0.8542 | | 0.999 |
| | | | K2 | 4*e* | 0.5766 | 0.9751 | 0.2887 | | 0.966 |
| | | $P2_1/c$ | K3 | 4*e* | 0.9456 | 0.8768 | 0.1147 | | 0.745 |
| **$K_3BO_3$** | ***mP*28-5** | a=5.5350, b=14.3019, | B1 | 4*e* | 0.0504 | 0.8760 | 0.7172 | -1.4142 | 2.720 |
| | | c=7.2498, α=γ=90°, | O1 | 4*e* | 0.3470 | 0.6290 | 0.3949 | | 1.913 |
| | | β=124.27° | O2 | 4*e* | 0.0620 | 0.3198 | 0.9741 | | 1.667 |
| | | | O3 | 4*e* | 0.8654 | 0.5603 | 0.2283 | | 1.850 |
| | | | K1 | 8*f* | 0.8595 | 0.5397 | 0.0770 | | 0.967 |
| | | $C2/c$ | K2 | 8*f* | 0.8611 | 0.8364 | 0.7341 | | 0.891 |
| **$K_4B_2O_5$** | ***mC*44** | a=11.7267, b=9.1359, | B1 | 8*f* | 0.0874 | 0.1790 | 0.6728 | -1.5636 | 2.772 |
| | | c=6.9802, α=γ=90°, | O1 | 8*f* | 0.0521 | 0.6985 | 0.0528 | | 1.833 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | | β=109.38° | O2 | 4*e* | 0.0000 | 0.8913 | 0.2500 | | 1.804 |
| | | | O3 | 8*f* | 0.6993 | 0.3849 | 0.2191 | | 1.895 |
| $K_4B_2O_5$ | ***aP*22** | $P\bar{1}$ a=5.5174, b=7.5099, c=10.3114, α=70.62°, β=75.21°, γ=77.19° | K1 | 2*i* | 0.2945 | 0.9668 | 0.1496 | -1.5087 | 0.951 |
| | | | K2 | 2*i* | 0.7144 | 0.1546 | 0.4692 | | 1.042 |
| | | | K3 | 2*i* | 0.7410 | 0.3082 | 0.0718 | | 0.886 |
| | | | K4 | 2*i* | 0.1831 | 0.4673 | 0.3430 | | 0.814 |
| | | | B1 | 2*i* | 0.7419 | 0.6458 | 0.1642 | | 2.773 |
| | | | B2 | 2*i* | 0.8006 | 0.8599 | 0.3000 | | 2.767 |
| | | | O1 | 2*i* | 0.4043 | 0.9997 | 0.7060 | | 1.940 |
| | | | O2 | 2*i* | 0.2939 | 0.5163 | 0.7276 | | 1.765 |
| | | | O3 | 2*i* | 0.1161 | 0.2209 | 0.8196 | | 1.885 |
| | | | O4 | 2*i* | 0.0508 | 0.2001 | 0.6002 | | 1.845 |
| | | | O5 | 2*i* | 0.3367 | 0.3064 | 0.9611 | | 1.666 |
| $K_2B_4O_7$ | ***aP*52** | $P\bar{1}$ a=6.9441, b=8.8709, c=11.6204, α=94.71°, β=94.87°, γ=92.33° | K1 | 2*i* | 0.6343 | 0.0524 | 0.1429 | -1.4211 | 1.038 |
| | | | K2 | 2*i* | 0.4913 | 0.5214 | 0.7793 | | 0.992 |
| | | | K3 | 2*i* | 0.8316 | 0.6704 | 0.9827 | | 0.912 |
| | | | K4 | 2*i* | 0.8582 | 0.8544 | 0.3985 | | 1.154 |
| | | | B1 | 2*i* | 0.6782 | 0.2578 | 0.5784 | | 2.924 |
| | | | B2 | 2*i* | 0.5651 | 0.7957 | 0.5870 | | 2.930 |
| | | | B3 | 2*i* | 0.9739 | 0.4517 | 0.2854 | | 2.929 |
| | | | B4 | 2*i* | 0.8436 | 0.0502 | 0.8447 | | 2.921 |
| | | | B5 | 2*i* | 0.8739 | 0.3071 | 0.7839 | | 3.135 |
| | | | B6 | 2*i* | 0.7891 | 0.2534 | 0.3773 | | 2.944 |
| | | | B7 | 2*i* | 0.9012 | 0.8084 | 0.7158 | | 2.912 |
| | | | B8 | 2*i* | 0.6784 | 0.2622 | 0.9484 | | 2.847 |
| | | | O1 | 2*i* | 0.9068 | 0.1479 | 0.3156 | | 1.948 |
| | | | O2 | 2*i* | 0.8223 | 0.2487 | 0.5058 | | 1.977 |
| | | | O3 | 2*i* | 0.1761 | 0.5898 | 0.6526 | | 1.996 |
| | | | O4 | 2*i* | 0.4225 | 0.7890 | 0.6613 | | 2.051 |
| | | | O5 | 2*i* | 0.2956 | 0.7104 | 0.3040 | | 1.934 |
| | | | O6 | 2*i* | 0.0429 | 0.8448 | 0.2030 | | 1.977 |
| | | | O7 | 2*i* | 0.2032 | 0.6364 | 0.1048 | | 2.035 |
| | | | O8 | 2*i* | 0.0320 | 0.4048 | 0.7540 | | 1.862 |
| | | | O9 | 2*i* | 0.4842 | 0.2327 | 0.5335 | | 2.039 |
| | | | O10 | 2*i* | 0.2891 | 0.8972 | 0.0779 | | 2.101 |
| | | | O11 | 2*i* | 0.4532 | 0.7000 | 0.9800 | | 1.753 |
| | | | O12 | 2*i* | 0.8854 | 0.6463 | 0.7441 | | 1.931 |
| | | | O13 | 2*i* | 0.7555 | 0.8318 | 0.6182 | | 1.951 |
| | | | O14 | 2*i* | 0.8536 | 0.8976 | 0.8250 | | 1.868 |

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