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# Supporting Information

## Structural and electronic configuration of medium-sized strontium doped magnesium $Sr_mMg_n$ clusters and their anions

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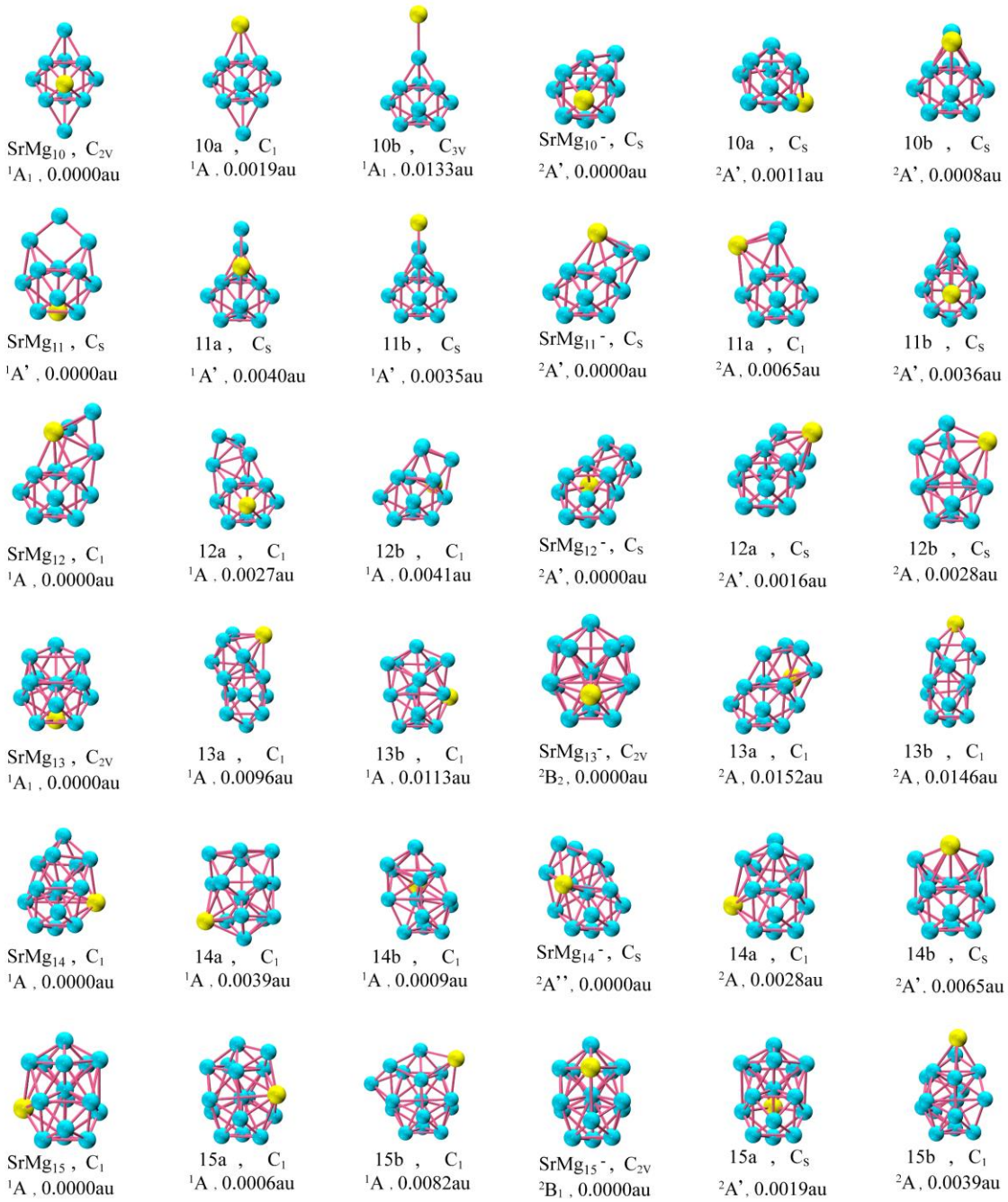
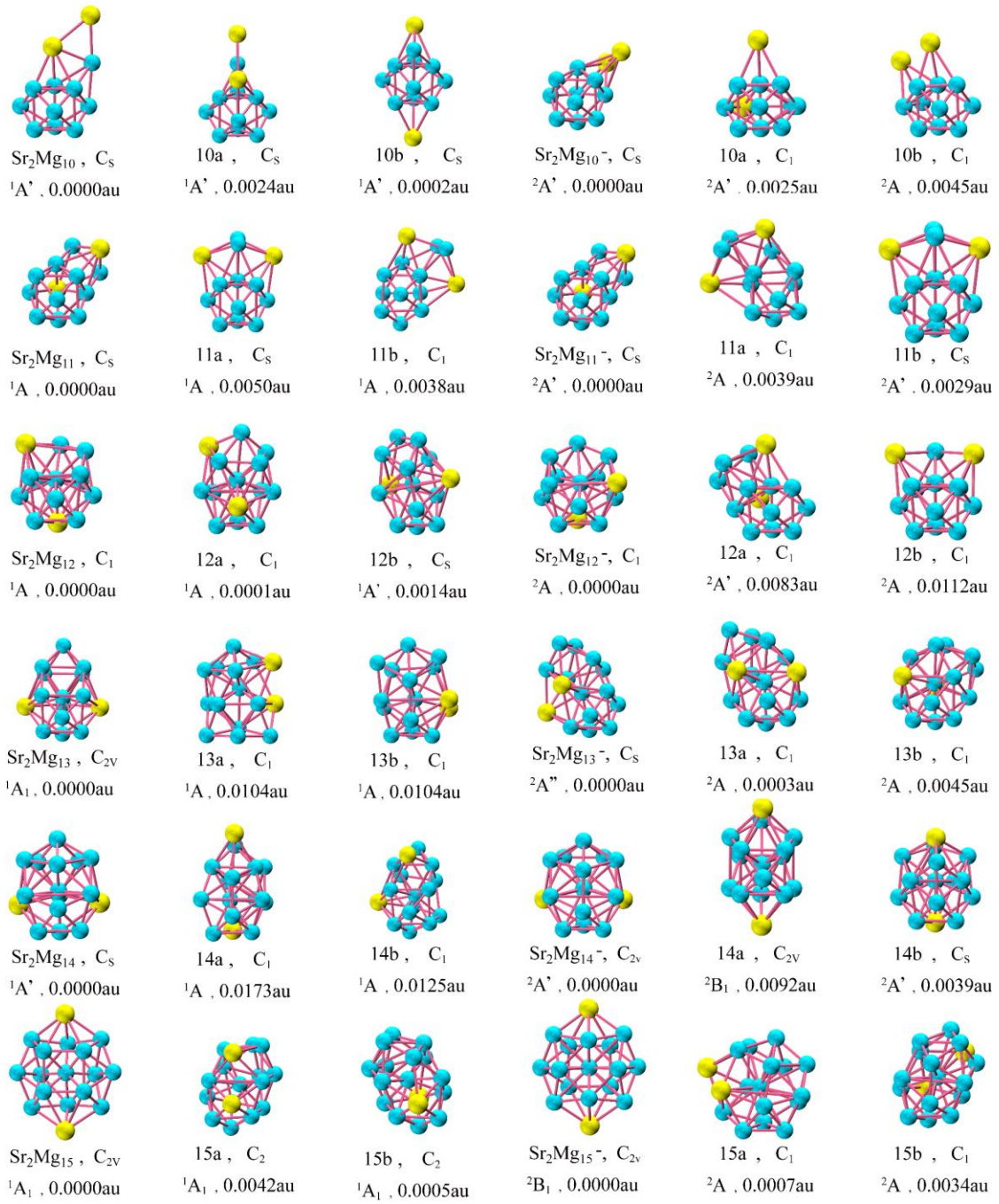
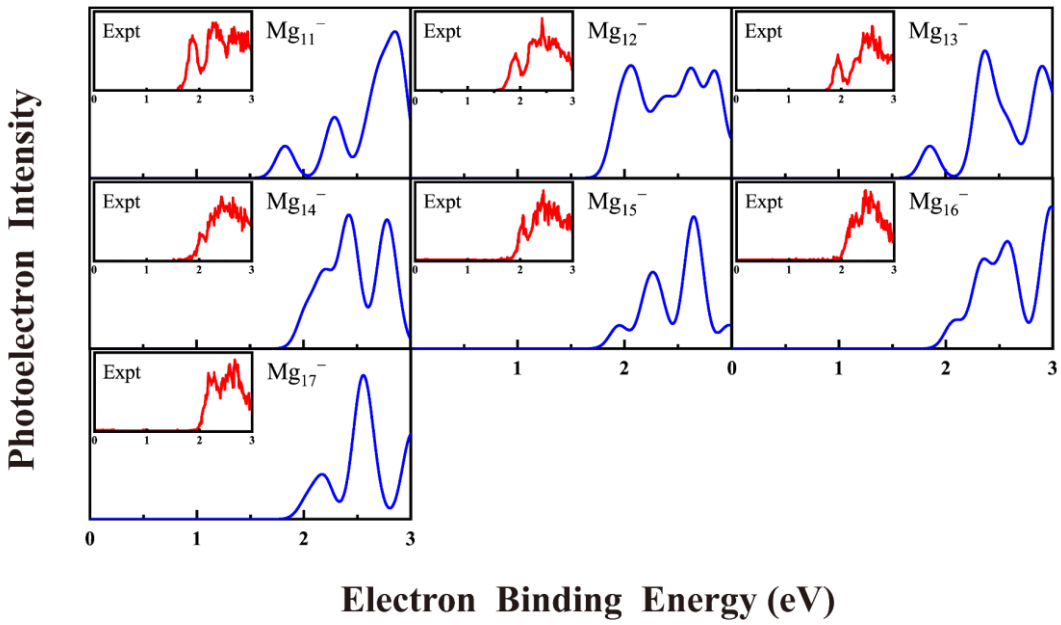



**S1.** Most stable structures of low-lying isomers of $SrMg_n^{0/-}$ (n=10–15) clusters, along with the electronic state, point group symmetry and relative energy (eV).




**S2.** Most stable structures of low-lying isomers of $Sr_2Mg_n^{0/-}$ (n=10–15) clusters, along with the electronic state, point group symmetry and relative energy (eV).




**S3.** Comparison of the simulated PES with experimental results of the most stable $Mg_n^-$ clusters.

**Table. S4** Electronic states, symmetries, average binding energies $E_b$ (eV), HOMO−LUMO energy gaps $E_g$ (eV), and the second-order difference of energies $\triangle_2E$ (eV) of the most stable $Mg_n^{0/-}$ ($n$=11–17) clusters.

| | $Mg_n$ | | | | | $Mg_n^-$ | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| **clusters** | **sta** | **sym** | $E_b$**(eV)** | $E_g$**(eV)** | $\triangle_2E$**(eV)** | **sta** | **sym** | $E_b$**(eV)** | $E_g$**(eV)** | $\triangle_2E$**(eV)** |
| $n$=11 | 1-A' | $C_{3H}$ | 0.525 | 2.045 | -0.096 | 2-A' | $C_S$ | 0.729 | 0.403 | -0.318 |
| $n$=12 | 1-A' | $C_S$ | 0.524 | 1.433 | -0.278 | 2-A' | $C_S$ | 0.729 | 0.134 | -0.117 |
| $n$=13 | 1-A' | $C_S$ | 0.545 | 1.457 | 0.177 | 2-A' | $C_S$ | 0.737 | 0.145 | 0.006 |
| $n$=14 | 1-A | $C_1$ | 0.550 | 1.215 | -0.639 | 2-A | $C_2$ | 0.745 | -0.062 | -0.319 |
| $n$=15 | 1-$A_1$' | $D_{3H}$ | 0.597 | 1.218 | 0.592 | 2-$A_2$" | $D_{3H}$ | 0.772 | -0.105 | 0.342 |
| $n$=16 | 1-$A_1$ | $C_{3V}$ | 0.601 | 1.462 | -0.869 | 2-$A_2$" | $C_1$ | 0.775 | -0.105 | -0.652 |
| $n$=17 | 1-$A_1$ | $D_{4D}$ | 0.656 | 1.106 | | 2-$B_2$ | $C_{2V}$ | 0.815 | -0.293 | |

**Table. S5** The HOMO energy level and LUMO energy level of neutral and anionic clusters. ($\triangle_{HOMO}$ (eV): it represents the difference value in the HOMO energy level between the neutral clusters and the corresponding anionic clusters; $\triangle_{LUMO}$ (eV): it represents the difference value in the LUMO energy level between the neutral clusters and the corresponding anionic clusters.)

| cluster | HOMO (eV) | LUMO (eV) | $\triangle_{HOMO}$ (eV) | $\triangle_{LUMO}$ (eV) | $E_g$ (eV) |
|---|---|---|---|---|---|
| $SrMg_{10}$ | -4.054 | -2.220 | 3.182 | 2.450 | 1.834 |
| $SrMg_{10}^-$ | -0.873 | 0.230 | | | 1.102 |
| $SrMg_{11}$ | -3.869 | -2.429 | 3.062 | 2.642 | 1.441 |
| $SrMg_{11}^-$ | -0.807 | 0.213 | | | 1.020 |
| $SrMg_{12}$ | -3.847 | -2.551 | 3.026 | 2.727 | 1.296 |
| $SrMg_{12}^-$ | -0.821 | 0.176 | | | 0.997 |
| $SrMg_{13}$ | -3.821 | -2.698 | 2.775 | 2.569 | 1.124 |
| $SrMg_{13}^-$ | -1.047 | -0.129 | | | 0.918 |
| $SrMg_{14}$ | -3.727 | -2.575 | 2.679 | 2.509 | 1.152 |
| $SrMg_{14}^-$ | -1.048 | -0.066 | | | 0.982 |
| $SrMg_{15}$ | -3.546 | -2.645 | 2.514 | 2.419 | 0.900 |
| $SrMg_{15}^-$ | -1.031 | -0.228 | | | 0.803 |
| $Sr_2Mg_{10}$ | -3.534 | -2.334 | 2.663 | 2.490 | 1.200 |
| $Sr_2Mg_{10}^-$ | -0.871 | 0.156 | | | 1.027 |
| $Sr_2Mg_{11}$ | -3.537 | -2.439 | 2.790 | 2.607 | 1.099 |
| $Sr_2Mg_{11}^-$ | -0.747 | 0.169 | | | 0.916 |
| $Sr_2Mg_{12}$ | -3.490 | -2.564 | 2.547 | 2.575 | 0.926 |
| $Sr_2Mg_{12}^-$ | -0.943 | 0.011 | | | 0.954 |
| $Sr_2Mg_{13}$ | -3.640 | -2.563 | 2.703 | 2.610 | 1.077 |
| $Sr_2Mg_{13}^-$ | -0.937 | 0.047 | | | 0.984 |
| $Sr_2Mg_{14}$ | -3.414 | -2.531 | 2.532 | 2.398 | 0.883 |
| $Sr_2Mg_{14}^-$ | -0.882 | -0.133 | | | 0.749 |

| | | | | | |
|---|---|---|---|---|---|
| $Sr_2Mg_{15}$ | -3.592 | -2.493 | 2.775 | 2.235 | 1.099 |
| $Sr_2Mg_{15}^-$ | -0.818 | -0.258 | | | 0.559 |

**Table. S6** The type and corresponding contribution of atomic orbitals for $SrMg_{13}^-$ cluster.

| **$SrMg_{13}^-$** | **α-electron** | | | | | **β-electron** | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| AOs | Sr-4d | Sr-5s | Sr-5p | Mg-3s | Mg-3p | Sr-4d | Sr-5s | Sr-5p | Mg-3s | Mg-3p |
| LUMO | 3.51% | | | 15.71% | 77.04% | 4.15% | | | 15.02% | 76.36% |
| HOMO | 3.18% | | | 21.21% | 72.18% | 8.35% | 8.66% | | 27.66% | 51.16% |
| HOMO-1 | 8.68% | 7.25% | | 30.53% | 48.19% | 13.42% | | | 44.80% | 38.03% |
| HOMO-2 | 6.03% | 15.16% | 1.10% | 15.07% | 55.88% | 6.77% | 14.14% | 1.12% | 17.07% | 65.21% |
| HOMO-3 | 12.65 % | | | 46.77% | 37.34% | | | | 34.77% | 58.84% |
| HOMO-4 | | | | 36.57% | 59.18% | | | | 36.33% | 57.54% |
| HOMO-5 | | | | 37.58% | 56.60% | 6.56% | | 0.97% | 55.63% | 33.95% |
| HOMO-6 | 5.87% | | 0.80% | 57.22% | 33.87% | 4.11% | | 5.49% | 54.47% | 32.54% |

**Table. S7** The type and corresponding contribution of atomic orbitals for $Sr_2Mg_{11}$ cluster.

| **$Sr_2Mg_{11}$ Molecular orbital** | | | | | |
|---|---|---|---|---|---|
| AOs | Sr-4d | Sr-5s | Sr-5p | Mg-3s | Mg-3p |
| LUMO | 8.16% | 15.34% | 4.76% | 1.47% | 63.67% |
| HOMO | 4.58% | 14.30% | 4.82% | 13.22% | 57.71% |
| HOMO-1 | 1.79% | 15.85% | 3.52% | 22.23% | 54.27% |
| HOMO-2 | 6.31% | | 0.67% | 37.65% | 51.58% |
| HOMO-3 | 5.26% | | 1.10% | 43.23% | 46.97% |
| HOMO-4 | 5.36% | | 1.96% | 40.05% | 48.38% |
| HOMO-5 | 7.40% | 5.18% | 1.13% | 38.21% | 43.24% |
| HOMO-6 | | 19.93% | | 22.68% | 54.06% |
| HOMO-7 | 9.30% | | 4.32% | 52.68% | 31.28% |
| HOMO-8 | 5.79% | 0.76% | 4.16% | 55.20% | 30.31% |

| $Mg_{11}$: | | | | $Mg_{11}^-$: | | | |
|---|---|---|---|---|---|---|---|
| Mg | 1.806 | 0.000 | 1.539 | Mg | -1.515 | -2.315 | 0.000 |
| Mg | -3.009 | 0.000 | 0.000 | Mg | 1.158 | 0.735 | 1.512 |
| Mg | 0.000 | 0.000 | -4.198 | Mg | 1.158 | 0.735 | -1.512 |
| Mg | 1.504 | 2.606 | 0.000 | Mg | -2.705 | 3.990 | 0.000 |
| Mg | -0.903 | 1.564 | 1.539 | Mg | -1.221 | -0.815 | -2.577 |
| Mg | -0.903 | -1.564 | -1.539 | Mg | -1.221 | -0.815 | 2.577 |
| Mg | 1.806 | 0.000 | -1.539 | Mg | 0.359 | 3.346 | 0.000 |
| Mg | -0.903 | 1.564 | -1.539 | Mg | -1.580 | 0.820 | 0.000 |
| Mg | -0.903 | -1.564 | 1.539 | Mg | 3.253 | -0.885 | 0.000 |
| Mg | 1.504 | -2.606 | 0.000 | Mg | 1.158 | -2.398 | -1.536 |
| Mg | 0.000 | 0.000 | 4.198 | Mg | 1.158 | -2.398 | 1.536 |

| $Mg_{12}$: | | | | $Mg_{12}^-$: | | | |
|---|---|---|---|---|---|---|---|
| Mg | -0.397 | 2.645 | 1.560 | Mg | 0.352 | 1.177 | 1.539 |
| Mg | -0.397 | -0.486 | -1.535 | Mg | -2.261 | -0.367 | 1.484 |
| Mg | -1.883 | -4.575 | 0.000 | Mg | 0.287 | 4.152 | 0.000 |
| Mg | 1.973 | 1.047 | 2.626 | Mg | -2.189 | 2.464 | 0.000 |
| Mg | -2.484 | 1.095 | 0.000 | Mg | 2.319 | -0.627 | 0.000 |
| Mg | -0.397 | 2.645 | -1.560 | Mg | -1.548 | -2.947 | 0.000 |
| Mg | 2.326 | -0.527 | 0.000 | Mg | 0.352 | 1.177 | -1.539 |
| Mg | 0.681 | -3.030 | 0.000 | Mg | -2.261 | -0.367 | -1.484 |
| Mg | -3.225 | -1.933 | 0.000 | Mg | 2.780 | 2.457 | 0.000 |
| Mg | 1.973 | 1.047 | -2.626 | Mg | 0.352 | -1.763 | 2.162 |
| Mg | 2.228 | 2.558 | 0.000 | Mg | 1.464 | -3.593 | 0.000 |
| Mg | -0.397 | -0.486 | 1.535 | Mg | 0.352 | -1.763 | -2.162 |

| $Mg_{13}$: | | | | $Mg_{13}^-$: | | | |
|---|---|---|---|---|---|---|---|
| Mg | -1.938 | -2.173 | 0.000 | Mg | -0.170 | -0.395 | 1.523 |
| Mg | 0.170 | -0.306 | 1.558 | Mg | -0.170 | -4.019 | 1.481 |
| Mg | 1.550 | 2.540 | 1.614 | Mg | 1.923 | -2.354 | 0.000 |
| Mg | -1.245 | 2.112 | -2.627 | Mg | -0.170 | -0.395 | -1.523 |
| Mg | 1.550 | 2.540 | -1.614 | Mg | -1.291 | 2.607 | -1.546 |
| Mg | -0.796 | 3.566 | 0.000 | Mg | -2.756 | 0.495 | 0.000 |
| Mg | -0.263 | -4.240 | 1.517 | Mg | -2.361 | -2.508 | 0.000 |
| Mg | 0.170 | -0.306 | -1.558 | Mg | -0.170 | -4.019 | -1.481 |
| Mg | 1.841 | -2.710 | 0.000 | Mg | 1.196 | 3.455 | 0.000 |
| Mg | -2.254 | 0.831 | 0.000 | Mg | -1.291 | 2.607 | 1.546 |
| Mg | -0.263 | -4.240 | -1.517 | Mg | 1.441 | 1.951 | 2.590 |
| Mg | 2.722 | 0.277 | 0.000 | Mg | 2.381 | 0.623 | 0.000 |
| Mg | -1.245 | 2.112 | 2.627 | Mg | 1.441 | 1.951 | -2.590 |

| $Mg_{14}$: | | | | $Mg_{14}^-$: | | | |
|---|---|---|---|---|---|---|---|
| Mg | 1.634 | 1.239 | 1.684 | Mg | 1.657 | 0.256 | 0.881 |
| Mg | -0.444 | -1.388 | -1.906 | Mg | 0.247 | -1.673 | 2.928 |
| Mg | -0.229 | -1.188 | 1.186 | Mg | -1.163 | 1.024 | -1.833 |
| Mg | -0.253 | 1.507 | -0.813 | Mg | 1.163 | -1.024 | -1.833 |
| Mg | 2.649 | 2.732 | -0.834 | Mg | 0.295 | -3.915 | -1.787 |
| Mg | 2.127 | -2.393 | -0.533 | Mg | -1.936 | -1.925 | -1.692 |
| Mg | -2.653 | -2.859 | -0.078 | Mg | -1.883 | 2.833 | 0.626 |
| Mg | -3.287 | 2.517 | -0.172 | Mg | -0.295 | 3.915 | -1.787 |
| Mg | -1.318 | 1.548 | 2.054 | Mg | 1.936 | 1.925 | -1.692 |
| Mg | -3.265 | -0.183 | -1.690 | Mg | 1.883 | -2.833 | 0.626 |
| Mg | 2.690 | -1.559 | 2.252 | Mg | -1.163 | -3.361 | 0.876 |
| Mg | 2.106 | 0.222 | -2.415 | Mg | -1.657 | -0.256 | 0.881 |
| Mg | 3.936 | 0.060 | -0.010 | Mg | -0.247 | 1.673 | 2.928 |
| Mg | -3.693 | -0.256 | 1.274 | Mg | 1.163 | 3.361 | 0.876 |

| $Mg_{15}$: | | | | $Mg_{15}^-$: | | | |
|---|---|---|---|---|---|---|---|
| Mg | 0.000 | 1.973 | 0.000 | Mg | 0.000 | 1.876 | 0.000 |
| Mg | 0.000 | 1.812 | 3.244 | Mg | 0.000 | 1.798 | 3.228 |
| Mg | -1.709 | -0.987 | 0.000 | Mg | -1.557 | -0.899 | -3.228 |
| Mg | 0.000 | 1.812 | -3.244 | Mg | -1.625 | -0.938 | 0.000 |
| Mg | 1.709 | -0.987 | 0.000 | Mg | 2.557 | 1.476 | 1.724 |
| Mg | -2.524 | 1.457 | 1.671 | Mg | 1.557 | -0.899 | 3.228 |
| Mg | -1.569 | -0.906 | 3.244 | Mg | 0.000 | -2.953 | -1.724 |
| Mg | 2.524 | 1.457 | -1.671 | Mg | 1.625 | -0.938 | 0.000 |
| Mg | 1.569 | -0.906 | -3.244 | Mg | 2.557 | 1.476 | -1.724 |
| Mg | 2.524 | 1.457 | 1.671 | Mg | -1.557 | -0.899 | 3.228 |
| Mg | 1.569 | -0.906 | 3.244 | Mg | 1.557 | -0.899 | -3.228 |
| Mg | -1.569 | -0.906 | -3.244 | Mg | 0.000 | -2.953 | 1.724 |
| Mg | -2.524 | 1.457 | -1.671 | Mg | 0.000 | 1.798 | -3.228 |
| Mg | 0.000 | -2.914 | -1.671 | Mg | -2.557 | 1.476 | 1.724 |
| Mg | 0.000 | -2.914 | 1.671 | Mg | -2.557 | 1.476 | -1.724 |

| $Mg_{16}$: | | | | $Mg_{16}^-$: | | | |
|---|---|---|---|---|---|---|---|
| Mg | 2.600 | -1.501 | 2.805 | Mg | -3.661 | 0.783 | 0.679 |
| Mg | -1.532 | -0.884 | -3.425 | Mg | -2.325 | 1.856 | -1.876 |
| Mg | 0.000 | 1.840 | -0.366 | Mg | -0.483 | -0.057 | -0.420 |
| Mg | -1.594 | -0.920 | -0.366 | Mg | 2.004 | -0.951 | -1.799 |
| Mg | 2.188 | 1.263 | 1.740 | Mg | -1.437 | 0.221 | 2.534 |
| Mg | 0.000 | -2.526 | 1.740 | Mg | -1.137 | 2.768 | 0.852 |
| Mg | 2.630 | 1.518 | -1.931 | Mg | -3.095 | -1.111 | -1.698 |
| Mg | -2.600 | -1.501 | 2.805 | Mg | 0.769 | 2.200 | -1.920 |
| Mg | 0.000 | 1.769 | -3.425 | Mg | -0.604 | -2.925 | -1.296 |
| Mg | 0.000 | 0.000 | 3.532 | Mg | 3.395 | 1.469 | -0.614 |
| Mg | 1.532 | -0.884 | -3.425 | Mg | 2.171 | -3.684 | -0.356 |
| Mg | 1.594 | -0.920 | -0.366 | Mg | 3.355 | -1.189 | 0.963 |
| Mg | -2.188 | 1.263 | 1.740 | Mg | -2.590 | -2.147 | 1.099 |
| Mg | 0.000 | -3.037 | -1.931 | Mg | 1.720 | 3.851 | 0.449 |
| Mg | 0.000 | 3.002 | 2.805 | Mg | 0.487 | -2.116 | 1.684 |
| Mg | -2.630 | 1.518 | -1.931 | Mg | 1.431 | 1.032 | 1.720 |

| $Mg_{17}$: | | | | $Mg_{17}^-$: | | | |
|---|---|---|---|---|---|---|---|
| Mg | -1.542 | 1.542 | 2.133 | Mg | -1.526 | 1.570 | 2.194 |
| Mg | -2.611 | -2.611 | -0.591 | Mg | 0.000 | 0.000 | 0.027 |
| Mg | -2.181 | 0.000 | -2.133 | Mg | 0.000 | 3.640 | 0.637 |
| Mg | 1.542 | -1.542 | 2.133 | Mg | -3.633 | 0.000 | 0.569 |
| Mg | 0.000 | 0.000 | 0.000 | Mg | 1.526 | -1.570 | 2.194 |
| Mg | 0.000 | 3.692 | 0.591 | Mg | 2.567 | 2.571 | -0.611 |
| Mg | 0.000 | -3.692 | 0.591 | Mg | -2.012 | 0.000 | -2.215 |
| Mg | 3.692 | 0.000 | 0.591 | Mg | 0.000 | -3.640 | 0.637 |
| Mg | 0.000 | 2.181 | -2.133 | Mg | 3.633 | 0.000 | 0.569 |
| Mg | 1.542 | 1.542 | 2.133 | Mg | 0.000 | 2.330 | -2.171 |
| Mg | 0.000 | -2.181 | -2.133 | Mg | -2.567 | -2.571 | -0.611 |
| Mg | -1.542 | -1.542 | 2.133 | Mg | 2.567 | -2.571 | -0.611 |
| Mg | -2.611 | 2.611 | -0.591 | Mg | 2.012 | 0.000 | -2.215 |
| Mg | -3.692 | 0.000 | 0.59 | Mg | 0.000 | -2.330 | -2.171 |
| Mg | 2.181 | 0.000 | -2.133 | Mg | 1.526 | 1.570 | 2.194 |
| Mg | 2.611 | 2.611 | -0.591 | Mg | -2.567 | 2.571 | -0.611 |
| Mg | 2.611 | -2.611 | -0.591 | Mg | -1.526 | -1.570 | 2.194 |

**S8.** The xyz data of each structure in $Mg_n^{0/-}$ ($n$=11-17) clusters.

| $SrMg_{10}$: | | | | 10a: | | | | 10b: | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Sr | 0.000 | 0.000 | 3.020 | Sr | -3.867 | 0.000 | 0.000 | Sr | 0.000 | 0.000 | 5.461 |
| Mg | 0.000 | 1.521 | -2.498 | Mg | 2.335 | -1.777 | 0.141 | Mg | 1.553 | -0.896 | -3.640 |
| Mg | 0.000 | -4.177 | -0.625 | Mg | -0.752 | -1.798 | 0.143 | Mg | 0.000 | 1.813 | -0.592 |
| Mg | 1.547 | 1.527 | 0.251 | Mg | 2.335 | 0.766 | -1.609 | Mg | -1.553 | -0.896 | -3.640 |
| Mg | -1.547 | 1.527 | 0.251 | Mg | 0.784 | -1.290 | 2.710 | Mg | 2.610 | 1.507 | -2.136 |
| Mg | 1.547 | -1.527 | 0.251 | Mg | -0.751 | 0.775 | -1.628 | Mg | 0.000 | 0.000 | 1.808 |
| Mg | -1.547 | -1.527 | 0.251 | Mg | -0.751 | 1.023 | 1.485 | Mg | -2.610 | 1.507 | -2.136 |
| Mg | 2.597 | 0.000 | -2.162 | Mg | 0.784 | -1.702 | -2.472 | Mg | 0.000 | -3.014 | -2.136 |
| Mg | 0.000 | -1.521 | -2.498 | Mg | 0.784 | 2.992 | -0.239 | Mg | 1.570 | -0.907 | -0.592 |
| Mg | 0.000 | 4.177 | -0.625 | Mg | 5.140 | 0.000 | 0.000 | Mg | 0.000 | 1.793 | -3.640 |
| Mg | -2.597 | 0.000 | -2.162 | Mg | 2.334 | 1.011 | 1.467 | Mg | -1.570 | -0.907 | -0.592 |
| $SrMg_{11}$: | | | | 11a: | | | | 11b: | | | |
| Sr | 1.644 | -2.680 | 0.000 | Sr | 0.030 | -3.539 | 0.000 | Sr | 2.877 | 3.856 | 0.000 |
| Mg | 0.646 | -0.306 | 2.677 | Mg | -0.124 | 2.869 | 2.625 | Mg | -2.851 | 0.753 | 0.000 |
| Mg | -1.474 | -2.076 | 1.487 | Mg | -0.124 | 0.058 | -1.518 | Mg | -0.401 | 2.807 | 0.000 |
| Mg | 1.539 | 4.731 | 0.000 | Mg | -2.955 | -0.373 | 0.000 | Mg | 2.353 | 0.445 | 0.000 |
| Mg | -1.474 | -2.076 | -1.487 | Mg | -3.434 | -3.314 | 0.000 | Mg | -0.413 | -2.952 | 2.624 |
| Mg | 0.914 | 0.798 | 0.000 | Mg | 1.020 | 3.938 | 0.000 | Mg | -3.067 | -1.829 | -1.554 |
| Mg | -1.796 | 1.176 | 1.543 | Mg | -0.124 | 2.869 | -2.625 | Mg | -0.413 | -0.166 | 1.525 |
| Mg | 0.646 | 2.965 | 2.229 | Mg | 2.506 | 1.786 | -1.557 | Mg | -3.067 | -1.829 | 1.554 |
| Mg | -3.705 | -0.558 | 0.000 | Mg | 2.506 | 1.786 | 1.557 | Mg | 1.112 | -2.369 | 0.000 |
| Mg | 0.646 | 2.965 | -2.229 | Mg | 2.359 | -0.789 | 0.000 | Mg | -0.413 | -2.952 | -2.624 |
| Mg | -1.796 | 1.176 | -1.543 | Mg | -0.124 | 0.058 | 1.518 | Mg | -1.538 | -3.953 | 0.000 |
| Mg | 0.646 | -0.306 | -2.677 | Mg | -1.597 | 2.320 | 0.000 | Mg | -0.413 | -0.166 | -1.525 |
| $SrMg_{12}$: | | | | 12a: | | | | 12b: | | | |
| Sr | 2.385 | -1.618 | -0.026 | Sr | -2.973 | -2.051 | -0.013 | Sr | -3.173 | -1.391 | -0.055 |
| Mg | -2.135 | -0.736 | 2.875 | Mg | 3.276 | 0.001 | 1.706 | Mg | -3.117 | 1.852 | 1.306 |
| Mg | -3.006 | 1.742 | 1.398 | Mg | 2.148 | -1.356 | -1.592 | Mg | 1.712 | -1.147 | 2.827 |
| Mg | 2.020 | 2.173 | -0.775 | Mg | -2.884 | 1.387 | -0.749 | Mg | -0.396 | 3.160 | 0.547 |
| Mg | -3.367 | 1.146 | -1.669 | Mg | -0.941 | 3.270 | 0.638 | Mg | 1.350 | 1.662 | -1.422 |
| Mg | 4.694 | 0.714 | -1.026 | Mg | 1.456 | 1.608 | -0.499 | Mg | 0.742 | -2.261 | 0.135 |
| Mg | -0.019 | 0.715 | 1.322 | Mg | 0.177 | -0.947 | 0.873 | Mg | 2.297 | 1.514 | 1.380 |
| Mg | 3.483 | 1.251 | 1.733 | Mg | -0.646 | 2.802 | -2.283 | Mg | 3.778 | -1.535 | 0.717 |
| Mg | -2.677 | -1.768 | -2.230 | Mg | -2.205 | 0.674 | 2.084 | Mg | 2.601 | -1.162 | -2.096 |
| Mg | -0.398 | 0.113 | -1.696 | Mg | 4.756 | 0.219 | -0.937 | Mg | 4.351 | 0.933 | -0.891 |
| Mg | -3.952 | -0.984 | 0.422 | Mg | 4.208 | -2.485 | 0.331 | Mg | -0.408 | -0.652 | -2.041 |
| Mg | -1.113 | 2.842 | -0.638 | Mg | -0.611 | -0.246 | -1.998 | Mg | -0.369 | 0.257 | 1.234 |
| Mg | -1.080 | -2.084 | 0.366 | Mg | 0.6810 | 1.567 | 2.469 | Mg | -2.490 | 1.785 | -1.522 |

| $SrMg_{13}$: | | | | 13a: | | | | 13b: | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Sr | 0.000 | 0.000 | 2.709 | Sr | 3.232 | -1.063 | -1.004 | Sr | -2.982 | -1.761 | -0.380 |
| Mg | 2.802 | 1.501 | 0.835 | Mg | -3.488 | -1.731 | -0.834 | Mg | -0.318 | -0.934 | 1.710 |
| Mg | 0.000 | 0.000 | -0.768 | Mg | -3.663 | 0.051 | 1.595 | Mg | -0.565 | 0.578 | -1.280 |
| Mg | 0.000 | -2.684 | 0.519 | Mg | -1.963 | 0.286 | -2.569 | Mg | -2.694 | 1.163 | 1.605 |
| Mg | 0.000 | 2.684 | 0.519 | Mg | -1.989 | 2.222 | -0.010 | Mg | 2.228 | -2.861 | 1.647 |
| Mg | -1.640 | 2.042 | -2.208 | Mg | -0.341 | -1.586 | -0.833 | Mg | 4.434 | 1.286 | -0.656 |
| Mg | 1.640 | -2.042 | -2.208 | Mg | 0.717 | 3.021 | 1.348 | Mg | 2.180 | 0.179 | -2.385 |
| Mg | -1.640 | -2.042 | -2.208 | Mg | 3.187 | 2.500 | -0.257 | Mg | -3.453 | 1.648 | -1.191 |
| Mg | 1.640 | 2.042 | -2.208 | Mg | 0.581 | 1.220 | -1.260 | Mg | 0.717 | -2.099 | -0.918 |
| Mg | -2.802 | 1.501 | 0.835 | Mg | 1.308 | -2.166 | 1.743 | Mg | 0.225 | 2.020 | 2.151 |
| Mg | 2.802 | -1.501 | 0.835 | Mg | 2.577 | 0.641 | 1.968 | Mg | 2.564 | 0.166 | 1.530 |
| Mg | -3.782 | 0.000 | -1.677 | Mg | -1.970 | -2.523 | 1.648 | Mg | -1.327 | 3.534 | 0.002 |
| Mg | 3.782 | 0.000 | -1.677 | Mg | -0.649 | 0.342 | 1.867 | Mg | 3.809 | -1.687 | -0.557 |
| Mg | -2.802 | -1.501 | 0.835 | Mg | -4.543 | 1.087 | -1.224 | Mg | 1.644 | 2.583 | -0.455 |
| $SrMg_{14}$: | | | | 14a: | | | | 14b: | | | |
| Sr | 0.506 | 2.762 | -0.535 | Sr | -2.925 | -1.652 | -0.385 | Sr | -0.880 | 2.953 | -0.599 |
| Mg | 0.077 | -0.387 | 0.197 | Mg | -0.070 | -1.913 | 2.068 | Mg | 0.605 | -0.048 | -0.402 |
| Mg | -3.543 | -0.825 | 1.336 | Mg | -2.488 | 0.425 | 2.282 | Mg | -1.118 | 0.359 | 2.081 |
| Mg | 3.834 | -2.003 | -0.734 | Mg | 1.942 | 2.533 | 1.063 | Mg | 0.094 | -2.262 | -2.209 |
| Mg | 1.371 | 0.907 | 2.646 | Mg | 1.936 | 1.009 | -1.836 | Mg | 1.727 | -1.083 | 2.524 |
| Mg | -0.966 | -0.160 | -2.549 | Mg | 4.470 | 1.191 | -0.036 | Mg | 1.798 | 1.851 | 1.802 |
| Mg | 3.325 | 0.711 | 0.483 | Mg | -3.022 | 1.848 | -0.460 | Mg | -2.401 | -0.316 | -1.493 |
| Mg | -1.834 | -2.665 | -0.304 | Mg | 2.239 | -3.390 | 0.705 | Mg | -0.522 | -2.684 | 1.045 |
| Mg | 1.079 | -2.780 | -1.334 | Mg | -1.197 | 0.555 | -2.460 | Mg | 2.569 | -2.686 | 0.141 |
| Mg | 2.235 | -1.902 | 1.862 | Mg | -1.076 | 3.131 | 1.640 | Mg | -3.701 | 1.305 | 0.652 |
| Mg | -1.811 | 1.490 | 2.145 | Mg | 2.750 | -0.541 | 1.643 | Mg | 2.722 | 2.070 | -1.025 |
| Mg | -2.797 | 1.422 | -0.672 | Mg | 0.629 | -1.863 | -1.400 | Mg | 3.950 | -0.093 | 0.785 |
| Mg | -0.965 | -1.459 | 2.750 | Mg | -0.383 | 3.240 | -1.254 | Mg | -2.535 | -3.337 | -1.108 |
| Mg | 2.202 | 0.009 | -2.272 | Mg | 3.632 | -1.491 | -1.187 | Mg | 2.963 | -0.775 | -2.152 |
| Mg | -3.808 | -1.106 | -1.858 | Mg | -0.098 | 0.497 | 0.451 | Mg | -3.363 | -1.653 | 1.255 |
| $SrMg_{15}$: | | | | 15a: | | | | 15b: | | | |
| Sr | 0.766 | 2.859 | -0.269 | Sr | 0.223 | 2.904 | 0.000 | Sr | 4.294 | -0.442 | 0.184 |
| Mg | -3.883 | -0.507 | -0.855 | Mg | 1.966 | 0.284 | 1.990 | Mg | -0.453 | -2.904 | -2.021 |
| Mg | -0.487 | -0.335 | 0.096 | Mg | -1.722 | 1.174 | 2.464 | Mg | 1.493 | -0.291 | -1.939 |
| Mg | 3.224 | -2.070 | -1.815 | Mg | 2.008 | -2.775 | 1.493 | Mg | 1.161 | 0.756 | 1.382 |
| Mg | 3.421 | 0.677 | -0.559 | Mg | -0.427 | -1.611 | 2.739 | Mg | -0.919 | -1.383 | 2.561 |
| Mg | -2.784 | 1.978 | 0.476 | Mg | -0.427 | -1.611 | -2.740 | Mg | -1.750 | -3.498 | 0.688 |
| Mg | 3.107 | -1.975 | 1.195 | Mg | -1.722 | 1.174 | -2.464 | Mg | -2.685 | 3.855 | -0.200 |
| Mg | -1.979 | 1.339 | -2.286 | Mg | 2.008 | -2.775 | -1.494 | Mg | -1.941 | 1.504 | 1.693 |
| Mg | 0.817 | -3.030 | -0.352 | Mg | -1.613 | -3.134 | -0.000 | Mg | -3.640 | -1.134 | 1.329 |
| Mg | -3.002 | -0.633 | 2.084 | Mg | 3.534 | 1.950 | -0.000 | Mg | -3.397 | -2.055 | -1.545 |
| Mg | 2.319 | 0.738 | 2.162 | Mg | -3.244 | 1.547 | 0.000 | Mg | -0.559 | 2.304 | -1.681 |
| Mg | -0.713 | 1.229 | 2.592 | Mg | 3.900 | -1.017 | -0.000 | Mg | -1.060 | -0.427 | -0.456 |
| Mg | 1.161 | -0.012 | -2.394 | Mg | -3.317 | -1.140 | 1.507 | Mg | 1.195 | -2.352 | 0.553 |
| Mg | -1.598 | -1.714 | -2.318 | Mg | 1.965 | 0.284 | -1.990 | Mg | -3.598 | 1.023 | -1.003 |
| Mg | 0.555 | -1.796 | 2.545 | Mg | -3.317 | -1.140 | -1.507 | Mg | 2.365 | 2.389 | -0.893 |
| Mg | -2.582 | -2.942 | 0.281 | Mg | -0.298 | -0.403 | 0.000 | Mg | 0.193 | 3.611 | 0.948 |

$SrMg_{10}^-$:

| | | | |
|---|---|---|---|
| Sr | -1.726 | 3.225 | 0.000 |
| Mg | -0.255 | 0.774 | 2.159 |
| Mg | 2.271 | -3.066 | 0.000 |
| Mg | -0.255 | -2.160 | -1.564 |
| Mg | 1.565 | 2.019 | 0.000 |
| Mg | -0.255 | 0.774 | -2.159 |
| Mg | -0.255 | -2.160 | 1.565 |
| Mg | 2.394 | -0.426 | 1.549 |
| Mg | -0.081 | -5.184 | 0.000 |
| Mg | 2.394 | -0.426 | -1.549 |
| Mg | -2.055 | -0.357 | 0.000 |

$SrMg_{11}^-$:

| | | | |
|---|---|---|---|
| Sr | -0.166 | -3.053 | 0.000 |
| Mg | -0.135 | 2.956 | 1.505 |
| Mg | 2.588 | 2.980 | 0.000 |
| Mg | -0.135 | -0.033 | 1.672 |
| Mg | -0.135 | -0.033 | -1.672 |
| Mg | 2.323 | 1.465 | 2.532 |
| Mg | 2.338 | -0.289 | 0.000 |
| Mg | -2.310 | 1.352 | 0.000 |
| Mg | -0.135 | 2.956 | -1.505 |
| Mg | -3.097 | -1.576 | 1.470 |
| Mg | -3.097 | -1.576 | -1.470 |
| Mg | 2.323 | 1.465 | -2.532 |

$SrMg_{12}^-$:

| | | | |
|---|---|---|---|
| Sr | -0.961 | -2.819 | 0.000 |
| Mg | -0.606 | 0.383 | 1.585 |
| Mg | -3.588 | -0.864 | -1.464 |
| Mg | 1.946 | -1.195 | 1.505 |
| Mg | -0.606 | 0.383 | -1.585 |
| Mg | -0.057 | 2.890 | 0.000 |
| Mg | -3.588 | -0.864 | 1.464 |
| Mg | -3.046 | 1.805 | 0.000 |
| Mg | 1.946 | 1.731 | 2.221 |
| Mg | 3.828 | 0.618 | 0.000 |
| Mg | 1.946 | 1.731 | -2.221 |
| Mg | 1.946 | -1.195 | -1.505 |
| Mg | 2.923 | 3.501 | 0.000 |

10a:

| | | | |
|---|---|---|---|
| Sr | 0.724 | 3.865 | 0.000 |
| Mg | -2.112 | 1.861 | 0.000 |
| Mg | -2.214 | -0.943 | 1.539 |
| Mg | 0.436 | 0.611 | -1.544 |
| Mg | -1.373 | -3.353 | 0.000 |
| Mg | -2.214 | -0.943 | -1.539 |
| Mg | 0.436 | -2.282 | -2.216 |
| Mg | 0.436 | 0.6114 | 1.544 |
| Mg | 0.436 | -2.282 | 2.216 |
| Mg | 2.262 | -1.217 | 0.000 |
| Mg | 1.615 | -4.304 | 0.000 |

11a:

| | | | |
|---|---|---|---|
| Sr | -3.182 | -1.045 | -0.005 |
| Mg | -3.297 | 2.277 | -0.838 |
| Mg | 0.147 | -2.203 | -1.293 |
| Mg | 3.924 | 0.528 | -0.006 |
| Mg | 2.829 | -0.418 | 2.619 |
| Mg | 2.793 | -2.247 | 0.190 |
| Mg | 2.175 | 2.394 | -1.630 |
| Mg | 0.158 | -0.861 | 1.412 |
| Mg | 2.364 | -0.519 | -2.345 |
| Mg | -1.990 | 1.671 | 1.856 |
| Mg | -0.323 | 0.815 | -1.203 |
| Mg | 1.299 | 1.872 | 1.254 |

12a:

| | | | |
|---|---|---|---|
| Sr | -1.647 | -3.004 | 0.000 |
| Mg | 0.128 | -0.323 | 1.625 |
| Mg | 1.626 | -3.135 | -1.465 |
| Mg | -2.383 | 3.679 | 0.000 |
| Mg | 2.954 | -0.743 | 0.000 |
| Mg | -0.763 | 2.446 | -2.202 |
| Mg | 2.118 | 1.926 | -1.490 |
| Mg | 1.626 | -3.135 | 1.465 |
| Mg | -2.195 | 0.635 | 0.000 |
| Mg | 2.118 | 1.926 | 1.490 |
| Mg | 0.618 | 4.112 | 0.000 |
| Mg | 0.126 | -0.323 | -1.625 |
| Mg | -0.763 | 2.446 | 2.202 |

10b:

| | | | |
|---|---|---|---|
| Sr | 0.615 | -3.811 | 0.000 |
| Mg | -0.869 | 3.853 | 0.000 |
| Mg | 0.271 | 2.737 | 2.563 |
| Mg | 0.271 | -0.130 | 1.534 |
| Mg | 2.852 | -1.031 | 0.000 |
| Mg | 0.271 | 2.737 | -2.563 |
| Mg | 1.748 | 2.000 | 0.000 |
| Mg | 0.271 | -0.130 | -1.534 |
| Mg | -2.310 | 1.560 | -1.51 |
| Mg | -2.144 | -1.087 | 0.000 |
| Mg | -2.310 | 1.560 | 1.510 |

11b:

| | | | |
|---|---|---|---|
| Sr | -0.580 | -3.591 | 0.000 |
| Mg | -3.178 | 1.429 | 0.000 |
| Mg | -0.710 | 2.780 | 1.489 |
| Mg | -3.439 | -1.530 | 0.000 |
| Mg | -0.710 | 2.780 | -1.489 |
| Mg | 3.985 | 1.306 | 0.000 |
| Mg | 1.851 | -0.900 | 0.000 |
| Mg | 1.803 | 1.280 | 2.184 |
| Mg | 1.854 | 3.493 | 0.000 |
| Mg | -0.710 | -0.273 | 1.524 |
| Mg | 1.803 | 1.280 | -2.184 |
| Mg | -0.710 | -0.273 | -1.524 |

12b:

| | | | |
|---|---|---|---|
| Sr | -3.045 | -1.533 | -0.021 |
| Mg | -2.238 | 1.398 | 1.808 |
| Mg | 3.103 | -2.242 | -0.012 |
| Mg | -0.303 | 0.476 | -1.113 |
| Mg | 3.005 | -0.613 | 2.554 |
| Mg | 2.479 | -0.460 | -2.388 |
| Mg | 0.417 | -2.430 | -1.295 |
| Mg | -3.347 | 1.847 | -0.888 |
| Mg | 1.975 | 2.402 | -1.375 |
| Mg | 4.013 | 0.627 | -0.037 |
| Mg | 1.256 | 1.598 | 1.422 |
| Mg | 0.243 | -1.231 | 1.474 |
| Mg | -0.960 | 3.482 | -0.086 |

| $SrMg_{13}^-$: | | | |
|---|---|---|---|
| Sr | 0.000 | 0.000 | 2.581 |
| Mg | 0.000 | 0.000 | -1.068 |
| Mg | 1.502 | 2.754 | 0.798 |
| Mg | -2.437 | 1.643 | -1.995 |
| Mg | 2.437 | -1.643 | -1.995 |
| Mg | -1.502 | -2.754 | 0.798 |
| Mg | 1.502 | -2.754 | 0.798 |
| Mg | -2.437 | -1.643 | -1.995 |
| Mg | 2.437 | 1.643 | -1.995 |
| Mg | -1.502 | 2.754 | 0.798 |
| Mg | 0.000 | -3.412 | -1.801 |
| Mg | 0.000 | 3.412 | -1.801 |
| Mg | -2.803 | 0.000 | 0.644 |
| Mg | 2.803 | 0.000 | 0.644 |

| $SrMg_{14}^-$: | | | |
|---|---|---|---|
| Sr | 2.496 | 0.129 | 0.000 |
| Mg | 2.053 | -0.753 | 3.416 |
| Mg | -2.895 | -1.452 | -1.729 |
| Mg | 0.225 | -2.316 | 1.586 |
| Mg | 2.053 | -0.753 | -3.416 |
| Mg | 0.663 | 1.787 | -2.675 |
| Mg | -0.311 | 2.862 | 0.000 |
| Mg | -2.392 | 1.641 | 2.228 |
| Mg | -0.994 | -0.553 | -3.823 |
| Mg | -2.392 | 1.641 | -2.228 |
| Mg | -0.913 | 0.023 | 0.000 |
| Mg | -2.895 | -1.452 | 1.729 |
| Mg | 0.225 | -2.316 | -1.586 |
| Mg | 0.663 | 1.787 | 2.675 |
| Mg | -0.994 | -0.553 | 3.823 |

| $SrMg_{15}^-$: | | | |
|---|---|---|---|
| Sr | 0.000 | 0.000 | 3.389 |
| Mg | 0.000 | 3.384 | 1.361 |
| Mg | 1.456 | -2.947 | -1.455 |
| Mg | 2.272 | 1.512 | 1.118 |
| Mg | 0.000 | -1.521 | -3.818 |
| Mg | -2.272 | -1.512 | 1.118 |
| Mg | 0.000 | 0.000 | -0.254 |
| Mg | 0.000 | -3.384 | 1.361 |
| Mg | 1.456 | 2.947 | -1.455 |
| Mg | -1.456 | 2.947 | -1.455 |
| Mg | 2.205 | 0.000 | -2.108 |
| Mg | -2.272 | 1.512 | 1.118 |
| Mg | -2.205 | 0.000 | -2.108 |
| Mg | 0.000 | 1.521 | -3.818 |
| Mg | -1.456 | -2.947 | -1.455 |
| Mg | 2.272 | -1.512 | 1.118 |

| 13a: | | | |
|---|---|---|---|
| Sr | -3.387 | -1.670 | 0.075 |
| Mg | 2.547 | -0.631 | -2.323 |
| Mg | 1.356 | -2.793 | -0.427 |
| Mg | 2.601 | 0.848 | 1.639 |
| Mg | -1.374 | 3.870 | -0.412 |
| Mg | -2.775 | 1.659 | 1.304 |
| Mg | 2.147 | -2.085 | 2.342 |
| Mg | -0.442 | -0.882 | -1.973 |
| Mg | 0.111 | 2.592 | 1.875 |
| Mg | 4.162 | 1.484 | -0.895 |
| Mg | -2.531 | 1.318 | -1.682 |
| Mg | 1.012 | 1.738 | -0.972 |
| Mg | -0.154 | -0.433 | 1.137 |
| Mg | 4.066 | -1.396 | 0.150 |

| 14a: | | | |
|---|---|---|---|
| Sr | 0.753 | 2.976 | -0.017 |
| Mg | 3.205 | -1.925 | -1.952 |
| Mg | 0.935 | 0.058 | -2.286 |
| Mg | -0.460 | -0.067 | 0.416 |
| Mg | -2.028 | 1.324 | -1.998 |
| Mg | 3.080 | -2.042 | 1.138 |
| Mg | -3.960 | -0.440 | -0.484 |
| Mg | 0.398 | -1.986 | 2.469 |
| Mg | -2.726 | -0.511 | 2.481 |
| Mg | 0.672 | -2.745 | -0.664 |
| Mg | -2.288 | -2.701 | 0.450 |
| Mg | 3.341 | 0.667 | -0.382 |
| Mg | -2.718 | 2.038 | 0.871 |
| Mg | 2.183 | 0.570 | 2.392 |
| Mg | -2.015 | -1.666 | -2.398 |

| 15a: | | | |
|---|---|---|---|
| Sr | 2.381 | -2.516 | 0.000 |
| Mg | -0.336 | 4.562 | 0.000 |
| Mg | -1.156 | 2.191 | 1.634 |
| Mg | -2.522 | -0.620 | 2.504 |
| Mg | -3.631 | 0.862 | 0.000 |
| Mg | -1.156 | 2.191 | -1.634 |
| Mg | -0.794 | -2.869 | 1.574 |
| Mg | -0.794 | -2.869 | -1.574 |
| Mg | 1.251 | 0.251 | -2.388 |
| Mg | 3.148 | 0.890 | 0.000 |
| Mg | 1.251 | 0.251 | 2.388 |
| Mg | -0.471 | -0.259 | 0.000 |
| Mg | -3.316 | -2.058 | 0.000 |
| Mg | -2.522 | -0.620 | -2.504 |
| Mg | 1.754 | 3.032 | -1.565 |
| Mg | 1.754 | 3.032 | 1.565 |

| 13b: | | | |
|---|---|---|---|
| Sr | 4.200 | -0.862 | -0.184 |
| Mg | -3.702 | -0.004 | 1.783 |
| Mg | -3.048 | 2.551 | 0.254 |
| Mg | -1.139 | 1.043 | -1.710 |
| Mg | -0.755 | 0.958 | 1.589 |
| Mg | -2.005 | -1.908 | -1.961 |
| Mg | -4.112 | 0.198 | -1.268 |
| Mg | -1.299 | -1.985 | 1.191 |
| Mg | 0.195 | 3.397 | -0.091 |
| Mg | 0.780 | -1.219 | -0.992 |
| Mg | 1.991 | 1.551 | -1.739 |
| Mg | 1.515 | -1.064 | 2.089 |
| Mg | 2.312 | 1.762 | 1.316 |
| Mg | -4.032 | -2.550 | 0.120 |

| 14b: | | | |
|---|---|---|---|
| Sr | -2.309 | -2.131 | 0.000 |
| Mg | 0.136 | -2.014 | 2.535 |
| Mg | 0.038 | 3.639 | 1.578 |
| Mg | 0.038 | 3.639 | -1.578 |
| Mg | 1.406 | 1.175 | 2.605 |
| Mg | -1.578 | 1.049 | 1.700 |
| Mg | 1.406 | 1.175 | -2.605 |
| Mg | 2.967 | -1.600 | 1.544 |
| Mg | 0.944 | -3.418 | 0.000 |
| Mg | 0.136 | -2.014 | -2.535 |
| Mg | -1.578 | 1.049 | -1.700 |
| Mg | 2.967 | -1.600 | -1.544 |
| Mg | 0.654 | -0.135 | 0.000 |
| Mg | -2.534 | 3.280 | 0.000 |
| Mg | 2.309 | 2.516 | 0.0000 |

| 15b: | | | |
|---|---|---|---|
| Sr | -4.268 | -0.232 | -0.184 |
| Mg | -1.092 | 0.812 | -1.497 |
| Mg | 1.515 | -3.580 | -0.666 |
| Mg | 0.717 | 2.258 | 1.758 |
| Mg | 3.619 | 0.816 | 1.132 |
| Mg | 2.950 | 3.617 | 0.180 |
| Mg | 0.112 | 3.565 | -0.963 |
| Mg | -1.556 | -0.203 | 2.030 |
| Mg | 2.151 | 1.397 | -1.762 |
| Mg | 3.612 | -1.321 | -1.235 |
| Mg | 3.097 | -2.219 | 1.621 |
| Mg | 0.094 | -2.858 | 1.960 |
| Mg | 0.947 | -0.402 | 0.428 |
| Mg | 0.900 | -1.380 | -2.527 |
| Mg | -1.388 | -2.278 | -0.709 |
| Mg | -2.164 | 2.505 | 0.833 |

**S9.** The xyz data of each structure in $SrMg_n^{0/-}$ ($n$=10-15) clusters.

| $Sr_2Mg_{10}$: | | | | 10a: | | | | 10b: | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Sr | 2.375 | 0.446 | 0.000 | Sr | -0.468 | 2.924 | 0.000 | Sr | 3.844 | 2.475 | 0.000 |
| Sr | 2.427 | 4.441 | 0.000 | Sr | 3.553 | 3.224 | 0.000 | Sr | -3.772 | -3.050 | 0.000 |
| Mg | -0.793 | -0.427 | 1.525 | Mg | -3.171 | -2.291 | 1.551 | Mg | -1.909 | -0.343 | 1.488 |
| Mg | -0.793 | -3.227 | -2.613 | Mg | -3.171 | -2.291 | -1.551 | Mg | 0.738 | 4.332 | 0.000 |
| Mg | -0.793 | -0.427 | -1.525 | Mg | -2.999 | 0.279 | 0.000 | Mg | -1.909 | -0.343 | -1.488 |
| Mg | -3.424 | -2.109 | -1.538 | Mg | -0.518 | -0.578 | -1.514 | Mg | -1.764 | 2.316 | 0.000 |
| Mg | 0.685 | -2.689 | 0.000 | Mg | -1.655 | -4.424 | 0.000 | Mg | 0.699 | 1.321 | -1.567 |
| Mg | -3.250 | 0.486 | 0.000 | Mg | -0.518 | -3.371 | -2.622 | Mg | -0.307 | -2.858 | 0.000 |
| Mg | -1.953 | -4.302 | 0.000 | Mg | -0.518 | -0.578 | 1.514 | Mg | 0.699 | -1.524 | 2.576 |
| Mg | -3.424 | -2.109 | 1.538 | Mg | 0.975 | -2.807 | 0.000 | Mg | 0.699 | -1.524 | -2.576 |
| Mg | -0.793 | -3.227 | 2.613 | Mg | 2.324 | -0.036 | 0.000 | Mg | 0.699 | 1.321 | 1.567 |
| Mg | -0.671 | 2.557 | 0.00 | Mg | -0.518 | -3.371 | 2.622 | Mg | 2.128 | -0.873 | 0.000 |

| $Sr_2Mg_{11}$: | | | | 11a: | | | | 11b: | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Sr | 1.829 | -3.006 | 0.000 | Sr | 0.056 | -1.985 | 2.939 | Sr | -2.739 | -2.347 | 0.067 |
| Sr | -3.117 | -0.415 | 0.000 | Sr | 0.056 | -1.985 | -2.940 | Sr | -0.794 | 3.302 | 0.134 |
| Mg | 3.244 | 3.480 | 0.000 | Mg | 1.383 | 1.435 | -2.439 | Mg | -0.135 | -1.233 | -2.071 |
| Mg | -1.372 | 2.298 | 1.522 | Mg | 1.383 | 1.435 | 2.439 | Mg | 3.870 | -1.566 | 0.998 |
| Mg | 0.378 | 4.263 | 0.000 | Mg | -2.631 | 3.259 | 0.000 | Mg | -2.746 | 0.786 | -1.710 |
| Mg | 1.512 | 2.371 | 2.262 | Mg | -0.049 | 3.943 | -1.479 | Mg | 4.467 | 0.735 | -0.832 |
| Mg | 0.178 | -0.234 | -1.622 | Mg | -1.881 | -2.406 | 0.000 | Mg | 2.902 | -1.571 | -1.933 |
| Mg | 2.565 | 0.484 | 0.000 | Mg | 0.816 | -3.649 | 0.000 | Mg | -0.248 | 0.033 | 0.846 |
| Mg | -1.372 | 2.298 | -1.522 | Mg | 2.412 | 2.916 | 0.000 | Mg | 1.489 | 1.227 | -1.570 |
| Mg | 1.512 | 2.371 | -2.262 | Mg | -1.435 | 0.936 | 1.503 | Mg | -3.333 | 0.955 | 1.160 |
| Mg | 0.178 | -0.234 | 1.622 | Mg | 1.129 | -0.180 | 0.000 | Mg | 1.553 | -1.147 | 2.892 |
| Mg | -1.372 | -3.132 | -1.472 | Mg | -0.049 | 3.943 | 1.479 | Mg | 2.307 | 1.389 | 1.319 |
| Mg | -1.372 | -3.132 | 1.472 | Mg | -1.435 | 0.936 | -1.503 | Mg | 1.061 | -2.633 | 0.265 |

| $Sr_2Mg_{12}$: | | | | 12a: | | | | 12b: | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Sr | -1.958 | -2.094 | -1.089 | Sr | 1.959 | -2.095 | -1.087 | Sr | 0.350 | -3.046 | 0.000 |
| Sr | 3.211 | 1.365 | -0.664 | Sr | -3.211 | 1.364 | -0.665 | Sr | 0.921 | 3.144 | 0.000 |
| Mg | -0.990 | 1.828 | 2.638 | Mg | 0.129 | 3.055 | -0.711 | Mg | 2.225 | -0.098 | -1.468 |
| Mg | 1.556 | -0.344 | 2.975 | Mg | -0.152 | 0.261 | 0.364 | Mg | -0.331 | 0.160 | 0.000 |
| Mg | 0.738 | -3.110 | 1.184 | Mg | -3.414 | -1.670 | 1.017 | Mg | 1.061 | -1.819 | 3.590 |
| Mg | 0.045 | 0.388 | -2.550 | Mg | -0.044 | 0.384 | -2.551 | Mg | 0.190 | 1.314 | -3.381 |
| Mg | -2.708 | 3.370 | 0.688 | Mg | 3.544 | 0.466 | 0.967 | Mg | 0.190 | 1.314 | 3.381 |
| Mg | 0.152 | 0.262 | 0.365 | Mg | 0.987 | 1.830 | 2.638 | Mg | -1.687 | -1.040 | -2.844 |
| Mg | -3.546 | 0.464 | 0.967 | Mg | 1.480 | -1.332 | 2.269 | Mg | -2.193 | 1.932 | 1.656 |
| Mg | -2.729 | 1.433 | -1.774 | Mg | -1.556 | -0.341 | 2.975 | Mg | -2.885 | -1.047 | 0.000 |
| Mg | -1.480 | -1.331 | 2.268 | Mg | -1.707 | -2.036 | -1.518 | Mg | -2.193 | 1.932 | -1.656 |
| Mg | -0.130 | 3.055 | -0.711 | Mg | 2.730 | 1.434 | -1.775 | Mg | -1.687 | -1.040 | 2.844 |
| Mg | 1.707 | -2.035 | -1.518 | Mg | 2.706 | 3.372 | 0.688 | Mg | 2.225 | -0.098 | 1.468 |
| Mg | 3.414 | -1.670 | 1.017 | Mg | -0.738 | -3.109 | 1.186 | Mg | 1.061 | -1.819 | -3.590 |

| $Sr_2Mg_{13}$: | | | | 13a: | | | | 13b: | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| Sr | 3.081 | 0.000 | -1.007 | Sr | -2.963 | -0.957 | -1.294 | Sr | -0.327 | -2.421 | 1.411 |
| Sr | -3.081 | 0.000 | -1.007 | Sr | -0.123 | -2.752 | 1.373 | Sr | -2.901 | -1.099 | -1.610 |
| Mg | 1.557 | 3.183 | -0.461 | Mg | 0.697 | -0.952 | -2.007 | Mg | 3.903 | -0.715 | -1.698 |
| Mg | -1.557 | 3.183 | -0.461 | Mg | -0.122 | 0.496 | 0.520 | Mg | 4.311 | 1.782 | -0.145 |
| Mg | 1.557 | -3.183 | -0.461 | Mg | 2.867 | -0.725 | 1.147 | Mg | 1.006 | -1.629 | -1.872 |
| Mg | -1.557 | -3.183 | -0.461 | Mg | -3.021 | 2.312 | -0.017 | Mg | -3.118 | 2.247 | -0.560 |
| Mg | 0.000 | -3.965 | 2.140 | Mg | 3.752 | -0.424 | -1.870 | Mg | 2.017 | 1.644 | -2.139 |
| Mg | -1.714 | -1.561 | 2.187 | Mg | -1.070 | 1.804 | -2.243 | Mg | 2.546 | -0.288 | 1.246 |
| Mg | 0.000 | 1.643 | -2.498 | Mg | -0.372 | 3.818 | -0.090 | Mg | 2.885 | -3.034 | 0.041 |
| Mg | -1.714 | 1.561 | 2.187 | Mg | 4.449 | 1.658 | 0.231 | Mg | -1.370 | 3.219 | 1.728 |
| Mg | 1.714 | -1.561 | 2.187 | Mg | 1.946 | 2.009 | -1.459 | Mg | 1.606 | 2.711 | 1.039 |
| Mg | 0.000 | 3.965 | 2.140 | Mg | -2.731 | -0.032 | 2.001 | Mg | -0.028 | 0.800 | 2.837 |
| Mg | 0.000 | 0.000 | 0.192 | Mg | 1.876 | 2.259 | 1.798 | Mg | -0.255 | 0.627 | -0.350 |
| Mg | 0.000 | -1.643 | -2.498 | Mg | -1.142 | 2.556 | 2.534 | Mg | -2.776 | 0.244 | 1.744 |
| Mg | 1.714 | 1.561 | 2.187 | Mg | 2.640 | -3.033 | -0.796 | Mg | -0.500 | 3.538 | -1.241 |
| $Sr_2Mg_{14}$: | | | | 14a: | | | | 14b: | | | |
| Sr | 0.064 | -1.333 | 2.990 | Sr | -3.941 | -0.628 | -0.656 | Sr | -4.166 | 0.000 | -0.302 |
| Sr | 0.064 | -1.333 | -2.990 | Sr | 4.793 | -0.033 | -0.087 | Sr | 1.915 | -0.000 | -2.470 |
| Mg | 0.065 | 0.245 | 0.000 | Mg | 2.025 | 2.312 | 0.397 | Mg | 0.617 | -0.000 | 0.638 |
| Mg | 3.146 | 2.311 | 0.000 | Mg | 1.732 | 0.123 | -1.957 | Mg | 1.183 | 2.647 | 2.184 |
| Mg | -3.334 | 2.063 | 0.000 | Mg | -0.726 | 0.612 | -0.406 | Mg | 3.568 | 1.531 | 0.498 |
| Mg | 3.244 | -0.332 | 1.531 | Mg | 0.089 | 1.623 | 2.617 | Mg | 1.378 | -3.020 | -0.827 |
| Mg | 1.807 | -2.414 | 0.000 | Mg | -0.606 | 3.836 | 0.800 | Mg | 2.714 | -0.000 | 2.908 |
| Mg | 3.244 | -0.332 | -1.531 | Mg | -0.516 | -2.235 | -1.437 | Mg | 3.567 | -1.532 | 0.498 |
| Mg | 1.579 | 1.911 | -2.424 | Mg | 2.498 | -2.616 | -0.909 | Mg | -1.165 | 3.976 | 0.411 |
| Mg | 1.579 | 1.911 | 2.424 | Mg | -2.772 | 2.768 | -1.172 | Mg | 1.182 | -2.647 | 2.184 |
| Mg | -3.226 | -0.577 | -1.528 | Mg | 1.656 | -0.748 | 1.321 | Mg | -1.270 | 1.545 | -1.456 |
| Mg | -1.742 | 1.765 | -2.428 | Mg | -2.767 | 1.813 | 1.721 | Mg | -1.793 | -1.533 | 1.806 |
| Mg | -0.249 | 3.172 | 0.000 | Mg | 0.179 | 2.957 | -2.040 | Mg | -1.167 | -3.975 | 0.411 |
| Mg | -1.742 | 1.765 | 2.428 | Mg | 0.453 | -3.545 | 1.164 | Mg | -1.270 | -1.545 | -1.456 |
| Mg | -3.226 | -0.577 | 1.528 | Mg | -2.480 | -3.676 | 0.326 | Mg | -1.793 | 1.534 | 1.805 |
| Mg | -1.553 | -2.466 | 0.000 | Mg | -1.465 | -1.132 | 1.928 | Mg | 1.379 | 3.019 | -0.827 |
| $Sr_2Mg_{15}$: | | | | 15a: | | | | 15b: | | | |
| Sr | 0.000 | 4.476 | -0.585 | Sr | -0.815 | 1.896 | -3.228 | Sr | 0.000 | 4.211 | -1.336 |
| Sr | 0.000 | -4.476 | -0.585 | Sr | 0.814 | -1.896 | -3.228 | Sr | 0.000 | -4.211 | -1.336 |
| Mg | 0.000 | 0.000 | 0.167 | Mg | -2.852 | -0.202 | 1.705 | Mg | 2.218 | -0.388 | 2.352 |
| Mg | 0.000 | 2.329 | 2.215 | Mg | 1.425 | -0.548 | 4.337 | Mg | 0.825 | -1.268 | -3.088 |
| Mg | -2.672 | 2.600 | 0.762 | Mg | -1.968 | -0.863 | -1.259 | Mg | -2.349 | 1.646 | -0.486 |
| Mg | -1.545 | 1.564 | -1.927 | Mg | 2.928 | -1.972 | -0.435 | Mg | 1.900 | 1.259 | -1.619 |
| Mg | 3.686 | 0.000 | -0.400 | Mg | 2.067 | -2.747 | 2.345 | Mg | 0.000 | 0.000 | 0.395 |
| Mg | 2.672 | 2.600 | 0.762 | Mg | -1.425 | 0.548 | 4.337 | Mg | -0.825 | 1.268 | -3.088 |
| Mg | -2.091 | 0.000 | 2.286 | Mg | 0.000 | 2.910 | 0.075 | Mg | 1.715 | 2.477 | 1.226 |
| Mg | -3.686 | 0.000 | -0.400 | Mg | 1.968 | 0.863 | -1.259 | Mg | 0.322 | 1.472 | 3.785 |
| Mg | -1.545 | -1.564 | -1.928 | Mg | 2.852 | 0.202 | 1.705 | Mg | -1.182 | 3.285 | 1.866 |
| Mg | 1.545 | 1.564 | -1.927 | Mg | -0.814 | -2.144 | 2.987 | Mg | -1.900 | -1.25 | -1.619 |
| Mg | 2.091 | 0.000 | 2.285 | Mg | 0.000 | 0.000 | 0.938 | Mg | 2.349 | -1.646 | -0.486 |
| Mg | 1.545 | -1.564 | -1.927 | Mg | 0.814 | 2.144 | 2.987 | Mg | -2.218 | 0.388 | 2.352 |
| Mg | 2.672 | -2.600 | 0.762 | Mg | -2.928 | 1.972 | -0.435 | Mg | -1.715 | -2.477 | 1.224 |
| Mg | 0.000 | -2.329 | 2.215 | Mg | 0.000 | -2.910 | 0.075 | Mg | 1.182 | -3.285 | 1.866 |
| Mg | -2.672 | -2.600 | 0.762 | Mg | -2.067 | 2.747 | 2.345 | Mg | -0.322 | -1.472 | 3.785 |

$Sr_2Mg_{10}^-$:

| | | | |
|---|---|---|---|
| Sr | 2.816 | 1.884 | 0.000 |
| Sr | 3.135 | -2.166 | 0.000 |
| Mg | -2.520 | -1.720 | 1.492 |
| Mg | -0.156 | -3.208 | 0.000 |
| Mg | -3.692 | 3.068 | 0.000 |
| Mg | -2.520 | -1.720 | -1.492 |
| Mg | 0.129 | -0.169 | 1.515 |
| Mg | -4.436 | 0.111 | 0.000 |
| Mg | 0.129 | -0.169 | -1.515 |
| Mg | -0.737 | 2.330 | 0.000 |
| Mg | -2.520 | 1.185 | -2.206 |
| Mg | -2.520 | 1.185 | 2.206 |

$Sr_2Mg_{11}^-$:

| | | | |
|---|---|---|---|
| Sr | -2.621 | -2.457 | 0.000 |
| Sr | 2.934 | -1.253 | 0.000 |
| Mg | -2.226 | 4.181 | 0.000 |
| Mg | -2.416 | 1.159 | 0.000 |
| Mg | 0.474 | -3.357 | 1.470 |
| Mg | 1.984 | 1.915 | -1.501 |
| Mg | -0.819 | 2.692 | 2.236 |
| Mg | -0.819 | 2.692 | -2.236 |
| Mg | 0.474 | -3.357 | -1.470 |
| Mg | -0.200 | -0.166 | -1.565 |
| Mg | -0.200 | -0.166 | 1.565 |
| Mg | 0.772 | 4.241 | 0.000 |
| Mg | 1.984 | 1.915 | 1.501 |

$Sr_2Mg_{12}^-$:

| | | | |
|---|---|---|---|
| Sr | -1.839 | -1.477 | -1.791 |
| Sr | 3.510 | 1.127 | -0.206 |
| Mg | 0.346 | 3.259 | -0.167 |
| Mg | -2.128 | -1.781 | 1.592 |
| Mg | -1.664 | 0.929 | 3.040 |
| Mg | -2.263 | 3.261 | 1.252 |
| Mg | -3.677 | 0.607 | 0.554 |
| Mg | 1.796 | -1.755 | -1.590 |
| Mg | 0.544 | 0.971 | -2.317 |
| Mg | 2.924 | -2.004 | 1.255 |
| Mg | 0.259 | -3.310 | 0.521 |
| Mg | -2.206 | 2.117 | -1.593 |
| Mg | 0.158 | 0.298 | 0.655 |
| Mg | 0.618 | -1.483 | 3.122 |

10a:

| | | | |
|---|---|---|---|
| Sr | 2.816 | 1.884 | 0.000 |
| Sr | 3.135 | -2.166 | 0.000 |
| Mg | -2.520 | -1.720 | 1.492 |
| Mg | -0.158 | -3.208 | 0.000 |
| Mg | -3.692 | 3.068 | 0.000 |
| Mg | -2.520 | -1.720 | -1.492 |
| Mg | 0.129 | -0.169 | 1.515 |
| Mg | -4.436 | 0.111 | 0.000 |
| Mg | 0.129 | -0.169 | -1.515 |
| Mg | -0.737 | 2.330 | 0.000 |
| Mg | -2.520 | 1.185 | -2.206 |
| Mg | -2.520 | 1.185 | 2.206 |

11a:

| | | | |
|---|---|---|---|
| Sr | 0.902 | 3.346 | 0.099 |
| Sr | 2.795 | -2.387 | 0.080 |
| Mg | -1.567 | -1.038 | 2.878 |
| Mg | 3.348 | 0.985 | 1.108 |
| Mg | 0.003 | -1.462 | -2.033 |
| Mg | -3.954 | -1.436 | 1.060 |
| Mg | -1.437 | 1.165 | -1.613 |
| Mg | -1.213 | -2.700 | 0.378 |
| Mg | 2.550 | 0.692 | -1.715 |
| Mg | 0.276 | -0.003 | 0.757 |
| Mg | -2.267 | 1.486 | 1.257 |
| Mg | -4.412 | 0.889 | -0.818 |
| Mg | -3.036 | -1.614 | -1.829 |

12a:

| | | | |
|---|---|---|---|
| Sr | -3.134 | -1.752 | -0.719 |
| Sr | 0.632 | 3.363 | -0.906 |
| Mg | 3.258 | -2.670 | -0.511 |
| Mg | -2.659 | 1.905 | -0.566 |
| Mg | 1.680 | 1.010 | 1.561 |
| Mg | -0.736 | -1.024 | 2.070 |
| Mg | 2.832 | 0.322 | -1.370 |
| Mg | -1.051 | 2.487 | 2.026 |
| Mg | 1.280 | -2.067 | -2.609 |
| Mg | 2.128 | -2.047 | 2.239 |
| Mg | -0.064 | -0.041 | -0.806 |
| Mg | -3.421 | 0.473 | 1.957 |
| Mg | 4.364 | -0.348 | 1.138 |
| Mg | 0.313 | -3.104 | 0.018 |

10b:

| | | | |
|---|---|---|---|
| Sr | 1.816 | 2.723 | 0.337 |
| Sr | 3.523 | -1.041 | -0.359 |
| Mg | -2.247 | -0.626 | 2.825 |
| Mg | -2.124 | -2.515 | 0.471 |
| Mg | -0.088 | -1.874 | -1.659 |
| Mg | -0.759 | 1.110 | -1.628 |
| Mg | -1.883 | 1.849 | 1.028 |
| Mg | 0.112 | -0.347 | 0.959 |
| Mg | -4.303 | -0.359 | 0.580 |
| Mg | -3.754 | 1.927 | -1.389 |
| Mg | 1.135 | -3.479 | 0.916 |
| Mg | -2.996 | -1.014 | -2.035 |

11b:

| | | | |
|---|---|---|---|
| Sr | -0.750 | -1.893 | 3.020 |
| Sr | -0.750 | -1.893 | -3.020 |
| Mg | 1.685 | 0.395 | -1.507 |
| Mg | -1.229 | 3.475 | 0.000 |
| Mg | 0.877 | -2.775 | 0.000 |
| Mg | -0.750 | 1.855 | 2.502 |
| Mg | 1.398 | 3.699 | 1.503 |
| Mg | -1.075 | 0.193 | 0.000 |
| Mg | -2.069 | -3.015 | 0.000 |
| Mg | -0.750 | 1.855 | -2.502 |
| Mg | 3.582 | 2.213 | 0.000 |
| Mg | 1.398 | 3.699 | -1.503 |
| Mg | 1.685 | 0.395 | 1.507 |

12b:

| | | | |
|---|---|---|---|
| Sr | 2.243 | -2.684 | -0.868 |
| Sr | 1.663 | 2.857 | -1.063 |
| Mg | -3.672 | -1.754 | 0.635 |
| Mg | -1.819 | -0.097 | 2.539 |
| Mg | -1.811 | 1.455 | -1.719 |
| Mg | -4.155 | -0.367 | -1.957 |
| Mg | -1.561 | -1.842 | -1.754 |
| Mg | 0.080 | -0.009 | 0.015 |
| Mg | 3.436 | 0.277 | 0.580 |
| Mg | 1.489 | 1.840 | 2.375 |
| Mg | 1.677 | -1.252 | 2.475 |
| Mg | -1.268 | 2.577 | 1.135 |
| Mg | -0.858 | -2.641 | 1.146 |
| Mg | -3.910 | 1.267 | 0.645 |

$Sr_2Mg_{13}^-$:

| | | | |
|---|---|---|---|
| Sr | 2.941 | -1.254 | 0.000 |
| Sr | -1.513 | -2.098 | 0.000 |
| Mg | -0.524 | 1.392 | 3.878 |
| Mg | -0.524 | 1.392 | -3.878 |
| Mg | 0.290 | 0.800 | 0.000 |
| Mg | -2.173 | -1.187 | -3.431 |
| Mg | -2.446 | 1.147 | -1.540 |
| Mg | -0.173 | 3.355 | -1.663 |
| Mg | 2.175 | 1.451 | -2.441 |
| Mg | 0.735 | -1.251 | -2.730 |
| Mg | -2.173 | -1.188 | 3.431 |
| Mg | -2.446 | 1.147 | 1.540 |
| Mg | -0.173 | 3.355 | 1.663 |
| Mg | 2.175 | 1.451 | 2.441 |
| Mg | 0.735 | -1.251 | 2.730 |

$Sr_2Mg_{14}^-$:

| | | | |
|---|---|---|---|
| Sr | 3.047 | 0.000 | -1.364 |
| Sr | -3.047 | 0.000 | -1.364 |
| Mg | 0.000 | 0.000 | 0.216 |
| Mg | 0.000 | 1.680 | -2.449 |
| Mg | -2.515 | 1.610 | 1.892 |
| Mg | 2.515 | 1.610 | 1.892 |
| Mg | -2.515 | -1.610 | 1.892 |
| Mg | 2.515 | -1.610 | 1.892 |
| Mg | 0.000 | -1.680 | -2.449 |
| Mg | -1.544 | -3.191 | -0.441 |
| Mg | 0.000 | -3.137 | 2.178 |
| Mg | 1.544 | -3.191 | -0.441 |
| Mg | -1.544 | 3.191 | -0.441 |
| Mg | 0.000 | 3.137 | 2.178 |
| Mg | 1.544 | 3.191 | -0.441 |
| Mg | 0.000 | 0.000 | 3.164 |

$Sr_2Mg_{15}^-$:

| | | | |
|---|---|---|---|
| Sr | 0.000 | 4.401 | -0.571 |
| Sr | 0.000 | -4.401 | -0.571 |
| Mg | 2.643 | -2.548 | 0.775 |
| Mg | 3.641 | 0.000 | -0.461 |
| Mg | -2.643 | 2.548 | 0.775 |
| Mg | 0.000 | -2.195 | 2.305 |
| Mg | 2.230 | 0.000 | 2.340 |
| Mg | -2.230 | 0.000 | 2.340 |
| Mg | 0.000 | 2.195 | 2.305 |
| Mg | 1.572 | 1.531 | -2.007 |
| Mg | 0.000 | 0.000 | 0.173 |
| Mg | 2.643 | 2.548 | 0.775 |
| Mg | -2.643 | -2.548 | 0.775 |
| Mg | -1.572 | -1.531 | -2.007 |
| Mg | -1.572 | 1.531 | -2.007 |
| Mg | 1.572 | -1.531 | -2.007 |
| Mg | -3.641 | 0.000 | -0.461 |

13a:

| | | | |
|---|---|---|---|
| Sr | -1.962 | 0.373 | -2.329 |
| Sr | 0.678 | -2.551 | -0.056 |
| Mg | -1.929 | -1.564 | 2.466 |
| Mg | 1.057 | 3.038 | -1.117 |
| Mg | 1.606 | 0.190 | -2.262 |
| Mg | 3.867 | -1.433 | -1.275 |
| Mg | 3.286 | -0.402 | 1.425 |
| Mg | 2.220 | 2.456 | 1.767 |
| Mg | -2.133 | 2.918 | 0.244 |
| Mg | 3.729 | 1.723 | -0.734 |
| Mg | -0.038 | 0.694 | 0.436 |
| Mg | 0.790 | -0.262 | 3.066 |
| Mg | -1.807 | 1.506 | 2.997 |
| Mg | -3.672 | 0.390 | 0.800 |
| Mg | -2.911 | -2.357 | -0.260 |

14a:

| | | | |
|---|---|---|---|
| Sr | 0.000 | 4.254 | 0.409 |
| Sr | 0.000 | -4.254 | 0.409 |
| Mg | 0.000 | 0.000 | 4.133 |
| Mg | -1.569 | -1.602 | 2.169 |
| Mg | 1.569 | 1.602 | 2.169 |
| Mg | 2.240 | -1.844 | -0.851 |
| Mg | 1.476 | 0.000 | -3.144 |
| Mg | 0.000 | 2.678 | -2.787 |
| Mg | -2.240 | 1.844 | -0.851 |
| Mg | -2.240 | -1.844 | -0.851 |
| Mg | 1.569 | -1.602 | 2.169 |
| Mg | 0.000 | 0.000 | -0.129 |
| Mg | -1.569 | 1.602 | 2.169 |
| Mg | 0.000 | -2.678 | -2.787 |
| Mg | 2.240 | 1.844 | -0.851 |
| Mg | -1.476 | 0.000 | -3.144 |

15a:

| | | | |
|---|---|---|---|
| Sr | 1.533 | -2.198 | -1.568 |
| Sr | 3.768 | 0.635 | 0.430 |
| Mg | -0.569 | 0.092 | 0.190 |
| Mg | -1.366 | 3.035 | 1.236 |
| Mg | -3.366 | -2.203 | 1.333 |
| Mg | -0.784 | 3.341 | -1.825 |
| Mg | -0.558 | -3.395 | 1.044 |
| Mg | 1.455 | 3.270 | 0.276 |
| Mg | 1.711 | -1.676 | 2.047 |
| Mg | 0.905 | 1.328 | 2.533 |
| Mg | -3.332 | 0.781 | 1.681 |
| Mg | -3.473 | 2.494 | -0.826 |
| Mg | -4.175 | -0.415 | -1.036 |
| Mg | -1.530 | 0.435 | -2.554 |
| Mg | -1.943 | -2.399 | -1.400 |
| Mg | 1.423 | 1.287 | -2.081 |
| Mg | -1.187 | -1.026 | 2.983 |

13b:

| | | | |
|---|---|---|---|
| Sr | -2.867 | 1.209 | -1.325 |
| Sr | 2.858 | -1.296 | -1.248 |
| Mg | -2.948 | -2.224 | -0.296 |
| Mg | -0.007 | -0.002 | 0.056 |
| Mg | -0.154 | -3.089 | 0.267 |
| Mg | -3.885 | -0.194 | 1.763 |
| Mg | 0.908 | 1.460 | -2.484 |
| Mg | 0.153 | 3.094 | 0.065 |
| Mg | -0.924 | -1.631 | -2.381 |
| Mg | -1.681 | -1.994 | 2.616 |
| Mg | 2.945 | 2.199 | -0.460 |
| Mg | -1.290 | 1.294 | 2.371 |
| Mg | 1.312 | -1.123 | 2.440 |
| Mg | 3.901 | 0.318 | 1.726 |
| Mg | 1.699 | 2.171 | 2.470 |

14b:

| | | | |
|---|---|---|---|
| Sr | -0.746 | 3.440 | 0.000 |
| Sr | -0.084 | -3.559 | 0.000 |
| Mg | -1.939 | 1.123 | 2.452 |
| Mg | 3.980 | 0.584 | 0.000 |
| Mg | 2.770 | 3.395 | 0.000 |
| Mg | -3.511 | 1.055 | 0.000 |
| Mg | 0.051 | -1.253 | -2.759 |
| Mg | 0.051 | -1.253 | 2.759 |
| Mg | -2.780 | -1.615 | 1.484 |
| Mg | 2.718 | -1.763 | -1.474 |
| Mg | -0.253 | -0.030 | 0.000 |
| Mg | 1.772 | 1.196 | -1.941 |
| Mg | 2.718 | -1.763 | 1.474 |
| Mg | -2.780 | -1.615 | -1.484 |
| Mg | -1.939 | 1.123 | -2.452 |
| Mg | 1.772 | 1.196 | 1.941 |

15b:

| | | | |
|---|---|---|---|
| Sr | 3.177 | 1.962 | 0.492 |
| Sr | 3.176 | -1.963 | -0.492 |
| Mg | -0.882 | 0.000 | 0.000 |
| Mg | -1.711 | -1.655 | 2.469 |
| Mg | -1.710 | 1.654 | -2.469 |
| Mg | 1.181 | -0.492 | 2.212 |
| Mg | 0.425 | -3.285 | 1.170 |
| Mg | -2.308 | -3.422 | -0.056 |
| Mg | -4.258 | -1.289 | 0.795 |
| Mg | -2.877 | 1.211 | 2.000 |
| Mg | -0.072 | 2.417 | 1.811 |
| Mg | -2.878 | -1.211 | -2.000 |
| Mg | -4.258 | 1.291 | -0.795 |
| Mg | -2.307 | 3.422 | 0.056 |
| Mg | 0.426 | 3.285 | -1.170 |
| Mg | 1.181 | 0.492 | -2.211 |
| Mg | -0.072 | -2.411 | -1.811 |

**S10.** The xyz data of each structure in $Sr_2Mg_n^{0/-}$ ($n$=10-15) clusters.