Electronic Supplementary Material (ESI) for Materials Advances.


# Supplemental information 2

The space-group, lattice parameters, relative energy and spin magnetic moment are shown in the following tables. T, H, and P represent the types of initial structures. X means the structure is not in the group "three stable structures" mentioned in the paper. The order of THP represents their stability. For example, "PTX" means the planar type initial structure is the most stable, the 1T type one is the second stable, and the 1H type one is much more unstable than the others. In other words, X represents a structure whose relative energy exceed 0.03 Hartree ($\approx$ 0.82 eV) per the unit cell including 12 atoms. The space-groups of the obtained final structures for each initial states are also shown. The definitions of relative energies $\Delta E_1$ and $\Delta E_2$ are as follows: $\Delta E_1 = E_{\text{the second stable structure}} - E_{\text{the most stable structure}}$, and $\Delta E_2 = E_{\text{the third stable structure}} - E_{\text{the most stable structure}}$.

Table 1: List of stable structures

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $LiLi_2$ | HTX | $Cmmm(65)$ | $Amm2(38)$ | – | 5.97 | 7.76 | 49.0 | 6.03 | 6.52 | 57.8 | – | – | – | 0.160 | 4.548 | 0.0 | 0.0 | – |
| $LiMg_2$ | THX | $C2/m(12)$ | $Amm2(38)$ | – | 6.15 | 6.61 | 56.9 | 6.60 | 6.17 | 57.5 | – | – | – | 0.152 | 3.972 | 0.0 | 0.0 | – |
| $LiAl_2$ | HTX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 5.46 | 5.45 | 59.9 | 5.45 | 5.45 | 60.0 | – | – | – | 0.046 | 3.644 | 0.0 | 0.0 | – |
| $LiCl_2$ | PXX | – | – | $P2/m(10)$ | – | – | – | – | – | – | 9.13 | 11.15 | 55.1 | 1.509 | 1.725 | – | – | 0.0 |
| $LiSc_2$ | PXX | – | – | $Pmma(51)$ | – | – | – | – | – | – | 7.23 | 7.23 | 52.5 | 3.306 | 3.363 | – | – | 0.0 |
| $LiMn_2$ | HXX | – | $P\bar{1}(2)$ | – | – | – | – | 7.75 | 10.43 | 29.6 | – | – | – | 2.707 | 5.736 | – | 32.3 | – |
| $LiAg_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.83 | 5.84 | 59.9 | – | – | – | 3.253 | 3.264 | – | 0.0 | – |
| $LiCd_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 6.00 | 9.16 | 40.2 | – | – | – | 2.170 | 2.316 | – | 0.0 | – |
| $LiIn_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.58 | 9.07 | 43.7 | – | – | – | 1.741 | 2.532 | – | 0.0 | – |
| $LiSn_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 8.75 | 6.47 | 42.0 | – | – | – | 3.741 | 3.823 | – | 0.0 | – |
| $LiCs_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 12.59 | 12.52 | 46.3 | – | – | – | 0.865 | 1.607 | – | 0.0 | – |
| $LiBa_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 12.24 | 8.58 | 44.8 | – | – | – | 1.109 | 6.245 | – | 0.0 | – |
| $LiHg_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.35 | 9.05 | 44.4 | – | – | – | 1.491 | 1.549 | – | 0.0 | – |
| $LiBi_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 10.80 | 8.20 | 39.4 | – | – | – | 1.327 | 1.585 | – | 0.0 | – |
| $BeBe_2$ | HTX | $Cmmm(65)$ | $P\bar{6}m2(187)$ | – | 4.24 | 4.73 | 56.1 | 4.39 | 4.39 | 120.0 | – | – | – | 0.167 | 6.772 | 0.0 | 0.0 | – |
| $BeB_2$ | PXX | – | – | $Pmmn(59)$ | – | – | – | – | – | – | 6.03 | 6.01 | 60.1 | 1.909 | 2.423 | – | – | 0.0 |
| $BeO_2$ | HXX | – | $P1(1)$ | – | – | – | – | 5.58 | 5.74 | 60.2 | – | – | – | 1.771 | 1.878 | – | 2.0 | – |
| $BeMg_2$ | THX | $P\bar{1}(2)$ | $Amm2(38)$ | – | 6.15 | 7.68 | 52.1 | 6.11 | 6.31 | 60.8 | – | – | – | 0.494 | 6.478 | 0.0 | 0.0 | – |
| $BeAl_2$ | HXX | – | $Pmm2(25)$ | – | – | – | – | 5.30 | 5.45 | 59.0 | – | – | – | 1.429 | 3.864 | – | 0.0 | – |
| $BeSi_2$ | HTX | $C2/m(12)$ | $Amm2(38)$ | – | 7.49 | 7.49 | 39.3 | 7.47 | 7.46 | 39.7 | – | – | – | 0.581 | 4.407 | 0.0 | 0.0 | – |
| $BeP_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 6.79 | 6.79 | 60.0 | – | – | – | 1.270 | 1.864 | – | 0.0 | – |
| $BeS_2$ | PHX | – | $C2(5)$ | $P1(1)$ | – | – | – | 7.15 | 7.16 | 78.3 | 8.85 | 6.88 | 51.6 | 0.065 | 3.706 | – | 0.0 | 0.0 |
| $BeCl_2$ | PHX | – | $P\bar{4}m2(115)$ | $Pccm(49)$ | – | – | – | 6.68 | 6.68 | 86.6 | 7.54 | 7.58 | 91.4 | 0.457 | 3.017 | – | 0.0 | 0.0 |
| $BeK_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 9.21 | 8.57 | 62.5 | 2.140 | 4.508 | – | – | 0.0 |
| $BeCa_2$ | PTH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 8.62 | 8.62 | 58.8 | 7.77 | 7.76 | 59.9 | 8.32 | 8.33 | 60.2 | 0.020 | 0.231 | 0.0 | 0.0 | 0.0 |
| $BeSc_2$ | HPX | – | $P4/mmm(123)$ | $P\bar{1}(2)$ | – | – | – | 6.24 | 8.83 | 45.1 | 6.32 | 7.48 | 54.7 | 0.259 | 0.904 | – | 0.0 | 2.3 |
| $BeV_2$ | HXX | – | $Pbcm(57)$ | – | – | – | – | 5.68 | 7.25 | 38.3 | – | – | – | 2.015 | 3.622 | – | 0.0 | – |
| $BeCr_2$ | TXX | $Cm(8)$ | – | – | 6.78 | 6.78 | 24.9 | – | – | – | – | – | – | 1.808 | 15.575 | 1.8 | – | – |
| $BeMn_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 7.38 | 5.24 | 45.2 | – | – | – | 0.953 | 8.523 | – | 29.3 | – |
| $BeGe_2$ | HTX | $P\bar{3}m1(164)$ | $Amm2(38)$ | – | 7.45 | 7.45 | 59.9 | 7.70 | 7.69 | 41.5 | – | – | – | 0.675 | 1.290 | 0.0 | 0.0 | – |
| $BeSe_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 10.46 | 6.44 | 52.1 | 2.049 | 3.159 | – | – | 0.0 |
| $BeRb_2$ | THX | $P\bar{3}m1(164)$ | $Amm2(38)$ | – | 10.74 | 10.74 | 56.9 | 10.59 | 10.59 | 49.0 | – | – | – | 0.542 | 2.225 | 0.0 | 0.0 | – |
| $BeZr_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 6.05 | 8.11 | 41.6 | 1.302 | 2.180 | – | – | 0.0 |
| $BeMo_2$ | HPX | – | $P\bar{1}(2)$ | $P\bar{1}(2)$ | – | – | – | 6.88 | 8.22 | 38.5 | 9.60 | 7.09 | 32.7 | 0.481 | 1.048 | – | 0.0 | 0.0 |
| $BeRu_2$ | TXX | $C2/m(12)$ | – | – | 8.70 | 7.49 | 30.6 | – | – | – | – | – | – | 1.128 | 9.799 | 0.0 | – | – |
| $BeRh_2$ | THX | $C2/m(12)$ | $P\bar{6}m2(187)$ | – | 6.32 | 5.43 | 49.5 | 5.32 | 5.32 | 59.8 | – | – | – | 0.239 | 1.681 | 0.0 | 0.0 | – |
| $BeAg_2$ | THX | $P4/mmm(123)$ | $Amm2(38)$ | – | 8.01 | 5.65 | 44.8 | 6.20 | 5.67 | 56.2 | – | – | – | 0.552 | 5.148 | 0.0 | 0.0 | – |
| $BeIn_2$ | HTX | $C2/m(12)$ | $P1(1)$ | – | 6.90 | 7.89 | 50.3 | 6.92 | 5.95 | 61.2 | – | – | – | 0.494 | 6.038 | 0.0 | 0.0 | – |
| $BeSb_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 7.71 | 7.71 | 59.2 | – | – | – | 1.290 | 1.822 | – | 0.0 | – |
| $BeTe_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{1}(2)$ | 7.05 | 7.05 | 56.5 | – | – | – | 10.97 | 8.25 | 67.0 | 0.282 | 1.756 | 0.0 | – | 0.0 |
| $BeI_2$ | HXX | – | $C222(21)$ | – | – | – | – | 7.77 | 10.22 | 49.1 | – | – | – | 2.537 | 3.411 | – | 0.0 | – |
| $BeCs_2$ | THX | $P\bar{3}m1(164)$ | $Amm2(38)$ | – | 10.99 | 10.99 | 59.2 | 11.24 | 11.25 | 50.2 | – | – | – | 0.787 | 2.815 | 0.0 | 0.0 | – |
| $BeBa_2$ | PTH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 10.03 | 10.03 | 57.0 | 8.97 | 8.96 | 58.2 | 9.87 | 9.85 | 58.8 | 0.007 | 0.278 | 0.0 | 0.0 | 0.0 |
| $BeHf_2$ | HXX | – | $P4mm(99)$ | – | – | – | – | 7.98 | 5.64 | 45.0 | – | – | – | 1.142 | 1.145 | – | 0.0 | – |
| $BeTa_2$ | HXX | – | $P2_1/m(11)$ | – | – | – | – | 6.35 | 5.61 | 55.3 | – | – | – | 7.349 | 8.785 | – | 0.0 | – |
| $BeW_2$ | HXX | – | $P\bar{1}(2)$ | – | – | – | – | 7.34 | 8.14 | 37.4 | – | – | – | 1.613 | 1.652 | – | 0.0 | – |
| $BeRe_2$ | TXX | $C2/m(12)$ | – | – | 6.98 | 6.98 | 41.2 | – | – | – | – | – | – | 1.327 | 3.902 | 0.0 | – | – |
| $BePt_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.51 | 5.52 | 60.0 | – | – | – | 1.509 | 11.273 | – | 0.0 | – |
| $BeAu_2$ | HTX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 6.13 | 6.10 | 54.9 | 6.08 | 6.09 | 55.7 | – | – | – | 0.104 | 0.949 | 0.0 | 0.0 | – |
| $BeTl_2$ | HTX | $P1(1)$ | $P1(1)$ | – | 6.29 | 8.79 | 48.2 | 7.00 | 6.15 | 59.0 | – | – | – | 0.040 | 4.767 | 0.0 | 0.0 | – |
| $BePb_2$ | PTH | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P\bar{3}m1(164)$ | 8.34 | 8.34 | 59.2 | 7.87 | 7.87 | 52.1 | 8.25 | 8.25 | 59.9 | 0.012 | 0.416 | 0.0 | 0.0 | 0.0 |
| $BeBi_2$ | HPX | – | $P\bar{6}m2(187)$ | $P1(1)$ | – | – | – | 7.90 | 7.89 | 59.7 | 8.65 | 8.01 | 47.7 | 0.342 | 1.070 | – | 0.0 | 0.0 |
| $BBe_2$ | TXX | $C2/m(12)$ | – | – | 4.04 | 5.97 | 59.4 | – | – | – | – | – | – | 1.451 | 1.965 | 0.0 | – | – |
| $BB_2$ | THX | $C2/m(12)$ | $Amm2(38)$ | – | 5.12 | 5.68 | 33.6 | 5.37 | 4.94 | 35.3 | – | – | – | 0.713 | 1.914 | 0.0 | 0.0 | – |
| $BF_2$ | TXX | $P\bar{1}(2)$ | – | – | 6.80 | 8.63 | 68.0 | – | – | – | – | – | – | 1.761 | 4.861 | 0.0 | – | – |
| $BMg_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.45 | 7.43 | 55.6 | – | – | – | 7.20 | 7.24 | 55.8 | 0.003 | 1.172 | 0.0 | – | 0.0 |
| $BAl_2$ | HTX | $C2/m(12)$ | $Amm2(38)$ | – | 6.48 | 6.65 | 59.2 | 6.66 | 6.34 | 45.2 | – | – | – | 0.492 | 2.832 | 0.0 | 0.0 | – |
| $BSi_2$ | TPX | $P\bar{3}m1(164)$ | – | $P2_1/m(11)$ | 6.43 | 6.42 | 60.0 | – | – | – | 7.80 | 7.16 | 89.9 | 0.443 | 1.111 | 0.0 | – | 0.0 |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $BP_2$ | TXX | $C2/m(12)$ | – | – | 7.19 | 7.19 | 52.4 | – | – | – | – | – | – | 3.719 | 4.235 | 0.0 | – | – |
| $BCl_2$ | HXX | – | $P1(1)$ | – | – | – | – | 8.10 | 7.03 | 79.3 | – | – | – | 5.713 | 5.724 | – | 0.0 | – |
| $BK_2$ | THX | $P\bar{3}m1(164)$ | $Amm2(38)$ | – | 10.11 | 10.12 | 57.7 | 9.22 | 9.21 | 52.3 | – | – | – | 0.565 | 2.933 | 11.1 | 3.4 | – |
| $BTi_2$ | PTX | $P\bar{3}m1(164)$ | – | $P1(1)$ | 6.16 | 6.17 | 60.1 | – | – | – | 7.35 | 7.10 | 36.3 | 0.451 | 3.307 | 0.0 | – | 0.0 |
| $BCr_2$ | HPX | – | $P2/m(10)$ | $P2_1/m(11)$ | – | – | – | 5.02 | 6.08 | 49.1 | 6.24 | 6.26 | 53.9 | 0.558 | 2.198 | – | 0.0 | 0.0 |
| $BMn_2$ | TXX | $P2_1/m(11)$ | – | – | 6.30 | 6.31 | 60.1 | – | – | – | – | – | – | 1.940 | 5.815 | 27.5 | – | – |
| $BNi_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 5.27 | 5.27 | 59.6 | 5.12 | 5.12 | 59.6 | – | – | – | 0.413 | 4.629 | 0.0 | 0.0 | – |
| $BGe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.71 | 6.71 | 60.0 | – | – | – | – | – | – | 0.916 | 1.964 | 0.0 | – | – |
| $BSe_2$ | HTX | $P1(1)$ | $Cm(8)$ | – | 8.00 | 6.40 | 49.8 | 6.32 | 6.18 | 77.4 | – | – | – | 0.665 | 5.197 | 0.0 | 0.0 | – |
| $BBr_2$ | TXX | $P1(1)$ | – | – | 9.54 | 7.93 | 73.5 | – | – | – | – | – | – | 3.011 | 3.019 | 0.0 | – | – |
| $BRb_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 10.45 | 10.46 | 58.3 | – | – | – | – | – | – | 2.549 | 3.286 | 11.0 | – | – |
| $BSr_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 16.42 | 15.21 | 16.1 | 3.136 | 4.685 | – | – | 0.0 |
| $BY_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.71 | 7.70 | 59.8 | – | – | – | – | – | – | 1.297 | 3.219 | 0.0 | – | – |
| $BNb_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.32 | 6.31 | 59.9 | – | – | – | – | – | – | 4.132 | 13.651 | 0.0 | – | – |
| $BRu_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.57 | 5.58 | 60.0 | – | – | – | 1.003 | 1.062 | – | 0.0 | – |
| $BRh_2$ | TPH | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 5.51 | 5.51 | 60.0 | 5.47 | 5.47 | 60.0 | 5.51 | 5.51 | 60.0 | 0.015 | 0.267 | 0.0 | 0.0 | 0.0 |
| $BPd_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 5.87 | 5.87 | 60.0 | 5.73 | 5.73 | 59.9 | – | – | – | 0.724 | 3.647 | 0.0 | 0.0 | – |
| $BAg_2$ | TXX | $Pmma(51)$ | – | – | 5.42 | 6.23 | 54.3 | – | – | – | – | – | – | 5.683 | 7.225 | 0.0 | – | – |
| $BCd_2$ | THX | $P\bar{1}(2)$ | $Pc(7)$ | – | 7.21 | 6.78 | 47.1 | 6.65 | 7.14 | 48.1 | – | – | – | 0.767 | 6.092 | 0.0 | 0.0 | – |
| $BSn_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.36 | 7.36 | 60.0 | – | – | – | – | – | – | 1.261 | 2.480 | 0.0 | – | – |
| $BSb_2$ | HXX | – | $Cm(8)$ | – | – | – | – | 7.20 | 8.84 | 51.6 | – | – | – | 1.994 | 2.447 | – | 0.0 | – |
| $BBa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.32 | 9.29 | 58.0 | – | – | – | 9.19 | 9.25 | 59.1 | 0.012 | 1.120 | 4.2 | – | 4.2 |
| $BHf_2$ | HTX | $P\bar{3}m1(164)$ | $Cm(8)$ | – | 6.59 | 6.59 | 60.0 | 6.32 | 6.33 | 53.9 | – | – | – | 0.060 | 2.799 | 0.0 | 0.0 | – |
| $BTa_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.25 | 6.25 | 60.0 | – | – | – | – | – | – | 1.487 | 4.771 | 0.0 | – | – |
| $BW_2$ | HTX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 6.16 | 6.16 | 60.0 | 5.77 | 5.77 | 59.9 | – | – | – | 0.647 | 4.847 | 0.0 | 0.0 | – |
| $BRe_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.66 | 5.66 | 60.0 | – | – | – | 4.914 | 7.263 | – | 0.0 | – |
| $BOs_2$ | HTX | $P2_1/m(11)$ | $Pmm2(25)$ | – | 5.50 | 5.41 | 59.4 | 5.48 | 5.42 | 59.6 | – | – | – | 0.517 | 11.452 | 0.0 | 0.0 | – |
| $BIr_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 5.43 | 5.43 | 60.0 | 5.46 | 5.46 | 60.0 | – | – | – | 0.226 | 13.691 | 0.0 | 0.0 | – |
| $BPt_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 5.71 | 5.72 | 60.0 | 5.68 | 5.69 | 60.0 | – | – | – | 0.524 | 2.810 | 0.0 | 0.0 | – |
| $BAu_2$ | PXX | – | – | $P4/mbm(127)$ | – | – | – | – | – | – | 11.00 | 8.09 | 47.1 | 1.297 | 1.488 | – | – | 0.0 |
| $BBi_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 8.53 | 8.92 | 57.6 | 0.982 | 1.241 | – | – | 0.0 |
| $CBe_2$ | PTX | $P\bar{3}m1(164)$ | – | $Pmmn(59)$ | 5.95 | 5.95 | 60.0 | – | – | – | 5.68 | 5.95 | 58.4 | 0.101 | 5.950 | 0.0 | – | 0.0 |
| $CB_2$ | TPX | $P\bar{1}(2)$ | – | $P1(1)$ | 5.21 | 5.53 | 36.1 | – | – | – | 5.28 | 6.63 | 83.9 | 0.085 | 3.588 | 0.0 | – | 0.0 |
| $CC_2$ | HXX | – | $Cm(8)$ | – | – | – | – | 4.27 | 4.94 | 30.1 | – | – | – | 4.542 | 4.575 | – | 0.0 | – |
| $CMg_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.16 | 7.16 | 59.6 | – | – | – | – | – | – | 2.292 | 3.812 | 0.0 | – | – |
| $CSi_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 7.72 | 8.38 | 74.2 | 1.633 | 1.697 | – | – | 0.0 |
| $CP_2$ | HXX | – | $P1(1)$ | – | – | – | – | 5.87 | 5.85 | 60.9 | – | – | – | 1.045 | 5.705 | – | 0.0 | – |
| $CS_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 11.20 | 10.63 | 100.3 | 2.451 | 2.971 | – | – | 0.0 |
| $CK_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 9.26 | 9.28 | 58.4 | – | – | – | – | – | – | 1.062 | 2.497 | 8.0 | – | – |
| $CCa_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.94 | 7.94 | 58.9 | – | – | – | – | – | – | 1.278 | 3.176 | 0.0 | – | – |
| $CTi_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.10 | 6.11 | 60.0 | – | – | – | – | – | – | 4.952 | 12.161 | 7.7 | – | – |
| $CV_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 5.76 | 5.77 | 60.0 | – | – | – | – | – | – | 3.652 | 4.154 | 0.0 | – | – |
| $CCr_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 5.62 | 5.65 | 59.8 | 5.27 | 5.26 | 59.8 | – | – | – | 0.352 | 7.427 | 0.0 | 0.0 | – |
| $CNi_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 5.80 | 5.80 | 59.7 | – | – | – | – | – | – | 2.230 | 2.701 | 0.0 | – | – |
| $CGe_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 6.25 | 6.26 | 60.0 | 6.19 | 6.19 | 60.0 | – | – | – | 0.382 | 1.232 | 0.0 | 0.0 | – |
| $CBr_2$ | PTH | $P1(1)$ | $Pmn2_1(31)$ | $Pc(7)$ | 8.51 | 8.37 | 66.6 | 8.16 | 8.17 | 72.3 | 10.68 | 10.70 | 103.8 | 0.047 | 0.084 | 0.0 | 0.0 | 0.0 |
| $CRb_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 9.55 | 9.56 | 58.4 | – | – | – | – | – | – | 0.985 | 2.050 | 8.1 | – | – |
| $CY_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{3}m1(164)$ | – | 7.10 | 7.11 | 60.1 | 7.10 | 7.11 | 60.1 | – | – | – | 0.003 | 5.500 | 0.0 | 0.0 | – |
| $CNb_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.25 | 6.26 | 60.0 | – | – | – | – | – | – | 3.403 | 8.561 | 0.0 | – | – |
| $CMo_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.73 | 5.71 | 59.6 | – | – | – | 0.933 | 6.554 | – | 0.0 | – |
| $CTc_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 6.57 | 5.77 | 48.7 | 1.882 | 2.940 | – | – | 0.0 |
| $CRu_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.55 | 5.56 | 59.5 | – | – | – | 1.540 | 3.671 | – | 0.0 | – |
| $CPd_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.24 | 6.24 | 59.9 | – | – | – | – | – | – | 1.217 | 1.591 | 0.0 | – | – |
| $CAg_2$ | HTX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 6.42 | 6.43 | 59.6 | 6.13 | 6.11 | 59.7 | – | – | – | 0.322 | 0.848 | 0.0 | 0.0 | – |
| $CCd_2$ | THX | $P2_1/m(11)$ | $Pmn2_1(31)$ | – | 7.22 | 6.86 | 58.1 | 6.80 | 6.80 | 52.1 | – | – | – | 0.346 | 2.386 | 0.0 | 0.0 | – |
| $CCs_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.98 | 9.99 | 58.0 | – | – | – | 9.78 | 9.77 | 59.7 | 0.035 | 0.996 | 8.1 | – | 8.1 |
| $CBa_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 8.49 | 8.49 | 59.8 | – | – | – | – | – | – | 1.533 | 2.727 | 0.0 | – | – |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | T | H | P |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | | | |
| $CHf_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.42 | 6.43 | 60.1 | – | – | – | – | – | – | 6.411 | 8.695 | 0.0 | – | – |
| $CTa_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{1}(2)$ | 6.16 | 6.16 | 59.9 | – | – | – | 7.15 | 5.86 | 54.3 | 0.107 | 3.898 | 0.0 | – | 0.0 |
| $CW_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.72 | 5.71 | 59.8 | – | – | – | 1.818 | 3.061 | – | 0.0 | – |
| $CRe_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.58 | 5.57 | 60.0 | – | – | – | 1.894 | 5.864 | – | 0.0 | – |
| $CPt_2$ | HXX | – | $Cm(8)$ | – | – | – | – | 5.73 | 5.37 | 74.5 | – | – | – | 1.432 | 2.786 | – | 0.0 | – |
| $CTl_2$ | TXX | $P3m1(156)$ | – | – | 7.80 | 7.80 | 59.6 | – | – | – | – | – | – | 1.855 | 2.813 | 0.0 | – | – |
| $CPb_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 7.28 | 7.29 | 59.9 | 7.15 | 7.16 | 59.8 | – | – | – | 0.592 | 3.316 | 0.0 | 0.0 | – |
| $CBi_2$ | HXX | – | $Cm(8)$ | – | – | – | – | 7.08 | 6.99 | 75.4 | – | – | – | 3.044 | 7.253 | – | 0.0 | – |
| $NLi_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 6.31 | 6.33 | 59.6 | – | – | – | 6.28 | 6.31 | 60.0 | 0.001 | 1.793 | 4.0 | – | 4.0 |
| $NBe_2$ | TPX | $C2/m(12)$ | – | $P\bar{1}(2)$ | 4.94 | 4.95 | 64.7 | – | – | – | 7.86 | 7.35 | 40.1 | 0.427 | 2.340 | 0.0 | – | 0.0 |
| $NC_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 5.22 | 5.51 | 86.1 | 5.134 | 10.406 | – | – | 0.0 |
| $NNa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.55 | 7.57 | 59.3 | – | – | – | 7.53 | 7.54 | 59.5 | 0.044 | 1.432 | 4.0 | – | 4.0 |
| $NAl_2$ | HXX | – | $Pmn2_1(31)$ | – | – | – | – | 5.34 | 5.34 | 65.7 | – | – | – | 3.125 | 4.334 | – | 0.0 | – |
| $NSi_2$ | HTP | $Pc(7)$ | $Cm(8)$ | $P1(1)$ | 5.53 | 5.65 | 60.7 | 5.63 | 5.62 | 59.9 | 8.28 | 7.51 | 59.9 | 0.007 | 0.722 | 0.0 | 0.0 | 0.0 |
| $NK_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 8.68 | 8.68 | 58.5 | – | – | – | – | – | – | 0.972 | 3.156 | 4.0 | – | – |
| $NCa_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.22 | 7.22 | 60.0 | – | – | – | – | – | – | 2.863 | 3.023 | 0.0 | – | – |
| $NTi_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 5.93 | 5.95 | 60.1 | – | – | – | – | – | – | 3.872 | 9.483 | 4.7 | – | – |
| $NV_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 5.75 | 5.76 | 60.0 | – | – | – | – | – | – | 1.010 | 1.398 | 0.0 | – | – |
| $NCr_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 5.67 | 5.67 | 60.7 | 5.25 | 5.22 | 59.6 | – | – | – | 0.144 | 3.984 | 7.2 | 0.0 | – |
| $NNi_2$ | TPX | $P\bar{3}m1(164)$ | – | $Cmmm(65)$ | 5.64 | 5.65 | 59.5 | – | – | – | 9.50 | 9.50 | 33.3 | 0.040 | 0.850 | 0.0 | – | 0.0 |
| $NRb_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 9.12 | 9.12 | 57.1 | – | – | – | – | – | – | 0.850 | 1.934 | 4.1 | – | – |
| $NSr_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.71 | 7.71 | 60.0 | – | – | – | – | – | – | 2.541 | 4.094 | 0.0 | – | – |
| $NY_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{3}m1(164)$ | – | 6.89 | 6.90 | 60.1 | 6.89 | 6.89 | 60.0 | – | – | – | 0.002 | 7.381 | 0.0 | 0.0 | – |
| $NZr_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.46 | 6.48 | 60.1 | – | – | – | – | – | – | 3.576 | 9.888 | 0.0 | – | – |
| $NNb_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 6.29 | 6.29 | 60.1 | 5.86 | 5.84 | 59.9 | – | – | – | 0.283 | 4.541 | 0.0 | 0.0 | – |
| $NPd_2$ | PXX | – | – | $P2/c(13)$ | – | – | – | – | – | – | 9.92 | 10.99 | 28.8 | 2.012 | 2.055 | – | – | 0.0 |
| $NCs_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.48 | 9.47 | 56.1 | – | – | – | 9.40 | 9.14 | 58.2 | 0.029 | 1.020 | 4.1 | – | 4.0 |
| $NHf_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.34 | 6.36 | 60.1 | – | – | – | – | – | – | 3.563 | 4.401 | 0.0 | – | – |
| $NTa_2$ | HTX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 6.16 | 6.17 | 60.0 | 5.79 | 5.78 | 59.9 | – | – | – | 0.657 | 2.060 | 0.0 | 0.0 | – |
| $NOs_2$ | HXX | – | $Pmc2_1(26)$ | – | – | – | – | 5.43 | 7.21 | 41.2 | – | – | – | 2.289 | 3.111 | – | 0.0 | – |
| $NIr_2$ | HXX | – | $Pmn2_1(31)$ | – | – | – | – | 5.28 | 5.44 | 59.1 | – | – | – | 1.975 | 4.578 | – | 0.0 | – |
| $NPt_2$ | HXX | – | $Pmn2_1(31)$ | – | – | – | – | 5.85 | 5.39 | 57.2 | – | – | – | 1.617 | 2.099 | – | 0.0 | – |
| $NPb_2$ | HTP | $P\bar{3}m1(164)$ | $Cm(8)$ | $P2_1/m(11)$ | 6.97 | 6.97 | 59.6 | 6.82 | 7.08 | 61.1 | 8.87 | 8.87 | 47.5 | 0.027 | 0.306 | 0.0 | 0.0 | 0.0 |
| $NBi_2$ | HTP | $P1(1)$ | $Pc(7)$ | $P1(1)$ | 7.90 | 6.84 | 53.8 | 6.58 | 7.43 | 59.5 | 11.59 | 10.80 | 32.0 | 0.405 | 0.811 | 0.0 | 0.0 | 0.0 |
| $OLi_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.19 | 6.21 | 60.0 | – | – | – | – | – | – | 1.274 | 3.622 | 0.0 | – | – |
| $OBe_2$ | TXX | $P2_1/m(11)$ | – | – | 5.17 | 4.95 | 58.5 | – | – | – | – | – | – | 1.114 | 3.420 | 0.0 | – | – |
| $ONa_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{1}(2)$ | 7.52 | 7.53 | 59.4 | – | – | – | 9.67 | 9.07 | 41.9 | 0.756 | 2.577 | 0.0 | – | 0.0 |
| $OMg_2$ | PTX | $P\bar{3}m1(164)$ | – | $Cmmm(65)$ | 6.14 | 6.14 | 59.2 | – | – | – | 11.46 | 11.46 | 29.6 | 0.770 | 1.747 | 0.0 | – | 0.0 |
| $OAl_2$ | HXX | – | $Pmn2_1(31)$ | – | – | – | – | 5.09 | 5.53 | 57.2 | – | – | – | 2.374 | 2.973 | – | 0.0 | – |
| $OSi_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 6.67 | 7.90 | 67.9 | 1.102 | 2.497 | – | – | 0.0 |
| $OK_2$ | TPX | $P\bar{3}m1(164)$ | – | $Pmmn(59)$ | 8.26 | 8.27 | 59.3 | – | – | – | 8.17 | 14.38 | 29.1 | 0.294 | 1.823 | 0.0 | – | 0.0 |
| $OCa_2$ | PXX | – | – | $P2/c(13)$ | – | – | – | – | – | – | 13.93 | 12.08 | 24.9 | 1.945 | 2.182 | – | – | 0.0 |
| $OSc_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.38 | 6.39 | 60.0 | – | – | – | – | – | – | 0.915 | 3.979 | 4.8 | – | – |
| $OTi_2$ | HTX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 5.96 | 5.98 | 59.9 | 5.60 | 5.60 | 59.9 | – | – | – | 0.164 | 1.350 | 0.0 | 0.0 | – |
| $OV_2$ | HTP | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P2/c(13)$ | 5.32 | 5.30 | 59.9 | 5.32 | 5.31 | 59.1 | 10.12 | 8.59 | 28.5 | 0.555 | 0.671 | 0.0 | 0.0 | 0.0 |
| $OCr_2$ | HTP | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P2/c(13)$ | 5.74 | 5.73 | 59.9 | 5.08 | 5.08 | 59.8 | 10.96 | 10.98 | 28.8 | 0.403 | 0.650 | 29.1 | 0.0 | 31.9 |
| $OFe_2$ | PHT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $Cmmm(65)$ | 5.37 | 5.37 | 59.8 | 5.33 | 5.32 | 59.8 | 10.08 | 10.07 | 30.6 | 0.083 | 0.553 | 26.4 | 25.4 | 24.2 |
| $ORb_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 8.36 | 8.36 | 59.7 | – | – | – | – | – | – | 1.533 | 1.866 | 0.0 | – | – |
| $OSr_2$ | PXX | – | – | $Pccm(49)$ | – | – | – | – | – | – | 13.71 | 12.22 | 27.0 | 1.619 | 2.157 | – | – | 0.0 |
| $OY_2$ | PXX | – | – | $Pccm(49)$ | – | – | – | – | – | – | 11.90 | 10.49 | 27.8 | 0.988 | 0.991 | – | – | 0.0 |
| $OZr_2$ | THX | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | – | 6.46 | 6.45 | 57.9 | 6.13 | 6.13 | 60.0 | – | – | – | 0.613 | 1.683 | 0.0 | 0.0 | – |
| $ONb_2$ | HTX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 5.84 | 5.85 | 57.8 | 5.83 | 5.83 | 58.3 | – | – | – | 0.242 | 1.484 | 0.0 | 0.0 | – |
| $OMo_2$ | TXX | $P2_1/m(11)$ | – | – | 6.79 | 6.55 | 50.1 | – | – | – | – | – | – | 1.871 | 7.775 | 0.0 | – | – |
| $ORu_2$ | HPX | – | $P1(1)$ | $Pc(7)$ | – | – | – | 5.02 | 5.38 | 56.6 | 9.62 | 9.32 | 30.4 | 0.143 | 0.846 | – | 0.0 | 0.0 |
| $OIn_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 6.64 | 6.63 | 60.2 | 6.60 | 6.58 | 60.2 | – | – | – | 0.488 | 2.401 | 0.0 | 0.0 | – |
| $OCs_2$ | PTX | $C2/m(12)$ | – | $P\bar{3}m1(164)$ | 9.81 | 9.81 | 50.4 | – | – | – | 8.54 | 8.53 | 59.4 | 0.733 | 1.339 | 0.0 | – | 0.0 |
| $OBa_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 9.20 | 9.19 | 59.2 | 2.125 | 2.135 | – | – | 0.0 |

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Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $OHf_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 5.03 | 8.57 | 91.0 | 2.913 | 3.990 | – | – | 0.0 |
| $OTa_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 7.81 | 7.79 | 59.9 | 0.937 | 1.474 | – | – | 0.0 |
| $OW_2$ | PHX | – | $Pmn2_1(31)$ | $P1(1)$ | – | – | – | 5.19 | 5.19 | 62.2 | 8.22 | 5.88 | 57.5 | 0.128 | 2.842 | – | 0.0 | 0.0 |
| $OPt_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 7.29 | 7.30 | 98.4 | 1.894 | 1.908 | – | – | 0.0 |
| $OAu_2$ | THP | $P2_1/m(11)$ | $Pmn2_1(31)$ | $P2/c(13)$ | 6.46 | 6.46 | 54.4 | 6.45 | 6.46 | 54.6 | 6.26 | 10.81 | 73.5 | 0.035 | 0.733 | 0.0 | 0.0 | 0.0 |
| $OTl_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 7.40 | 7.39 | 58.7 | 7.17 | 7.16 | 59.4 | – | – | – | 0.417 | 1.002 | 0.0 | 0.0 | – |
| $OPb_2$ | TXX | $C222(21)$ | – | – | 7.28 | 6.85 | 57.6 | – | – | – | – | – | – | 1.078 | 4.459 | 0.0 | – | – |
| $FLi_2$ | PHX | – | $Pmmn(59)$ | $Cmmm(65)$ | – | – | – | 4.92 | 4.92 | 73.3 | 11.48 | 11.46 | 27.6 | 0.134 | 1.185 | – | 0.0 | 0.0 |
| $FNa_2$ | PTH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $Cmmm(65)$ | 7.04 | 7.03 | 59.0 | 6.84 | 6.85 | 59.1 | 13.89 | 13.93 | 26.9 | 0.347 | 0.787 | 0.0 | 0.0 | 0.0 |
| $FK_2$ | PTH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $Cmmm(65)$ | 8.42 | 8.42 | 56.0 | 8.30 | 8.30 | 55.6 | 16.17 | 16.20 | 27.0 | 0.070 | 0.574 | 0.0 | 0.0 | 0.0 |
| $FRb_2$ | PTH | $P\bar{3}m1(164)$ | $C2/m(12)$ | $Cmmm(65)$ | 8.94 | 8.93 | 55.9 | 10.25 | 10.22 | 46.2 | 17.12 | 17.14 | 27.1 | 0.007 | 0.138 | 0.0 | 0.0 | 0.0 |
| $FSr_2$ | HTX | $P1(1)$ | $P1(1)$ | – | 8.16 | 9.88 | 54.2 | 8.63 | 8.62 | 60.6 | – | – | – | 0.101 | 1.923 | 0.0 | 0.0 | – |
| $FCd_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 6.19 | 6.19 | 58.3 | 6.26 | 6.25 | 56.7 | – | – | – | 0.085 | 1.061 | 0.0 | 0.0 | – |
| $FIn_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 6.56 | 6.56 | 60.2 | 6.54 | 6.54 | 60.1 | – | – | – | 0.072 | 1.818 | 0.0 | 0.0 | – |
| $FTa_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 5.99 | 5.71 | 62.9 | 10.357 | 10.429 | – | – | 0.0 |
| $FAu_2$ | PTH | $Pmmn(59)$ | $Pmmn(59)$ | $P2/m(10)$ | 4.95 | 4.95 | 72.4 | 5.86 | 4.96 | 53.7 | 13.06 | 5.77 | 72.8 | 0.662 | 0.666 | 0.0 | 0.0 | 0.0 |
| $FTl_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 7.19 | 7.19 | 58.3 | 7.08 | 7.07 | 59.0 | – | – | – | 0.183 | 2.788 | 0.0 | 0.0 | – |
| $NaN_2$ | THP | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $Cmmm(65)$ | 8.21 | 8.27 | 59.1 | 7.59 | 7.59 | 56.0 | 10.65 | 10.56 | 44.8 | 0.466 | 0.542 | 20.0 | 20.0 | 20.0 |
| $NaSi_2$ | TPX | $Cmmm(65)$ | – | $Cmmm(65)$ | 12.29 | 12.29 | 36.3 | – | – | – | 11.82 | 11.81 | 38.2 | 0.281 | 6.475 | 0.0 | – | 0.0 |
| $NaCl_2$ | PTX | $C2/m(12)$ | – | $P1(1)$ | 8.40 | 10.16 | 51.8 | – | – | – | 12.18 | 10.56 | 43.9 | 0.731 | 0.955 | 4.0 | – | 2.0 |
| $NaGe_2$ | HXX | – | $Cmme(67)$ | – | – | – | – | 11.17 | 10.02 | 25.7 | – | – | – | 2.678 | 3.000 | – | 0.0 | – |
| $NaBr_2$ | PXX | – | – | $P2/m(10)$ | – | – | – | – | – | – | 13.42 | 12.62 | 45.0 | 1.067 | 1.295 | – | – | 0.0 |
| $NaI_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 10.89 | 14.27 | 64.5 | 0.969 | 1.287 | – | – | 0.0 |
| $NaAu_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 5.81 | 9.01 | 38.3 | – | – | – | 1.783 | 1.787 | – | 0.0 | – |
| $MgO_2$ | HPX | – | $P\bar{6}m2(187)$ | $P2/c(13)$ | – | – | – | 6.61 | 6.63 | 59.7 | 7.91 | 5.99 | 47.3 | 0.056 | 4.414 | – | 0.0 | 0.0 |
| $MgF_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 6.29 | 6.29 | 59.8 | – | – | – | 6.28 | 6.29 | 59.6 | 0.003 | 3.879 | 0.0 | – | 0.0 |
| $MgSi_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 9.92 | 7.60 | 38.3 | – | – | – | 1.732 | 2.165 | – | 0.0 | – |
| $MgCl_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.42 | 7.42 | 59.5 | – | – | – | 7.43 | 7.43 | 59.4 | 0.049 | 2.430 | 0.0 | – | 0.0 |
| $MgSc_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.73 | 9.54 | 44.8 | – | – | – | 3.061 | 9.615 | – | 0.0 | – |
| $MgGe_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 10.26 | 8.38 | 33.9 | – | – | – | 1.749 | 3.081 | – | 0.0 | – |
| $MgBr_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.81 | 7.82 | 59.5 | – | – | – | 7.81 | 7.82 | 59.5 | 0.005 | 2.072 | 0.0 | – | 0.0 |
| $MgRh_2$ | THX | $C2/m(12)$ | $Amm2(38)$ | – | 9.63 | 9.64 | 33.2 | 9.07 | 9.07 | 33.3 | – | – | – | 0.102 | 1.958 | 3.6 | 0.0 | – |
| $MgIn_2$ | HXX | – | $Pmmm(47)$ | – | – | – | – | 10.52 | 8.51 | 35.3 | – | – | – | 2.379 | 2.923 | – | 0.0 | – |
| $MgSn_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.89 | 9.95 | 37.1 | – | – | – | 1.742 | 2.456 | – | 0.0 | – |
| $MgI_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{3}m1(164)$ | – | 8.44 | 8.45 | 59.5 | 8.44 | 8.44 | 59.5 | – | – | – | 0.002 | 1.141 | 0.0 | 0.0 | – |
| $MgBa_2$ | PTH | $C2/m(12)$ | $Amm2(38)$ | $P\bar{1}(2)$ | 11.05 | 8.90 | 51.5 | 8.84 | 8.86 | 59.6 | 12.04 | 11.07 | 44.4 | 0.101 | 0.322 | 0.0 | 0.0 | 0.0 |
| $MgIr_2$ | HXX | – | $Cm(8)$ | – | – | – | – | 9.92 | 9.91 | 28.9 | – | – | – | 5.421 | 6.766 | – | 0.0 | – |
| $AlBe_2$ | TXX | $C2/m(12)$ | – | – | 6.08 | 6.96 | 42.4 | – | – | – | – | – | – | 2.495 | 3.435 | 0.0 | – | – |
| $AlB_2$ | THX | $P\bar{1}(2)$ | $Pmn2_1(31)$ | – | 5.33 | 6.15 | 54.6 | 5.26 | 6.11 | 54.5 | – | – | – | 0.066 | 1.212 | 0.0 | 0.0 | – |
| $AlC_2$ | HTP | $P\bar{1}(2)$ | $P1(1)$ | $Cmme(67)$ | 6.99 | 6.75 | 39.5 | 6.26 | 5.90 | 41.9 | 8.45 | 8.45 | 40.0 | 0.144 | 0.327 | 0.0 | 0.0 | 0.0 |
| $AlN_2$ | PXX | – | – | $P2(3)$ | – | – | – | – | – | – | 8.22 | 10.27 | 37.9 | 0.943 | 3.355 | – | – | 0.0 |
| $AlO_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 5.71 | 5.71 | 64.4 | – | – | – | – | – | – | 2.061 | 2.775 | 4.0 | – | – |
| $AlF_2$ | HTX | $C2/m(12)$ | $P1(1)$ | – | 6.76 | 5.18 | 59.3 | 6.79 | 5.75 | 65.4 | – | – | – | 0.168 | 2.742 | 0.0 | 0.0 | – |
| $AlAl_2$ | THX | $P\bar{3}m1(164)$ | $P4/mmm(123)$ | – | 5.51 | 5.51 | 62.7 | 5.48 | 5.48 | 87.5 | – | – | – | 0.676 | 6.286 | 0.0 | 0.0 | – |
| $AlSi_2$ | HTX | $P\bar{1}(2)$ | $Pc(7)$ | – | 7.44 | 7.78 | 56.2 | 7.02 | 7.35 | 54.3 | – | – | – | 0.623 | 4.540 | 0.0 | 0.0 | – |
| $AlP_2$ | TXX | $P\bar{1}(2)$ | – | – | 7.62 | 7.84 | 41.5 | – | – | – | – | – | – | 1.290 | 1.807 | 0.0 | – | – |
| $AlS_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 6.71 | 8.14 | 56.4 | 1.041 | 1.615 | – | – | 0.0 |
| $AlK_2$ | HTX | $C2/m(12)$ | $Pmma(51)$ | – | 11.42 | 10.98 | 43.8 | 9.37 | 9.78 | 61.1 | – | – | – | 0.706 | 6.459 | 0.0 | 0.0 | – |
| $AlCa_2$ | HPX | – | $P4/mmm(123)$ | $P\bar{1}(2)$ | – | – | – | 10.35 | 7.31 | 45.0 | 9.17 | 7.55 | 53.0 | 0.024 | 2.832 | – | 0.0 | 0.0 |
| $AlSc_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 8.77 | 6.20 | 45.0 | – | – | – | 1.330 | 1.376 | – | 0.0 | – |
| $AlCr_2$ | TXX | $P2/c(13)$ | – | – | 7.23 | 7.98 | 39.4 | – | – | – | – | – | – | 4.443 | 11.654 | 0.0 | – | – |
| $AlGe_2$ | HTX | $C2/m(12)$ | $Pc(7)$ | – | 8.95 | 8.97 | 36.6 | 8.00 | 8.07 | 46.4 | – | – | – | 0.389 | 5.203 | 0.0 | 0.0 | – |
| $AlSe_2$ | TXX | $C2/m(12)$ | – | – | 7.29 | 7.29 | 49.9 | – | – | – | – | – | – | 2.444 | 2.936 | 0.0 | – | – |
| $AlBr_2$ | HXX | – | $P2(3)$ | – | – | – | – | 11.39 | 7.31 | 65.4 | – | – | – | 0.908 | 2.623 | – | 0.0 | – |
| $AlRb_2$ | THX | $C2/m(12)$ | $Cmmm(65)$ | – | 11.40 | 11.84 | 44.1 | 10.18 | 13.18 | 40.0 | – | – | – | 0.424 | 5.631 | 0.0 | 0.0 | – |
| $AlSr_2$ | HXX | – | $Pmmm(47)$ | – | – | – | – | 7.86 | 11.03 | 44.7 | – | – | – | 2.095 | 2.108 | – | 0.0 | – |
| $AlY_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 9.56 | 6.76 | 45.1 | – | – | – | 0.888 | 4.155 | – | 0.0 | – |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $\Delta E_1$ [eV] | $\Delta E_2$ [eV] | T | H | P |
| $AlZr_2$ | HXX | – | $Pbcm(57)$ | – | – | – | – | 8.90 | 7.23 | 35.7 | – | – | – | 1.093 | 2.313 | – | 0.0 | – |
| $AlMo_2$ | PHX | – | $P2/c(13)$ | $P\bar{1}(2)$ | – | – | – | 7.39 | 10.20 | 30.8 | 7.46 | 7.73 | 41.3 | 0.309 | 0.821 | – | 0.0 | 0.0 |
| $AlRu_2$ | HXX | – | $C2/m(12)$ | – | – | – | – | 7.72 | 6.69 | 43.7 | – | – | – | 7.612 | 8.751 | – | 0.0 | – |
| $AlRh_2$ | PHX | – | $P4/mmm(123)$ | $C2/m(12)$ | – | – | – | 7.78 | 5.50 | 45.0 | 6.78 | 7.81 | 43.0 | 0.265 | 1.125 | – | 0.0 | 0.0 |
| $AlPd_2$ | THX | $C2/m(12)$ | $P\bar{6}m2(187)$ | – | 6.96 | 5.63 | 53.2 | 5.88 | 5.88 | 59.9 | – | – | – | 0.287 | 1.642 | 0.0 | 0.0 | – |
| $AlAg_2$ | THX | $C2/m(12)$ | $P4/mmm(123)$ | – | 7.19 | 8.24 | 43.0 | 5.82 | 8.36 | 44.1 | – | – | – | 0.366 | 3.429 | 0.0 | 0.0 | – |
| $AlCd_2$ | THX | $P2/c(13)$ | $P2/c(13)$ | – | 7.45 | 8.76 | 40.6 | 5.80 | 8.30 | 60.3 | – | – | – | 0.531 | 3.763 | 0.0 | 0.0 | – |
| $AlIn_2$ | THX | $P1(1)$ | $P1(1)$ | – | 6.16 | 7.74 | 50.9 | 7.37 | 6.28 | 53.4 | – | – | – | 0.041 | 5.934 | 0.0 | 0.0 | – |
| $AlSn_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 8.68 | 8.68 | 45.5 | – | – | – | 1.491 | 5.250 | – | 0.0 | – |
| $AlSb_2$ | HTP | $P\bar{1}(2)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 10.18 | 8.75 | 44.0 | 8.25 | 8.26 | 59.2 | 10.29 | 8.07 | 50.1 | 0.176 | 0.251 | 0.0 | 0.0 | 0.0 |
| $AlBa_2$ | HPX | – | $P4/mmm(123)$ | $C2/m(12)$ | – | – | – | 11.80 | 8.34 | 45.0 | 9.58 | 10.87 | 47.6 | 0.688 | 2.324 | – | 0.0 | 0.0 |
| $AlHf_2$ | TXX | $C2/m(12)$ | – | – | 7.70 | 7.69 | 45.9 | – | – | – | – | – | – | 2.870 | 4.085 | 0.0 | – | – |
| $AlW_2$ | THP | $P2_1/c(14)$ | $P2/c(13)$ | $P2/c(13)$ | 9.17 | 7.79 | 30.9 | 8.03 | 7.39 | 40.6 | 10.11 | 7.34 | 31.2 | 0.293 | 0.613 | 0.0 | 0.0 | 0.0 |
| $AlIr_2$ | HXX | – | $C2/m(12)$ | – | – | – | – | 7.81 | 6.82 | 42.6 | – | – | – | 1.127 | 6.685 | – | 0.0 | – |
| $AlPt_2$ | THX | $P4/mmm(123)$ | $P\bar{6}m2(187)$ | – | 8.00 | 5.65 | 44.7 | 5.81 | 5.82 | 60.1 | – | – | – | 0.212 | 6.625 | 0.0 | 0.0 | – |
| $AlAu_2$ | THX | $C2/m(12)$ | $P4/mmm(123)$ | – | 8.03 | 6.92 | 43.7 | 5.85 | 8.32 | 46.1 | – | – | – | 0.701 | 2.688 | 0.0 | 0.0 | – |
| $AlHg_2$ | THP | $P2_1/m(11)$ | $Pc(7)$ | $P\bar{1}(2)$ | 8.03 | 8.04 | 44.1 | 7.97 | 7.84 | 44.3 | 9.74 | 8.70 | 49.4 | 0.042 | 0.795 | 0.0 | 0.0 | 0.0 |
| $AlTl_2$ | HXX | – | $Pm(6)$ | – | – | – | – | 7.10 | 7.12 | 55.6 | – | – | – | 1.199 | 2.662 | – | 0.0 | – |
| $AlPb_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 8.86 | 8.86 | 46.7 | – | – | – | 1.361 | 2.072 | – | 0.0 | – |
| $AlBi_2$ | TXX | $P\bar{1}(2)$ | – | – | 9.06 | 8.59 | 43.3 | – | – | – | – | – | – | 1.782 | 1.864 | 0.0 | – | – |
| $SiBe_2$ | TXX | $Cmme(67)$ | – | – | 7.70 | 7.03 | 29.8 | – | – | – | – | – | – | 2.089 | 5.750 | 0.0 | – | – |
| $SiB_2$ | HTP | $Cm(8)$ | $C2(5)$ | $P\bar{1}(2)$ | 7.35 | 7.35 | 48.3 | 6.88 | 6.87 | 43.4 | 5.96 | 7.86 | 60.7 | 0.471 | 0.528 | 0.0 | 0.0 | 0.0 |
| $SiO_2$ | THP | $P\bar{3}m1(164)$ | $P\bar{3}m1(164)$ | $Amm2(38)$ | 5.41 | 5.41 | 60.0 | 5.41 | 5.41 | 60.0 | 8.79 | 4.95 | 92.6 | 0.010 | 0.562 | 0.0 | 0.0 | 0.0 |
| $SiNa_2$ | PTX | $C2/m(12)$ | – | $P\bar{1}(2)$ | 9.31 | 9.86 | 43.7 | – | – | – | 10.15 | 9.47 | 42.4 | 0.679 | 1.723 | 0.0 | – | 0.0 |
| $SiAl_2$ | HXX | – | $Pmn2_1(31)$ | – | – | – | – | 7.52 | 7.52 | 41.7 | – | – | – | 2.678 | 4.125 | – | 0.0 | – |
| $SiP_2$ | PHX | – | $Cm(8)$ | $P2/c(13)$ | – | – | – | 7.60 | 7.60 | 51.1 | 7.44 | 8.45 | 41.2 | 0.713 | 3.531 | – | 0.0 | 0.0 |
| $SiS_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{4}m2(115)$ | – | 6.62 | 6.62 | 60.0 | 9.57 | 6.78 | 45.1 | – | – | – | 0.016 | 2.884 | 0.0 | 0.0 | – |
| $SiCl_2$ | TPH | $P\bar{1}(2)$ | $Amm2(38)$ | $P\bar{1}(2)$ | 7.11 | 9.49 | 72.3 | 8.64 | 8.69 | 86.9 | 8.82 | 9.42 | 93.9 | 0.153 | 0.713 | 0.0 | 0.0 | 0.0 |
| $SiK_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.75 | 10.41 | 46.2 | – | – | – | 3.611 | 3.632 | – | 0.0 | – |
| $SiCa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.44 | 9.44 | 59.8 | – | – | – | 9.41 | 9.41 | 60.1 | 0.000 | 2.665 | 0.0 | – | 0.0 |
| $SiTi_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 7.96 | 8.13 | 37.9 | 1.712 | 3.520 | – | – | 0.0 |
| $SiCr_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 4.84 | 6.22 | 49.9 | – | – | – | 2.504 | 5.007 | – | 0.0 | – |
| $SiGe_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 7.45 | 7.45 | 60.0 | – | – | – | 0.902 | 1.448 | – | 0.0 | – |
| $SiBr_2$ | TPX | $P\bar{1}(2)$ | – | $P1(1)$ | 9.79 | 7.24 | 65.0 | – | – | – | 8.55 | 9.41 | 88.0 | 0.336 | 1.155 | 0.0 | – | 0.0 |
| $SiRb_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 10.13 | 10.81 | 46.4 | – | – | – | 3.591 | 5.384 | – | 0.0 | – |
| $SiSr_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.90 | 9.90 | 59.6 | – | – | – | 9.84 | 9.84 | 60.0 | 0.003 | 2.382 | 0.0 | – | 0.0 |
| $SiZr_2$ | HPT | $C2/m(12)$ | $Cmmm(65)$ | $P\bar{1}(2)$ | 7.94 | 8.03 | 59.0 | 5.96 | 7.48 | 51.1 | 6.72 | 7.11 | 64.7 | 0.030 | 0.736 | 0.0 | 0.0 | 0.0 |
| $SiPd_2$ | HTP | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 7.11 | 7.08 | 48.2 | 6.11 | 6.11 | 59.7 | 7.15 | 7.20 | 59.7 | 0.083 | 0.668 | 0.0 | 0.0 | 0.0 |
| $SiSn_2$ | HPX | – | $P\bar{6}m2(187)$ | $P\bar{1}(2)$ | – | – | – | 8.03 | 8.04 | 59.5 | 8.18 | 8.04 | 61.6 | 0.724 | 0.855 | – | 0.0 | 0.0 |
| $SiI_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{1}(2)$ | 8.37 | 8.37 | 60.4 | – | – | – | 10.77 | 8.54 | 91.5 | 0.482 | 0.976 | 0.0 | – | 0.0 |
| $SiCs_2$ | PTX | $P\bar{3}m1(164)$ | – | $P2_1/m(11)$ | 11.81 | 11.79 | 58.3 | – | – | – | 11.48 | 11.52 | 59.8 | 0.013 | 1.126 | 8.0 | – | 8.0 |
| $SiBa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.28 | 10.27 | 59.0 | – | – | – | 10.14 | 10.14 | 60.1 | 0.013 | 1.590 | 0.0 | – | 0.0 |
| $SiPt_2$ | THX | $C2/m(12)$ | $P\bar{6}m2(187)$ | – | 6.46 | 6.49 | 52.7 | 5.96 | 6.44 | 57.4 | – | – | – | 0.390 | 1.688 | 0.0 | 0.0 | – |
| $SiPb_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $C2/m(12)$ | 8.80 | 8.80 | 58.1 | 8.38 | 8.38 | 57.9 | 8.09 | 9.08 | 55.7 | 0.653 | 0.740 | 0.0 | 0.0 | 0.0 |
| $PLi_2$ | TXX | $C2/m(12)$ | – | – | 8.24 | 8.01 | 42.9 | – | – | – | – | – | – | 1.238 | 3.853 | 0.0 | – | – |
| $PBe_2$ | PXX | – | – | $P3m1(156)$ | – | – | – | – | – | – | 3.99 | 6.92 | 90.0 | 2.887 | 4.350 | – | – | 0.0 |
| $PNa_2$ | TXX | $C2/m(12)$ | – | – | 9.39 | 9.01 | 43.0 | – | – | – | – | – | – | 0.865 | 2.517 | 0.0 | – | – |
| $PAl_2$ | PHX | – | $P1(1)$ | $P2/c(13)$ | – | – | – | 7.23 | 6.55 | 60.2 | 7.55 | 6.17 | 72.3 | 0.725 | 0.921 | – | 0.0 | 0.0 |
| $PSi_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 8.81 | 8.81 | 49.0 | 1.687 | 4.190 | – | – | 0.0 |
| $PP_2$ | HPX | – | $P1(1)$ | $P1(1)$ | – | – | – | 6.57 | 6.49 | 60.8 | 7.52 | 7.88 | 61.4 | 0.183 | 2.348 | – | 0.0 | 0.0 |
| $PS_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.59 | 6.59 | 60.0 | – | – | – | – | – | – | 1.396 | 1.559 | 0.0 | – | – |
| $PCl_2$ | THX | $P\bar{1}(2)$ | $Pc(7)$ | – | 8.05 | 10.81 | 55.7 | 9.58 | 7.78 | 60.3 | – | – | – | 0.248 | 3.548 | 0.0 | 0.0 | – |
| $PK_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.24 | 10.24 | 58.2 | – | – | – | 10.09 | 10.08 | 59.5 | 0.031 | 1.049 | 4.0 | – | 4.0 |
| $PCa_2$ | PTX | $P\bar{3}m1(164)$ | – | $C2/m(12)$ | 8.42 | 8.42 | 59.9 | – | – | – | 8.45 | 8.47 | 59.9 | 0.082 | 1.612 | 0.0 | – | 0.0 |
| $PSc_2$ | PTX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 7.57 | 7.30 | 61.2 | – | – | – | 7.55 | 7.30 | 61.2 | 0.000 | 2.459 | 0.0 | – | 0.0 |
| $PTi_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 7.28 | 6.79 | 62.1 | 0.856 | 3.023 | – | – | 0.0 |
| $PV_2$ | TXX | $P2_1/m(11)$ | – | – | 6.91 | 6.13 | 63.4 | – | – | – | – | – | – | 3.931 | 5.400 | 0.0 | – | – |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | T | H | P |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | | | |
| $PCr_2$ | TPX | $P2_1/m(11)$ | – | $Pmmn(59)$ | 7.17 | 7.04 | 60.5 | – | – | – | 6.76 | 7.40 | 56.7 | 0.187 | 2.486 | 27.8 | – | 27.4 |
| $PMn_2$ | TXX | $P2_1/m(11)$ | – | – | 6.78 | 6.77 | 57.9 | – | – | – | – | – | – | 2.465 | 6.119 | 23.4 | – | – |
| $PFe_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 7.94 | 7.94 | 60.0 | 5.69 | 5.67 | 59.9 | – | – | – | 0.202 | 1.151 | 18.0 | 11.8 | – |
| $PCo_2$ | TXX | $P2_1/m(11)$ | – | – | 6.46 | 6.46 | 47.9 | – | – | – | – | – | – | 2.829 | 4.078 | 7.8 | – | – |
| $PNi_2$ | PTX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 6.63 | 6.63 | 58.5 | – | – | – | 7.00 | 6.53 | 57.0 | 0.214 | 2.323 | 0.0 | – | 0.0 |
| $PGe_2$ | PHT | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $Cm(8)$ | 6.75 | 6.75 | 59.4 | 7.03 | 7.40 | 58.4 | 8.92 | 8.89 | 52.0 | 0.002 | 0.320 | 0.0 | 0.0 | 0.0 |
| $PSe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.99 | 6.99 | 60.0 | – | – | – | – | – | – | 0.943 | 2.920 | 0.0 | – | – |
| $PRb_2$ | TPX | $P\bar{3}m1(164)$ | – | $Pmmn(59)$ | 10.75 | 10.76 | 58.1 | – | – | – | 10.20 | 10.44 | 60.0 | 0.295 | 0.931 | 4.0 | – | 4.0 |
| $PSr_2$ | PTX | $P\bar{3}m1(164)$ | – | $P2_1/m(11)$ | 8.94 | 8.94 | 59.4 | – | – | – | 8.93 | 8.92 | 59.7 | 0.005 | 1.668 | 0.0 | – | 0.0 |
| $PY_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.63 | 7.63 | 60.0 | – | – | – | 7.64 | 7.63 | 60.0 | 0.037 | 2.802 | 0.0 | – | 0.0 |
| $PNb_2$ | TXX | $P2_1/m(11)$ | – | – | 6.68 | 7.58 | 63.8 | – | – | – | – | – | – | 2.057 | 4.823 | 0.0 | – | – |
| $PMo_2$ | TXX | $P2_1/m(11)$ | – | – | 7.24 | 7.24 | 49.2 | – | – | – | – | – | – | 3.085 | 3.334 | 0.0 | – | – |
| $PTc_2$ | TXX | $P2_1/m(11)$ | – | – | 7.10 | 5.63 | 66.6 | – | – | – | – | – | – | 3.599 | 7.906 | 0.0 | – | – |
| $PRu_2$ | TXX | $P2_1/m(11)$ | – | – | 7.02 | 7.02 | 47.1 | – | – | – | – | – | – | 1.103 | 4.425 | 0.0 | – | – |
| $PRh_2$ | PTX | $P2_1/m(11)$ | – | $Pmmn(59)$ | 7.21 | 6.95 | 58.7 | – | – | – | 9.06 | 7.11 | 38.3 | 0.760 | 1.307 | 0.0 | – | 0.0 |
| $PPd_2$ | PTX | $P2_1/m(11)$ | – | $P\bar{1}(2)$ | 7.19 | 7.19 | 60.5 | – | – | – | 7.29 | 7.27 | 56.1 | 0.089 | 1.098 | 0.0 | – | 0.0 |
| $PAg_2$ | HPX | – | $P2/c(13)$ | $Cm(8)$ | – | – | – | 7.99 | 7.19 | 43.5 | 7.91 | 8.54 | 61.8 | 0.677 | 1.887 | – | 0.0 | 0.0 |
| $PCd_2$ | HPX | – | $Aem2(39)$ | $C2/m(12)$ | – | – | – | 7.24 | 7.25 | 63.0 | 8.33 | 11.24 | 55.2 | 0.111 | 1.459 | – | 0.0 | 0.0 |
| $PSn_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 7.39 | 7.39 | 59.6 | 7.52 | 7.52 | 59.9 | – | – | – | 0.222 | 1.592 | 0.0 | 0.0 | – |
| $PTe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.50 | 7.51 | 59.8 | – | – | – | – | – | – | 1.708 | 1.971 | 0.0 | – | – |
| $PI_2$ | HXX | – | $P2/m(10)$ | – | – | – | – | 9.55 | 9.95 | 51.9 | – | – | – | 2.502 | 2.885 | – | 0.0 | – |
| $PCs_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 11.24 | 11.25 | 58.4 | – | – | – | 11.05 | 11.06 | 59.4 | 0.013 | 0.944 | 4.0 | – | 4.0 |
| $PBa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.32 | 9.31 | 59.4 | – | – | – | 9.26 | 12.25 | 40.9 | 0.103 | 1.678 | 0.0 | – | 2.6 |
| $PHf_2$ | PTX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 7.69 | 7.70 | 52.4 | – | – | – | 7.83 | 6.91 | 63.8 | 0.077 | 1.660 | 0.0 | – | 0.0 |
| $PPt_2$ | HTP | $P2_1/m(11)$ | $Pmn2_1(31)$ | $Pc(7)$ | 6.86 | 6.86 | 49.2 | 6.44 | 6.44 | 53.1 | 9.12 | 9.79 | 43.4 | 0.060 | 0.541 | 0.0 | 0.0 | 0.0 |
| $PTl_2$ | TPH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{1}(2)$ | 8.73 | 8.73 | 59.5 | 8.33 | 8.33 | 59.3 | 9.18 | 7.67 | 76.7 | 0.359 | 0.726 | 0.0 | 0.0 | 0.0 |
| $PPb_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 7.71 | 7.72 | 59.6 | 7.93 | 7.92 | 59.4 | – | – | – | 0.271 | 1.080 | 0.0 | 0.0 | – |
| $SLi_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.89 | 7.87 | 59.8 | – | – | – | 7.86 | 7.86 | 59.9 | 0.025 | 2.651 | 0.0 | – | 0.0 |
| $SBe_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 6.83 | 5.30 | 90.0 | 2.333 | 4.987 | – | – | 0.0 |
| $SNa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.01 | 9.02 | 59.5 | – | – | – | 9.02 | 9.03 | 59.6 | 0.033 | 2.464 | 0.0 | – | 0.0 |
| $SAl_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 8.09 | 7.99 | 54.2 | 2.727 | 2.786 | – | – | 0.0 |
| $SS_2$ | HXX | – | $Pc(7)$ | – | – | – | – | 8.20 | 11.18 | 43.5 | – | – | – | 2.451 | 2.703 | – | 0.0 | – |
| $SCl_2$ | HTP | $P\bar{1}(2)$ | $P1(1)$ | $P2/c(13)$ | 7.47 | 8.27 | 78.4 | 7.16 | 9.40 | 96.0 | 9.96 | 10.57 | 96.2 | 0.379 | 0.641 | 0.0 | 0.0 | 0.0 |
| $SK_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.17 | 10.17 | 57.5 | – | – | – | 9.92 | 9.91 | 59.6 | 0.063 | 1.948 | 0.0 | – | 0.0 |
| $SCa_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 7.82 | 7.81 | 60.0 | 7.73 | 7.73 | 59.8 | – | – | – | 0.798 | 2.382 | 0.4 | 0.0 | – |
| $SSc_2$ | TPH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P3m1(156)$ | 7.04 | 7.03 | 60.0 | 6.79 | 6.79 | 60.0 | 6.95 | 6.98 | 60.2 | 0.224 | 0.717 | 0.0 | 0.0 | 0.0 |
| $STi_2$ | PTX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 6.56 | 7.28 | 63.1 | – | – | – | 6.57 | 7.29 | 63.1 | 0.014 | 3.411 | 0.0 | – | 0.0 |
| $SV_2$ | PTX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 6.89 | 6.89 | 53.0 | – | – | – | 6.89 | 6.89 | 53.1 | 0.008 | 5.997 | 0.0 | – | 0.0 |
| $SGe_2$ | HTP | $P1(1)$ | $P1(1)$ | $P1(1)$ | 6.73 | 6.89 | 60.9 | 6.72 | 6.90 | 60.6 | 7.33 | 8.51 | 78.8 | 0.002 | 0.771 | 0.0 | 0.0 | 0.0 |
| $SSe_2$ | HPX | – | $Pc(7)$ | $P1(1)$ | – | – | – | 8.81 | 11.67 | 41.4 | 8.54 | 8.91 | 76.9 | 0.744 | 2.519 | – | 0.0 | 0.0 |
| $SBr_2$ | THP | $P2_1/c(14)$ | $Pm(6)$ | $P1(1)$ | 8.48 | 8.48 | 73.3 | 7.93 | 8.36 | 65.1 | 11.15 | 11.13 | 72.1 | 0.222 | 0.350 | 0.0 | 0.0 | 0.0 |
| $SRb_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.37 | 10.37 | 59.1 | – | – | – | 10.21 | 10.23 | 60.1 | 0.019 | 1.635 | 0.0 | – | 0.0 |
| $SSr_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 8.35 | 8.35 | 59.7 | – | – | – | – | – | – | 0.977 | 2.337 | 0.0 | – | – |
| $SY_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{1}(2)$ | 7.49 | 7.49 | 59.9 | – | – | – | 8.89 | 7.20 | 54.2 | 0.273 | 1.130 | 0.0 | – | 0.0 |
| $SZr_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 7.97 | 7.04 | 63.8 | 1.250 | 2.169 | – | – | 0.0 |
| $SNb_2$ | TXX | $P\bar{1}(2)$ | – | – | 7.56 | 7.30 | 50.3 | – | – | – | – | – | – | 1.868 | 3.667 | 0.0 | – | – |
| $STc_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 4.62 | 6.99 | 64.7 | 4.769 | 11.245 | – | – | 0.0 |
| $SSn_2$ | TPH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P1(1)$ | 7.14 | 7.16 | 59.7 | 7.02 | 7.02 | 59.1 | 8.69 | 8.33 | 85.7 | 0.037 | 0.309 | 0.0 | 0.0 | 0.0 |
| $SI_2$ | HPT | $P1(1)$ | $Amm2(38)$ | $P\bar{1}(2)$ | 7.91 | 9.57 | 75.7 | 7.96 | 9.56 | 64.8 | 9.98 | 12.93 | 55.3 | 0.019 | 0.038 | 0.0 | 0.0 | 0.0 |
| $SCs_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.67 | 10.69 | 58.8 | – | – | – | 10.51 | 10.52 | 59.8 | 0.020 | 1.312 | 0.0 | – | 0.0 |
| $SBa_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 8.84 | 8.84 | 59.6 | – | – | – | – | – | – | 1.845 | 2.529 | 0.0 | – | – |
| $SAu_2$ | TXX | $P42_12(90)$ | – | – | 8.04 | 11.46 | 44.3 | – | – | – | – | – | – | 1.498 | 2.257 | 0.0 | – | – |
| $STl_2$ | TPH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 8.54 | 8.54 | 59.0 | 8.33 | 8.33 | 59.4 | 8.62 | 8.54 | 58.5 | 0.008 | 0.169 | 0.0 | 0.0 | 0.0 |
| $SPb_2$ | PHT | $P\bar{3}m1(164)$ | $Pmmn(59)$ | $P2_1/m(11)$ | 7.45 | 7.44 | 59.7 | 7.54 | 6.88 | 56.4 | 10.21 | 10.26 | 43.9 | 0.289 | 0.527 | 0.0 | 0.0 | 0.0 |
| $SBi_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 9.73 | 10.66 | 56.2 | 1.536 | 1.745 | – | – | 0.0 |
| $ClCl_2$ | PHX | – | $P1(1)$ | $P2/c(13)$ | – | – | – | 10.28 | 6.52 | 94.6 | 10.76 | 10.84 | 98.2 | 0.715 | 2.022 | – | 0.0 | 0.0 |
| $ClK_2$ | TPH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 9.24 | 9.26 | 57.9 | 9.08 | 9.10 | 57.3 | 10.37 | 10.65 | 89.6 | 0.130 | 0.236 | 0.0 | 0.0 | 0.0 |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | T | H | P |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | | | |
| $ClCa_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 7.63 | 7.62 | 59.7 | 7.59 | 7.59 | 59.7 | – | – | – | 0.303 | 1.497 | 0.0 | 0.0 | – |
| $ClSc_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 6.41 | 6.73 | 73.6 | 5.835 | 6.699 | – | – | 0.0 |
| $ClBr_2$ | PHX | – | $P1(1)$ | $P2/c(13)$ | – | – | – | 8.78 | 7.23 | 80.9 | 10.62 | 10.63 | 94.8 | 0.159 | 2.528 | – | 0.0 | 0.0 |
| $ClRb_2$ | THP | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P1(1)$ | 9.82 | 9.83 | 58.0 | 9.69 | 9.71 | 56.6 | 11.98 | 11.99 | 91.3 | 0.278 | 0.393 | 0.0 | 0.0 | 0.0 |
| $ClSr_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 8.25 | 8.24 | 59.6 | 8.33 | 8.33 | 57.7 | – | – | – | 0.343 | 2.532 | 0.0 | 0.0 | – |
| $ClY_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P2_12_12(18)$ | 7.08 | 7.08 | 60.1 | 7.05 | 7.04 | 60.1 | 8.72 | 8.72 | 81.4 | 0.622 | 0.748 | 0.0 | 0.0 | 0.0 |
| $ClIn_2$ | THP | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P1(1)$ | 7.02 | 7.02 | 60.6 | 6.97 | 6.98 | 60.4 | 10.11 | 7.62 | 85.3 | 0.043 | 0.467 | 0.0 | 0.0 | 0.0 |
| $ClSn_2$ | PHX | – | $Amm2(38)$ | $P1(1)$ | – | – | – | 6.81 | 6.81 | 59.8 | 8.91 | 9.05 | 65.3 | 0.211 | 1.219 | – | 0.0 | 0.0 |
| $ClCs_2$ | TPH | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P1(1)$ | 10.58 | 10.58 | 56.8 | 10.64 | 10.65 | 54.1 | 11.64 | 10.89 | 78.7 | 0.183 | 0.436 | 0.0 | 0.0 | 0.0 |
| $ClBa_2$ | TPH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $Pmna(53)$ | 8.71 | 8.71 | 59.9 | 8.57 | 8.57 | 59.8 | 12.62 | 7.36 | 90.0 | 0.026 | 0.085 | 0.0 | 0.0 | 0.9 |
| $ClTl_2$ | THX | $P\bar{3}m1(164)$ | $Amm2(38)$ | – | 7.71 | 7.69 | 57.7 | 7.69 | 7.67 | 55.8 | – | – | – | 0.235 | 2.120 | 0.0 | 0.0 | – |
| $ClPb_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 6.71 | 13.42 | 46.4 | 1.535 | 1.646 | – | – | 0.0 |
| $KN_2$ | TPX | $P\bar{3}m1(164)$ | – | $P6/mmm(191)$ | 9.79 | 10.30 | 58.5 | – | – | – | 10.07 | 10.07 | 61.7 | 0.006 | 1.103 | 20.0 | – | 20.0 |
| $KF_2$ | THX | $P4mm(99)$ | $P\bar{6}m2(187)$ | – | 7.36 | 10.45 | 44.6 | 8.83 | 8.81 | 56.8 | – | – | – | 0.434 | 1.186 | 4.0 | 4.0 | – |
| $KSi_2$ | PXX | – | – | $P2/c(13)$ | – | – | – | – | – | – | 11.24 | 11.25 | 39.7 | 3.311 | 9.007 | – | – | 0.0 |
| $KS_2$ | TPX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 10.37 | 12.11 | 38.8 | – | – | – | 7.57 | 12.14 | 57.7 | 0.016 | 1.904 | 0.0 | – | 0.0 |
| $KCl_2$ | THX | $P4/mmm(123)$ | – | $P\bar{6}m2(187)$ | 8.54 | 12.06 | 45.0 | 10.13 | 10.20 | 57.7 | – | – | – | 0.294 | 1.368 | 4.0 | 4.0 | – |
| $KSe_2$ | PTX | $C2/m(12)$ | – | $P\bar{1}(2)$ | 12.40 | 12.43 | 41.7 | – | – | – | 12.07 | 10.58 | 41.8 | 0.400 | 1.789 | 0.0 | – | 0.0 |
| $KBr_2$ | PTX | $P4/mmm(123)$ | – | $P2/m(10)$ | 9.94 | 9.94 | 53.0 | – | – | – | 12.65 | 12.78 | 57.8 | 0.683 | 1.014 | 4.0 | – | 0.0 |
| $KSr_2$ | HXX | – | $P1(1)$ | – | – | – | – | 14.90 | 12.22 | 34.9 | – | – | – | 4.308 | 4.310 | – | 0.0 | – |
| $KAg_2$ | HXX | – | $Aem2(39)$ | – | – | – | – | 13.20 | 12.24 | 20.9 | – | – | – | 2.265 | 2.295 | – | 0.0 | – |
| $KSn_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 12.42 | 12.46 | 43.5 | 1.599 | 6.654 | – | – | 0.0 |
| $KI_2$ | TPH | $P2/c(13)$ | $Amm2(38)$ | $P2/m(10)$ | 10.94 | 10.95 | 53.3 | 11.37 | 11.37 | 56.3 | 13.32 | 13.26 | 56.3 | 0.171 | 0.227 | 4.0 | 4.0 | 0.0 |
| $KBa_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 14.40 | 14.44 | 34.8 | – | – | – | 1.099 | 1.172 | – | 0.0 | – |
| $KBi_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 12.35 | 14.81 | 29.2 | – | – | – | 1.424 | 3.286 | – | 0.0 | – |
| $CaB_2$ | TPX | $Pmma(51)$ | – | $Pmma(51)$ | 8.29 | 10.25 | 35.9 | – | – | – | 8.26 | 10.19 | 36.0 | 0.005 | 15.069 | 0.0 | – | 0.0 |
| $CaN_2$ | PXX | – | – | $Pmmn(59)$ | – | – | – | – | – | – | 6.97 | 7.94 | 55.9 | 2.686 | 21.815 | – | – | 0.0 |
| $CaO_2$ | PHX | – | $P\bar{6}m2(187)$ | $P4/mmm(123)$ | – | – | – | 7.49 | 7.48 | 60.6 | 6.41 | 7.17 | 63.4 | 0.615 | 7.585 | – | 0.0 | 0.0 |
| $CaF_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.24 | 7.25 | 60.0 | – | – | – | 7.24 | 7.24 | 60.1 | 0.028 | 3.153 | 0.0 | – | 0.0 |
| $CaSi_2$ | TPX | $C2/m(12)$ | – | $Pmmn(59)$ | 11.52 | 11.52 | 39.0 | – | – | – | 11.42 | 11.42 | 39.4 | 0.030 | 5.564 | 0.0 | – | 0.0 |
| $CaS_2$ | PHX | – | $P\bar{6}m2(187)$ | $P4/mmm(123)$ | – | – | – | 9.02 | 9.01 | 58.4 | 8.58 | 7.66 | 63.3 | 0.388 | 7.064 | – | 0.0 | 0.0 |
| $CaCl_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 8.29 | 8.29 | 60.0 | – | – | – | 8.29 | 8.29 | 59.9 | 0.001 | 1.980 | 0.0 | – | 0.0 |
| $CaK_2$ | HXX | – | $P2/m(10)$ | – | – | – | – | 8.35 | 13.97 | 33.5 | – | – | – | 4.431 | 4.483 | – | 0.0 | – |
| $CaCr_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 6.42 | 10.52 | 34.3 | – | – | – | 3.709 | 3.723 | – | 36.4 | – |
| $CaGe_2$ | TPX | $C2/m(12)$ | – | $Pmmn(59)$ | 11.48 | 11.48 | 40.7 | – | – | – | 11.27 | 11.27 | 41.4 | 0.007 | 4.591 | 0.0 | – | 0.0 |
| $CaSe_2$ | THX | $P4/mmm(123)$ | $P\bar{6}m2(187)$ | – | 8.00 | 11.36 | 44.9 | 9.37 | 9.38 | 58.2 | – | – | – | 0.335 | 1.768 | 0.0 | 0.0 | – |
| $CaBr_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 8.62 | 8.61 | 59.4 | – | – | – | 8.55 | 8.55 | 59.9 | 0.005 | 1.548 | 0.0 | – | 0.0 |
| $CaRb_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 13.13 | 8.80 | 41.5 | – | – | – | 3.612 | 3.733 | – | 0.0 | – |
| $CaSr_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 8.12 | 11.93 | 42.7 | – | – | – | 5.908 | 6.058 | – | 0.0 | – |
| $CaAg_2$ | HXX | – | $P4/nmm(129)$ | – | – | – | – | 7.29 | 10.38 | 45.1 | – | – | – | 2.068 | 2.099 | – | 0.0 | – |
| $CaSn_2$ | PTX | $C2/m(12)$ | – | $Pmmn(59)$ | 11.94 | 11.94 | 44.0 | – | – | – | 11.99 | 12.00 | 43.6 | 0.053 | 4.749 | 0.0 | – | 0.0 |
| $CaSb_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 9.52 | 11.96 | 36.0 | – | – | – | 1.402 | 4.121 | – | 0.0 | – |
| $CaTe_2$ | THX | $C2/m(12)$ | $P\bar{6}m2(187)$ | – | 11.55 | 9.01 | 49.8 | 9.86 | 9.90 | 59.2 | – | – | – | 0.410 | 2.140 | 0.0 | 0.0 | – |
| $CaI_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.13 | 9.14 | 59.4 | – | – | – | 9.07 | 9.08 | 59.8 | 0.005 | 1.259 | 0.0 | – | 0.0 |
| $CaBa_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 8.41 | 13.79 | 34.9 | – | – | – | 5.809 | 6.597 | – | 0.0 | – |
| $CaIr_2$ | HXX | – | $P1(1)$ | – | – | – | – | 10.09 | 8.92 | 30.6 | – | – | – | 7.678 | 7.791 | – | 0.0 | – |
| $CaAu_2$ | HXX | – | $Pmn2_1(31)$ | – | – | – | – | 7.61 | 8.88 | 54.2 | – | – | – | 1.218 | 1.219 | – | 0.0 | – |
| $CaHg_2$ | HPT | $C2/m(12)$ | $Amm2(38)$ | $P6/mmm(191)$ | 11.48 | 11.50 | 37.9 | 10.67 | 10.75 | 41.0 | 10.98 | 10.99 | 59.6 | 0.088 | 0.094 | 0.0 | 0.0 | 0.0 |
| $CaTl_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 8.22 | 12.19 | 36.0 | – | – | – | 2.239 | 2.264 | – | 0.0 | – |
| $CaBi_2$ | HXX | – | $Pmmm(47)$ | – | – | – | – | 12.04 | 9.66 | 36.2 | – | – | – | 1.884 | 1.930 | – | 0.0 | – |
| $ScC_2$ | PXX | – | – | $Pmmn(59)$ | – | – | – | – | – | – | 6.80 | 8.20 | 52.8 | 1.291 | 6.761 | – | – | 0.0 |
| $ScN_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 7.35 | 7.36 | 49.7 | 1.883 | 14.128 | – | – | 0.0 |
| $ScO_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 5.77 | 7.32 | 55.5 | 2.577 | 3.186 | – | – | 0.0 |
| $ScF_2$ | PHX | – | $P\bar{6}m2(187)$ | $P\bar{1}(2)$ | – | – | – | 6.28 | 6.29 | 60.0 | 6.30 | 6.83 | 63.1 | 0.652 | 0.827 | – | 4.0 | 0.0 |
| $ScS_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 9.53 | 8.94 | 46.3 | 1.311 | 1.457 | – | – | 0.0 |
| $ScCl_2$ | HTX | $C2/m(12)$ | $P\bar{6}m2(187)$ | – | 7.28 | 7.28 | 59.7 | 7.11 | 7.11 | 59.9 | – | – | – | 0.085 | 2.970 | 0.7 | 3.7 | – |
| $ScCa_2$ | HTX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 7.35 | 10.44 | 44.6 | 7.32 | 10.32 | 45.2 | – | – | – | 0.003 | 9.863 | 0.0 | 0.0 | – |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $ScSc_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.56 | 9.28 | 45.0 | – | – | – | 5.445 | 12.533 | – | 0.0 | – |
| $ScCr_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 6.02 | 9.89 | 34.7 | – | – | – | 5.287 | 8.769 | – | 32.2 | – |
| $ScGe_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 7.97 | 10.15 | 38.2 | – | – | – | 2.631 | 2.774 | – | 0.0 | – |
| $ScSe_2$ | TXX | $P\bar{1}(2)$ | – | – | 7.56 | 8.62 | 56.9 | – | – | – | – | – | – | 0.967 | 2.324 | 0.0 | – | – |
| $ScBr_2$ | HTX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 7.61 | 7.61 | 59.4 | 7.43 | 7.42 | 59.9 | – | – | – | 0.156 | 2.274 | 0.0 | 3.8 | – |
| $ScTc_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 7.27 | 10.03 | 35.5 | – | – | – | 2.727 | 8.818 | – | 0.0 | – |
| $ScAg_2$ | HTX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 6.11 | 8.71 | 44.6 | 6.10 | 8.67 | 44.7 | – | – | – | 0.005 | 6.321 | 0.0 | 0.0 | – |
| $ScIn_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.75 | 9.55 | 45.2 | – | – | – | 5.359 | 5.523 | – | 0.0 | – |
| $ScSn_2$ | PHX | – | $Pmmm(47)$ | $Pmmm(47)$ | – | – | – | 10.92 | 8.91 | 35.2 | 10.98 | 8.93 | 35.0 | 0.109 | 4.083 | – | 0.0 | 0.0 |
| $ScTe_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{1}(2)$ | 7.92 | 7.54 | 58.5 | – | – | – | 9.18 | 8.25 | 56.4 | 0.464 | 2.029 | 0.0 | – | 0.0 |
| $ScI_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 8.16 | 8.16 | 59.9 | 8.00 | 7.99 | 59.9 | – | – | – | 0.125 | 0.956 | 0.0 | 3.7 | – |
| $ScPt_2$ | HTX | $Cmme(67)$ | $P4/mmm(123)$ | – | 8.24 | 10.28 | 29.8 | 5.91 | 8.33 | 45.1 | – | – | – | 0.742 | 6.458 | 0.0 | 0.0 | – |
| $ScAu_2$ | HTX | $C2/m(12)$ | $P4/mmm(123)$ | – | 8.12 | 6.79 | 51.1 | 6.47 | 9.14 | 44.9 | – | – | – | 0.019 | 4.427 | 0.0 | 0.0 | – |
| $ScHg_2$ | THX | $P4/mmm(123)$ | $P\bar{6}m2(187)$ | – | 6.60 | 9.37 | 44.8 | 7.03 | 6.76 | 58.3 | – | – | – | 0.457 | 3.630 | 0.0 | 0.0 | – |
| $ScPb_2$ | PHT | $Pmmm(47)$ | $Pmma(51)$ | $Pmmn(59)$ | 10.98 | 8.71 | 37.3 | 10.97 | 8.67 | 37.5 | 10.56 | 7.36 | 45.2 | 0.502 | 0.573 | 0.0 | 0.0 | 0.0 |
| $ScBi_2$ | THP | $Pmmm(47)$ | $P4/mmm(123)$ | $Pmmm(47)$ | 11.21 | 8.36 | 40.9 | 8.35 | 11.21 | 41.0 | 8.38 | 8.50 | 59.7 | 0.028 | 0.076 | 0.0 | 0.0 | 0.0 |
| $TiBe_2$ | THP | $P4/mmm(123)$ | $P4/mmm(123)$ | $P1(1)$ | 5.26 | 7.31 | 43.8 | 7.30 | 5.26 | 43.9 | 6.65 | 5.28 | 53.9 | 0.027 | 0.467 | 0.0 | 0.0 | 0.0 |
| $TiB_2$ | PXX | – | – | $P2/c(13)$ | – | – | – | – | – | – | 8.32 | 8.29 | 42.5 | 1.852 | 1.853 | – | – | 0.0 |
| $TiC_2$ | PXX | – | – | $Cm(8)$ | – | – | – | – | – | – | 7.09 | 7.08 | 47.9 | 3.522 | 5.376 | – | – | 0.0 |
| $TiN_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 6.50 | 6.52 | 60.3 | – | – | – | 1.634 | 7.641 | – | 0.0 | – |
| $TiF_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.70 | 5.69 | 60.0 | – | – | – | 2.451 | 2.491 | – | 0.0 | – |
| $TiMg_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 6.14 | 8.75 | 44.4 | 6.04 | 8.60 | 44.5 | – | – | – | 0.025 | 10.966 | 0.0 | 0.0 | – |
| $TiAl_2$ | HTX | $Pmma(51)$ | $P4/mmm(123)$ | – | 9.02 | 6.93 | 39.8 | 8.08 | 5.57 | 43.5 | – | – | – | 0.695 | 8.486 | 0.0 | 0.0 | – |
| $TiS_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.80 | 6.79 | 60.0 | – | – | – | – | – | – | 1.138 | 1.607 | 0.0 | – | – |
| $TiCl_2$ | HPX | – | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | – | – | – | 6.55 | 6.55 | 59.9 | 6.51 | 6.71 | 60.9 | 0.179 | 1.369 | – | 0.0 | 0.0 |
| $TiCa_2$ | HTX | $Pmma(51)$ | $P4/mmm(123)$ | – | 10.20 | 7.09 | 45.9 | 10.33 | 7.30 | 44.9 | – | – | – | 0.530 | 11.273 | 8.6 | 9.6 | – |
| $TiGe_2$ | THX | $Pmmm(47)$ | $Pmmm(47)$ | – | 9.73 | 8.02 | 34.4 | 8.02 | 9.72 | 34.5 | – | – | – | 0.003 | 1.876 | 0.0 | 0.0 | – |
| $TiSe_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.01 | 6.99 | 59.8 | – | – | – | 7.00 | 6.99 | 60.0 | 0.001 | 1.296 | 0.0 | – | 0.0 |
| $TiBr_2$ | HTP | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 7.36 | 7.64 | 58.7 | 6.94 | 6.93 | 60.0 | 9.56 | 6.77 | 69.3 | 0.670 | 0.720 | 7.8 | 0.0 | 0.0 |
| $TiIn_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 6.24 | 8.81 | 45.0 | 9.05 | 6.39 | 45.2 | – | – | – | 0.062 | 8.034 | 0.0 | 0.0 | – |
| $TiSn_2$ | THX | $Pmmm(47)$ | $Pmmm(47)$ | – | 8.37 | 10.36 | 35.7 | 8.37 | 10.33 | 35.8 | – | – | – | 0.013 | 9.388 | 0.0 | 0.0 | – |
| $TiTe_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.51 | 7.50 | 59.8 | – | – | – | 7.53 | 7.52 | 59.5 | 0.046 | 1.148 | 0.0 | – | 0.0 |
| $TiHf_2$ | PHX | – | $P4/mmm(123)$ | $P\bar{1}(2)$ | – | – | – | 6.01 | 8.51 | 45.0 | 5.48 | 7.03 | 49.3 | 0.179 | 6.492 | – | 0.0 | 0.0 |
| $TiTl_2$ | HTX | $P4/mmm(123)$ | $Cmmm(65)$ | – | 6.71 | 9.49 | 44.8 | 9.77 | 7.01 | 43.5 | – | – | – | 0.061 | 6.409 | 0.0 | 0.0 | – |
| $TiBi_2$ | PTX | $P\bar{1}(2)$ | – | $C2/m(12)$ | 7.59 | 8.85 | 39.9 | – | – | – | 6.56 | 7.85 | 51.3 | 0.501 | 2.761 | 0.0 | – | 0.0 |
| $VBe_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 4.80 | 6.81 | 44.4 | 6.81 | 4.81 | 44.8 | – | – | – | 0.003 | 9.537 | 0.0 | 0.0 | – |
| $VB_2$ | HPX | – | $Cmmm(65)$ | $Cmmm(65)$ | – | – | – | 6.29 | 7.98 | 37.9 | 8.18 | 8.18 | 42.6 | 0.806 | 2.263 | – | 0.0 | 4.0 |
| $VN_2$ | PHX | – | $Cm(8)$ | $P\bar{1}(2)$ | – | – | – | 6.08 | 6.10 | 59.8 | 6.49 | 5.78 | 58.2 | 0.561 | 3.376 | – | 0.0 | 0.0 |
| $VO_2$ | TPX | $P2_1/m(11)$ | – | $P2/c(13)$ | 5.77 | 5.77 | 60.6 | – | – | – | 7.19 | 7.26 | 43.1 | 0.555 | 1.228 | 4.0 | – | 4.0 |
| $VF_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 6.43 | 6.45 | 60.0 | – | – | – | 6.42 | 6.44 | 60.1 | 0.014 | 2.829 | 12.0 | – | 12.0 |
| $VAl_2$ | HTX | $Pmmm(47)$ | $Pmmm(47)$ | – | 6.68 | 8.71 | 39.9 | 8.70 | 6.68 | 39.9 | – | – | – | 0.002 | 8.146 | 0.0 | 0.0 | – |
| $VP_2$ | PHX | – | $P\bar{6}m2(187)$ | $P1(1)$ | – | – | – | 7.25 | 7.25 | 60.0 | 7.26 | 6.71 | 45.4 | 0.214 | 1.818 | – | 1.3 | 0.0 |
| $VS_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 6.35 | 6.34 | 59.9 | 6.34 | 6.34 | 60.0 | 6.34 | 6.34 | 60.0 | 0.327 | 0.329 | 1.9 | 3.7 | 1.9 |
| $VCl_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.21 | 7.21 | 59.8 | – | – | – | 7.19 | 7.19 | 60.0 | 0.001 | 1.961 | 12.0 | – | 12.0 |
| $VSc_2$ | PXX | – | – | $P4/mmm(123)$ | – | – | – | – | – | – | 6.36 | 9.05 | 44.6 | 0.966 | 1.508 | – | – | 0.0 |
| $VTi_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 5.89 | 8.37 | 44.3 | 5.88 | 8.31 | 44.9 | – | – | – | 0.228 | 4.235 | 0.0 | 0.0 | – |
| $VV_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 8.01 | 5.10 | 35.3 | – | – | – | 6.097 | 19.320 | – | 0.0 | – |
| $VMn_2$ | HTX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 5.79 | 8.22 | 44.9 | 5.77 | 8.22 | 44.6 | – | – | – | 0.023 | 16.527 | 21.1 | 21.1 | – |
| $VGe_2$ | PTH | $Pmmm(47)$ | $Pmmm(47)$ | $Pmmm(47)$ | 9.32 | 7.61 | 35.5 | 9.25 | 7.60 | 35.8 | 9.46 | 7.79 | 34.4 | 0.548 | 0.549 | 0.0 | 0.0 | 2.7 |
| $VAs_2$ | HTX | $C2/m(12)$ | $P\bar{6}m2(187)$ | – | 8.60 | 8.63 | 42.2 | 7.50 | 7.48 | 59.8 | – | – | – | 0.205 | 1.563 | 5.1 | 4.0 | – |
| $VSe_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 6.61 | 6.61 | 59.9 | 6.64 | 6.63 | 59.9 | 6.61 | 6.60 | 60.0 | 0.333 | 0.335 | 2.3 | 3.9 | 2.3 |
| $VBr_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.58 | 7.58 | 60.0 | – | – | – | 7.58 | 7.57 | 60.0 | 0.007 | 1.825 | 12.0 | – | 12.0 |
| $VSr_2$ | TXX | $C2/m(12)$ | – | – | 7.76 | 10.28 | 48.5 | – | – | – | – | – | – | 2.329 | 2.557 | 1.4 | – | – |
| $VY_2$ | PTH | $P4/mmm(123)$ | $Pmmm(47)$ | $P2_1/m(11)$ | 9.96 | 7.04 | 44.8 | 6.99 | 9.84 | 44.7 | 7.04 | 7.03 | 62.2 | 0.366 | 0.558 | 9.8 | 6.2 | 0.0 |
| $VZr_2$ | TPH | $P4/mmm(123)$ | $P4/mmm(123)$ | $P4/mmm(123)$ | 6.31 | 8.91 | 45.0 | 6.30 | 8.91 | 45.1 | 6.31 | 8.94 | 44.9 | 0.001 | 0.004 | 0.0 | 0.0 | 0.0 |
| $VCd_2$ | HTX | $Cmmm(65)$ | $Cmmm(65)$ | – | 6.93 | 9.05 | 39.6 | 8.64 | 5.99 | 43.7 | – | – | – | 0.725 | 8.211 | 0.0 | 0.0 | – |
| $VSn_2$ | HXX | – | $P\bar{1}(2)$ | – | – | – | – | 8.31 | 6.11 | 45.9 | – | – | – | 7.157 | 10.323 | – | 1.1 | – |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $VSb_2$ | PTH | $C2/m(12)$ | $Amm2(38)$ | $C2/m(12)$ | 9.16 | 9.17 | 43.4 | 8.88 | 8.90 | 43.6 | 9.19 | 9.18 | 43.1 | 0.058 | 0.300 | 8.3 | 10.3 | 8.4 |
| $VTe_2$ | PTH | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 7.42 | 7.45 | 57.1 | 7.26 | 7.25 | 59.9 | 7.49 | 7.50 | 56.0 | 0.062 | 0.215 | 5.3 | 4.0 | 5.5 |
| $VI_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 8.17 | 8.18 | 59.9 | – | – | – | – | – | – | 1.407 | 3.176 | 12.0 | – | – |
| $VPb_2$ | PHX | – | $P4/mmm(123)$ | $C2/m(12)$ | – | – | – | 6.92 | 9.80 | 44.9 | 8.97 | 6.97 | 48.7 | 0.758 | 4.917 | – | 12.5 | 0.5 |
| $VBi_2$ | PTH | $C2/m(12)$ | $Amm2(38)$ | $C2/m(12)$ | 9.46 | 9.46 | 42.2 | 9.12 | 9.13 | 44.1 | 9.48 | 9.46 | 42.0 | 0.004 | 0.007 | 9.9 | 10.4 | 10.0 |
| $CrC_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 6.61 | 7.26 | 47.4 | 1.637 | 5.024 | – | – | 7.6 |
| $CrO_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 5.74 | 5.73 | 60.0 | 5.23 | 5.23 | 60.0 | 5.73 | 5.73 | 60.0 | 0.416 | 0.437 | 8.0 | 0.0 | 8.0 |
| $CrMg_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 6.26 | 9.01 | 43.8 | 6.25 | 8.95 | 44.1 | – | – | – | 0.060 | 5.738 | 14.8 | 14.8 | – |
| $CrAl_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 6.35 | 8.44 | 41.2 | 5.94 | 8.41 | 45.0 | – | – | – | 0.061 | 5.287 | 0.0 | 0.0 | – |
| $CrP_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 6.88 | 6.79 | 42.4 | 0.835 | 1.359 | – | – | 1.8 |
| $CrS_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 6.08 | 6.08 | 59.9 | – | – | – | 1.347 | 1.351 | – | 0.0 | – |
| $CrK_2$ | HXX | – | $P2_1/m(11)$ | – | – | – | – | 8.68 | 10.18 | 53.9 | – | – | – | 1.711 | 3.942 | – | 20.3 | – |
| $CrCa_2$ | THX | $P2_1/m(11)$ | $P4/mmm(123)$ | – | 7.62 | 8.88 | 54.4 | 7.42 | 10.52 | 44.9 | – | – | – | 0.640 | 8.018 | 16.0 | 17.7 | – |
| $CrSc_2$ | PHT | $P4/mmm(123)$ | $P4/mmm(123)$ | $P\bar{1}(2)$ | 6.42 | 9.09 | 45.0 | 6.42 | 9.09 | 44.9 | 7.40 | 6.70 | 52.5 | 0.209 | 0.213 | 7.0 | 7.0 | 0.0 |
| $CrMn_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 8.00 | 5.65 | 44.9 | – | – | – | 11.904 | 16.133 | – | 23.7 | – |
| $CrGa_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 5.95 | 8.45 | 44.8 | 5.97 | 8.46 | 44.7 | – | – | – | 0.039 | 5.490 | 10.4 | 10.3 | – |
| $CrGe_2$ | PXX | – | – | $Pmma(51)$ | – | – | – | – | – | – | 6.68 | 6.68 | 50.7 | 0.941 | 1.385 | – | – | 8.8 |
| $CrSe_2$ | TPH | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 6.86 | 6.81 | 59.5 | 6.76 | 6.75 | 59.8 | 6.81 | 6.87 | 59.4 | 0.016 | 0.811 | 8.6 | 8.0 | 8.6 |
| $CrBr_2$ | THX | $C2/m(12)$ | $Cmmm(65)$ | – | 8.07 | 8.07 | 53.5 | 8.02 | 8.02 | 53.5 | – | – | – | 0.554 | 2.069 | 16.0 | 16.0 | – |
| $CrSr_2$ | PHX | – | $P4/mmm(123)$ | $P\bar{1}(2)$ | – | – | – | 7.97 | 11.30 | 44.9 | 10.01 | 8.10 | 52.3 | 0.577 | 1.952 | – | 19.1 | 17.3 |
| $CrY_2$ | HTP | $C2/m(12)$ | $P4/mmm(123)$ | $P2_1/c(14)$ | 8.81 | 6.98 | 53.0 | 6.86 | 9.72 | 44.9 | 10.19 | 7.21 | 44.0 | 0.498 | 0.712 | 7.6 | 6.1 | 7.8 |
| $CrZr_2$ | PHT | $P4/mmm(123)$ | $P4/mmm(123)$ | $P4/mmm(123)$ | 8.68 | 6.38 | 45.3 | 6.29 | 8.64 | 46.4 | 9.15 | 6.28 | 43.3 | 0.094 | 0.119 | 0.0 | 0.0 | 0.0 |
| $CrRu_2$ | HXX | – | $C2/m(12)$ | – | – | – | – | 6.88 | 7.84 | 41.6 | – | – | – | 1.187 | 5.058 | – | 0.0 | – |
| $CrSn_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 8.80 | 6.45 | 42.3 | – | – | – | 4.969 | 7.754 | – | 14.5 | – |
| $CrSb_2$ | PXX | – | – | $Pmmm(47)$ | – | – | – | – | – | – | 6.31 | 9.98 | 49.5 | 0.975 | 1.011 | – | – | 13.6 |
| $CrI_2$ | HTX | $C2/m(12)$ | $C2/m(12)$ | – | 8.68 | 8.68 | 53.8 | 8.57 | 8.57 | 54.6 | – | – | – | 0.001 | 3.470 | 16.0 | 16.0 | – |
| $CrCs_2$ | THX | $P\bar{3}m1(164)$ | $Amm2(38)$ | – | 11.35 | 11.40 | 58.3 | 11.95 | 11.92 | 48.4 | – | – | – | 0.599 | 2.505 | 22.1 | 21.2 | – |
| $CrBa_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 8.70 | 9.16 | 58.2 | 1.423 | 2.977 | – | – | 0.0 |
| $CrHf_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.24 | 8.82 | 45.0 | – | – | – | 2.721 | 5.543 | – | 0.0 | – |
| $CrPb_2$ | PXX | – | – | $Pmmn(59)$ | – | – | – | – | – | – | 6.65 | 8.87 | 67.5 | 0.910 | 1.161 | – | – | 18.2 |
| $CrBi_2$ | HPT | $C2/m(12)$ | $Amm2(38)$ | $C2/m(12)$ | 9.44 | 9.44 | 42.1 | 9.27 | 9.30 | 42.3 | 9.44 | 9.46 | 42.0 | 0.055 | 0.058 | 14.2 | 14.6 | 14.2 |
| $MnBe_2$ | HTX | $P4/mmm(123)$ | $Cmmm(65)$ | – | 5.15 | 7.25 | 45.2 | 4.60 | 7.51 | 35.3 | – | – | – | 0.801 | 7.736 | 7.7 | 0.0 | – |
| $MnB_2$ | PXX | – | – | $Cmmm(65)$ | – | – | – | – | – | – | 7.88 | 7.88 | 44.5 | 1.841 | 4.105 | – | – | 11.0 |
| $MnO_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 5.75 | 5.75 | 60.0 | – | – | – | 5.75 | 5.74 | 60.0 | 0.014 | 4.768 | 12.0 | – | 12.0 |
| $MnF_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 6.73 | 6.73 | 59.8 | – | – | – | 6.73 | 6.73 | 59.8 | 0.004 | 2.553 | 20.0 | – | 20.0 |
| $MnAl_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 6.66 | 8.60 | 39.0 | – | – | – | 0.941 | 5.969 | – | 10.9 | – |
| $MnSi_2$ | HTX | $Pmmm(47)$ | $Pmmm(47)$ | – | 7.44 | 9.01 | 34.0 | 9.01 | 7.45 | 34.0 | – | – | – | 0.017 | 2.663 | 11.0 | 11.1 | – |
| $MnP_2$ | PHT | $C2/m(12)$ | $P\bar{6}m2(187)$ | $C2/m(12)$ | 8.01 | 8.01 | 42.7 | 7.33 | 7.36 | 58.7 | 6.80 | 6.61 | 59.0 | 0.219 | 0.766 | 10.0 | 12.0 | 0.0 |
| $MnS_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 6.70 | 6.71 | 60.1 | – | – | – | 6.70 | 6.71 | 60.1 | 0.003 | 1.757 | 11.8 | – | 11.8 |
| $MnCl_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.45 | 7.46 | 59.8 | – | – | – | – | – | – | 0.942 | 1.647 | 20.0 | – | – |
| $MnCa_2$ | TPH | $P2_1/m(11)$ | $P4/mmm(123)$ | $P\bar{1}(2)$ | 7.55 | 8.78 | 54.5 | 7.37 | 10.46 | 44.7 | 7.99 | 9.55 | 50.0 | 0.441 | 0.589 | 14.7 | 17.2 | 14.8 |
| $MnSc_2$ | PHT | $P\bar{1}(2)$ | $P4/mmm(123)$ | $P2_1/m(11)$ | 6.56 | 8.25 | 53.2 | 6.30 | 8.92 | 44.9 | 6.81 | 8.28 | 52.2 | 0.107 | 0.154 | 5.8 | 0.0 | 5.1 |
| $MnCr_2$ | HXX | – | $Pccm(49)$ | – | – | – | – | 5.00 | 7.11 | 45.0 | – | – | – | 16.040 | 17.407 | – | 8.2 | – |
| $MnMn_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 5.56 | 7.87 | 45.0 | – | – | – | 9.663 | 13.770 | – | 27.3 | – |
| $MnSe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.02 | 7.03 | 60.0 | – | – | – | – | – | – | 1.765 | 2.984 | 11.5 | – | – |
| $MnBr_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.79 | 7.80 | 59.8 | – | – | – | – | – | – | 0.941 | 1.621 | 20.0 | – | – |
| $MnZr_2$ | THP | $P4/mmm(123)$ | $P4/mmm(123)$ | $P\bar{1}(2)$ | 6.23 | 8.86 | 44.6 | 6.24 | 8.80 | 45.1 | 6.83 | 6.35 | 58.3 | 0.015 | 0.188 | 0.0 | 0.0 | 0.0 |
| $MnIn_2$ | HTX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 6.36 | 9.06 | 45.4 | 9.07 | 6.39 | 45.3 | – | – | – | 0.000 | 4.674 | 15.2 | 15.2 | – |
| $MnSn_2$ | HXX | – | $Pmmm(47)$ | – | – | – | – | 9.98 | 7.95 | 36.9 | – | – | – | 3.872 | 7.001 | – | 15.3 | – |
| $MnOs_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 7.02 | 8.72 | 36.5 | – | – | – | 5.890 | 6.289 | – | 5.9 | – |
| $MnAu_2$ | HTX | $P\bar{3}m1(164)$ | $P4/mmm(123)$ | – | 5.96 | 5.96 | 59.3 | 6.68 | 6.68 | 52.5 | – | – | – | 0.711 | 3.227 | 17.2 | 18.0 | – |
| $MnPb_2$ | PHX | – | $P4/mmm(123)$ | $P4/mmm(123)$ | – | – | – | 7.17 | 10.13 | 43.5 | 7.18 | 7.84 | 62.6 | 0.124 | 3.399 | – | 15.7 | 15.9 |
| $FeBe_2$ | HTX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 7.37 | 5.21 | 45.0 | 7.29 | 5.15 | 45.0 | – | – | – | 0.475 | 9.512 | 0.0 | 5.0 | – |
| $FeB_2$ | TXX | $C2/m(12)$ | – | – | 5.59 | 5.97 | 36.8 | – | – | – | – | – | – | 4.107 | 4.694 | 0.0 | – | – |
| $FeO_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 5.58 | 5.58 | 60.0 | – | – | – | 5.59 | 5.58 | 60.0 | 0.005 | 3.965 | 8.0 | – | 8.0 |
| $FeF_2$ | TPH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 6.35 | 6.39 | 59.6 | 5.85 | 5.86 | 59.7 | 6.33 | 6.34 | 59.6 | 0.001 | 0.566 | 16.0 | 16.0 | 16.0 |
| $FeAl_2$ | HTX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 5.68 | 8.05 | 45.0 | 5.68 | 8.05 | 45.0 | – | – | – | 0.092 | 7.347 | 0.0 | 1.8 | – |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $FeP_2$ | PTH | $C2/m(12)$ | $Amm2(38)$ | $P\bar{1}(2)$ | 7.74 | 7.75 | 42.3 | 7.31 | 7.34 | 50.7 | 7.38 | 7.68 | 50.5 | 0.161 | 0.538 | 6.3 | 8.1 | 1.9 |
| $FeS_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 6.37 | 6.40 | 60.2 | 6.31 | 6.30 | 60.0 | – | – | – | 0.666 | 1.421 | 7.1 | 5.9 | – |
| $FeSc_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 6.20 | 8.77 | 45.1 | 6.20 | 8.79 | 44.9 | – | – | – | 0.002 | 1.286 | 0.0 | 0.0 | – |
| $FeGe_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 6.08 | 7.02 | 47.5 | 1.728 | 1.741 | – | – | 7.6 |
| $FeAs_2$ | THX | $C2/m(12)$ | $Amm2(38)$ | – | 8.04 | 8.10 | 43.2 | 7.62 | 7.64 | 50.7 | – | – | – | 0.444 | 7.230 | 7.7 | 9.2 | – |
| $FeSe_2$ | PTH | $C2/m(12)$ | $P\bar{6}m2(187)$ | $Cm(8)$ | 6.60 | 6.60 | 59.7 | 6.60 | 6.58 | 59.7 | 6.63 | 6.71 | 59.3 | 0.037 | 0.674 | 3.9 | 8.0 | 2.0 |
| $FeZr_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 8.22 | 6.70 | 50.2 | 1.057 | 1.825 | – | – | 0.0 |
| $FeTc_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 5.31 | 7.92 | 59.9 | 3.152 | 7.289 | – | – | 0.0 |
| $FePd_2$ | HTX | $Cmmm(65)$ | $P\bar{6}m2(187)$ | – | 5.54 | 8.18 | 41.8 | 5.48 | 5.48 | 59.9 | – | – | – | 0.217 | 1.393 | 15.4 | 15.7 | – |
| $FeSn_2$ | THX | $Pmmm(47)$ | $Pmmm(47)$ | – | 6.41 | 8.64 | 42.0 | 8.64 | 6.42 | 42.0 | – | – | – | 0.018 | 8.822 | 9.7 | 9.7 | – |
| $FeBi_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 7.01 | 8.44 | 50.6 | 2.146 | 2.272 | – | – | 8.0 |
| $CoB_2$ | PXX | – | – | $Pmmn(59)$ | – | – | – | – | – | – | 6.68 | 6.69 | 53.2 | 1.582 | 1.617 | – | – | 0.0 |
| $CoC_2$ | TXX | $C2/m(12)$ | – | – | 5.89 | 5.61 | 44.4 | – | – | – | – | – | – | 2.261 | 3.502 | 0.0 | – | – |
| $CoO_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 5.65 | 5.64 | 59.7 | – | – | – | 5.65 | 5.64 | 59.7 | 0.010 | 5.514 | 3.3 | – | 3.3 |
| $CoF_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 6.30 | 6.30 | 59.3 | – | – | – | 6.32 | 6.30 | 59.4 | 0.032 | 2.104 | 12.0 | – | 12.0 |
| $CoAl_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 5.72 | 7.87 | 43.2 | 5.43 | 7.82 | 45.7 | – | – | – | 0.020 | 6.863 | 0.0 | 0.0 | – |
| $CoSi_2$ | HXX | – | $Pbcm(57)$ | – | – | – | – | 8.55 | 7.06 | 34.0 | – | – | – | 1.204 | 1.329 | – | 0.0 | – |
| $CoS_2$ | TPX | $P\bar{1}(2)$ | – | $P2/c(13)$ | 6.67 | 6.63 | 53.8 | – | – | – | 7.57 | 7.06 | 43.4 | 0.041 | 1.218 | 0.0 | – | 0.0 |
| $CoSe_2$ | TPX | $P\bar{1}(2)$ | – | $P2_1/m(11)$ | 7.00 | 7.04 | 53.3 | – | – | – | 6.68 | 6.82 | 59.7 | 0.153 | 1.557 | 0.0 | – | 0.0 |
| $CoBr_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.47 | 7.48 | 59.6 | – | – | – | – | – | – | 1.436 | 2.428 | 11.9 | – | – |
| $CoZr_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 7.79 | 6.52 | 52.6 | 2.502 | 2.631 | – | – | 0.0 |
| $CoSb_2$ | HXX | – | $Pmm2(25)$ | – | – | – | – | 6.95 | 6.94 | 55.2 | – | – | – | 1.237 | 9.025 | – | 0.6 | – |
| $CoHf_2$ | TPX | $C2/m(12)$ | – | $C2/m(12)$ | 6.43 | 7.81 | 51.7 | – | – | – | 7.82 | 6.45 | 51.7 | 0.000 | 2.055 | 0.0 | – | 0.0 |
| $CoIr_2$ | HTX | $C2/m(12)$ | $Amm2(38)$ | – | 8.38 | 8.39 | 35.6 | 8.23 | 8.24 | 35.8 | – | – | – | 0.363 | 0.833 | 5.0 | 6.3 | – |
| $NiBe_2$ | THX | $P\bar{3}m1(164)$ | $P4/mmm(123)$ | – | 7.41 | 6.38 | 29.8 | 5.12 | 7.26 | 44.9 | – | – | – | 0.315 | 6.864 | 0.0 | 0.0 | – |
| $NiO_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{3}m1(164)$ | – | 5.67 | 5.67 | 59.7 | 5.69 | 5.67 | 59.8 | – | – | – | 0.002 | 2.454 | 0.0 | 0.0 | – |
| $NiP_2$ | HPT | $P\bar{1}(2)$ | $Pc(7)$ | $C2/m(12)$ | 7.54 | 7.82 | 40.9 | 7.62 | 7.67 | 40.8 | 7.87 | 7.87 | 47.2 | 0.405 | 0.553 | 0.0 | 0.0 | 0.0 |
| $NiS_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.72 | 6.72 | 59.7 | – | – | – | – | – | – | 1.559 | 1.922 | 0.0 | – | – |
| $NiSc_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 7.47 | 7.51 | 59.4 | 6.82 | 6.85 | 59.7 | 7.46 | 7.49 | 59.6 | 0.008 | 0.030 | 0.0 | 0.0 | 0.0 |
| $NiAs_2$ | HTX | $C2/m(12)$ | $Amm2(38)$ | – | 8.09 | 7.79 | 43.3 | 7.94 | 7.94 | 41.8 | – | – | – | 0.030 | 2.912 | 0.0 | 0.0 | – |
| $NiSe_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.16 | 7.18 | 58.9 | – | – | – | 7.16 | 7.16 | 59.1 | 0.016 | 1.992 | 0.0 | – | 0.0 |
| $NiBr_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.40 | 7.39 | 59.6 | – | – | – | – | – | – | 1.535 | 1.574 | 8.0 | – | – |
| $NiY_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 8.04 | 8.08 | 59.7 | – | – | – | 8.07 | 8.09 | 59.3 | 0.002 | 0.841 | 0.0 | – | 0.0 |
| $NiIn_2$ | HXX | – | $Pmmm(47)$ | – | – | – | – | 9.15 | 6.93 | 39.5 | – | – | – | 2.741 | 4.089 | – | 0.0 | – |
| $NiSn_2$ | HTP | $P2_1/m(11)$ | $Pmmm(47)$ | $P\bar{1}(2)$ | 8.32 | 6.49 | 49.8 | 7.04 | 7.04 | 49.5 | 6.70 | 8.17 | 52.9 | 0.383 | 0.556 | 0.0 | 0.0 | 0.0 |
| $NiI_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.96 | 7.95 | 59.6 | – | – | – | – | – | – | 2.497 | 3.016 | 7.8 | – | – |
| $NiHf_2$ | PTX | $C2/m(12)$ | – | $C2/m(12)$ | 6.43 | 8.31 | 54.4 | – | – | – | 8.32 | 6.42 | 54.6 | 0.023 | 1.233 | 0.0 | – | 0.0 |
| $NiIr_2$ | HPT | $C2/m(12)$ | $Amm2(38)$ | $Pmmn(59)$ | 8.49 | 8.49 | 34.7 | 8.41 | 8.44 | 34.6 | 8.69 | 8.69 | 53.7 | 0.275 | 0.300 | 0.0 | 0.0 | 2.6 |
| $NiHg_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 8.51 | 5.99 | 43.8 | – | – | – | 3.814 | 3.885 | – | 0.0 | – |
| $NiBi_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 8.51 | 6.89 | 50.3 | – | – | – | 1.937 | 1.956 | – | 0.0 | – |
| $GaCa_2$ | PTH | $P4/mmm(123)$ | $P4/mmm(123)$ | $P2_1/m(11)$ | 7.31 | 10.40 | 44.8 | 10.38 | 7.30 | 44.6 | 7.60 | 8.94 | 53.3 | 0.226 | 0.265 | 0.0 | 0.0 | 0.0 |
| $GaTi_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 6.10 | 8.18 | 63.1 | 3.154 | 3.531 | – | – | 0.0 |
| $GaCr_2$ | TXX | $P4/mmm(123)$ | – | – | 6.04 | 8.64 | 43.3 | – | – | – | – | – | – | 0.958 | 5.749 | 33.7 | – | – |
| $GaMn_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 5.78 | 8.35 | 41.9 | – | – | – | 3.209 | 4.275 | – | 31.7 | – |
| $GaY_2$ | PHX | – | $P4/mmm(123)$ | $C2/m(12)$ | – | – | – | 7.03 | 9.96 | 44.9 | 8.50 | 9.40 | 46.9 | 0.142 | 2.547 | – | 0.0 | 0.0 |
| $GaSn_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.90 | 9.94 | 36.7 | – | – | – | 3.145 | 5.782 | – | 0.2 | – |
| $GeBe_2$ | HPT | $P6mm(183)$ | $Pmn2_1(31)$ | $Pmmn(59)$ | 7.51 | 7.53 | 60.0 | 6.45 | 6.45 | 47.0 | 7.59 | 7.34 | 58.9 | 0.620 | 0.717 | 0.0 | 0.0 | 0.0 |
| $GeC_2$ | PXX | – | – | $P\bar{4}2_1m(113)$ | – | – | – | – | – | – | 6.49 | 6.48 | 90.0 | 2.928 | 5.387 | – | – | 0.0 |
| $GeO_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{3}m1(164)$ | – | 5.81 | 5.81 | 60.0 | 5.81 | 5.81 | 60.0 | – | – | – | 0.005 | 2.317 | 0.0 | 0.0 | – |
| $GeMg_2$ | PTX | $P\bar{3}m1(164)$ | – | $Pmmn(59)$ | 8.89 | 8.90 | 59.6 | – | – | – | 9.01 | 8.04 | 55.4 | 0.432 | 1.688 | 0.0 | – | 0.0 |
| $GeAl_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 8.11 | 8.10 | 39.7 | – | – | – | 1.794 | 2.666 | – | 0.0 | – |
| $GeCl_2$ | TPX | $P\bar{3}m1(164)$ | – | $P1(1)$ | 7.86 | 7.86 | 60.6 | – | – | – | 8.29 | 8.29 | 79.8 | 0.279 | 0.979 | 0.0 | – | 0.0 |
| $GeK_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 10.57 | 9.90 | 46.0 | – | – | – | 2.766 | 3.054 | – | 0.0 | – |
| $GeCa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.50 | 9.50 | 59.6 | – | – | – | 9.43 | 9.44 | 60.1 | 0.005 | 2.573 | 0.0 | – | 0.0 |
| $GeCr_2$ | THX | $P2_1/m(11)$ | $P4/mmm(123)$ | – | 7.43 | 7.87 | 58.0 | 5.95 | 8.44 | 44.8 | – | – | – | 0.593 | 2.554 | 31.9 | 32.5 | – |
| $GeGe_2$ | HPX | – | $P\bar{6}m2(187)$ | $P1(1)$ | – | – | – | 7.72 | 7.73 | 60.0 | 8.18 | 6.15 | 69.2 | 0.126 | 1.722 | – | 0.0 | 0.0 |
| $GeSe_2$ | HTX | $P\bar{3}m1(164)$ | $C222(21)$ | – | 7.28 | 7.28 | 59.7 | 7.47 | 7.47 | 78.8 | – | – | – | 0.394 | 1.030 | 0.0 | 0.0 | – |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $GeBr_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 8.10 | 8.10 | 60.6 | – | – | – | 8.16 | 7.06 | 90.0 | 0.045 | 1.381 | 0.0 | – | 0.0 |
| $GeRb_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 10.96 | 10.28 | 46.3 | – | – | – | 2.719 | 4.539 | – | 0.0 | – |
| $GeSr_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.92 | 9.92 | 59.6 | – | – | – | 9.86 | 9.87 | 59.9 | 0.003 | 2.266 | 0.0 | – | 0.0 |
| $GePd_2$ | PTH | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 7.57 | 7.59 | 45.3 | 6.11 | 6.11 | 59.9 | 5.78 | 7.27 | 66.1 | 0.230 | 0.630 | 0.0 | 0.0 | 0.0 |
| $GeCd_2$ | HTX | $P\bar{3}m1(164)$ | $Amm2(38)$ | – | 9.08 | 9.08 | 59.8 | 8.87 | 8.84 | 38.0 | – | – | – | 0.761 | 0.863 | 0.0 | 0.0 | – |
| $GeIn_2$ | HXX | – | $Pm(6)$ | – | – | – | – | 8.81 | 8.97 | 40.7 | – | – | – | 0.867 | 0.879 | – | 0.0 | – |
| $GeSn_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 8.21 | 8.23 | 60.0 | – | – | – | 0.915 | 1.077 | – | 0.0 | – |
| $GeTe_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{1}(2)$ | 7.84 | 7.84 | 59.0 | – | – | – | 9.44 | 9.40 | 69.4 | 0.284 | 0.953 | 0.0 | – | 0.0 |
| $GeCs_2$ | PTH | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P\bar{3}m1(164)$ | 11.87 | 11.83 | 58.2 | 11.13 | 11.12 | 48.6 | 11.60 | 11.60 | 59.4 | 0.015 | 0.776 | 8.0 | 5.3 | 8.0 |
| $GeBa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.28 | 10.28 | 59.2 | – | – | – | 10.16 | 10.16 | 60.2 | 0.010 | 1.539 | 0.0 | – | 0.0 |
| $GePt_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.95 | 5.97 | 60.1 | – | – | – | 0.991 | 2.490 | – | 0.0 | – |
| $GeAu_2$ | THX | $P2_1/m(11)$ | $Pmn2_1(31)$ | – | 7.84 | 7.85 | 42.0 | 7.78 | 7.78 | 42.5 | – | – | – | 0.120 | 1.981 | 0.0 | 0.0 | – |
| $GeTl_2$ | HXX | – | $Pm(6)$ | – | – | – | – | 8.49 | 7.08 | 51.7 | – | – | – | 1.926 | 1.934 | – | 0.0 | – |
| $AsS_2$ | TPX | $P\bar{3}m1(164)$ | – | $P1(1)$ | 7.00 | 7.01 | 59.5 | – | – | – | 6.59 | 10.23 | 67.7 | 0.402 | 3.003 | 0.0 | – | 0.0 |
| $AsCa_2$ | PTX | $P\bar{3}m1(164)$ | – | $Cm(8)$ | 8.66 | 8.68 | 59.8 | – | – | – | 8.71 | 8.73 | 59.6 | 0.154 | 1.572 | 0.0 | – | 0.0 |
| $AsSc_2$ | TPX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 7.89 | 7.47 | 61.3 | – | – | – | 7.97 | 7.52 | 61.6 | 0.008 | 2.161 | 0.0 | – | 0.0 |
| $AsTi_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 6.16 | 8.05 | 48.4 | – | – | – | 5.888 | 8.074 | – | 1.9 | – |
| $AsV_2$ | TXX | $P2_1/m(11)$ | – | – | 6.21 | 6.96 | 62.8 | – | – | – | – | – | – | 7.718 | 8.634 | 0.0 | – | – |
| $AsCr_2$ | TXX | $P\bar{1}(2)$ | – | – | 7.05 | 7.27 | 60.7 | – | – | – | – | – | – | 2.208 | 4.659 | 15.9 | – | – |
| $AsSe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.33 | 7.34 | 59.3 | – | – | – | – | – | – | 1.864 | 1.925 | 0.0 | – | – |
| $AsRb_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 9.67 | 12.74 | 36.5 | – | – | – | 2.480 | 2.557 | – | 0.0 | – |
| $AsSr_2$ | PTX | $P\bar{3}m1(164)$ | – | $P2_1/m(11)$ | 9.11 | 9.12 | 60.0 | – | – | – | 9.13 | 9.21 | 59.6 | 0.033 | 1.587 | 0.0 | – | 1.8 |
| $AsZr_2$ | TPX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 8.17 | 8.22 | 51.8 | – | – | – | 7.26 | 8.15 | 63.3 | 0.078 | 2.960 | 0.0 | – | 0.0 |
| $AsPd_2$ | HTP | $C2/m(12)$ | $Pmn2_1(31)$ | $P\bar{3}m1(164)$ | 8.55 | 8.54 | 40.6 | 7.31 | 6.09 | 65.1 | 8.60 | 8.60 | 59.4 | 0.242 | 0.782 | 0.0 | 0.0 | 0.0 |
| $AsSn_2$ | PTH | $P\bar{3}m1(164)$ | $P3m1(156)$ | $P\bar{1}(2)$ | 7.43 | 7.39 | 59.4 | 7.89 | 7.88 | 59.2 | 7.95 | 9.70 | 54.5 | 0.071 | 0.233 | 0.0 | 0.0 | 0.0 |
| $AsTe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.81 | 7.78 | 58.8 | – | – | – | – | – | – | 1.290 | 1.502 | 0.0 | – | – |
| $AsCs_2$ | TPX | $P\bar{3}m1(164)$ | – | $Cm(8)$ | 11.37 | 11.31 | 59.6 | – | – | – | 11.44 | 11.32 | 58.7 | 0.116 | 0.844 | 4.0 | – | 4.0 |
| $AsBa_2$ | TPX | $P\bar{3}m1(164)$ | – | $P2_1/m(11)$ | 9.46 | 9.52 | 60.2 | – | – | – | 9.67 | 9.56 | 59.2 | 0.018 | 1.636 | 0.0 | – | 0.1 |
| $AsHf_2$ | PTX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 6.99 | 8.10 | 64.3 | – | – | – | 8.14 | 8.16 | 50.3 | 0.155 | 2.724 | 0.0 | – | 0.0 |
| $SeLi_2$ | TPX | $P\bar{3}m1(164)$ | – | $P2_1/m(11)$ | 8.32 | 8.31 | 59.8 | – | – | – | 8.33 | 8.31 | 59.8 | 0.043 | 2.199 | 0.0 | – | 0.0 |
| $SeBe_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 5.42 | 7.01 | 69.5 | 1.058 | 1.540 | – | – | 0.0 |
| $SeNa_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 9.39 | 9.40 | 59.6 | – | – | – | – | – | – | 2.205 | 2.205 | 0.0 | – | – |
| $SeS_2$ | PTX | $P\bar{3}m1(164)$ | – | $P1(1)$ | 7.14 | 7.14 | 60.3 | – | – | – | 9.50 | 8.02 | 80.9 | 0.729 | 4.000 | 0.0 | – | 0.0 |
| $SeK_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.65 | 10.65 | 57.2 | – | – | – | 10.35 | 10.34 | 59.7 | 0.075 | 1.818 | 0.0 | – | 0.0 |
| $SeCa_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 8.06 | 8.06 | 60.0 | 8.00 | 7.99 | 59.8 | – | – | – | 0.534 | 1.206 | 0.0 | 0.0 | – |
| $SeSc_2$ | TPH | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 8.11 | 8.12 | 52.2 | 6.98 | 6.97 | 60.0 | 8.12 | 8.12 | 52.1 | 0.003 | 0.776 | 0.0 | 0.0 | 0.0 |
| $SeV_2$ | TXX | $P\bar{1}(2)$ | – | – | 6.59 | 6.77 | 60.4 | – | – | – | – | – | – | 9.914 | 10.090 | 0.0 | – | – |
| $SeSe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.47 | 7.47 | 60.3 | – | – | – | – | – | – | 0.859 | 2.830 | 0.0 | – | – |
| $SeBr_2$ | HXX | – | $P1(1)$ | – | – | – | – | 8.07 | 7.30 | 76.7 | – | – | – | 0.853 | 0.872 | – | 0.0 | – |
| $SeRb_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.88 | 10.87 | 58.8 | – | – | – | 10.72 | 10.71 | 59.6 | 0.015 | 1.665 | 0.0 | – | 0.0 |
| $SeSr_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 8.59 | 8.58 | 59.5 | 8.53 | 8.53 | 59.4 | – | – | – | 0.726 | 2.660 | 0.0 | 0.0 | – |
| $SeY_2$ | HTP | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 7.66 | 7.65 | 60.0 | 7.39 | 7.38 | 59.9 | 7.53 | 8.63 | 64.1 | 0.058 | 0.150 | 0.0 | 0.0 | 0.0 |
| $SeZr_2$ | PTX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 8.16 | 8.15 | 52.1 | – | – | – | 7.17 | 8.16 | 63.9 | 0.023 | 3.252 | 0.0 | – | 0.0 |
| $SeIn_2$ | HTX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 8.13 | 8.11 | 60.6 | 7.98 | 7.97 | 60.6 | – | – | – | 0.285 | 2.427 | 0.0 | 0.0 | – |
| $SeSn_2$ | PTX | $P2_1/m(11)$ | – | $P1(1)$ | 7.46 | 7.46 | 59.0 | – | – | – | 8.39 | 9.21 | 80.6 | 0.327 | 0.868 | 0.0 | – | 0.0 |
| $SeSb_2$ | PTX | $P\bar{1}(2)$ | – | $P1(1)$ | 7.56 | 7.90 | 59.6 | – | – | – | 11.69 | 10.10 | 42.7 | 0.546 | 2.176 | 0.0 | – | 0.0 |
| $SeI_2$ | HTX | $P\bar{1}(2)$ | $Cmmm(65)$ | – | 7.92 | 10.24 | 76.2 | 9.54 | 7.92 | 65.7 | – | – | – | 0.078 | 0.890 | 0.0 | 0.0 | – |
| $SeCs_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 11.22 | 11.19 | 58.8 | – | – | – | 11.06 | 11.04 | 59.8 | 0.018 | 1.302 | 0.0 | – | 0.0 |
| $SeBa_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 9.11 | 9.10 | 59.5 | – | – | – | – | – | – | 1.546 | 1.697 | 0.0 | – | – |
| $SeTl_2$ | PTH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 9.00 | 9.00 | 58.8 | 8.70 | 8.70 | 58.1 | 8.99 | 8.98 | 58.6 | 0.005 | 0.055 | 0.0 | 0.0 | 0.0 |
| $SePb_2$ | PHT | $P2_1/m(11)$ | $Pmmn(59)$ | $P2_1/m(11)$ | 7.94 | 7.94 | 57.5 | 7.02 | 7.77 | 55.9 | 10.61 | 10.61 | 43.2 | 0.379 | 0.517 | 0.0 | 0.0 | 0.0 |
| $SeBi_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 11.73 | 8.77 | 58.6 | 1.572 | 1.751 | – | – | 0.0 |
| $BrLi_2$ | TPH | $C2/m(12)$ | $Pc(7)$ | $P2_1/m(11)$ | 7.43 | 7.77 | 57.0 | 6.71 | 6.66 | 72.0 | 8.01 | 7.42 | 89.9 | 0.103 | 0.215 | 0.0 | 0.0 | 0.0 |
| $BrF_2$ | HTP | $P2/m(10)$ | $P\bar{1}(2)$ | $P\bar{1}(2)$ | 8.04 | 5.93 | 90.6 | 8.79 | 5.94 | 62.1 | 7.31 | 8.37 | 74.4 | 0.070 | 0.577 | 0.0 | 0.0 | 0.0 |
| $BrAl_2$ | PXX | – | – | $P2(3)$ | – | – | – | – | – | – | 6.99 | 7.56 | 83.1 | 5.015 | 5.034 | – | – | 0.0 |
| $BrCl_2$ | PHT | $P\bar{1}(2)$ | $P\bar{1}(2)$ | $P1(1)$ | 8.01 | 8.38 | 80.5 | 8.06 | 8.01 | 70.2 | 11.19 | 11.29 | 102.7 | 0.218 | 0.228 | 0.0 | 0.0 | 0.0 |
| $BrK_2$ | THP | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 9.59 | 9.57 | 58.4 | 9.58 | 9.55 | 56.4 | 11.19 | 11.15 | 90.5 | 0.245 | 0.281 | 0.0 | 0.0 | 0.0 |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | T | H | P |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | | | |
| $BrCa_2$ | THX | $P\bar{3}m1(164)$ | $P6m2(187)$ | – | 7.79 | 7.79 | 59.7 | 7.77 | 7.77 | 60.0 | – | – | – | 0.200 | 2.747 | 0.0 | 0.0 | – |
| $BrSc_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 6.24 | 6.51 | 79.3 | 6.190 | 7.243 | – | – | 0.0 |
| $BrTi_2$ | TXX | $Pmma(51)$ | – | – | 7.80 | 5.55 | 45.2 | – | – | – | – | – | – | 14.720 | 20.222 | 0.0 | – | – |
| $BrGe_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 7.85 | 7.74 | 73.6 | 1.999 | 2.060 | – | – | 0.0 |
| $BrSe_2$ | PHX | – | $P1(1)$ | $P1(1)$ | – | – | – | 8.53 | 6.62 | 56.6 | 8.08 | 8.51 | 109.5 | 0.617 | 2.111 | – | 0.0 | 0.0 |
| $BrBr_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 11.50 | 10.75 | 95.9 | 1.125 | 1.130 | – | – | 0.0 |
| $BrRb_2$ | THP | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P2_1/m(11)$ | 10.19 | 10.17 | 58.1 | 10.14 | 10.12 | 56.1 | 11.31 | 11.73 | 90.6 | 0.241 | 0.304 | 0.0 | 0.0 | 0.0 |
| $BrSr_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 8.38 | 8.38 | 59.6 | 8.30 | 8.30 | 59.7 | – | – | – | 0.198 | 1.454 | 0.0 | 0.0 | – |
| $BrSn_2$ | PTX | $P2_1/m(11)$ | – | $Pm(6)$ | 6.19 | 6.18 | 71.5 | – | – | – | 9.74 | 7.25 | 67.7 | 0.121 | 1.408 | 0.0 | – | 0.0 |
| $BrI_2$ | PXX | – | – | $Pc(7)$ | – | – | – | – | – | – | 13.24 | 11.46 | 66.2 | 1.177 | 3.073 | – | – | 0.0 |
| $BrCs_2$ | THP | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{4}m2(115)$ | 10.65 | 10.61 | 59.4 | 10.61 | 10.59 | 57.1 | 13.20 | 13.24 | 90.0 | 0.309 | 0.629 | 0.0 | 0.0 | 0.0 |
| $BrBa_2$ | HTX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 8.85 | 8.85 | 59.8 | 8.72 | 8.72 | 59.7 | – | – | – | 0.055 | 3.475 | 0.0 | 0.0 | – |
| $BrHf_2$ | THP | $P2_1/m(11)$ | $Pm(6)$ | $Pm(6)$ | 6.60 | 6.70 | 59.5 | 6.59 | 6.58 | 60.3 | 8.66 | 5.58 | 49.6 | 0.551 | 0.623 | 0.0 | 0.0 | 0.0 |
| $BrRe_2$ | PXX | – | – | $Cm(8)$ | – | – | – | – | – | – | 5.65 | 5.65 | 60.0 | 4.136 | 47.650 | – | – | 0.0 |
| $BrTl_2$ | PTH | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P\bar{1}(2)$ | 7.88 | 7.87 | 58.6 | 8.04 | 8.06 | 54.7 | 9.87 | 8.39 | 83.2 | 0.056 | 0.449 | 0.0 | 0.0 | 0.0 |
| $BrPb_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 10.47 | 9.88 | 38.8 | 1.434 | 2.317 | – | – | 0.0 |
| $RbN_2$ | TPX | $P2/c(13)$ | – | $P6/mmm(191)$ | 10.37 | 10.37 | 57.5 | – | – | – | 10.50 | 10.89 | 58.1 | 0.029 | 0.851 | 20.0 | – | 20.0 |
| $RbF_2$ | THX | $P4/mmm(123)$ | $P\bar{6}m2(187)$ | – | 7.81 | 11.09 | 44.7 | 9.37 | 9.36 | 57.0 | – | – | – | 0.508 | 1.140 | 4.0 | 4.0 | – |
| $RbS_2$ | TPX | $P\bar{1}(2)$ | – | $C2(5)$ | 10.76 | 12.97 | 37.0 | – | – | – | 8.51 | 11.35 | 68.2 | 0.082 | 1.896 | 0.0 | – | 0.0 |
| $RbCl_2$ | THX | $P4/mmm(123)$ | $P\bar{6}m2(187)$ | – | 8.99 | 12.73 | 45.1 | 10.82 | 10.87 | 56.7 | – | – | – | 0.349 | 1.122 | 4.0 | 4.0 | – |
| $RbK_2$ | TPX | $P\bar{3}m1(164)$ | – | $P6/mmm(191)$ | 16.29 | 16.29 | 59.5 | – | – | – | 16.99 | 16.99 | 57.9 | 0.042 | 2.192 | 0.0 | – | 0.0 |
| $RbCa_2$ | HXX | – | $P2_1/m(11)$ | – | – | – | – | 14.39 | 15.13 | 16.3 | – | – | – | 7.929 | 7.954 | – | 0.0 | – |
| $RbGe_2$ | PXX | – | – | $P2/c(13)$ | – | – | – | – | – | – | 12.98 | 11.83 | 30.7 | 0.890 | 6.183 | – | – | 0.0 |
| $RbSe_2$ | PXX | – | – | $P2_1(4)$ | – | – | – | – | – | – | 10.60 | 13.06 | 36.9 | 0.841 | 2.222 | – | – | 0.0 |
| $RbBr_2$ | THX | $P4/mmm(123)$ | $P\bar{6}m2(187)$ | – | 9.35 | 13.21 | 44.9 | 11.21 | 11.16 | 57.6 | – | – | – | 0.346 | 1.251 | 4.0 | 4.0 | – |
| $RbSr_2$ | HTP | $P6/mmm(191)$ | $Amm2(38)$ | $P6/mmm(191)$ | 15.62 | 15.61 | 60.1 | 16.32 | 16.39 | 30.0 | 15.95 | 15.95 | 58.0 | 0.754 | 0.786 | 0.0 | 0.0 | 0.0 |
| $RbY_2$ | HXX | – | $Cmm2(35)$ | – | – | – | – | 14.19 | 15.63 | 24.9 | – | – | – | 7.531 | 7.609 | – | 0.0 | – |
| $RbI_2$ | PTX | $P4/mmm(123)$ | – | $P2/m(10)$ | 9.83 | 13.90 | 45.4 | – | – | – | 13.39 | 13.96 | 65.6 | 0.748 | 1.166 | 4.0 | – | 0.0 |
| $RbBa_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 15.30 | 15.34 | 33.0 | – | – | – | 0.831 | 0.907 | – | 0.0 | – |
| $RbAu_2$ | PTX | $Cmmm(65)$ | – | $Cmmm(65)$ | 13.37 | 13.42 | 46.9 | – | – | – | 13.40 | 13.44 | 46.8 | 0.003 | 4.908 | 0.0 | – | 0.0 |
| $SrB_2$ | PTX | $Cmmm(65)$ | – | $Cmmm(65)$ | 10.86 | 10.88 | 34.3 | – | – | – | 10.88 | 10.87 | 34.2 | 0.005 | 12.283 | 0.0 | – | 0.0 |
| $SrC_2$ | PXX | – | – | $Pmmn(59)$ | – | – | – | – | – | – | 8.26 | 10.52 | 50.3 | 2.001 | 34.056 | – | – | 0.0 |
| $SrN_2$ | PXX | – | – | $Pmmn(59)$ | – | – | – | – | – | – | 8.47 | 7.45 | 56.0 | 1.588 | 21.284 | – | – | 0.9 |
| $SrF_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.82 | 7.83 | 60.1 | – | – | – | 7.81 | 7.82 | 60.2 | 0.004 | 2.693 | 0.0 | – | 0.0 |
| $SrAl_2$ | PXX | – | – | $P6mm(183)$ | – | – | – | – | – | – | 9.20 | 9.20 | 60.0 | 3.037 | 8.347 | – | – | 0.0 |
| $SrSi_2$ | TPX | $C2/m(12)$ | – | $P2/c(13)$ | 12.31 | 12.31 | 37.3 | – | – | – | 12.47 | 12.48 | 36.9 | 0.055 | 4.898 | 0.0 | – | 0.0 |
| $SrP_2$ | TPX | $C2/m(12)$ | – | $Cmmm(65)$ | 11.14 | 11.14 | 37.4 | – | – | – | 11.31 | 11.31 | 43.7 | 0.600 | 2.113 | 0.0 | – | 0.0 |
| $SrS_2$ | PXX | – | – | $P4/mmm(123)$ | – | – | – | – | – | – | 8.10 | 11.48 | 45.0 | 0.837 | 7.807 | – | – | 0.0 |
| $SrCl_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 8.93 | 8.93 | 59.9 | – | – | – | 8.92 | 8.92 | 60.1 | 0.001 | 1.839 | 0.0 | – | 0.0 |
| $SrK_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 14.81 | 8.76 | 32.3 | – | – | – | 4.385 | 4.424 | – | 0.0 | – |
| $SrCa_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 7.90 | 13.16 | 34.6 | – | – | – | 6.178 | 6.180 | – | 0.0 | – |
| $SrSc_2$ | PXX | – | – | $P4mm(99)$ | – | – | – | – | – | – | 10.27 | 7.19 | 44.3 | 6.776 | 7.510 | – | – | 0.0 |
| $SrGe_2$ | TPX | $C2/m(12)$ | – | $Cmmm(65)$ | 12.13 | 12.13 | 39.3 | – | – | – | 12.45 | 12.45 | 38.9 | 0.256 | 4.014 | 0.0 | – | 0.0 |
| $SrSe_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 9.99 | 9.99 | 57.9 | – | – | – | 2.071 | 5.736 | – | 0.0 | – |
| $SrBr_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.18 | 9.19 | 59.9 | – | – | – | 9.17 | 9.17 | 60.0 | 0.001 | 1.447 | 0.0 | – | 0.0 |
| $SrSr_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 8.55 | 14.45 | 31.6 | – | – | – | 6.433 | 6.440 | – | 0.0 | – |
| $SrY_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 8.66 | 13.98 | 28.0 | – | – | – | 11.818 | 12.121 | – | 0.0 | – |
| $SrPd_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 8.94 | 6.47 | 43.0 | – | – | – | 5.686 | 7.687 | – | 0.0 | – |
| $SrAg_2$ | HXX | – | $P4/nmm(129)$ | – | – | – | – | 7.87 | 11.16 | 44.7 | – | – | – | 2.038 | 2.070 | – | 0.0 | – |
| $SrCd_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 8.32 | 11.91 | 43.6 | – | – | – | 1.436 | 2.675 | – | 0.0 | – |
| $SrIn_2$ | HXX | – | $C2/m(12)$ | – | – | – | – | 12.52 | 11.36 | 24.8 | – | – | – | 3.379 | 4.365 | – | 0.0 | – |
| $SrSn_2$ | TPX | $C2/m(12)$ | – | $Cmmm(65)$ | 12.68 | 12.68 | 42.2 | – | – | – | 13.25 | 13.26 | 41.5 | 0.389 | 4.638 | 0.0 | – | 0.0 |
| $SrSb_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 10.03 | 12.61 | 36.5 | – | – | – | 1.128 | 3.870 | – | 0.0 | – |
| $SrI_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.74 | 9.74 | 59.1 | – | – | – | 9.61 | 9.61 | 60.1 | 0.010 | 1.111 | 0.0 | – | 0.0 |
| $SrCs_2$ | HXX | – | $P2/m(10)$ | – | – | – | – | 9.91 | 15.60 | 36.5 | – | – | – | 3.320 | 3.326 | – | 0.0 | – |
| $SrBa_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 8.63 | 14.42 | 33.6 | – | – | – | 6.319 | 6.612 | – | 0.0 | – |
| $SrAu_2$ | TPH | $P6/mmm(191)$ | $P\bar{6}m2(187)$ | $Cmmm(65)$ | 10.80 | 10.84 | 60.1 | 8.49 | 8.59 | 60.0 | 11.38 | 11.38 | 53.5 | 0.060 | 0.644 | 0.0 | 0.0 | 0.0 |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $SrHg_2$ | HXX | – | $Pmmn(59)$ | – | – | – | – | 9.48 | 12.86 | 41.3 | – | – | – | 1.553 | 1.834 | – | 0.0 | – |
| $SrTl_2$ | HXX | – | $Pmna(53)$ | – | – | – | – | 8.22 | 11.78 | 45.1 | – | – | – | 2.209 | 2.225 | – | 0.0 | – |
| $SrPb_2$ | TPX | $C2/m(12)$ | – | $Cmmm(65)$ | 12.83 | 12.83 | 43.5 | – | – | – | 12.72 | 12.73 | 48.5 | 0.402 | 3.960 | 0.0 | – | 0.0 |
| $SrBi_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 10.24 | 12.70 | 35.8 | – | – | – | 1.319 | 1.366 | – | 0.0 | – |
| $YB_2$ | TPX | $Cmmm(65)$ | – | $Cmmm(65)$ | 9.96 | 9.96 | 37.0 | – | – | – | 9.95 | 9.95 | 37.0 | 0.002 | 9.924 | 0.0 | – | 0.0 |
| $YC_2$ | PXX | – | – | $Pmmn(59)$ | – | – | – | – | – | – | 8.76 | 7.27 | 53.1 | 3.385 | 6.174 | – | – | 0.0 |
| $YN_2$ | PXX | – | – | $P4/mmm(123)$ | – | – | – | – | – | – | 7.32 | 7.31 | 53.3 | 1.584 | 13.358 | – | – | 0.0 |
| $YO_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 6.76 | 6.19 | 74.2 | 3.184 | 3.324 | – | – | 0.0 |
| $YF_2$ | HPX | – | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | – | – | – | 6.85 | 6.85 | 60.0 | 7.86 | 7.88 | 60.1 | 0.756 | 0.865 | – | 4.0 | 3.6 |
| $YSi_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 10.27 | 7.92 | 39.4 | – | – | – | 3.207 | 3.681 | – | 0.0 | – |
| $YP_2$ | HPX | – | $P4/mmm(123)$ | $P1(1)$ | – | – | – | 10.63 | 7.74 | 43.2 | 8.52 | 7.76 | 63.5 | 0.602 | 1.434 | – | 0.0 | 0.0 |
| $YS_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 9.29 | 7.83 | 49.2 | 3.022 | 3.234 | – | – | 0.0 |
| $YCl_2$ | HPX | – | $P\bar{6}m2(187)$ | $P3m1(156)$ | – | – | – | 7.53 | 7.52 | 59.8 | 7.60 | 7.62 | 60.0 | 0.685 | 0.867 | – | 3.9 | 0.0 |
| $YGe_2$ | PTX | $C2/m(12)$ | – | $P2/c(13)$ | 10.75 | 10.75 | 42.9 | – | – | – | 10.61 | 10.31 | 43.3 | 0.387 | 4.699 | 0.0 | – | 0.0 |
| $YAs_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 7.85 | 11.13 | 42.7 | – | – | – | 2.041 | 2.109 | – | 0.0 | – |
| $YSe_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 9.82 | 7.90 | 53.8 | 1.937 | 1.979 | – | – | 0.0 |
| $YBr_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $C2/m(12)$ | 7.91 | 7.90 | 58.4 | 7.77 | 7.77 | 59.6 | 7.87 | 7.86 | 60.4 | 0.601 | 0.698 | 0.0 | 3.9 | 0.9 |
| $YY_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 10.21 | 11.25 | 34.0 | 3.582 | 4.649 | – | – | 0.0 |
| $YZr_2$ | HTX | $Cmme(67)$ | $Cmme(67)$ | – | 11.03 | 9.78 | 27.6 | 9.77 | 11.02 | 27.6 | – | – | – | 0.007 | 2.366 | 0.0 | 0.0 | – |
| $YSn_2$ | HXX | – | $Pmmm(47)$ | – | – | – | – | 9.40 | 11.44 | 34.7 | – | – | – | 3.455 | 5.582 | – | 0.0 | – |
| $YI_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $C2/m(12)$ | 8.39 | 8.39 | 58.9 | 8.25 | 8.25 | 59.6 | 8.33 | 8.34 | 60.3 | 0.339 | 0.412 | 0.0 | 3.7 | 0.8 |
| $YPb_2$ | PTH | $Pmmm(47)$ | $Pmmm(47)$ | $P2/c(13)$ | 11.67 | 9.46 | 35.7 | 9.48 | 11.69 | 35.6 | 11.57 | 10.45 | 31.2 | 0.012 | 0.023 | 0.0 | 0.0 | 0.0 |
| $YBi_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 8.65 | 11.78 | 41.7 | 8.63 | 11.77 | 41.9 | – | – | – | 0.003 | 2.813 | 0.0 | 0.0 | – |
| $ZrBe_2$ | PXX | – | – | $P4/nmm(129)$ | – | – | – | – | – | – | 5.07 | 7.18 | 45.0 | 6.083 | 6.270 | – | – | 0.0 |
| $ZrB_2$ | PHT | $P2/c(13)$ | $P2/c(13)$ | $P2/c(13)$ | 8.79 | 8.74 | 41.0 | 8.78 | 8.74 | 41.1 | 8.80 | 8.76 | 41.0 | 0.003 | 0.004 | 0.0 | 0.0 | 0.0 |
| $ZrC_2$ | PTX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 7.66 | 8.50 | 44.5 | – | – | – | 7.03 | 7.33 | 51.5 | 0.479 | 5.712 | 0.0 | – | 0.0 |
| $ZrN_2$ | HPX | – | $P\bar{6}m2(187)$ | $P1(1)$ | – | – | – | 7.01 | 7.04 | 60.2 | 6.67 | 6.05 | 69.1 | 0.260 | 7.170 | – | 0.0 | 0.0 |
| $ZrO_2$ | HXX | – | $Pmmn(59)$ | – | – | – | – | 5.19 | 6.59 | 50.6 | – | – | – | 1.087 | 1.287 | – | 0.0 | – |
| $ZrF_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 6.23 | 6.23 | 60.0 | – | – | – | 0.876 | 0.892 | – | 0.0 | – |
| $ZrMg_2$ | TXX | $P4/mmm(123)$ | – | – | 6.58 | 9.37 | 42.1 | – | – | – | – | – | – | 1.262 | 14.651 | 0.0 | – | – |
| $ZrSi_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 9.67 | 7.38 | 40.2 | – | – | – | 2.408 | 7.072 | – | 0.0 | – |
| $ZrP_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 8.14 | 8.13 | 59.8 | – | – | – | 1.562 | 9.368 | – | 0.0 | – |
| $ZrS_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.38 | 7.38 | 59.9 | – | – | – | – | – | – | 0.872 | 2.041 | 0.0 | – | – |
| $ZrCl_2$ | HTP | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 7.11 | 6.71 | 61.8 | 6.84 | 6.84 | 60.1 | 7.11 | 7.11 | 56.3 | 0.436 | 0.440 | 0.0 | 0.0 | 0.0 |
| $ZrCa_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 7.16 | 10.14 | 45.0 | 10.16 | 7.18 | 44.9 | – | – | – | 0.017 | 13.243 | 0.0 | 0.0 | – |
| $ZrTi_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 5.76 | 9.53 | 35.4 | – | – | – | 2.361 | 6.522 | – | 0.0 | – |
| $ZrCr_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 6.06 | 9.42 | 39.0 | – | – | – | 7.350 | 13.581 | – | 29.3 | – |
| $ZrGe_2$ | HPX | – | $Pmmm(47)$ | $P2(3)$ | – | – | – | 8.50 | 10.32 | 34.5 | 9.13 | 8.88 | 40.2 | 0.736 | 4.903 | – | 0.0 | 0.0 |
| $ZrSe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.58 | 7.58 | 60.0 | – | – | – | – | – | – | 1.099 | 1.565 | 0.0 | – | – |
| $ZrBr_2$ | HTP | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 7.01 | 7.40 | 61.6 | 7.13 | 7.13 | 60.1 | 7.40 | 7.40 | 56.6 | 0.024 | 0.028 | 0.0 | 0.0 | 0.0 |
| $ZrNb_2$ | HTX | $P\bar{1}(2)$ | $P2/c(13)$ | – | 10.55 | 8.26 | 31.9 | 11.36 | 8.50 | 28.5 | – | – | – | 0.765 | 14.293 | 0.0 | 0.0 | – |
| $ZrPd_2$ | TPH | $P4/mmm(123)$ | $P4/mmm(123)$ | $P4/mmm(123)$ | 8.79 | 6.31 | 42.6 | 6.19 | 8.63 | 43.9 | 6.97 | 6.98 | 50.3 | 0.238 | 0.516 | 0.0 | 0.0 | 0.0 |
| $ZrIn_2$ | HPT | $P4/mmm(123)$ | $Pmma(51)$ | $P4/mmm(123)$ | 6.32 | 8.90 | 45.2 | 7.29 | 9.78 | 42.0 | 6.58 | 9.34 | 44.9 | 0.014 | 0.372 | 0.0 | 0.0 | 0.0 |
| $ZrSn_2$ | PTH | $Pmmm(47)$ | $Pmmm(47)$ | $P\bar{1}(2)$ | 8.90 | 10.88 | 35.0 | 9.42 | 9.42 | 38.7 | 8.07 | 9.15 | 40.0 | 0.061 | 0.091 | 0.0 | 0.0 | 0.0 |
| $ZrTe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.95 | 7.94 | 59.9 | – | – | – | – | – | – | 1.091 | 1.342 | 0.0 | – | – |
| $ZrI_2$ | TPH | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 7.57 | 7.88 | 61.3 | 7.69 | 7.69 | 60.0 | 7.88 | 7.57 | 61.3 | 0.035 | 0.337 | 0.0 | 0.0 | 0.0 |
| $ZrHf_2$ | HPX | – | $C2/m(12)$ | $Cm(8)$ | – | – | – | 8.59 | 9.71 | 40.1 | 9.25 | 7.52 | 51.6 | 0.404 | 3.838 | – | 0.0 | 0.0 |
| $ZrAu_2$ | HTX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 8.64 | 6.12 | 45.1 | 8.63 | 6.11 | 45.0 | – | – | – | 0.009 | 7.649 | 0.0 | 0.0 | – |
| $ZrTl_2$ | THX | $P4/mmm(123)$ | $Pmma(51)$ | – | 9.89 | 7.07 | 43.7 | 10.12 | 7.58 | 41.4 | – | – | – | 0.755 | 9.882 | 0.0 | 0.0 | – |
| $ZrPb_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 6.49 | 7.75 | 51.3 | 0.916 | 0.927 | – | – | 0.0 |
| $ZrBi_2$ | PXX | – | – | $Cmmm(65)$ | – | – | – | – | – | – | 8.00 | 6.69 | 54.5 | 1.087 | 4.002 | – | – | 0.0 |
| $NbBe_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 7.84 | 5.43 | 43.8 | 5.43 | 7.85 | 43.7 | – | – | – | 0.001 | 4.217 | 0.0 | 0.0 | – |
| $NbC_2$ | PXX | – | – | $P2/c(13)$ | – | – | – | – | – | – | 6.49 | 6.65 | 46.5 | 3.852 | 11.023 | – | – | 0.0 |
| $NbO_2$ | THX | $C2/m(12)$ | $P\bar{6}m2(187)$ | – | 6.21 | 6.18 | 60.2 | 6.01 | 5.96 | 60.4 | – | – | – | 0.651 | 1.777 | 0.0 | 0.0 | – |
| $NbF_2$ | HXX | – | $P\bar{1}(2)$ | – | – | – | – | 6.58 | 6.46 | 52.4 | – | – | – | 2.240 | 4.478 | – | 0.8 | – |
| $NbAl_2$ | HTX | $Pmmm(47)$ | $Pmmm(47)$ | – | 9.41 | 7.43 | 37.8 | 7.44 | 9.41 | 37.8 | – | – | – | 0.004 | 8.037 | 0.0 | 0.0 | – |
| $NbP_2$ | THX | $P\bar{1}(2)$ | $P\bar{6}m2(187)$ | – | 7.57 | 7.86 | 44.9 | 7.80 | 7.80 | 57.8 | – | – | – | 0.163 | 1.567 | 0.0 | 0.0 | – |

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Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $NbS_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $C2/m(12)$ | 6.77 | 6.77 | 60.0 | 6.72 | 6.73 | 59.7 | 6.13 | 7.70 | 55.4 | 0.379 | 0.410 | 0.0 | 0.0 | 0.0 |
| $NbCl_2$ | HXX | – | $Pmm2(25)$ | – | – | – | – | 6.74 | 6.60 | 60.6 | – | – | – | 3.274 | 3.278 | – | 0.0 | – |
| $NbCa_2$ | THX | $P2_1/m(11)$ | $Pmma(51)$ | – | 6.86 | 10.30 | 48.0 | 6.92 | 10.11 | 46.5 | – | – | – | 0.468 | 14.491 | 0.0 | 0.0 | – |
| $NbV_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 6.48 | 6.49 | 49.9 | 0.861 | 1.278 | – | – | 0.0 |
| $NbGa_2$ | THX | $Pmmm(47)$ | $Pmmm(47)$ | – | 7.41 | 9.47 | 38.3 | 7.46 | 9.50 | 38.1 | – | – | – | 0.109 | 10.646 | 0.0 | 0.0 | – |
| $NbSe_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $C2/m(12)$ | 6.96 | 6.96 | 59.9 | 6.95 | 6.94 | 60.0 | 6.35 | 6.85 | 74.3 | 0.171 | 0.417 | 0.0 | 0.0 | 0.0 |
| $NbBr_2$ | HXX | – | $Pmm2(25)$ | – | – | – | – | 7.09 | 7.09 | 57.9 | – | – | – | 2.904 | 2.906 | – | 0.0 | – |
| $NbNb_2$ | HTX | $P2/c(13)$ | $P2/c(13)$ | – | 8.44 | 8.19 | 38.4 | 8.44 | 8.19 | 38.4 | – | – | – | 0.005 | 3.812 | 0.0 | 0.0 | – |
| $NbRu_2$ | TXX | $P2_1/m(11)$ | – | – | 9.02 | 7.79 | 30.2 | – | – | – | – | – | – | 2.016 | 2.038 | 0.0 | – | – |
| $NbTe_2$ | HTX | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | – | 7.52 | 7.51 | 54.3 | 7.40 | 7.40 | 60.0 | – | – | – | 0.124 | 1.416 | 0.0 | 0.0 | – |
| $NbI_2$ | HXX | – | $Pmm2(25)$ | – | – | – | – | 7.65 | 7.65 | 57.4 | – | – | – | 1.714 | 1.715 | – | 0.0 | – |
| $NbBi_2$ | TPX | $C2/m(12)$ | – | $P\bar{1}(2)$ | 7.07 | 7.08 | 54.3 | – | – | – | 8.09 | 8.85 | 44.5 | 0.312 | 4.848 | 0.0 | – | 0.0 |
| $MoBe_2$ | HTX | $Cmmm(65)$ | $Pmm2(25)$ | – | 5.16 | 8.03 | 38.9 | 8.81 | 8.21 | 21.2 | – | – | – | 0.355 | 6.371 | 0.0 | 0.0 | – |
| $MoN_2$ | TXX | $P\bar{1}(2)$ | – | – | 6.49 | 6.50 | 55.7 | – | – | – | – | – | – | 1.347 | 2.470 | 0.0 | – | – |
| $MoO_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.69 | 5.68 | 60.0 | – | – | – | 2.347 | 2.376 | – | 0.0 | – |
| $MoF_2$ | HXX | – | $P2/m(10)$ | – | – | – | – | 7.42 | 5.75 | 52.0 | – | – | – | 6.516 | 6.522 | – | 0.0 | – |
| $MoSi_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 7.58 | 6.86 | 38.4 | 1.556 | 1.700 | – | – | 0.0 |
| $MoP_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 6.14 | 6.91 | 63.6 | 1.389 | 3.230 | – | – | 0.0 |
| $MoS_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 6.39 | 6.39 | 60.0 | – | – | – | 2.625 | 3.668 | – | 0.0 | – |
| $MoCl_2$ | PTH | $C2/m(12)$ | $Cmmm(65)$ | $P2_1/c(14)$ | 8.81 | 8.81 | 49.2 | 8.21 | 8.21 | 52.9 | 7.99 | 8.00 | 64.2 | 0.039 | 0.176 | 16.0 | 16.0 | 16.0 |
| $MoMn_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 6.15 | 8.72 | 43.9 | 6.07 | 8.59 | 45.0 | – | – | – | 0.406 | 12.003 | 26.2 | 26.1 | – |
| $MoSe_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 6.65 | 6.65 | 60.1 | – | – | – | 1.444 | 1.489 | – | 0.0 | – |
| $MoBr_2$ | THP | $C2/m(12)$ | $Cmmm(65)$ | $C2/m(12)$ | 8.92 | 8.92 | 50.9 | 8.32 | 8.31 | 54.8 | 14.76 | 7.59 | 74.9 | 0.198 | 0.629 | 16.0 | 16.0 | 16.0 |
| $MoY_2$ | PHX | – | $Pmmm(47)$ | $P\bar{1}(2)$ | – | – | – | 6.81 | 9.50 | 44.0 | 8.88 | 7.07 | 53.3 | 0.460 | 0.934 | – | 0.0 | 0.0 |
| $MoIn_2$ | HXX | – | $P\bar{1}(2)$ | – | – | – | – | 6.42 | 9.25 | 38.8 | – | – | – | 9.001 | 9.719 | – | 0.0 | – |
| $MoSb_2$ | HTX | $C2/m(12)$ | $P\bar{6}m2(187)$ | – | 9.19 | 9.19 | 42.4 | 7.84 | 7.94 | 59.2 | – | – | – | 0.638 | 7.676 | 0.0 | 0.0 | – |
| $MoTe_2$ | THP | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 7.29 | 7.28 | 57.3 | 7.16 | 7.16 | 60.1 | 7.31 | 7.31 | 57.0 | 0.006 | 0.064 | 0.0 | 0.0 | 0.0 |
| $MoI_2$ | THX | $C2/m(12)$ | $Cmmm(65)$ | – | 9.33 | 9.33 | 51.8 | 8.96 | 8.97 | 54.0 | – | – | – | 0.269 | 2.477 | 15.9 | 16.0 | – |
| $MoTl_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 8.14 | 9.52 | 27.5 | – | – | – | 12.878 | 12.901 | – | 0.0 | – |
| $MoBi_2$ | TXX | $P\bar{1}(2)$ | – | – | 6.70 | 7.90 | 51.7 | – | – | – | – | – | – | 0.960 | 1.056 | 0.0 | – | – |
| $TcBe_2$ | HTX | $P\bar{1}(2)$ | $Pmma(51)$ | – | 7.50 | 6.57 | 33.5 | 7.99 | 6.00 | 41.4 | – | – | – | 0.715 | 3.892 | 0.0 | 0.0 | – |
| $TcC_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 7.13 | 7.91 | 41.1 | 5.542 | 6.515 | – | – | 0.0 |
| $TcN_2$ | PTH | $P1(1)$ | $P\bar{6}m2(187)$ | $Pc(7)$ | 6.34 | 6.09 | 59.0 | 5.74 | 5.75 | 60.1 | 6.98 | 6.22 | 59.9 | 0.406 | 0.515 | 0.0 | 0.3 | 0.0 |
| $TcO_2$ | TPX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 5.77 | 5.70 | 59.9 | – | – | – | 5.70 | 5.77 | 60.0 | 0.022 | 3.508 | 0.0 | – | 0.0 |
| $TcF_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 6.92 | 6.66 | 60.7 | 0.992 | 2.717 | – | – | 16.0 |
| $TcSi_2$ | THX | $C2/m(12)$ | $Amm2(38)$ | – | 8.59 | 8.59 | 40.4 | 7.47 | 7.49 | 51.3 | – | – | – | 0.278 | 0.964 | 0.0 | 0.0 | – |
| $TcP_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 7.28 | 7.28 | 52.2 | – | – | – | 1.228 | 1.912 | – | 0.0 | – |
| $TcS_2$ | PTX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 6.60 | 6.54 | 58.6 | – | – | – | 6.43 | 6.60 | 60.2 | 0.000 | 1.813 | 0.0 | – | 0.0 |
| $TcTi_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 8.64 | 6.11 | 45.0 | – | – | – | 2.445 | 2.569 | – | 0.0 | – |
| $TcV_2$ | PXX | – | – | $P2/c(13)$ | – | – | – | – | – | – | 9.01 | 7.21 | 35.2 | 2.589 | 2.619 | – | – | 0.0 |
| $TcMn_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 8.44 | 5.97 | 44.9 | 8.32 | 5.82 | 45.4 | – | – | – | 0.042 | 11.865 | 29.7 | 12.6 | – |
| $TcSe_2$ | TPX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 6.67 | 6.86 | 60.3 | – | – | – | 6.67 | 6.80 | 61.2 | 0.004 | 1.746 | 0.0 | – | 0.0 |
| $TcY_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 9.74 | 6.89 | 45.0 | – | – | – | 1.260 | 1.275 | – | 0.0 | – |
| $TcSb_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 6.65 | 6.65 | 60.0 | – | – | – | 3.596 | 11.384 | – | 0.0 | – |
| $TcTe_2$ | TPX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 7.31 | 7.27 | 58.5 | – | – | – | 7.32 | 7.29 | 58.2 | 0.013 | 1.768 | 0.0 | – | 0.0 |
| $TcI_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 8.19 | 8.19 | 57.3 | – | – | – | – | – | – | 2.457 | 3.271 | 4.0 | – | – |
| $TcTa_2$ | THX | $C2/m(12)$ | $P2/c(13)$ | – | 8.15 | 8.89 | 35.1 | 7.50 | 9.08 | 38.3 | – | – | – | 0.488 | 0.844 | 0.0 | 0.0 | – |
| $TcBi_2$ | PHX | – | $P\bar{6}m2(187)$ | $P\bar{1}(2)$ | – | – | – | 6.89 | 6.88 | 60.1 | 7.30 | 8.47 | 46.4 | 0.659 | 4.313 | – | 0.0 | 0.0 |
| $RuBe_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 5.71 | 8.08 | 45.0 | – | – | – | 1.933 | 5.762 | – | 0.0 | – |
| $RuC_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 7.23 | 8.98 | 36.9 | 3.319 | 7.440 | – | – | 0.0 |
| $RuN_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 6.80 | 7.22 | 76.4 | 4.664 | 5.141 | – | – | 0.0 |
| $RuO_2$ | TPX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 6.19 | 5.77 | 57.7 | – | – | – | 5.78 | 6.19 | 57.6 | 0.066 | 3.979 | 0.0 | – | 0.0 |
| $RuF_2$ | PTX | $P\bar{1}(2)$ | – | $Cm(8)$ | 7.14 | 6.99 | 51.8 | – | – | – | 6.59 | 6.17 | 60.9 | 0.793 | 0.962 | 15.9 | – | 12.0 |
| $RuAl_2$ | HTX | $P4/nmm(129)$ | $P4/nmm(129)$ | – | 8.44 | 5.97 | 45.0 | 8.41 | 5.95 | 45.0 | – | – | – | 0.178 | 8.136 | 0.0 | 0.0 | – |
| $RuP_2$ | PHT | $P2_1/m(11)$ | $Pmn2_1(31)$ | $Pmmn(59)$ | 7.89 | 7.89 | 43.4 | 7.58 | 7.59 | 45.9 | 5.88 | 8.04 | 68.5 | 0.004 | 0.305 | 0.0 | 0.0 | 0.0 |
| $RuS_2$ | TPX | $P2_1/m(11)$ | – | $C2/m(12)$ | 6.94 | 6.60 | 58.3 | – | – | – | 6.91 | 6.57 | 58.3 | 0.210 | 3.164 | 0.0 | – | 0.0 |
| $RuCl_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.24 | 7.24 | 59.9 | – | – | – | – | – | – | 3.699 | 4.041 | 0.0 | – | – |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $RuCa_2$ | TXX | $P2_1/m(11)$ | – | – | 8.83 | 7.22 | 52.3 | – | – | – | – | – | – | 1.040 | 1.344 | 0.0 | – | – |
| $RuSc_2$ | HPX | – | $P4/mmm(123)$ | $P4/mmm(123)$ | – | – | – | 6.40 | 9.05 | 45.0 | 7.17 | 7.16 | 53.1 | 0.053 | 1.564 | – | 0.0 | 0.0 |
| $RuTi_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 5.93 | 8.40 | 44.6 | – | – | – | 0.919 | 1.873 | – | 0.0 | – |
| $RuV_2$ | THX | $C2/m(12)$ | $C2/m(12)$ | – | 7.53 | 8.24 | 34.8 | 6.46 | 7.59 | 46.1 | – | – | – | 0.353 | 1.832 | 0.0 | 0.0 | – |
| $RuMn_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 8.41 | 5.93 | 44.4 | – | – | – | 2.015 | 11.563 | – | 33.2 | – |
| $RuSe_2$ | TXX | $P2_1/m(11)$ | – | – | 7.22 | 6.86 | 58.2 | – | – | – | – | – | – | 2.201 | 2.763 | 0.0 | – | – |
| $RuBr_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.63 | 7.63 | 59.9 | – | – | – | – | – | – | 1.206 | 4.004 | 0.0 | – | – |
| $RuY_2$ | HPX | – | $P4/mmm(123)$ | $C2/m(12)$ | – | – | – | 6.79 | 9.60 | 45.0 | 8.98 | 7.56 | 50.4 | 0.414 | 1.389 | – | 0.0 | 0.0 |
| $RuTc_2$ | TXX | $C2/m(12)$ | – | – | 8.15 | 9.42 | 30.0 | – | – | – | – | – | – | 4.418 | 5.983 | 0.0 | – | – |
| $RuRu_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 8.06 | 6.89 | 38.8 | – | – | – | 1.030 | 5.235 | – | 0.0 | – |
| $RuPd_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.51 | 5.51 | 59.8 | – | – | – | 6.269 | 7.276 | – | 0.0 | – |
| $RuSb_2$ | TXX | $P\bar{1}(2)$ | – | – | 7.19 | 7.32 | 59.7 | – | – | – | – | – | – | 0.833 | 11.598 | 0.0 | – | – |
| $RuTe_2$ | PTX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 7.30 | 7.69 | 58.3 | – | – | – | 7.33 | 7.72 | 57.9 | 0.017 | 1.365 | 0.0 | – | 0.0 |
| $RuTa_2$ | HTX | $C2/m(12)$ | $C2/m(12)$ | – | 8.83 | 8.10 | 35.0 | 6.93 | 8.12 | 45.8 | – | – | – | 0.412 | 7.279 | 0.0 | 0.0 | – |
| $RuOs_2$ | TXX | $P2_1/m(11)$ | – | – | 8.36 | 8.36 | 37.6 | – | – | – | – | – | – | 2.801 | 5.282 | 0.0 | – | – |
| $RhLi_2$ | PTH | $P4/mmm(123)$ | $P4/mmm(123)$ | $C2/m(12)$ | 5.54 | 7.85 | 45.2 | 5.54 | 7.84 | 45.1 | 6.85 | 5.78 | 49.1 | 0.133 | 0.149 | 0.0 | 0.0 | 0.0 |
| $RhBe_2$ | PXX | – | – | $P4/nmm(129)$ | – | – | – | – | – | – | 4.58 | 4.58 | 90.0 | 1.291 | 2.630 | – | – | 0.0 |
| $RhB_2$ | TPX | $Pmmn(59)$ | – | $Cmmm(65)$ | 7.53 | 7.53 | 48.0 | – | – | – | 7.97 | 7.97 | 44.7 | 0.399 | 8.642 | 0.0 | – | 0.0 |
| $RhO_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 6.17 | 6.16 | 59.9 | – | – | – | 6.16 | 6.17 | 60.0 | 0.026 | 4.539 | 0.0 | – | 0.0 |
| $RhF_2$ | PXX | – | – | $Cmmm(65)$ | – | – | – | – | – | – | 15.14 | 15.34 | 22.8 | 2.132 | 4.657 | – | – | 4.0 |
| $RhP_2$ | THP | $P\bar{1}(2)$ | $Pc(7)$ | $P1(1)$ | 7.66 | 8.15 | 50.3 | 7.93 | 7.92 | 40.0 | 7.29 | 7.83 | 51.8 | 0.007 | 0.413 | 0.0 | 0.0 | 0.0 |
| $RhS_2$ | PTX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 7.13 | 7.06 | 54.0 | – | – | – | 7.13 | 7.06 | 54.0 | 0.000 | 2.867 | 0.0 | – | 0.0 |
| $RhSc_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 7.09 | 8.58 | 51.0 | 0.904 | 2.281 | – | – | 0.0 |
| $RhGa_2$ | THX | $C2/m(12)$ | $Amm2(38)$ | – | 7.96 | 7.94 | 42.9 | 7.56 | 7.50 | 45.0 | – | – | – | 0.346 | 4.161 | 0.0 | 0.0 | – |
| $RhAs_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 7.00 | 7.05 | 58.4 | 1.109 | 1.242 | – | – | 0.0 |
| $RhSe_2$ | TXX | $P\bar{1}(2)$ | – | – | 7.46 | 7.39 | 53.3 | – | – | – | – | – | – | 2.124 | 2.438 | 0.0 | – | – |
| $RhY_2$ | PTX | $P\bar{3}m1(164)$ | – | $P2_1/m(11)$ | 8.22 | 8.23 | 59.9 | – | – | – | 10.37 | 8.57 | 33.8 | 0.349 | 2.516 | 0.0 | – | 0.0 |
| $RhAg_2$ | HXX | – | $Pmmm(47)$ | – | – | – | – | 8.14 | 5.75 | 43.3 | – | – | – | 8.602 | 8.637 | – | 0.0 | – |
| $RhIn_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 6.43 | 6.38 | 58.1 | – | – | – | 1.550 | 1.883 | – | 0.0 | – |
| $RhTe_2$ | TXX | $P\bar{1}(2)$ | – | – | 7.97 | 7.92 | 52.7 | – | – | – | – | – | – | 1.716 | 3.389 | 0.0 | – | – |
| $RhI_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{3}m1(164)$ | – | 8.07 | 8.07 | 60.0 | 8.08 | 8.08 | 59.9 | – | – | – | 0.004 | 2.418 | 3.5 | 3.5 | – |
| $RhAu_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 7.96 | 5.61 | 44.3 | – | – | – | 5.785 | 5.794 | – | 0.0 | – |
| $RhHg_2$ | TXX | $P4/mmm(123)$ | – | – | 6.61 | 9.22 | 43.2 | – | – | – | – | – | – | 1.278 | 6.618 | 0.0 | – | – |
| $RhBi_2$ | TPX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 8.80 | 7.19 | 52.5 | – | – | – | 7.22 | 8.79 | 52.3 | 0.006 | 1.307 | 0.0 | – | 0.0 |
| $PdB_2$ | PTH | $Cmmm(65)$ | $Cmmm(65)$ | $Cmmm(65)$ | 8.13 | 8.13 | 44.4 | 8.13 | 8.13 | 44.4 | 8.13 | 8.13 | 44.4 | 0.013 | 0.016 | 0.0 | 0.0 | 0.0 |
| $PdO_2$ | HTP | $P\bar{3}m1(164)$ | $P\bar{3}m1(164)$ | $P\bar{3}m1(164)$ | 6.20 | 6.19 | 59.8 | 6.18 | 6.18 | 60.1 | 6.18 | 6.18 | 59.9 | 0.004 | 0.009 | 0.0 | 0.0 | 0.0 |
| $PdF_2$ | PTH | $P\bar{3}m1(164)$ | $C2/m(12)$ | $P2_1/c(14)$ | 6.83 | 6.84 | 59.9 | 6.54 | 7.64 | 48.8 | 6.98 | 6.98 | 72.0 | 0.177 | 0.237 | 8.0 | 3.9 | 0.0 |
| $PdAl_2$ | HXX | – | $C2/m(12)$ | – | – | – | – | 7.11 | 5.87 | 50.2 | – | – | – | 3.293 | 3.299 | – | 0.0 | – |
| $PdP_2$ | HTX | $Pc(7)$ | $Pc(7)$ | – | 9.07 | 9.08 | 42.3 | 8.49 | 8.52 | 38.4 | – | – | – | 0.395 | 1.051 | 0.0 | 0.0 | – |
| $PdS_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.14 | 7.14 | 60.0 | – | – | – | – | – | – | 0.888 | 2.958 | 0.0 | – | – |
| $PdCl_2$ | HTX | $P\bar{3}m1(164)$ | $Cmmm(65)$ | – | 7.48 | 7.48 | 59.9 | 8.56 | 8.54 | 47.4 | – | – | – | 0.753 | 3.561 | 8.0 | 0.0 | – |
| $PdK_2$ | HPT | $P\bar{3}m1(164)$ | $Pmmm(47)$ | $P\bar{3}m1(164)$ | 10.58 | 10.59 | 57.8 | 8.38 | 11.28 | 41.7 | 10.26 | 10.28 | 59.7 | 0.480 | 0.512 | 0.0 | 0.0 | 0.0 |
| $PdCa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 8.53 | 8.54 | 59.8 | – | – | – | 8.51 | 8.52 | 60.0 | 0.006 | 1.685 | 0.0 | – | 0.0 |
| $PdSc_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 7.99 | 7.97 | 59.6 | 6.91 | 6.93 | 60.1 | 7.97 | 7.95 | 60.0 | 0.376 | 0.382 | 0.0 | 0.0 | 0.0 |
| $PdAs_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.09 | 8.78 | 37.4 | – | – | – | 2.195 | 7.320 | – | 0.0 | – |
| $PdSe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.51 | 7.51 | 59.8 | – | – | – | – | – | – | 2.841 | 4.700 | 0.0 | – | – |
| $PdBr_2$ | PHT | $P\bar{3}m1(164)$ | $Cmmm(65)$ | $P\bar{1}(2)$ | 7.84 | 7.84 | 59.8 | 8.63 | 8.63 | 49.7 | 15.26 | 6.63 | 60.1 | 0.020 | 0.475 | 7.9 | 0.0 | 0.0 |
| $PdRb_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.86 | 10.89 | 58.4 | – | – | – | 10.62 | 10.64 | 60.2 | 0.019 | 1.091 | 0.0 | – | 0.0 |
| $PdSr_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 9.14 | 9.14 | 59.2 | – | – | – | – | – | – | 2.115 | 4.412 | 0.0 | – | – |
| $PdZr_2$ | HXX | – | $C2/m(12)$ | – | – | – | – | 8.73 | 7.47 | 45.6 | – | – | – | 0.831 | 4.247 | – | 0.0 | – |
| $PdRu_2$ | PXX | – | – | $Pmmn(59)$ | – | – | – | – | – | – | 8.34 | 8.33 | 36.9 | 3.878 | 3.891 | – | – | 0.0 |
| $PdAg_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 5.83 | 8.37 | 43.3 | – | – | – | 6.189 | 6.315 | – | 0.0 | – |
| $PdIn_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 6.36 | 6.35 | 60.1 | – | – | – | 1.708 | 1.943 | – | 0.0 | – |
| $PdSb_2$ | THX | $C2/m(12)$ | $Amm2(38)$ | – | 8.93 | 8.93 | 54.1 | 8.87 | 8.87 | 42.2 | – | – | – | 0.077 | 5.364 | 0.0 | 0.0 | – |
| $PdTe_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 8.08 | 8.08 | 59.8 | – | – | – | 6.98 | 8.06 | 90.0 | 0.025 | 2.028 | 0.0 | – | 0.0 |
| $PdI_2$ | THP | $C2/m(12)$ | $Cmmm(65)$ | $P\bar{1}(2)$ | 10.07 | 10.07 | 45.5 | 8.96 | 8.96 | 51.8 | 14.21 | 7.29 | 75.9 | 0.153 | 0.225 | 0.0 | 0.0 | 0.0 |
| $PdCs_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 10.85 | 10.91 | 59.8 | – | – | – | – | – | – | 0.882 | 2.308 | 0.0 | – | – |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $PdIr_2$ | PHX | – | $Amm2(38)$ | $Pmmn(59)$ | – | – | – | 9.21 | 9.21 | 32.4 | 8.73 | 8.72 | 55.8 | 0.795 | 1.191 | – | 0.0 | 0.0 |
| $PdPt_2$ | TPX | $C2/m(12)$ | – | $Pmmn(59)$ | 9.36 | 9.36 | 33.0 | – | – | – | 9.04 | 9.03 | 57.0 | 0.607 | 0.845 | 0.0 | – | 0.0 |
| $PdAu_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.72 | 5.71 | 59.6 | – | – | – | 5.169 | 5.185 | – | 0.0 | – |
| $PdHg_2$ | HTX | $C2/m(12)$ | $Pmmm(47)$ | – | 8.86 | 8.87 | 40.0 | 9.71 | 7.61 | 37.8 | – | – | – | 0.741 | 2.403 | 0.0 | 0.0 | – |
| $PdTl_2$ | HTP | $P\bar{3}m1(164)$ | $Amm2(38)$ | $C2/m(12)$ | 8.85 | 8.83 | 56.7 | 8.37 | 8.29 | 44.7 | 9.41 | 9.42 | 44.6 | 0.489 | 0.506 | 0.0 | 0.0 | 0.0 |
| $AgB_2$ | HTP | $Cmmm(65)$ | $P1(1)$ | $Cmmm(65)$ | 8.90 | 8.90 | 40.6 | 8.41 | 7.22 | 31.9 | 8.88 | 8.89 | 40.6 | 0.222 | 0.245 | 0.0 | 0.0 | 0.0 |
| $AgO_2$ | PXX | – | – | $Cmme(67)$ | – | – | – | – | – | – | 10.94 | 8.10 | 38.4 | 3.783 | 7.092 | – | – | 0.0 |
| $AgF_2$ | HTX | $C2/m(12)$ | $P\bar{1}(2)$ | – | 7.74 | 7.75 | 50.8 | 11.61 | 11.31 | 34.2 | – | – | – | 0.309 | 1.359 | 3.7 | 0.0 | – |
| $AgAl_2$ | TPH | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P6/mmm(191)$ | 9.05 | 9.05 | 60.0 | 8.48 | 8.48 | 36.2 | 9.11 | 9.11 | 60.0 | 0.025 | 0.098 | 0.0 | 0.0 | 0.0 |
| $AgSi_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 9.06 | 9.98 | 29.1 | – | – | – | 1.521 | 3.989 | – | 0.0 | – |
| $AgP_2$ | TPX | $P2/m(10)$ | – | $P\bar{1}(2)$ | 11.30 | 8.95 | 37.0 | – | – | – | 11.25 | 6.60 | 52.2 | 0.402 | 1.672 | 0.0 | – | 0.0 |
| $AgS_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 9.42 | 12.17 | 37.6 | 2.184 | 4.385 | – | – | 0.0 |
| $AgCl_2$ | THP | $C2/m(12)$ | $Cmmm(65)$ | $Cmmm(65)$ | 8.35 | 8.34 | 52.2 | 8.09 | 8.09 | 54.0 | 12.12 | 12.12 | 36.2 | 0.354 | 0.505 | 3.0 | 2.8 | 0.0 |
| $AgK_2$ | THX | $C2/m(12)$ | $Amm2(38)$ | – | 10.05 | 10.04 | 56.1 | 10.08 | 10.29 | 50.5 | – | – | – | 0.348 | 2.338 | 0.0 | 0.0 | – |
| $AgCa_2$ | THX | $P\bar{3}m1(164)$ | $Amm2(38)$ | – | 8.98 | 8.97 | 59.5 | 7.78 | 7.80 | 60.9 | – | – | – | 0.101 | 1.069 | 0.0 | 0.0 | – |
| $AgSc_2$ | TPH | $C2/m(12)$ | $P4/mmm(123)$ | $C2/m(12)$ | 9.29 | 6.62 | 57.6 | 6.51 | 9.21 | 45.0 | 9.30 | 6.64 | 57.5 | 0.003 | 0.219 | 0.0 | 0.0 | 0.0 |
| $AgMn_2$ | THX | $C2/m(12)$ | $P1(1)$ | – | 8.19 | 5.68 | 57.8 | 7.79 | 8.67 | 39.0 | – | – | – | 0.126 | 6.400 | 33.0 | 34.4 | – |
| $AgGe_2$ | PHX | – | $P\bar{1}(2)$ | $P1(1)$ | – | – | – | 9.05 | 9.47 | 35.7 | 6.07 | 6.72 | 75.7 | 0.406 | 2.470 | – | 0.0 | 0.0 |
| $AgSe_2$ | PXX | – | – | $Cmme(67)$ | – | – | – | – | – | – | 10.39 | 13.02 | 35.2 | 2.171 | 3.360 | – | – | 0.0 |
| $AgSr_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 9.53 | 9.53 | 59.8 | – | – | – | – | – | – | 0.860 | 4.582 | 0.0 | – | – |
| $AgY_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 7.85 | 10.58 | 33.5 | 1.843 | 2.438 | – | – | 0.0 |
| $AgPd_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 10.12 | 5.58 | 46.0 | 1.479 | 3.669 | – | – | 0.0 |
| $AgIn_2$ | HXX | – | $C2/m(12)$ | – | – | – | – | 8.95 | 7.89 | 42.5 | – | – | – | 2.390 | 3.107 | – | 0.0 | – |
| $AgSb_2$ | THX | $P\bar{1}(2)$ | $Pc(7)$ | – | 9.50 | 13.53 | 38.5 | 9.52 | 9.55 | 40.5 | – | – | – | 0.095 | 4.273 | 0.0 | 0.0 | – |
| $AgI_2$ | THP | $C2/m(12)$ | $C2/m(12)$ | $P2/m(10)$ | 9.23 | 9.23 | 50.7 | 9.35 | 9.35 | 50.1 | 10.18 | 14.09 | 66.1 | 0.005 | 0.026 | 0.0 | 0.0 | 0.0 |
| $AgCs_2$ | TPH | $P\bar{3}m1(164)$ | $Amm2(38)$ | $Cm(8)$ | 11.02 | 11.02 | 60.0 | 10.98 | 10.94 | 54.6 | 15.91 | 15.99 | 38.2 | 0.267 | 0.523 | 0.0 | 0.0 | 0.0 |
| $AgBa_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.97 | 9.96 | 59.7 | – | – | – | 9.87 | 10.08 | 58.9 | 0.019 | 1.129 | 0.0 | – | 0.0 |
| $AgHf_2$ | HXX | – | $P1(1)$ | – | – | – | – | 6.06 | 10.15 | 34.5 | – | – | – | 2.380 | 7.840 | – | 0.0 | – |
| $AgTl_2$ | HXX | – | $P2/m(10)$ | – | – | – | – | 10.80 | 7.64 | 37.6 | – | – | – | 0.855 | 3.872 | – | 0.0 | – |
| $AgPb_2$ | TXX | $C2/m(12)$ | – | – | 8.87 | 9.45 | 43.8 | – | – | – | – | – | – | 1.367 | 1.829 | 0.0 | – | – |
| $AgBi_2$ | THX | $P\bar{1}(2)$ | $Amm2(38)$ | – | 13.84 | 9.79 | 39.2 | 9.49 | 9.48 | 42.9 | – | – | – | 0.078 | 0.890 | 0.0 | 0.0 | – |
| $CdO_2$ | PXX | – | – | $P2/m(10)$ | – | – | – | – | – | – | 9.14 | 7.13 | 90.0 | 1.962 | 2.804 | – | – | 2.0 |
| $CdF_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.15 | 7.15 | 59.8 | – | – | – | 7.17 | 7.18 | 59.8 | 0.031 | 2.285 | 0.0 | – | 0.0 |
| $CdP_2$ | TXX | $C2/m(12)$ | – | – | 11.38 | 11.29 | 34.1 | – | – | – | – | – | – | 0.824 | 2.323 | 0.0 | – | – |
| $CdS_2$ | PHX | – | $Pc(7)$ | $P1(1)$ | – | – | – | 9.47 | 9.49 | 54.0 | 9.68 | 8.44 | 55.2 | 0.408 | 5.042 | – | 0.0 | 0.0 |
| $CdCl_2$ | HTP | $P\bar{3}m1(164)$ | $P\bar{3}m1(164)$ | $C222(21)$ | 7.91 | 7.91 | 58.7 | 7.83 | 7.83 | 59.7 | 8.08 | 8.08 | 79.4 | 0.006 | 0.771 | 0.0 | 0.0 | 0.0 |
| $CdK_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 8.43 | 11.95 | 44.6 | – | – | – | 1.278 | 2.679 | – | 0.0 | – |
| $CdCa_2$ | PTH | $C2/m(12)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 8.05 | 8.07 | 59.1 | 7.91 | 7.90 | 59.5 | 7.80 | 9.10 | 54.1 | 0.438 | 0.706 | 0.0 | 0.0 | 0.0 |
| $CdCr_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 7.69 | 10.38 | 34.0 | – | – | – | 2.805 | 3.215 | – | 36.1 | – |
| $CdGe_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.22 | 9.22 | 36.9 | – | – | – | 1.601 | 1.654 | – | 0.0 | – |
| $CdSe_2$ | PHX | – | $C2(5)$ | $Cm(8)$ | – | – | – | 11.60 | 8.63 | 47.4 | 9.39 | 9.40 | 54.1 | 0.364 | 4.240 | – | 0.0 | 0.0 |
| $CdBr_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 8.21 | 8.21 | 58.9 | – | – | – | – | – | – | 0.874 | 1.427 | 0.0 | – | – |
| $CdRb_2$ | HXX | – | $P1(1)$ | – | – | – | – | 8.85 | 13.29 | 41.6 | – | – | – | 1.561 | 2.875 | – | 0.0 | – |
| $CdY_2$ | PHT | $C2/m(12)$ | $P4/mmm(123)$ | $C2/m(12)$ | 9.02 | 9.89 | 46.7 | 9.81 | 6.93 | 45.0 | 10.05 | 7.29 | 56.9 | 0.040 | 0.730 | 0.0 | 0.0 | 1.5 |
| $CdPd_2$ | HTX | $C2/m(12)$ | $Pmmm(47)$ | – | 10.32 | 10.33 | 31.8 | 10.31 | 8.33 | 34.1 | – | – | – | 0.203 | 3.136 | 0.0 | 0.0 | – |
| $CdAg_2$ | PXX | – | – | $P6/mmm(191)$ | – | – | – | – | – | – | 9.96 | 9.96 | 59.8 | 1.025 | 1.245 | – | – | 0.0 |
| $CdSn_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.63 | 9.78 | 37.6 | – | – | – | 1.492 | 2.923 | – | 0.0 | – |
| $CdBa_2$ | HPT | $C2/m(12)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 10.64 | 10.61 | 56.1 | 9.24 | 9.19 | 58.5 | 10.29 | 10.26 | 60.1 | 0.497 | 0.549 | 0.0 | 0.0 | 0.0 |
| $CdAu_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 8.60 | 7.54 | 41.5 | – | – | – | 1.506 | 1.517 | – | 0.0 | – |
| $CdTl_2$ | THX | $C2/m(12)$ | $Amm2(38)$ | – | 9.39 | 9.40 | 41.4 | 9.32 | 9.26 | 40.5 | – | – | – | 0.451 | 2.846 | 0.0 | 0.0 | – |
| $CdBi_2$ | THX | $C2/m(12)$ | $P\bar{6}m2(187)$ | – | 12.89 | 12.88 | 39.4 | 9.20 | 9.20 | 58.2 | – | – | – | 0.525 | 2.600 | 0.0 | 0.0 | – |
| $InLi_2$ | HTX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 6.32 | 9.04 | 45.6 | 9.15 | 6.45 | 45.0 | – | – | – | 0.051 | 4.573 | 0.0 | 0.0 | – |
| $InO_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 6.67 | 6.69 | 65.5 | – | – | – | 7.17 | 6.69 | 57.8 | 0.154 | 1.285 | 4.0 | – | 4.0 |
| $InNa_2$ | THX | $Cmmm(65)$ | $Pmma(51)$ | – | 8.86 | 11.40 | 38.1 | 8.85 | 11.33 | 37.7 | – | – | – | 0.056 | 3.600 | 0.0 | 0.0 | – |
| $InAl_2$ | PHX | – | $Amm2(38)$ | $Cm(8)$ | – | – | – | 9.28 | 9.28 | 35.3 | 8.68 | 8.47 | 59.6 | 0.071 | 2.307 | – | 0.0 | 0.0 |
| $InS_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 8.90 | 8.91 | 60.3 | 1.836 | 2.242 | – | – | 0.0 |
| $InK_2$ | HTP | $C2/m(12)$ | $Pmma(51)$ | $P\bar{1}(2)$ | 11.36 | 10.25 | 48.2 | 10.39 | 9.49 | 57.2 | 10.57 | 10.48 | 51.1 | 0.234 | 0.567 | 0.0 | 0.0 | 0.0 |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | T | H | P |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | | | |
| $InCa_2$ | TXX | $P4/mmm(123)$ | – | – | 7.57 | 10.75 | 44.6 | – | – | – | – | – | – | 1.123 | 6.594 | 0.0 | – | – |
| $InSc_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.65 | 9.46 | 45.0 | – | – | – | 3.680 | 6.339 | – | 0.0 | – |
| $InTi_2$ | TXX | $C2/m(12)$ | – | – | 10.64 | 10.63 | 31.5 | – | – | – | – | – | – | 1.117 | 5.256 | 0.0 | – | – |
| $InV_2$ | TXX | $C2/m(12)$ | – | – | 10.66 | 10.65 | 31.1 | – | – | – | – | – | – | 3.078 | 3.226 | 0.0 | – | – |
| $InCr_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.11 | 8.63 | 45.1 | – | – | – | 1.595 | 2.770 | – | 35.6 | – |
| $InMn_2$ | PXX | – | – | $P6/mmm(191)$ | – | – | – | – | – | – | 9.24 | 9.20 | 59.8 | 2.572 | 2.657 | – | – | 22.2 |
| $InY_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.81 | 9.62 | 45.1 | – | – | – | 2.618 | 3.690 | – | 0.0 | – |
| $InPd_2$ | PXX | – | – | $P\bar{3}m1(164)$ | – | – | – | – | – | – | 8.97 | 9.04 | 59.4 | 3.730 | 4.080 | – | – | 0.0 |
| $InIn_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.65 | 9.57 | 37.4 | – | – | – | 2.065 | 3.373 | – | 0.0 | – |
| $InTe_2$ | HTP | $C2/m(12)$ | $C222(21)$ | $P2_1/m(11)$ | 8.51 | 8.50 | 47.8 | 8.53 | 8.53 | 46.2 | 9.24 | 9.24 | 68.7 | 0.058 | 0.390 | 0.0 | 0.0 | 0.0 |
| $InBa_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 8.51 | 12.04 | 45.1 | – | – | – | 2.067 | 2.487 | – | 0.0 | – |
| $InOs_2$ | PXX | – | – | $P6/mmm(191)$ | – | – | – | – | – | – | 8.97 | 8.96 | 60.0 | 7.610 | 8.673 | – | – | 0.0 |
| $InAu_2$ | TPX | $P6/mmm(191)$ | – | $P6/mmm(191)$ | 9.88 | 9.87 | 60.1 | – | – | – | 9.90 | 9.87 | 60.1 | 0.001 | 1.107 | 0.0 | – | 0.0 |
| $InTl_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 6.94 | 6.95 | 59.9 | – | – | – | 3.251 | 4.456 | – | 0.0 | – |
| $SnBe_2$ | HXX | – | $Pma2(28)$ | – | – | – | – | 7.19 | 8.34 | 30.2 | – | – | – | 4.465 | 4.815 | – | 0.0 | – |
| $SnO_2$ | PXX | – | – | $P\bar{3}m1(164)$ | – | – | – | – | – | – | 6.18 | 6.19 | 60.1 | 2.221 | 2.222 | – | – | 0.0 |
| $SnAl_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 6.54 | 6.69 | 55.2 | 3.860 | 5.502 | – | – | 0.0 |
| $SnS_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.46 | 7.46 | 60.0 | – | – | – | – | – | – | 1.498 | 3.010 | 0.0 | – | – |
| $SnCl_2$ | TPX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 8.91 | 8.91 | 57.2 | – | – | – | 8.91 | 8.94 | 57.1 | 0.024 | 1.262 | 0.0 | – | 0.0 |
| $SnK_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 10.55 | 11.48 | 45.0 | – | – | – | 2.288 | 2.307 | – | 0.0 | – |
| $SnCa_2$ | TPH | $P\bar{3}m1(164)$ | $P4/mmm(123)$ | $P\bar{3}m1(164)$ | 10.12 | 10.12 | 60.0 | 7.62 | 10.79 | 44.8 | 10.11 | 10.11 | 60.0 | 0.018 | 0.590 | 0.0 | 0.0 | 0.0 |
| $SnV_2$ | HXX | – | $P\bar{1}(2)$ | – | – | – | – | 5.42 | 9.17 | 39.5 | – | – | – | 11.665 | 12.496 | – | 0.0 | – |
| $SnCr_2$ | HTX | $P2_1/m(11)$ | $C2/m(12)$ | – | 8.19 | 8.23 | 45.0 | 7.40 | 8.58 | 44.3 | – | – | – | 0.589 | 1.785 | 34.3 | 33.5 | – |
| $SnBr_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{1}(2)$ | 8.77 | 8.77 | 59.9 | – | – | – | 8.88 | 8.41 | 75.8 | 0.806 | 1.045 | 0.0 | – | 0.0 |
| $SnRb_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 10.89 | 11.68 | 45.6 | – | – | – | 2.089 | 2.099 | – | 0.0 | – |
| $SnSr_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.51 | 10.53 | 60.0 | – | – | – | 10.49 | 10.54 | 60.1 | 0.070 | 2.162 | 0.0 | – | 0.0 |
| $SnY_2$ | PXX | – | – | $Cmme(67)$ | – | – | – | – | – | – | 8.74 | 5.79 | 70.5 | 2.673 | 3.095 | – | – | 0.7 |
| $SnIn_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.54 | 9.31 | 39.1 | – | – | – | 1.481 | 1.499 | – | 0.0 | – |
| $SnI_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.18 | 9.18 | 59.7 | – | – | – | 9.14 | 9.12 | 59.8 | 0.004 | 0.937 | 0.0 | – | 0.0 |
| $SnCs_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 10.34 | 13.50 | 39.4 | – | – | – | 2.435 | 2.463 | – | 0.0 | – |
| $SnBa_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.86 | 10.91 | 59.6 | – | – | – | 10.95 | 10.84 | 59.7 | 0.029 | 1.678 | 0.0 | – | 0.0 |
| $SnHg_2$ | HXX | – | $P2/m(10)$ | – | – | – | – | 10.65 | 13.41 | 26.7 | – | – | – | 2.336 | 3.721 | – | 0.0 | – |
| $SnPb_2$ | PHX | – | $P\bar{6}m2(187)$ | $P\bar{1}(2)$ | – | – | – | 9.08 | 9.09 | 59.6 | 8.45 | 10.32 | 49.2 | 0.438 | 1.695 | – | 0.0 | 0.0 |
| $SbLi_2$ | THX | $P\bar{1}(2)$ | $Amm2(38)$ | – | 9.10 | 9.50 | 41.1 | 9.25 | 9.22 | 41.5 | – | – | – | 0.694 | 2.421 | 0.0 | 0.0 | – |
| $SbS_2$ | TPX | $P\bar{3}m1(164)$ | – | $P1(1)$ | 7.58 | 7.58 | 59.7 | – | – | – | 12.71 | 6.94 | 63.5 | 0.467 | 2.805 | 0.0 | – | 0.0 |
| $SbK_2$ | HPX | – | $Pm(6)$ | $P\bar{3}m1(164)$ | – | – | – | 10.75 | 11.36 | 43.9 | 11.21 | 11.14 | 58.3 | 0.737 | 0.960 | – | 0.0 | 4.0 |
| $SbCa_2$ | PTX | $C2/m(12)$ | – | $C2/m(12)$ | 9.29 | 9.28 | 60.5 | – | – | – | 9.38 | 9.31 | 59.7 | 0.075 | 1.341 | 0.0 | – | 1.4 |
| $SbV_2$ | HXX | – | $Pmn2_1(31)$ | – | – | – | – | 7.55 | 7.53 | 47.0 | – | – | – | 4.077 | 4.090 | – | 0.0 | – |
| $SbSe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.84 | 7.84 | 59.6 | – | – | – | – | – | – | 0.925 | 2.376 | 0.0 | – | – |
| $SbBr_2$ | HXX | – | $Pm(6)$ | – | – | – | – | 8.58 | 8.89 | 55.8 | – | – | – | 2.203 | 2.925 | – | 0.0 | – |
| $SbRb_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 10.78 | 11.48 | 45.7 | – | – | – | 1.195 | 2.554 | – | 0.0 | – |
| $SbSr_2$ | PTX | $C2/m(12)$ | – | $C2/m(12)$ | 9.82 | 9.78 | 60.4 | – | – | – | 9.78 | 9.90 | 59.3 | 0.004 | 1.210 | 0.0 | – | 0.0 |
| $SbPd_2$ | HXX | – | $Pmn2_1(31)$ | – | – | – | – | 7.79 | 7.78 | 48.3 | – | – | – | 0.833 | 1.455 | – | 0.0 | – |
| $SbCd_2$ | PXX | – | – | $P2/c(13)$ | – | – | – | – | – | – | 11.86 | 9.43 | 39.4 | 1.297 | 3.037 | – | – | 0.0 |
| $SbIn_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.02 | 9.00 | 43.2 | – | – | – | 0.937 | 3.263 | – | 0.0 | – |
| $SbTe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 8.33 | 8.32 | 58.5 | – | – | – | – | – | – | 1.259 | 1.772 | 0.0 | – | – |
| $SbI_2$ | HXX | – | $Pm(6)$ | – | – | – | – | 9.45 | 9.00 | 56.4 | – | – | – | 1.739 | 2.914 | – | 0.0 | – |
| $SbCs_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 11.27 | 11.95 | 44.4 | – | – | – | 1.231 | 1.308 | – | 0.0 | – |
| $SbBa_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 10.03 | 10.07 | 59.9 | – | – | – | – | – | – | 1.313 | 6.828 | 0.0 | – | – |
| $SbTl_2$ | HPX | – | $Amm2(38)$ | $P2/c(13)$ | – | – | – | 9.69 | 9.65 | 41.1 | 9.76 | 7.23 | 68.4 | 0.209 | 1.189 | – | 0.0 | 0.0 |
| $SbBi_2$ | PTX | $P1(1)$ | – | $P1(1)$ | 9.16 | 9.21 | 41.9 | – | – | – | 9.81 | 9.91 | 67.2 | 0.195 | 2.661 | 0.0 | – | 0.0 |
| $TeLi_2$ | PTX | $P\bar{3}m1(164)$ | – | $P2_1/m(11)$ | 9.17 | 9.17 | 59.3 | – | – | – | 9.11 | 9.13 | 59.5 | 0.038 | 1.715 | 0.0 | – | 0.0 |
| $TeB_2$ | PXX | – | – | $P2/c(13)$ | – | – | – | – | – | – | 6.22 | 8.93 | 79.7 | 17.621 | 18.239 | – | – | 0.0 |
| $TeNa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.19 | 10.20 | 59.5 | – | – | – | 10.21 | 10.21 | 59.4 | 0.005 | 2.006 | 0.0 | – | 0.0 |
| $TeS_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.71 | 7.71 | 59.8 | – | – | – | – | – | – | 2.292 | 2.634 | 0.0 | – | – |
| $TeK_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 11.31 | 11.33 | 58.6 | – | – | – | 11.19 | 11.20 | 59.7 | 0.013 | 1.709 | 0.0 | – | 0.0 |
| $TeCa_2$ | THX | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | – | 8.45 | 9.16 | 62.8 | 8.41 | 8.37 | 59.7 | – | – | – | 0.767 | 0.919 | 0.0 | 0.0 | – |

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Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | T | H | P |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | | | |
| $TeSc_2$ | TPX | $P\bar{1}(2)$ | – | $P2_1/m(11)$ | 7.64 | 8.55 | 63.8 | – | – | – | 8.62 | 7.54 | 63.9 | 0.150 | 2.466 | 0.5 | – | 0.0 |
| $TeSe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.97 | 7.97 | 59.8 | – | – | – | – | – | – | 0.931 | 2.325 | 0.0 | – | – |
| $TeRb_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 11.86 | 11.88 | 58.1 | – | – | – | 11.64 | 11.67 | 59.6 | 0.032 | 1.515 | 0.0 | – | 0.0 |
| $TeSr_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 8.91 | 8.95 | 60.3 | 8.94 | 8.88 | 59.3 | – | – | – | 0.500 | 2.067 | 0.0 | 0.0 | – |
| $TeCd_2$ | PXX | – | – | $P2(3)$ | – | – | – | – | – | – | 10.08 | 12.42 | 49.0 | 1.789 | 1.844 | – | – | 0.0 |
| $TeTe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 8.57 | 8.57 | 59.3 | – | – | – | – | – | – | 1.102 | 1.829 | 0.0 | – | – |
| $TeCs_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 12.04 | 12.14 | 59.4 | – | – | – | – | – | – | 1.228 | 2.144 | 0.0 | – | – |
| $TeTl_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 9.79 | 9.80 | 58.4 | 9.28 | 9.32 | 58.4 | 9.76 | 9.77 | 58.2 | 0.032 | 0.034 | 0.0 | 0.0 | 0.0 |
| $TePb_2$ | PHX | – | $Pc(7)$ | $P\bar{1}(2)$ | – | – | – | 9.27 | 13.39 | 42.8 | 10.57 | 10.84 | 48.5 | 0.103 | 1.349 | – | 0.0 | 0.0 |
| $IN_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 9.18 | 9.72 | 78.0 | 21.899 | 22.768 | – | – | 0.0 |
| $IS_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 11.21 | 9.66 | 71.1 | 4.600 | 5.349 | – | – | 1.9 |
| $ICl_2$ | THP | $P\bar{1}(2)$ | $P1(1)$ | $P\bar{1}(2)$ | 9.36 | 8.62 | 80.0 | 7.93 | 8.97 | 75.1 | 13.63 | 8.65 | 81.4 | 0.112 | 0.159 | 0.0 | 0.0 | 0.0 |
| $IK_2$ | TPH | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P\bar{1}(2)$ | 9.84 | 9.86 | 59.0 | 10.00 | 9.98 | 56.2 | 11.61 | 12.07 | 90.0 | 0.041 | 0.189 | 0.0 | 0.0 | 0.0 |
| $ISe_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 9.35 | 12.58 | 70.5 | 4.298 | 4.658 | – | – | 0.0 |
| $IBr_2$ | TPH | $P\bar{1}(2)$ | $P1(1)$ | $P1(1)$ | 9.08 | 9.40 | 76.7 | 8.93 | 9.22 | 78.3 | 10.74 | 10.83 | 87.9 | 0.019 | 0.075 | 0.0 | 0.0 | 0.0 |
| $IRb_2$ | HPX | – | $Amm2(38)$ | $P1(1)$ | – | – | – | 10.57 | 10.55 | 55.9 | 13.18 | 12.60 | 89.9 | 0.072 | 0.937 | – | 0.0 | 0.0 |
| $ISr_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | – | 8.54 | 8.55 | 59.8 | 8.57 | 8.57 | 59.0 | – | – | – | 0.115 | 1.645 | 0.0 | 0.0 | – |
| $II_2$ | PHT | $P\bar{1}(2)$ | $P\bar{1}(2)$ | $P2/m(10)$ | 9.69 | 9.61 | 84.7 | 9.73 | 9.58 | 62.4 | 11.74 | 13.03 | 94.1 | 0.444 | 0.501 | 0.0 | 0.0 | 0.0 |
| $ICs_2$ | THP | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P1(1)$ | 10.99 | 10.96 | 58.9 | 11.22 | 11.18 | 55.7 | 12.27 | 12.09 | 74.1 | 0.245 | 0.271 | 0.0 | 0.0 | 0.0 |
| $CsN_2$ | TPH | $P2/c(13)$ | $Amm2(38)$ | $Pmma(51)$ | 10.96 | 10.42 | 61.7 | 10.37 | 10.34 | 55.0 | 11.21 | 11.19 | 57.8 | 0.169 | 0.689 | 20.0 | 20.0 | 20.0 |
| $CsF_2$ | HPX | – | $Amm2(38)$ | $Cmmm(65)$ | – | – | – | 10.12 | 10.13 | 55.1 | 11.40 | 9.82 | 53.9 | 0.512 | 1.732 | – | 4.0 | 4.0 |
| $CsAl_2$ | PTX | $Cmmm(65)$ | – | $Cmme(67)$ | 15.07 | 15.07 | 36.6 | – | – | – | 14.58 | 14.59 | 37.7 | 0.159 | 6.625 | 0.0 | – | 0.0 |
| $CsK_2$ | PTX | $P6/mmm(191)$ | – | $P6/mmm(191)$ | 17.01 | 16.99 | 57.9 | – | – | – | 16.95 | 16.91 | 59.2 | 0.034 | 2.466 | 0.0 | – | 0.0 |
| $CsCa_2$ | TPX | $P6/mmm(191)$ | – | $Cmmm(65)$ | 15.19 | 15.20 | 58.9 | – | – | – | 15.56 | 15.57 | 56.4 | 0.044 | 3.461 | 0.0 | – | 0.0 |
| $CsCr_2$ | PTX | $Cmmm(65)$ | – | $Cmmm(65)$ | 14.19 | 14.18 | 46.0 | – | – | – | 14.19 | 14.19 | 46.0 | 0.016 | 3.209 | 42.2 | – | 42.1 |
| $CsSe_2$ | PTX | $C2/m(12)$ | – | $P1(1)$ | 13.71 | 13.70 | 40.2 | – | – | – | 11.90 | 12.37 | 39.3 | 0.598 | 1.834 | 0.0 | – | 0.0 |
| $CsBr_2$ | TXX | $P4/mmm(123)$ | – | – | 9.84 | 13.95 | 45.2 | – | – | – | – | – | – | 0.919 | 1.134 | 4.0 | – | – |
| $CsRb_2$ | PTX | $P6/mmm(191)$ | – | $P6/mmm(191)$ | 17.64 | 17.65 | 59.0 | – | – | – | 17.85 | 17.84 | 58.6 | 0.012 | 2.173 | 0.0 | – | 0.0 |
| $CsSr_2$ | TPX | $P6/mmm(191)$ | – | $Cmmm(65)$ | 16.14 | 16.13 | 59.2 | – | – | – | 16.59 | 16.57 | 56.7 | 0.069 | 3.214 | 0.0 | – | 0.0 |
| $CsY_2$ | PTX | $C2/m(12)$ | – | $Cmmm(65)$ | 15.79 | 15.78 | 43.4 | – | – | – | 15.56 | 15.55 | 45.8 | 0.040 | 4.966 | 14.0 | – | 13.4 |
| $CsAg_2$ | PTX | $Cmmm(65)$ | – | $Cmmm(65)$ | 14.23 | 14.22 | 44.8 | – | – | – | 14.23 | 14.25 | 44.8 | 0.028 | 3.849 | 0.0 | – | 0.0 |
| $CsIn_2$ | HTP | $C2/m(12)$ | $P1(1)$ | $Cmmm(65)$ | 15.03 | 15.01 | 41.2 | 13.63 | 12.06 | 43.9 | 15.17 | 15.15 | 40.9 | 0.504 | 0.543 | 0.0 | 0.0 | 0.0 |
| $CsTe_2$ | TPX | $C2/m(12)$ | – | $Cmmm(65)$ | 14.54 | 14.54 | 41.5 | – | – | – | 14.33 | 14.36 | 45.4 | 0.384 | 1.809 | 0.0 | – | 0.0 |
| $CsI_2$ | PTX | $P4/mmm(123)$ | – | $P\bar{1}(2)$ | 10.42 | 14.74 | 44.9 | – | – | – | 13.76 | 15.04 | 61.7 | 0.796 | 1.746 | 4.0 | – | 0.0 |
| $CsCs_2$ | PTX | $P\bar{3}m1(164)$ | – | $P6/mmm(191)$ | 18.62 | 18.63 | 58.2 | – | – | – | 18.82 | 18.97 | 58.7 | 0.027 | 2.081 | 0.0 | – | 0.0 |
| $CsAu_2$ | PTX | $Cmmm(65)$ | – | $Cmmm(65)$ | 13.95 | 13.95 | 45.0 | – | – | – | 13.95 | 13.96 | 45.0 | 0.002 | 4.896 | 0.0 | – | 0.0 |
| $CsTl_2$ | TPX | $C2/m(12)$ | – | $P2_1/m(11)$ | 15.60 | 15.58 | 41.9 | – | – | – | 15.61 | 15.60 | 41.8 | 0.041 | 4.172 | 0.0 | – | 0.0 |
| $CsPb_2$ | TPX | $P\bar{1}(2)$ | – | $Cmmm(65)$ | 15.50 | 15.51 | 37.4 | – | – | – | 15.45 | 15.45 | 38.3 | 0.152 | 4.817 | 0.0 | – | 0.0 |
| $CsBi_2$ | TXX | $C2/m(12)$ | – | – | 15.08 | 15.10 | 35.0 | – | – | – | – | – | – | 1.192 | 4.126 | 0.0 | – | – |
| $BaB_2$ | PXX | – | – | $Pmma(51)$ | – | – | – | – | – | – | 8.97 | 10.87 | 34.1 | 2.298 | 16.736 | – | – | 0.0 |
| $BaC_2$ | PXX | – | – | $Pmmn(59)$ | – | – | – | – | – | – | 8.72 | 11.72 | 47.6 | 24.445 | 34.444 | – | – | 0.0 |
| $BaN_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 9.18 | 9.23 | 60.7 | – | – | – | 19.750 | 19.780 | – | 3.8 | – |
| $BaF_2$ | TPX | $P\bar{3}m1(164)$ | – | $Pmmn(59)$ | 8.52 | 8.53 | 59.3 | – | – | – | 8.09 | 8.53 | 58.4 | 0.025 | 2.175 | 0.0 | – | 0.0 |
| $BaAl_2$ | PXX | – | – | $Cmm2(35)$ | – | – | – | – | – | – | 8.48 | 8.48 | 58.3 | 1.492 | 9.809 | – | – | 0.0 |
| $BaSi_2$ | PTX | $P2/c(13)$ | – | $P2/c(13)$ | 12.20 | 12.21 | 37.3 | – | – | – | 12.25 | 12.29 | 37.3 | 0.017 | 5.115 | 0.0 | – | 0.0 |
| $BaP_2$ | TXX | $P\bar{1}(2)$ | – | – | 11.20 | 10.66 | 34.9 | – | – | – | – | – | – | 1.981 | 3.218 | 0.0 | – | – |
| $BaS_2$ | PHX | – | $P\bar{6}m2(187)$ | $P4/mmm(123)$ | – | – | – | 10.15 | 10.14 | 60.1 | 9.65 | 9.65 | 53.2 | 0.814 | 8.564 | – | 0.0 | 0.0 |
| $BaCl_2$ | TPX | $P\bar{3}m1(164)$ | – | $Pmmn(59)$ | 9.70 | 9.73 | 59.5 | – | – | – | 9.55 | 9.31 | 59.0 | 0.213 | 1.705 | 0.0 | – | 0.0 |
| $BaK_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 15.14 | 8.97 | 32.4 | – | – | – | 5.288 | 5.295 | – | 0.0 | – |
| $BaCa_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 13.20 | 13.23 | 34.5 | – | – | – | 1.951 | 1.981 | – | 0.0 | – |
| $BaCr_2$ | PTH | $Cmmm(65)$ | $Pmmm(47)$ | $Cmmm(65)$ | 12.36 | 12.35 | 51.8 | 10.35 | 12.66 | 34.6 | 12.37 | 12.37 | 51.7 | 0.012 | 0.318 | 40.8 | 38.5 | 40.8 |
| $BaGe_2$ | TPX | $P\bar{1}(2)$ | – | $P2/c(13)$ | 12.23 | 12.08 | 38.8 | – | – | – | 12.26 | 12.47 | 39.0 | 0.066 | 4.080 | 0.0 | – | 0.0 |
| $BaSe_2$ | PTX | $P4/mmm(123)$ | – | $P4/mmm(123)$ | 8.90 | 12.61 | 45.0 | – | – | – | 8.91 | 12.62 | 45.0 | 0.022 | 0.868 | 0.0 | – | 0.0 |
| $BaBr_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.03 | 10.02 | 59.4 | – | – | – | 9.92 | 9.91 | 59.9 | 0.009 | 1.318 | 0.0 | – | 0.0 |
| $BaRb_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 9.25 | 11.07 | 52.8 | – | – | – | 4.754 | 4.775 | – | 0.0 | – |
| $BaSr_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 13.70 | 13.69 | 35.6 | – | – | – | 1.993 | 2.024 | – | 0.0 | – |
| $BaY_2$ | TXX | $C2/m(12)$ | – | – | 14.17 | 14.16 | 30.4 | – | – | – | – | – | – | 4.497 | 11.981 | 0.0 | – | – |

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Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $BaPd_2$ | TPX | $C2/m(12)$ | – | $Cmmm(65)$ | 11.56 | 11.56 | 46.8 | – | – | – | 11.61 | 11.62 | 48.4 | 0.173 | 1.447 | 0.0 | – | 0.0 |
| $BaAg_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 6.90 | 9.76 | 44.1 | – | – | – | 4.854 | 4.883 | – | 0.0 | – |
| $BaSn_2$ | HXX | – | $Pc(7)$ | – | – | – | – | 8.68 | 9.40 | 75.0 | – | – | – | 1.507 | 1.720 | – | 0.0 | – |
| $BaSb_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 10.96 | 13.78 | 34.8 | – | – | – | 2.519 | 4.322 | – | 0.0 | – |
| $BaTe_2$ | TPX | $P4/mmm(123)$ | – | $P4/mmm(123)$ | 9.43 | 13.37 | 44.8 | – | – | – | 9.43 | 13.37 | 44.8 | 0.004 | 1.146 | 0.0 | – | 0.0 |
| $BaI_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.50 | 10.51 | 59.1 | – | – | – | 10.35 | 10.34 | 59.8 | 0.012 | 0.973 | 0.0 | – | 0.0 |
| $BaCs_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 15.57 | 15.52 | 35.9 | – | – | – | 1.937 | 2.001 | – | 0.0 | – |
| $BaBa_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 14.13 | 14.12 | 34.9 | – | – | – | 2.303 | 2.377 | – | 0.0 | – |
| $BaAu_2$ | HXX | – | $Pmn2_1(31)$ | – | – | – | – | 9.83 | 8.33 | 54.0 | – | – | – | 1.867 | 1.871 | – | 0.0 | – |
| $BaPb_2$ | TPX | $C2/m(12)$ | – | $Cmmm(65)$ | 13.51 | 13.52 | 42.2 | – | – | – | 13.58 | 13.58 | 44.3 | 0.021 | 4.013 | 0.0 | – | 0.0 |
| $BaBi_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 13.57 | 11.01 | 34.7 | – | – | – | 1.568 | 3.780 | – | 0.0 | – |
| $HfBe_2$ | PHX | – | $P4/mmm(123)$ | $Cmm2(35)$ | – | – | – | 8.00 | 5.79 | 43.7 | 6.93 | 7.58 | 46.5 | 0.718 | 3.790 | – | 0.0 | 0.0 |
| $HfB_2$ | PTX | $P2/c(13)$ | – | $P2/c(13)$ | 8.80 | 8.82 | 40.6 | – | – | – | 8.82 | 8.81 | 40.6 | 0.008 | 2.755 | 0.0 | – | 0.0 |
| $HfC_2$ | PXX | – | – | $Pmmn(59)$ | – | – | – | – | – | – | 7.56 | 6.48 | 54.2 | 4.052 | 8.259 | – | – | 0.0 |
| $HfN_2$ | HXX | – | $Pmn2_1(31)$ | – | – | – | – | 6.81 | 6.88 | 59.9 | – | – | – | 1.434 | 6.335 | – | 0.0 | – |
| $HfO_2$ | HXX | – | $Pmmn(59)$ | – | – | – | – | 5.09 | 6.52 | 50.2 | – | – | – | 1.359 | 1.371 | – | 0.0 | – |
| $HfF_2$ | HTP | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $Pm(6)$ | 6.99 | 6.98 | 50.7 | 6.08 | 6.08 | 59.9 | 5.97 | 7.04 | 64.7 | 0.463 | 0.726 | 0.0 | 0.0 | 0.0 |
| $HfSi_2$ | PHX | – | $Pmma(51)$ | $Pmma(51)$ | – | – | – | 7.33 | 9.57 | 40.0 | 9.57 | 7.33 | 39.9 | 0.002 | 6.863 | – | 0.0 | 0.0 |
| $HfP_2$ | THX | $P\bar{1}(2)$ | $P\bar{6}m2(187)$ | – | 8.16 | 7.93 | 48.6 | 8.03 | 8.02 | 59.5 | – | – | – | 0.106 | 1.575 | 0.0 | 0.0 | – |
| $HfS_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.30 | 7.29 | 59.8 | – | – | – | – | – | – | 1.150 | 2.406 | 0.0 | – | – |
| $HfCl_2$ | HTP | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 6.57 | 6.98 | 61.8 | 6.69 | 6.69 | 60.2 | 6.98 | 6.98 | 56.1 | 0.536 | 0.536 | 0.0 | 0.0 | 0.0 |
| $HfCa_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 9.97 | 7.05 | 45.0 | 7.08 | 9.99 | 44.8 | – | – | – | 0.011 | 13.950 | 0.0 | 0.0 | – |
| $HfV_2$ | THX | $Cmme(67)$ | $Cmme(67)$ | – | 10.52 | 9.63 | 23.2 | 9.62 | 10.50 | 23.3 | – | – | – | 0.008 | 14.503 | 0.0 | 0.0 | – |
| $HfGe_2$ | PXX | – | – | $Pmma(51)$ | – | – | – | – | – | – | 7.57 | 9.82 | 39.6 | 0.955 | 0.956 | – | – | 0.0 |
| $HfSe_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.49 | 7.48 | 60.0 | – | – | – | 7.49 | 7.48 | 60.0 | 0.001 | 1.854 | 0.0 | – | 0.0 |
| $HfBr_2$ | TPH | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 6.88 | 7.28 | 61.8 | 6.99 | 6.99 | 60.1 | 7.28 | 7.28 | 56.4 | 0.001 | 0.039 | 0.0 | 0.0 | 0.0 |
| $HfY_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 10.14 | 7.15 | 44.6 | 9.39 | 6.75 | 45.8 | – | – | – | 0.502 | 5.011 | 0.0 | 2.5 | – |
| $HfTe_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.91 | 7.91 | 60.0 | – | – | – | 7.90 | 7.90 | 60.0 | 0.005 | 1.351 | 0.0 | – | 0.0 |
| $HfI_2$ | PTH | $C2/m(12)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 7.59 | 7.84 | 59.7 | 7.56 | 7.56 | 59.8 | 7.76 | 7.75 | 57.3 | 0.231 | 0.516 | 0.0 | 0.0 | 0.0 |
| $HfAu_2$ | THX | $C2/m(12)$ | $P\bar{6}m2(187)$ | – | 7.35 | 6.29 | 50.1 | 6.18 | 6.19 | 60.1 | – | – | – | 0.297 | 7.760 | 0.0 | 0.0 | – |
| $HfTl_2$ | THX | $P4/mmm(123)$ | $P4/mmm(123)$ | – | 9.49 | 6.71 | 44.9 | 6.72 | 9.51 | 44.9 | – | – | – | 0.018 | 9.804 | 0.0 | 0.0 | – |
| $HfPb_2$ | PXX | – | – | $Pmmm(47)$ | – | – | – | – | – | – | 9.16 | 11.20 | 34.3 | 0.916 | 3.420 | – | – | 0.0 |
| $HfBi_2$ | TXX | $Cmmm(65)$ | – | – | 8.41 | 6.60 | 50.4 | – | – | – | – | – | – | 2.365 | 4.070 | 0.0 | – | – |
| $TaBe_2$ | THX | $Pmm2(25)$ | $P4/mmm(123)$ | – | 8.54 | 9.17 | 21.4 | 5.47 | 7.80 | 44.5 | – | – | – | 0.199 | 5.207 | 0.0 | 0.0 | – |
| $TaC_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 6.84 | 7.07 | 49.0 | 4.651 | 10.043 | – | – | 0.0 |
| $TaN_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 6.32 | 6.32 | 60.0 | – | – | – | – | – | – | 1.284 | 5.132 | 3.7 | – | – |
| $TaO_2$ | TPH | $C2/m(12)$ | $P\bar{6}m2(187)$ | $Pmmn(59)$ | 6.14 | 6.13 | 60.0 | 5.95 | 5.92 | 60.4 | 6.01 | 6.00 | 60.2 | 0.239 | 0.595 | 0.0 | 0.0 | 0.0 |
| $TaF_2$ | HXX | – | $Pmmn(59)$ | – | – | – | – | 6.09 | 6.11 | 52.2 | – | – | – | 4.641 | 8.674 | – | 0.0 | – |
| $TaP_2$ | TXX | $P\bar{1}(2)$ | – | – | 7.30 | 7.71 | 50.3 | – | – | – | – | – | – | 1.257 | 11.721 | 0.0 | – | – |
| $TaS_2$ | HTP | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $C2/m(12)$ | 6.76 | 6.76 | 60.1 | 6.68 | 6.68 | 60.0 | 6.57 | 7.69 | 50.1 | 0.242 | 0.728 | 0.0 | 0.0 | 0.0 |
| $TaAs_2$ | TPX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 7.58 | 7.59 | 51.6 | – | – | – | 7.68 | 6.65 | 63.8 | 0.173 | 1.714 | 0.0 | – | 0.0 |
| $TaSe_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 7.00 | 7.00 | 59.8 | 6.94 | 6.94 | 60.0 | 6.99 | 7.00 | 59.9 | 0.282 | 0.284 | 0.0 | 0.0 | 0.0 |
| $TaY_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.98 | 9.88 | 44.9 | – | – | – | 0.849 | 4.248 | – | 0.0 | – |
| $TaIn_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 6.69 | 6.07 | 45.2 | 2.749 | 2.836 | – | – | 0.0 |
| $TaTe_2$ | PTH | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $C2/m(12)$ | 7.50 | 7.50 | 54.7 | 7.44 | 7.43 | 59.9 | 6.88 | 8.65 | 55.4 | 0.111 | 0.115 | 0.0 | 0.0 | 0.0 |
| $TaI_2$ | HTX | $P\bar{1}(2)$ | $Cm(8)$ | – | 7.63 | 7.43 | 61.3 | 7.81 | 7.79 | 60.1 | – | – | – | 0.119 | 5.416 | 0.0 | 0.0 | – |
| $TaBi_2$ | TPX | $C2/m(12)$ | – | $P2_1/m(11)$ | 7.10 | 7.11 | 53.7 | – | – | – | 8.00 | 8.00 | 47.9 | 0.322 | 5.303 | 0.0 | – | 0.0 |
| $WBe_2$ | THX | $Pm(6)$ | $Cmmm(65)$ | – | 7.49 | 8.17 | 23.4 | 5.20 | 8.09 | 38.9 | – | – | – | 0.512 | 3.976 | 0.0 | 0.0 | – |
| $WB_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 6.08 | 7.90 | 39.7 | – | – | – | 2.009 | 2.281 | – | 0.0 | – |
| $WN_2$ | TXX | $P3(143)$ | – | – | 6.22 | 6.22 | 60.1 | – | – | – | – | – | – | 2.445 | 3.081 | 0.0 | – | – |
| $WO_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 5.70 | 5.70 | 60.0 | – | – | – | 2.620 | 2.722 | – | 0.0 | – |
| $WAl_2$ | THX | $Pmmm(47)$ | $Pmmm(47)$ | – | 9.22 | 7.38 | 36.8 | 7.90 | 7.90 | 40.9 | – | – | – | 0.033 | 10.429 | 0.0 | 0.0 | – |
| $WP_2$ | PXX | – | – | $P2_1/m(11)$ | – | – | – | – | – | – | 7.13 | 6.50 | 62.8 | 1.196 | 3.803 | – | – | 0.0 |
| $WS_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 6.40 | 6.40 | 60.0 | – | – | – | 2.345 | 4.115 | – | 0.0 | – |
| $WCl_2$ | HXX | – | $P2/m(10)$ | – | – | – | – | 8.60 | 7.59 | 46.7 | – | – | – | 10.252 | 10.470 | – | 0.0 | – |
| $WAs_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 7.39 | 7.43 | 60.2 | – | – | – | 2.084 | 10.262 | – | 0.0 | – |
| $WSe_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 6.66 | 6.66 | 59.9 | – | – | – | 1.257 | 1.281 | – | 0.0 | – |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | T | H | P |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | | | |
| $WBr_2$ | HTP | $C2/m(12)$ | $Cmmm(65)$ | $C2/m(12)$ | 9.46 | 9.46 | 47.9 | 8.60 | 8.57 | 53.1 | 7.67 | 14.49 | 74.5 | 0.039 | 0.356 | 15.9 | 15.9 | 15.9 |
| $WSr_2$ | HPT | $P2_1/m(11)$ | $P\bar{1}(2)$ | $P2_1/m(11)$ | 8.17 | 7.80 | 58.5 | 7.99 | 9.00 | 53.0 | 8.23 | 7.87 | 58.2 | 0.192 | 0.208 | 0.0 | 0.0 | 0.0 |
| $WNb_2$ | HXX | – | $P\bar{1}(2)$ | – | – | – | – | 6.80 | 8.14 | 41.9 | – | – | – | 1.420 | 1.877 | – | 0.0 | – |
| $WSn_2$ | HXX | – | $P\bar{1}(2)$ | – | – | – | – | 6.14 | 9.01 | 40.7 | – | – | – | 5.683 | 15.239 | – | 0.0 | – |
| $WSb_2$ | TPX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 7.99 | 7.13 | 46.8 | – | – | – | 7.40 | 6.81 | 63.7 | 0.049 | 4.571 | 0.0 | – | 0.0 |
| $WTe_2$ | TPH | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P2_1/m(11)$ | 7.05 | 7.27 | 61.0 | 7.18 | 7.18 | 60.0 | 7.27 | 7.04 | 61.0 | 0.004 | 0.473 | 0.0 | 0.0 | 0.0 |
| $WI_2$ | HXX | – | $P\bar{1}(2)$ | – | – | – | – | 11.12 | 10.24 | 35.6 | – | – | – | 7.959 | 9.436 | – | 0.0 | – |
| $WTa_2$ | HPT | $C2/m(12)$ | $P\bar{1}(2)$ | $P1(1)$ | 9.13 | 8.16 | 32.9 | 8.94 | 7.45 | 38.0 | 6.10 | 8.07 | 59.2 | 0.614 | 0.738 | 0.0 | 0.0 | 0.0 |
| $ReB_2$ | THP | $P2/c(13)$ | $Pmma(51)$ | $Cmmm(65)$ | 7.83 | 6.85 | 44.1 | 5.75 | 5.83 | 59.6 | 8.26 | 8.26 | 42.0 | 0.213 | 0.278 | 0.0 | 0.0 | 4.3 |
| $ReN_2$ | THX | $P1(1)$ | $P\bar{6}m2(187)$ | – | 6.36 | 6.10 | 57.8 | 5.76 | 5.77 | 60.1 | – | – | – | 0.018 | 1.863 | 0.0 | 0.0 | – |
| $ReO_2$ | TPX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 5.70 | 5.78 | 60.1 | – | – | – | 5.78 | 5.74 | 59.3 | 0.013 | 3.965 | 0.0 | – | 0.0 |
| $ReSi_2$ | TXX | $C2/m(12)$ | – | – | 8.56 | 8.56 | 40.3 | – | – | – | – | – | – | 0.861 | 1.573 | 0.0 | – | – |
| $ReS_2$ | PTX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 6.60 | 6.54 | 58.7 | – | – | – | 6.44 | 6.60 | 60.2 | 0.004 | 2.516 | 0.0 | – | 0.0 |
| $ReSc_2$ | PHT | $P4/mmm(123)$ | $P4/mmm(123)$ | $P4/mmm(123)$ | 6.49 | 9.16 | 45.0 | 6.48 | 9.17 | 45.0 | 6.48 | 9.17 | 45.0 | 0.001 | 0.001 | 0.0 | 0.0 | 0.0 |
| $ReTi_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.12 | 8.66 | 45.0 | – | – | – | 2.452 | 3.638 | – | 0.0 | – |
| $ReSe_2$ | TPX | $C2/m(12)$ | – | $P\bar{1}(2)$ | 6.86 | 6.67 | 60.3 | – | – | – | 6.86 | 6.68 | 60.2 | 0.093 | 2.313 | 0.0 | – | 0.0 |
| $ReTe_2$ | TPX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 7.13 | 7.31 | 60.4 | – | – | – | 7.30 | 7.26 | 58.6 | 0.007 | 1.876 | 0.0 | – | 0.0 |
| $ReCs_2$ | TXX | $C2/m(12)$ | – | – | 10.91 | 11.87 | 45.3 | – | – | – | – | – | – | 10.951 | 11.154 | 6.0 | – | – |
| $ReBi_2$ | TPX | $P2_1/m(11)$ | – | $P\bar{1}(2)$ | 7.38 | 7.37 | 54.4 | – | – | – | 7.37 | 7.32 | 54.2 | 0.382 | 1.551 | 0.0 | – | 0.0 |
| $OsBe_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 5.72 | 8.07 | 44.9 | – | – | – | 2.085 | 7.582 | – | 0.0 | – |
| $OsB_2$ | PXX | – | – | $P2/c(13)$ | – | – | – | – | – | – | 7.99 | 7.79 | 40.5 | 1.783 | 5.686 | – | – | 0.0 |
| $OsN_2$ | THX | $P1(1)$ | $P\bar{6}m2(187)$ | – | 6.17 | 6.49 | 58.1 | 5.65 | 5.64 | 59.8 | – | – | – | 0.049 | 0.888 | 0.0 | 0.0 | – |
| $OsF_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 5.58 | 6.86 | 48.1 | – | – | – | 2.329 | 12.030 | – | 0.0 | – |
| $OsMg_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.01 | 6.25 | 44.6 | – | – | – | 1.045 | 12.251 | – | 0.0 | – |
| $OsSi_2$ | PXX | – | – | $Pmmn(59)$ | – | – | – | – | – | – | 6.82 | 5.82 | 64.7 | 2.880 | 3.261 | – | – | 0.0 |
| $OsS_2$ | TPX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 6.63 | 7.11 | 57.6 | – | – | – | 7.11 | 6.62 | 57.6 | 0.005 | 3.611 | 0.0 | – | 0.0 |
| $OsSc_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 9.06 | 6.40 | 45.0 | – | – | – | 1.942 | 5.550 | – | 0.0 | – |
| $OsTi_2$ | HPX | – | $P4/mmm(123)$ | $P4/mmm(123)$ | – | – | – | 5.96 | 8.44 | 44.7 | 6.66 | 5.97 | 63.4 | 0.005 | 2.918 | – | 0.0 | 0.0 |
| $OsV_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 9.15 | 7.17 | 36.0 | – | – | – | 1.739 | 6.933 | – | 0.0 | – |
| $OsMn_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 8.30 | 5.87 | 45.0 | – | – | – | 1.335 | 12.451 | – | 32.3 | – |
| $OsSe_2$ | TPX | $P2_1/m(11)$ | – | $P2_1/m(11)$ | 6.87 | 7.37 | 57.6 | – | – | – | 7.37 | 6.87 | 57.6 | 0.005 | 3.117 | 0.0 | – | 0.0 |
| $OsBr_2$ | HTX | $P\bar{3}m1(164)$ | $Cm(8)$ | – | 7.70 | 7.70 | 60.0 | 7.15 | 7.16 | 55.5 | – | – | – | 0.714 | 5.472 | 0.0 | 0.0 | – |
| $OsZr_2$ | TPH | $P\bar{1}(2)$ | $P\bar{6}m2(187)$ | $P\bar{1}(2)$ | 8.12 | 8.43 | 49.5 | 7.09 | 7.13 | 61.1 | 9.30 | 8.10 | 43.7 | 0.125 | 0.816 | 0.0 | 0.0 | 0.0 |
| $OsNb_2$ | HTX | $C2/m(12)$ | $Pmmm(47)$ | – | 7.99 | 8.64 | 46.1 | 9.59 | 7.60 | 37.6 | – | – | – | 0.293 | 2.822 | 0.0 | 0.0 | – |
| $OsSb_2$ | TPX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 7.32 | 7.18 | 59.6 | – | – | – | 7.21 | 7.18 | 61.1 | 0.007 | 1.738 | 0.0 | – | 0.0 |
| $OsTe_2$ | TPX | $P2_1/m(11)$ | – | $C2/m(12)$ | 7.80 | 7.32 | 57.8 | – | – | – | 7.79 | 7.32 | 57.6 | 0.221 | 3.032 | 0.0 | – | 0.0 |
| $OsI_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 8.13 | 8.13 | 60.1 | – | – | – | – | – | – | 2.659 | 5.434 | 0.0 | – | – |
| $OsCs_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 12.42 | 9.66 | 40.3 | – | – | – | 5.639 | 5.702 | – | 8.2 | – |
| $OsBa_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 10.04 | 9.05 | 47.4 | 1.409 | 3.666 | – | – | 2.5 |
| $OsHf_2$ | TPX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 7.95 | 8.40 | 50.1 | – | – | – | 7.87 | 8.40 | 50.4 | 0.007 | 0.966 | 0.0 | – | 0.0 |
| $OsPb_2$ | HXX | – | $Pm(6)$ | – | – | – | – | 7.65 | 6.39 | 51.9 | – | – | – | 4.336 | 4.336 | – | 0.0 | – |
| $OsBi_2$ | PTH | $P\bar{1}(2)$ | $Pmm2(25)$ | $P\bar{1}(2)$ | 7.32 | 7.31 | 61.0 | 7.32 | 7.32 | 52.2 | 7.42 | 7.32 | 59.6 | 0.001 | 0.655 | 0.0 | 0.0 | 0.0 |
| $IrBe_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 5.65 | 8.00 | 45.0 | – | – | – | 3.811 | 6.232 | – | 0.0 | – |
| $IrB_2$ | TPX | $Pmmn(59)$ | – | $Pmmn(59)$ | 7.61 | 7.61 | 47.7 | – | – | – | 7.61 | 7.61 | 47.7 | 0.002 | 6.441 | 0.0 | – | 0.0 |
| $IrN_2$ | TPX | $C2/m(12)$ | – | $C2/m(12)$ | 6.08 | 6.12 | 59.9 | – | – | – | 6.12 | 6.09 | 59.9 | 0.001 | 1.903 | 0.0 | – | 0.0 |
| $IrO_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 6.35 | 6.37 | 55.1 | – | – | – | 6.29 | 6.29 | 60.4 | 0.059 | 2.606 | 0.0 | – | 0.0 |
| $IrF_2$ | HTP | $Pmma(51)$ | $Pmmm(47)$ | $Pbcm(57)$ | 6.24 | 6.23 | 62.0 | 8.41 | 6.40 | 39.9 | 9.04 | 7.26 | 36.1 | 0.084 | 0.743 | 0.0 | 0.0 | 0.0 |
| $IrMg_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 9.00 | 6.35 | 44.8 | – | – | – | 3.230 | 10.834 | – | 0.0 | – |
| $IrAl_2$ | THX | $P2_1/m(11)$ | $Pmmm(47)$ | – | 8.48 | 6.52 | 49.5 | 8.80 | 6.84 | 39.0 | – | – | – | 0.307 | 2.068 | 0.0 | 0.0 | – |
| $IrSi_2$ | HTX | $P\bar{1}(2)$ | $Pc(7)$ | – | 8.20 | 7.97 | 51.6 | 8.00 | 6.78 | 42.8 | – | – | – | 0.639 | 1.006 | 0.0 | 0.0 | – |
| $IrP_2$ | TPX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 7.53 | 8.02 | 51.0 | – | – | – | 8.03 | 7.53 | 51.1 | 0.010 | 0.974 | 0.0 | – | 0.0 |
| $IrS_2$ | TXX | $P\bar{1}(2)$ | – | – | 7.16 | 7.23 | 53.7 | – | – | – | – | – | – | 2.809 | 3.443 | 0.0 | – | – |
| $IrCa_2$ | PHX | – | $P4/mmm(123)$ | $P2_1/m(11)$ | – | – | – | 6.95 | 9.83 | 45.0 | 8.85 | 7.32 | 52.8 | 0.250 | 2.053 | – | 0.0 | 0.0 |
| $IrSc_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.97 | 7.96 | 59.7 | – | – | – | 7.93 | 7.93 | 60.0 | 0.002 | 1.432 | 0.0 | – | 0.0 |
| $IrTi_2$ | HXX | – | $P2/m(10)$ | – | – | – | – | 8.77 | 6.56 | 40.4 | – | – | – | 2.498 | 2.506 | – | 6.4 | – |
| $IrGe_2$ | HXX | – | $Aem2(39)$ | – | – | – | – | 7.04 | 7.04 | 47.0 | – | – | – | 1.108 | 1.459 | – | 0.0 | – |
| $IrSe_2$ | TXX | $P\bar{1}(2)$ | – | – | 7.46 | 7.54 | 53.3 | – | – | – | – | – | – | 2.084 | 3.579 | 0.0 | – | – |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $IrBr_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 7.41 | 9.03 | 52.7 | – | – | – | 1.219 | 1.663 | – | 0.0 | – |
| $IrSr_2$ | HTX | $P\bar{3}m1(164)$ | $P4/mmm(123)$ | – | 8.93 | 8.95 | 59.5 | 7.46 | 10.57 | 44.9 | – | – | – | 0.362 | 1.981 | 0.0 | 0.0 | – |
| $IrY_2$ | PTX | $P\bar{3}m1(164)$ | – | $C2/m(12)$ | 8.37 | 8.37 | 59.6 | – | – | – | 7.75 | 9.08 | 50.1 | 0.156 | 2.223 | 0.0 | – | 0.0 |
| $IrZr_2$ | HTP | $P\bar{3}m1(164)$ | $P4/mmm(123)$ | $P\bar{3}m1(164)$ | 8.28 | 8.25 | 60.0 | 8.47 | 5.99 | 45.0 | 8.28 | 8.26 | 59.9 | 0.648 | 0.649 | 0.0 | 0.0 | 0.0 |
| $IrIn_2$ | HPT | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P\bar{3}m1(164)$ | 8.28 | 8.27 | 60.2 | 8.14 | 8.15 | 43.4 | 8.18 | 8.18 | 60.5 | 0.330 | 0.337 | 0.0 | 0.0 | 0.0 |
| $IrSb_2$ | TXX | $P2_1/m(11)$ | – | – | 7.25 | 8.03 | 56.3 | – | – | – | – | – | – | 0.937 | 1.265 | 0.0 | – | – |
| $IrTe_2$ | TXX | $P\bar{1}(2)$ | – | – | 7.96 | 8.03 | 53.1 | – | – | – | – | – | – | 2.618 | 2.666 | 0.0 | – | – |
| $IrI_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 8.10 | 8.10 | 59.8 | – | – | – | – | – | – | 1.852 | 2.785 | 0.0 | – | – |
| $IrBa_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 9.28 | 9.29 | 59.5 | – | – | – | – | – | – | 0.965 | 2.130 | 0.0 | – | – |
| $IrHf_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 6.66 | 8.17 | 52.1 | 1.216 | 1.762 | – | – | 0.0 |
| $IrOs_2$ | HXX | – | $P2/c(13)$ | – | – | – | – | 8.11 | 6.97 | 39.2 | – | – | – | 7.871 | 9.036 | – | 0.0 | – |
| $IrTl_2$ | HPT | $P\bar{3}m1(164)$ | $Pm(6)$ | $P\bar{3}m1(164)$ | 8.66 | 8.63 | 59.2 | 8.32 | 8.40 | 44.5 | 8.57 | 8.55 | 60.0 | 0.682 | 0.691 | 0.0 | 0.0 | 0.0 |
| $IrPb_2$ | TPX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 7.34 | 7.05 | 61.7 | – | – | – | 7.37 | 7.06 | 60.9 | 0.051 | 0.971 | 0.0 | – | 0.0 |
| $PtBe_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 6.41 | 8.39 | 40.2 | – | – | – | 2.567 | 2.855 | – | 0.0 | – |
| $PtB_2$ | TPX | $Cmmm(65)$ | – | $Cmmm(65)$ | 8.01 | 8.01 | 45.8 | – | – | – | 8.01 | 8.01 | 45.8 | 0.008 | 10.620 | 0.0 | – | 0.0 |
| $PtO_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 6.30 | 6.30 | 60.1 | – | – | – | 6.31 | 6.31 | 60.0 | 0.002 | 4.501 | 0.0 | – | 0.0 |
| $PtF_2$ | HXX | – | $Pmmm(47)$ | – | – | – | – | 8.83 | 6.67 | 39.2 | – | – | – | 0.865 | 3.365 | – | 2.4 | – |
| $PtAl_2$ | HXX | – | $C2/m(12)$ | – | – | – | – | 7.62 | 6.51 | 46.1 | – | – | – | 2.256 | 2.423 | – | 0.0 | – |
| $PtSi_2$ | HXX | – | $Pmc2_1(26)$ | – | – | – | – | 7.68 | 9.04 | 31.8 | – | – | – | 1.233 | 1.760 | – | 0.0 | – |
| $PtP_2$ | TPH | $C2/m(12)$ | $Pm(6)$ | $C2/m(12)$ | 7.99 | 7.99 | 53.2 | 7.78 | 7.73 | 51.1 | 7.98 | 7.98 | 53.4 | 0.007 | 0.282 | 0.0 | 0.0 | 0.0 |
| $PtS_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.20 | 7.20 | 60.0 | – | – | – | 7.20 | 7.20 | 60.0 | 0.007 | 2.936 | 0.0 | – | 0.0 |
| $PtCl_2$ | PTH | $P1(1)$ | $Cmmm(65)$ | $Pmna(53)$ | 10.87 | 10.48 | 36.1 | 8.74 | 8.63 | 47.1 | 7.80 | 7.82 | 68.6 | 0.189 | 0.364 | 0.0 | 0.0 | 0.0 |
| $PtK_2$ | TPX | $P\bar{3}m1(164)$ | – | $Pmmn(59)$ | 10.23 | 10.22 | 59.1 | – | – | – | 9.82 | 10.05 | 59.2 | 0.380 | 1.658 | 0.0 | – | 0.0 |
| $PtSc_2$ | PTH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 8.13 | 8.11 | 59.0 | 7.26 | 7.28 | 60.1 | 8.02 | 8.07 | 59.7 | 0.019 | 0.447 | 0.0 | 0.0 | 0.0 |
| $PtTi_2$ | HXX | – | $Pmmm(47)$ | – | – | – | – | 9.50 | 7.72 | 35.7 | – | – | – | 2.145 | 2.147 | – | 0.0 | – |
| $PtV_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 7.51 | 6.20 | 45.1 | 3.050 | 5.944 | – | – | 0.0 |
| $PtGa_2$ | HTX | $P\bar{3}m1(164)$ | $Amm2(38)$ | – | 8.10 | 8.10 | 59.8 | 7.80 | 7.78 | 41.5 | – | – | – | 0.189 | 2.943 | 0.0 | 0.0 | – |
| $PtAs_2$ | TPH | $C2/m(12)$ | $Amm2(38)$ | $C2/m(12)$ | 8.31 | 8.31 | 53.4 | 8.32 | 8.32 | 40.4 | 8.31 | 8.31 | 53.4 | 0.052 | 0.125 | 0.0 | 0.0 | 0.0 |
| $PtSe_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 7.53 | 7.53 | 60.1 | – | – | – | – | – | – | 3.643 | 5.429 | 0.0 | – | – |
| $PtRb_2$ | TPX | $P\bar{3}m1(164)$ | – | $Pmmn(59)$ | 10.62 | 10.61 | 58.8 | – | – | – | 10.24 | 10.23 | 60.6 | 0.306 | 1.460 | 0.0 | – | 0.0 |
| $PtSr_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 9.07 | 9.07 | 59.5 | – | – | – | – | – | – | 2.234 | 5.942 | 0.0 | – | – |
| $PtY_2$ | TPH | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 8.43 | 8.45 | 60.0 | 7.69 | 7.75 | 59.7 | 8.42 | 8.46 | 60.1 | 0.002 | 0.602 | 0.0 | 0.0 | 0.0 |
| $PtZr_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 8.68 | 6.52 | 55.6 | 1.498 | 3.438 | – | – | 0.0 |
| $PtNb_2$ | PHX | – | $P\bar{1}(2)$ | $Cmmm(65)$ | – | – | – | 9.95 | 8.57 | 34.2 | 9.67 | 7.29 | 41.3 | 0.740 | 2.650 | – | 0.0 | 0.0 |
| $PtRu_2$ | THP | $C2/m(12)$ | $Amm2(38)$ | $Pmmn(59)$ | 9.42 | 9.42 | 33.1 | 9.04 | 9.04 | 33.5 | 8.86 | 8.86 | 50.4 | 0.224 | 0.255 | 5.8 | 0.0 | 0.0 |
| $PtRh_2$ | TXX | $C2/m(12)$ | – | – | 9.23 | 9.23 | 33.5 | – | – | – | – | – | – | 1.102 | 3.120 | 0.0 | – | – |
| $PtCd_2$ | HXX | – | $Pmmm(47)$ | – | – | – | – | 9.56 | 7.53 | 37.9 | – | – | – | 2.899 | 2.922 | – | 0.0 | – |
| $PtIn_2$ | HTX | $P\bar{3}m1(164)$ | $Amm2(38)$ | – | 8.56 | 8.53 | 60.2 | 8.10 | 8.10 | 42.5 | – | – | – | 0.408 | 3.977 | 0.0 | 0.0 | – |
| $PtTe_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 8.06 | 8.06 | 60.0 | – | – | – | 8.07 | 8.07 | 59.9 | 0.033 | 3.900 | 0.0 | – | 0.0 |
| $PtI_2$ | THX | $C2/m(12)$ | $Cmmm(65)$ | – | 10.27 | 10.31 | 44.7 | 9.81 | 9.74 | 47.3 | – | – | – | 0.019 | 2.617 | 0.0 | 0.0 | – |
| $PtCs_2$ | THX | $P\bar{3}m1(164)$ | $P\bar{3}m1(164)$ | – | 10.67 | 10.67 | 60.0 | 10.67 | 10.67 | 60.0 | – | – | – | 0.038 | 0.939 | 0.0 | 0.0 | – |
| $PtHf_2$ | TXX | $C2/m(12)$ | – | – | 6.43 | 8.63 | 56.0 | – | – | – | – | – | – | 1.333 | 2.460 | 0.0 | – | – |
| $PtIr_2$ | HTX | $C2/m(12)$ | $Amm2(38)$ | – | 9.25 | 9.25 | 33.1 | 9.09 | 9.10 | 33.2 | – | – | – | 0.235 | 1.098 | 0.0 | 0.0 | – |
| $PtAu_2$ | HXX | – | $C2/m(12)$ | – | – | – | – | 7.88 | 6.77 | 44.4 | – | – | – | 3.958 | 3.996 | – | 0.0 | – |
| $PtHg_2$ | HTX | $P\bar{3}m1(164)$ | $Amm2(38)$ | – | 8.73 | 8.72 | 59.8 | 8.89 | 8.87 | 38.3 | – | – | – | 0.655 | 1.251 | 0.0 | 0.0 | – |
| $PtTl_2$ | PHT | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P2_1/m(11)$ | 8.73 | 8.72 | 58.9 | 8.37 | 8.39 | 43.6 | 8.63 | 8.37 | 58.9 | 0.035 | 0.093 | 0.0 | 0.0 | 0.0 |
| $PtPb_2$ | TPH | $P2_1/m(11)$ | $P\bar{6}(174)$ | $P2_1/m(11)$ | 7.39 | 8.04 | 57.0 | 7.24 | 7.22 | 60.0 | 7.38 | 8.03 | 57.0 | 0.005 | 0.141 | 0.0 | 0.0 | 0.0 |
| $PtBi_2$ | HTP | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P\bar{3}m1(164)$ | 8.76 | 8.68 | 58.8 | 7.10 | 8.60 | 52.6 | 8.70 | 8.64 | 59.6 | 0.545 | 0.554 | 0.0 | 0.0 | 0.0 |
| $AuBe_2$ | PXX | – | – | $P6/mmm(191)$ | – | – | – | – | – | – | 8.17 | 8.16 | 60.0 | 2.167 | 5.488 | – | – | 0.0 |
| $AuB_2$ | TPH | $P2/c(13)$ | $P2/c(13)$ | $P2/c(13)$ | 8.66 | 8.40 | 42.2 | 8.42 | 8.67 | 42.2 | 8.65 | 8.40 | 42.3 | 0.004 | 0.005 | 0.0 | 0.0 | 0.0 |
| $AuO_2$ | PTH | $C2/m(12)$ | $C2/m(12)$ | $P2/m(10)$ | 6.93 | 6.93 | 53.9 | 6.14 | 7.79 | 66.7 | 6.91 | 6.91 | 54.5 | 0.278 | 0.371 | 3.3 | 4.0 | 0.0 |
| $AuNa_2$ | THX | $P2_1/m(11)$ | $Cmmm(65)$ | – | 9.75 | 7.58 | 48.7 | 7.50 | 10.43 | 42.6 | – | – | – | 0.527 | 3.404 | 0.0 | 0.0 | – |
| $AuAl_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 8.87 | 8.88 | 59.9 | – | – | – | 8.88 | 8.88 | 60.0 | 0.008 | 0.908 | 0.0 | – | 0.0 |
| $AuSi_2$ | HXX | – | $Pmma(51)$ | – | – | – | – | 9.64 | 8.43 | 31.2 | – | – | – | 1.789 | 3.293 | – | 0.0 | – |
| $AuP_2$ | TPX | $P2/m(10)$ | – | $C2/m(12)$ | 11.09 | 7.68 | 46.9 | – | – | – | 9.01 | 9.00 | 50.4 | 0.664 | 1.583 | 0.0 | – | 0.0 |
| $AuS_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 10.41 | 7.81 | 62.5 | 1.049 | 1.253 | – | – | 0.0 |
| $AuCl_2$ | THP | $C2/m(12)$ | $Cmmm(65)$ | $P2/m(10)$ | 9.06 | 9.08 | 47.6 | 8.19 | 8.16 | 53.3 | 14.73 | 7.34 | 64.9 | 0.056 | 0.313 | 3.2 | 3.1 | 0.0 |

(Continued on next page)

Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | [eV] | [eV] | T | H | P |
| $AuK_2$ | PTH | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P\bar{1}(2)$ | 9.75 | 9.76 | 59.6 | 10.01 | 10.08 | 50.6 | 9.73 | 11.17 | 51.1 | 0.142 | 0.621 | 0.0 | 0.0 | 0.0 |
| $AuCa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 8.88 | 8.88 | 59.2 | – | – | – | 8.79 | 8.78 | 59.9 | 0.007 | 0.922 | 0.0 | – | 0.0 |
| $AuSc_2$ | HTP | $C2/m(12)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 8.70 | 8.65 | 55.4 | 6.98 | 6.98 | 60.0 | 8.68 | 8.60 | 56.4 | 0.216 | 0.241 | 0.0 | 0.0 | 0.0 |
| $AuCr_2$ | HXX | – | $C2/m(12)$ | – | – | – | – | 8.58 | 7.43 | 42.8 | – | – | – | 3.104 | 3.114 | – | 36.8 | – |
| $AuMn_2$ | TXX | $P\bar{1}(2)$ | – | – | 8.41 | 7.57 | 39.5 | – | – | – | – | – | – | 4.828 | 5.453 | 33.6 | – | – |
| $AuGa_2$ | THX | $C2/m(12)$ | $Amm2(38)$ | – | 8.84 | 8.84 | 35.9 | 8.86 | 8.82 | 35.7 | – | – | – | 0.157 | 0.838 | 0.0 | 0.0 | – |
| $AuGe_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 8.91 | 8.89 | 36.1 | – | – | – | 0.908 | 0.962 | – | 0.0 | – |
| $AuSe_2$ | HPT | $P\bar{3}m1(164)$ | $Pmm2(25)$ | $C2/m(12)$ | 7.62 | 7.61 | 60.0 | 7.83 | 11.25 | 44.2 | 9.54 | 9.89 | 66.3 | 0.426 | 0.545 | 0.0 | 0.0 | 0.0 |
| $AuBr_2$ | THX | $C2/m(12)$ | $Cmmm(65)$ | – | 9.13 | 9.14 | 49.1 | 8.48 | 8.48 | 53.4 | – | – | – | 0.020 | 0.853 | 0.0 | 0.0 | – |
| $AuRb_2$ | THP | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P2_1/m(11)$ | 10.14 | 10.17 | 60.1 | 10.04 | 10.00 | 55.1 | 13.99 | 13.98 | 40.8 | 0.437 | 0.491 | 0.0 | 0.0 | 0.0 |
| $AuSr_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 9.34 | 9.35 | 59.4 | – | – | – | – | – | – | 1.124 | 1.688 | 0.0 | – | – |
| $AuY_2$ | HPT | $C2/m(12)$ | $P\bar{6}m2(187)$ | $C2/m(12)$ | 9.06 | 9.01 | 55.0 | 7.58 | 7.60 | 60.2 | 9.01 | 8.97 | 55.0 | 0.274 | 0.282 | 0.0 | 0.0 | 0.0 |
| $AuPd_2$ | THX | $C2/m(12)$ | $Amm2(38)$ | – | 9.68 | 9.67 | 32.9 | 9.40 | 9.42 | 33.5 | – | – | – | 0.742 | 2.001 | 0.0 | 0.0 | – |
| $AuAg_2$ | PTH | $P6/mmm(191)$ | $Amm2(38)$ | $P6/mmm(191)$ | 9.75 | 9.75 | 59.9 | 9.14 | 9.10 | 35.8 | 9.75 | 9.75 | 59.9 | 0.028 | 0.460 | 0.0 | 0.0 | 0.0 |
| $AuIn_2$ | THX | $P\bar{3}m1(164)$ | $Pmm2(25)$ | – | 7.33 | 7.31 | 61.8 | 7.13 | 7.03 | 51.4 | – | – | – | 0.403 | 1.982 | 0.0 | 0.0 | – |
| $AuSn_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.49 | 8.83 | 42.3 | – | – | – | 2.861 | 2.870 | – | 0.0 | – |
| $AuSb_2$ | HTX | $P\bar{3}m1(164)$ | $Pc(7)$ | – | 8.60 | 8.57 | 59.3 | 9.04 | 9.05 | 44.3 | – | – | – | 0.171 | 1.440 | 0.0 | 0.0 | – |
| $AuTe_2$ | TPX | $P\bar{3}m1(164)$ | – | $P2_1/m(11)$ | 8.11 | 8.10 | 59.9 | – | – | – | 10.47 | 10.47 | 61.3 | 0.024 | 0.917 | 0.0 | – | 0.0 |
| $AuI_2$ | THX | $C2/m(12)$ | $Cmmm(65)$ | – | 9.66 | 9.68 | 48.9 | 9.12 | 9.12 | 52.3 | – | – | – | 0.111 | 0.875 | 0.0 | 0.0 | – |
| $AuCs_2$ | THP | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P\bar{1}(2)$ | 10.73 | 10.72 | 59.6 | 10.62 | 10.69 | 55.1 | 14.80 | 15.03 | 37.9 | 0.621 | 0.654 | 0.0 | 0.0 | 0.0 |
| $AuIr_2$ | PTX | $Pmmn(59)$ | – | $Pmmn(59)$ | 8.35 | 8.87 | 57.9 | – | – | – | 8.38 | 8.37 | 63.9 | 0.161 | 2.445 | 0.0 | – | 0.0 |
| $AuHg_2$ | HTX | $P\bar{3}m1(164)$ | $Amm2(38)$ | – | 9.44 | 9.43 | 58.5 | 9.11 | 9.09 | 36.8 | – | – | – | 0.323 | 0.914 | 0.0 | 0.0 | – |
| $AuPb_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 7.20 | 10.40 | 43.9 | – | – | – | 0.933 | 0.981 | – | 0.0 | – |
| $AuBi_2$ | HPT | $P\bar{3}m1(164)$ | $Amm2(38)$ | $P1(1)$ | 8.89 | 8.88 | 57.7 | 9.23 | 9.23 | 45.5 | 9.27 | 8.77 | 46.1 | 0.112 | 0.325 | 0.0 | 0.0 | 0.0 |
| $HgLi_2$ | HXX | – | $P4/mmm(123)$ | – | – | – | – | 6.66 | 9.44 | 44.7 | – | – | – | 1.596 | 3.332 | – | 0.0 | – |
| $HgBe_2$ | PHT | $P6/mmm(191)$ | $P6/mmm(191)$ | $P6/mmm(191)$ | 8.29 | 8.29 | 60.0 | 8.29 | 8.29 | 60.0 | 8.29 | 8.30 | 59.9 | 0.016 | 0.018 | 0.0 | 0.0 | 0.0 |
| $HgO_2$ | PXX | – | – | $P2/m(10)$ | – | – | – | – | – | – | 9.53 | 7.97 | 59.4 | 2.593 | 4.809 | – | – | 0.0 |
| $HgF_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 7.45 | 7.46 | 59.4 | – | – | – | 7.45 | 7.45 | 59.6 | 0.001 | 1.882 | 0.0 | – | 0.0 |
| $HgP_2$ | PTX | $P2/m(10)$ | – | $P1(1)$ | 12.10 | 8.10 | 46.7 | – | – | – | 9.72 | 9.46 | 58.5 | 0.798 | 3.283 | 0.0 | – | 0.0 |
| $HgCl_2$ | HTX | $P\bar{3}m1(164)$ | $C2/m(12)$ | – | 8.21 | 8.22 | 57.2 | 9.88 | 8.34 | 53.0 | – | – | – | 0.350 | 1.827 | 0.0 | 0.0 | – |
| $HgCa_2$ | THP | $P2_1/m(11)$ | $P\bar{6}m2(187)$ | $P\bar{3}m1(164)$ | 7.78 | 9.09 | 54.1 | 8.01 | 7.99 | 59.8 | 8.14 | 8.10 | 59.8 | 0.167 | 0.272 | 0.0 | 0.0 | 0.0 |
| $HgGe_2$ | PXX | – | – | $P3m1(156)$ | – | – | – | – | – | – | 8.12 | 8.13 | 59.9 | 2.224 | 3.213 | – | – | 0.0 |
| $HgSe_2$ | PHX | – | $C2/m(12)$ | $P1(1)$ | – | – | – | 8.58 | 8.56 | 86.4 | 11.54 | 9.97 | 45.2 | 0.539 | 4.257 | – | 0.0 | 0.0 |
| $HgBr_2$ | THX | $C2/m(12)$ | $C2/m(12)$ | – | 8.49 | 9.57 | 54.9 | 8.43 | 8.41 | 68.4 | – | – | – | 0.079 | 0.926 | 0.0 | 0.0 | – |
| $HgSr_2$ | HPT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P\bar{1}(2)$ | 9.00 | 8.90 | 59.5 | 8.75 | 8.70 | 59.2 | 9.17 | 9.58 | 56.6 | 0.022 | 0.108 | 0.0 | 0.0 | 0.0 |
| $HgAg_2$ | PTX | $P6/mmm(191)$ | – | $P6/mmm(191)$ | 10.01 | 10.02 | 59.7 | – | – | – | 10.01 | 10.01 | 59.7 | 0.055 | 1.936 | 0.0 | – | 0.0 |
| $HgSn_2$ | HPX | – | $Amm2(38)$ | $Pm(6)$ | – | – | – | 9.70 | 9.71 | 38.1 | 9.31 | 9.34 | 59.7 | 0.567 | 1.287 | – | 0.0 | 0.0 |
| $HgI_2$ | HTX | $C2/m(12)$ | $P\bar{4}m2(115)$ | – | 10.21 | 9.10 | 54.9 | 9.01 | 9.02 | 87.1 | – | – | – | 0.295 | 1.328 | 0.0 | 0.0 | – |
| $HgCs_2$ | TXX | $P\bar{3}m1(164)$ | – | – | 11.55 | 11.43 | 57.4 | – | – | – | – | – | – | 1.902 | 3.325 | 0.0 | – | – |
| $HgBa_2$ | PHX | – | $P\bar{6}m2(187)$ | $C2/m(12)$ | – | – | – | 9.26 | 9.17 | 58.8 | 8.96 | 11.04 | 50.6 | 0.760 | 1.059 | – | 0.0 | 0.0 |
| $HgPt_2$ | PTX | $P6mm(183)$ | – | $Pmmn(59)$ | 9.18 | 9.18 | 60.0 | – | – | – | 9.20 | 9.14 | 60.2 | 0.055 | 2.866 | 0.0 | – | 0.0 |
| $HgBi_2$ | TXX | $C2/m(12)$ | – | – | 13.27 | 13.23 | 38.3 | – | – | – | – | – | – | 2.268 | 3.304 | 0.0 | – | – |
| $TlBe_2$ | PTH | $P6/mmm(191)$ | $P6/mmm(191)$ | $P6/mmm(191)$ | 8.40 | 8.40 | 60.0 | 8.39 | 8.39 | 60.0 | 8.40 | 8.40 | 59.9 | 0.005 | 0.006 | 0.0 | 0.0 | 0.0 |
| $TlN_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 11.28 | 9.45 | 61.4 | 17.897 | 18.774 | – | – | 0.0 |
| $TlNa_2$ | THX | $Pmmm(47)$ | $Pmmm(47)$ | – | 8.95 | 11.56 | 37.8 | 8.91 | 11.53 | 37.9 | – | – | – | 0.024 | 3.001 | 0.0 | 0.0 | – |
| $TlS_2$ | PXX | – | – | $P2(3)$ | – | – | – | – | – | – | 7.82 | 8.95 | 94.4 | 5.582 | 5.834 | – | – | 0.0 |
| $TlCa_2$ | HPX | – | $P4/mmm(123)$ | $C2/m(12)$ | – | – | – | 7.66 | 10.85 | 45.0 | 9.88 | 8.16 | 51.4 | 0.389 | 1.984 | – | 0.0 | 0.0 |
| $TlCr_2$ | HXX | – | $P\bar{1}(2)$ | – | – | – | – | 11.10 | 7.66 | 33.2 | – | – | – | 5.563 | 5.653 | – | 26.6 | – |
| $TlBr_2$ | HPT | $P2/m(10)$ | $P2(3)$ | $P\bar{1}(2)$ | 9.39 | 8.65 | 62.1 | 11.31 | 11.75 | 41.1 | 8.42 | 13.59 | 55.8 | 0.204 | 0.207 | 0.0 | 0.0 | 0.0 |
| $TlSr_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 8.58 | 10.54 | 51.4 | 1.108 | 1.465 | – | – | 0.0 |
| $TlIn_2$ | HPX | – | $Amm2(38)$ | $Cm(8)$ | – | – | – | 6.97 | 6.64 | 58.4 | 6.74 | 7.77 | 64.0 | 0.448 | 4.086 | – | 0.0 | 0.0 |
| $TlI_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{1}(2)$ | 9.18 | 9.17 | 57.7 | – | – | – | 10.73 | 11.54 | 71.8 | 0.527 | 1.204 | 0.0 | – | 0.0 |
| $TlBa_2$ | HPX | – | $P4/mmm(123)$ | $P2_1/m(11)$ | – | – | – | 8.60 | 12.17 | 45.0 | 8.96 | 10.88 | 52.3 | 0.492 | 1.832 | – | 0.0 | 0.0 |
| $TlTl_2$ | HXX | – | $P\bar{6}m2(187)$ | – | – | – | – | 7.10 | 7.09 | 58.7 | – | – | – | 2.866 | 3.135 | – | 0.0 | – |
| $PbBe_2$ | PTX | $P6mm(183)$ | – | $P6mm(183)$ | 8.03 | 8.03 | 60.0 | – | – | – | 8.03 | 8.03 | 60.0 | 0.000 | 6.908 | 0.0 | – | 0.0 |
| $PbN_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 8.61 | 8.11 | 80.3 | 17.363 | 17.365 | – | – | 0.0 |
| $PbO_2$ | TPX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 6.88 | 6.88 | 60.0 | – | – | – | 6.88 | 6.88 | 59.9 | 0.006 | 4.286 | 0.0 | – | 0.0 |

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Table 1: List of stable structures

(Continued from previous page)

| species | Initial structure indices | space group | | | lattice parameters | | | | | | | | | | relative energy | | spin moment [$\mu_B$/unit cell] | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | | T | H | P | T | | | H | | | P | | | | $\Delta E_1$ | $\Delta E_2$ | | | |
| | | | | | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | $a$ [Å] | $b$ [Å] | $\gamma$ [deg] | | | [eV] | [eV] | T | H | P |
| $PbF_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 8.05 | 8.06 | 59.8 | – | – | – | 8.06 | 8.07 | 59.6 | | | 0.013 | 1.893 | 0.0 | – | 0.0 |
| $PbS_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 8.63 | 8.17 | 84.5 | | | 2.214 | 2.219 | – | – | 0.0 |
| $PbCl_2$ | TPX | $P\bar{3}m1(164)$ | – | $Pmmn(59)$ | 8.81 | 8.81 | 59.9 | – | – | – | 8.99 | 8.70 | 58.2 | | | 0.336 | 1.116 | 0.0 | – | 0.0 |
| $PbCa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.26 | 10.26 | 59.7 | – | – | – | 10.22 | 10.21 | 60.0 | | | 0.006 | 2.093 | 0.0 | – | 0.0 |
| $PbSc_2$ | PXX | – | – | $C2/m(12)$ | – | – | – | – | – | – | 8.07 | 6.17 | 67.4 | | | 2.664 | 6.488 | – | – | 0.0 |
| $PbGe_2$ | TXX | $P\bar{1}(2)$ | – | – | 11.49 | 8.02 | 39.4 | – | – | – | – | – | – | | | 0.906 | 3.153 | 0.0 | – | – |
| $PbSe_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 10.24 | 8.22 | 73.1 | | | 1.315 | 3.941 | – | – | 0.0 |
| $PbBr_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 8.95 | 8.94 | 60.2 | – | – | – | 8.94 | 8.94 | 59.9 | | | 0.004 | 0.939 | 0.0 | – | 0.0 |
| $PbRb_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 10.96 | 11.95 | 46.2 | – | – | – | | | 1.818 | 3.099 | – | 0.0 | – |
| $PbSr_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 10.69 | 10.68 | 59.7 | – | – | – | 10.64 | 10.63 | 59.9 | | | 0.004 | 1.946 | 0.0 | – | 0.0 |
| $PbIn_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.90 | 9.90 | 38.4 | – | – | – | | | 1.235 | 1.498 | – | 0.0 | – |
| $PbI_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 9.33 | 9.33 | 59.4 | – | – | – | 9.26 | 9.26 | 60.0 | | | 0.002 | 0.862 | 0.0 | – | 0.0 |
| $PbCs_2$ | HXX | – | $Cmmm(65)$ | – | – | – | – | 10.34 | 13.60 | 40.1 | – | – | – | | | 2.093 | 3.761 | – | 0.0 | – |
| $PbBa_2$ | PTX | $P\bar{3}m1(164)$ | – | $P\bar{3}m1(164)$ | 11.06 | 11.04 | 59.4 | – | – | – | 10.96 | 10.94 | 59.7 | | | 0.007 | 1.629 | 0.0 | – | 0.0 |
| $PbTl_2$ | HXX | – | $P2/m(10)$ | – | – | – | – | 12.44 | 9.42 | 33.2 | – | – | – | | | 2.366 | 3.528 | – | 0.0 | – |
| $BiLi_2$ | THX | $P\bar{1}(2)$ | $Amm2(38)$ | – | 10.13 | 9.04 | 39.2 | 9.50 | 9.45 | 41.8 | – | – | – | | | 0.802 | 2.355 | 0.0 | 0.0 | – |
| $BiBe_2$ | PTX | $P\bar{1}(2)$ | – | $P\bar{1}(2)$ | 5.67 | 7.92 | 66.9 | – | – | – | 5.31 | 8.06 | 53.2 | | | 0.032 | 10.589 | 0.0 | – | 0.0 |
| $BiO_2$ | PXX | – | – | $P1(1)$ | – | – | – | – | – | – | 7.52 | 6.43 | 59.3 | | | 0.895 | 3.859 | – | – | 0.0 |
| $BiAl_2$ | PHT | $P\bar{3}m1(164)$ | $P\bar{6}m2(187)$ | $P6/mmm(191)$ | 8.84 | 8.84 | 59.7 | 8.63 | 8.60 | 58.5 | 10.25 | 10.25 | 62.2 | | | 0.564 | 0.719 | 0.0 | 0.0 | 0.0 |
| $BiSi_2$ | PTX | $P\bar{1}(2)$ | – | $P2_1/m(11)$ | 10.50 | 13.65 | 30.6 | – | – | – | 9.28 | 9.28 | 50.1 | | | 0.606 | 6.198 | 0.0 | – | 0.0 |
| $BiP_2$ | PXX | – | – | $P\bar{1}(2)$ | – | – | – | – | – | – | 9.70 | 7.16 | 67.1 | | | 1.029 | 10.019 | – | – | 0.0 |
| $BiS_2$ | PTX | $P\bar{3}m1(164)$ | – | $P2_1/m(11)$ | 7.87 | 7.86 | 59.6 | – | – | – | 9.95 | 8.55 | 63.7 | | | 0.397 | 2.636 | 0.0 | – | 0.0 |
| $BiCl_2$ | HXX | – | $Pm(6)$ | – | – | – | – | 8.48 | 7.95 | 64.7 | – | – | – | | | 1.887 | 2.316 | – | 0.0 | – |
| $BiK_2$ | HXX | – | $Pmmm(47)$ | – | – | – | – | 9.43 | 9.69 | 58.6 | – | – | – | | | 1.483 | 2.678 | – | 0.0 | – |
| $BiCa_2$ | TPX | $C2/m(12)$ | – | $C2/m(12)$ | 9.52 | 9.42 | 59.6 | – | – | – | 9.41 | 9.44 | 60.7 | | | 0.001 | 1.141 | 0.0 | – | 0.0 |
| $BiSc_2$ | TXX | $P\bar{1}(2)$ | – | – | 8.76 | 8.31 | 62.9 | – | – | – | – | – | – | | | 1.271 | 3.748 | 1.8 | – | – |
| $BiV_2$ | HXX | – | $Pm(6)$ | – | – | – | – | 7.64 | 9.06 | 31.0 | – | – | – | | | 13.294 | 13.298 | – | 0.0 | – |
| $BiGe_2$ | PXX | – | – | $Pc(7)$ | – | – | – | – | – | – | 10.82 | 7.27 | 47.6 | | | 1.002 | 2.791 | – | – | 0.0 |
| $BiSe_2$ | PXX | – | – | $Cm(8)$ | – | – | – | – | – | – | 8.04 | 9.24 | 64.0 | | | 0.884 | 2.750 | – | – | 0.0 |
| $BiBr_2$ | HXX | – | $Pm(6)$ | – | – | – | – | 8.66 | 9.05 | 54.8 | – | – | – | | | 1.745 | 2.808 | – | 0.0 | – |
| $BiRb_2$ | HXX | – | $Pmmm(47)$ | – | – | – | – | 9.89 | 12.97 | 39.9 | – | – | – | | | 1.454 | 2.790 | – | 0.0 | – |
| $BiSr_2$ | TPX | $C2/m(12)$ | – | $P\bar{1}(2)$ | 10.03 | 9.93 | 59.8 | – | – | – | 9.92 | 10.01 | 59.9 | | | 0.009 | 1.115 | 0.0 | – | 0.0 |
| $BiY_2$ | TPX | $P2_1/m(11)$ | – | $Cm(8)$ | 9.36 | 8.46 | 63.0 | – | – | – | 9.48 | 8.47 | 55.8 | | | 0.565 | 1.703 | 0.0 | – | 1.7 |
| $BiIn_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.32 | 9.28 | 42.6 | – | – | – | | | 1.375 | 2.254 | – | 0.0 | – |
| $BiTe_2$ | THX | $P\bar{3}m1(164)$ | $P1(1)$ | – | 8.59 | 8.59 | 56.1 | 9.56 | 10.21 | 51.3 | – | – | – | | | 0.370 | 0.993 | 0.0 | 0.0 | – |
| $BiI_2$ | HXX | – | $Pm(6)$ | – | – | – | – | 9.05 | 8.79 | 62.4 | – | – | – | | | 0.896 | 1.507 | – | 0.0 | – |
| $BiCs_2$ | HXX | – | $Pm(6)$ | – | – | – | – | 11.35 | 12.72 | 42.6 | – | – | – | | | 1.364 | 2.997 | – | 0.0 | – |
| $BiBa_2$ | TPX | $P\bar{3}m1(164)$ | – | $P2_1/m(11)$ | 10.20 | 10.20 | 59.7 | – | – | – | 10.36 | 10.18 | 60.7 | | | 0.022 | 1.152 | 0.0 | – | 0.0 |
| $BiRe_2$ | HXX | – | $Aem2(39)$ | – | – | – | – | 10.43 | 10.45 | 23.7 | – | – | – | | | 5.278 | 16.490 | – | 0.0 | – |
| $BiHg_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 10.97 | 10.95 | 33.0 | – | – | – | | | 0.957 | 1.721 | – | 0.0 | – |
| $BiTl_2$ | HXX | – | $Amm2(38)$ | – | – | – | – | 9.88 | 9.86 | 41.5 | – | – | – | | | 1.495 | 1.525 | – | 0.0 | – |
| $BiPb_2$ | THP | $P\bar{1}(2)$ | $Pmn2_1(31)$ | $P1(1)$ | 11.60 | 12.02 | 33.3 | 9.73 | 9.74 | 53.9 | 10.41 | 9.97 | 50.7 | | | 0.090 | 0.223 | 0.0 | 0.0 | 0.0 |
| $BiBi_2$ | TPX | $P\bar{1}(2)$ | – | $P1(1)$ | 8.12 | 12.03 | 72.0 | – | – | – | 8.98 | 12.04 | 56.4 | | | 0.133 | 2.147 | 0.0 | – | 0.0 |