# GBRV14/QE

GBRV 1.4 USPP dataset / Quantum ESPRESSO 5.1

`name and version of the code:` Quantum ESPRESSO 5.1
`type of basis set:` plane waves
`method:` ultrasoft pseudopotentials (GBRV 1.4)

## GENERAL INFORMATION

| | |
|---|---|
| `exchange-correlation functional` | PBE |
| `relativistic scheme` | core and valence scalar relativistic (Koelling-Harmon) |
| `assignment of core / valence states` | see table ($Z_{val}$) |
| `basis set size` | wave function cutoff = 100 Ry |
| `k-mesh density` | see table (k-point mesh in the full 1st Brillouin zone of the conventional cell *kpts*, and number of irreducible k-points # *k*) |
| `reciprocal-space integration method` | Gaussian smearing with a fictitious temperature corresponding to 0.01 eV |

## METHOD-SPECIFIC INFORMATION

| | |
|---|---|
| `wave function cutoff` | 100 Ry |
| `density cutoff` | 400 Ry |

## ADDITIONAL COMMENTS

none

## REFERENCES

`potentials`


[1] http://www.physics.rutgers.edu/gbrv/
[2] K. F. Garrity, J. W. Bennett, K. M. Rabe and D. Vanderbilt, *Comput. Mater. Sci.* **81** 446–452 (2014).


`code`


[3] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari and R. M. Wentzcovitch, *J. Phys.: Condens. Matter* **21**, 395502 (2009).


`scalar relativity`


[4] D. D. Koelling and B. N. Harmon, *J. Phys. C: Solid State* **10**, 3107–3114 (1977).

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**Table I.** Calculation settings and results per element: valence $Z_{val}$, k-point mesh in the full 1st Brillouin zone of the conventional cell *kpts* and number of irreducible k-points # $k$, equilibrium volume per atom $V_0$, bulk modulus $B_0$, pressure derivative of the bulk modulus $B_1$.

| | $Z_{val}$ [–] | *kpts* [–] | # $k$ [–] | $V_0$ [Å$^3$/atom] | $B_0$ [GPa] | $B_1$ [–] |
|---|---|---|---|---|---|---|
| H | 1 | 28×28×20 | 6 020 | 18.177 | 10.368 | 2.832 |
| He | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Li | 3 | 38×38×38 | 27 436 | 20.224 | 13.84 | 3.346 |
| Be | 4 | 52×52×28 | 9 828 | 7.941 | 123.371 | 3.327 |
| B | 3 | 26×26×24 | 12 324 | 7.225 | 236.568 | 3.453 |
| C | 4 | 48×48×12 | 10 512 | 11.633 | 208.087 | 3.563 |
| N | 5 | 16×16×16 | 688 | 29.263 | 54.732 | 3.840 |
| O | 6 | 26×24×24 | 7 488 | 18.780 | 50.921 | 4.100 |
| F | 7 | 16×28×14 | 3 136 | 19.357 | 34.093 | 4.107 |
| Ne | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Na | 9 | 32×32×32 | 16 384 | 37.106 | 7.737 | 3.674 |
| Mg | 10 | 36×36×20 | 9 900 | 22.930 | 36.062 | 4.018 |
| Al | 3 | 24×24×24 | 364 | 16.489 | 77.513 | 4.990 |
| Si | 4 | 32×32×32 | 8 448 | 20.433 | 88.607 | 4.311 |
| P | 5 | 30×8×22 | 1 320 | 21.724 | 67.181 | 4.332 |
| S | 6 | 38×38×38 | 27 436 | 17.189 | 84.045 | 4.071 |
| Cl | 7 | 12×24×12 | 864 | 38.770 | 19.005 | 4.381 |
| Ar | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| K | 9 | 20×20×20 | 220 | 73.686 | 3.588 | 3.776 |
| Ca | 10 | 18×18×18 | 165 | 42.221 | 17.638 | 3.375 |
| Sc | 11 | 34×34×20 | 8 840 | 24.607 | 54.578 | 3.384 |
| Ti | 12 | 40×40×22 | 4 620 | 17.386 | 112.115 | 3.602 |
| V | 13 | 34×34×34 | 969 | 13.438 | 182.370 | 3.899 |
| Cr | 14 | 36×36×36 | 2 280 | 11.862 | 172.279 | 7.128 |
| Mn | 15 | 28×28×28 | 5 488 | 11.681 | 122.189 | −0.026 |
| Fe | 16 | 36×36×36 | 2 280 | 11.436 | 175.772 | 7.489 |
| Co | 17 | 46×46×24 | 13 248 | 10.862 | 213.021 | 5.032 |
| Ni | 18 | 28×28×28 | 1 120 | 10.889 | 198.741 | 4.695 |
| Cu | 19 | 28×28×28 | 560 | 11.991 | 141.011 | 5.032 |
| Zn | 20 | 44×44×20 | 14 740 | 15.213 | 74.869 | 5.314 |
| Ga | 19 | 22×12×22 | 1 452 | 20.337 | 48.984 | 5.466 |
| Ge | 14 | 30×30×30 | 6 975 | 23.875 | 59.266 | 4.878 |
| As | 5 | 30×30×10 | 6 825 | 22.700 | 68.757 | 4.327 |
| Se | 6 | 26×26×20 | 3 510 | 29.737 | 47.300 | 4.489 |
| Br | 7 | 12×24×12 | 864 | 39.605 | 22.381 | 4.877 |
| Kr | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Rb | 9 | 18×18×18 | 165 | 91.037 | 2.792 | 3.739 |
| Sr | 10 | 16×16×16 | 120 | 54.502 | 11.235 | 5.218 |
| Y | 11 | 32×32×18 | 2 448 | 32.849 | 41.359 | 3.157 |
| Zr | 12 | 36×36×20 | 9 900 | 23.383 | 93.885 | 3.269 |
| Nb | 13 | 30×30×30 | 680 | 18.106 | 170.280 | 3.693 |
| Mo | 14 | 32×32×32 | 816 | 15.767 | 260.081 | 4.328 |
| Tc | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Ru | 16 | 42×42×24 | 5 544 | 13.743 | 313.054 | 4.877 |
| Rh | 15 | 26×26×26 | 455 | 14.073 | 258.078 | 5.212 |
| Pd | 16 | 26×26×26 | 455 | 15.365 | 169.929 | 5.513 |
| Ag | 19 | 24×24×24 | 364 | 17.869 | 91.355 | 6.057 |
| Cd | 12 | 38×38×18 | 9 918 | 22.917 | 44.215 | 7.064 |

| | | | | | | |
|---|---|---|---|---|---|---|
| In | 13 | 30×30×20 | 1 200 | 27.518 | 35.898 | 5.040 |
| Sn | 14 | 26×26×26 | 4 563 | 36.765 | 35.918 | 4.934 |
| Sb | 15 | 26×26×8 | 4 108 | 31.776 | 50.444 | 4.548 |
| Te | 6 | 26×26×16 | 8 216 | 34.930 | 45.254 | 4.739 |
| I | 7 | 12×22×10 | 660 | 50.205 | 18.711 | 5.073 |
| Xe | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Cs | 9 | 16×16×16 | 120 | 116.906 | 1.965 | 3.608 |
| Ba | 10 | 20×20×20 | 220 | 63.381 | 8.793 | 2.131 |
| Lu | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Hf | 12 | 36×36×20 | 3 420 | 22.596 | 107.949 | 3.329 |
| Ta | 13 | 30×30×30 | 680 | 18.273 | 195.688 | 3.569 |
| W | 14 | 32×32×32 | 816 | 16.146 | 304.758 | 4.203 |
| Re | 15 | 42×42×22 | 5 082 | 14.951 | 365.321 | 4.435 |
| Os | 16 | 42×42×24 | 5 544 | 14.264 | 398.853 | 4.817 |
| Ir | 15 | 26×26×26 | 455 | 14.500 | 347.418 | 5.131 |
| Pt | 16 | 26×26×26 | 455 | 15.602 | 250.194 | 5.475 |
| Au | 11 | 24×24×24 | 364 | 17.924 | 140.123 | 5.999 |
| Hg | 12 | 24×24×28 | 1 092 | 29.717 | 7.677 | 10.066 |
| Tl | 13 | 32×32×18 | 7 056 | 31.406 | 26.756 | 5.451 |
| Pb | 14 | 20×20×20 | 220 | 31.869 | 40.031 | 5.574 |
| Bi | 15 | 26×26×8 | 4 108 | 36.820 | 42.741 | 4.649 |
| Po | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |
| Rn | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* | *N/A* |