

# ONCVSP (SG15) 2/CASTEP

SG15 ONCVSP 2015-05-20 NCPP dataset / CASTEP 9.0

name and version of the code: CASTEP 9.0 (Hg revision 6666 Jun 05 2015)

type of basis set: plane waves

method: norm-conserving pseudopotentials (Schlipf-Gygi ONCVSP 2015-05-20)

## GENERAL INFORMATION

exchange-correlation functional	PBE
relativistic scheme	core and valence scalar relativistic (Koelling-Harmon)
assignment of core / valence states	see table
basis set size	cutoff energy = 952 eV
k-mesh density	see table for grid values and number of k-points in the irreducible wedge of the 1st Brillouin zone (# $k$ ); this choice achieves spacing $\Delta k <$ $0.0754 \text{ \AA}^{-1}$
reciprocal-space integration method	Gaussian smearing with a fictitious temperature corresponding to 0.2 eV

## METHOD-SPECIFIC INFORMATION

size of FFT grid for augmentation	N/A
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## ADDITIONAL COMMENTS

Basis set, “fine” FFT grid,  $k$ -point density and plane-wave cutoff were chosen uniformly across the periodic table to achieve high convergence. Less stringent criteria, determined individually per element will still give high convergence in almost all cases at substantially reduced computational cost.

## REFERENCES

### potentials

- [1] D. R. Hamann, *Phys. Rev. B* **88**, 085117 (2013).
- [2] M. Schlipf and F. Gygi, *Comput. Phys. Commun.* (2015). doi: 10.1016/j.cpc.2015.05.011

### code

- [3] S. J. Clark, M. D. Segall, C. J. Pickard, P. J. Hasnip, M. I. J. Probert, K. Refson and M. C. Payne, *Z. Kristall.*, **220**, 567–570 (2005).

### 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, Monkhorst-Pack 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  $B_1$ .

	Valence	$kpts$	$\# k$	$V_0$ [ $\text{\AA}^3/\text{atom}$ ]	$B_0$ [GPa]	$B_1$ [-]
H	$1s^1$	$24 \times 24 \times 17$	1404	17.357	10.297	2.691
He	$1s^2$	$33 \times 33 \times 18$	972	17.711	0.882	6.404
Li	$1s^2 2s^1$	$31 \times 31 \times 4$	352	20.264	13.798	3.366
Be	$1s^2 2s^2$	$42 \times 42 \times 23$	5544	7.933	124.158	3.309
B	$2s^2 2p^1$	$21 \times 21 \times 20$	2310	7.180	235.389	3.405
C	$2s^2 2p^2$	$39 \times 39 \times 10$	735	11.587	208.587	3.549
N	$2s^2 2p^3$	$14 \times 14 \times 14$	119	28.777	53.174	3.663
O	$2s^2 2p^4$	$21 \times 20 \times 20$	2100	18.607	50.062	3.649
F	$2s^2 2p^5$	$14 \times 23 \times 12$	1008	19.281	33.791	4.081
Ne	$2s^2 2p^6$	$18 \times 18 \times 18$	165	24.271	1.344	7.261
Na	$2s^2 2p^6 3s^1$	$26 \times 26 \times 3$	533	37.174	7.739	3.684
Mg	$2s^2 2p^6 3s^2$	$30 \times 30 \times 16$	1920	22.973	36.398	4.344
Al	$2s^2 2p^6 3s^2 3p^1$	$21 \times 21 \times 21$	286	16.542	77.143	4.264
Si	$3s^2 3p^2$	$26 \times 26 \times 26$	1638	20.543	87.433	4.265
P	$3s^2 3p^3$	$25 \times 8 \times 18$	468	21.476	67.780	4.314
S	$3s^2 3p^4$	$32 \times 32 \times 32$	2992	17.285	86.250	3.916
Cl	$3s^2 3p^5$	$11 \times 19 \times 10$	300	39.340	18.699	4.364
Ar	$3s^2 3p^6$	$14 \times 14 \times 14$	84	52.471	0.755	7.945
K	$3s^2 3p^6 4s^1$	$16 \times 16 \times 16$	120	73.844	3.581	3.133
Ca	$3s^2 3p^6 4s^2$	$15 \times 15 \times 15$	120	42.150	17.405	3.318
Sc	$3s^2 3p^6 3d^1 4s^2$	$29 \times 29 \times 16$	680	24.716	53.956	3.349
Ti	$3s^2 3p^6 3d^2 4s^2$	$33 \times 33 \times 18$	972	17.422	111.583	3.504
V	$3s^2 3p^6 3d^3 4s^2$	$28 \times 28 \times 28$	560	13.489	181.719	3.864
Cr	$3s^2 3p^6 3d^5 4s^1$	$29 \times 29 \times 29$	680	12.430	116.331	6.841
Mn	$3s^2 3p^6 3d^5 4s^2$	$23 \times 23 \times 23$	936	11.912	124.007	3.996
Fe	$3s^2 3p^6 3d^6 4s^2$	$29 \times 29 \times 29$	680	11.463	171.168	8.576
Co	$3s^2 3p^6 3d^7 4s^2$	$38 \times 38 \times 21$	4180	10.932	209.487	4.731
Ni	$3s^2 3p^6 3d^8 4s^2$	$24 \times 24 \times 24$	364	10.960	194.124	4.866
Cu	$3s^2 3p^6 3d^{10} 4s^1$	$23 \times 23 \times 23$	364	11.971	135.520	5.366
Zn	$3s^2 3p^6 3d^{10} 4s^2$	$36 \times 36 \times 17$	3078	15.177	75.431	5.622
Ga	$3d^{10} 4s^2 4p^1$	$18 \times 11 \times 18$	486	20.341	49.091	5.378
Ge	$3d^{10} 4s^2 4p^2$	$25 \times 25 \times 25$	455	23.992	58.657	4.849
As	$4s^2 4p^3$	$25 \times 25 \times 8$	468	22.672	67.892	4.190
Se	$4s^2 4p^4$	$21 \times 21 \times 17$	728	29.806	46.930	4.430
Br	$4s^2 4p^5$	$10 \times 20 \times 10$	250	39.671	22.387	4.837
Kr	$4s^2 4p^6$	$13 \times 13 \times 13$	84	65.975	0.645	7.299
Rb	$4s^2 4p^6 5s^1$	$15 \times 15 \times 15$	120	91.165	2.764	3.769
Sr	$4s^2 4p^6 5s^2$	$14 \times 14 \times 14$	84	54.942	11.778	3.213
Y	$4s^2 4p^6 4d^1 5s^2$	$26 \times 26 \times 15$	1456	32.919	40.516	3.072
Zr	$4s^2 4p^6 4d^2 5s^2$	$30 \times 30 \times 16$	1920	23.400	93.780	3.342
Nb	$4s^2 4p^6 4d^4 5s^1$	$25 \times 25 \times 25$	455	18.166	169.438	3.743
Mo	$4s^2 4p^6 4d^5 5s^1$	$26 \times 26 \times 26$	455	15.784	259.481	4.239
Tc	$4s^2 4p^6 4d^6 5s^1$	$35 \times 35 \times 19$	1200	14.443	297.773	4.491
Ru	$4s^2 4p^6 4d^7 5s^1$	$35 \times 35 \times 20$	1200	13.776	311.240	4.841
Rh	$4s^2 4p^6 4d^8 5s^1$	$22 \times 22 \times 22$	286	14.065	255.184	5.188
Pd	$4s^2 4p^6 4d^{10}$	$21 \times 21 \times 21$	286	15.342	167.685	5.585
Ag	$4s^2 4p^6 4d^{10} 5s^1$	$20 \times 20 \times 20$	220	17.833	90.812	5.848

