JTH01/ABINIT

JTH1 PAW dataset / ABINIT 7.5.3

`name and version of the code:` ABINIT 7.5.3
`type of basis set:` plane waves
`method:` projector-augmented wave (JTH1)

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 = 20 Ha
`k-mesh density`	$6\,750/N$ k-points in the full first Brillouin zone of an N-atom cell
`reciprocal-space integration method`	Fermi-Dirac smearing with a fictitious temperature corresponding to 0.002 Ha

METHOD-SPECIFIC INFORMATION

`PAW radii`	see table (R_{PAW})
`PAW cutoff energy`	20 Ha
`PAW cutoff augmentation energy`	40 Ha
`Partial-wave basis size`	2 elements per ℓ-value except for H, He, Li (one p element) and Ga, Ge, In, K, Kr, Pb and Sn (one d element)

ADDITIONAL COMMENTS

`PAW dataset generator`	ATOMPAW 3.1.0.2

REFERENCES

`PAW dataset`

[1] http://pwpaw.wfu.edu
[2] http://www.abinit.org/downloads/PAW2
[3] F. Jollet, M. Torrent and N. Holzwarth, *Comput. Phys. Commun.* **185**, 1246–1254 (2014).

`code`

[4] X. Gonze, J.-M. Beuken, R. Caracas, F. Detraux, M. Fuchs, G.-M. Rignanese, L. Sindic, M. Verstraete, G. Zerah, F. Jollet, M. Torrent, A. Roy, M. Mikami, Ph. Ghosez, J.-Y. Raty and D. C. Allan, *Comput. Mater. Sci.* **25**, 478–492 (2002).
[5] X. Gonze, B. Amadon, P.-M. Anglade, J.-M. Beuken, F. Bottin, P. Boulanger, F. Bruneval, D. Caliste, R. Caracas, M. Côté, T. Deutsch, L. Genovese, Ph. Ghosez, M. Giantomassi, S. Goedecker, D. R. Hamann, P. Hermet, F. Jollet, G. Jomard, S. Leroux, M. Mancini, S. Mazevet, M. J. T. Oliveira, G. Onida, Y. Pouillon, T. Rangel, G.-M. Rignanese, D. Sangalli, R. Shaltaf, M. Torrent, M. J. Verstraete, G. Zerah and J. W. Zwanziger, *Comput. Phys. Commun.* **180**, 2582–2615 (2009).
[6] M. Torrent, F. Jollet, F. Bottin, G. Zérah, X. Gonze, *Comput. Mater. Sci.* **42**, 337–351, (2008).

`scalar relativity`

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

Table I. Calculation settings and results per element: valence, PAW radius R_{PAW}, equilibrium volume per atom V_0, bulk modulus B_0, pressure derivative of the bulk modulus B_1.

	valence	R_{PAW} [a.u.]	V_0 [Å^3/atom]	B_0 [GPa]	B_1 [–]
H	$1s^1\ 2p^0$	1.0	17.42891	10.28346	3.719
He	$1s^2\ 2p^0$	1.3	17.82441	0.83567	6.413
Li	$1s^2\ 2s^1\ 2p^0$	1.6	20.23673	13.80591	3.344
Be	$1s^2\ 2s^2$	1.3	7.90902	122.23427	2.891
B	$2s^2\ 2p^1$	1.7	7.24585	237.21331	3.487
C	$2s^2\ 2p^2$	1.55	11.66043	213.85783	2.594
N	$2s^2\ 2p^3$	1.2	28.93696	55.05401	2.963
O	$2s^2\ 2p^4$	1.4	18.58836	51.34026	3.880
F	$2s^2\ 2p^5$	1.4	19.29223	35.23528	4.276
Ne	$2s^2\ 2p^6$	1.8	24.23408	1.33457	13.286
Na	$2s^2\ 2p^6\ 3s^1$	1.8	37.11691	7.99425	3.227
Mg	$2s^2\ 2p^6\ 3s^2$	1.9	22.99185	35.65583	4.271
Al	$3s^2\ 3p^1$	1.9	16.47564	77.73267	4.560
Si	$3s^2\ 3p^2$	1.9	20.53424	88.13173	4.364
P	$3s^2\ 3p^3$	1.9	21.57113	67.40838	4.364
S	$3s^2\ 3p^4$	1.9	17.31878	80.58862	3.863
Cl	$3s^2\ 3p^5$	1.8	39.16074	18.46534	4.448
Ar	$3s^2\ 3p^6$	1.8	52.23071	0.74955	6.567
K	$3s^2\ 3p^6\ 4s^1\ 3d^0$	2.1	73.77139	3.62522	3.658
Ca	$3s^2\ 3p^6\ 4s^2\ 3d^0$	1.9	42.13974	17.44360	3.823
Sc	$3s^2\ 3p^6\ 4s^2\ 3d^1$	2.4	24.64343	54.20351	3.356
Ti	$3s^2\ 3p^6\ 4s^1\ 3d^3$	2.3	17.43943	111.33248	3.582
V	$3s^2\ 3p^6\ 4s^2\ 3d^3$	2.2	13.50749	180.77544	3.818
Cr	$3s^2\ 3p^6\ 4s^1\ 3d^5$	2.1	11.89846	174.61933	6.518
Mn	$3s^2\ 3p^6\ 4s^1\ 3d^6$	2.1	11.58353	110.57780	2.073
Fe	$3s^2\ 3p^6\ 4s^1\ 3d^7$	2.1	11.46507	185.27502	4.325
Co	$3s^2\ 3p^6\ 4s^1\ 3d^8$	2.1	10.94555	209.20659	5.147
Ni	$3s^2\ 3p^6\ 4s^2\ 3d^8$	2.1	10.98538	195.04959	4.806
Cu	$3s^2\ 3p^6\ 4s^1\ 3d^{10}$	2.2	12.00941	139.35753	5.169
Zn	$4s^2\ 4p^0\ 3d^{10}$	2.3	15.31269	74.63335	5.868
Ga	$4s^2\ 4p^1\ 3d^{10}$	2.31	20.39324	49.90232	5.286
Ge	$4s^2\ 4p^2\ 3d^{10}$	2.3	24.16805	59.14874	4.895
As	$4s^2\ 4p^3$	2.2	22.55430	68.80630	4.400
Se	$4s^2\ 4p^4$	2.2	29.96519	46.92162	4.420
Br	$4s^2\ 4p^5$	2.2	39.76958	22.16956	4.958
Kr	$4s^2\ 4p^6\ 4d^0$	2.2	65.61745	0.66575	7.041
Rb	$4s^2\ 4p^6\ 5s^1\ 4d^0$	2.3	91.11045	2.75660	3.576
Sr	$4s^2\ 4p^6\ 5s^1\ 4d^1$	2.21	54.63677	11.62676	3.449
Y	$4s^2\ 4p^6\ 5s^2\ 4d^1$	2.21	32.88362	40.84671	3.093
Zr	$4s^2\ 4p^6\ 5s^1\ 4d^3$	2.21	23.39812	93.38537	3.308
Nb	$4s^2\ 4p^6\ 5s^1\ 4d^4$	2.21	18.13594	169.36451	3.672
Mo	$4s^2\ 4p^6\ 5s^1\ 4d^5$	2.2	15.81129	259.30147	4.058
Tc	$4s^2\ 4p^6\ 5s^1\ 4d^6$	2.2	14.46649	301.41262	4.603
Ru	$4s^2\ 4p^6\ 5s^1\ 4d^7$	2.2	13.82013	307.96378	4.297
Rh	$4s^2\ 4p^6\ 5s^1\ 4d^8$	2.4	14.08022	261.48262	5.066
Pd	$4s^2\ 4p^6\ 5s^1\ 4d^9$	2.5	15.32170	166.63735	5.830
Ag	$5s^1\ 5p^0\ 4d^{10}$	2.5	17.82260	91.32391	5.846
Cd	$5s^2\ 5p^0\ 4d^{9.5}$	2.5	22.76797	44.17371	6.759
In	$5s^2\ 5p^1\ 5d^0$	2.9	27.56282	36.88450	5.224

Sn	$5s^2\ 5p^2\ 5d^0$	2.7	36.90882	36.05080	4.883
Sb	$5s^2\ 5p^3$	2.3	31.81352	50.68865	4.654
Te	$5s^2\ 5p^4$	2.3	34.97375	45.13662	4.735
I	$5s^2\ 5p^5$	2.3	50.41409	18.72654	5.018
Xe	$5s^2\ 5p^6$	2.4	87.14873	0.53582	4.918
Cs	$5s^2\ 5p^6\ 6s^1\ 5d^0$	2.45	117.82868	2.05877	1.843
Ba	$5s^2\ 5p^6\ 6s^2\ 5d^0$	2.3	63.23845	8.77715	2.243
Lu	$5s^2\ 5p^6\ 6s^2\ 5d^1\ 4f^{14}$	2.5	29.05223	47.68307	3.519
Hf	$5s^2\ 5p^6\ 6s^2\ 5d^2$	2.41	22.54013	107.62002	3.303
Ta	$5s^2\ 5p^6\ 6s^2\ 5d^3$	2.41	18.30301	195.94631	3.794
W	$5s^2\ 5p^6\ 6s^2\ 5d^4$	2.41	16.17507	303.98275	4.152
Re	$5s^2\ 5p^6\ 6s^2\ 5d^5$	2.4	14.98499	364.96449	4.376
Os	$5p^6\ 6s^1\ 5d^7$	2.5	14.32062	425.11571	4.549
Ir	$5p^6\ 6s^1\ 5d^8$	2.5	14.55237	347.21064	5.034
Pt	$6s^1\ 6p^0\ 5d^9$	2.5	15.68200	250.05791	5.560
Au	$6s^1\ 6p^0\ 5d^{10}$	2.5	18.01243	140.30702	5.501
Hg	$6s^2\ 6p^0\ 5d^{10}$	2.4	29.65450	8.84950	12.145
Tl	$6s^2\ 6p^1$	2.9	31.42413	27.78389	5.431
Pb	$6s^2\ 6p^2\ 6d^0$	2.9	32.02008	41.11044	5.147
Bi	$6s^2\ 6p^3$	2.9	36.92694	43.22333	4.717
Po	$6s^2\ 6p^4$	2.9	37.57228	46.07731	4.848
Rn	$6s^2\ 6p^6$	2.3	92.80198	0.61546	8.807