Testing of JTH2 PAW table for ABINIT

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A new version of the JTH table (JTHv0.2, named here JTH2) is now available. It has been tested both against the Δ and Δ_1 factors ([1],[2]) and against the lattice parameter of fcc and bcc structures, following the GBRV testing suite [3].

I. JTH2 PAW TABLE FOR ABINIT

A new version of the JTH table (JTHv0.2, named here JTH2) is now available. It has been generated with the code ATOMPAW (v4.0.0.8) [4]. This new version follows the XML format defined in [5]. Compared with the JTHv0.1 version, some paw radii have been reduced (especially d ones) to take into account the work of Garrity et al. [6]. With these modifications, we obtain a table that gives good results both for the fcc and bcc structures, and for the Δ and Δ_1 factors.

II. PAW ATOMIC DATA VALIDATION AGAINST THE DELTA FACTOR

We have used the delta calculation package (version 3.0 [7]) to validate our new atomic data against the Wien2k code. The electronic structure calculations have been performed thanks to the ABINIT code [8]. For this we have used the recommended values [1] for the k-point sampling (6750/N k-points in the Brillouin zone for a N-atom cell). A Fermi-Dirac broadenning of 0.002 Ha has been used. As indicated in [1], we have used the cystallographic data (CIF's files) provided with the delta calculation package. The Equation of State (EOS) of each element has been adjusted to a Birch-Murnaghan one thanks to seven calculations at seven different volumes, ranging from 0.94 to 1.06 V_S, where V_S is the equilibrium volume deduced from the CIF's file, without geometry optimisation to be exactly in the same conditions as the Wien2k calculations.

The version 3.0 of the delta calculation package gives both the delta factor and the modified delta1 factor proposed by [2]. For the JTH2 table, we obtain the mean values of Δ=0.56 meV and Δ_1=1.32 meV for a 20 Ha cutoff, which are very good results (see [7] for comparison with other PAW data).
The detailed results for each elements are given here:

```
#--------------------
# Delta values of JTH2.txt with respect to WIEN2k.txt (in meV/atom)
# (71 elements of 71 included)
# calculated with calcDelta.py version 3.0
# from left to right: Delta [meV/atom] - relative Delta [%] - Delta1 [meV/atom]
#--------------------
 H  0.249  27.5 4.187
He  0.008  10.8 1.662
Li  0.052   3.7 0.562
Be  0.056   1.1 0.173
 B  0.244   2.8 0.426
 C  1.806  14.5 2.206
 N  0.499   6.2 0.947
 O  0.244   5.1 0.768
```

F	0.139	4.1	0.623
Ne	0.014	7.7	1.227
Na	0.552	37.5	5.748
Mg	0.449	10.7	1.637
Al	0.098	1.5	0.229
Si	0.307	3.3	0.507
P	0.488	6.6	1.003
S	0.304	4.2	0.636
Cl	0.062	1.7	0.252
Ar	0.032	16.0	2.459
K	0.069	5.1	0.778
Ca	0.205	5.5	0.842
Sc	0.023	0.3	0.052
Ti	1.252	12.7	1.930
V	1.688	13.6	2.074
Cr	0.723	6.7	1.024
Mn	0.892	13.6	2.050
Fe	0.557	5.0	0.763
Co	1.235	10.4	1.584
Ni	1.604	14.6	2.230
Cu	0.821	9.5	1.444
Zn	0.092	1.6	0.242
Ga	0.530	10.4	1.594
Ge	0.555	7.7	1.181
As	0.519	6.6	1.005
Se	0.238	3.3	0.510
Br	0.109	2.4	0.369
Kr	0.021	9.3	1.441
Rb	0.288	22.4	3.415
Sr	0.785	24.7	3.772
Y	0.333	4.9	0.737
Zr	0.245	2.2	0.336
Nb	0.198	1.3	0.193
Mo	1.561	7.5	1.144
Tc	1.031	4.7	0.715
Ru	0.344	1.6	0.241
Rh	0.944	5.1	0.781
Pd	1.161	8.9	1.360
Ag	0.325	3.9	0.602
Cd	2.015	38.0	5.886
In	0.839	16.6	2.547
Sn	0.726	10.7	1.638
Sb	0.931	11.4	1.740
Te	0.069	0.9	0.131
I	0.727	15.2	2.319
Xe	0.010	4.2	0.645
Cs	0.115	9.9	1.500
Ba	0.836	29.5	4.488
Lu	0.211	3.1	0.464
Hf	0.192	1.6	0.239
Ta	0.781	4.3	0.656
W	1.362	5.5	0.835
Re	0.885	3.2	0.487
Os	1.049	3.6	0.552

```
Ir  0.568   2.2 0.337
Pt  2.105  10.6 1.616
Au  1.108   8.6 1.323
Hg  0.206  15.4 2.420
Tl  0.261   6.0 0.912
Pb  0.355   5.4 0.824
Bi  0.236   2.9 0.446
Po  0.194   2.2 0.338
Rn  0.033  11.8 1.835
#--------------------
#np.mean  0.560  8.6 1.322
#np.std   0.520  7.9 1.214
#np.max   2.105  38.0 5.886   (Pt, Cd, Cd)
#np.min   0.008  0.3 0.052   (He, Sc, Sc)
#--------------------
```

We have also studied the convergency of the delta factor with the energy cutoff. We have calculated the delta factor for each element for Ecut=10 Ha, 12 Ha, 15 Ha, 17.5 Ha, 20 Ha, 25 Ha and 40 Ha. The following table shows the absolute difference of the Δ_1 factor in meV compared to the converged value at Ecut=40 Ha.

# Ecut	10 Ha	12 Ha	15 Ha	17.5 Ha	20 Ha	25 Ha	40 Ha
H	17.325	15.781	12.047	7.064	3.670	0.291	0.000
He	26.637	75.749	2.172	3.652	1.206	3.253	0.000
Li	1.061	1.086	0.761	0.304	0.271	0.199	0.000
Be	11.198	-0.376	1.525	-0.077	-0.299	-0.116	0.000
B	0.072	1.029	0.986	0.367	0.099	0.040	0.000
C	4.127	0.588	0.513	0.458	0.493	0.002	0.000
N	5.949	15.606	13.675	4.024	0.781	0.098	0.000
O	70.776	31.858	9.273	0.866	0.351	0.282	0.000
F	108.920	12.951	8.662	0.561	0.320	-0.232	0.000
Ne	5.777	10.853	9.952	19.122	-1.171	2.584	0.000
Na	-6.505	7.646	-2.084	0.475	-0.757	-1.092	0.000
Mg	0.062	0.351	0.267	0.355	0.174	0.191	0.000
Al	3.095	1.192	-0.168	-0.210	-0.171	-0.026	0.000
Si	-0.375	-0.277	-0.070	-0.090	-0.026	-0.018	0.000
P	4.953	2.296	-1.333	-1.013	-0.591	-0.044	0.000
S	5.416	4.192	0.911	-0.659	-0.573	-0.047	0.000
Cl	9.561	8.118	2.845	0.196	-0.813	-0.112	0.000
Ar	13.592	7.560	3.548	3.788	1.662	-0.080	0.000
K	4.136	4.020	0.680	-0.046	-0.012	-0.224	0.000
Ca	0.106	0.106	-0.592	-0.291	-0.048	-0.089	0.000
Sc	0.781	0.467	0.109	-0.001	-0.032	-0.022	0.000
Ti	-0.620	0.333	0.003	-0.007	0.014	-0.021	0.000
V	0.335	-0.034	0.008	-0.035	-0.003	-0.027	0.000
Cr	4.227	8.864	5.156	0.205	-3.626	-0.780	0.000
Mn	49.221	1.189	0.293	1.564	-0.026	0.306	0.000
Fe	19.818	-0.151	0.010	-0.193	-0.056	0.209	0.000
Co	30.284	1.326	0.097	1.766	0.939	0.328	0.000
Ni	452.240	39.614	18.881	21.212	-1.858	-0.565	0.000
Cu	12.597	13.509	1.787	2.840	1.095	-0.027	0.000

Zn	43.927	1.891	0.572	0.737	0.214	0.141	0.000
Ga	20.330	3.419	0.402	0.006	0.038	-0.038	0.000
Ge	22.142	4.919	1.008	0.328	0.038	-0.021	0.000
As	0.144	0.559	0.083	0.100	0.016	-0.001	0.000
Se	0.103	1.198	0.129	0.377	0.043	0.007	0.000
Br	-0.335	0.499	-0.234	-0.293	-0.046	0.011	0.000
Kr	0.783	2.318	0.215	0.565	0.242	-0.127	0.000
Rb	1.886	0.008	-0.711	-0.157	-0.178	0.067	0.000
Sr	-0.773	-0.456	0.132	0.100	0.150	0.110	0.000
Y	0.362	1.018	0.079	0.054	-0.076	-0.020	0.000
Zr	3.456	0.270	0.035	0.054	0.164	0.038	0.000
Nb	1.303	0.820	-0.145	-0.173	-0.229	0.016	0.000
Mo	1.004	-0.019	-0.066	0.056	-0.093	0.007	0.000
Tc	1.047	-0.534	-0.229	-0.116	-0.062	-0.011	0.000
Ru	0.298	0.454	-0.056	-0.140	-0.070	0.061	0.000
Rh	1.606	1.432	-0.814	0.293	-0.296	-0.337	0.000
Pd	21.532	14.000	5.090	0.018	0.351	0.295	0.000
Ag	1.357	-0.216	-0.233	-0.195	-0.143	-0.014	0.000
Cd	29.805	-1.707	-0.676	-0.291	0.179	0.029	0.000
In	-0.015	0.006	-0.009	0.009	0.012	-0.002	0.000
Sn	0.066	0.061	0.013	0.014	0.005	-0.004	0.000
Sb	2.467	1.211	0.319	0.169	0.159	0.148	0.000
Te	0.505	0.151	-0.108	-0.033	-0.021	-0.010	0.000
I	0.296	0.046	0.075	0.066	-0.011	0.007	0.000
Xe	3.969	8.409	7.455	4.665	-1.216	1.554	0.000
Cs	5.666	4.324	7.542	-0.026	0.861	0.182	0.000
Ba	2.482	0.390	0.580	-0.424	0.183	0.154	0.000
Lu	8.428	1.500	0.670	0.133	0.051	0.061	0.000
Hf	1.692	0.080	0.053	0.011	0.062	0.019	0.000
Ta	-0.372	1.324	0.141	0.160	0.058	0.004	0.000
W	0.386	0.688	0.379	0.479	0.469	0.073	0.000
Re	1.769	0.692	0.108	0.078	0.245	0.015	0.000
Os	20.535	9.966	0.492	0.166	0.197	-0.098	0.000
Ir	1.566	0.265	0.070	0.247	0.022	0.030	0.000
Pt	18.814	5.866	0.787	0.724	0.343	0.101	0.000
Au	29.222	7.812	1.280	0.992	0.318	0.122	0.000
Hg	122.942	23.485	1.260	0.955	0.292	0.080	0.000
Tl	0.395	0.146	0.042	0.064	0.067	-0.009	0.000
Pb	0.071	0.031	0.015	0.026	0.008	0.003	0.000
Bi	0.106	0.020	0.025	-0.004	0.008	0.005	0.000
Po	0.035	0.056	0.164	-0.054	0.004	0.028	0.000
Rn	2.597	1.358	2.817	1.210	1.222	0.069	0.000

From this table we have calculated recommended values for the cutoff energy:
Low value: abs(Δ_1-$\Delta_1(40Ha)$) < 5 meV
Medium value: abs(Δ_1-$\Delta_1(40Ha)$) < 2 meV
High value: abs(Δ_1-$\Delta_1(40Ha)$) < 1 meV

These values are given here and are inserted inside each PAW data XML file for each element.

```
# Ecut low medium high

 H  20.00  25.00  25.00
He  15.00  25.00  25.00
```

```
Li  10.00  10.00  15.00
Be  12.00  12.00  17.50
 B  10.00  10.00  15.00
 C  10.00  12.00  12.00
 N  17.50  20.00  20.00
 O  17.50  17.50  17.50
 F  17.50  17.50  17.50
Ne  20.00  25.00  25.00
Na  15.00  17.50  25.00
Mg  10.00  10.00  10.00
Al  10.00  12.00  15.00
Si  10.00  10.00  10.00
 P  10.00  15.00  20.00
 S  12.00  15.00  15.00
Cl  15.00  17.50  17.50
Ar  15.00  20.00  25.00
 K  10.00  15.00  15.00
Ca  10.00  10.00  10.00
Sc  10.00  10.00  10.00
Ti  10.00  10.00  10.00
 V  10.00  10.00  10.00
Cr  17.50  25.00  25.00
Mn  12.00  12.00  20.00
Fe  12.00  12.00  12.00
Co  12.00  12.00  20.00
Ni  20.00  20.00  25.00
Cu  15.00  20.00  25.00
Zn  12.00  12.00  15.00
Ga  12.00  15.00  15.00
Ge  12.00  15.00  17.50
As  10.00  10.00  10.00
Se  10.00  10.00  15.00
Br  10.00  10.00  10.00
Kr  10.00  15.00  15.00
Rb  10.00  10.00  12.00
Sr  10.00  10.00  10.00
 Y  10.00  10.00  15.00
Zr  10.00  12.00  12.00
Nb  10.00  10.00  12.00
Mo  10.00  10.00  12.00
Tc  10.00  10.00  12.00
Ru  10.00  10.00  10.00
Rh  10.00  10.00  15.00
Pd  17.50  17.50  17.50
Ag  10.00  10.00  12.00
Cd  12.00  12.00  15.00
In  10.00  10.00  10.00
Sn  10.00  10.00  10.00
Sb  10.00  12.00  15.00
Te  10.00  10.00  10.00
 I  10.00  10.00  10.00
Xe  17.50  20.00  25.00
Cs  17.50  17.50  17.50
Ba  10.00  12.00  12.00
```

```
Lu  12.00  12.00  15.00
Hf  10.00  10.00  12.00
Ta  10.00  10.00  15.00
 W  10.00  10.00  10.00
Re  10.00  10.00  12.00
Os  15.00  15.00  15.00
Ir  10.00  10.00  12.00
Pt  15.00  15.00  15.00
Au  15.00  15.00  17.50
Hg  15.00  15.00  17.50
Tl  10.00  10.00  10.00
Pb  10.00  10.00  10.00
Bi  10.00  10.00  10.00
Po  10.00  10.00  10.00
Rn  10.00  17.50  25.00
#n_low(10)= 42 n_low(12)= 10 n_low(15)=  9 n_low(17.5)=  7 n_low(20)=  3 n_low(25)=  0
#n_med(10)= 33 n_med(12)= 12 n_med(15)= 10 n_med(17.5)=  7 n_med(20)=  5 n_med(25)=  4
#n_high(10)= 19 n_high(12)= 12 n_high(15)= 17 n_high(17.5)=  9 n_high(20)=  5 n_high(25)=  9
```

III. PAW ATOMIC DATA VALIDATION AGAINST FCC AND BCC STRUCTURE

Following [6], we have calculated the lattice parameters for fcc and bcc structures and compare the results to a WIEN2k calculation in the same conditions. The calculations were performed with the ABINIT code with the following input files:
For fcc structures (example for Al):

```
ndtset 7
nsym 0
occopt 3
pawovlp -1
prteig 0
prtden 0
prtcif 1
tsmear 0.001
ecutsm 0.5
ecut 20
pawecutdg 40
chkprim 0
usexcnhat -1
ngkpt 8 8 8
shiftk 0.0 0.0 0.0
chksymbreak 0
paral_kgb 0
nstep 99
toldfe 1.0d-8

getwfk2 -1
getwfk3 -1
getwfk4 -1
getwfk5 -1
getwfk6 -1
getwfk7 -1
```

```
scalecart3 3*0.9932883883792687
scalecart2 3*0.986484829732188
scalecart1 3*0.9795861087155615
scalecart5 3*1.006622709560113
scalecart6 3*1.0131594038201772
scalecart7 3*1.0196128224222163

acell  4.040210000000    4.040210000000    4.040210000000  angstrom
xred 0 0 0
rprim 0.0 0.5 0.5
      0.5 0.0 0.5
      0.5 0.5 0.0
natom 1 typat 1
ntypat 1
znucl  13
nband 8
```

For bcc structures(example for Al):

```
ndtset 7
nsym 0
occopt 3
pawovlp -1
prteig 0
prtden 0
prtcif 1
tsmear 0.001
ecutsm 0.5
ecut 20
pawecutdg 40
chkprim 0
usexcnhat -1
ngkpt 8 8 8
shiftk 0.5 0.5 0.5
chksymbreak 0
paral_kgb 0
nstep 99
toldfe 1.0d-8

getwfk2 -1
getwfk3 -1
getwfk4 -1
getwfk5 -1
getwfk6 -1
getwfk7 -1

scalecart3 3*0.9932883883792687
scalecart2 3*0.986484829732188
scalecart1 3*0.9795861087155615
scalecart5 3*1.006622709560113
scalecart6 3*1.0131594038201772
scalecart7 3*1.0196128224222163
```

```
acell  3.240000000000    3.240000000000    3.240000000000  angstrom
xred 0 0 0
rprim -0.5 0.5 0.5
      0.5 -0.5 0.5
      0.5 0.5 -0.5
natom 1 typat 1
ntypat 1
znucl  13
nband 8
```

A summary of the results is presented Table I. The values for GBRV in ABINIT and the values used for AE reference calculations come from [6].

Test	GBRV-Abinit	JTH2-Abinit
fcc latt. const. (%)	0.13	0.13
bcc latt. const. (%)	0.14	0.14

Table I: Summary of PAW data files testing (RMS errors reltaive to AE calculations)

The detailed results for each element is given on fig.1 for fcc structures and fig.2 for bcc structures. On these figures, the results for noble gases have been set to zero as we have no AE reference calculations. They have not been taken into account for RMS error calculations.

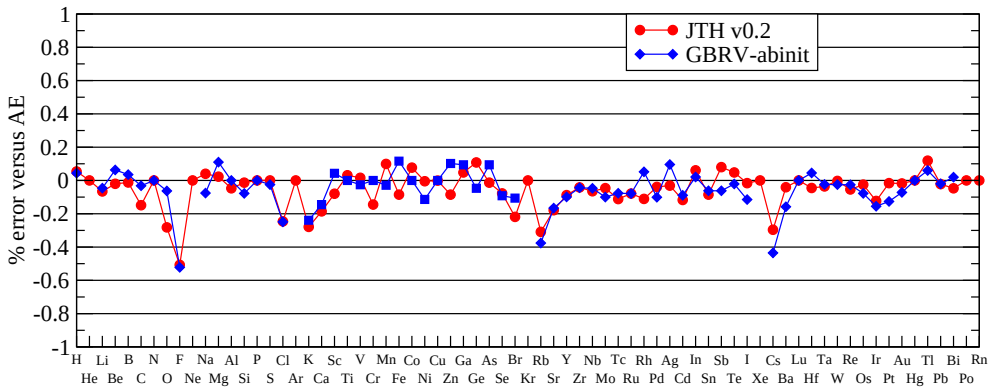

Figure 1: Percent difference in AE versus PAW data calculations for fcc lattice constant

Following [6], we have also calculated magnetic moments of transition metal oxides with non-zero magnetic moments at the AE non-spin polarized lattice constant. The magnetic moments are given in μ_B per primitive cell. The AE results come from [6]. The calculations have been done with a 12x12x12 k-point mesh.

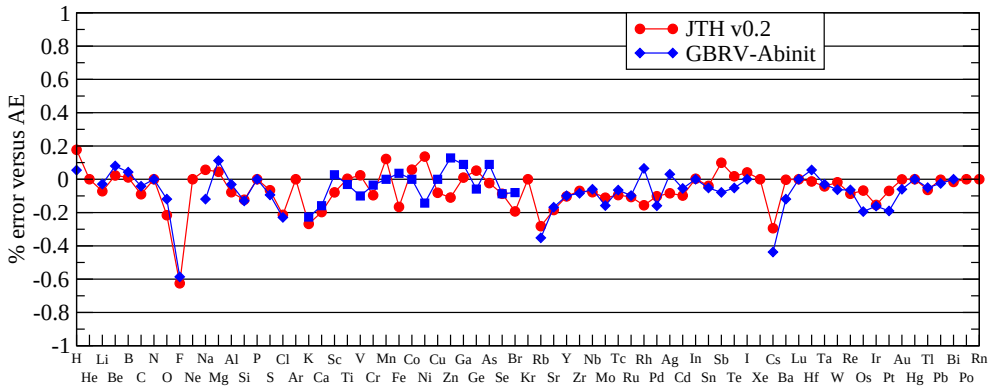

Figure 2: Percent difference in AE versus PAW data calculations for bcc lattice constant

Compound	μ_{AE}	$\mu_{GBRV-Abinit}$	$\mu_{JTH2-Abinit}$
VO	1.32	1.27	1.24
CrO	2.99	3.04	3.05
MnO	3.85	3.84	3.86
FeO	3.83	3.84	3.86
CoO	2.42	2.53	2.56
NiO	1.68	1.47	1.36
MoO	0.54	0.53	0.49
TcO	1.92	1.90	1.95
RuO	1.64	1.63	1.67
OsO	1.56	1.50	1.50
IrO	0.62	0.62	0.75

Table II: Summary of PAW data files testing (RMS errors reltaive to AE calculations)

IV. CONCLUSIONS

The JTH2 table has good accuracy and efficiency compared to other packages makes it a good candidate for high-throughput calculations. This new table is provided as XML files, that makes it easily readable by all the PAW codes. It is distributed on the ABINIT web site [9].

V. ACKNOWLEDGMENTS

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