

*TABLES OF PARAMETERS  
FOR EXTENDED HÜCKEL  
CALCULATIONS*

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## General Observations

References are to the original paper which first reported EH calculations with the given  $H_{ii}$  for a related set of molecules or solids. For some elements, when no EH calculations have been reported, the experimental ionization potentials are given and the references correspond to those experimental values. Although these tables are intended to be of some use in locating atomic parameters, reference to the original work is encouraged.

### Ionization potentials ( $H_{ii}$ )

a) All energies are in eV.  $H_{ii}$ 's for most transition metals are charge-iterated for model compounds like metal carbonyls or typical organometallic molecules with Cp,  $CH_3$ , CO, etc. Exceptions, including bulk metals are conveniently indicated. For cases in which charge-iterated  $H_{ii}$ 's are not available, the standard sources are the Hinze and Jaffé's tables of ionization potentials.<sup>1</sup>

b) When alternative sets of  $H_{ii}$ 's were available for the same element, the one which fits better with the trend along a group or a period of the periodic table has been chosen. If two sets correspond to markedly different environments (e.g., an organometallic molecule and a bulk metal), both sets are displayed in the table.

c) As the ionization energies collected in these tables are of empirical origin, theoretical values are not included for consistency. However, orbital energies calculated for atoms can be useful to check trends along the periodic table and also to find orientative values for the elements missing in these tables. One such collection corresponds to Herman and Skillman,<sup>2</sup> and can also be found in Harrison's table.<sup>3</sup> A comprehensive listing of Dirac-Fock orbital energies was published by Desclaux<sup>4</sup> and can also be found in a paper by Pyykko and Lohr.<sup>5</sup> A particularly useful collection of parameters was obtained by Vela and Gázquez from atomic calculations using density functional theory.<sup>6</sup>

d) *Relativistic* values are averages of the spin-orbital energies from relativistic atomic calculations.<sup>7</sup>

e) More information on  $H_{ii}$ 's and charge iteration parameters can be found in McGlynn et al.<sup>8</sup> and references therein.

The orbital energies adopted here are based in the well-behaved parameters calculated by Vela and Gázquez for those elements for which such energies were reported. No parameters were reported for noble gases, but the standard parameters are seen to represent a good extrapolation for the VG set and are adopted here. Also parameters for

rare earths have been taken from the standard set, if somewhat modified to adapt to the periodic trends. All in all, the new parameter set is not very different from the previously used ones, but is intended to better reproduce the periodic variations in atomic properties. Such parameter set presents also similar trends as orbital energies from other sources, such as Harrison's empirical parameters or the VG ones.

### Trends in s and p Orbital Energies

For any element, the energy order for the valence orbitals is

$$(n-1)d < ns < np$$

The orbital energies show a clear dependence on the atomic number (Fig.), with a practically linear decrease along a period for **ns** and **np** orbitals in main group elements and a similar trend but with a smaller slope for the transition elements and rare earths. Hence, the smallest ionization potential within each period corresponds to the alkaline element and the largest one to the noble gas. Furthermore, the variations are smaller for each row of the periodic table. Such trends are consistent with the relative electronegativity of the elements. In the next Figure we show the  $H_{ii}$ 's as a function of the Pauling electronegativity, that clearly indicates that the nice connection between orbital energies and electronegativity.

It must be noted, however that the parameters adopted here are close to those pertaining to the zero oxidation state according to the charge dependence formula

$$H_{ii} = Aq^2 + Bq + C$$

and do not take into account differences in orbital energies associated to different oxidation states.

For transition metals the energies of ns and np orbitals change little along each transition series. The energies of the (n-1)d orbitals decrease linearly from group 3 to group 12, but fall drastically for group 12 elements. As for the vertical relationships, the orbital energies decrease from the first to the second transition series, but remain practically unaltered from the second to the third transition periods, in excellent agreement with photoelectron spectral data.

For rare earths, the energy of the **(n-1)d** orbitals, deduced from the charge iteration parameters A, B, C, is practically constant.

### Orbital Energies: Trends within a Group

The s and p energies increase from second to third row, then change little, showing the same trend as the Pauling electronegativities.

The s energies show a bump for the 4th row, maybe associated to d shell.<sup>9</sup>

Variations in s-p gap discussed later.

### **Orbital Energies: Trends along a Period**

For s and p orbitals,  $H_{ii}$  decreases linearly down the group. The change is larger for s than for p orbitals. The variation is less pronounced as we move from left to right of the periodic table.

### **Orbital Gaps**

The s/p gap for Main Group elements increase from left to right of the periodic table (similar trend for all rows) and change little down a group for the more electropositive elements (Groups 1, 2, 13, 14). It decreases from period 2 to 3 and from period 4 to 5 for the more electronegative elements (Groups 15, 16, 17).

The s/p gap for transition metals increase from left to right in a row, but less than for main group elements.

The d/s gap for transition metals show an important increase from left to right, probably related to an increased tendency to lower coordination numbers.

That gap shows a dramatic jump for post-transition elements (Group 12), which may have some relationship with the tendency to form M...M contacts.

The Hartree-Fock atomic calculations of Vanquickenborne et al<sup>10</sup> indicate that the 3d-4s gap increases with increasing atomic number, and also with oxidation state, resulting in the largest gap for Cu<sup>2+</sup>.

The theoretical (Vela) and empirical (Alvarez) parameters for alkaline and alkaline earth elements are practically coincident.

The trend for main group elements is the same in the theoretical and standard parameters, with the latter slightly shifted to more negative energies. Large fluctuations around the main trend are observed in the empirical parameters for the heavier elements (Hg - Bi).

By looking at the trend shown by the empirical parameters, a reasonable guess can be given for the ionization potentials of noble gases that were not provided by Vela and Gásquez, by a simple extrapolation.

The general trend in the theoretical parameters within a transition series indicates a weaker dependence on the atomic number than for the main group elements. A similar trend is shown by the empirical parameters, although the energies are lower by about X eV, and some fluctuations can be seen, specially for second and third row transition elements. Such fluctuations are undoubtedly due to the different criteria with which such parameters have been chosen by different authors.

The theoretical parameters for transition elements are practically coincident with those obtained from expression YY (dependencia de  $H_{ii}$  con q) for a zero atomic charge, whereas the empirical ones are midway between these and the ones calculated for  $q = +1$ .

No theoretical values have been reported for lanthanides. The empirically proposed parameters suggest a behavior similar to that of the transition metal elements, consistent with interpolation between the alkaline-earth element and the group 4 element of the corresponding period.

### **Trends in d Orbital Energies**

The trend along a transition series should be consistent with the results of Hartree-Fock calculations reported by Vanquickenborne et al<sup>10</sup> which show a steeper decrease in the energy of the 3d than of the 4s orbitals.

The ionization potentials of the d orbitals in the set of parameters included here increase from the first row to the second row transition metal of the same periodic group, and the difference increases from left to right of the periodic table (Figure). This trend is consistent with the experimental binding energies from photoelectron spectra of organometallic and coordination compounds,<sup>9</sup> as seen in Figure X, where an excellent agreement is found between the difference in binding energies deduced from the EH parameters and the experimentally reported values.

In contrast, the d orbital energies are practically unchanged from the second to the third row transition metal of the same group, both in the EH parameters and in the experimental binding energies.<sup>9</sup> Furthermore, such energy difference remains practically constant when moving from left to right of the periodic table (see Figure).

### **Slater exponents**

The Slater exponent for ns and np orbitals increases from left to right in each row of the periodic table, reaching a maximum (i.e., most contracted orbitals) for the noble gas, as expected from the increasing effective nuclear charge. Currently the p orbitals of P and Cl seem to have a too small exponent (maybe also S and Ar too large) **check**. The s orbital of Rb has a too small exponent, and Sr p orbital a too large one.

a) Slater exponents and coefficients are those used in the quoted paper. When the reference in the table is to experimental ionization potentials, the exponents and coefficients are from standard sources.<sup>11</sup>

b) An alternative basis set for Slater orbitals has been reported by Fitzpatrick and Murphy.<sup>12</sup> Wheeler suggests that this set reproduce better the overlap behavior of the Herman and Skillman's SCF orbitals.<sup>13</sup>

c) Additional sources of Slater exponents, including the original paper from Slater, can be found in the literature.<sup>2,14</sup>

d) Slater exponents for relativistic calculations have been reported by Pyykko *et al.*, both at the single- $\zeta^5$  and double- $\zeta^{15}$  levels.

e) For lanthanides, Slater exponents of Sm or Lu can be used, since the spatial extent of the atomic orbitals change little across the series.

f) Anderson's parameters for alkaline elements,<sup>16</sup> reported for diatomic  $M_2$  molecules, appear to be too diffuse for use in calculations of solid state compounds of the corresponding cations.

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atom	orbital	$H_{ii}$ (eV)	$\zeta_{i1}$	( $c_1$ )	$\zeta_{i2}$	( $c_2$ )	Ref.
<b>Ac</b>	7s	-4.381	1.433				6,82
	7p	-3.098	1.253				
	6d	-6.843	2.120				
<b>Ag</b>	5s	-11.1	2.244				80
	5p	-5.8	2.202				
	4d	-14.5	6.07	(0.5591)	2.663	(0.6048)	
Ag metal	5s	-7.56	2.244				74
	5p	-3.83	2.244				
	4d	-11.58	6.07	(0.5889)	2.663	(0.6370)	
<b>Al</b>	3s	-12.3	1.167				25
	3p	-6.5	1.167				
<b>Am</b>	7s	-4.399	1.462				82
	7p						
	6d	-7.407	2.358				
	5f	-17.178	4.682				
<b>Ar</b>	3s	-27.63	2.585				71
	3p	-15.76	2.255				
<b>As</b>	<b>33</b>	4s	-16.22	2.23			26
		4p	-12.16	1.89			
<b>At</b>	<b>85</b>	6s	-20.827	2.870			82
		6p	-10.337	2.405			
<b>Au</b>	<b>79</b>	6s	-10.92	2.602			27
		6p	-5.55	2.584			
		5d	-15.07	6.163	(0.6851)	2.794	
<b>B</b>	<b>5</b>	2s	-15.2	1.3			25
		2p	-8.5	1.3			
<b>Ba</b>	<b>56</b>	6s	-5.486	2.1			79
		6p	-3.559	2.1			
<b>Be</b>	<b>4</b>	2s	-10.0	0.975			68
		2p	-6.0	0.975			

atom	orbital	$H_{ii}(\text{eV})$	$\zeta_{i1}$	$(c_1)$	$\zeta_{i2}$	$(c_2)$	Ref.
<b>Bh</b>	<b>107</b>	7s	-9.260	2.501			82
		7p	-3.547	1.646			
		6d	-7.863	2.900			
<b>Bi</b>	<b>83</b>	6s	-15.19	2.560			28
		6p	-7.79	2.072			
Bi		6s	-21.20	2.760			77
		6p	-12.60	2.29			
<b>Bk</b>		7s	-4.473	1.486			82
		7p					
		6d	-7.430	2.409			
		5f	-19.858	5.012			
<b>Br</b>		4s	-22.07	2.588			29
		4p	-13.10	2.131			
<b>C</b>		2s	-21.4	1.625			30
		2p	-11.4	1.625			
<b>Ca</b>		4s	-7.0	1.2			31
		4p	-4.0	1.2			
Ca		4s	-6.111	1.2			73
		4p	-4.219	1.2			
		3d	-5.0	4.0 (0.4000)	1.3 (0.7000)		
<b>Cd</b>		5s	-11.8	1.64			32
		5p	-8.2	1.60			
<b>Ce</b>		6s	-4.97	1.799			6
		6p	-4.97				
		5d	-6.43				
<i>relativistic values</i>							
<b>Cf</b>		7s	-4.508	1.498			82
		7p					
		6d	-7.425	2.431			
		5f	-21.163	5.169			
<b>Cl</b>		3s	-26.3	2.183			33
		3p	-14.2	1.733			

atom	orbital	$H_{ii}(\text{eV})$	$\zeta_{i1}$	$(c_1)$	$\zeta_{i2}$	$(c_2)$	Ref.
<b>Cm</b>	7s	-4.712	1.543				82
	7p						
	6d	-7.424	2.385				
	5f	-23.673	5.007				
<b>Co</b>	4s	-9.21	2.0				33
	4p	-5.29	2.0				
	3d	-13.18	5.55	(0.5680)	2.10	(0.6060)	
Co metal	4s	-7.8	2.0				34
	4p	-3.8	2.0				
	3d	-9.7	5.55	(0.5550)	1.90	(0.6678)	
<b>Cr</b>	4s	-8.66	1.7				33
	4p	-5.24	1.7				
	3d	-11.22	4.95	(0.5060)	1.80	(0.6750)	
Cr metal	4s	-7.3	1.70				33
	4p	-3.6	1.70				
	3d	-7.9	4.95	(0.4876)	1.60	(0.7205)	
<b>Cs</b>	6s	-3.88	1.06				29
	6p	-2.49	1.06				
<b>Cu</b>	4s	-11.4	2.2				35
	4p	-6.06	2.2				
	3d	-14.0	5.95	(0.5933)	2.30	(0.5744)	
<b>Db</b>	<b>105</b>	7s	-8.076	2.287			82
		7p	-3.415	1.548			
		6d	-6.090	2.530			
<b>Es</b>	<b>99</b>	7s	-4.542	1.509			82
		7p	-				
		6d	-7.411	2.450			
		5f	-22.450	5.323			
<b>F</b> (F <sub>2</sub> )	<b>9</b>	2s	-40.0	2.425			25
		2p	-18.1	2.425			

atom	orbital	$H_{ii}$ (eV)	$\zeta_{i1}$	$(c_1)$	$\zeta_{i2}$	$(c_2)$	Ref.
<b>Fe</b>	<b>26</b>	4s	-9.10	1.9			33
		4p	-5.32	1.9			
		3d	-12.6	5.35	(0.5505)	2.00	
Fe metal		4s	-7.6	1.90			34
		4p	-3.8	1.90			
		3d	-9.2	5.35	(0.5366)	1.80	
<b>Fm</b>	<b>100</b>	7s	-4.575	1.521			82
		7p					
		6d	-7.388	2.468			
		5f	-23.720	5.473			
<b>Fr</b>	<b>87</b>	7s	-3.209	1.131			82
		7p	-2.205	0.939			
		6d	-1.931	1.258			
<b>Ga</b>	<b>31</b>	4s	-14.58	1.77			36
		4p	-6.75	1.55			
<b>Gd</b>	<b>64</b>	6s	-5.44	1.369			6
		6p	-5.44				
		5d	-6.06				
<i>relativistic values</i>							
<b>Ge</b>	<b>32</b>	4s	-16.0	2.16			37
		4p	-9.0	1.85			
<b>H</b>		1s	-13.6	1.3			30
<b>He</b>		1s	-23.4	1.688			3
<b>Hf</b>		6s	-4.84	1.527			6
		6p	-4.84				
		5d	-6.56				
<i>relativistic values</i>							
<b>Hg</b>	<b>80</b>	6s	-13.68	2.649			38
		6p	-8.47	2.631			
		5d	-17.50	6.436	(0.6438)	3.032	
<b>Hs</b>	<b>108</b>	7s	-9.841	2.603			82
		7p	-3.594	1.688			
		6d	-8.712	3.061			

atom	orbital	$H_{ii}$ (eV)	$\zeta_{i1}$	$(c_1)$	$\zeta_{i2}$	$(c_2)$	Ref.	
<b>I</b>	<b>53</b>	5s	-18.0	2.679			39	
		5p	-12.7	2.322				
<b>In</b>	<b>49</b>	5s	-12.60	1.903			36	
		5p	-6.19	1.677				
<b>Ir</b>	<b>77</b>	6s	-11.36	2.50			40	
		6p	-4.50	2.20				
		5d	-12.17	5.796	(0.6698)	2.557		(0.5860)
<b>K</b>	<b>19</b>	4s	-4.34	0.874			29	
		4p	-2.73	0.874				
<b>Kr</b>	<b>36</b>	4s	-24.36	2.829			71	
		4p	-13.99	2.442				
<b>La</b>		6s	-7.67	2.14			41	
		6p	-5.01	2.08				
		5d	-8.21	3.78	(0.7765)	1.381		(0.4586)
<i>La, relativistic values</i>								
		6s	-4.89				6	
		6p	-4.89					
		5d	-6.41					
<b>Li</b>		2s	-5.4	1.0			75	
		2p	-3.5	1.0				
Li metal		2s	-9.0	0.703			42	
		2p	-8.0	0.703				
<b>Lr</b>	<b>103</b>	7s	-6.738	2.041			82	
		7p						
		6d	-3.985	5.527				
		5f	-19.452	5.527				
<b>Lu</b>		6s	-6.05	1.666			6	
		6p	-6.05	1.666				
		5d	-5.12	2.813	(0.7044)	1.210		(0.4880)
		4f	-22.40	9.136	(0.7330)	3.666		(0.4459)
<i>relativistic values</i>								

atom	orbital	$H_{ii}$ (eV)	$\zeta_{i1}$	( $c_1$ )	$\zeta_{i2}$	( $c_2$ )	Ref.
<b>Lw</b>	7s	-6.74					6
	7p	-6.74					
	6d	-4.11					
<i>relativistic values</i>							
<b>Md</b>	<b>101</b>	7s	-5.622	1.838			82
		7p					
		6d	-4.538	4.261			
		5f	-12.194	5.061			
<b>Mg</b>	<b>12</b>	3s	-9.0	1.1			43
		3p	-4.5	1.1			
<b>Mn</b>	<b>25</b>	4s	-9.75	0.97			44
		4p	-5.89	0.97			
		3d	-11.67	5.15	(0.5139)	1.70	
Mn		4s		1.8			33
		4p		1.8			
		3d		5.15	(0.5320)	1.90	
Mn metal		4s	-7.5	1.80			34
		4p	-3.8	1.80			
		3d	-8.7	5.15	(0.5140)	1.70	
<b>Mo</b>	<b>42</b>	5s	-8.34	1.96			33
		5p	-5.24	1.90			
		4d	-10.50	4.54	(0.6097)	1.90	
<b>Mt</b>	<b>109</b>	7s	-10.427	2.703			82
		7p	-3.633	1.725			
		6d	-9.550	3.211			
<b>N</b>	<b>7</b>	2s	-26.0	1.950			30
		2p	-13.4	1.950			
<b>Na</b> in Na <sub>2</sub>	<b>11</b>	3s	-5.1	0.733			25
		3p	-3.0	0.733			
Na metal		3s	-8.5	0.815			42
		3p	-6.25	0.815			

atom	orbital	$H_{ii}(\text{eV})$	$\zeta_{i1}$	$(c_1)$	$\zeta_{i2}$	$(c_2)$	Ref.
<b>Nb</b>	5s	-10.10	1.89				33
	5p	-6.86	1.85				
	4d	-12.10	4.08	(0.6401)	1.64	(0.5516)	
<b>Ne</b>	2s	-43.20	2.879				3
	2p	-20.00	2.879				
Ne	2s	-40.96	2.879				71
	2p	-21.56	2.879				
<b>Ni</b>	4s	-10.95	2.10				33, 45
	4p	-6.27	2.10				
	3d	-14.2	5.75	(0.5683)	2.30	(0.6292)	
Ni metal	4s	-7.8	2.10				34
	4p	-3.7	2.10				
	3d	-9.9	5.75	(0.5683)	2.00	(0.6292)	
<b>No</b> <b>102</b>	7s	-5.696	1.861				82
	7p						
	6d	-4.127	2.002				
	5f	-12.770	5.200				
<b>Np</b>	7s	-4.583	1.500				6, 82
	7p	-					
	6d	-7.324	2.297				
	5f	-18.928	4.502				
<b>O</b>	2s	-32.3	2.275				30
	2p	-14.8	2.275				
<b>Os</b>	6s	-8.17	2.452				46
	6p	-4.81	2.429				
	5d	-11.84	5.571	(0.6372)	2.416	(0.5598)	
Os	6s	-8.492	"	"	"	"	47
	6p	-3.479					
	5d	-10.946					
<b>P</b>	3s	-18.6	1.75				33
	3p	-14.0	1.30				



atom	orbital	$H_{ii}$ (eV)	$\zeta_{i1}$	( $c_1$ )	$\zeta_{i2}$	( $c_2$ )	Ref.
<b>Pa</b>	7s	-4.489	1.469				82
	7p						
	6d	-7.156	2.220				
	5f	-15.537	4.123				
<b>Pb</b>	6s	-15.7	2.35				48
	6p	-8.0	2.06				
<b>Pd</b>	5s	-7.32	2.19				49
	5p	-3.75	2.152				
	4d	-12.02	5.983	(0.5535)	2.613	(0.6701)	
<i>caution: the exponents used for Pd are probably too contracted.</i>							
<b>Po</b>	6s	-17.96	2.720				5
	6p	-9.05	2.245				
<b>Pr</b>	6s	-7.42	1.40				72
	6p	-4.65	1.40				
	5d	-8.08	2.753	(0.7187)	1.267	(0.4449)	
<b>Pt</b>	6s	-9.077	2.554				33
	6p	-5.475	2.554				
	5d	-12.59	6.013	(0.6334)	2.696	(0.5513)	
<b>Pu</b>	7s	-4.360	1.449				82
	7p						
	6d	-7.374	2.329				
	6f	-15.794	4.507				
<b>Ra</b>	7s	-4.048	1.346				82
	7p	-2.934	1.177				
	6d	-4.108	2.113				
<b>Rb</b>	5s	-4.18	0.997				1
	5p	-2.60	0.997				
<b>Re</b>	6s	-9.36	2.398				50
	6p	-5.96	2.372				
	5d	-12.66	5.343	(0.6662)	2.277	(0.5910)	
<b>Rf</b>	104	7s	-7.443	2.171			82
		7p	-3.320	1.489			
		6d	-5.121	2.297			

atom	orbital	$H_{ii}$ (eV)	$\zeta_{i1}$	( $c_1$ )	$\zeta_{i2}$	( $c_2$ )	Ref.
<b>Rh</b>	<b>45</b>	5s	-8.09	2.135			33
		5p	-4.57	2.10			
		4d	-12.50	4.29	(0.5807)	1.97	
in $ML_4$ chains		5s	-9.01				51
		5p	-4.53				
		4d	-12.73				
<b>Rn</b>	<b>86</b>	6s	-23.783	3.014			82
		6p	-11.647	2.556			
<b>Ru</b>	<b>44</b>	5s	-10.4	2.08			37
		5p	-6.87	2.04			
		4d	-14.90	5.38	(0.5340)	2.30	
Ru in $[Ru(NH_3)_6]^{2+}$							52
		5s	-7.73				
		5p	-4.44				
		4d	-11.23				
<b>S</b>	<b>16</b>	3s	-20.0	2.122			53
		3p	-11.0	1.827			
		[3d	-8.0	1.500]			
<b>Sb</b>		5s	-18.8	2.323			54
		5p	-11.7	1.999			
<b>Sc</b>		4s	-8.87	1.30			55
		4p	-2.75	1.30			
		3d	-8.51	4.35	(0.4228)	1.70	
<b>Se</b>		4s	-20.5	2.44			56
		4p	-14.4	2.07			
	[	4d	-7.0	. ]			57
<b>Sg</b>	<b>106</b>	7s	-8.675	2.397			82
		7p	-3.489	2.726			
		6d	-6.994	2.726			
<b>Si</b>		3s	-17.30	1.383			58
		3p	-9.20	1.383			
		3d	-6.00				
<b>Sm</b>		6s	-4.86	1.400			6
		6p	-4.86	1.400			

atom	orbital	$H_{ii}(\text{eV})$	$\zeta_{i1}$	$(c_1)$	$\zeta_{i2}$	$(c_2)$	Ref.
	5d	-6.06	2.747	(0.7184)	1.267	(0.4447)	
	4f	-11.28	6.907	(0.7354)	2.639	(0.4597)	
<b>Sn</b>	5s	-16.16	2.12				1
	5p	-8.32	1.82				
<b>Sr</b>	5s	-6.62	1.214				1
	5p	-3.92	1.214				
<b>Ta</b>	6s	-10.10	2.28				59
	6p	-6.86	2.241				
	5d	-12.10	4.762	(0.6815)	1.938	(0.6815)	
<b>Tc</b>	5s	-10.07	2.018				60
	5p	-5.40	1.984				
	4d	-12.82	4.90	(0.5715)	2.094	(0.6012)	
<b>Te</b>	5s	-20.8	2.51				61
	5p	-14.8	2.16				
<b>Th</b>	7s	-5.39	1.834				62
	7p	-5.39	1.834				
	6d	-10.11	2.461	(0.7612)	1.165	(0.4071)	
	5f	-9.64	4.477	(0.7682)	1.837	(0.4267)	
	6p	-27.83	3.806				
<b>Ti</b>	4s	-8.97	1.075				63
	4p	-5.44	0.675				
	3d	-10.81	4.55	(0.4206)	1.40	(0.7839)	
Ti metal	4s	-6.3	1.50				34
	4p	-3.2	1.50				
	3d	-5.9	4.55	(0.4206)	1.40	(0.7839)	
<b>Tl</b>	6s	-11.60	2.30				69
	6p	-5.80	1.60				
<b>U</b>	7s	-5.50	1.914				62
	7p	-5.50	1.914				
	6d	-9.19	2.581	(0.7608)	1.207	(0.4126)	
	5f	-10.62	4.943	(0.7844)	2.106	(0.3908)	
	6p	-30.03	4.033				

atom	orbital	$H_{ii}(\text{eV})$	$\zeta_{i1}$	$(c_1)$	$\zeta_{i2}$	$(c_2)$	Ref.
	6d	-5.12					
<b>V</b>	4s	-8.81	1.30				64
	4p	-5.52	1.30				
	3d	-11.0	4.75	(0.4755)	1.70	(0.7052)	
<b>V</b> metal	4s	-6.7	1.60				34
	4p	-3.4	1.60				
	3d	-6.7	4.75	(0.4560)	1.50	(0.7520)	
<b>W</b>	6s	-8.26	2.341				50
	6p	-5.17	2.309				
	5d	-10.37	4.982	(0.6940)	2.068	(0.5631)	
<b>Xe</b>	5s	-21.21	2.844				70, 71
	5p	-12.13	2.485				
<b>Y</b>	5s	-7.02	1.74				76
	5p	-4.40	1.70				
	d	-6.80	1.56	(0.8316)	3.55	(0.3041)	
<b>Yb</b>	6s	-5.35	1.54				65
	6p	-5.35	1.54				
	5d	-5.21	2.810	(0.7063)	1.216	(0.4834)	
	4f	-13.86	8.629	(0.7460)	3.198	(0.4564)	
<b>Zn</b>	4s	-12.41	2.01				66
	4p	-6.53	1.70				
<b>Zn</b>	3d	-17.302	6.15	(0.5900)	2.60	(0.5700)	73
	4s	-9.391	2.01				
	4p	-5.163	1.70				
<b>Zr</b>	5s	-9.87	1.817				67
	5p	-6.76	1.776				
	4d	-11.18	3.835	(0.6210)	1.505	(0.5769)	

atom	orbital	$H_{ii}(\text{eV})$	$\zeta_{i1}$	$(c_1)$	$\zeta_{i2}$	$(c_2)$	Ref.
<b>Rf</b>	7s	-6.75					6
	7p	-6.75					
	6d	-4.11					
<i>relativistic values</i>							

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