Table of experimental and calculated static dipole polarizabilities for the electronic ground states of the neutral elements (in atomic units)

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Table of static (scalar) dipole polarizabilities (in atomic units) for neutral atoms. If not otherwise indicated by the state symmetry, $M_L(M_J)$ - averaged polarizabilities are listed; M_L (M_J) res. denotes that the polarizability for each M_L (M_J) state can be found in the reference given. Abbreviations used: exp.: experimentally determined value (set in bold letters, uncertainties given here consistently as ± values); NR: nonrelativistic; R: Relativistic, DK: Scalar relativistic Douglas-Kroll; MVD: mass-velocity-Darwin; SO: Spin-orbit coupled; SF: Dyall's spin-free formalism (scalar relativistic); PP: relativistic pseudopotential; LDA: local (spin) density approximation; PW91: Perdew-Wang 91 functional; RPA: Random phase approximation; PolPot: Polarization potential; MBPT: many-body perturbation theory; CI: configuration interaction; CCSD(T): coupled cluster singles doubles (SD) with perturbative triples; FS Fock-space; CEPA: coupled electron pair approximation; MR: multi-reference; CAS: complete active space; VPA: variational perturbation approach [1]. For all other abbreviations see text or references. If the symmetry of the state is not clearly specified as in Doolen's calculations, the calculation was most likely set at a specific configuration (orbital occupancy) as listed in the Desclaux tables [2], reflecting the ground state symmetry of the specific atom. Nonrelativistic HF values up to element No have been published by Fraga et al and are not listed here [3]. NB: 1 a.u.=0.14818474 $Å^3$= 1.6487773×10^{-41} C m^2/V.
Remarks: Not all published values are listed, only the most accurate ones. *If you have more accurate polarizability data available, please provide the necessary information with a proper reference*. NB: There is some confusion about the experimental data listed in the *CRC Handbook of Chemistry and Physics* taken from Miller and Bederson. Some of the data are not experimental values as indicated, but from LDA calculations of Doolen, which are listed here as well. Concerning older literature, in 1971 the polarizabilities have been listed up to the element Radon by Teachout and Pack giving 138 references [4]. A more recent review by Mitroy, Safronova and Clark is highly recommended [5]. The present list started in 2006 and the first version was published in Ref.6. The correct citation is therefore ref.6 with the addition: Updated static dipole polarizabilities are available as *pdf* file from the CTCP website at Massey University: http://ctcp.massey.ac.nz/dipole-polarizabilities. If we should provide ionic polarizabilities as well, please let us know.

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Z	Atom	Refs.	State	α_D	comments
1	H	[7]	^{2}S	4.5	NR, exact
		[7,8]	$^2S_{1/2}$	4.49975149589	R, Dirac, variational, Slater basis/B-splines (more digits are given in ref.8)
		[9]	$^2S_{1/2}$	4.49975149518	R, Dirac, Lagrange mesh method (more digits are given in this paper)
		[8,10]	$^2S_{1/2}$	4.50710742367	R, Dirac (as above), but with finite mass correction added for ^{1}H
2	He	[11]	$^1S_0$	1.383191	R, Dirac, Breit-Pauli, QED, mass pol., correlated basis (^{4}He)
		[12]	$^1S_0$	1.38376079(23)	R, Dirac, Breit-Pauli, QED, mass pol., exponentially correlated Slater functions (^{4}He)
		[13]	$^1S_0$	1.3837295330(1)	R, Dirac, Breit, QED, recoil, … (^{4}He)
		[14,15]	$^1S_0$	**1.383746(7)**	***exp***.
3	Li	[16,17]	^{2}S	164.05	NR, exponentially correlated Gaussians [21] + R/DK
		[18]	$^2S_{1/2}$	164.084	R, Dirac, MBPT, Breit, QED, recoil (^{7}Li)
		[19]	$^2S_{1/2}$	164.1125(5)	Hylleraas basis, R(MV+Darwin+Breit), QED, recoil (^{7}Li)
		[20]	$^2S_{1/2}$	**164.0±3.4**	***exp.***
4	Be	[16]	^{1}S	37.755	NR, exponentially correlated Gaussians [21]
		[22]	$^1S_0$	37.80	R, Dirac, coupled cluster
		[23]	$^1S_0$	37.71	R, Dirac, CI+MBPT+ experimental data
5	B	[24]	^{2}P	20.5	NR, PNO-CEPA, M_L res.
		[25]	^{2}P	20.43	NR, CCSD(T), M_L res.
		[26]	^{2}P	20.59	R, SF, MRCI, M_L res.
		[26]	$^2P_{1/2}/^2P_{3/2}$	20.53/20.54	R, Dirac, MRCI, M_J res.
6	C	[27]	^{3}P	11.0	NR, CASPT2, M_L res.
		[25]	^{3}P	11.67	NR, CCSD(T), M_L res.
		[28]	$^3P_0$	11.26	R, Dirac+Gaunt, CCSD(T)
7	N	[24]	^{4}S	7.43	NR, PNO-CEPA
		[29]	^{4}S	7.41	R, DK, CASPT2
		[25]	^{4}S	7.26	NR, CCSD(T)
		[20,30]	$^4S_{3/2}$	**7.6±0.4**	***exp.***

Z	Atom	Refs.	State	α_D	comments
8	O	[24]	^{3}P	6.04	NR, PNO-CEPA, M_L res.
		[27]	^{3}P	6.1	NR, CASPT2, M_L res.
		[25]	^{3}P	5.24	NR, CCSD(T), M_L res.
9	F	[24]	^{2}P	3.76	NR, PNO-CEPA, M_L res.
		[31]	^{2}P	3.76	NR, CASPT2, M_L res.
		[25]	^{2}P	3.70	NR, CCSD(T), M_L res.
10	Ne	[32]	^{1}S	2.68	NR, CCSD(T)
		[33]	^{1}S	2.665	NR, CC3
		[33-35]	^{1}S	2.666	R, CC3+FCI+DK3 correction
		[36]	$^1S_0$	2.6772	R, Dirac-Coulomb, non-linear PRCC
		[37]	$^1S_0$	**2.670±0.005**	***exp***.
11	Na	[38]	$^2S_{1/2}$	162.6	R, SD all orders + exp. data
		[39]	$^2S_{1/2}$	**162.7±0.8**	***exp.***
		[40]	$^2S_{1/2}$	**162.7±0.1/±1.2**	***exp.*** (values in parentheses correspond to statistical and systematic uncertainties resp.)
		[41]	$^2S_{1/2}$	**161±7.5**	***exp.***
12	Mg	[42]	^{1}S	71.7	NR, MBPT4
		[43]	^{1}S	71.8	NR, MBPT4
		[44]	^{1}S	70.9	R, DK, CASPT2
		[22]	$^1S_0$	73.41	R, Dirac, coupled cluster
		[23,45]	$^1S_0$	70.89	R, Dirac, CI+MBPT+ experimental data
		[46]	$^1S_0$	70.76	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[41]	$^1S_0$	**59±16**	***exp.***
13	Al	[47]	^{2}P	56.3	NR, PNO-CEPA
		[48]	^{2}P	62.0	NR, numerical MCSCF, M_L res.
		[49]	^{2}P	57.74	NR, CCSD(T), M_L res.
		[26]	^{2}P	55.5	R, SF, MRCI, M_L res.
		[26]	$^2P_{1/2}/^2P_{3/2}$	55.4/55.9	R, Dirac, MRCI, M_J res.
		[50,51]	$^2P_{1/2}$	**46±2**	***exp.*** (see also ref.41)

Z	Atom	Refs.	State	α_D	comments
14	Si	[47]	^{3}P	36.7	NR, PNO-CEPA, M_L res.
		[27]	^{3}P	36.5	NR, CASPT2, M_L res.
		[52]	^{3}P	37.4	NR, CCSD(T), M_L res.
		[49]	^{3}P	37.17	NR, CCSD(T), M_L res.
		[28]	$^3P_0$	37.31	R, Dirac+Gaunt, CCSD(T)
15	P	[47]	^{4}S	24.7	NR, PNO-CEPA
		[27]	^{4}S	24.6	NR, CASPT2
		[29]	^{4}S	24.9	R, DK, CASPT2
		[49]	^{4}S	24.93	NR, CCSD(T)
16	S	[47]	^{3}P	19.6	NR, PNO-CEPA, M_L res.
		[27]	^{3}P	19.6	NR, CASPT2, M_L res.
		[31]	^{3}P	19.6	NR, CASPT2, M_L res.
		[49]	^{3}P	19.37	NR, CCSD(T), M_L res.
17	Cl	[47]	^{2}P	14.7	NR, PNO-CEPA, M_L res.
		[27]	^{2}P	14.6	NR, CASPT2, M_L res.
		[31]	^{2}P	14.73	NR, CASPT2, M_L res.
		[49]	^{2}P	14.57	NR, CCSD(T), M_L res.
18	Ar	[47]	^{1}S	11.10	NR, PNO-CEPA
		[53]	^{1}S	11.084	NR, CCSD(T)
		[29]	^{1}S	11.1	R, DK, CASPT2
		[35,53]	^{1}S	11.10	R, CCSD(T) + DK3 correction
		[54,55]	$^1S_0$	**11.070(7)**	***exp.***
19	K	[38]	$^2S_{1/2}$	289.1	R, SD all orders, + exp. data for electronic transitions
		[56]	^{2}S	291.1	R, DK, CCSD(T)
		[20]	$^2S_{1/2}$	**293±6**	***exp.***
		[40]	$^2S_{1/2}$	**290.6±1.4**	***exp.*** (for hyperfine effects see ref.57)
		[92]	$^2S_{1/2}$	**289.7(1)(5)**	***exp.***

Z	Atom	Refs.	State	α_D	comments
20	Ca	[58]	$^1S_0$	160	R, CI, MBPT
		[59]	^1S	152.0	R, MVD, CCSD+T
		[44]	^1S	163	R, DK, CASPT2
		[60]	$^1S_0$	158.6	R, DK+SO, CCSD(T)
		[22]	$^1S_0$	154.58	R, Dirac, coupled cluster
		[23,45]	$^1S_0$	155.9	R, Dirac, CI+MBPT+ experimental data
		[46]	$^1S_0$	160.77	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[61,62]	$^1S_0$	**169±17**	***exp.***
21	Sc	[63,64]	$^2D_{3/2}$	120	R, Dirac, LDA
		[65,66]	^2D	107	NR, small CI, VPA
		[67]	^2D	142.28	NR, MCPF
		[41]	$^2D_{3/2}$	**97.2±9.5**	***exp.***
22	Ti	[63]	$^3F_2$	99	R, Dirac, LDA
		[65]	^3F	92	NR, small CI, VPA
		[67]	^3F	114.34	NR, MCPF
		[41]	$^3F_2$	**63.4±3.4**	***exp.***
23	V	[63]	$^4F_{3/2}$	84	R, Dirac, LDA
		[65]	^4F	81	NR, small CI, VPA
		[67]	^4F	97.34	NR, MCPF
		[41]	$^4F_{3/2}$	**68.2±5.4**	***exp.***
24	Cr	[63]	$^7S_3$	78	R, Dirac, LDA
		[67]	^7S	94.72	NR, MCPF
		[68]	^7S	78.4	DK,CASPT2
		[41]	$^7S_3$	**60±24**	***exp.***
25	Mn	[63]	$^6S_{5/2}$	63	R, Dirac, LDA
		[65]	^6S	65	NR, small CI, VPA
		[67]	^6S	75.52	NR, MCPF
		[68]	^6S	66.8	DK,CASPT2

Z	Atom	Refs.	State	α_D	comments
26	Fe	[63]	$^5D_4$	57	R, Dirac, LDA
		[65]	^5D	58	NR, small CI, VPA
		[67]	^5D	63.93	NR, MCPF
		[69]	^5D	62.65	NR, GGA(PW86)
27	Co	[63]	$^4F_{9/2}$	51	R, Dirac, LDA
		[65]	^4F	53	NR, small CI, VPA
		[67]	^4F	57.71	NR, MCPF
28	Ni	[63]	$^3F_4$	46	R, Dirac, LDA
		[65]	^3F	48	NR, small CI, VPA
		[67]	^3F	51.10	NR, MCPF
29	Cu	[67]	^2S	53.44	NR, MCPF
		[70]	^2S	45.0	R, PP, QCISD(T)
		[71]	^2S	46.5	R, DK, CCSD(T)
		[68]	^2S	40.7	R, DK,CASPT2
		[41]	$^2S_{1/2}$	**58.7±4.7**	***exp.***
30	Zn	[72]	^1S	39.2	NR, CCSD(T), MP2 basis correction
		[73]	^1S	38.0	R, PP, CCSD(T)
		[74]	^1S	37.6	R, MVD, CCSD(T)
		[68]	^1S	38.4	R, DK,CASPT2
		[75]	$^1S_0$	38.666	R, Dirac, CCSDT
		[72]	$^1S_0$	**38.8±0.3**	***exp.***
31	Ga	[76]	^2P	54.9	NR, PNO-CEPA, M_L res.
		[26]	^2P	50.7	R, SF, MRCI, M_L res.
		[26]	$^2P_{1/2}/^2P_{3/2}$	49.9/51.6	R, Dirac, MRCI, M_J res.
		[77]	$^2P_{1/2}/^2P_{3/2}$	51.4/53.4	R, Dirac, FSCC, M_J res. (J=3/2: M_J=3/2: 41.9, M_J=1/2: 65.0)
		[41]	$^2P_{1/2}$	**46.6±4.0**	***exp.***
32	Ge	[76]	^3P	41.0	NR, PNO-CEPA, M_L res.
		[28]	^3P	40.16	R, DK, CCSD(T), M_L res. (M_L=0: 32.83, M_L=1: 43.83)
		[28]	$^3P_0$	39.43	R, Dirac_Gaunt, CCSD(T),

Z	Atom	Refs.	State	α_D	comments
33	As	[76]	^4S	29.1	NR, PNO-CEPA
		[29]	^4S	29.8	R, DK, CASPT2
34	Se	[30]	^3P	26.24	R, MVD, CASPT2, M_L res.
35	Br	[78]	$^2P_{1/2}$	21.9	R, DK, SO-CI
		[78]	$^2P_{3/2}$	21.8	R, DK, SO-CI, *M_J res.*
		[31]	^2P	21.03	R, MVD, CASPT2, *M_L res.*
36	Kr	[54]	^1S	16.8	R, DK3, CCSD(T)
		[29]	^1S	16.6	R, DK, CASPT2
		[79]	$^1S_0$	16.012	R, Dirac, CCSD/T
		[80]	$^1S_0$	16.5	R, RPA, PolPot
		[54]	$^1S_0$	**17.075**	***exp.***
37	Rb	[38]	$^2S_{1/2}$	318.6	R, SD all orders + exp. data
		[56]	^2S	316.2	R, DK, CCSD(T)
		[20]	$^2S_{1/2}$	**316(6)**	***exp.***
		[40]	$^2S_{1/2}$	**318.8±1.4**	***exp.***
		[92]	$^2S_{1/2}$	**319.8(2)(5)**	***exp.***
38	Sr	[58]	^1S	199	R, CI, MBPT
		[60]	$^1S_0$	199.4	R, DK+SO, CCSD(T)
		[22]	$^1S_0$	199.71	R, Dirac, coupled cluster
		[45,81]	$^1S_0$	197.2(3.6)	R, Dirac, CI+MBPT+ experimental data
		[82]	$^1S_0$	197.6	CI+ core polarization (corrected to exp. term energies)
		[46]	$^1S_0$	190.82	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[64]	$^1S_0$	**186±15**	***exp.***
39	Y	[63]	$^2D_{3/2}$	153	R, Dirac, LDA
		[41]	$^2D_{3/2}$	**163±12**	***exp.***
40	Zr	[63]	$^3F_2$	121	R, Dirac, LDA
		[41]	$^3F_2$	**112±13**	***exp.***

Z	Atom	Refs.	State	α_D	comments
41	Nb	[63]	$^6D_{1/2}$	106	R, Dirac, LDA
		[41]	$^6D_{1/2}$	**97.9±7.4**	***exp.***
42	Mo	[63]	$^7S_3$	86	R, Dirac, LDA
		[68]	^7S	72.5	R, DK,CASPT2
		[41]	$^7S_3$	**87.1±6.1**	***exp.***
43	Tc	[63]	$^6S_{5/2}$	77	R, Dirac, LDA
		[68]	^6S	80.4	R, DK,CASPT2
44	Ru	[63]	$^5F_5$	65	R, Dirac, LDA
45	Rh	[63]	$^4F_{9/2}$	58	R, Dirac, LDA
		[41]	$^4F_{9/2}$	**11±22**	***exp.*** (an unusually low value was obtained)
46	Pd	[63]	$^1S_0$	32	R, Dirac, LDA
47	Ag	[70]	^2S	52.2	R, PP, QCISD(T)
		[71]	^2S	52.5	R, DK, CCSD(T)
		[68]	^2S	36.7	R, DK, CCSD(T)
		[41]	$^2S_{1/2}$	**45.9±7.4**	***exp.***
48	Cd	[73]	^1S	46.3	R, PP, CCSD(T)
		[74]	^1S	46.8	R, MVD, CCSD(T)
		[68]	^1S	46.9	R, DK,CASPT2
		[83]	$^1S_0$	**49.65±1.46**	***exp.***
49	In	[84]	$^2P_{1/2}$	65.2	R, DFT
		[26]	^2P	66.7	R, SF, MRCI, M_L *res.*
		[26]	$^2P_{1/2}/^2P_{3/2}$	61.9/69.6	R, Dirac, MRCI, M_J res.
		[77]	$^2P_{1/2}/^2P_{3/2}$	62.0/69.8	R, Dirac, FSCC, M_J res. (J=3/2: M_J=3/2: 55.1, M_J=1/2: 84.6)
		[85]	$^2P_{1/2}$	62.4	R, Dirac+Breit, CI+all-order
		[86]	$^2P_{1/2}$	**68.7±8.1**	***exp.***
		[41]	$^2P_{1/2}$	**62.1±6.1**	***exp.***

Z	Atom	Refs.	State	α_D	comments
50	Sn	[63]	^{3}P	52	R, Dirac, LDA
		[28]	^{3}P	53.3	R, PP, 2nd order MBPT
		[28]	^{3}P	56.34	R, PP, CCSD(T), M_L res. (M_L=0: 54.28, M_L=±1: 59.36)
		[28]	^{3}P$_0$	52.91	R, Dirac+Gaunt
		[28]	^{3}P$_0$	**42.4±11**	***exp.***
		[41]	^{3}P$_0$	**67.5±8.8**	***exp.***
51	Sb	[63]	^{4}S	45	R, Dirac, LDA
		[29]	^{4}S	42.2	R, DK, CASPT2
		[87]	^{4}S	42.55	NR,CCSD(T)
52	Te	[63]	^{3}P	37	R, LDA
53	I	[78]	^{2}P$_{1/2}$	35.1	R, DK, SO-CI
		[78]	^{2}P$_{3/2}$	34.6	R, DK, SO-CI, M_J res.
54	Xe	[35]	^{1}S	27.06	R, DK3, CCSD(T)
		[88]	^{1}S$_0$	27.36	R, SOPP, CCSD(T) + MP2 basis set correction
		[29]	^{1}S	26.7	R, DK, CASPT2
		[79]	^{1}S$_0$	25.297	R, Dirac, CCSD/T
		[89]	^{1}S$_0$	27.42	R, DK3, CCSD(T)
		[80]	^{1}S$_0$	26.7	R, RPA, PolPot
		[54]	^{1}S$_0$	**27.815**	***exp.***
55	Cs	[38]	^{2}S$_{1/2}$	399.9	R, Dirac, SD, all orders + exp. data
		[56]	^{2}S	396.0	R, DK, CCSD(T)
		[90]	^{2}S$_{1/2}$	399.0	R, Dirac, CCSD(T)
		[91]	^{2}S$_{1/2}$	**401.0±0.6**	***exp.***
		[92]	^{2}S$_{1/2}$	**400.8(2)(6)**	***exp.***

Z	Atom	Refs.	State	α_D	comments
56	Ba	[23,58]	^1S	262.2	R, CI, MBPT
		[60]	$^1S_0$	273.5	R, DK+SO, CCSD(T)
		[22]	$^1S_0$	268.19	R, Dirac, coupled cluster
		[93]	$^1S_0$	272.7	R, Dirac+Gaunt, CCSD(T)
		[46]	$^1S_0$	275.68	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[80]	$^1S_0$	251	R, RPA, PolPot
		[61]	$^1S_0$	**268±22**	***exp.***
57	La	[63]	$^2D_{3/2}$, $5d^1$	210	R, Dirac, LDA
		[94]	$^2D_{3/2}$	213.7	R, Dirac, CI+MBPT+CP(RPA); (α_D =218.7 for the $5d^26s^1$ configuration)
		[41]	$^2D_{3/2}$	**170.7±8.1**	***exp.***
58	Ce	[63]	$4f^15d^1$	200	R, Dirac, LDA
		[94]	$4f^15d^1$	204.7	R, Dirac, CI+MBPT+CP(RPA); (α_D =223.4 for the $4f^2$ configuration)
		[41]	$^1G_4$	**191.7±20.2**	***exp.***
59	Pr	[63]	$4f^3$	190	R, Dirac, LDA
		[94]	$4f^3$	215.8	R, Dirac, CI+MBPT+CP(RPA); (α_D =195.7 for the $4f^25d^1$ configuration)
		[41]	^4I	**238.9±27.7**	***exp.***
60	Nd	[63]	$4f^4$	212	R, Dirac, LDA
		[94]	$4f^4$	208.4	R, Dirac, CI+MBPT+CP(RPA); (α_D =187.5 for the $4f^35d^1$ configuration)
		[41]	$^5I_4$	**183.6±19.6**	***exp.***
61	Pm	[63]	$4f^5$	203	R, Dirac, LDA
		[94]	$4f^5$	200.2	R, Dirac, CI+MBPT+CP(RPA); (α_D =179.3 for the $4f^45d^1$ configuration)
62	Sm	[63]	$4f^6$	194	R, Dirac, LDA
		[94]	$4f^6$	192.1	R, Dirac, CI+MBPT+CP(RPA); (α_D =171.7 for the $4f^55d^1$ configuration)
		[41]	$^7F_0$	**156.6±16.2**	***exp.***
63	Eu	[63]	$4f^7$	187	R, Dirac, LDA
		[94]	$4f^7$	184.2	R, Dirac, CI+MBPT+CP(RPA); (α_D =164.7 for the $4f^65d^1$ configuration)
		[41]	$^8S_{7/2}$	**154.8±25.0**	***exp.***

Z	Atom	Refs.	State	α_D	comments
64	Gd	[63] [94] [41]	$4f^7 5d^1$ $4f^7 5d^1$ $^9D_2$	159 158.3 **176.1±26.3**	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); (α_D =194.5 for the $4f^7 5d^2 6s^1$ configuration) ***exp.***
65	Tb	[63] [94] [41]	$4f^9$ $4f^9$ $^6H_{15/2}$	172 169.5 **158.6±10.8**	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); (α_D =152.4 for the $4f^8 5d^1$ configuration) ***exp.***
66	Dy	[63] [94] [80] [41]	$4f^{10}$ $4f^{10}$ $4f^{10}$ $^5I_8$	165 162.7 168 **157.2±10.8**	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); (α_D =148.3 for the $4f^9 5d^1$ configuration) R, RPA, PolPot ***exp.***
67	Ho	[63] [94] [80] [41]	$4f^{11}$ $4f^{11}$ $4f^{11}$ $^4I_{15/2}$	159 156.3 161 **145.1±11.5**	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); (α_D =142.9 for the $4f^{10} 5d^1$ configuration) R, RPA, PolPot ***exp.***
68	Er	[63] [94] [80] [41]	$4f^{12}$ $4f^{12}$ $4f^{12}$ $^3H_6$	153 150.2 154 **217.3±38.5**	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); (α_D =139.4 for the $4f^{11} 5d^1$ configuration) R, RPA, PolPot ***exp.***
69	Tm	[63] [94] [80] [41]	$4f^{13}$ $4f^{13}$ $4f^{13}$ $^2F_{7/2}$	147 144.3 147 **129.6±16.2**	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); (α_D =137.8 for the $4f^{12} 5d^1$ configuration) R, RPA, PolPot ***exp.***

Z	Atom	Refs.	State	α_D	comments
70	Yb	[63]	$^1S_0$, $4f^{14}$	142	R, Dirac, LDA
		[22]	$^1S_0$	144.59	R, Dirac, coupled cluster
		[95]	$^1S_0$	140.7	R, Dirac+Gaunt, CCSD(T)
		[96]	$^1S_0$	141(6)	R, Dirac, CI+MBPT+ experimental data, see also ref.98 for error estimates
		[97]	$^1S_0$	142.6	ECP, CCSD(T)
		[94]	$^1S_0$	138.9	R, Dirac, CI+MBPT+CP(RPA); (α_D =312.2 for the $4f^{14}6s^16p^1$ configuration)
		[80]	$^1S_0$	142	R, RPA, PolPot
		[41]	$^1S_0$	**147.1±19.6**	***exp.***
71	Lu	[63]	$^2D_{3/2}$, $5d^1$	148	R, Dirac, LDA
		[94]	$^2D_{3/2}$	137.2	R, Dirac, CI+MBPT+CP(RPA); (α_D =61.3 for the $4f^{14}6s^26p^1$ configuration)
		[41]	$^2D_{3/}$	**123.5±18.2**	***exp.***
72	Hf	[63]	$^3F_2$, $5d^3$	109	R, Dirac, LDA
		[41]	$^3F_2$	**83.7±18.9**	***exp.***
73	Ta	[63]	$^4F_{3/2}$, $5d^3$	88	R, Dirac, LDA
		[80]	$5d^3$	73.7	R, RPA, PolPot
		[41]	$^4F_{3/2}$	**58.0±12.1**	***exp.***
74	W	[63]	$^5D_0$	75	R, Dirac, LDA
		[80]	$5d^4$	68.1	R, RPA, PolPot
75	Re	[63]	$^6S_{5/2}$	65	R, Dirac, LDA
		[68]	^6S	61.1	DK, CASPT2
		[80]	$5d^5$	65.6	R, RPA, PolPot
76	Os	[63]	$^5D_4$	57	R, Dirac, LDA
		[80]	$5d^6$	57.8	R, RPA, PolPot
77	Ir	[63]	$^4F_{9/2}$	51	R, Dirac, LDA
		[80]	$5d^7$	51.7	R, RPA, PolPot
78	Pt	[63]	$^3D_3$	44	R, Dirac, LDA

Z	Atom	Refs.	State	α_D	comments
79	Au	[70]	^2S	35.1	R, PP, QCISD(T)
		[71]	^2S	36.1	R, DK, CCSD(T)
		[68]	^2S	27.9	R, DK, CASPT2
80	Hg	[73]	^1S	34.4	R, PP, CCSD(T)
		[74]	^1S	31.2	R, MVD, CCSD(T)
		[68]	^1S	33.3	R, DK, CASPT2
		[99]	$^1S_0$	34.15	R, Dirac, CCSD(T)
		[100]	$^1S_0$	34.27	R, Dirac, CCSDT+QED
		[80]	$^1S_0$	39.1	R, RPA, PolPot
		[101]	$^1S_0$	**33.91±0.34**	***exp.***
81	Tl	[26]	^2P	70.0	R, SF, MRCI, M_L res.
		[26]	$^2P_{1/2}/^2P_{3/2}$	51.6/81.2	R, Dirac, MRCI, M_J res.
		[102]	$^2P_{1/2}$	52.3	R, Dirac, FS-CCSD
		[77]	$^2P_{1/2}/^2P_{3/2}$	50.3/80.9	R, Dirac, FSCC, M_J res. (J=3/2: M_J=3/2: 56.7, M_J=1/2: 105.1)
		[64]	$^2P_{1/2}$	**51±7**	***exp.***
82	Pb	[63]	^3P	46	R, Dirac, LDA
		[103]	$^3P_0$	51.0	R, SOPP, CCSD(T)
		[28]	$^3P_0$	47.71	R, Dirac+Gaunt, CCSD(T)
		[99]	$^3P_0$	46.96	R, Dirac, CCSD(T)
		[28]	$^3P_0$	**47.1±7**	***exp.***
		[41]	$^3P_0$	**56.0±18.2**	***exp.***
83	Bi	[63]	^4S	50	R, Dirac, LDA
		[29]	^4S	48.6	R, DK, CASPT2
		[104]	^4S	52.85	R, Cowan-Griffin, HF only
		[41]	$^4S_{3/2}$	**54.7±11.5**	***exp.***
84	Po	[63]	^3P	46	R, R, Dirac, LDA
		[104]	^3P	46.8	R, Cowan-Griffin, HF only, M_L res.

Z	Atom	Refs.	State	α_D	comments
85	At	[78]	$^2P_{1/2}$	45.6	R, DK, SO-CI
		[78]	$^2P_{3/2}$	43.0	R, DK, SO-CI, M_J res.
86	Rn	[35]	^1S	33.18	R, DK3, CCSD(T)
		[88]	$^1S_0$	34.33	R, SOPP, CCSD(T) + MP2 basis set correction
		[103]	$^1S_0$	28.6	R, SOPP, CCSD(T)
		[29]	^1S	32.6	R, DK, CASPT2
		[80]	$^1S_0$	34.2	R, RPA, PolPot
87	Fr	[38]	$^2S_{1/2}$	317.8	R, Dirac, SD all orders + experimental data
		[56]	^2S	315.2	R, DK, CCSD(T)
		[90]	$^2S_{1/2}$	311.5	R, Dirac, CCSD(T)
		[105]		316.8	
88	Ra	[60]	$^1S_0$	246.2	R, DK+SO, CCSD(T)
		[93]	$^1S_0$	242.8	R, Dirac+Gaunt, CCSD(T)
		[46]	$^1S_0$	242.42	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[80]	$^1S_0$	232	R, RPA, PolPot
89	Ac	[63]	$^2D_{3/2},6d^1$	217	R, Dirac, LDA
		[94]	$^2D_{3/2},6d^1$	203.3	R, Dirac, CI+MBPT+CP(RPA); (α_D =141.9 for the $7s^27p^1$ configuration)
90	Th	[63]	$6d^2$	217	R, Dirac, LDA
91	Pa	[63]	$5f^26d^1$	171	R, Dirac, LDA
		[94]	$5f^26d^1$	154.4	R, Dirac, CI+MBPT+CP(RPA); (α_D =151.9 for the $5f^26d^27s^1$ configuration)
92	U	[63]	$5f^36d^1$	152.7	R, Dirac, LDA
		[94]	$5f^36d^1$	127.8	R, Dirac, CI+MBPT+CP(RPA); (α_D =153.2 for the $5f^4$ configuration)
		[106]	$^5L_6$	**137±9**	***exp.***
93	Np	[63]	$5f^46d^1$	167	R, Dirac, LDA
		[94]	$5f^46d^1$	150.5	R, Dirac, CI+MBPT+CP(RPA); (α_D =127.5 for the $5f^5$ configuration)
94	Pu	[63]	$5f^6$	165	R, Dirac, LDA
		[94]	$5f^6$	132.2	R, Dirac, CI+MBPT+CP(RPA); (α_D =147.6 for the $5f^56d^1$ configuration)

Z	Atom	Refs.	State	α_D	comments
95	Am	[63]	$5f^7$	157	R, Dirac, LDA
		[107]	$5f^7$	116	R, DK, CASPT2
		[94]	$5f^7$	131.2	R, Dirac, CI+MBPT+CP(RPA); (α_D =144.7 for the $5f^6 6d^1$ configuration)
96	Cm	[63]	$5f^7 6d^1$	155	R, Dirac, LDA
		[94]	$5f^7 6d^1$	143.6	R, Dirac, CI+MBPT+CP(RPA); (α_D =128.6 for the $5f^8$ configuration)
97	Bk	[63]	$5f^9$	153	R, Dirac, LDA
		[94]	$5f^9$	125.3	R, Dirac, CI+MBPT+CP(RPA); (α_D =141.6 for the $5f^8 6d^1$ configuration)
98	Cf	[63]	$5f^{10}$	138	R, Dirac, LDA
		[94]	$5f^{10}$	121.5	R, Dirac, CI+MBPT+CP(RPA); (α_D =142.3 for the $5f^9 6d^1$ configuration)
99	Es	[63]	$5f^{11}$	133	R, Dirac, LDA
		[94]	$5f^{11}$	117.5	R, Dirac, CI+MBPT+CP(RPA); (α_D =146.1 for the $5f^{10} 6d^1$ configuration)
100	Fm	[63]	$5f^{12}$	161	R, Dirac, LDA
		[94]	$5f^{12}$	113.4	R, Dirac, CI+MBPT+CP(RPA); (α_D =155.6 for the $5f^{11} 6d^1$ configuration)
101	Md	[63]	$5f^{13}$	123	R, Dirac, LDA
		[94]	$5f^{13}$	109.4	R, Dirac, CI+MBPT+CP(RPA); (α_D =179.6 for the $5f^{12} 6d^1$configuration)
102	No	[63]	$^1S_0$, $5f^{14}$	118	R, Dirac, LDA
		[95]	$^1S_0$, $5f^{14}$	110.8	R, Dirac+Gaunt, CCSD(T)
		[94]	$^1S_0$, $5f^{14}$	105.4	R, Dirac, CI+MBPT+CP(RPA); (α_D =267.8 for the $5f^{14} 7s^1 7p^1$ configuration)
		[80]	$^1S_0$, $5f^{14}$	114	R, RPA, PolPot
105	Db	[80]	$6d^3 7s^2$	42.5	R, RPA, PolPot
106	Sg	[80]	$6d^4 7s^2$	40.7	R, RPA, PolPot
107	Bh	[80]	$6d^5 7s^2$	38.4	R, RPA, PolPot
108	Hs	[80]	$6d^6 7s^2$	36.2	R, RPA, PolPot
109	Mt	[80]	$6d^7 7s^2$	34.2	R, RPA, PolPot
110	Ds	[80]	$6d^8 7s^2$	32.3	R, RPA, PolPot

Z	Atom	Refs.	State	α_D	comments
111	Rg	[80]	$6d^97s^2$	30.6	R, RPA, PolPot
112	Cn	[73]	^1S	25.8	R, PP, CCSD(T)
		[103]	$^1S_0$	28.7	R, SOPP, CCSD(T)
		[99]	$^1S_0$	27.64	R, Dirac, CCSD(T)
		[80]	$^1S_0$	29.0/28.2	R, RPA, PolPot
113	Nh	[102]	$^2P_{1/2}$	29.9	R, Dirac, FS-CCSD
114	Fl	[103]	$^3P_0$	34.4	R, SOPP, CCSD(T)
		[28]	$^3P_0$	31.98	R, Dirac+Gaunt, CCSD(T)
		[99]	$^3P_0$	30.59	R, Dirac, CCSD(T)
118	Og	[103]	$^1S_0$	52.4	R, SOPP, CCSD(T)
		[108]	$^1S_0$	46.33	R, Dirac, CCSD(T)
		[80]	$^1S_0$	59.0/57.2	R, RPA, PolPot
		[109]	$^1S_0$	57.98	R, Dirac+Gaunt, CCSD(T)
119		[56]	^2S	163.8	R, DK, CCSD(T)
		[90]	$^2S_{1/2}$	169.7	R, Dirac, CCSD(T)
120		[93]	$^1S_0$	162.6	R, Dirac+Gaunt, CCSD(T)
		[80]	$^1S_0$	147	R, RPA, PolPot

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