

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 \pm 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.= $0.14818474 \text{ \AA}^3 = 1.6487773 \times 10^{-41} \text{ C m}^2/\text{V}$. **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]	2S	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 1H
2	He	[11]	1S_0	1.383191	R, Dirac, Breit-Pauli, QED, mass pol., correlated basis (4He)
		[12]	1S_0	1.38376079(23)	R, Dirac, Breit-Pauli, QED, mass pol., exponentially correlated Slater functions (4He)
		[13,14]	1S_0	1.383746(7)	<i>exp.</i>
3	Li	[15,16]	2S	164.05	NR, exponentially correlated Gaussians [20] + R/DK
		[17]	$^2S_{1/2}$	164.084	R, Dirac, MBPT, Breit, QED, recoil (7Li)
		[18]	$^2S_{1/2}$	164.1125(5)	Hylleraas basis, R(MV+Darwin+Breit), QED, recoil (7Li)
		[19]	$^2S_{1/2}$	164.0±3.4	<i>exp.</i>
4	Be	[15]	1S	37.755	NR, exponentially correlated Gaussians [20]
		[21]	1S_0	37.80	R, Dirac, coupled cluster
		[22]	1S_0	37.71	R, Dirac, CI+MBPT+ experimental data
5	B	[23]	2P	20.5	NR, PNO-CEPA, M_L res.
		[24]	2P	20.43	NR, CCSD(T), M_L res.
		[25]	2P	20.59	R, SF, MRCI, M_L res.
		[25]	$^2P_{1/2}/^2P_{3/2}$	20.53/20.54	R, Dirac, MRCI, M_J res.
6	C	[26]	3P	11.0	NR, CASPT2, M_L res.
		[24]	3P	11.67	NR, CCSD(T), M_L res.
		[27]	3P_0	11.26	R, Dirac+Gaunt, CCSD(T)
7	N	[23]	4S	7.43	NR, PNO-CEPA
		[28]	4S	7.41	R, DK, CASPT2
		[24]	4S	7.26	NR, CCSD(T)
		[19,29]	$^4S_{3/2}$	7.6±0.4	<i>exp.</i>
8	O	[23]	3P	6.04	NR, PNO-CEPA, M_L res.
		[26]	3P	6.1	NR, CASPT2, M_L res.
		[24]	3P	5.24	NR, CCSD(T), M_L res.

Z	Atom	Refs.	State	α_D	comments
9	F	[23]	2P	3.76	NR, PNO-CEPA, M_L res.
		[30]	2P	3.76	NR, CASPT2, M_L res.
		[24]	2P	3.70	NR, CCSD(T), M_L res.
10	Ne	[31]	1S	2.68	NR, CCSD(T)
		[32]	1S	2.665	NR, CC3
		[32-34]	1S	2.666	R, CC3+FCI+DK3 correction
		[35]	1S_0	2.6772	R, Dirac-Coulomb, non-linear PRCC
		[36]	1S_0	2.670±0.005	<i>exp.</i>
11	Na	[37]	$^2S_{1/2}$	162.6	R, SD all orders + exp. data
		[38]	$^2S_{1/2}$	162.7±0.8	<i>exp.</i>
		[39]	$^2S_{1/2}$	162.7±0.1/±1.2	<i>exp.</i> (values in parentheses correspond to statistical and systematic uncertainties respectively)
		[40]	$^2S_{1/2}$	161±7.5	<i>exp.</i>
12	Mg	[41]	1S	71.7	NR, MBPT4
		[42]	1S	71.8	NR, MBPT4
		[43]	1S	70.9	R, DK, CASPT2
		[21]	1S_0	73.41	R, Dirac, coupled cluster
		[22,44]	1S_0	70.89	R, Dirac, CI+MBPT+ experimental data
		[45]	1S_0	70.76	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[40]	1S_0	59±16	<i>exp.</i>
13	Al	[46]	2P	56.3	NR, PNO-CEPA
		[47]	2P	62.0	NR, numerical MCSCF, M_L res.
		[48]	2P	57.74	NR, CCSD(T), M_L res.
		[25]	2P	55.5	R, SF, MRCI, M_L res.
		[25]	$^2P_{1/2}/^2P_{3/2}$	55.4/55.9	R, Dirac, MRCI, M_J res.
		[49,50]	$^2P_{1/2}$	46±2	<i>exp.</i> (see also ref.40)

Z	Atom	Refs.	State	α_D	comments
14	Si	[46] [26] [51] [48] [27]	³ P ³ P ³ P ³ P ³ P ₀	36.7 36.5 37.4 37.17 37.31	NR, PNO-CEPA, M_L res. NR, CASPT2, M_L res. NR, CCSD(T), M_L res. NR, CCSD(T), M_L res. R, Dirac+Gaunt, CCSD(T)
15	P	[46] [26] [28] [48]	⁴ S ⁴ S ⁴ S ⁴ S	24.7 24.6 24.9 24.93	NR, PNO-CEPA NR, CASPT2 R, DK, CASPT2 NR, CCSD(T)
16	S	[46] [26] [30] [48]	³ P ³ P ³ P ³ P	19.6 19.6 19.6 19.37	NR, PNO-CEPA, M_L res. NR, CASPT2, M_L res. NR, CASPT2, M_L res. NR, CCSD(T), M_L res.
17	Cl	[46] [26] [30] [48]	² P ² P ² P ² P	14.7 14.6 14.73 14.57	NR, PNO-CEPA, M_L res. NR, CASPT2, M_L res. NR, CASPT2, M_L res. NR, CCSD(T), M_L res.
18	Ar	[46] [52] [28] [34,52] [53,54]	¹ S ¹ S ¹ S ¹ S ¹ S ₀	11.10 11.084 11.1 11.10 11.070(7)	NR, PNO-CEPA NR, CCSD(T) R, DK, CASPT2 R, CCSD(T) + DK3 correction <i>exp.</i>
19	K	[37] [55] [19] [39] [91]	² S _{1/2} ² S ² S _{1/2} ² S _{1/2} ² S _{1/2}	289.1 291.1 293±6 290.6±1.4 289.7(1)(5)	R, SD all orders, + exp. data for electronic transitions R, DK, CCSD(T) <i>exp.</i> <i>exp.</i> (for hyperfine effects see ref.56) <i>exp.</i>

Z	Atom	Refs.	State	α_D	comments
20	Ca	[57]	1S_0	160	R, CI, MBPT
		[58]	1S	152.0	R, MVD, CCSD+T
		[43]	1S	163	R, DK, CASPT2
		[59]	1S_0	158.6	R, DK+SO, CCSD(T)
		[21]	1S_0	154.58	R, Dirac, coupled cluster
		[22,44]	1S_0	155.9	R, Dirac, CI+MBPT+ experimental data
		[45]	1S_0	160.77	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[60,61]	1S_0	169±17	<i>exp.</i>
21	Sc	[62,63]	$^2D_{3/2}$	120	R, Dirac, LDA
		[64,65]	2D	107	NR, small CI, VPA
		[66]	2D	142.28	NR, MCPF
		[40]	$^2D_{3/2}$	97.2±9.5	<i>exp.</i>
22	Ti	[62]	3F_2	99	R, Dirac, LDA
		[64]	3F	92	NR, small CI, VPA
		[66]	3F	114.34	NR, MCPF
		[40]	3F_2	63.4±3.4	<i>exp.</i>
23	V	[62]	$^4F_{3/2}$	84	R, Dirac, LDA
		[64]	4F	81	NR, small CI, VPA
		[66]	4F	97.34	NR, MCPF
		[40]	$^4F_{3/2}$	68.2±5.4	<i>exp.</i>
24	Cr	[62]	7S_3	78	R, Dirac, LDA
		[66]	7S	94.72	NR, MCPF
		[67]	7S	78.4	DK,CASPT2
		[40]	7S_3	60±24	<i>exp.</i>
25	Mn	[62]	$^6S_{5/2}$	63	R, Dirac, LDA
		[64]	6S	65	NR, small CI, VPA
		[66]	6S	75.52	NR, MCPF
		[67]	6S	66.8	DK,CASPT2

Z	Atom	Refs.	State	α_D	comments
26	Fe	[62]	5D_4	57	R, Dirac, LDA
		[64]	5D	58	NR, small CI, VPA
		[66]	5D	63.93	NR, MCPF
		[68]	5D	62.65	NR, GGA(PW86)
27	Co	[62]	$^4F_{9/2}$	51	R, Dirac, LDA
		[64]	4F	53	NR, small CI, VPA
		[66]	4F	57.71	NR, MCPF
28	Ni	[62]	3F_4	46	R, Dirac, LDA
		[64]	3F	48	NR, small CI, VPA
		[66]	3F	51.10	NR, MCPF
29	Cu	[66]	2S	53.44	NR, MCPF
		[69]	2S	45.0	R, PP, QCISD(T)
		[70]	2S	46.5	R, DK, CCSD(T)
		[67]	2S	40.7	R, DK, CASPT2
		[40]	$^2S_{1/2}$	58.7±4.7	exp.
30	Zn	[71]	1S	39.2	NR, CCSD(T), MP2 basis correction
		[72]	1S	38.0	R, PP, CCSD(T)
		[73]	1S	37.6	R, MVD, CCSD(T)
		[67]	1S	38.4	R, DK, CASPT2
		[74]	1S_0	38.666	R, Dirac, CCSDT
		[71]	1S_0	38.8±0.3	exp.
31	Ga	[75]	2P	54.9	NR, PNO-CEPA, M_L res.
		[25]	2P	50.7	R, SF, MRCI, M_L res.
		[25]	$^2P_{1/2}/^2P_{3/2}$	49.9/51.6	R, Dirac, MRCI, M_J res.
		[76]	$^2P_{1/2}/^2P_{3/2}$	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)
		[40]	$^2P_{1/2}$	46.6±4.0	exp.
32	Ge	[75]	3P	41.0	NR, PNO-CEPA, M_L res.
		[27]	3P	40.16	R, DK, CCSD(T), M_L res. ($M_L=0$: 32.83, $M_L=1$: 43.83)
		[27]	3P_0	39.43	R, Dirac Gaunt, CCSD(T),

Z	Atom	Refs.	State	α_D	comments
33	As	[75]	4S	29.1	NR, PNO-CEPA
		[28]	4S	29.8	R, DK, CASPT2
34	Se	[29]	3P	26.24	R, MVD, CASPT2, M_L res.
35	Br	[77]	$^2P_{1/2}$	21.9	R, DK, SO-CI
		[77]	$^2P_{3/2}$	21.8	R, DK, SO-CI, M_J res.
		[30]	2P	21.03	R, MVD, CASPT2, M_L res.
36	Kr	[53]	1S	16.8	R, DK3, CCSD(T)
		[28]	1S	16.6	R, DK, CASPT2
		[78]	1S_0	16.012	R, Dirac, CCSD/T
		[79]	1S_0	16.5	R, RPA, PolPot
		[53]	1S_0	17.075	<i>exp.</i>
37	Rb	[37]	$^2S_{1/2}$	318.6	R, SD all orders + exp. data
		[55]	2S	316.2	R, DK, CCSD(T)
		[19]	$^2S_{1/2}$	316(6)	<i>exp.</i>
		[39]	$^2S_{1/2}$	318.8±1.4	<i>exp.</i>
		[91]	$^2S_{1/2}$	319.8(2)(5)	<i>exp.</i>
38	Sr	[57]	1S	199	R, CI, MBPT
		[59]	1S_0	199.4	R, DK+SO, CCSD(T)
		[21]	1S_0	199.71	R, Dirac, coupled cluster
		[44,80]	1S_0	197.2(3.6)	R, Dirac, CI+MBPT+ experimental data
		[81]	1S_0	197.6	CI+ core polarization (corrected to exp. term energies)
		[45]	1S_0	190.82	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[63]	1S_0	186±15	<i>exp.</i>
39	Y	[62]	$^2D_{3/2}$	153	R, Dirac, LDA
		[40]	$^2D_{3/2}$	163±12	<i>exp.</i>
40	Zr	[62]	3F_2	121	R, Dirac, LDA
		[40]	3F_2	112±13	<i>exp.</i>

41	Nb	[62] [40]	${}^6D_{1/2}$ ${}^6D_{1/2}$	106 97.9±7.4	R, Dirac, LDA <i>exp.</i>
Z	Atom	Refs.	State	α_D	comments
42	Mo	[62] [67] [40]	7S_3 7S 7S_3	86 72.5 87.1±6.1	R, Dirac, LDA R, DK,CASPT2 <i>exp.</i>
43	Tc	[62] [67]	${}^6S_{5/2}$ 6S	77 80.4	R, Dirac, LDA R, DK,CASPT2
44	Ru	[62]	5F_5	65	R, Dirac, LDA
45	Rh	[62] [40]	${}^4F_{9/2}$ ${}^4F_{9/2}$	58 11±22	R, Dirac, LDA <i>exp.</i> (an unusually low value was obtained)
46	Pd	[62]	1S_0	32	R, Dirac, LDA
47	Ag	[69] [70] [67] [40]	2S 2S 2S ${}^2S_{1/2}$	52.2 52.5 36.7 45.9±7.4	R, PP, QCISD(T) R, DK, CCSD(T) R, DK, CCSD(T) <i>exp.</i>
48	Cd	[72] [73] [67] [82]	1S 1S 1S 1S_0	46.3 46.8 46.9 49.65±1.46	R, PP, CCSD(T) R, MVD, CCSD(T) R, DK,CASPT2 <i>exp.</i>
49	In	[83] [25] [25] [76] [84] [85] [40]	${}^2P_{1/2}$ 2P ${}^2P_{1/2}/{}^2P_{3/2}$ ${}^2P_{1/2}/{}^2P_{3/2}$ ${}^2P_{1/2}$ ${}^2P_{1/2}$ ${}^2P_{1/2}$	65.2 66.7 61.9/69.6 62.0/69.8 62.4 68.7±8.1 62.1±6.1	R, DFT R, SF, MRCI, M_L res. R, Dirac, MRCI, M_J res. R, Dirac, FSCC, M_J res. ($J=3/2$: $M_J=3/2$: 55.1, $M_J=1/2$: 84.6) R, Dirac+Breit, CI+all-order <i>exp.</i> <i>exp.</i>

Z	Atom	Refs.	State	α_D	comments
50	Sn	[62]	3P	52	R, Dirac, LDA
		[27]	3P	53.3	R, PP, 2 nd order MBPT
		[27]	3P	56.34	R, PP, CCSD(T), M_L res. ($M_L=0$: 54.28, $M_L=\pm 1$: 59.36)
		[27]	3P_0	52.91	R, Dirac+Gaunt
		[27]	3P_0	42.4±11	<i>exp.</i>
		[40]	3P_0	67.5±8.8	<i>exp.</i>
51	Sb	[62]	4S	45	R, Dirac, LDA
		[28]	4S	42.2	R, DK, CASPT2
		[86]	4S	42.55	NR,CCSD(T)
52	Te	[62]	3P	37	R, LDA
53	I	[77]	$^2P_{1/2}$	35.1	R, DK, SO-CI
		[77]	$^2P_{3/2}$	34.6	R, DK, SO-CI, M_J res.
54	Xe	[34]	1S	27.06	R, DK3, CCSD(T)
		[87]	1S_0	27.36	R, SOPP, CCSD(T) + MP2 basis set correction
		[28]	1S	26.7	R, DK, CASPT2
		[78]	1S_0	25.297	R, Dirac, CCSD/T
		[88]	1S_0	27.42	R, DK3, CCSD(T)
		[79]	1S_0	26.7	R, RPA, PolPot
[53]	1S_0	27.815	<i>exp.</i>		
55	Cs	[37]	$^2S_{1/2}$	399.9	R, Dirac, SD, all orders + exp. data
		[55]	2S	396.0	R, DK, CCSD(T)
		[89]	$^2S_{1/2}$	399.0	R, Dirac, CCSD(T)
		[90]	$^2S_{1/2}$	401.0±0.6	<i>exp.</i>
		[91]	$^2S_{1/2}$	400.8(2)(6)	<i>exp.</i>

Z	Atom	Refs.	State	α_D	comments
56	Ba	[22,57] [59] [21] [92] [45] [79] [60]	1S 1S_0 1S_0 1S_0 1S_0 1S_0 1S_0	262.2 273.5 268.19 272.7 275.68 251 268±22	R, CI, MBPT R, DK+SO, CCSD(T) R, Dirac, coupled cluster R, Dirac+Gaunt, CCSD(T) R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC) R, RPA, PolPot <i>exp.</i>
57	La	[62] [93] [40]	$^2D_{3/2}, 5d^1$ $^2D_{3/2}$ $^2D_{3/2}$	210 213.7 170.7±8.1	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 218.7$ for the $5d^2 6s^1$ configuration) <i>exp.</i>
58	Ce	[62] [93] [40]	$4f^1 5d^1$ $4f^1 5d^1$ 1G_4	200 204.7 191.7±20.2	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 223.4$ for the $4f^2$ configuration) <i>exp.</i>
59	Pr	[62] [93] [40]	$4f^3$ $4f^3$ 4I	190 215.8 238.9±27.7	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 195.7$ for the $4f^2 5d^1$ configuration) <i>exp.</i>
60	Nd	[62] [93] [40]	$4f^4$ $4f^4$ 5I_4	212 208.4 183.6±19.6	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 187.5$ for the $4f^3 5d^1$ configuration) <i>exp.</i>
61	Pm	[62] [93]	$4f^5$ $4f^5$	203 200.2	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 179.3$ for the $4f^4 5d^1$ configuration)
62	Sm	[62] [93] [40]	$4f^6$ $4f^6$ 7F_0	194 192.1 156.6±16.2	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 171.7$ for the $4f^5 5d^1$ configuration) <i>exp.</i>
63	Eu	[62] [93] [40]	$4f^7$ $4f^7$ $^8S_{7/2}$	187 184.2 154.8±25.0	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 164.7$ for the $4f^6 5d^1$ configuration) <i>exp.</i>

Z	Atom	Refs.	State	α_D	comments
64	Gd	[62] [93] [40]	$4f^7 5d^1$ $4f^7 5d^1$ 9D_2	159 158.3 176.1±26.3	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 194.5$ for the $4f^7 5d^2 6s^1$ configuration) <i>exp.</i>
65	Tb	[62] [93] [40]	$4f^9$ $4f^9$ $^6H_{15/2}$	172 169.5 158.6±10.8	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 152.4$ for the $4f^8 5d^1$ configuration) <i>exp.</i>
66	Dy	[62] [93] [79] [40]	$4f^{10}$ $4f^{10}$ $4f^{10}$ 5I_8	165 162.7 168 157.2±10.8	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 148.3$ for the $4f^9 5d^1$ configuration) R, RPA, PolPot <i>exp.</i>
67	Ho	[62] [93] [79] [40]	$4f^{11}$ $4f^{11}$ $4f^{11}$ $^4I_{15/2}$	159 156.3 161 145.1±11.5	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 142.9$ for the $4f^{10} 5d^1$ configuration) R, RPA, PolPot <i>exp.</i>
68	Er	[62] [93] [79] [40]	$4f^{12}$ $4f^{12}$ $4f^{12}$ 3H_6	153 150.2 154 217.3±38.5	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 139.4$ for the $4f^{11} 5d^1$ configuration) R, RPA, PolPot <i>exp.</i>
69	Tm	[62] [93] [79] [40]	$4f^{13}$ $4f^{13}$ $4f^{13}$ $^2F_{7/2}$	147 144.3 147 129.6±16.2	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 137.8$ for the $4f^{12} 5d^1$ configuration) R, RPA, PolPot <i>exp.</i>

Z	Atom	Refs.	State	α_D	comments
70	Yb	[62] [21] [94] [95] [96] [93] [79] [40]	$^1S_0, 4f^{14}$ 1S_0 1S_0 1S_0 1S_0 1S_0 1S_0 1S_0	142 144.59 140.7 141(6) 142.6 138.9 142 147.1±19.6	R, Dirac, LDA R, Dirac, coupled cluster R, Dirac+Gaunt, CCSD(T) R, Dirac, CI+MBPT+ experimental data, see also ref.97 for error estimates ECP, CCSD(T) R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D=312.2$ for the $4f^{14}6s^16p^1$ configuration) R, RPA, PolPot <i>exp.</i>
71	Lu	[62] [93] [40]	$^2D_{3/2}, 5d^1$ $^2D_{3/2}$ $^2D_{3/2}$	148 137.2 123.5±18.2	R, Dirac, LDA R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D=61.3$ for the $4f^{14}6s^26p^1$ configuration) <i>exp.</i>
72	Hf	[62] [40]	$^3F_2, 5d^3$ 3F_2	109 83.7±18.9	R, Dirac, LDA <i>exp.</i>
73	Ta	[62] [79] [40]	$^4F_{3/2}, 5d^3$ $5d^3$ $^4F_{3/2}$	88 73.7 58.0±12.1	R, Dirac, LDA R, RPA, PolPot <i>exp.</i>
74	W	[62] [79]	5D_0 $5d^4$	75 68.1	R, Dirac, LDA R, RPA, PolPot
75	Re	[62] [67] [79]	$^6S_{5/2}$ 6S $5d^5$	65 61.1 65.6	R, Dirac, LDA DK, CASPT2 R, RPA, PolPot
76	Os	[62] [79]	5D_4 $5d^6$	57 57.8	R, Dirac, LDA R, RPA, PolPot
77	Ir	[62] [79]	$^4F_{9/2}$ $5d^7$	51 51.7	R, Dirac, LDA R, RPA, PolPot
78	Pt	[62]	3D_3	44	R, Dirac, LDA

Z	Atom	Refs.	State	α_D	comments
79	Au	[69]	2S	35.1	R, PP, QCISD(T)
		[70]	2S	36.1	R, DK, CCSD(T)
		[67]	2S	27.9	R, DK, CASPT2
80	Hg	[72]	1S	34.4	R, PP, CCSD(T)
		[73]	1S	31.2	R, MVD, CCSD(T)
		[67]	1S	33.3	R, DK, CASPT2
		[98]	1S_0	34.15	R, Dirac, CCSD(T)
		[99]	1S_0	34.27	R, Dirac, CCSDT+QED
		[79]	1S_0	39.1	R, RPA, PolPot
	[100]	1S_0	33.91±0.34	<i>exp.</i>	
81	Tl	[25]	2P	70.0	R, SF, MRCI, M_L res.
		[25]	$^2P_{1/2}/^2P_{3/2}$	51.6/81.2	R, Dirac, MRCI, M_J res.
		[101]	$^2P_{1/2}$	52.3	R, Dirac, FS-CCSD
		[76]	$^2P_{1/2}/^2P_{3/2}$	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)
		[63]	$^2P_{1/2}$	51±7	<i>exp.</i>
82	Pb	[62]	3P	46	R, Dirac, LDA
		[102]	3P_0	51.0	R, SOPP, CCSD(T)
		[27]	3P_0	47.71	R, Dirac+Gaunt, CCSD(T)
		[98]	3P_0	46.96	R, Dirac, CCSD(T)
		[27]	3P_0	47.1±7	<i>exp.</i>
	[40]	3P_0	56.0±18.2	<i>exp.</i>	
83	Bi	[62]	4S	50	R, Dirac, LDA
		[28]	4S	48.6	R, DK, CASPT2
		[103]	4S	52.85	R, Cowan-Griffin, HF only
		[40]	$^4S_{3/2}$	54.7±11.5	<i>exp.</i>
84	Po	[62]	3P	46	R, R, Dirac, LDA
		[103]	3P	46.8	R, Cowan-Griffin, HF only, M_L res.

Z	Atom	Refs.	State	α_D	comments
85	At	[77]	$^2P_{1/2}$	45.6	R, DK, SO-CI
		[77]	$^2P_{3/2}$	43.0	R, DK, SO-CI, M_J res.
86	Rn	[34]	1S	33.18	R, DK3, CCSD(T)
		[87]	1S_0	34.33	R, SOPP, CCSD(T) + MP2 basis set correction
		[102]	1S_0	28.6	R, SOPP, CCSD(T)
		[28]	1S	32.6	R, DK, CASPT2
		[79]	1S_0	34.2	R, RPA, PolPot
87	Fr	[37]	$^2S_{1/2}$	317.8	R, Dirac, SD all orders + experimental data
		[55]	2S	315.2	R, DK, CCSD(T)
		[89]	$^2S_{1/2}$	311.5	R, Dirac, CCSD(T)
88	Ra	[59]	1S_0	246.2	R, DK+SO, CCSD(T)
		[92]	1S_0	242.8	R, Dirac+Gaunt, CCSD(T)
		[45]	1S_0	242.42	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[79]	1S_0	232	R, RPA, PolPot
89	Ac	[62]	$^2D_{3/2}, 6d^1$	217	R, Dirac, LDA
		[93]	$^2D_{3/2}, 6d^1$	203.3	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 141.9$ for the $7s^27p^1$ configuration)
90	Th	[62]	$6d^2$	217	R, Dirac, LDA
91	Pa	[62]	$5f^26d^1$	171	R, Dirac, LDA
		[93]	$5f^26d^1$	154.4	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 151.9$ for the $5f^26d^27s^1$ configuration)
92	U	[62]	$5f^36d^1$	152.7	R, Dirac, LDA
		[93]	$5f^36d^1$	127.8	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 153.2$ for the $5f^4$ configuration)
		[104]	5L_6	137±9	<i>exp.</i>
93	Np	[62]	$5f^46d^1$	167	R, Dirac, LDA
		[93]	$5f^46d^1$	150.5	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 127.5$ for the $5f^5$ configuration)
94	Pu	[62]	$5f^6$	165	R, Dirac, LDA
		[93]	$5f^6$	132.2	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 147.6$ for the $5f^56d^1$ configuration)

Z	Atom	Refs.	State	α_D	comments
95	Am	[62]	$5f^7$	157	R, Dirac, LDA
		[105]	$5f^7$	116	R, DK, CASPT2
		[93]	$5f^7$	131.2	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 144.7$ for the $5f^6 6d^1$ configuration)
96	Cm	[62]	$5f^7 6d^1$	155	R, Dirac, LDA
		[93]	$5f^7 6d^1$	143.6	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 128.6$ for the $5f^8$ configuration)
97	Bk	[62]	$5f^9$	153	R, Dirac, LDA
		[93]	$5f^9$	125.3	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 141.6$ for the $5f^8 6d^1$ configuration)
98	Cf	[62]	$5f^{10}$	138	R, Dirac, LDA
		[93]	$5f^{10}$	121.5	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 142.3$ for the $5f^9 6d^1$ configuration)
99	Es	[62]	$5f^{11}$	133	R, Dirac, LDA
		[93]	$5f^{11}$	117.5	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 146.1$ for the $5f^{10} 6d^1$ configuration)
100	Fm	[62]	$5f^{12}$	161	R, Dirac, LDA
		[93]	$5f^{12}$	113.4	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 155.6$ for the $5f^{11} 6d^1$ configuration)
101	Md	[62]	$5f^{13}$	123	R, Dirac, LDA
		[93]	$5f^{13}$	109.4	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 179.6$ for the $5f^{12} 6d^1$ configuration)
102	No	[62]	$^1S_0, 5f^{14}$	118	R, Dirac, LDA
		[94]	$^1S_0, 5f^{14}$	110.8	R, Dirac+Gaunt, CCSD(T)
		[93]	$^1S_0, 5f^{14}$	105.4	R, Dirac, CI+MBPT+CP(RPA); ($\alpha_D = 267.8$ for the $5f^{14} 7s^1 7p^1$ configuration)
		[79]	$^1S_0, 5f^{14}$	114	R, RPA, PolPot
105	Db	[79]	$6d^3 7s^2$	42.5	R, RPA, PolPot
106	Sg	[79]	$6d^4 7s^2$	40.7	R, RPA, PolPot
107	Bh	[79]	$6d^5 7s^2$	38.4	R, RPA, PolPot
108	Hs	[79]	$6d^6 7s^2$	36.2	R, RPA, PolPot
109	Mt	[79]	$6d^7 7s^2$	34.2	R, RPA, PolPot
110	Ds	[79]	$6d^8 7s^2$	32.3	R, RPA, PolPot

Z	Atom	Refs.	State	α_D	comments
111	Rg	[79]	$6d^9 7s^2$	30.6	R, RPA, PolPot
112	Cn	[72] [102] [98] [79]	1S 1S_0 1S_0 1S_0	25.8 28.7 27.64 29.0/28.2	R, PP, CCSD(T) R, SOPP, CCSD(T) R, Dirac, CCSD(T) R, RPA, PolPot
113		[101]	$^2P_{1/2}$	29.9	R, Dirac, FS-CCSD
114	Fl	[102] [27] [98]	3P_0 3P_0 3P_0	34.4 31.98 30.59	R, SOPP, CCSD(T) R, Dirac+Gaunt, CCSD(T) R, Dirac, CCSD(T)
118		[102] [106] [79]	1S_0 1S_0 1S_0	52.4 46.33 59.0/57.2	R, SOPP, CCSD(T) R, Dirac, CCSD(T) R, RPA, PolPot
119		[55] [89]	2S $^2S_{1/2}$	163.8 169.7	R, DK, CCSD(T) R, Dirac, CCSD(T)
120		[92] [79]	1S_0 1S_0	162.6 147	R, Dirac+Gaunt, CCSD(T) R, RPA, PolPot

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