2018 Table of Polarizabilities

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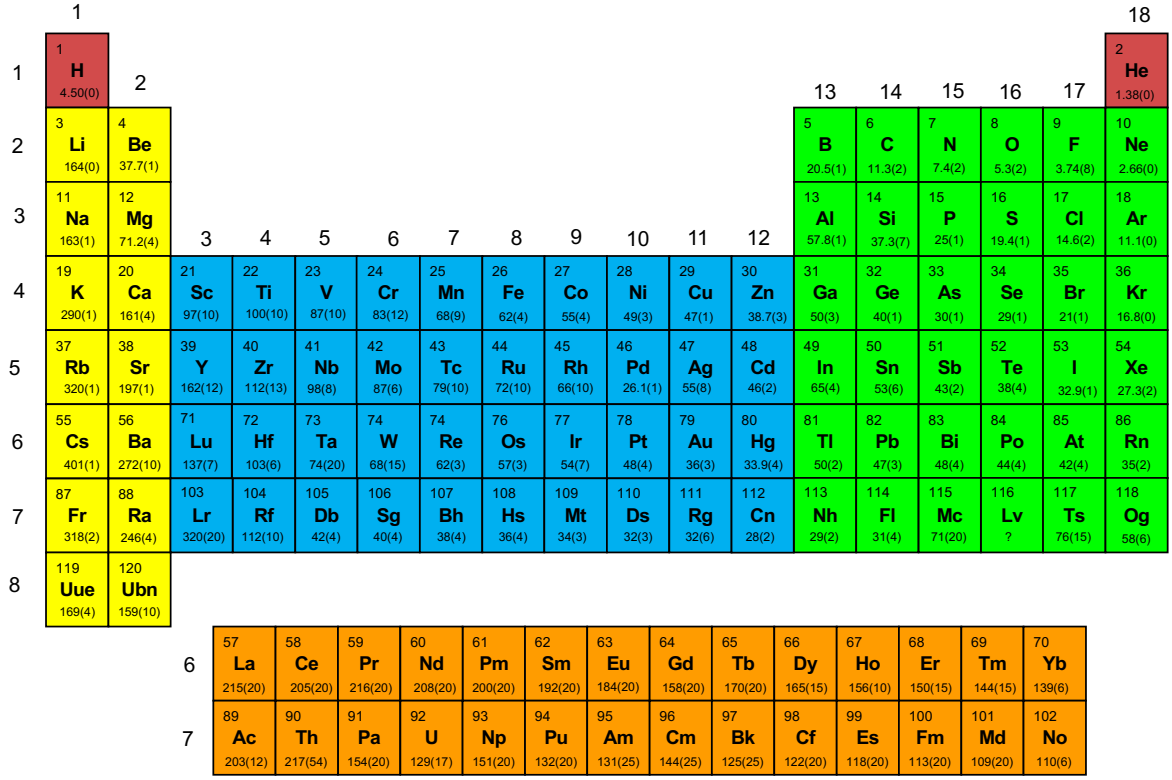

Figure 1. Recommended values from Table 1 for the atomic polarizabilities (atomic units; estimated uncertainties in parentheses) of elements Z = 1-120. The various blocks of elements are color-coded: *s*-block, yellow; *p*-block, green; *d*-block, blue; *f*-block, orange.

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Table 1. 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) respectively denotes that the polarizability for each M_L (M_J) state can be found in the reference given. Abbreviations used (uncertainties given here consistently as ± values): exp.: experimentally determined value; 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. 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 [1], reflecting the ground state symmetry of the specific atom. NB: 1 a.u. = 0.14818471 $Å^3$ = 1.6487773 $\times 10^{-41}$ C m^2/V.

Z	Atom	Refs.	State	α_D	Comments
1	H	[2]	^2S	4.5	NR, exact
		[2,3]	$^2S_{1/2}$	4.49975149589	R, Dirac, variational, Slater basis/B-splines (more digits are given in ref 3)
		[4]	$^2S_{1/2}$	4.49975149518	R, Dirac, Lagrange mesh method (more digits are given in this paper)
		[3]	$^2S_{1/2}$	4.507107623	R, Dirac (as above), but with finite mass correction added for the ^{1}H isotope
			$^2S_{1/2}$	**4.50711±0.00003**	**recommended**
2	He	[5]	$^1S_0$	1.383191	R, Dirac, Breit-Pauli, QED, mass pol., correlated basis (^{4}He)
		[6]	$^1S_0$	1.38376079 ±0.00000023	R, Dirac, Breit-Pauli, QED, mass pol., exponentially correlated Slater functions (^{4}He)
		[7]	$^1S_0$	1.3837295330 ±0.0000000001	R, Dirac, Breit, QED, recoil, … (^{4}He)
		[8,9]	$^1S_0$	1.383746±0.000007	exp.
		[10]	$^1S_0$	1.383759±0.000013	exp.
			$^1S_0$	**1.38375±0.00002**	**recommended**
3	Li	[11,12]	^2S	164.05	NR, exponentially correlated Gaussians [18] + R/DK
		[13]	$^2S_{1/2}$	164.084	R, Dirac, MBPT, Breit, QED, recoil (^{7}Li)
		[14]	$^2S_{1/2}$	164.1125±0.0005	Hylleraas basis, R(MV+Darwin+Breit), QED, recoil (^{7}Li)
		[15]	$^2S_{1/2}$	164.21	Frozen core Hamiltonian, semi-empirical polarization potential
		[16]	$^2S_{1/2}$	164.0±3.4	exp.
		[17]	$^2S_{1/2}$	164.2±1.1	exp.
			$^2S_{1/2}$	**164.1125±0.0005**	**recommended**

Z	Atom	Refs.	State	α_D	Comments
4	Be	[11]	^1S	37.755	NR, exponentially correlated Gaussians [18]
		[19]	$^1S_0$	37.80±0.47	R, Dirac, coupled cluster
		[20]	$^1S_0$	37.76±0.22	R, Dirac, CI+MBPT+ experimental data
		[11,21]	$^1S_0$	37.739±0.030	R correction of –0.016 applied to value from ref [11]
		[22]	$^1S_0$	37.86±0.17	R, Dirac, MBPT, CCSD
		[23]	$^1S_0$	37.73±0.05	CCSD(T)
		[24]	$^1S_0$	37.807	CI, expanded London formula
		[25]	$^1S_0$	37.69	Combination of *ab initio* and semi-empirical methods
		[26]	$^1S_0$	37.29	All-electron SCF plus valence CI
		[27]	$^1S_0$	37.9	Model potential
				37.74±0.03	**recommended**
5	B	[28]	^2P	20.47	NR, PNO-CEPA, M_L res.
		[29]	^2P	20.43±0.11	NR, CCSD(T), M_L res.
		[30]	^2P	20.59	R, SF, MRCI, M_L res.
		[30]	$^2P_{1/2}/^2P_{3/2}$	20.53/20.54	R, Dirac, MRCI, M_J res.
				20.5±0.1	**recommended**
6	C	[31]	^3P	11.39	NR, CASPT2, M_L res.
		[29]	^3P	11.67±0.07	NR, CCSD(T), M_L res.
		[32]	$^3P_0$	11.26±0.20	R, Dirac+Gaunt, CCSD(T)
				11.3±0.2	**recommended**
7	N	[28]	^4S	7.43	NR, PNO-CEPA
		[33]	^4S	7.41	R, DK, CASPT2
		[29]	^4S	7.26±0.05	NR, CCSD(T)
		[16,34]	$^4S_{3/2}$	7.6±0.4	exp.
		[35,36]	$^4S_{3/2}$	7.28	exp.
				7.4±0.2	**recommended**

Z	Atom	Refs.	State	α_D	Comments
8	O	[28,86]	^3P	5.41±0.11	NR, PNO-CEPA, M_L res.
		[31]	^3P	5.4±0.7	NR, CASPT2, M_L res.
		[21,29]	^3P	5.24±0.04	NR, CCSD(T), M_L res.
		[34]	$^3P_2$	5.2±0.4	exp.
				5.3±0.2	**recommended**
9	F	[28]	^2P	3.76	NR, PNO-CEPA, M_L res.
		[37]	^2P	3.76±0.06	NR, CASPT2, M_L res.
		[29]	^2P	3.70±0.03	NR, CCSD(T), M_L res.
				3.74±0.08	**recommended**
10	Ne	[38]	^1S	2.68	NR, CCSD(T)
		[39]	^1S	2.665	NR, CC3
		[39,40,41]	^1S	2.666	R, CC3+FCI+DK3 correction
		[42,43]	$^1S_0$	2.677±0.070	R, Dirac-Coulomb, non-linear PRCC
		[44]	$^1S_0$	2.66063±0.00001	CCSD(T), ECP
		[21]	$^1S_0$	2.661±0.005	R, CCSD(T)
		[45]	$^1S_0$	2.663	exp.
		[46]	$^1S_0$	2.6669±0.0008	exp.
		[47]	$^1S_0$	2.66110±0.00003	exp.
				2.66110±0.00003	**recommended**
11	Na	[48]	$^2S_{1/2}$	162.6±0.3	R, SD all orders + exp. data
		[21,49]	$^2S_{1/2}$	162.88±0.60	R, CCSD(T)
		[50]	$^2S_{1/2}$	162.7±0.5	exp.
		[51]	$^2S_{1/2}$	162.7±0.1/±1.2	exp. (values in parentheses correspond to statistical and systematic uncertainties resp.)
		[52]	$^2S_{1/2}$	161±7.5	exp.
				162.7±0.5	**recommended**

Z	Atom	Refs.	State	α_D	Comments
12	Mg	[53]	^1S	71.7	NR, MBPT4
		[54]	^1S	71.8	NR, MBPT4
		[55]	^1S	70.90	R, DK, CASPT2
		[19]	$^1S_0$	73.4±2.3	R, Dirac, coupled cluster
		[20,56]	$^1S_0$	70.89	R, Dirac, CI+MBPT+ experimental data
		[57]	$^1S_0$	70.76	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[21]	$^1S_0$	71.22±0.36	R, DK, CCSD(T)
		[20]	$^1S_0$	71.33	R, Dirac, CI+MBPT
		[20]	$^1S_0$	71.3±0.7	R, Dirac, CI+MBPT, recommended
		[27]	$^1S_0$	72.0	Model potential
		[25]	$^1S_0$	71.35	Combination of *ab initio* and semi-empirical methods
		[63]	^1S	71.32	NR, PNO-CEPA
		[58]	^1S	70.5	NR, CI+pseudo-potential
		[22]	$^1S_0$	72.54±0.50	R, Dirac, MBPT, CCSD
		[124]	$^1S_0$	71.4	CI, oscillator strength correction
		[48]	$^1S_0$	74.9±2.7	Hybrid-RCI+MBPT sum rule
		[52]	$^1S_0$	59±16	exp.
		[59]	$^1S_0$	77.6±7.8	exp.
		[60,61]	$^1S_0$	75.0±3.5	exp.
		[62]	$^1S_0$	71.5±3.5	exp.
				71.2±0.4	**recommended**

Z	Atom	Refs.	State	α_D	Comments
13	Al	[63]	^2P	56.27	NR, PNO-CEPA
		[60]	^2P	62.0	NR, numerical MCSCF, M_L res.
		[64]	^2P	57.74	NR, CCSD(T), M_L res.
		[30]	^2P	55.5	R, SF, MRCI, M_L res.
		[30]	$^2P_{1/2}/^2P_{3/2}$	55.4/55.9	R, Dirac, MRCI, M_J res.
		[21]	^2P	57.79±0.30	R, DK, CCSD(T)
		[65]	^2P	59.47	NR, MRCI
		[66]	^2P	61	SIC-DFT
		[67]	$^2P_{1/2}/^2P_{3/2}$	57.8±1.0/58.0±1.0	SI-SOCI, M_J res.
		[68]	^2P	58.0±0.4	CCSD(T)
		[69,70]	^2P	46±2	exp. (see also ref 52)
		[59,71]	^2P	55.3±5.5	exp.
				57.8±1.0	**recommended**
14	Si	[63]	^3P	36.32	NR, PNO-CEPA, M_L res.
		[31]	^3P	36.54	NR, CASPT2, M_L res.
		[72]	^3P	37.4±0.1	NR, CCSD(T), M_L res.
		[64]	^3P	37.17±0.21	NR, CCSD(T), M_L res.
		[32]	$^3P_0$	37.31±0.70	R, Dirac+Gaunt, CCSD(T)
		[66]	^3P	38.9	SIC-DFT
		[65]	^3P	36.95	NR, MRCI
				37.3±0.7	**recommended**
15	P	[63]	^4S	24.7±0.5	NR, PNO-CEPA
		[31]	^4S	24.6±0.2	NR, CASPT2
		[33]	^4S	24.9	R, DK, CASPT2
		[64]	^4S	24.93±0.15	NR, CCSD(T)
		[66]	^4S	26.11	SIC-DFT
		[36]	^4S	25.06	R, DK, CASPT2
				25±1	**recommended**

Z	Atom	Refs.	State	α_D	Comments
16	S	[63]	^3P	19.60	NR, PNO-CEPA, M_L res.
		[31]	^3P	19.6	NR, CASPT2, M_L res.
		[37]	^3P	19.6	NR, CASPT2, M_L res.
		[66]	^3P	19.72	SIC-DFT
		[64]	^3P	19.37±0.12	NR, CCSD(T), M_L res.
				19.4±0.1	**recommended**
17	Cl	[63]	^2P	14.71	NR, PNO-CEPA, M_L res.
		[31]	^2P	14.6	NR, CASPT2, M_L res.
		[37]	^2P	14.73	NR, CASPT2, M_L res.
		[66]	^2P	14.7	SIC-DFT
		[64]	^2P	14.57±0.10	NR, CCSD(T), M_L res.
				14.6±0.1	**recommended**
18	Ar	[63]	^1S	11.10	NR, PNO-CEPA
		[44]	^1S	11.08401±0.00004	NR, CCSD(T)
		[33]	^1S	11.1	R, DK, CASPT2
		[41,44]	^1S	11.10	R, CCSD(T) + DK3 correction
		[22]	^1S	11.089±0.004	R, CCDS(T)
		[21,59,64]	^1S	11.085±0.060	R, CCSD(T)
		[45]	$^1S_0$	11.080	exp.
		[73,74]	$^1S_0$	11.070±0.007	exp.
		[43]	$^1S_0$	11.081±0.005	exp.
		[8]	$^1S_0$	11.083±0.002	exp.
		[75]	$^1S_0$	11.091	exp.
		[21]	$^1S_0$	11.078±0.010	exp.
				11.083±0.007	**recommended**

Z	Atom	Refs.	State	α_D	Comments
19	K	[48]	$^2S_{1/2}$	289.1	RLCCSD
		[76]	^2S	291.1±1.5	R, DK, CCSD(T), AE
		[77]	$^2S_{1/2}$	290.2	Combination of theoretical and experimental data
		[48]	$^2S_{1/2}$	290.2±0.8	R, SD all orders + exp. data for electronic transitions
		[25]	$^2S_{1/2}$	290.0	Combination of *ab initio* and semi-empirical methods
		[78]	$^2S_{1/2}$	290.05	Oscillator-strength sum rule
		[16]	$^2S_{1/2}$	292.9±6.1	exp.
		[51]	$^2S_{1/2}$	290.6±1.4	exp. (for hyperfine effects see ref 78)
		[79,80]	$^2S_{1/2}$	289.7±0.3	exp.
				289.7±0.3	**recommended**
20	Ca	[81]	$^1S_0$	160	R, CI, MBPT
		[82]	^{1}S	152.0	R, MVD, CCSD+T
		[55]	^1S	163	R, DK, CASPT2
		[83]	$^1S_0$	158.0	R, DK+SO, CCSD(T)
		[19]	$^1S_0$	154.58	R, Dirac, coupled cluster
		[20,56]	$^1S_0$	155.9	R, Dirac, CI+MBPT+ experimental data
		[57]	$^1S_0$	160.77	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[22]	$^1S_0$	157.03±0.80	R, Dirac, MBPT, CCSD
		[20]	$^1S_0$	157.1±1.3	Hybrid-RCI+MBPT sum rule
		[20]	$^1S_0$	159.0	R, Dirac, CI+MBPT
		[25]	^1S	159.4	Combination of *ab initio* and semi-empirical methods
		[53]	^1S	157	NR, MBPT4
		[77]	$^1S_0$	157.1	Combination of theoretical and experimental data
		[58]	^1S	153.7	NR, CI+pseudo-potential
		[21]	$^1S_0$	157.9±0.8	R, DK, CCSD(T)
		[124]	^1S	158.6	CI, oscillator strength correction
		[84,86]	$^1S_0$	169±17	exp.
				160.8±4.0	**recommended**

Z	Atom	Refs.	State	α_D	Comments
21	Sc	[85,86]	$^2D_{3/2}$, $3d^1$	120±30	R, Dirac, LDA
		[87,88]	^2D, $3d^1$	107.1	NR, small CI, VPA
		[89]	^2D, $3d^1$	138.8	NR, small CI, VPA
		[90]	^2D, $3d^1$	142±21	NR, MCPF
		[91]	^2D, $3d^1$	115.46	DFT
		[92]	^2D, $3d^1$	121±12	R, DK, MRCI
		[93]	^2D, $3d^1$	105.88	TD-DFT
		[94]	^2D, $3d^1$	114.00	Interacting-induced-dipoles polarization model
		[95]	^2D, $3d^1$	123	TD-DFT (LEXX)
		[66,96]	$^2D_{3/2}$, $3d^1$	106.0	SIC-DFT (RXH)
		[96]	^2D, $3d^1$	134.6	TD-DFT (PGG)
		[52]	$^2D_{3/2}$, $3d^1$	97.2±9.5	exp.
				97±10	**recommended**
22	Ti	[85,86]	$^3F_2$, $3d^2$	99±25	R, Dirac, LDA
		[87]	^3F, $3d^2$	91.8	NR, small CI, VPA
		[90]	^3F, $3d^2$	114±17	NR, MCPF
		[92]	$^3F_2$, $3d^2$	102±10	R, DK, MRCI
		[93]	^3F, $3d^2$	94.69	TD-DFT
		[87]	^3F, $3d^2$	91.4	NR, small CI, VPA
		[66]	^3F, $3d^2$	85.7	SIC-DFT
		[52]	$^3F_2$, $3d^2$	63.4±3.4	exp.
				100±10	**recommended**
23	V	[85,86]	$^4F_{3/2}$, $3d^3$	84±21	R, Dirac, LDA
		[87]	^4F, $3d^3$	80.6	NR, small CI, VPA
		[90]	^4F, $3d^3$	97±15	NR, MCPF
		[92]	$^4F_{3/2}$, $3d^3$	87.3±8.7	R, DK, MRCI
		[66]	^4F, $3d^3$	72.8	SIC-DFT
		[52]	$^4F_{3/2}$, $3d^{13}$	68.2±5.4	exp.
				87±10	**recommended**

Z	Atom	Refs.	State	α_D	Comments
24	Cr	[85,86]	$^7S_3$, $3d^5$	78±20	R, Dirac, LDA
		[90]	^7S, $3d^5$	95±15	NR, MCPF
		[97]	$^7S_3$, $3d^5$	78.4±7.8	DK, CASPT2
		[36]	$^7S_3$, $3d^5$	83.2	R, CCSD(T)
		[66]	^7S, $3d^5$	60.7	SIC-DFT
		[52]	$^7S_3$, $3d^5$	60±24	exp.
				83±12	**recommended**
25	Mn	[85,86]	$^6S_{5/2}$, $3d^5$	63±16	R, Dirac, LDA
		[87]	^6S, $3d^5$	65.4	NR, small CI, VPA
		[66]	^6S, $3d^5$	56.8	SIC-DFT
		[90]	^6S, $3d^5$	76±11	NR, MCPF
		[97]	$^6S_{5/2}$, $3d^5$	66.8±6.7	DK, CASPT2
		[36]	$^6S_{5/2}$, $3d^5$	68.5	R, CCSD(T)
				68±9	**recommended**
26	Fe	[85,86]	$^5D_4$, $3d^6$	57±14	R, Dirac, LDA
		[66]	$^5D_4$, $3d^6$	54.4	SIC-DFT
		[87]	^5D, $3d^6$	58.4	NR, small CI, VPA
		[90]	^5D, $3d^6$	63.93	NR, MCPF
		[98]	^5D, $3d^6$	62.65	NR, GGA(PW86)
				62±4	**recommended**
27	Co	[85,86]	$^4F_{9/2}$, $3d^7$	51±13	R, Dirac, LDA
		[87]	^4F, $3d^7$	52.3	NR, small CI, VPA
		[90]	^4F, $3d^7$	57.71	NR, MCPF
		[66]	$^4F_{9/2}$, $3d^7$	48.9	SIC-DFT
				55±4	**recommended**

Z	Atom	Refs.	State	α_D	Comments
28	Ni	[85,86]	$^3F_4$, $3d^8$	46±11	R, Dirac, LDA
		[87]	^3F, $3d^8$	48.3	NR, small CI, VPA
		[90]	^3F, $3d^8$	51.1±7.7	NR, MCPF
		[92]	$^3F_4$, $3d^8$	47.4±4.7	R, DK, MRCI
		[66]	$^3F_4$, $3d^8$	44.5	SIC-DFT
				49±3	**recommended**
29	Cu	[85,86]	$^2S_{1/2}$, $3d^{10}$	41±10	R, Dirac, LDA
		[90]	^2S, $3d^{10}$	53.44	NR, MCPF
		[99]	$^2S_{1/2}$, $3d^{10}$	45.0	R, PP, QCISD(T)
		[21,100]	$^2S_{1/2}$, $3d^{10}$	46.50±0.35	R, DK, CCSD(T)
		[97]	$^2S_{1/2}$, $3d^{10}$	40.7±4.1	R, DK, CASPT2
		[92]	$^2S_{1/2}$, $3d^{10}$	43.7±4.4	R, DK, MRCI
		[101]	^2S, $3d^{10}$	51.8	semi-empirical
		[102]	$^2S_{1/2}$, $3d^{10}$	46.98	R, DK, CCSD(T)
		[66]	$^2S_{1/2}$, $3d^{10}$	39.5	SIC-DFT
		[103,104]	$^2S_{1/2}$, $3d^{10}$	41.65	CICP
		[105]	$^2S_{1/2}$, $3d^{10}$	42.6	B3LYP/aug-cc-pVDZ
		[59,71]	$^2S_{1/2}$, $3d^{10}$	54.7±5.5	exp.
		[52]	$^2S_{1/2}$, $3d^{10}$	58.7±4.7	exp.
				46.5±0.5	**recommended**

Z	Atom	Refs.	State	α_D	Comments
30	Zn	[85,86]	$^1S_0$, $3d^{10}$	38±9	R, Dirac, LDA
		[106]	^1S, $3d^{10}$	39.2±0.8	NR, CCSD(T), MP2 basis correction
		[107]	^1S, $3d^{10}$	38.01	R, PP, CCSD(T)
		[108]	^1S, $3d^{10}$	37.6	R, MVD, CCSD(T)
		[97]	^1S, $3d^{10}$	38.4	R, DK, CASPT2
		[109]	$^1S_0$, $3d^{10}$	38.666±0.096	R, Dirac, CCSDT
		[21,108]	$^1S_0$, $3d^{10}$	38.35±0.29	R, MVD, CCSD(T)
		[110]	$^1S_0$, $3d^{10}$	38.75	R, PRCC(T)
		[66]	$^1S_0$, $3d^{10}$	37.7	SIC-DFT
		[111]	$^1S_0$, $3d^{10}$	39.12	R, MRCI, pseudo-potential
		[110,112]	$^1S_0$, $3d^{10}$	38.92	exp.
		[106]	$^1S_0$, $3d^{10}$	38.8±0.8	exp.
				38.67±0.30	**recommended**
31	Ga	[113]	^2P	54.9±1.0	NR, PNO-CEPA, M_L res.
		[30]	^2P	50.7	R, SF, MRCI, M_L res.
		[30]	$^2P_{1/2}/^2P_{3/2}$	49.9/51.6	R, Dirac, MRCI, M_J res.
		[114]	$^2P_{1/2}/^2P_{3/2}$	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)
		[115]	^2P	52.91±0.40	R, DK, CCSD(T)
		[67]	$^2P_{1/2}/^2P_{3/2}$	51.3±2.0/53.0±2.0	SI-SOCI, M_J res.
		[52]	$^2P_{1/2}$	46.6±4.0	exp.
				50±3	**recommended**
32	Ge	[113]	^3P	41.0	NR, PNO-CEPA, M_L res.
		[32]	^3P	40.16	R, DK, CCSD(T), M_L res. (M_L = 0: 32.83, M_L = 1: 43.83)
		[32]	$^3P_0$	39.43±0.80	R, Dirac Gaunt, CCSD(T)
		[66]	^3P	41.6	SIC-DFT
		[21]	$^3P_0$	40.80±0.82	R, PNO-CEPA
				40±1	**recommended**

Z	Atom	Refs.	State	α_D	Comments
33	As	[113]	^4S	29.1	NR, PNO-CEPA
		[33]	^4S	29.8±0.6	R, DK, CASPT2
		[36]	^4S	29.92	R, DK, CCSD(T)
		[66]	^4S	31.52	SIC-DFT
		[36]	^4S	29.81	ECP, CCSD(T)
				30±1	**recommended**
34	Se	[34]	^3P	26.24±0.52	R, MVD, CASPT2, M_L res.
		[66]	^3P	26.65	SIC-DFT
		[116]	$^3P_2$	28.9±1.0	exp.
				28.9±1.0	**recommended**
35	Br	[117]	$^2P_{1/2}$	21.9	R, DK, SO-CI
		[117]	$^2P_{3/2}$	21.8	R, DK, SO-CI, M_J *res.*
		[37]	^2P	21.03	R, MVD, CASPT2, M_L *res.*
		[21,37]	^2P	21.13±0.42	R, MVD, CASPT2
		[66]	^2P	21.5	SIC-DFT
				21±1	**recommended**
36	Kr	[73]	^1S	16.80±0.13	R, DK3, CCSD(T)
		[33]	^1S	16.6	R, DK, CASPT2
		[118]	$^1S_0$	16.012	R, Dirac, CCSD/T
		[119]	$^1S_0$	16.47	R, RPA, PolPot
		[120]	$^1S_0$	16.79	DOSD (constrained dipole oscillator strength distribution)
		[148]	$^1S_0$	16.736	R, DK3, CCSD(T)
		[121]	$^1S_0$	16.782±0.005	exp.
		[43]	$^1S_0$	16.766±0.008	exp.
		[45,73]	$^1S_0$	16.740	exp.
		[45]	$^1S_0$	16.734	exp.
				16.78±0.02	**recommended**

Z	Atom	Refs.	State	α_D	Comments
37	Rb	[48,77]	$^2S_{1/2}$	318.6±0.6	R, SD all orders + exp. data
		[76]	^2S	316.2±3.2	R, DK, CCSD(T), AE
		[16]	$^2S_{1/2}$	319±6	exp.
		[51]	$^2S_{1/2}$	318.8±1.4	exp.
		[79,80]	$^2S_{1/2}$	319.8±0.3	exp.
		[21]	$^2S_{1/2}$	319.2±6.1	exp.
				319.8±0.3	**recommended**
38	Sr	[21,81]	^1S	199.0±2.0	R, CI, MBPT
		[83]	$^1S_0$	199.4	R, DK+SO, CCSD(T)
		[19]	$^1S_0$	199.71	R, Dirac, coupled cluster
		[56,122]	$^1S_0$	197.2±3.6	R, Dirac, CI+MBPT+ experimental data
		[123]	$^1S_0$	197.6	CI+ core polarization (corrected to exp. term energies)
		[57]	$^1S_0$	190.82	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[22]	$^1S_0$	186.98±0.85	R, Dirac, MBPT, CCSD
		[124]	$^1S_0$	198.5±1.3	CI, oscillator strength correction
		[83]	$^1S_0$	198.85	R, DK, CCSD(T)
		[20]	$^1S_0$	202.0	Hybrid-RCI+MBPT sum rule
		[20,77]	$^1S_0$	197.2±0.2	Hybrid-RCI+MBPT sum rule
		[25]	$^1S_0$	201.2	Combination of *ab initio* and semi-empirical methods
		[27]	$^1S_0$	193.2	Model potential
		[86]	$^1S_0$	186±15	exp.
				197.2±0.2	**recommended**

Z	Atom	Refs.	State	α_D	Comments
39	Y	[85,86]	$^2D_{3/2}$, $4d^1$	153±38	R, Dirac, LDA
		[125]	$^2D_{3/2}$, $4d^1$	140.94	DFT, ECP
		[59,126]	$^2D_{3/2}$, $4d^1$	139±28	TD-DFT
		[96]	$^2D_{3/2}$, $4d^1$	134.9	SIC-DFT (RXH)
		[127]	$^2D_{3/2}$, $4d^1$	126.74	LR-CCSD
		[52]	$^2D_{3/2}$, $4d^1$	163±12	exp.
				162±12	**recommended**
40	Zr	[85,86]	$^3F_2$, $4d^2$	121±30	R, Dirac, LDA
		[127]	$^3F_2$, $4d^2$	119.97	LR-CCSD
		[52]	$^3F_2$, $4d^2$	112±13	exp.
				112±13	**recommended**
41	Nb	[85,86]	$^6D_{1/2}$, $4d^4$	106±27	R, Dirac, LDA
		[127]	$^6D_{1/2}$, $4d^4$	101.60	LR-CCSD
		[52]	$^6D_{1/2}$, $4d^4$	97.9±7.4	exp.
				98±8	**recommended**
42	Mo	[85,86]	$^7S_3$, $4d^5$	86±22	R, Dirac, LDA
		[59,97]	^7S, $4d^5$	73±11	R, DK, CASPT2
		[36]	$^7S_3$, $4d^5$	84	R, CCSD(T)
		[36]	$^7S_3$, $4d^5$	79	MRCI
		[127]	$^7S_3$, $4d^5$	88.42	LR-CCSD
		[52]	$^7S_3$, $4d^5$	87.1±6.1	exp.
		[128]	$^7S_3$, $4d^5$	61±10	exp.
				87±6	**recommended**
43	Tc	[85,86]	$^6S_{5/2}$, $4d^5$	77±20	R, Dirac, LDA
		[59,97]	^6S, $4d^5$	80±12	R, DK, CASPT2
		[95]	$^6S_{5/2}$, $4d^5$	79.6	TD-DFT (LEXX)
		[36]	$^6S_{5/2}$, $4d^5$	78.6	R, CCSD(T)
		[127]	$^6S_{5/2}$, $4d^5$	80.08	LR-CCSD
				79±10	**recommended**

Z	Atom	Refs.	State	α_D	Comments
44	Ru	[85,86]	$^5F_5$, $4d^7$	65±16	R, Dirac, LDA
		[95]	$^5F_5$, $4d^7$	72.3	TD-DFT (LEXX)
		[127]	$^5F_5$, $4d^7$	65.89	LR-CCSD
				72±10	**recommended**
45	Rh	[85,86]	$^4F_{9/2}$, $4d^8$	58±15	R, Dirac, LDA
		[95]	$^4F_{9/2}$, $4d^8$	66.4	TD-DFT (LEXX)
		[127]	$^4F_{9/2}$, $4d^8$	56.10	LR-CCSD
		[52]	$^4F_{9/2}$, $4d^8$	11±22	exp. (an unusually low value was obtained)
				66±10	**recommended**
46	Pd	[85,86]	$^1S_0$, $4d^{10}$	32±8	R, Dirac, LDA
		[129]	$^1S_0$, $4d^{10}$	26.14±0.10	CCSDTQP, DKH2+Gaunt, CBS
		[130]	^1S, $4d^{10}$	26.612	NR, ECP, CCSD(T)
		[131]	$^1S_0$, $4d^{10}$	24.581	R, DK
		[127]	$^1S_0$, $4d^{10}$	23.68	LR-CCSD
				26.14±0.10	**recommended**
47	Ag	[99,102]	^2S, $4d^{10}$	52.2	R, PP, QCISD(T)
		[21,100]	^2S, $4d^{10}$	52.46±0.52	R, DK, CCSD(T)
		[97]	^2S, $4d^{10}$	36.7±5.5	R, DK, CCSD(T)
		[101]	^2S, $4d^{10}$	55.2	Semi-empirical
		[100]	$^2S_{1/2}$, $4d^{10}$	55.3±0.5	R, DK, CCSD(T)
		[132]	$^2S_{1/2}$, $4d^{10}$	46.17	CICP
		[127]	$^2S_{1/2}$, $4d^{10}$	50.60	LR-CCSD
		[52]	$^2S_{1/2}$, $4d^{10}$	45.9±7.4	exp.
		[59]	$^2S_{1/2}$, $4d^{10}$	63.1±6.3	exp.
				55±8	**recommended**

Z	Atom	Refs.	State	α_D	Comments
48	Cd	[107]	^1S, $4d^{10}$	46.25	R, PP, CCSD(T)
		[108]	^1S, $4d^{10}$	46.8	R, MVD, CCSD(T)
		[97]	^1S, $4d^{10}$	46.9	R, DK, CASPT2
		[133]	$^1S_0$, $4d^{10}$	46.02±0.50	R, DHF, CCSD(T)
		[21,108]	$^1S_0$, $4d^{10}$	47.55±0.48	R, MVD, CCSD(T)
		[134]	$^1S_0$, $4d^{10}$	44.63	R, DHF, CPMP
		[109]	$^1S_0$, $4d^{10}$	45.86±0.15	R, DF, CCSD(T), MBPT3
		[127]	$^2S_{1/2}$, $4d^{10}$	39.70	LR-CCSD
		[135]	$^1S_0$, $4d^{10}$	49.7±1.6	exp.
		[136,137]	$^1S_0$, $4d^{10}$	45.3±1.4	exp.
		[137]	$^1S_0$, $4d^{10}$	48.2 ±1.1	exp.
				46±2	**recommended**
49	In	[138]	$^2P_{1/2}$	65.2	R, DFT
		[30]	^2P	66.7	R, SF, MRCI, M_L *res.*
		[30]	$^2P_{1/2}/^2P_{3/2}$	61.9/69.6	R, Dirac, MRCI, M_J res.
		[114]	$^2P_{1/2}/^2P_{3/2}$	62.0±1.9/69.8	R, Dirac, FSCC, M_J res. (J = 3/2: M_J = 3/2: 55.1, M_J = 1/2: 84.6)
		[139]	$^2P_{1/2}$	62.4	R, Dirac+Breit, CI+all-order
		[115]	$^2P_{1/2}$	68.67±0.69	R, DK, CCSD(T)
		[30,114]	$^2P_{1/2}$	61.5	CCSD(T)
		[67]	$^2P_{1/2}$	66.4±5.0/74.4±8.0	SI-SOCI, M_J res.
		[127]	$^2P_{1/2}$	70.22	LR-CCSD
		[140]	$^2P_{1/2}/^2P_{3/2}$	68.7±8.1	exp.
		[52]	$^2P_{1/2}$	62.1±6.1	exp.
				65±4	**recommended**

Z	Atom	Refs.	State	α_D	Comments
50	Sn	[85,86]	^3P	52±13	R, Dirac, LDA
		[32]	^3P	53.3±5.7	R, PP, 2nd order MBPT
		[32]	^3P	56.34	R, PP, CCSD(T), M_L res. (M_L = 0: 54.28, M_L = ±1: 59.36)
		[32]	$^3P_0$	52.9±2.1	R, Dirac+Gaunt, CCSD(T)
		[141]	$^3P_0$	54.48	R, PP, DFT, BP386
		[66]	^3P	57.5	SIC-DFT
		[127]	$^3P_0$	55.95	LR-CCSD
		[32]	$^3P_0$	42.4±11	exp.
		[52]	$^3P_0$	67.5±8.8	exp.
				53±6	**recommended**
51	Sb	[85,86]	^4S	45±11	R, Dirac, LDA
		[33]	^4S	42.2±1.3	R, DK, CASPT2
		[142]	^4S	42.55	NR, CCSD(T)
		[36]	^4S	43.03	ECP, CCSD(T)
		[66]	^4S	47.07	SIC-DFT
		[127]	$^3P_0$	43.67	LR-CCSD
				43±2	**recommended**
52	Te	[85,86]	^3P	37±4	R, LDA
		[21,143]	^3P	38.1±3.8	QR, MVD-HF, GTO basis set
		[66]	^3P	40.06	SIC-DFT
		[127]	^3P	37.65	LR-CCSD
				38±4	**recommended**

53	I	[117]	$^2P_{1/2}$	35.1	R, DK, SO-CI
		[117]	$^2P_{3/2}$	34.6	R, DK, SO-CI, M_J res.
		[21,117,143]	$^2P_{3/2}$	33.0±1.7	R, DK, SO-CI
		[66]	^2P	33.6	SIC-DFT
		[127]	^3P	35.00	LR-CCSD
		[144]	$^2P_{3/2}$	32.9±1.3	exp.
		[145]	$^2P_{3/2}$	33.4	exp.
				32.9±1.3	**recommended**
54	Xe	[41]	^1S	27.06±0.27	R, DK3, CCSD(T)
		[146]	$^1S_0$	27.36	R, SOPP, CCSD(T) + MP2 basis set correction
		[120]	$^1S_0$	27.16	DOSD (constrained dipole oscillator strength distribution)
		[33]	^1S	26.7	R, DK, CASPT2
		[118]	$^1S_0$	25.297	R, Dirac, CCSD/T
		[147]	$^1S_0$	27.42	R, DK3, CCSD(T)
		[119]	$^1S_0$	26.7	R, RPA, PolPot
		[148]	$^1S_0$	26.432	R, DK3, CCSD
		[44]	$^1S_0$	27.2937±0.0003	CCSD(T), ECP
		[149]	$^1S_0$	28.4±0.5	R, CCSD(T)
		[150]	$^1S_0$	27.508	R, CCSD(T)
		[127]	$^1S_0$	27.30	LR-CCSD
		[46]	$^1S_0$	27.078±0.050	exp.
		[75]	$^1S_0$	27.342	exp.
		[45]	$^1S_0$	27.292	exp.
				27.32±0.20	**recommended**

Z	Atom	Refs.	State	α_D	Comments
55	Cs	[48]	$^2S_{1/2}$	399.9±1.9	R, Dirac, SD, all orders + exp. data
		[76]	^2S	396.0±5.9	R, DK, CCSD(T), AE
		[151]	$^2S_{1/2}$	399.0	R, Dirac, CCSD(T)
		[152]	$^2S_{1/2}$	399.5±0.8	R, Dirac, RCC-SD
		[77]	$^2S_{1/2}$	399.8	Combination of theoretical and experimental data
		[153]	$^2S_{1/2}$	398.2±0.9	R, Dirac, SDpT
		[154]	$^2S_{1/2}$	398.4±0.7	R, DF, RPA, SD-all order
		[48]	$^2S_{1/2}$	401.5	R, SD all orders + exp. data for electronic transitions
		[155]	$^2S_{1/2}$	401.0±0.6	exp.
		[79,80]	$^2S_{1/2}$	400.8±0.4	exp.
				400.9±0.7	**recommended**
56	Ba	[20,81]	^1S	262.2	R, CI, MBPT
		[21,83]	$^1S_0$	273.5±4.1	R, DK+SO, CCSD(T)
		[19]	$^1S_0$	268.19	R, Dirac, coupled cluster
		[156]	$^1S_0$	272.7	R, Dirac+Gaunt, CCSD(T)
		[57]	$^1S_0$	274.68	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[119]	$^1S_0$	251	R, RPA, PolPot
		[27]	$^1S_0$	261.2	Model potential
		[157]	$^1S_0$	275.5±5.5	R, DK, CCSD(T)
		[20,77]	$^1S_0$	273.5±2.0	Hybrid-RCI+MBPT sum rule, recommended
		[20]	$^1S_0$	272.1	Hybrid-RCI+MBPT sum rule
		[127]	$^1S_0$	275	LR-CCSD
		[84]	$^1S_0$	268±22	exp.
				272±10	**recommended**

Z	Atom	Refs.	State	α_D	Comments
57	La	[85,86]	$^2D_{3/2}$, $5d^1$	210±52	R, Dirac, LDA
		[158]	$^2D_{3/2}$, $5d^1$	213.7	R, Dirac, CI+MBPT+CP(RPA); (α_D = 218.7 for the $5d^26s^1$ configuration)
		[126]	$^2D_{3/2}$, $5d^1$	201±40	TD-DFT
		[59,159]	$^2D_{3/2}$, $5d^1$	220±22	R, CASSCF, ECP
		[159]	$^2D_{3/2}$, $5d^1$	219.8	R, CASSCF, ECP
		[52]	$^2D_{3/2}$, $5d^1$	170.7±8.1	exp.
				215±20	**recommended**
58	Ce	[85,86]	$4f^15d^1$	200±50	R, Dirac, LDA
		[158]	$4f^15d^1$	204.7	R, Dirac, CI+MBPT+CP(RPA); (α_D = 223.4 for the $4f^2$ configuration)
		[126]	$4f^15d^1$	194±39	TD-DFT
		[52]	$^1G_4$, $4f^15d^1$	192±20	exp.
				205±20	**recommended**
59	Pr	[85,86]	$4f^3$	190±48	R, Dirac, LDA
		[158]	$4f^3$	215.8	R, Dirac, CI+MBPT+CP(RPA); (α_D = 195.7 for the $4f^25d^1$ configuration)
		[126]	$4f^3$	220±44	TD-DFT
		[52]	$^4I_{9/2}$, $4f^3$	239±28	exp.
				216±20	**recommended**
60	Nd	[85,86]	$4f^4$	212±53	R, Dirac, LDA
		[158]	$4f^4$	208.4	R, Dirac, CI+MBPT+CP(RPA); (α_D = 187.5 for the $4f^35d^1$ configuration)
		[126]	$4f^4$	213±43	TD-DFT
		[52]	$^5I_4$, $4f^4$	184±20	exp.
				208±20	**recommended**
61	Pm	[85,86]	$4f^5$	203±51	R, Dirac, LDA
		[158]	$4f^5$	200.2	R, Dirac, CI+MBPT+CP(RPA); (α_D = 179.3 for the $4f^45d^1$ configuration)
		[126]	$4f^5$	206±41	TD-DFT
				200±20	**recommended**

Z	Atom	Refs.	State	α_D	Comments
62	Sm	[85,86]	$4f^6$	194±48	R, Dirac, LDA
		[158]	$4f^6$	192.1	R, Dirac, CI+MBPT+CP(RPA); (α_D = 171.7 for the $4f^5 5d^1$ configuration)
		[126]	$4f^6$	200±40	TD-DFT
		[159]	$4f^6$	196.8	R, CASSCF, ECP
		[59,159]	$4f^6$	197±20	R, CASSCF, ECP
		[52]	$^7F_0$, $4f^6$	157±16	exp.
				192±20	**recommended**
63	Eu	[85,86]	$4f^7$	187±47	R, Dirac, LDA
		[158]	$4f^7$	184.2	R, Dirac, CI+MBPT+CP(RPA); (α_D = 164.7 for the $4f^6 5d^1$ configuration)
		[126]	$4f^7$	194±39	TD-DFT
		[159]	$4f^7$	189.4	R, CASSCF, ECP
		[59,159]	$4f^7$	189±19	R, CASSCF, ECP
		[52]	$^8S_{7/2}$, $4f^7$	155±25	exp.
				184±20	**recommended**
64	Gd	[85,86]	$4f^7 5d^1$	159±40	R, Dirac, LDA
		[158]	$4f^7 5d^1$	158.3	R, Dirac, CI+MBPT+CP(RPA); (α_D = 194.5 for the $4f^7 5d^2 6s^1$ configuration)
		[126]	$4f^7 5d^1$	161±32	TD-DFT
		[52]	$^9D_2$, $4f^7 5d^1$	176±26	exp.
				158±20	**recommended**
65	Tb	[85,86]	$4f^9$	172±43	R, Dirac, LDA
		[158]	$4f^9$	169.5	R, Dirac, CI+MBPT+CP(RPA); (α_D = 152.4 for the $4f^8 5d^1$ configuration)
		[126]	$4f^9$	181±36	TD-DFT
		[52]	$^6H_{15/2}$, $4f^9$	159±11	exp.
				170±20	**recommended**

Z	Atom	Refs.	State	α_D	Comments
66	Dy	[85,86]	$4f^{10}$	165±41	R, Dirac, LDA
		[158]	$4f^{10}$	162.7	R, Dirac, CI+MBPT+CP(RPA); (α_D = 148.3 for the $4f^9 5d^1$ configuration)
		[158]	$4f^{10}$	165	R, RPA, PolPot
		[119]	$4f^{10}$	168	R, RPA, PolPot
		[126]	$4f^{10}$	175±35	TD-DFT
		[160]	$^5I_8$, $4f^{10}$	164	exp.
		[52]	$^5I_8$, $4f^{10}$	157±11	exp.
				163±15	**recommended**
67	Ho	[85,86]	$4f^{11}$	159±40	R, Dirac, LDA
		[158]	$4f^{11}$	156.3	R, Dirac, CI+MBPT+CP(RPA); (α_D = 142.9 for the $4f^{10}5d^1$ configuration)
		[119]	$4f^{11}$	161	R, RPA, PolPot
		[126]	$4f^{11}$	170±34	TD-DFT
		[161]	$^4I_{15/2}$, $4f^{11}$	160	exp.
		[52]	$^4I_{15/2}$, $4f^{11}$	145±12	exp.
				156±10	**recommended**
68	Er	[85,86]	$4f^{12}$	153±38	R, Dirac, LDA
		[158]	$4f^{12}$	150.2	R, Dirac, CI+MBPT+CP(RPA); (α_D = 139.4 for the $4f^{11}5d^1$ configuration)
		[158]	$4f^{12}$	169	R, RPA, PolPot
		[119]	$4f^{12}$	154	R, RPA, PolPot
		[126]	$4f^{12}$	166±33	TD-DFT
		[162]	$4f^{12}$	141±7	R, HF, Darwin, SO
		[163]	$4f^{12}$	149	R, HF, Darwin, SO
		[163]	$^3H_6$, $4f^{12}$	155	exp.
		[52]	$^3H_6$, $4f^{12}$	217±39	exp.
				150±10	**recommended**

Z	Atom	Refs.	State	α_D	Comments
69	Tm	[85,86]	$4f^{13}$	147±37	R, Dirac, LDA
		[158]	$4f^{13}$	144.3	R, Dirac, CI+MBPT+CP(RPA); (α_D = 137.8 for the $4f^{12}5d^1$ configuration)
		[119]	$4f^{13}$	147	R, RPA, PolPot
		[126]	$4f^{13}$	161±32	TD-DFT
		[59,164]	$4f^{13}$	152±15	R, MR-ACQQ, ECP
		[159]	$4f^{13}$	152.2	R, CASSCF, ECP
		[52]	$^2F_{7/2}$, $4f^{13}$	130±16	exp.
				144±15	**recommended**
70	Yb	[85,86]	$^1S_0$, $4f^{14}$	142±36	R, Dirac, LDA
		[19]	$^1S_0$, $4f^{14}$	144.6±5.6	R, Dirac, coupled cluster
		[165]	$^1S_0$, $4f^{14}$	140.7±7.0	R, Dirac+Gaunt, CCSD(T)
		[166]	$^1S_0$, $4f^{14}$	141±6	R, Dirac, CI+MBPT+ experimental data, see also ref 173 for error estimates
		[167]	$^1S_0$, $4f^{14}$	142.6	ECP, CCSD(T)
		[158]	$^1S_0$, $4f^{14}$	138.9	R, Dirac, CI+MBPT+CP(RPA); (α_D = 312.2 for the $4f^{14}6s^16p^1$ configuration)
		[119]	$^1S_0$, $4f^{14}$	142	R, RPA, PolPot
		[168]	$^1S_0$, $4f^{14}$	144	R, CCSD, PolPot
		[169]	$^1S_0$, $4f^{14}$	141±2	R, CI+MBPT+RPA
		[170]	$^1S_0$, $4f^{14}$	141±4	R, DHF+Breit+QED, PP
		[59,164]	$^1S_0$, $4f^{14}$	145.3±4.4	R, Dirac, CCSD(T)
		[171]	$^1S_0$, $4f^{14}$	135.73	R, DFT, CAM-B3LYP, 2c-NESC
		[171]	$^1S_0$, $4f^{14}$	147.26	R, DFT, PBE0, 2c-NESC
		[165]	$^1S_0$, $4f^{14}$	140.44	R, Dirac, CCSD(T)
		[164]	$^1S_0$, $4f^{14}$	152.9	R, Dirac, CCSD(T)
		[172]	$^1S_0$, $4f^{14}$	143	R, DCHF, CCSD(T), ECP
		[126]	$^1S_0$, $4f^{14}$	157.3	TD-DFT
		[159]	$^1S_0$, $4f^{14}$	151.0	R, CASSCF, ECP
		[149]	$^1S_0$, $4f^{14}$	136±5	R, CCSD(T)
		[52]	$^1S_0$, $4f^{14}$	147±20	exp.
		[173]	$^1S_0$, $4f^{14}$	139.3±5.9	exp.
				139±6	**recommended**

Z	Atom	Refs.	State	α_D	Comments
71	Lu	[85,86]	$^2D_{3/2}$, $5d^1$	148±17	R, Dirac, LDA
		[158]	$^2D_{3/2}$, $5d^1$	137±7	R, Dirac, CI+MBPT+CP(RPA); (α_D = 61.3 for the $4f^{14}6s^26p^1$ configuration)
		[174]	$^2D_{3/2}$, $5d^1$	145	R, DF, CI+all-order+Breit+QED
		[126]	$^2D_{3/2}$, $5d^1$	131±26	TD-DFT
		[52]	$^2D_{3/2}$, $5d^1$	124±18	exp.
				137±7	**recommended**
72	Hf	[85,86]	$^3F_2$, $5d^2$	109±27	R, Dirac, LDA
		[174]	$^3F_2$, $5d^2$	97	R, DF, CI+all-order+Breit+QED
		[158,174]	$^3F_2$, $5d^2$	103±5	R, DF, CI+MBPT+Breit+QED
		[54,95]	$^3F_2$, $5d^2$	83.7	NR, MBPT4
		[127]	$^3F_2$, $5d^2$	99.52	LR-CCSD
		[52]	$^3F_2$, $5d^2$	84±19	exp.
				103±6	**recommended**
73	Ta	[85,86]	$^4F_{3/2}$, $5d^3$	88±22	R, Dirac, LDA
		[119]	$5d^3$	73.7	R, RPA, PolPot
		[95]	$^4F_{3/2}$, $5d^3$	73.9	TD-DFT (LEXX)
		[127]	$^4F_{3/2}$, $5d^3$	82.53	LR-CCSD
		[52]	$^4F_{3/2}$, $5d^3$	58±12	exp.
		[175]	$^4F_{3/2}$, $5d^3$	128±20	exp.
		[128]	$^4F_{3/2}$, $5d^3$	115±20	exp.
		[175]	$^4F_{3/2}$, $5d^3$	108±20	exp.
				74±20	**recommended**
74	W	[85,86]	$^5D_0$, $5d^4$	75±19	R, Dirac, LDA
		[119]	$5d^4$	68.1	R, RPA, PolPot
		[95]	$^5D_0$, $5d^4$	65.8	TD-DFT (LEXX)
		[127]	$^5D_0$, $5d^4$	71.04	LR-CCSD
		[128]	$^5D_0$, $5d^4$	47±7	exp.
				68±15	**recommended**

Z	Atom	Refs.	State	α_D	Comments
75	Re	[85,86]	$^6S_{5/2}$, $5d^5$	65±16	R, Dirac, LDA
		[97]	^6S, $5d^5$	61.1	DK, CASPT2
		[119]	$5d^5$	65.6	R, RPA, PolPot
		[95]	$^6S_{5/2}$, $5d^5$	60.2	TD-DFT (LEXX)
		[36]	$^6S_{5/2}$, $5d^5$	61.9	R, CCSD(T)
		[127]	$^6S_{5/2}$, $5d^5$	63.04	LR-CCSD
				62±3	**recommended**
76	Os	[85,86]	$^5D_4$, $5d^6$	57	R, Dirac, LDA
		[119]	$5d^6$	57.8	R, RPA, PolPot
		[95]	$^5D_4$, $5d^6$	55.3	TD-DFT (LEXX)
		[127]	$^5D_4$, $5d^6$	55.06	LR-CCSD
				57±3	**recommended**
77	Ir	[85,86]	$^4F_{9/2}$, $5d^7$	51±13	R, Dirac, LDA
		[119]	$5d^7$	51.7	R, RPA, PolPot
		[95]	$^4F_{9/2}$, $5d^7$	51.3	TD-DFT (LEXX)
		[127]	$^4F_{9/2}$, $5d^7$	42.51	LR-CCSD
		[175,176]	$^4F_{9/2}$, $5d^7$	54.0±6.7	exp.
				54±7	**recommended**
78	Pt	[85,86]	$^3D_3$, $5d^9$	44±11	R, Dirac, LDA
		[95]	$^3D_3$, $5d^9$	48.0	TD-DFT (LEXX)
		[127]	$^3D_3$, $5d^9$	39.68	LR-CCSD
				48±4	**recommended**

Z	Atom	Refs.	State	α_D	Comments
79	Au	[99,102,177]	^2S, $5d^{10}$	35.1	R, PP, QCISD(T)
		[21,100]	^2S, $5d^{10}$	36.06±0.54	R, DK, CCSD(T)
		[59,97]	^2S, $5d^{10}$	27.9±4.2	R, DK, CASPT2
		[178]	^2S, $5d^{10}$	34.9	R, DK, CCSD(T)
		[95]	$^2S_{1/2}$, $5d^{10}$	45.4	TD-DFT (LEXX)
		[179]	$^2S_{1/2}$, $5d^{10}$	30±4	R, HFR, HS, CI, CACP
		[127]	$^2S_{1/2}$, $5d^{10}$	36.50	LR-CCSD
		[59,71]	$^2S_{1/2}$, $5d^{10}$	49.1±4.1	exp.
		[97]	$^2S_{1/2}$, $5d^{10}$	39.1±9.8	exp.
				36±3	**recommended**
80	Hg	[107]	^1S, $5d^{10}$	34.42	R, PP, CCSD(T)
		[108]	^1S, $5d^{10}$	31.24	R, MVD, CCSD(T)
		[101]	^1S, $5d^{10}$	32.9	semi-empirical
		[97]	^1S, $5d^{10}$	33.3	R, DK, CASPT2
		[180]	$^1S_0$, $5d^{10}$	34.15	R, Dirac, CCSD(T)
		[181]	$^1S_0$, $5d^{10}$	34.27	R, Dirac, CCSDT+QED
		[119]	$^1S_0$, $5d^{10}$	39.1	R, RPA, PolPot
		[21,182]	$^1S_0$, $5d^{10}$	34.73±0.52	R, DK, CCSD(T)
		[183]	$^1S_0$, $5d^{10}$	34.1	R, Dirac, CCSD(T)
		[110]	$^1S_0$, $5d^{10}$	33.59	R, PRCC(T)
		[184]	$^1S_0$, $5d^{10}$	34.2±0.5	R, CCSD(T)+Breit
		[149]	$^1S_0$, $5d^{10}$	34.5±0.8	R, CCSD(T)
		[127]	$^1S_0$, $5d^{10}$	33.90	LR-CCSD
		[108,112,185]	$^1S_0$, $5d^{10}$	33.75	exp.
		[186]	$^1S_0$, $5d^{10}$	33.91±0.34	exp.
				33.91±0.34	**recommended**

Z	Atom	Refs.	State	α_D	Comments
81	Tl	[30]	^2P	70.0	R, SF, MRCI, M_L res.
		[30]	$^2P_{1/2}/^2P_{3/2}$	51.6/81.2	R, Dirac, MRCI, M_J res.
		[187]	$^2P_{1/2}$	52.3	R, Dirac, FS-CCSD
		[114]	$^2P_{1/2}/^2P_{3/2}$	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)
		[59,115]	^2P	71.7±1.1	R, DK, CCSD(T)
		[183,187]	^2P	51.3	R, Dirac, FS-CCSD
		[188,189]	^2P	49.2	RCI + MBPT
		[190]	^2P	48.81	R, Dirac, CI+MBPT
		[191]	^2P	47.78	R, Dirac+Breit+QED, SD+CI, RPA
		[192]	^2P	50.0±3.0	R, CC
		[192]	^2P	50.7	R, CI + all-order
		[114]	^2P	52.1±1.6	R, Dirac, FSCC
		[193]	^2P	50.4	R, DHF, SD, MBPT all-order
		[115]	^2P	50.48	R, DK, CCSD(T)
		[115]	^2P	50.62	R, DK, CCSD(T)
		[67]	$^2P_{1/2}/^2P_{3/2}$	50.7±5.0/78.5±6.0	SI-SOCI, M_J res.
		[127]	^2P	69.92	LR-CCSD
		[86]	$^2P_{1/2}$	51.3±5.4	exp.
				50±2	**recommended**
82	Pb	[85]	^3P	46±11	R, Dirac, LDA
		[194]	$^3P_0$	51.0	R, SOPP, CCSD(T)
		[32]	$^3P_0$	47.70	R, Dirac+Gaunt, CCSD(T)
		[180]	$^3P_0$	46.96	R, Dirac, CCSD(T)
		[32]	$^3P_0$	47.3±0.9	R, Dirac+Gaunt, CCSD(T)
		[183]	$^3P_0$	47.0	R, Dirac, FS-CCSD
		[191]	$^3P_0$	44.04	R, Dirac+Breit+QED, SD+CI, RPA
		[195]	$^3P_0$	46.5	R, CI + all-order, RPA
		[127]	$^3P_0$	61.80	LR-CCSD
		[32,86]	$^3P_0$	47.1±7.1	exp.
		[52]	$^3P_0$	56±18	exp.
				47±3	**recommended**

Z	Atom	Refs.	State	α_D	Comments
83	Bi	[85,86]	^4S	50±12	R, Dirac, LDA
		[33]	^4S	48.6	R, DK, CASPT2
		[196]	^4S	52.85	R, Cowan-Griffin, HF only
		[36]	^4S	48.75	ECP, CCSD(T)
		[191]	^4S	44.62	R, Dirac+Breit+QED, SD+CI, RPA
		[127]	^4S	49.02	LR-CCSD
		[52]	$^4S_{3/2}$	55±11	exp.
				48±4	**recommended**
84	Po	[85,86]	$^3P_2$	46	R, R, Dirac, LDA
		[196]	$^3P_2$	46.8	R, Cowan-Griffin, HF only, M_L res.
		[21,59,196]	$^3P_2$	43.6±4.4	R, Cowan-Griffin, HF only
		[127]	$^3P_2$	45.01	LR-CCSD
				44±4	**recommended**
85	At	[117]	$^2P_{1/2}$	45.6	R, DK, SO-CI
		[117]	$^2P_{3/2}$	43.0	R, DK, SO-CI, M_J res.
		[21,59,196]	$^2P_{3/2}$	40.7±2.0	R, Cowan-Griffin, HF only
		[127]	$^2P_{3/2}$	38.93	LR-CCSD
				42±4	**recommended**

Z	Atom	Refs.	State	α_D	Comments
86	Rn	[41]	^1S	33.18	R, DK3, CCSD(T)
		[146]	$^1S_0$	34.33	R, SOPP, CCSD(T) + MP2 basis set correction
		[194]	$^1S_0$	28.6	R, SOPP, CCSD(T)
		[33]	^1S	32.6	R, DK, CASPT2
		[119]	$^1S_0$	34.2	R, RPA, PolPot
		[178,197]	$^1S_0$	35.77	R, DK, CCSD(T)
		[197]	$^1S_0$	35.47	CCSD, ECP
		[148]	$^1S_0$	35.391	R, RPA, PolPot
		[183]	$^1S_0$	35.0	R, Dirac, CCSD(T)
		[85,86]	$^1S_0$	36±5	R, Dirac, LDA
		[198]	$^1S_0$	35.87	R, DFT, DC, PBE38
		[199]	$^1S_0$	34.89	R, DKH2, B3LYP, SARC
		[199]	$^1S_0$	34.70	R, DKH2, B3LYP, UGBS
		[146]	$^1S_0$	34.60	R, SOPP, CCSD(T) + MP2 basis set correction
		[198]	$^1S_0$	33.62	R, DFT, sfDC, PBE38
		[44]	$^1S_0$	34.4374±0.0001	CCSD(T), ECP
		[59,200]	$^1S_0$	35.04±1.8	R, Dirac, CCSD(T)
		[149]	$^1S_0$	37.0±0.5	R, CCSD(T)
		[201]	$^1S_0$	35.3	R, Dirac-Gaunt, CCSD(T)
		[127]	$^1S_0$	33.54	LR-CCSD
				35±2	**recommended**
87	Fr	[48,77]	$^2S_{1/2}$	317.8±2.4	R, Dirac, SD all orders + experimental data
		[76]	^2S	315.2	R, DK, CCSD(T), AE
		[151]	$^2S_{1/2}$	311.5	R, Dirac, CCSD(T)
		[127]	$^2S_{1/2}$	317.80	LR-CCSD
		[202]	$^2S_{1/2}$	316.8	exp.
				317.8±2.4	**recommended**

Z	Atom	Refs.	State	α_D	Comments
88	Ra	[21,83]	$^1S_0$	246.2±4.9	R, DK+SO, CCSD(T)
		[156]	$^1S_0$	242.8	R, Dirac+Gaunt, CCSD(T)
		[57]	$^1S_0$	242.42	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[119]	$^1S_0$	232	R, RPA, PolPot
		[83]	$^1S_0$	248.56	R, DK+SO, CCSD(T)
		[149]	$^1S_0$	236±15	R, CCSD(T)
		[127]	$^1S_0$	246.20	
				246±4	**recommended**
89	Ac	[85,86]	$^2D_{3/2}$, $6d^1$	217±44	R, Dirac, LDA
		[158]	$^2D_{3/2}$, $6d^1$	203.3	R, Dirac, CI+MBPT+CP(RPA); (α_D = 141.9 for the $7s^27p^1$ configuration)
				203±12	**recommended**
90	Th	[85,86]	$6d^2$	217±54	R, Dirac, LDA
				217±54	**recommended**
91	Pa	[85,86]	$5f^26d^1$	171±34	R, Dirac, LDA
		[158]	$5f^26d^1$	154.4	R, Dirac, CI+MBPT+CP(RPA); (α_D = 151.9 for the $5f^26d^27s^1$ configuration)
				154±20	**recommended**
92	U	[85,86]	$5f^36d^1$	153±38	R, Dirac, LDA
		[158]	$5f^36d^1$	127.8	R, Dirac, CI+MBPT+CP(RPA); (α_D = 153.2 for the $5f^4$ configuration)
		[203]	$^5L_6$, $5f^36d^1$	137±9	exp.
				129±17	**recommended**
93	Np	[85,86]	$5f^46d^1$	167±42	R, Dirac, LDA
		[158]	$5f^46d^1$	150.5	R, Dirac, CI+MBPT+CP(RPA); (α_D = 127.5 for the $5f^5$ configuration)
				151±20	**recommended**
94	Pu	[85,86]	$5f^6$	165±41	R, Dirac, LDA
		[158]	$5f^6$	132.2	R, Dirac, CI+MBPT+CP(RPA); (α_D = 147.6 for the $5f^56d^1$ configuration)
				132±20	**recommended**

Z	Atom	Refs.	State	α_D	Comments
95	Am	[85,86]	$5f^7$	157±39	R, Dirac, LDA
		[204]	$5f^7$	116±29	R, DK, CASPT2
		[158]	$5f^7$	131.2	R, Dirac, CI+MBPT+CP(RPA); (α_D = 144.7 for the $5f^6 6d^1$ configuration)
		[205]	$5f^7$	122.4	R, DFT, DKH, B3LYP
				131±25	**recommended**
96	Cm	[85,86]	$5f^7 6d^1$	155±39	R, Dirac, LDA
		[158]	$5f^7 6d^1$	143.6	R, Dirac, CI+MBPT+CP(RPA); (α_D = 128.6 for the $5f^8$ configuration)
				144±25	**recommended**
97	Bk	[85,86]	$5f^9$	153±38	R, Dirac, LDA
		[158]	$5f^9$	125.3	R, Dirac, CI+MBPT+CP(RPA); (α_D = 141.6 for the $5f^8 6d^1$ configuration)
				125±25	**recommended**
98	Cf	[85,86]	$5f^{10}$	138±34	R, Dirac, LDA
		[158]	$5f^{10}$	121.5	R, Dirac, CI+MBPT+CP(RPA); (α_D = 142.3 for the $5f^9 6d^1$ configuration)
				122±20	**recommended**
99	Es	[85,86]	$5f^{11}$	133±33	R, Dirac, LDA
		[158]	$5f^{11}$	117.5	R, Dirac, CI+MBPT+CP(RPA); (α_D = 146.1 for the $5f^{10} 6d^1$ configuration)
				118±20	**recommended**
100	Fm	[85,86]	$5f^{12}$	161±40	R, Dirac, LDA
		[158]	$5f^{12}$	113.4	R, Dirac, CI+MBPT+CP(RPA); (α_D = 155.6 for the $5f^{11} 6d^1$ configuration)
				113±20	**recommended**
101	Md	[85,86]	$5f^{13}$	123±31	R, Dirac, LDA
		[158]	$5f^{13}$	109.4	R, Dirac, CI+MBPT+CP(RPA); (α_D = 179.6 for the $5f^{12} 6d^1$configuration)
				109±20	**recommended**

Z	Atom	Refs.	State	α_D	Comments
102	No	[85,86]	$^1S_0$, $5f^{14}$	118±30	R, Dirac, LDA
		[165]	$^1S_0$, $5f^{14}$	110.8±5.5	R, Dirac+Gaunt, CCSD(T)
		[158]	$^1S_0$, $5f^{14}$	105.4	R, Dirac, CI+MBPT+CP(RPA); (α_D = 267.8 for the $5f^{14}7s^17p^1$ configuration)
		[119]	$^1S_0$, $5f^{14}$	114	R, RPA, PolPot
		[158,174]	$^1S_0$, $5f^{14}$	112±6	R, DF, CI+MBPT+Breit+QED
		[158,174]	$^1S_0$, $5f^{14}$	110±8	R, DF, CI+all-order+Breit+QED
		[171]	$^1S_0$, $5f^{14}$	107.77	R, DFT, CAM-B3LYP, 2c-NESC
		[165]	$^1S_0$, $5f^{14}$	115.64	R, DK, CCSD(T)
		[205]	$^1S_0$, $5f^{14}$	115.6	R, DFT, DKH, B3LYP
				110±6	**recommended**
103	Lr	[174]	$7p^1$	323±80	R, DF, CI+all-order+Breit+QED
		[174]	$7p^1$	320±80	R, DF, CI+MBPT+Breit+QED
		[206]	$7p^1$	225.2	R, DK, DFT, CAM-B3LYP
				320±20	**recommended**
104	Rf	[174]	$6d^2$	107±5	R, DF, CI+MBPT+Breit+QED
		[174]	$6d^2$	115±13	R, DF, CI+all-order+Breit+QED
				112±10	**recommended**
105	Db	[119]	$6d^3$	42.5	R, RPA, PolPot
		[119]	$6d^3$	42±4	R, RPA, PolPot (value recommended by authors)
				42±4	**recommended**
106	Sg	[119]	$6d^4$	40.7	R, RPA, PolPot
		[119]	$6d^4$	40±4	R, RPA, PolPot (value recommended by authors)
				40±4	**recommended**
107	Bh	[119]	$6d^5$	38.4	R, RPA, PolPot
		[119]	$6d^5$	38±4	R, RPA, PolPot (value recommended by authors)
				38±4	**recommended**
108	Hs	[119]	$6d^6$	36.2	R, RPA, PolPot
		[119]	$6d^6$	36±4	R, RPA, PolPot (value recommended by authors)
				36±4	**recommended**

Z	Atom	Refs.	State	α_D	Comments
109	Mt	[119]	$6d^7$	34.2	R, RPA, PolPot
		[119]	$6d^7$	34±3	R, RPA, PolPot (value recommended by authors)
				34±3	**recommended**
110	Ds	[119]	$6d^8$	32.3	R, RPA, PolPot
		[119]	$6d^8$	32±3	R, RPA, PolPot (recommended value by authors)
				32±3	**recommended**
111	Rg	[119]	$6d^9$	30.6	R, RPA, PolPot
		[119]	$6d^9$	30±3	R, RPA, PolPot (value recommended by authors)
		[207]	$6d^9$	31.6	ARPP CCSD(T)
				32±6	**recommended**
112	Cn	[107]	$^1S_0$, $6d^{10}$	25.82	R, PP, CCSD(T)
		[194]	$^1S_0$, $6d^{10}$	28.68	R, SOPP, CCSD(T)
		[180]	$^1S_0$, $6d^{10}$	27.64	R, Dirac, CCSD(T)
		[119]	$^1S_0$, $6d^{10}$	28.2	R, RPA, PolPot
		[180]	$^1S_0$, $6d^{10}$	27.40	R, Dirac, CCSD(T)
		[119]	$^1S_0$, $6d^{10}$	28±4	R, RPA, PolPot (value recommended by authors)
				28±2	**recommended**
113	Nh	[187]	$^2P_{1/2}$	29.85	R, Dirac, FS-CCSD
		[191]	$^2P_{1/2}$	28.8	R, Dirac+Breit+QED, SD+CI, RPA
				29±2	**recommended**
114	Fl	[194]	$^3P_0$	34.35	R, SOPP, CCSD(T)
		[32]	$^3P_0$	31.98	R, Dirac+Gaunt, CCSD(T)
		[180]	$^3P_0$	30.59	R, Dirac, CCSD(T)
		[180]	$^3P_0$	29.52	estimate
		[191]	$^3P_0$	31.4	R, Dirac+Breit+QED, SD+CI, RPA
		[32]	$^3P_0$	31.0	R, Dirac+Gaunt, CCSD(T)
				31±4	**recommended**

115	Mc	[191]	$^4S_{3/2}$	70.5 **71±20**	R, Dirac+Breit+QED, SD+CI, RPA **recommended**
116	Lv		$^3P_2$	-	No value currently available
117	Ts	[208]	$^2P_{3/2}$	76.3 **76±15**	empirical estimate **recommended**
118	Og	[194] [200] [119] [209] [119]	$^1S_0$ $^1S_0$ $^1S_0$ $^1S_0$ $^1S_0$	52.4 46.33 59.0/57.2 57.98 57±3 **58±6**	R, SOPP, CCSD(T) R, Dirac, CCSD(T) R, RPA, PolPot R, Dirac+Gaunt, CCSD(T) R, RPA, PolPot **recommended**
119	Uue	[76] [151] [76] [12]	^2S $^2S_{1/2}$ ^2S ^2S	163.7 169.7 166.0 169 **169±4**	R, DK, CCSD(T), ARPP R, Dirac, CCSD(T) R, DK, CCSD(T), AE R, Dirac, CCSD(T) **recommended**
120	Ubn	[156] [119] [119]	$^1S_0$ $^1S_0$ $^1S_0$	162.6 147 159±10 **159±10**	R, Dirac+Gaunt, CCSD(T) R, RPA, PolPot R, RPA, PolPot **recommended**

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