2023 Table of Dipole Polarizability

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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 $\pm$ 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. $= 0.1481847113\,\text{Å}^3 = 1.6487773 \times 10^{-41}\,\text{C m}^2/\text{V}$.

Z	Atom	Refs.	State	α	Year	Comments
1	H	[2]	^2S	4.5	1989	NR, exact
		[2,3]	$^2S_{1/2}$	4.49975145989	2012	R, Dirac, variational, Slater/B-splines (more digits are given in Ref. 3)
		[3]	$^2S_{1/2}$	4.500170623	2012	R, Dirac (as above), but with finite mass correction added for the ^{1}H isotope
		[4]	$^2S_{1/2}$	4.4997519518	2014	R, Dirac, Lagrange mesh method (more digits are given in this paper)
		[5]	$^2S_{1/2}$	4.50711 ± 0.00003	2019	recommended
		[6]	$^2S_{1/2}$	4.511 ± 0.004	2024	NR, neural network QMC, DS (DeepSolid) method
2	He	[7,8]	$^1S_0$	1.383746 ± 0.000007	1992	exp.

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Z	Atom	Refs.	State	α	Year	Comments
		[9]	$^1S_0$	1.383191	2000	R, Dirac, Breit-Pauli, QED, mass pol, correlated basis (^{4}He)
		[10]	$^1S_0$	$1.38376079 \pm 0.00000023$	2004	R, Dirac, Breit-Pauli, QED, mass pol, exponentially correlated Slater functions (^{4}He)
		[11]	$^1S_0$	1.383759 ± 0.000013	2007	exp.
		[12]	$^1S_0$	$1.3837295330 \pm 0.000000001$	2016	R, Dirac, Breit, QED, recoil, ... (^{4}He)
		[13]	$^1S_0$	1.3837616 ± 0.0000027	2018	exp.
		[5]	$^1S_0$	1.38375 ± 0.00002	2019	recommended
		[14]	$^1S_0$	$1.38376078 \pm 0.00000014$	2020	R, Dirac, Breit-Pauli, QED + finite nuclear size correction
3	Li	[15]	$^2S_{1/2}$	164.0 ± 3.4	1974	exp.
		[16,17]	^2S	164.05	2001	NR, exponentially correlated Gaussians [18] + R/DK
		[19]	$^2S_{1/2}$	164.2 ± 1.1	2006	exp.
		[20]	$^2S_{1/2}$	164.21	2007	Frozen core Hamiltonian, semi-empirical polarisation potential
		[21]	$^2S_{1/2}$	164.084	2008	R, Dirac, MBPT, Breit, QED, recoil (^{7}Li)
		[22]	$^2S_{1/2}$	164.1125 ± 0.0005	2011	Hyleraas basis, RMW + Darwin + Breit, QED, recoil (^{7}Li)
		[5]	$^2S_{1/2}$	164.1125 ± 0.0005	2019	recommended
		[23]	$^2S_{1/2}$	164.2	2021	NR, CCSD(T)
		[24]	$^2S_{1/2}$	162.00 ± 0.24	2022	R, Dirac-HF, pertubative singles + doubles method, RPA
		[6]	$^2S_{1/2}$	165.0 ± 0.1	2024	NR, neural network QMC, DS (DeepSolid) method
4	Be	[1]	$^1S_0$	37.29	1984	All-electron SCF plus valence CI
		[25]	$^1S_0$	37.73 ± 0.05	1997	CCSD(T)
		[26]	$^1S_0$	37.9	2000	Model potential
		[16]	^1S	37.755	2001	NR, exponentially correlated Gaussians [18]
		[27]	$^1S_0$	37.69	2003	Combination of ab initio and semi-empirical methods
		[28]	$^1S_0$	37.807	2004	CI, expanded London formula
		[29]	$^1S_0$	37.76 ± 0.22	2006	R, Dirac, CI + MBPT2 + experimental data

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Z	Atom	Refs.	State	α	Year	Comments
		[16,30]	$^1S_0$	37.739 ± 0.030	2006	R correction of -0.016 applied to value from ref [16]
		[31]	$^1S_0$	37.80 ± 0.47	2008	R, Dirac, CCSD
		[32]	$^1S_0$	37.86 ± 0.17	2013	R, Dirac, MBPT, CCSD
		[33,34]	$^1S_0$	37.73 ± 0.04	2015	Combination of theoretical (CICP) and experimental data
		[35]	$^1S_0$	37.75	2019	NR, CCSD
		[36]	$^1S_0$	37.69/37.71	2019	CCSD(T), R X2C-0/NR-0
		[5]	$--$	37.74 ± 0.03	2019	recommended
		[23]	$^1S_0$	37.7	2021	NR, CCSD(T)
		[37]	$^1S_0$	37.614	2021	R, MCDHF
		[38]	$^1S_0$	37.787	2023	R, DF, CICP (CP: core polarization)
		[6]	$^1S_0$	37.58 ± 0.03	2024	NR, neural network QMC, DS (DeepSolid) method
5	B	[39]	^2P	20.47	1976	NR, PNO-CEPA, M_L res.
		[40]	^2P	20.43 ± 0.11	1998	NR, CCSD(T), M_L res.
		[41]	^2P	20.59	2005	R, SF, MRCI, M_L res.
		[41]	$^2P_{1/2}/^2P_{3/2}$	20.53/20.54	2005	R, Dirac, MRCI, M_J res.
		[35]	^2P	20.42	2019	NR, CCSD
		[5]	$--$	20.5 ± 0.1	2019	recommended
		[42]	^2P	20.480	2021	NR, CCSD(T), CBS(T, Q), CBS(Q, 5)
		[43]	^2P	20.30 ± 0.26	2021	NR, CCSD(T)
6	C	[44]	^3P	11.39	1992	NR, CASPT2, M_L res.
		[40]	^3P	11.67 ± 0.07	1998	NR, CCSD(T), M_L res.
		[45]	$^3P_0$	11.26 ± 0.20	2008	R, Dirac + Gaunt, CCSD(T)
		[35]	^3P	11.63	2019	NR, CCSD
		[5]	$--$	11.3 ± 0.2	2019	recommended
		[43]	^3P	11.64 ± 0.15	2021	NR, CCSD(T)

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Z	Atom	Refs.	State	α	Year	Comments
		[42]	^3P	11.683	2021	NR, CCSD(T), CBS(T, Q)
		[42]	^3P	11.324	2021	NR, CCSD(T), CBS(Q, 5)
		[46]	^3P	11.542	2021	R, CCSD(T)
		[47]	^3P	11.61	2023	R, CCC (convergent close-coupling method)
7	N	[15,48]	$^4S_{3/2}$	7.6 ± 0.4	1974	exp.
		[39]	^4S	7.43	1976	NR, PNO-CEPA
		[49]	^4S	7.36	1995	NR, numerical MCSCF, M. res.
		[40]	^4S	7.26 ± 0.05	1998	NR, CCSD(T)
		[50]	^4S	7.41	2004	R, DK, CASPT2
		[51,52]	$^4S_{3/2}$	7.28	2010	exp.
		[35]	^4S	7.21	2019	NR, CCSD
		[5]	$--$	7.4 ± 0.2	2019	recommended
		[53]	^4S	7.2	2020	AE, CCSD(T)
		[43]	^4S	7.25 ± 0.09	2021	NR, CCSD(T)
		[42]	^4S	7.367	2021	NR, CCSD(T), CBS(T, Q)
		[42]	^4S	7.153	2021	NR, CCSD(T), CBS(Q, 5)
		[46]	^4S	7.178	2021	R, CCSD(T)
		[6]	^4S	7.189 ± 0.008	2024	NR, neural network QMC, DS (DeepSolid) method
8	O	[48]	$^3P_2$	5.2 ± 0.4	1959	exp.
		[44]	^3P	5.4	1992	NR, CASPT2, M_L res.
		[39,54]	^3P	5.41 ± 0.11	2004	NR, PNO-CEPA, M_L res.
		[30,40]	^3P	5.24 ± 0.04	2006	NR, CCSD(T), M_L res.
		[35]	^3P	5.15	2019	NR, CCSD
		[5]	$--$	5.3 ± 0.2	2019	recommended
		[43]	^3P	5.21 ± 0.07	2021	NR, CCSD(T)

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Z	Atom	Refs.	State	α	Year	Comments
		[42]	^3P	5.145	2021	NR, CCSD(T), CBS(T, Q)
		[6]	^3P	5.236 ± 0.008	2024	NR, neural network QMC, DS (DeepSolid) method
9	F	[39]	^2P	3.76	1976	NR, PNO-CEPA, M_L res.
		[40]	^2P	3.70 ± 0.03	1998	NR, CCSD(T), M_L res.
		[55]	^2P	3.76 ± 0.06	2000	NR, CASPT2, M_L res.
		[35]	^2P	3.62	2019	NR, CCSD
		[5]	$--$	3.74 ± 0.08	2019	recommended
		[43]	^2P	3.68 ± 0.05	2021	NR, CCSD(T)
		[42]	^2P	3.701	2021	NR, CCSD(T), CBS(T, Q)
		[42]	^2P	3.655	2021	NR, CCSD(T), CBS(Q, 5)
		[6]	^2P	3.776 ± 0.007	2024	NR, neural network QMC, DS (DeepSolid) method
10	Ne	[39]	^1S	2.676	1976	NR, PNNO-CEPA, M_L res.
		[56]	$^1S_0$	2.6669 ± 0.0008	1991	exp.
		[57]	^1S	2.68	1992	NR, CCSD(T)
		[58]	$^1S_0$	2.663	1997	exp.
		[59]	$^1S_0$	2.66053 ± 0.00001	2001	CCSD(T), ECP
		[60]	^1S	2.665	2003	NR, CC3
		[60–62]	^1S	2.666	2003	R, CC3 + FCI + DK3 correction
		[30]	$^1S_0$	2.661 ± 0.005	2006	R, CCSD(T)
		[63]	$^1S_0$	2.66110 ± 0.00003	2010	exp.
		[64,65]	$^1S_0$	2.677 ± 0.070	2012	R, Dirac-Coulomb, non-linear PRCC
		[13]	$^1S_0$	2.6610570 ± 0.0000064	2018	exp.
		[5]	$--$	2.66110 ± 0.00003	2019	recommended
		[66]	$^1S_0$	2.66080 ± 0.00036	2020	R, QED, AE-CCSD(T), finite nucl. mass & size corrections
		[43]	^1S	2.662 ± 0.034	2021	NR, CCSD(T)

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Z	Atom	Refs.	State	α	Year	Comments
		[67]	$^1S_0$	2.661067 ± 0.000077	2022	R, QED, AE-CCSDT(Q), finite nucl. mass & size corrections
		[47]	$^1S_0$	2.661 ± 0.005	2023	R, CCSD(T)
11	Na	[68]	$^2S_{1/2}$	162.7 ± 0.5	1995	exp.
		[69]	$^2S_{1/2}$	162.6 ± 0.3	1999	R, SD all orders + exp. data
		[30,70]	$^2S_{1/2}$	162.88 ± 0.60	2006	R, CCSD(T)
		[71]	$^2S_{1/2}$	$162.7 \pm 0.1/ \pm 1.2$	2010	exp.
		[72]	$^2S_{1/2}$	161 ± 7.5	2015	exp.
		[5]	$--$	162.7 ± 0.5	2019	recommended
		[23]	$^2S_{1/2}$	163.9	2021	NR, CCSD(T)
		[24]	$^2S_{1/2}$	162.44 ± 0.16	2022	R, Dirac-HF, pertubative singles + doubles method, RPA
12	Mg	[73]	$^1S_0$	71.5 ± 3.5	1973	exp.
		[74]	^1S	71.32	1976	NR, PNO-CEPA
		[75]	$^1S_0$	70.5	1979	NR, CI + pseudo-potential
		[76]	^1S	71.7	1991	NR, MBPT4
		[77]	^1S	71.8	1991	NR, MBPT4
		[49,78]	$^1S_0$	75.0 ± 3.5	1995	exp.
		[69]	$^1S_0$	74.9 ± 2.7	1999	Hybrid-RCI + MBPT sum rule
		[26]	$^1S_0$	72.0	2000	Model potential
		[79]	$^1S_0$	71.4	2002	CI, oscillator strength correction
		[27]	$^1S_0$	71.35	2003	Combination of ab initio and semi-empirical methods
		[80]	^1S	70.90	2004	R, DK, CASPT2
		[29,81]	$^1S_0$	70.89	2006	R, Dirac, CI + MBPT2 + experimental data
		[30]	$^1S_0$	71.22 ± 0.36	2006	R, DK, CCSD(T)
		[29]	$^1S_0$	71.33	2006	R, Dirac, CI + MBPT2
		[29]	$^1S_0$	71.3 ± 0.7	2006	R, Dirac, CI + MBPT2, recommended

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Z	Atom	Refs.	State	α	Year	Comments
		[31]	$^1S_0$	73.4 ± 2.3	2008	R, Dirac, CCSD
		[82]	$^1S_0$	77.6 ± 7.8	2012	exp.
		[32]	$^1S_0$	72.54 ± 0.50	2013	R, Dirac, MBPT, CCSD
		[83]	$^1S_0$	70.76	2014	R, Dirac + Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[72]	$^1S_0$	59 ± 16	2015	exp.
		[36]	$^1S_0$	71.15/71.63	2019	CCSD(T), R X2C-0/NR-0
		[36]	$^1S_0$	71.02/71.01	2019	CCSD(T), R X2C-2/NR-2
		[84]	$^1S_0$	73.0	2019	R, KRCISD/aug-QZ
		[5]	$--$	71.2 ± 0.4	2019	recommended
		[85]	$^1S_0$	71.9	2020	R, MCDF
		[46]	$^1S_0$	72.121	2021	R, CCSD(T)
		[86]	$^1S_0$	71.643	2021	R, CCSD(T)
		[23]	$^1S_0$	71.5	2021	NR, CCSD(T)
		[87]	$^1S_0$	81 ± 17	2022	exp.
13	Al	[78]	^2P	62.0	1971	NR, numerical MCSCF, M_L res.
		[74]	^2P	56.27	1976	NR, PNO-CEPA
		[88]	^2P	59.47	1980	NR, MRCI
		[89][92]	^2P	46 ± 2	1990	exp. (see also ref [72])
		[90]	^2P	61.0	2004	SIC-DFT
		[91]	^2P	58.0 ± 0.4	2004	CCSD(T)
		[92]	^2P	57.74	2005	NR, CCSD(T), M_L res.
		[41]	^2P	55.5	2005	R, SF, MRCI, M_L res.
		[41]	$^2P_{1/2}/^2P_{3/2}$	$55.4 \pm 2.2/55.9 \pm 2.2$	2005	R, Dirac, MRCI, M_J res.
		[30]	^2P	57.79 ± 0.30	2006	R, DK, CCSD(T)

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Z	Atom	Refs.	State	α	Year	Comments
		[93]	$^2P_{1/2}/^2P_{3/2}$	$57.8 \pm 1.0/58.0 \pm 1.0$	2010	SI-SOCI, M_L res.
		[82,94]	^2P	55.3 ± 5.5	2012	exp.
		[95]	^2P	58.3	2016	SIC-DFT (RXH)
		[35]	^2P	57.85	2019	NR, CCSD
		[5]	$--$	57.8 ± 1.0	2019	recommended
		[46]	^2P	58.089	2021	R, CCSD(T)
		[86]	^2P	48.455	2021	R, CCSD(T)
		[96]	$^2P_{1/2}/^2P_{3/2}$	$58.8 \pm 1.2/64.7 \pm 1.3$	2022	R, Breit+QED, CCSD
		[87]	^2P	54 ± 11	2022	exp.
		[97]	^2P	54.9 ± 5.3	2022	exp.
		[43,98]	^2P	47.69 ± 0.82	2023	NR, CCSD(T)
14	Si	[74]	^3P	36.32	1976	NR, PNO-CEPA, M_L res.
		[88]	^3P	36.95	1980	NR, MRCI
		[44]	^3P	36.54	1992	NR, CASPT2, M_L res.
		[49]	^3P	38.8	1995	NR, numerical MCSCF, M_L res.
		[99]	^3P	37.4 ± 0.1	2003	NR, CCSD(T), M_L res.
		[90]	^3P	38.9	2004	SIC-DFT
		[92]	^3P	37.17 ± 0.21	2005	NR, CCSD(T), M_L res.
		[45]	$^3P_0$	37.31 ± 0.70	2008	R, Dirac + Gaunt, CCSD(T)
		[95]	^3P	37.8	2016	SIC-DFT (RXH)
		[35]	^3P	37.16	2019	NR, CCSD
		[5]	$--$	37.3 ± 0.7	2019	recommended
		[43]	^3P	36.90 ± 0.63	2021	NR, CCSD(T)
		[46]	^3P	36.803	2021	R, CCSD(T)
15	P	[74]	^4S	24.7 ± 0.5	1976	NR, PNO-CEPA

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Z	Atom	Refs.	State	α	Year	Comments
		[44]	^4S	24.6 ± 0.2	1992	NR, CASPT2
		[49]	^4S	25.5	1995	NR, numerical MCSCF, M_L res.
		[50]	^4S	24.9	2004	R, DK, CASPT2
		[90]	^4S	26.11	2004	SIC-DFT
		[92]	^4S	24.93 ± 0.15	2005	NR, CCSD(T)
		[52]	^4S	25.06	2010	R, DK, CASPT2
		[95]	^4S	25.3	2016	SIC-DFT (RXH)
		[35]	^4S	24.88	2019	NR, CCSD
		[5]	$--$	25 ± 1	2019	recommended
		[53]	^4S	25.0	2020	AE, CCSD(T)
		[43]	^4S	24.95 ± 0.43	2021	NR, CCSD(T)
		[46]	^4S	24.980	2021	R, CCSD(T)
16	S	[74]	^3P	19.60	1976	NR, PNO-CEPA, M_L res.
		[44]	^3P	19.6	1992	NR, CASPT2, M_L res.
		[55]	^3P	19.6	2000	NR, CASPT2, M_L res.
		[90]	^3P	19.72	2004	SIC-DFT
		[92]	^3P	19.37 ± 0.12	2005	NR, CCSD(T), M_L res.
		[35]	^3P	19.22	2019	NR, CCSD(T)
		[5]	$--$	19.4 ± 0.1	2019	recommended
		[43]	^3P	19.38 ± 0.33	2021	NR, CCSD(T)
17	Cl	[74]	^2P	14.71	1976	NR, PNO-CEPA, M_L res.
		[44]	^2P	14.6	1992	NR, CASPT2, M_L res.
		[55]	^2P	14.73	2000	NR, CASPT2, M_L res.
		[90]	^2P	14.7	2004	SIC-DFT
		[92]	^2P	14.57 ± 0.10	2005	NR, CCSD(T), M_L res.

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Z	Atom	Refs.	State	α	Year	Comments
		[5]	$--$	14.6 ± 0.1	2019	recommended
		[43]	^2P	14.59 ± 0.25	2021	NR, CCSD(T)
		[46]	^2P	14.582	2021	R, CCSD(T)
18	Ar	[7]	$^1S_0$	11.083 ± 0.002	1965	exp.
		[65]	$^1S_0$	11.081 ± 0.005	1967	exp.
		[100]	$^1S_0$	11.091	1969	exp.
		[74]	^1S	11.10	1976	NR, PNO-CEPA
		[101,102]	$^1S_0$	11.070 ± 0.007	1990	exp.
		[58]	$^1S_0$	11.080	1997	exp.
		[59]	^1S	11.08401 ± 0.00004	2001	NR, CCSD(T)
		[59,62]	^1S	11.10	2001	R, CCSD(T) + DK3 correction
		[50]	^1S	11.1	2004	R, DK, CASPT2
		[30]	$^1S_0$	11.078 ± 0.010	2006	exp.
		[30,82,92]	^1S	11.085 ± 0.060	2012	R, CCSD(T)
		[32]	^1S	11.089 ± 0.004	2013	R, CCSD(T)
		[13]	$^1S_0$	11.07718 ± 0.00064	2018	exp.
		[5]	$--$	11.083 ± 0.007	2019	recommended
		[43]	^1S	11.08 ± 0.19	2021	NR, CCSD(T)
		[103]	^1S	11.0775 ± 0.0019	2023	R, DKH2, CCSD(T) + Breit-Pauli + QED + finite nuclear mass and size
19	K	[15]	$^2S_{1/2}$	292.9 ± 6.1	1974	exp.
		[69]	$^2S_{1/2}$	289.1	1999	RLCCSD
		[69]	$^2S_{1/2}$	290.2 ± 0.8	1999	R, SD all orders + exp. data for electronic transitions
		[27]	$^2S_{1/2}$	290.0	2003	Combination of ab initio and semi-empirical methods
		[104]	^2S	291.1 ± 1.5	2005	R, DK, CCSD(T), AE

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Z	Atom	Refs.	State	α	Year	Comments
		[105]	$^2S_{1/2}$	290.2	2010	Combination of theoretical and experimental data
		[71]	$^2S_{1/2}$	290.6 ± 1.4	2010	exp. (for hyperfine effects see ref [106])
		[106]	$^2S_{1/2}$	290.05	2013	Oscillator-strength sum rule
		[107,108]	$^2S_{1/2}$	289.7 ± 0.3	2016	exp.
		[5]	$--$	289.7 ± 0.3	2019	recommended
		[23]	$^2S_{1/2}$	289.6	2021	SR, CCSD(T), ECP
		[24]	$^2S_{1/2}$	290.30 ± 0.23	2022	R, Dirac-HF, pertubative singles + doubles method, RPA
20	Ca	[75]	^1S	153.7	1979	NR, CI + pseudo-potential
		[109]	^1S	152.0	1991	R, MVD, CCSD + T
		[76]	^1S	157	1991	NR, MBPT4
		[110]	$^1S_0$	160	2002	R, CI+MBPT
		[79]	^1S	158.6	2002	CI, oscillator strength correction
		[27]	^1S	159.4	2003	Combination of ab initio and semi-empirical methods
		[111]	$^1S_0$	155.3/157.7	2003	CCSD R/NR
		[80]	^1S	163	2004	R, DK, CASPT2
		[112]	$^1S_0$	158.0	2004	R, DK + SO, CCSD(T)
		[54,113]	$^1S_0$	169 ± 17	2004	exp.
		[29,81]	$^1S_0$	155.9	2006	R, Dirac, CI + MBPT2 + experimental data
		[29]	$^1S_0$	157.1 ± 1.3	2006	Hybrid-RCI + MBPT sum rule + experimental data
		[29]	$^1S_0$	159.0	2006	R, Dirac, CI + MBPT
		[30]	$^1S_0$	157.9 ± 0.8	2006	R, DK, CCSD(T)
		[31]	$^1S_0$	154.58	2008	R, Dirac, coupled cluster
		[31]	$^1S_0$	154.6 ± 5.4	2008	R, Dirac, CCSD
		[114]	$^1S_0$	154.7	2008	ab initio + experimental data
		[105]	$^1S_0$	157.1	2010	Combination of theoretical and experimental data

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Z	Atom	Refs.	State	α	Year	Comments
		[32]	$^1S_0$	157.03 ± 0.80	2013	R, Dirac, MBPT, CCSD
		[83]	$^1S_0$	160.77	2014	R, Dirac + Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[36]	$^1S_0$	156.10	2019	CCSD(T), ECP
		[36]	$^1S_0$	157.61/159.81	2019	CCSD(T), R X2C-10/NR-10
		[84]	$^1S_0$	157.5	2019	R, KRCISD/aug-QZ
		[5]	$--$	160.8 ± 4.0	2019	recommended
		[85]	$^1S_0$	158.2	2020	R, MCDF
		[23]	$^1S_0$	156.2	2021	SR, CCSD(T), ECP
		[115]	$^1S_0$	159.43 ± 0.97	2023	R, CI+MBPT
21	Sc	[116,117]	$^2D^{,3d1}$	107.1	1987	NR, small CI, VPA
		[117,118]	$^2D^{,3d1}$	138.8	1987	NR, small CI, VPA
		[119]	$^2D^{,3d1}$	142 ± 21	1995	NR, MCPF
		[120]	$^2D^{,3d1}$	114.00	2002	Interacting-induced-dipoles polarisation model
		[54,121]	$^2D^{,3d1}_{3/2}$	120 ± 30	2004	R, Dirac, LDA
		[122]	$^2D^{,3d1}_{3/2}$	121 ± 12	2005	R, DK, MRCI
		[123]	$^2D^{,3d1}$	105.88	2005	TD-DFT
		[124]	$^2D^{,3d1}$	115.46	2009	DFT
		[72]	$^2D^{,3d1}$	97.2 ± 9.5	2015	exp.
		[125]	$^2D^{,3d1}$	123	2016	TD-DFT (LEXX)
		[90,95]	$^2D^{,3d1}_{3/2}$	106.0	2016	SIC-DFT (RXH)
		[95]	$^2D^{,3d1}$	134.6	2016	TD-DFT (PGG)
		[35]	$^2D^{,3d1}$	125.84	2019	NR, CCSD
		[126]	$^2D^{,3d1}_{3/2}$	138.39	2019	R, CCSD(T)/ANO-RCC
		[5]	$--$	97 ± 10	2019	recommended

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Z	Atom	Refs.	State	α	Year	Comments
22	Ti	[116]	$^3F,3d2$	91.8	1987	NR, small CI, VPA
		[116]	$^3F,3d2$	91.4	1987	NR, small CI, VPA
		[119]	$^3F,3d2$	114 ± 17	1995	NR, MCPF
		[54,121]	$^3F_2^{3d2}$	99 ± 25	2004	R, Dirac, LDA
		[90]	$^3F,3d2$	85.7	2004	SIC-DFT
		[122]	$^3F_2^{3d2}$	102 ± 10	2005	R, DK, MRCI
		[123]	$^3F,3d2$	94.69	2005	TD-DFT
		[72]	$^3F_2^{3d2}$	63.4 ± 3.4	2015	exp.
		[125]	$^3F, 3d^2$	102	2016	TD-DFT (LEXX)
		[95]	$^3F, 3d^2$	89.4	2016	SIC-DFT (RXH)
		[95]	$^3F, 3d^2$	111.4	2016	TD-DFT (PGG)
		[35]	$^3F, 3d^2$	86.92	2019	NR, CCSD
		[126]	$^3F, 3d^2$	104.01	2019	R, CCSD(T)/ANO-RCC
		[5]	$--$	100 ± 10	2019	recommended
		[46]	$^3F, 3d^2$	106.22	2021	R, CCSD(T)
		[86]	$^3F, 3d^2$	98.373	2021	R, CCSD(T)
		[127]	$^3F_4, 3d^2$	100.4 ± 1.8	2023	R, Dirac-HF, CI + all-order
23	V	[116]	$^4F, 3d^3$	80.6	1987	NR, small CI, VPA
		[116]	$^4F, 3d^3$	84.6	1987	NR, small CI, VPA
		[119]	$^4F, 3d^3$	97 ± 15	1995	NR, MCPF
		[54,121]	$^4F_{3/2}, 3d^3$	84 ± 21	2004	R, Dirac, LDA
		[90]	$^4F, 3d^3$	72.8	2004	SIC-DFT
		[122]	$^4F_{3/2}, 3d^3$	87.3 ± 8.7	2005	R, DK, MRCI
		[72]	$^4F_{3/2}, 3d^3$	68.2 ± 5.4	2015	exp.
		[125]	$^4F, 3d^3$	87.3	2016	TD-DFT (LEXX)

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Z	Atom	Refs.	State	α	Year	Comments
		[95]	$^4F, 3d^3$	78.2	2016	SIC-DFT (RXH)
		[95]	$^4F, 3d^3$	96.2	2016	TD-DFT (PGG)
		[35]	$^4F, 3d^3$	86.85	2019	NR, CCSD
		[126]	$^4F, 3d^3$	94.30	2019	R, CCSD(T)/ANO-RCC
		[5]	$--$	87 ± 10	2019	recommended
		[46]	$^4F, 3d^3$	90.298	2021	R, CCSD(T)
		[86]	$^4F, 3d^3$	86.798	2021	R, CCSD(T)
24	Cr	[119]	$^7S, 3d^5$	95 ± 15	1995	NR, MCPF
		[54,121]	$^7S_3, 3d^5$	78 ± 20	2004	R, Dirac, LDA
		[90]	$^7S, 3d^5$	60.7	2004	SIC-DFT
		[128]	$^7S_3, 3d^5$	78.4 ± 7.8	2005	DK, CASPT2
		[52]	$^7S_3, 3d^5$	83.2	2010	R, CCSD(T)
		[72]	$^7S_3, 3d^5$	60 ± 24	2015	exp.
		[125]	$^7S_3, 3d^5$	78.4	2016	TD-DFT (LEXX)
		[95]	$^7S_3, 3d^5$	70.4	2016	TD-DFT (PGG)
		[95]	$^7S_3, 3d^5$	69.8	2016	SIC-DFT (RXH)
		[35]	$^7S, 3d^5$	87.77	2019	NR, CCSD
		[126]	$^7S, 3d^5$	96.20	2019	R, CCSD(T)/ANO-RCC
		[5]	$--$	83 ± 12	2019	recommended
25	Mn	[116]	$^6S, 3d^5$	65.4	1987	NR, small CI, VPA
		[119]	$^6S, 3d^5$	76 ± 11	1995	NR, MCPF
		[54,121]	$^6S_{5/2}, 3d^5$	63 ± 16	2004	R, Dirac, LDA
		[90]	$^6S, 3d^5$	56.8	2004	SIC-DFT
		[128]	$^6S_{5/2}, 3d^5$	66.8 ± 6.7	2005	DK, CASPT2
		[52]	$^6S_{5/2}, 3d^5$	68.5	2010	R, CCSD(T)

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Z	Atom	Refs.	State	α	Year	Comments
		[125]	$^6S, 3d^5$	66.8	2016	TD-DFT (LEXX)
		[95]	$^6S, 3d^5$	76.3	2016	TD-DFT (PGG)
		[95]	$^6S, 3d^5$	63.1	2016	SIC-DFT (RXH)
		[35]	$^6S_{5/2}, 3d^5$	83.98	2019	NR, CCSD
		[126]	$^6S_{5/2}, 3d^5$	73.55	2019	R, CCSD(T)/ANO-RCC
		[5]	$--$	68 ± 9	2019	recommended
		[46]	$^6S, 3d^5$	70.154	2021	R, CCSD(T)
		[86]	$^6S, 3d^5$	63.476	2021	R, CCSD(T)
26	Fe	[116]	$^5D, 3d^6$	58.4	1987	NR, small CI, VPA
		[119]	$^5D, 3d^6$	63.93	1995	NR, MCPF
		[54,121]	$^5D_4, 3d^6$	57 ± 14	2004	R, Dirac, LDA
		[90]	$^5D_4, 3d^6$	54.4	2004	SIC-DFT
		[129]	$^5D, 3d^6$	62.65	2004	NR, DFT, GGA(PW86)
		[125]	$^5D_4, 3d^6$	60.4	2016	TD-DFT (LEXX)
		[95]	$^5D_4, 3d^6$	67.8	2016	TD-DFT (PGG)
		[95]	$^5D_4, 3d^6$	56.3	2016	SIC-DFT (RXH)
		[35]	$^5D, 3d^6$	67.96	2019	NR, CCSD
		[126]	$^5D, 3d^6$	63.82	2019	R, CCSD(T)/ANO-RCC
		[5]	$--$	62 ± 4	2019	recommended
27	Co	[116]	$^4F, 3d^7$	52.3	1987	NR, small CI, VPA
		[119]	$^4F, 3d^7$	57.71	1995	NR, MCPF
		[54,121]	$^4F_{9/2}, 3d^7$	51 ± 13	2004	R, Dirac, LDA
		[90]	$^4F_{9/2}, 3d^7$	48.9	2004	SIC-DFT
		[125]	$^4F, 3d^7$	53.9	2016	TD-DFT (LEXX)
		[95]	$^4F, 3d^7$	60.9	2016	TD-DFT (PGG)

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Z	Atom	Refs.	State	α	Year	Comments
		[95]	$^4F, 3d^7$	50.8	2016	SIC-DFT (RXH)
		[35]	$^4F_{9/2}, 3d^7$	62.03	2019	NR, CCSD
		[126]	$^4F_{9/2}, 3d^7$	56.66	2019	R, CCSD(T)/ANO-RCC
		[5]	$--$	55 ± 4	2019	recommended
28	Ni	[116]	$^3F, 3d^8$	48.3	1987	NR, small CI, VPA
		[119]	$^3F, 3d^8$	51.10	1995	NR, MCPF
		[54,121]	$^3F_4, 3d^8$	46 ± 11	2004	R, Dirac, LDA
		[90]	$^3F_4, 3d^8$	44.5	2004	SIC-DFT
		[122]	$^3F_4, 3d^8$	47.4 ± 4.7	2005	R, DK, MRCI
		[125]	$^3F, 3d^8$	48.4	2016	TD-DFT (LEXX)
		[95]	$^3F, 3d^8$	55.3	2016	TD-DFT (PGG)
		[95]	$^3F, 3d^8$	46.2	2016	SIC-DFT (RXH)
		[35]	$^3F_4, 3d^8$	57.32	2019	NR, CCSD
		[126]	$^3F_4, 3d^8$	56.57	2019	R, CCSD(T)/ANO-RCC
		[5]	$--$	49 ± 3	2019	recommended
		[46]	$^3F, 3d^8$	50.849	2021	R, CCSD(T)
		[86]	$^3F, 3d^8$	46.919	2021	R, CCSD(T)
29	Cu	[130]	$^2S_{1/2}, 3d10$	45.0	1994	R, PP, QCISD(T)
		[119]	$^2S, 3d^{10}$	53.44	1995	NR, MCPF
		[54,121]	$^2S_{1/2}, 3d^{10}$	41 ± 10	2004	R, Dirac, LDA
		[90]	$^2S_{1/2}, 3d^{10}$	39.5	2004	SIC-DFT
		[128]	$^2S_{1/2}, 3d10$	40.7 ± 4.1	2005	R, DK, CASPT2
		[122]	$^2S_{1/2}, 3d10$	43.7 ± 4.4	2005	R, DK, MRCI
		[30,131]	$^2S_{1/2}, 3d10$	46.50 ± 0.35	2006	R, DK, CCSD(T)
		[132]	$^2S_{1/2}, 3d^{10}$	46.98	2009	R, DK, CCSD(T)

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Z	Atom	Refs.	State	α	Year	Comments
		[133,134]	$^2S_{1/2}, 3d^{10}$	41.65	2010	CICP
		[82,94]	$^2S_{1/2}, 3d^{10}$	54.7 ± 5.5	2012	exp.
		[72]	$^2S_{1/2}, 3d^{10}$	58.7 ± 4.7	2015	exp.
		[135]	$^2S, 3d^{10}$	51.8	2016	semi-empirical
		[136]	$^2S_{1/2}, 3d^{10}$	42.6 ± 4.3	2016	DFT B3LYP/aug-cc-pVDZ
		[125]	$^2S_{1/2}, 3d10$	41.7	2016	TD-DFT (LEXX)
		[95]	$^2S_{1/2}, 3d10$	46.1	2016	TD-DFT (PGG)
		[95]	$^2S_{1/2}, 3d10$	41.2	2016	SIC-DFT (RXH)
		[5]	$--$	46.5 ± 0.5	2019	recommended
30	Zn	[137]	$^1S, 3d^{10}$	37.6	1995	R, MVD, CCSD(T)
		[138]	$^1S, 3d^{10}$	39.2 ± 0.8	1996	NR, CCSD(T), MP2 basis correction
		[138]	$^1S_0, 3d^{10}$	38.8 ± 0.8	1996	exp.
		[139]	$^1S, 3d^{10}$	38.01	1997	R, PP, CCSD(T)
		[140]	$^1S_0, 3d^{10}$	39.12	2001	R, MRCI, pseudo-potential
		[54,121]	$^1S_0, 3d^{10}$	38 ± 9	2004	R, Dirac, LDA
		[90]	$^1S_0, 3d^{10}$	37.7	2004	SIC-DFT
		[128]	$^1S, 3d^{10}$	38.4	2005	R, DK, CASPT2
		[30,137]	$^1S_0, 3d^{10}$	38.35 ± 0.29	2006	R, MVD, CCSD(T)
		[141]	$^1S_0, 3d^{10}$	38.666 ± 0.096	2014	R, Dirac, CCSDT
		[142]	$^1S_0, 3d^{10}$	38.75	2015	R, PRCC(T)
		[142,143]	$^1S_0, 3d^{10}$	38.92	2015	exp.+fitting
		[95]	$^1S_0, 3d^{10}$	39.2	2016	SIC-DFT (RXH)
		[126]	$^1S_0, 3d^{10}$	41.50	2019	R, CCSD(T)/ANO-RCC
		[5]	$--$	38.67 ± 0.30	2019	recommended
		[144]	$^1S, 3d^{10}$	37.7	2021	ECP, CCSD(T)

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Z	Atom	Refs.	State	α	Year	Comments
		[145]	$^1S_0, 3d^{10}$	38.99 ± 0.31	2022	R, NCCSD
31	Ga	[49]	^2P	54.9 ± 1.0	1995	NR, PNO-CEPA, M_L res.
		[146]	^2P	52.91 ± 0.40	2003	R, DK, CCSD(T)
		[41]	^2P	50.7	2005	R, SF, MRCI, M_L res.
		[41]	$^2P_{1/2}/^2P_{3/2}$	49.9/51.6	2005	R, Dirac, MRCI, M_J res.
		[93]	$^2P_{1/2}/^2P_{3/2}$	$51.3 \pm 2.0/53.0 \pm 2.0$	2010	SI-SOCI, M_J res.
						R, Dirac, FSCC, M_J res.
		[147]	$^2P_{1/2}/^2P_{3/2}$	$51.1 \pm 1.5/53.4 \pm 3.0$	2012	($J = 3/2$: $M_J = 3/2$: 41.9,
						$M_J = 1/2$: 65.0)
		[72]	$^2P_{1/2}$	46.6 ± 4.0	2015	exp.
		[125]	$^2P_{1/2}$	52.1	2016	TD-DFT (LEXX)
		[95]	$^2P_{1/2}$	56.0	2016	SIC-DFT (RXH)
		[35]	$^2P_{1/2}$	53.01	2019	NR, CCSD
		[5]	$--$	50 ± 3	2019	recommended
		[46]	$^2P_{1/2}$	40.899	2021	R, CCSD(T)
32	Ge	[49]	^3P	41.0	1995	NR, PNO-CEPA, M_L res.
		[90]	^3P	41.6	2004	SIC-DFT
		[30]	$^3P_0$	40.80 ± 0.82	2006	R, PNO-CEPA
		[45]	^3P	39.97	2008	R, DK, CCSD(T), M_L res. ($M_L = 0$: 32.11, $M_L = 1$: 43.90)
		[45]	$^3P_0$	39.43 ± 0.80	2008	R, Dirac Gaunt, CCSD(T)
		[95]	^3P	41.2	2016	SIC-DFT (RXH)
		[35]	$^3P_0$	39.78	2019	NR, CCSD
		[5]	$--$	40 ± 1	2019	recommended
33	As	[49]	^4S	29.1	1995	NR, PNO-CEPA

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Z	Atom	Refs.	State	α	Year	Comments
		[49]	^4S	30.5	1995	NR, numerical MCSCF
		[50]	^4S	29.8 ± 0.6	2004	R, DK, CASPT2
		[90]	^4S	31.52	2004	SIC-DFT
		[52]	^4S	29.92	2010	R, DK, CCSD(T)
		[52]	^4S	29.81	2010	ECP, CCSD(T)
		[125]	^4S	29.6	2016	TD-DFT (LEXX)
		[95]	^4S	30.7	2016	SIC-DFT (RXH)
		[35]	^4S	29.65	2019	NR, CCSD
		[5]	$--$	30 ± 1	2019	recommended
		[53]	^4S	29.6	2020	ECP, CCSD(T)
34	Se	[48]	^3P	26.24 ± 0.52	1959	R, MVD, CASPT2, M_L res.
		[148]	$^3P_2$	28.9 ± 1.0	1997	exp.
		[90]	^3P	26.65	2004	SIC-DFT
		[95]	^3P	29.3	2016	TD-DFT (PGG)
		[95]	^3P	24.0	2016	SIC-DFT (RXH)
		[35]	^3P	25.03	2019	NR, CCSD
		[5]	$--$	28.9 ± 1.0	2019	recommended
35	Br	[55]	^2P	21.03	2000	R, MVD, CASPT2, M_L res.
		[149]	$^2P_{1/2}$	21.9	2002	R, DK, SO-CI
		[149]	$^2P_{3/2}$	21.7	2002	R, DK, SO-CI, M_J res.
		[90]	^2P	21.5	2004	SIC-DFT
		[30,55]	^2P	21.13 ± 0.42	2006	R, MVD, CASPT2
		[95]	^2P	21.6	2016	TD-DFT (LEXX)
		[35]	^2P	20.4	2019	NR, CCSD
		[5]	$--$	21 ± 1	2019	recommended

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Z	Atom	Refs.	State	α	Year	Comments
36	Kr	[65]	$^1S_0$	16.766 ± 0.008	1967	exp.
		[101]	^1S	16.80 ± 0.13	1990	R, DK3, CCSD(T)
		[56]	$^1S_0$	16.782 ± 0.005	1991	exp.
		[150]	$^1S_0$	16.79	1992	DOSD (constrained dipole oscillator strength distribution)
		[58,101]	$^1S_0$	16.740	1997	exp.
		[58]	$^1S_0$	16.734	1997	exp.
		[50]	^1S	16.6	2004	R, DK, CASPT2
		[151]	$^1S_0$	16.012	2009	R, Dirac, CCSD/T
		[152]	$^1S_0$	16.736	2012	R, DK3, CCSD(T)
		[153]	$^1S_0$	16.47	2016	R, RPA, PolPot
		[5]	$--$	16.78 ± 0.02	2019	recommended
		[154]	$^1S_0$	16.800	2020	R, DHF, MBPT
37	Rb	[15]	$^2S_{1/2}$	319 ± 6	1974	exp.
		[27]	^2S	315.7	2003	Combination of ab initio and semi-empirical methods
		[104]	^2S	316.2 ± 3.2	2005	R, DK, CCSD(T), AE
		[30]	$^2S_{1/2}$	319.2 ± 6.1	2006	exp.
		[69,105]	$^2S_{1/2}$	318.6 ± 0.6	2010	R, SD all orders + exp. data
		[71]	$^2S_{1/2}$	318.8 ± 1.4	2010	exp.
		[33]	^2S	317.0	2015	Oscillator-strength sum rule
		[107,108]	$^2S_{1/2}$	319.8 ± 0.3	2016	exp.
		[5]	$--$	319.8 ± 0.3	2019	recommended
		[23]	$^2S_{1/2}$	317.4	2021	SR, CCSD(T), ECP
		[155]	$^2S_{1/2}$	318.5 ± 0.6	2022	R, DHF, all orders
		[24]	$^2S_{1/2}$	318.38 ± 0.38	2022	R, Dirac-HF, pertubative singles + doubles method, RPA

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Z	Atom	Refs.	State	α	Year	Comments
		[156]	$^2S_{1/2}$	319.5 ± 1.5	2023	R, TDHF + Breit + QED + scaling + structure radiation + normaliz.
38	Sr	[26]	$^1S_0$	193.2	2000	Model potential
		[79]	$^1S_0$	198.5 ± 1.3	2002	CI, oscillator strength correction
		[27]	$^1S_0$	201.2	2003	Combination of ab initio and semi-empirical methods
		[112]	$^1S_0$	199.4	2004	R, DK + SO, CCSD(T)
		[112]	$^1S_0$	198.85	2004	R, DK, CCSD(T)
		[54]	$^1S_0$	186 ± 15	2004	exp.
		[30,110]	^1S	199.0 ± 2.0	2006	R, CI, MBPT2
		[29]	$^1S_0$	202.0	2006	Hybrid-RCI + MBPT sum rule
		[31]	$^1S_0$	199.71	2008	R, Dirac, coupled cluster
		[81,157]	$^1S_0$	197.2 ± 3.6	2008	R, Dirac, CI + MBPT + experimental data
		[114]	$^1S_0$	201.6	2008	Combination of ab initio and experimental results
		[158]	$^1S_0$	197.6	2010	CI + core polarisation (corrected to exp. term energies)
		[29,105]	$^1S_0$	197.2 ± 0.2	2010	Hybrid-RCI + MBPT sum rule
		[32]	$^1S_0$	186.98 ± 0.85	2013	R, Dirac, MBPT, CCSD
		[34]	$^1S_0$	197.8	2013	Combination of theoretical (CICP) and experimental methods
		[159]	$^1S_0$	197.14 ± 0.2	2013	CI + MBPT and experimental results
		[159]	$^1S_0$	198.9 ± 2.0	2013	CI + MBPT-SD and experimental results
		[83]	$^1S_0$	190.82	2014	R, Dirac + Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[33]	$^1S_0$	197.9	2015	Oscillator-strength sum rule
		[36]	$^1S_0$	198.62/198.93	2019	CCSD(T), ECP/R X2C-28
		[84]	$^1S_0$	196.5	2019	R, KRCISD/aug-QZ
		[5]	$--$	197.2 ± 0.2	2019	recommended

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Z	Atom	Refs.	State	α	Year	Comments
		[85]	$^1S_0$	214.5	2020	R, MCDF
		[46]	$^1S_0$	203.16	2021	R, CCSD(T)
39	Y	[54,121]	$^2D_{3/2}, 4d^1$	153 ± 38	2004	R, Dirac, LDA
		[160]	$^2D_{3/2}, 4d^1$	140.94	2009	DFT, ECP
		[82,161]	$^2D_{3/2}, 4d^1$	139 ± 28	2012	TD-DFT
		[72]	$^2D_{3/2}, 4d^1$	163 ± 12	2015	exp.
		[95]	$^2D_{3/2}, 4d^1$	134.9	2016	SIC-DFT (RXH)
		[125]	$^2D_{3/2}, 4d^1$	163	2016	TD-DFT (LEXX)
		[95]	$^2D_{3/2}, 4d^1$	134.9	2016	SIC-DFT (RXH)
		[95]	$^2D_{3/2}, 4d^1$	126.74	2016	TD-DFT (PGG)
		[162]	$^2D_{3/2}, 4d^1$	163 ± 12	2016	LR-CCSD
		[5]	$--$	162 ± 12	2019	recommended
40	Zr	[54,121]	$^3F_2, 4d^2$	121 ± 30	2004	R, Dirac, LDA
		[72]	$^3F_2, 4d^2$	112 ± 13	2015	exp.
		[162]	$^3F_2, 4d^2$	119.97	2016	LR-CCSD
		[125]	$^3F_2, 4d^2$	112	2016	TD-DFT (LEXX)
		[95]	$^3F_2, 4d^2$	109.8	2016	SIC-DFT (RXH)
		[95]	$^3F_2, 4d^2$	130.5	2016	TD-DFT (PGG)
		[5]	$--$	112 ± 13	2019	recommended
41	Nb	[54,121]	$^6D_{1/2}, 4d^4$	106 ± 27	2004	R, Dirac, LDA
		[72]	$^6D_{1/2}, 4d^4$	97.9 ± 7.4	2015	exp.
		[162]	$^6D_{1/2}, 4d^4$	101.60	2016	LR-CCSD
		[125]	$^6D_{1/2}, 4d^4$	97.9	2016	TD-DFT (LEXX)
		[95]	$^6D_{1/2}, 4d^4$	99.6	2016	TD-DFT (PGG)
		[95]	$^6D_{1/2}, 4d^4$	95.5	2016	SIC-DFT (RXH)

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Z	Atom	Refs.	State	α	Year	Comments
		[35]	$^6D_{1/2}, 4d^4$	106.43	2019	ECP, CCSD
		[5]	$--$	98 ± 8	2019	recommended
42	Mo	[163]	$^7S_3, 4d^5$	61 ± 10	1956	exp.
		[54,121]	$^7S_3, 4d^5$	86 ± 22	2004	R, Dirac, LDA
		[52]	$^7S_3, 4d^5$	84	2010	R, CCSD(T)
		[52]	$^7S_3, 4d^5$	79	2010	MRCI
		[82,128]	$^7S, 4d^5$	73 ± 11	2012	R, DK, CASPT2
		[72]	$^7S_3, 4d^5$	87.1 ± 6.1	2015	exp.
		[162]	$^7S_3, 4d^5$	88.42	2016	LR-CCSD
		[125]	$^7S_3, 4d^5$	87.1	2016	TD-DFT (LEXX)
		[95]	$^7S_3, 4d^5$	82.7	2016	TD-DFT (PGG)
		[95]	$^7S_3, 4d^5$	79.0	2016	SIC-DFT (RXH)
		[35]	$^7S_3, 4d^5$	85.93	2019	ECP, CCSD
		[5]	$--$	87 ± 6	2019	recommended
		[86]	$^7S_3, 4d^5$	84.355	2021	R, CCSD(T)
		[87]	$^7S_3, 4d^5$	76 ± 15	2022	exp.
43	Tc	[54,121]	$^6S_{5/2}, 4d^5$	77 ± 20	2004	R, Dirac, LDA
		[52]	$^6S_{5/2}, 4d^5$	78.6	2010	R, CCSD(T)
		[82,128]	$^6S, 4d^5$	80 ± 12	2012	R, DK, CASPT2
		[125]	$^6S_{5/2}, 4d^5$	79.6	2016	TD-DFT (LEXX)
		[95]	$^6S_{5/2}, 4d^5$	93.9	2016	TD-DFT (PGG)
		[95]	$^6S_{5/2}, 4d^5$	78.5	2016	SIC-DFT (RXH)
		[162]	$^6S_{5/2}, 4d^5$	80.08	2016	LR-CCSD
		[35]	$^6S_{5/2}, 4d^5$	80.9	2019	ECP, CCSD
		[5]	$--$	79 ± 10	2019	recommended

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Z	Atom	Refs.	State	α	Year	Comments
		[46]	$^6S_{5/2}, 4d^5$	71.113	2021	R, CCSD(T)
		[86]	$^6S_{5/2}, 4d^5$	65.158	2021	R, CCSD(T)
44	Ru	[54,121]	$^5F_5, 4d^7$	65 ± 16	2004	R, Dirac, LDA
		[125]	$^5F_5, 4d^7$	72.3	2016	TD-DFT (LEXX)
		[95]	$^5F_5, 4d^7$	69.5	2016	TD-DFT (PGG)
		[95]	$^5F_5, 4d^7$	71.4	2016	SIC-DFT (RXH)
		[162]	$^5F_5, 4d^7$	65.89	2016	LR-CCSD
		[35]	$^5F_5, 4d^7$	71.27	2019	ECP, CCSD
		[5]	$--$	72 ± 10	2019	recommended
45	Rh	[54,121]	$^4F_{9/2}, 4d^8$	58 ± 15	2004	R, Dirac, LDA
		[72]	$^4F_{9/2}, 4d^8$	11 ± 22	2015	exp. (an unusually low value was obtained)
		[125]	$^4F_{9/2}, 4d^8$	66.4	2016	TD-DFT (LEXX)
		[95]	$^4F_{9/2}, 4d^8$	66.2	2016	TD-DFT (PGG)
		[95]	$^4F_{9/2}, 4d^8$	65.7	2016	SIC-DFT (RXH)
		[162]	$^4F_{9/2}, 4d^8$	56.10	2016	LR-CCSD
		[35]	$^4F_{9/2}, 4d^8$	61.94	2019	ECP, CCSD
		[5]	$--$	66 ± 10	2019	recommended
46	Pd	[54,121]	$^1S_0, 4d^{10}$	32 ± 8	2004	R, Dirac, LDA
		[164]	$^1S_0, 4d^{10}$	26.612	2008	NR, ECP, CCSD(T)
		[165]	$^1S_0, 4d^{10}$	24.581	2011	R, DK
		[125]	$^1S_0, 4d^{10}$	61.7	2016	TD-DFT (LEXX)
		[95]	$^1S_0, 4d^{10}$	20.0	2016	TD-DFT (PGG)
		[95]	$^1S_0, 4d^{10}$	61.1	2016	SIC-DFT (RXH)
		[162]	$^1S_0, 4d^{10}$	23.68	2016	LR-CCSD
		[166]	$^1S_0, 4d^{10}$	26.14 ± 0.10	2018	CCSDTQDP, DKH2 + Gaunt, CBS

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Z	Atom	Refs.	State	α	Year	Comments
		[35]	$^1S_0, 4d^{10}$	24.36	2019	ECP, CCSD
		[5]	$--$	26.14 ± 0.10	2019	recommended
		[87]	$^1S_0, 4d^{10}$	43 ± 9	2022	exp.
47	Ag	[131]	$^2S_{1/2}, 4d^{10}$	55.3 ± 0.5	1997	R, DK, CCSD(T)
		[128]	$^2S, 4d^{10}$	36.7	2005	R, DK, CCSD(T)
		[30,131]	$^2S, 4d^{10}$	52.46 ± 0.52	2006	R, DK, CCSD(T)
		[134]	$^2S_{1/2}, 4d^{10}$	46.17	2008	CICP
		[130,132]	$^2S, 4d^{10}$	52.2	2009	R, PP, QCISD(T)
		[167]	$^2S_{1/2}, 4d^{10}$	56 ± 14	2010	exp.
		[82]	$^2S_{1/2}, 4d^{10}$	63.1 ± 6.3	2012	exp.
		[72]	$^2S_{1/2}, 4d^{10}$	45.9 ± 7.4	2015	exp.
		[135]	$^2S, 4d^{10}$	55.2	2016	Semi-empirical
		[125]	$^2S_{1/2}, 4d^{10}$	46.2	2016	TD-DFT (LEXX)
		[95]	$^2S_{1/2}, 4d^{10}$	63.3	2016	TD-DFT (PGG)
		[95]	$^2S_{1/2}, 4d^{10}$	57.3	2016	SIC-DFT (RXH)
		[162]	$^2S_{1/2}, 4d^{10}$	50.60	2016	LR-CCSD
		[35]	$^2S_{1/2}, 4d^{10}$	55	2019	ECP, CCSD
		[5]	$--$	55 ± 8	2019	recommended
		[23,168]	$^2S_{1/2}, 4d^{10}$	50.2	2021	SR, ECP, CCSD(T)
		[169]	$^2S_{1/2}, 4d^{10}$	50.6	2021	R, CI+MBPT
		[54,170][2023114]	$^2S_{1/2}, 4d^{10}$	48.4	2023	R, Dirac, LDA
48	Cd	[137]	$^1S, 4d^{10}$	46.8	1995	R, MVD, CCSD(T)
		[171]	$^1S_0, 4d^{10}$	49.7 ± 1.6	1995	exp.
		[172]	$^1S_0, 4d^{10}$	48.2 ± 1.1	1995	exp.
		[139]	$^1S, 4d^{10}$	46.25	1997	R, PP, CCSD(T)

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Z	Atom	Refs.	State	α	Year	Comments
		[172,173]	$^1S_0, 4d^{10}$	45.3 ± 1.4	2002	exp.
		[111]	$^1S_0, 4d^{10}$	45.91/53.99	2003	CCSD R/NR
		[128]	$^1S, 4d^{10}$	46.9	2005	R, DK, CASPT2
		[30,137]	$^1S_0, 4d^{10}$	47.55 ± 0.48	2006	R, MVD, CCSD(T)
		[174]	$^1S_0, 4d^{10}$	44.63	2008	R, DHF, CPMP
		[141]	$^1S_0, 4d^{10}$	45.86 ± 0.15	2014	R, DF, CCSD(T), MBPT3
		[125]	$^1S_0, 4d^{10}$	46.7	2016	TD-DFT (LEXX)
		[175]	$^1S_0, 4d^{10}$	46.02 ± 0.50	2018	R, DHF, CCSD(T)
		[35]	$^1S_0, 4d^{10}$	48.3	2019	ECP, CCSD
		[5]	$--$	46 ± 2	2019	recommended
		[154]	$^1S_0, 4d^{10}$	39.79	2020	LR-CCSD
		[176]	$^1S_0, 4d^{10}$	45.92 ± 0.10	2021	R, CCSD(T)
		[144]	$^1S_0, 4d^{10}$	45.8	2021	ECP, CCSD(T)
		[177]	$^1S_0, 4d^{10}$	46 ± 2	2021	R, DFCP+RCI
		[178]	$^1S_0, 4d^{10}$	47.5 ± 2.0	2022	exp.
49	In	[179]	$^2P_{1/2}$	68.7 ± 8.1	1984	exp.
		[146]	$^2P_{1/2}$	68.67 ± 0.69	2003	R, DK, CCSD(T)
		[90]	$^2P_{1/2}$	70.3	2004	SIC-DFT
		[41]	^2P	66.7	2005	R, SF, MRCI, M_L res.
		[41]	$^2P_{1/2}/^2P_{3/2}$	$61.9 \pm 1.2/69.6 \pm 1.4$	2005	R, Dirac, MRCI, M_J res.
		[93]	$^2P_{1/2}/^2P_{3/2}$	$66.4 \pm 5.0/74.4 \pm 8.0$	2010	SI-SOCI, M_J res.
		[147]	$^2P_{1/2}/^2P_{3/2}$	$62.0 \pm 1.9/69.7 \pm 4.0$	2012	R, Dirac, FSCC, M_J res. ($J = 3/2$: $M_J = 3/2$: 55.1, $M_J = 1/2$: 84.6)
		[41,147]	$^2P_{1/2}$	61.5 ± 5.6	2012	CCSD(T)

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Z	Atom	Refs.	State	α	Year	Comments
		[180]	$^2P_{1/2}$	62.4	2013	R, Dirac + Breit, CI + all-order
		[72]	$^2P_{1/2}$	62.1 ± 6.1	2015	exp.
		[95]	$^2P_{1/2}$	73.1	2016	SIC-DFT (RXH)
		[162]	$^2P_{1/2}$	70.22	2016	LR-CCSD
		[5][155]	$^2P_{1/2}$	65.2	2019	R, DFT
		[35]	$^2P_{1/2}$	67.9	2019	ECP, CCSD
		[5]	$--$	65 ± 4	2019	recommended
		[86]	$^2P_{1/2}$	70.070	2021	R, CCSD(T)
		[96]	$^2P_{1/2}$	$64.3 \pm 1.3/82.3 \pm 1.7$	2022	R, Breit+QED, CCSD
		[35][2023185]	$^2P_{1/2}$	64.5	2023	R, (D)BSR
50	Sn	[54,121]	^3P	52 ± 13	2004	R, Dirac, LDA
		[90]	^3P	57.5	2004	SIC-DFT
		[45]	$^3P_0$	52.9 ± 2.1	2008	R, Dirac + Gaunt, CCSD(T)
		[45]	$^3P_0$	42.4 ± 11	2008	exp.
		[181]	$^3P_0$	54.48	2009	R, PP, DFT, BP386
		[72]	$^3P_0$	67.5 ± 8.8	2015	exp.
		[95]	$^3P_0$	57.9	2016	SIC-DFT (RXH)
		[90,125]	$^3P_0$	60.0	2016	TD-DFT (LEXX)
		[162]	$^3P_0$	55.95	2016	LR-CCSD
		[35]	$^3P_0$	54.29	2019	ECP, CCSD
		[5]	$--$	53 ± 6	2019	recommended
		[46]	$^3P_0$	60.115	2021	R, CCSD(T)
		[86]	$^3P_0$	61.063	2021	R, CCSD(T)
51	Sb	[54,121]	^4S	45 ± 11	2004	R, Dirac, LDA
		[50]	^4S	42.2 ± 1.3	2004	R, DK, CASPT2

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Z	Atom	Refs.	State	α	Year	Comments
		[90]	^4S	47.07	2004	SIC-DFT
		[182]	^4S	42.26	2007	NR, CCSD(T)
		[52]	^4S	43.03	2010	ECP, CCSD(T)
		[95]	^4S	45.7	2016	SIC-DFT (RXH)
		[90,125]	^4S	44.0	2016	TD-DFT (LEXX)
		[35]	^4S	42.78	2019	ECP, CCSD
		[5]	$--$	43 ± 2	2019	recommended
		[53]	^4S	42.8	2020	ECP, CCSD(T)
52	Te	[54,121]	^3P	37 ± 4	2004	R, LDA
		[90]	^3P	40.06	2004	SIC-DFT
		[30,183]	^3P	38.1 ± 3.8	2006	QR, MVD-HF, GTO basis set
		[95]	^3P	36.9	2016	SIC-DFT (RXH)
		[162]	^3P	37.65	2016	LR-CCSD
		[35]	^3P	37.51	2019	ECP, CCSD
		[5]	$--$	38 ± 4	2019	recommended
		[184]	^3P	37.3	2022	R, Dirac, CIPT+SD (RPA)
53	I	[185]	$^2P_{3/2}$	32.9 ± 1.3	1997	exp.
		[185][162]	$^2P_{3/2}$	33.4	1997	exp.
		[149]	$^2P_{1/2}$	35.1	2002	R, DK, SO-CI
		[149]	$^2P_{3/2}$	34.1	2002	R, DK, SO-CI, M_J res.
		[90]	^2P	33.6	2004	SIC-DFT
		[30,149,183]	$^2P_{3/2}$	33.0 ± 1.7	2006	R, DK, SO-CI
		[95]	^2P	30.5	2016	SIC-DFT (RXH)
		[162]	^2P	35.00	2016	LR-CCSD
		[35]	^2P	31.57	2019	ECP, CCSD

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Z	Atom	Refs.	State	α	Year	Comments
		[5]	$--$	32.9 ± 1.3	2019	recommended
		[46]	^2P	31.101	2021	R, CCSD(T)
		[86]	^2P	31.114	2021	R, CCSD(T)
54	Xe	[100]	$^1S_0$	27.342	1969	exp.
		[56]	$^1S_0$	27.078 ± 0.050	1991	exp.
		[150]	$^1S_0$	27.16	1992	DOSD (constrained dipole oscillator strength distribution)
		[58]	$^1S_0$	27.292	1997	exp.
		[186]	$^1S_0$	27.36	1998	R, SOPP, CCSD(T) + MP2 basis set correction
		[62]	^1S	27.06 ± 0.27	2001	R, DK3, CCSD(T)
		[59]	$^1S_0$	27.2937 ± 0.0003	2001	CCSD(T), ECP
		[50]	^1S	26.7	2004	R, DK, CASPT2
		[151]	$^1S_0$	25.297	2009	R, Dirac, CCSD/T
		[167]	$^1S_0$	27.42	2010	R, DK3, CCSD(T)
		[152]	$^1S_0$	26.432	2012	R, DK3, CCSD
		[153]	$^1S_0$	26.7	2016	R, RPA, PolPot
		[95]	$^1S_0$	25.4	2016	SIC-DFT (RXH)
		[162]	$^1S_0$	27.30	2016	LR-CCSD
		[187]	$^1S_0$	28.4 ± 0.5	2018	R, CCSD(T)
		[188]	$^1S_0$	27.508	2018	R, CCSD(T)
		[35]	$^1S_0$	26.6	2019	ECP, CCSD
		[5]	$--$	27.32 ± 0.20	2019	recommended
		[154]	$^1S_0$	27.099	2020	R, DHF, MBPT
		[189]	$^1S_0$	27.55 ± 0.30	2023	CCSD + hyperfine-induced contributions
55	Cs	[69]	$^2S_{1/2}$	399.9 ± 1.9	1999	R, Dirac, SD, all orders + exp. data
		[69]	$^2S_{1/2}$	401.5	1999	R, SD all orders + exp. data for electronic transitions

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Z	Atom	Refs.	State	α	Year	Comments
		[190]	$^2S_{1/2}$	401.0 ± 0.6	2003	exp.
		[191]	$^2S_{1/2}$	398.2 ± 0.9	2004	R, Dirac, SDpT
		[104]	^2S	396.0 ± 5.9	2005	R, DK, CCSD(T), AE
		[192]	$^2S_{1/2}$	398.4 ± 0.7	2008	R, DF, RPA, SD-all order
		[105]	$^2S_{1/2}$	399.8	2010	Combination of theoretical and experimental data
		[193]	$^2S_{1/2}$	399.0	2013	R, Dirac, CCSD(T)
		[33]	$^2S_{1/2}$	396.7 ± 7.9	2015	Combination of theoretical and experimental data
		[194]	$^2S_{1/2}$	399.5 ± 0.8	2016	R, Dirac, RCC-SD
		[107,108]	$^2S_{1/2}$	400.8 ± 0.4	2016	exp.
		[5]	$--$	400.9 ± 0.7	2019	recommended
		[23]	$^2S_{1/2}$	391.1	2021	SR, CCSD(T), ECP
		[155]	$^2S_{1/2}$	399.9 ± 0.6	2022	R, DHF, all order
		[24]	$^2S_{1/2}$	399.74 ± 0.55	2022	R, Dirac-HF, pertubative singles + doubles method, RPA
56	Ba	[113]	$^1S_0$	268 ± 22	1974	exp.
		[26]	$^1S_0$	261.2	2000	Model potential
		[29,110]	^1S	262.2	2006	R, CI, MBPT
		[30,112]	$^1S_0$	273.5 ± 4.1	2006	R, DK + SO, CCSD(T)
		[29]	$^1S_0$	272.1	2006	Hybrid-RCI + MBPT sum rule
		[195]	$^1S_0$	275.5 ± 5.5	2007	R, DK, CCSD(T)
		[31]	$^1S_0$	268.19	2008	R, Dirac, coupled cluster
		[29,105]	$^1S_0$	273.5 ± 2.0	2010	Hybrid-RCI + MBPT sum rule, recommended
		[196]	$^1S_0$	272.7	2013	R, Dirac + Gaunt, CCSD(T)
		[83]	$^1S_0$	274.68	2014	R, Dirac + Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[33]	$^1S_0$	278.1 ± 5.6	2015	Combination of theoretical and experimental data

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Z	Atom	Refs.	State	α	Year	Comments
		[153]	$^1S_0$	251	2016	R, RPA, PolPot
		[162]	$^1S_0$	275.0	2016	LR-CCSD
		[197]	$^1S_0$	274.92 ± 0.01	2018	CCSD(T), R DKH ECP/CBS
		[36]	$^1S_0$	273.90/276.98	2019	CCSD(T), R, ECP-46/X2C-46
		[84]	$^1S_0$	269.0	2019	R, KRCISD/aug-QZ
		[5]	$--$	272 ± 10	2019	recommended
		[85]	$^1S_0$	276.2	2020	R, MCDF
57	La	[54,121]	$^2D_{3/2}, 5d^1$	210 ± 52	2004	R, Dirac, LDA
		[161]	$^2D_{3/2}, 5d^1$	201 ± 40	2007	TD-DFT
		[198]	$^2D_{3/2}, 5d^1$	219.8	2007	R, CASSCF, ECP
		[82,198]	$^2D_{3/2}, 5d^1$	220 ± 22	2012	R, CASSCF, ECP
		[199]	$^2D_{3/2}, 5d^1$	213.7	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 218.7$ for the $5d^26s^1$ configuration)
		[72]	$^2D_{3/2}, 5d^1$	170.7 ± 8.1	2015	exp.
		[35]	$^2D_{3/2}, 5d^1$	214.72	2019	ECP, CCSD
		[5]	$--$	215 ± 20	2019	recommended
		[200]	$^2D_{3/2}, 5d^1$	190.9	2022	R (ZORA), DFT (B3LYP)
58	Ce	[54,121]	$4f^15d^1$	200 ± 50	2004	R, Dirac, LDA
		[161]	$4f^15d^1$	194 ± 39	2007	TD-DFT
		[199]	$4f^15d^1$	204.7	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 223.4$ for the $4f^2$ configuration)
		[72]	$^1G_4, 4f^15d^1$	192 ± 20	2015	exp.
		[5]	$--$	205 ± 20	2019	recommended
		[201]	$4f^15d^1$	206.51	2020	R, DKH2-B3LYP/ADZP
		[201]	$4f^15d^1$	219.66	2020	R, DKH2-B3LYP/ADZP-DKH

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Z	Atom	Refs.	State	α	Year	Comments
59	Pr	[54,121]	$4f^3$	190 ± 48	2004	R, Dirac, LDA
		[161]	$4f^3$	220 ± 44	2007	TD-DFT
		[199]	$4f^3$	215.8	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 195.7$ for the $4f^2 5d^1$ configuration)
		[72]	${}^4I_{9/2}, 4f^3$	239 ± 28	2015	exp.
		[5]	$--$	216 ± 20	2019	recommended
60	Nd	[54,121]	$4f^4$	212 ± 53	2004	R, Dirac, LDA
		[161]	$4f^4$	213 ± 43	2007	TD-DFT
		[199]	$4f^4$	208.4	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 187.5$ for the $4f^3 5d^1$ configuration)
		[72]	${}^5I_4, 4f^4$	184 ± 20	2015	exp.
		[5]	$--$	208 ± 20	2019	recommended
		[201]	$4f^4$	194.56	2020	R, DKH2-B3LYP/ADZP
		[201]	$4f^4$	203.07	2020	R, DKH2-B3LYP/ADZP-DKH
61	Pm	[54,121]	$4f^5$	203 ± 51	2004	R, Dirac, LDA
		[161]	$4f^5$	206 ± 41	2007	TD-DFT
		[199]	$4f^5$	200.2	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 179.3$ for the $4f^4 5d^1$ configuration)
		[5]	$--$	200 ± 20	2019	recommended
62	Sm	[54,121]	$4f^6$	194 ± 48	2004	R, Dirac, LDA
		[161]	$4f^6$	200 ± 40	2007	TD-DFT
		[198]	$4f^6$	196.8	2007	R, CASSCF, ECP
		[82,198]	$4f^6$	197 ± 20	2012	R, CASSCF, ECP
		[199]	$4f^6$	192.1	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 171.7$ for the $4f^5 5d^1$ configuration)

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Z	Atom	Refs.	State	α	Year	Comments
		[72]	$^7F_0, 4f^6$	157 ± 16	2015	exp.
		[5]	$--$	192 ± 20	2019	recommended
63	Eu	[54,121]	$4f^7$	187 ± 47	2004	R, Dirac, LDA
		[161]	$4f^7$	194 ± 39	2007	TD-DFT
		[198]	$4f^7$	189.4	2007	R, CASSCF, ECP
		[82,198]	$4f^7$	189 ± 19	2012	R, CASSCF, ECP
		[199]	$4f^7$	184.2	2014	R, Dirac, CI + MBPT + CP(RPA); (α_D = 164.7 for the $4f^6 5d^1$ configuration)
		[72]	$^8S_{7/2}, 4f^7$	155 ± 25	2015	exp.
		[5]	$--$	184 ± 20	2019	recommended
		[202]	$4f^7$	188	2020	r, CI+MBPT
64	Gd	[54,121]	$4f^7 5d^1$	159 ± 40	2004	R, Dirac, LDA
		[161]	$4f^7 5d^1$	161 ± 32	2007	TD-DFT
		[199]	$4f^7 5d^1$	158.3	2014	R, Dirac, CI + MBPT + CP(RPA); (α_D = 194.5 for the $4f^7 5d^2 6s^1$ configuration)
		[72]	$^9D_2, 4f^7 5d^1$	176 ± 26	2015	exp.
		[5]	$--$	158 ± 20	2019	recommended
		[202]	$4f^7 5d^1$	159	2020	R, CI+MBPT
		[201]	$4f^7 5d^1$	171.40	2020	R, DKH2-B3LYP/ADZP
		[201]	$4f^7 5d^1$	145.74	2020	R, DKH2-B3LYP/ADZP-DKH
65	Tb	[54,121]	$4f^9$	172 ± 43	2004	R, Dirac, LDA
		[161]	$4f^9$	181 ± 36	2007	TD-DFT
		[199]	$4f^9$	169.5	2014	R, Dirac, CI + MBPT + CP(RPA); (α_D = 152.4 for the $4f^8 5d^1$ configuration)
		[72]	$^6H_{15/2}, 4f^9$	159 ± 11	2015	exp.

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Z	Atom	Refs.	State	α	Year	Comments
		[5]	$--$	170 ± 20	2019	recommended
66	Dy	[54,121]	$4f^{10}$	165 ± 41	2004	R, Dirac, LDA
		[161]	$4f^{10}$	175 ± 35	2007	TD-DFT
		[199]	$4f^{10}$	162.7	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 148.3$ for the $4f^9 5d^1$ configuration)
		[199]	$4f^{10}$	165	2014	R, RPA, PolPot
		[72]	${}^5I_8, 4f^{10}$	157 ± 11	2015	exp.
		[153]	$4f^{10}$	168	2016	R, RPA, PolPot
		[203]	${}^5I_8, 4f^{10}$	164	2016	exp.
		[5]	$--$	163 ± 15	2019	recommended
		[202]	$4f^{10}$	164	2020	R, CI+MBPT
		[201]	$4f^{10}$	169.69	2020	R, DKH2-B3LYP/ADZP
		[201]	$4f^{10}$	157.20	2020	R, DKH2-B3LYP/ADZP-DKH
67	Ho	[54,121]	$4f^{11}$	159 ± 40	2004	R, Dirac, LDA
		[161]	$4f^{11}$	170 ± 34	2007	TD-DFT
		[199]	$4f^{11}$	156.3	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 142.9$ for the $4f^{10} 5d^1$ configuration)
		[72]	${}^4I_{15/2}, 4f^{11}$	145 ± 12	2015	exp.
		[153]	$4f^{11}$	161	2016	R, RPA, PolPot
		[203]	${}^4I_{15/2}, 4f^{11}$	160	2016	exp.
		[5]	$--$	156 ± 10	2019	recommended
68	Er	[54,121]	$4f^{12}$	153 ± 38	2004	R, Dirac, LDA
		[161]	$4f^{12}$	166 ± 33	2007	TD-DFT
		[199]	$4f^{12}$	150.2	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 139.4$ for the $4f^{11} 5d^1$ configuration)

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Z	Atom	Refs.	State	α	Year	Comments
		[199]	$4f^{12}$	169	2014	R, RPA, PolPot
		[204]	$4f^{12}$	141 ± 7	2014	R, HF, Darwin, SO
		[72]	$^3H_6, 4f^{12}$	217 ± 39	2015	exp.
		[153]	$4f^{12}$	154	2016	R, RPA, PolPot
		[205]	$4f^{12}$	149	2018	R, HF, Darwin, SO
		[205]	$^3H_6, 4f^{12}$	155	2018	exp.
		[5]	$--$	150 ± 10	2019	recommended
		[201]	$4f^{12}$	143.98	2020	R, DKH2-B3LYP/ADZP
		[201]	$4f^{12}$	145.01	2020	R, DKH2-B3LYP/ADZP-DKH
		[206]	$^3H_6, 4f^{12}$	166.67	2020	R, Dirac, CIPT+HF+RPA
69	Tm	[54,121]	$4f^{13}$	147 ± 37	2004	R, Dirac, LDA
		[161]	$4f^{13}$	161 ± 32	2007	TD-DFT
		[198]	$4f^{13}$	152.2	2007	R, CASSCF, ECP
		[82,207]	$4f^{13}$	152 ± 15	2012	R, MR-ACQQ, ECP
		[199]	$4f^{13}$	144.3	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 137.8$ for the $4f^{12}5d^1$ configuration)
		[72]	$^2F_{7/2}, 4f^{13}$	130 ± 16	2015	exp.
		[153]	$4f^{13}$	147	2016	R, RPA, PolPot
		[5]	$--$	144 ± 15	2019	recommended
		[206]	$^2F^0_{7/2}, 4f^{13}$	153.02	2020	R, Dirac, CIPT+HF+RPA
70	Yb	[208]	$^1S_0, 4f^{14}$	141 ± 4	1998	R, DHF + Breit + QED, PP
		[54,121]	$^1S_0, 4f^{14}$	142 ± 36	2004	R, Dirac, LDA
		[207]	$^1S_0, 4f^{14}$	152.9	2006	R, Dirac, CCSD(T)
		[209]	$^1S_0, 4f^{14}$	143	2007	R, DCHF, CCSD(T), ECP
		[161]	$^1S_0, 4f^{14}$	157.3	2007	TD-DFT

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Z	Atom	Refs.	State	α	Year	Comments
		[198]	$^1S_0, 4f^{14}$	151.0	2007	R, CASSCF, ECP
		[31]	$^1S_0, 4f^{14}$	144.6 ± 5.6	2008	R, Dirac, coupled cluster
		[210]	$^1S_0, 4f^{14}$	140.7 ± 7.0	2009	R, Dirac + Gaunt, CCSD(T)
		[211]	$^1S_0, 4f^{14}$	144	2009	R, CCSD, PolPot
		[210]	$^1S_0, 4f^{14}$	140.44	2009	R, Dirac, CCSD(T)
		[212]	$^1S_0, 4f^{14}$	142.6	2010	ECP, CCSD(T)
		[213]	$^1S_0, 4f^{14}$	141 ± 6	2011	R, Dirac, CI + MBPT + experimental data, see also ref [214] for error estimates
		[215]	$^1S_0, 4f^{14}$	141 ± 2	2012	R, Dirac, CI + MBPT + RPA
		[82,207]	$^1S_0, 4f^{14}$	145.3 ± 4.4	2012	R, Dirac, CCSD(T)
		[214]	$^1S_0, 4f^{14}$	139.3 ± 5.9	2012	exp.
		[199]	$^1S_0, 4f^{14}$	138.9	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 312.2$ for the $4f^1 46s^1 6p^1$ configuration)
		[72]	$^1S_0, 4f^{14}$	147 ± 20	2015	exp.
		[153]	$^1S_0, 4f^{14}$	142	2016	R, RPA, PolPot
		[216]	$^1S_0, 4f^{14}$	135.73	2016	R, DFT, CAM-B3LYP, 2c-NESC
		[216]	$^1S_0, 4f^{14}$	147.26	2016	R, DFT, PBE0, 2c-NESC
		[217]	$^1S_0, 4f^{14}$	135.50	2017	R, CCSD
		[187]	$^1S_0, 4f^{14}$	136 ± 5	2018	R, CCSD(T)
		[218]	$^1S_0, 4f^{14}$	135 ± 3	2018	R, CI+MBPT+FC
		[219]	$^1S_0, 4f^{14}$	150 ± 9	2018	R, CIPT
		[36]	$^1S_0, 4f^{14}$	140.54	2019	R, CCSD(T)
		[5]	$--$	139 ± 6	2019	recommended
		[202]	$^1S_0, 4f^{14}$	147	2020	R, CI+MBPT

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Z	Atom	Refs.	State	α	Year	Comments
		[201]	$^1S_0, 4f^{14}$	133.65	2020	R, DKH2-B3LYP/ADZP
		[201]	$^1S_0, 4f^{14}$	134.44	2020	R, DKH2-B3LYP/ADZP
		[206]	$^1S_0, 4f^{14}$	143	2020	R, Dirac, CIPT+HF+RPA
		[168]	$^1S_0, 4f^{14}$	136.0	2021	SR, ECP, CCSD(T)
		[220]	$^1S_0, 4f^{14}$	139 ± 3	2023	MCDHF+Breit+QED
71	Lu	[54,121]	$^2D_{3/2}, 5d^1$	148 ± 17	2004	R, Dirac, LDA
		[161]	$^2D_{3/2}, 5d^1$	131 ± 26	2007	TD-DFT
		[199]	$^2D_{3/2}, 5d^1$	137 ± 7	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 61.3$ for the $4f^{14}6s^26p^1$ configuration)
		[221]	$^2D_{3/2}, 5d^1$	145	2014	R, DF, CI + all-order + Breit + QED
		[72]	$^2D_{3/2}, 5d^1$	124 ± 18	2015	exp.
		[5]	$--$	137 ± 7	2019	recommended
72	Hf	[54,121]	$^3F_2, 5d^2$	109 ± 27	2004	R, Dirac, LDA
		[221]	$^3F_2, 5d^2$	97	2014	R, DF, CI + all-order + Breit + QED
		[199,221]	$^3F_2, 5d^2$	103 ± 5	2014	R, DF, CI + MBPT + Breit + QED
		[72]	$^3F_2, 5d^2$	84 ± 19	2015	exp.
		[77,125]	$^3F_2, 5d^2$	83.7	2016	NR, MBPT4
		[162]	$^3F_2, 5d^2$	99.52	2016	LR-CCSD
		[35]	$^3F_2, 5d^2$	102.55	2019	ECP, CCSD
		[5]	$--$	103 ± 6	2019	recommended
		[200]	$^3F_2, 5d^2$	95.6	2022	R (ZORA), DFT (B3LYP)
		[222]	$^3F_2, 5d^2$	94.2	2023	R (ATZP-ZORA), DFT (B3LYP)
73	Ta	[163]	$^4F_{3/2}, 5d^3$	115 ± 20	1956	exp.
		[223]	$^4F_{3/2}, 5d^3$	128 ± 20	1986	exp.

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Z	Atom	Refs.	State	α	Year	Comments
		[223]	$^4F_{3/2}, 5d^3$	108 ± 20	1986	exp.
		[54,121]	$^4F_{3/2}, 5d^3$	88 ± 22	2004	R, Dirac, LDA
		[72]	$^4F_{3/2}, 5d^3$	58 ± 12	2015	exp.
		[153]	$^4F_{3/2}, 5d^3$	73.7	2016	R, RPA, PolPot
		[125]	$^4F_{3/2}, 5d^3$	73.9	2016	TD-DFT (LEXX)
		[162]	$^4F_{3/2}, 5d^3$	82.53	2016	LR-CCSD
		[35]	$^4F_{3/2}, 5d^3$	84.22	2019	ECP, CCSD
		[5]	$--$	74 ± 20	2019	recommended
		[200]	$^4F_{3/2}, 5d^3$	79.6	2022	R (ZORA), DFT (B3LYP)
74	W	[163]	$^5D_0, 5d^4$	47 ± 7	1956	exp.
		[54,121]	$^5D_0, 5d^4$	75 ± 19	2004	R, Dirac, LDA
		[153]	$^5d^4$	68.1	2016	R, RPA, PolPot
		[125]	$^5D_0, 5d^4$	65.8	2016	TD-DFT (LEXX)
		[162]	$^5D_0, 5d^4$	68.5	2016	LR-CCSD
		[35]	$^5D_0, 5d^4$	71.04	2019	ECP, CCSD
		[5]	$--$	68 ± 15	2019	recommended
		[200]	$^5D_0, 5d^4$	65 ± 13	2022	R (ZORA), DFT (B3LYP)
		[200]	$^5D_0, 5d^4$	73.2	2022	R (ZORA), CCSD(T)
		[87]	$^5D_0, 5d^4$	68.98	2022	exp.
75	Re	[54,121]	$^6S_{5/2}, 5d^5$	65 ± 16	2004	R, Dirac, LDA
		[128]	$^6S_{5/2}, 5d^5$	61.1	2005	DK, CASPT2
		[52]	$^6S_{5/2}, 5d^5$	61.9	2010	R, CCSD(T)
		[153]	$^5d^5$	65.6	2016	R, RPA, PolPot
		[125]	$^6S_{5/2}, 5d^5$	60.2	2016	TD-DFT (LEXX)
		[162]	$^6S_{5/2}, 5d^5$	63.04	2016	LR-CCSD

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Z	Atom	Refs.	State	α	Year	Comments
		[35]	$^6S_{5/2}, 5d^5$	65.55	2019	ECP, CCSD
		[5]	$--$	62 ± 3	2019	recommended
76	Os	[54,121]	$^5D_4, 5d^6$	57	2004	R, Dirac, LDA
		[153]	$^5d^6$	57.8	2016	R, RPA, PolPot
		[125]	$^5D_4, 5d^6$	55.3	2016	TD-DFT (LEXX)
		[162]	$^5D_4, 5d^6$	55.06	2016	LR-CCSD
		[35]	$^5D_4, 5d^6$	56.56	2019	ECP, CCSD
		[5]	$--$	57 ± 3	2019	recommended
		[200]	$^5D_4, 5d^6$	53.1	2022	R (ZORA), DFT (B3LYP)
		[222]	$^5D_4, 5d^6$	54.1	2023	R (ATZP-ZORA), DFT (B3LYP)
77	Ir	[223,224]	$^4F_{9/2}, 5d^7$	54.0 ± 6.7	1986	exp.
		[54,121]	$^4F_{9/2}, 5d^7$	51 ± 13	2004	R, Dirac, LDA
		[153]	$^5d^7$	51.7	2016	R, RPA, PolPot
		[125]	$^4F_{9/2}, 5d^7$	51.3	2016	TD-DFT (LEXX)
		[125]	$^4F_{9/2}, 5d^7$	51.3	2016	TD-DFT (LEXX)
		[162]	$^4F_{9/2}, 5d^7$	42.51	2016	LR-CCSD
		[35]	$^4F_{9/2}, 5d^7$	49.48	2019	ECP, CCSD
		[5]	$--$	54 ± 7	2019	recommended
		[200]	$^4F_{9/2}, 5d^7$	40.0	2022	R (ZORA), DFT (B3LYP)
		[222]	$^4F_{9/2}, 5d^7$	39.8	2023	R (ATZP-ZORA), DFT (B3LYP)
78	Pt	[54,121]	$^3D_3, 5d^9$	44 ± 11	2004	R, Dirac, LDA
		[125]	$^3D_3, 5d^9$	48.0	2016	TD-DFT (LEXX)
		[162]	$^3D_3, 5d^9$	39.68	2016	LR-CCSD
		[35]	$^3D_3, 5d^9$	43.83	2019	ECP, CCSD
		[5]	$--$	48 ± 4	2019	recommended

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Z	Atom	Refs.	State	α	Year	Comments
		[225]	$^3D_3, 5d^9$	41.2 ± 1.1	2021	ECP, CCSD(T)
		[200]	$^3D_3, 5d^9$	37.5	2022	R (ZORA), DFT (B3LYP)
		[87]	$^3D_3, 5d^9$	38 ± 8	2022	exp.
		[222]	$^3D_3, 5d^9$	40.9	2023	R (ATZP-ZORA), DFT (B3LYP)
79	Au	[226]	$^2S_{1/2}, 5d^{10}$	30 ± 4	1997	R, HFR, HS, CI, CACP
		[227]	$^2S, 5d^{10}$	34.9	2000	R, DK, CCSD(T)
		[128]	$^2S_{1/2}, 5d^{10}$	39.1 ± 9.8	2005	exp.
		[30,131]	$^2S, 5d^{10}$	36.06 ± 0.54	2006	R, DK, CCSD(T)
		[130,132,228]	$^2S, 5d^{10}$	35.1	2009	R, PP, QCISD(T)
		[82,128]	$^2S, 5d^{10}$	27.9 ± 4.2	2012	R, DK, CASPT2
		[82,94]	$^2S_{1/2}, 5d^{10}$	49.1 ± 4.9	2012	exp.
		[125]	$^2S_{1/2}, 5d^{10}$	45.4	2016	TD-DFT (LEXX)
		[162]	$^2S_{1/2}, 5d^{10}$	36.50	2016	LR-CCSD
		[35]	$^2S_{1/2}, 5d^{10}$	39.56	2019	ECP, CCSD
		[5]	$--$	36 ± 3	2019	recommended
		[169]	$^2S_{1/2}, 5d^{10}$	34.0	2021	R, CI+MBPT
		[168]	$^2S_{1/2}, 5d^{10}$	36.3	2021	SR, ECP, CCSD(T)
		[200]	$^2S_{1/2}, 5d^{10}$	34.2	2022	R (ZORA), DFT (B3LYP)
		[87]	$^2S_{1/2}, 5d^{10}$	40 ± 8	2022	exp.
		[222]	$^2S_{1/2}, 5d^{10}$	34.1	2023	R (ATZP-ZORA), DFT (B3LYP)
80	Hg	[137]	$^1S, 5d^{10}$	31.24	1995	R, MVD, CCSD(T)
		[229]	$^1S_0, 5d^{10}$	33.91 ± 0.34	1996	exp.
		[139]	$^1S, 5d^{10}$	34.42	1997	R, PP, CCSD(T)
		[128]	$^1S, 5d^{10}$	33.3	2005	R, DK, CASPT2
		[30,230]	$^1S_0, 5d^{10}$	34.73 ± 0.52	2006	R, DK, CCSD(T)

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Z	Atom	Refs.	State	α	Year	Comments
		[231]	$^1S_0, 5d^{10}$	34.15	2008	R, Dirac, CCSD(T)
		[137,143,232]	$^1S_0, 5d^{10}$	33.75	2012	exp.
		[233]	$^1S_0, 5d^{10}$	34.27	2015	R, Dirac, CCSDT + QED
		[234]	$^1S_0, 5d^{10}$	34.1	2015	R, Dirac, CCSD(T)
		[142]	$^1S_0, 5d^{10}$	33.59	2015	R, PRCC(T)
		[135]	$^1S, 5d^{10}$	32.9	2016	semi-empirical
		[153]	$^1S_0, 5d^{10}$	39.1	2016	R, RPA, PolPot
		[162]	$^1S_0, 5d^{10}$	33.90	2016	LR-CCSD
		[125]	$^1S_0, 5d^{10}$	33.5	2016	TD-DFT (LEXX)
		[235]	$^1S_0, 5d^{10}$	34.2 ± 0.5	2018	R, CCSD(T) + Breit
		[187]	$^1S_0, 5d^{10}$	34.5 ± 0.8	2018	R, CCSD(T)
		[35]	$^1S_0, 5d^{10}$	35.45	2019	ECP, CCSD
		[5]	$--$	33.91 ± 0.34	2019	recommended
		[236]	$^1S_0, 5d^{10}$	33.69 ± 0.34	2021	PRCC(T)+Breitt+QED
		[200]	$^1S_0, 5d^{10}$	36.1	2022	R (ZORA), DFT (B3LYP)
		[222]	$^1S_0, 5d^{10}$	34.9	2023	R (ATZP-ZORA), DFT (B3LYP)
81	Tl	[146]	^2P	50.48	2003	R, DK, CCSD(T)
		[146]	^2P	50.62	2003	R, DK, CCSD(T)
		[54]	$^2P_{1/2}$	51.3 ± 5.4	2004	exp.
		[41]	^2P	70.0	2005	R, SF, MRCI, M_L res.
		[41]	$^2P_{1/2}/^2P_{3/2}$	51.6/81.2	2005	R, Dirac, MRCI, M_J res.
		[237]	^2P	50.4	2006	R, DHF, SD, MBPT all-order
		[238]	$^2P_{1/2}$	52.3	2008	R, Dirac, FS-CCSD
		[239]	^2P	48.81	2009	R, Dirac, CI+MBPT
		[133,240]	^2P	49.2	2010	RCI + MBPT

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Z	Atom	Refs.	State	α	Year	Comments
		[93]	$^2P_{1/2}/^2P_{3/2}$	$50.7 \pm 5.0/78.5 \pm 6.0$	2010	SI-SOCI, M_J res.
						R, Dirac, FSCC, M_J res.
		[147]	$^2P_{1/2}/^2P_{3/2}$	50.3/80.9	2012	($J = 3/2$: $M_J = 3/2$: 56.7,
						$M_J = 1/2$: 105.1)
		[82,146]	^2P	71.7 ± 1.1	2012	R, DK, CCSD(T)
		[147]	^2P	$52.1 \pm 1.6/80.4 \pm 4.0$	2012	R, Dirac, FSCC
		[241]	^2P	50.0 ± 1.0	2013	R, CC
		[241]	^2P	50.7	2013	R, CI + all-order
		[234,238]	^2P	51.3	2015	R, Dirac, FS-CCSD
		[242]	^2P	47.78	2016	R, Dirac+Breit+QED, SD+CI, RPA
		[125]	^2P	51.4	2016	TD-DFT (LEXX)
		[162]	^2P	69.92	2016	LR-CCSD
		[243]	^2P	49.2 ± 2.0	2018	R, Dirac+Breit, CCSD
		[35]	^2P	70.06	2019	ECP, CCSD
		[5]	$--$	50 ± 2	2019	recommended
82	Pb	[121]	^3P	46 ± 11	1987	R, Dirac, LDA
		[244]	$^3P_0$	51.0	2005	R, SOPP, CCSD(T)
		[45]	$^3P_0$	47.70	2008	R, Dirac + Gaunt, CCSD(T)
		[231]	$^3P_0$	46.96	2008	R, Dirac, CCSD(T)
		[45]	$^3P_0$	47.3 ± 1.9	2008	R, Dirac + Gaunt, CCSD(T)
		[45,54]	$^3P_0$	47.1 ± 7.1	2008	exp.
		[234]	$^3P_0$	47.0	2015	R, Dirac, FS-CCSD
		[72]	$^3P_0$	56 ± 18	2015	exp.
		[242]	$^3P_0$	44.04	2016	R, Dirac + Breit + QED, SD + CI, RPA
		[245]	$^3P_0$	46.5	2016	R, CI + all-order, RPA

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Z	Atom	Refs.	State	α	Year	Comments
		[125]	$^3P_0$	47.9	2016	TD-DFT (LEXX)
		[162]	$^3P_0$	61.80	2016	LR-CCSD
		[35]	$^3P_0$	60.07	2019	EP, CCSD
		[5]	$--$	47 ± 3	2019	recommended
		[202]	$^3P_0$	46	2020	R, CI+MBPT
		[246]	$^3P_0$	47.0	2020	R, FS-RCCSD(T)
		[222]	$^3P_0$	56.3	2023	R (ATZP-ZORA), DFT(B3LYP)
83	Bi	[247]	^4S	52.85	1992	R, Cowan-Griffin, HF only
		[54,121]	^4S	50 ± 12	2004	R, Dirac, LDA
		[50]	^4S	48.6	2004	R, DK, CASPT2
		[52]	^4S	48.75	2010	ECP, CCSD(T)
		[72]	$^4S_{3/2}$	55 ± 11	2015	exp.
		[242]	^4S	44.62	2016	R, Dirac + Breit + QED, SD + CI, RPA
		[125]	^4S	43.2	2016	TD-DFT (LEXX)
		[162]	^4S	49.02	2016	LR-CCSD
		[35]	^4S	48.88	2019	ECP, CCSD
		[5]	$--$	48 ± 4	2019	recommended
		[53]	^4S	48.8	2020	ECP, CCSD(T)
		[200]	^4S	44.36	2022	R (ZORA), CCSD(T)
		[200]	^4S	53.1	2022	R (ATZP-ZORA), DFT (B3LYP)
		[222]	^4S	46.6	2023	R (ZORA), DFT (B3LYP)
84	Po	[247]	$^3P_2$	46.8	1992	R, Cowan-Griffin, HF only, M_L res.
		[54,121]	$^3P_2$	46	2004	R, Dirac, LDA
		[30,82,247]	$^3P_2$	43.6 ± 4.4	2012	R, Cowan-Griffin, HF only
		[162]	$^3P_2$	45.01	2016	LR-CCSD

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Z	Atom	Refs.	State	α	Year	Comments
		[35]	$^3P_2$	44.22	2019	ECP, CCSD
		[5]	$--$	44 ± 4	2019	recommended
		[200]	$^3P_2$	44.77	2022	R (ZORA), CCSD(T)
		[200]	$^3P_2$	47.1	2022	R (ZORA), DFT (B3LYP)
		[222]	$^3P_2$	46.5	2023	R (ATZP-ZORA), DFT (B3LYP)
85	At	[149]	$^2P_{1/2}$	45.6	2002	R, DK, SO-CI
		[149]	$^2P_{3/2}$	41.9	2002	R, DK, SO-CI, M_J res.
		[30,82,247]	$^2P_{3/2}$	40.7 ± 2.0	2012	R, Cowan-Griffin, HF only
		[162]	$^2P_{3/2}$	38.93	2016	LR-CCSD
		[35]	$^2P_{3/2}$	38.15	2019	ECP, CCSD
		[5]	$--$	42 ± 4	2019	recommended
		[200]	$^2P_{3/2}$	40.4	2022	R (ZORA), DFT (B3LYP)
		[222]	$^2P_{3/2}$	41.1	2023	R (ATZP-ZORA), DFT (B3LYP)
86	Rn	[186]	$^1S_0$	34.33	1998	R, SOPP, CCSD(T) + MP2 basis set correction
		[186]	$^1S_0$	34.60	1998	R, SOPP, CCSD(T) + MP2 basis set correction
		[62]	^1S	33.18	2001	R, DK3, CCSD(T)
		[59]	$^1S_0$	34.4374 ± 0.0001	2001	CCSD(T), ECP
		[50]	^1S	32.6	2004	R, DK, CASPT2
		[54,121]	$^1S_0$	36 ± 5	2004	R, Dirac, LDA
		[244]	$^1S_0$	28.6	2005	R, SOPP, CCSD(T)
		[227,248]	$^1S_0$	35.77	2005	R, DK, CCSD(T)
		[248]	$^1S_0$	35.47	2005	CCSD, ECP
		[152]	$^1S_0$	35.391	2012	R, RPA, PolPot
		[249]	$^1S_0$	35.87	2012	R, DFT, DC, PBE38
		[250]	$^1S_0$	34.89	2012	R, DKH2, B3LYP, SARC

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Z	Atom	Refs.	State	α	Year	Comments
		[250]	$^1S_0$	34.70	2012	R, DKH2, B3LYP, UGBS
		[249]	$^1S_0$	33.62	2012	R, DFT, sfDC, PBE38
		[82,251]	$^1S_0$	35.04 ± 1.8	2012	R, Dirac, CCSD(T)
		[234]	$^1S_0$	35.0	2015	R, Dirac, CCSD(T)
		[153]	$^1S_0$	34.2	2016	R, RPA, PolPot
		[125]	$^1S_0$	32.2	2016	TD-DFT (LEXX)
		[162]	$^1S_0$	33.54	2016	LR-CCSD
		[187,252]	$^1S_0$	37.0 ± 0.5	2018	R, CCSD(T)
		[252]	$^1S_0$	35.3	2018	R, Dirac-Gaunt, CCSD(T)
		[253]	$^1S_0$	35.00	2018	R, RPA
		[35]	$^1S_0$	32.8	2019	ECP, CCSD
		[5]	$--$	35 ± 2	2019	recommended
		[202]	$^1S_0$	35	2020	R, RPA
		[154]	$^1S_0$	34.66	2020	R, DHF, MBPT
		[254]	$^1S_0$	36.14	2020	R, DK, CCSD(T)
		[236]	$^1S_0$	35.53 ± 0.36	2021	PRCC(T)+Breit+QED
		[200]	$^1S_0$	34.6	2022	R (ZORA), DFT (B3LYP)
		[222]	$^1S_0$	30.9	2023	R (ATZP-ZORA), DFT (B3LYP)
87	Fr	[104]	^2S	315.2	2005	R, DK, CCSD(T), AE
		[255]	$^2S_{1/2}$	313.7	2007	R, DF, RPA, MBPT
		[69,105]	$^2S_{1/2}$	317.8 ± 2.4	2010	R, Dirac, SD all orders + experimental data
		[193]	$^2S_{1/2}$	311.5	2013	R, Dirac, CCSD(T)
		[162]	$^2S_{1/2}$	317.8	2016	LR-CCSD
		[256]	$^2S_{1/2}$	316.8	2016	R, Dirac-Fock, CCSD(T)
		[5]	$--$	317.8 ± 2.4	2019	recommended

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Z	Atom	Refs.	State	α	Year	Comments
		[257]	$^2S_{1/2}$	317.1 ± 1.3	2021	R, Dirac-HF, CCSD
		[23]	$^2S_{1/2}$	325.8	2021	SR, CCSD(T), ECP
		[258]	$^2S_{1/2}$	316.6 ± 2.4	2022	R, all orders, Dirac-Fock, RPA
		[24]	$^2S_{1/2}$	316.6 ± 1.5	2022	R, Dirac-HF, perturbative singles + doubles method, RPA
88	Ra	[112]	$^1S_0$	248.56	2004	R, DK + SO, CCSD(T)
		[30,112]	$^1S_0$	246.2 ± 4.9	2006	R, DK + SO, CCSD(T)
		[196]	$^1S_0$	242.8	2013	R, Dirac + Gaunt, CCSD(T)
		[83]	$^1S_0$	242.42	2014	R, Dirac + Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[153]	$^1S_0$	232	2016	R, RPA, PolPot
		[162]	$^1S_0$	246.2	2016	LR-CCSD
		[187]	$^1S_0$	236 ± 15	2018	R, CCSD(T)
		[84]	$^1S_0$	248.5	2019	R, KRCISD/aug-QZ
		[5]	$--$	246 ± 4	2019	recommended
		[154]	$^1S_0$	247.838	2020	R, DHF, MBPT
		[202]	$^1S_0$	250	2020	R, CI+MBPT
		[23]	$^1S_0$	250.5	2021	SR, CCSD(T), ECP
89	Ac	[54,121]	$^2D_{3/2}, 6d^1$	217 ± 44	2004	R, Dirac, LDA
		[199]	$^2D_{3/2}, 6d^1$	203.3	2014	R, Dirac, CI + MBPT + CP(RPA); (α_D = 141.9 for the $7s^2 7p^1$ configuration)
		[5]	$--$	203 ± 12	2019	recommended
		[202]	$^2D_{3/2}, 6d^1$	195	2020	R, CI+MBPT
90	Th	[54,121]	$6d^2$	217 ± 54	2004	R, Dirac, LDA
		[82]	$6d^2$	166.7	2012	Estimated from correlation with ionization energies
		[5]	$--$	217 ± 54	2019	recommended
91	Pa	[54,121]	$5f^2 6d^1$	171 ± 34	2004	R, Dirac, LDA

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Z	Atom	Refs.	State	α	Year	Comments
		[199]	$5f^26d^1$	154.4	2014	R, Dirac, CI + MBPT + CP(RPA); (α_D = 151.9 for the $5f^26d^27s^1$ configuration)
		[5]	$--$	154 ± 20	2019	recommended
		[202]	$5f^26d^1$	170	2020	R, CI+MBPT
92	U	[259]	${}^5L_6, 5f^36d^1$	137 ± 9	1994	exp.
		[54,121]	$5f^36d^1$	153 ± 38	2004	R, Dirac, LDA
		[199]	$5f^36d^1$	127.8	2014	R, Dirac, CI + MBPT + CP(RPA); (α_D = 153.2 for the $5f^4$ configuration)
		[5]	$--$	129 ± 17	2019	recommended
		[202]	$5f^36d^1$	165	2020	R, CI+MBPT
93	Np	[54,121]	$5f^46d^1$	167 ± 42	2004	R, Dirac, LDA
		[199]	$5f^46d^1$	150.5	2014	R, Dirac, CI + MBPT + CP(RPA); (α_D = 127.5 for the $5f^5$ configuration)
		[5]	$--$	151 ± 20	2019	recommended
		[202]	$5f^46d^1$	160	2020	R, CI+MBPT
94	Pu	[54,121]	$5f^6$	165 ± 41	2004	R, Dirac, LDA
		[199]	$5f^6$	132.2	2014	R, Dirac, CI + MBPT + CP(RPA); (α_D = 147.6 for the $5f^56d^1$ configuration)
		[5]	$--$	132 ± 20	2019	recommended
		[202]	$5f^6$	144	2020	R, CI+MBPT
95	Am	[54,121]	$5f^7$	157 ± 39	2004	R, Dirac, LDA
		[260]	$5f^7$	116 ± 29	2005	R, DK, CASPT2
		[199]	$5f^7$	131.2	2014	R, Dirac, CI + MBPT + CP(RPA); (α_D = 144.7 for the $5f^66d^1$ configuration)
		[261]	$5f^7$	122.4	2016	R, DFT, DKH, B3LYP
		[5]	$--$	131 ± 25	2019	recommended

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Z	Atom	Refs.	State	α	Year	Comments
96	Cm	[54,121]	$5f^7 6d^1$	155 ± 39	2004	R, Dirac, LDA
		[199]	$5f^7 6d^1$	143.6	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 128.6$ for the $5f^8$ configuration)
		[5]	$--$	144 ± 25	2019	recommended
97	Bk	[54,121]	$5f^9$	153 ± 38	2004	R, Dirac, LDA
		[199]	$5f^9$	125.3	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 141.6$ for the $5f^8 6d^1$ configuration)
		[5]	$--$	125 ± 25	2019	recommended
98	Cf	[54,121]	$5f^{10}$	138 ± 34	2004	R, Dirac, LDA
		[199]	$5f^{10}$	121.5	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 142.3$ for the $5f^9 6d^1$ configuration)
		[5]	$--$	122 ± 20	2019	recommended
99	Es	[54,121]	$5f^{11}$	133 ± 33	2004	R, Dirac, LDA
		[199]	$5f^{11}$	117.5	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 146.1$ for the $5f^{10} 6d^1$ configuration)
		[5]	$--$	118 ± 20	2019	recommended
100	Fm	[54,121]	$5f^{12}$	161 ± 40	2004	R, Dirac, LDA
		[199]	$5f^{12}$	113.4	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 155.6$ for the $5f^{11} 6d^1$ configuration)
		[5]	$--$	113 ± 20	2019	recommended
101	Md	[54,121]	$5f^{13}$	123 ± 31	2004	R, Dirac, LDA
		[199]	$5f^{13}$	109.4	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 179.6$ for the $5f^{12} 6d^1$ configuration)
		[5]	$--$	109 ± 20	2019	recommended
102	No	[54,121]	$^1S_0, 5f^{14}$	118 ± 30	2004	R, Dirac, LDA

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Z	Atom	Refs.	State	α	Year	Comments
		[210]	$^1S_0, 5f^{14}$	110.8 ± 5.5	2009	R, Dirac + Gaunt, CCSD(T)
		[210]	$^1S_0, 5f^{14}$	115.64	2009	R, DK, CCSD(T)
		[199]	$^1S_0, 5f^{14}$	105.4	2014	R, Dirac, CI + MBPT + CP(RPA); ($\alpha_D = 267.8$ for the $5f^{14}7s7p^1$ configuration)
		[199,221]	$^1S_0, 5f^{14}$	112 ± 6	2014	R, DF, CI + MBPT + Breit + QED
		[199,221]	$^1S_0, 5f^{14}$	110 ± 8	2014	R, DF, CI + all-order + Breit + QED
		[153]	$^1S_0, 5f^{14}$	114	2016	R, RPA, PolPot
		[216]	$^1S_0, 5f^{14}$	107.77	2016	R, DFT, CAM-B3LYP, 2c-NESC
		[261]	$^1S_0, 5f^{14}$	115.6	2016	R, DFT, DKH, B3LYP
		[5]	$--$	110 ± 6	2019	recommended
103	Lr	[221]	$7p^1$	323 ± 80	2014	R, DF, CI + all-order + Breit + QED
		[221]	$7p^1$	320 ± 80	2014	R, DF, CI + MBPT + Breit + QED
		[262]	$7p^1$	225.2	2016	R, DK, DFT, CAM-B3LYP
		[5]	$--$	320 ± 20	2019	recommended
104	Rf	[221]	$6d^2$	107 ± 5	2014	R, DF, CI + MBPT + Breit + QED
		[221]	$6d^2$	115 ± 13	2014	R, DF, CI + all-order + Breit + QED
		[5]	$--$	112 ± 10	2019	recommended
105	Db	[153]	$6d^3$	42.5	2016	R, RPA, PolPot
		[153]	$6d^3$	42 ± 4	2016	R, RPA, PolPot (value recommended by authors)
		[5]	$--$	42 ± 4	2019	recommended
106	Sg	[153]	$6d^4$	40.7	2016	R, RPA, PolPot
		[153]	$6d^4$	40 ± 4	2016	R, RPA, PolPot (value recommended by authors)
		[5]	$--$	40 ± 4	2019	recommended
107	Bh	[153]	$6d^5$	38.4	2016	R, RPA, PolPot
		[153]	$6d^5$	38 ± 4	2016	R, RPA, PolPot (value recommended by authors)

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Z	Atom	Refs.	State	α	Year	Comments
		[5]	$--$	38 ± 4	2019	recommended
108	Hs	[153]	$6d^6$	36.2	2016	R, RPA, PolPot
		[153]	$6d^6$	36 ± 4	2016	R, RPA, PolPot (value recommended by authors)
		[5]	$--$	36 ± 4	2019	recommended
109	Mt	[153]	$6d^7$	34.2	2016	R, RPA, PolPot
		[153]	$6d^7$	34 ± 3	2016	R, RPA, PolPot (value recommended by authors)
		[5]	$--$	34 ± 3	2019	recommended
110	Ds	[153]	$6d^8$	32.3	2016	R, RPA, PolPot
		[153]	$6d^8$	32 ± 3	2016	R, RPA, PolPot (recommended value by authors)
		[5]	$--$	32 ± 3	2019	recommended
111	Rg	[263]	$6d^9$	31.6	1996	ARPP, CCSD(T)
		[153]	$6d^9$	30.6	2016	R, RPA, PolPot
		[153]	$6d^9$	30 ± 3	2016	R, RPA, PolPot (value recommended by authors)
		[5]	$--$	32 ± 6	2019	recommended
112	Cn	[139]	$^1S_0, 6d^{10}$	25.82	1997	R, PP, CCSD(T)
		[244]	$^1S_0, 6d^{10}$	28.68	2005	R, SOPP, CCSD(T)
		[231]	$^1S_0, 6d^{10}$	27.64	2008	R, Dirac, CCSD(T)
		[231]	$^1S_0, 6d^{10}$	27.40	2008	R, Dirac, CCSD(T)
		[153]	$^1S_0, 6d^{10}$	28.2	2016	R, RPA, PolPot
		[153]	$^1S_0, 6d^{10}$	28 ± 4	2016	R, RPA, PolPot (value recommended by authors)
		[5]	$--$	28 ± 2	2019	recommended
		[236]	$^1S_0, 6d^{10}$	27.44 ± 0.88	2021	PRCC(T)+Breit+QED
113	Nh	[238]	$^2P_{1/2}$	29.85	2008	R, Dirac, FS-CCSD
		[242]	$^2P_{1/2}$	28.8	2016	R, Dirac+Breit+QED, SD+CI, RPA
		[5]	$--$	29 ± 2	2019	recommended

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Z	Atom	Refs.	State	α	Year	Comments
114	Fl	[244]	$^3P_0$	34.35	2005	R, SOPP, CCSD(T)
		[45]	$^3P_0$	31.87	2008	R, Dirac + Gaunt, CCSD(T)
		[231]	$^3P_0$	30.59	2008	R, Dirac, CCSD(T)
		[231]	$^3P_0$	29.52	2008	estimate
		[45]	$^3P_0$	31.0	2008	R, Dirac + Gaunt, CCSD(T)
		[242]	$^3P_0$	31.4	2016	R, Dirac + Breit + QED, SD + CI, RPA
		[5]	$--$	31 ± 4	2019	recommended
115	Mc	[264]	$^4S_{3/2}$	66	2014	Estimated via correlation with $R_{\max}(np_{3/2})$
		[242]	$^4S_{3/2}$	70.5	2016	R, Dirac + Breit + QED, SD + CI, RPA
		[5]	$--$	71 ± 20	2019	recommended
116	Lv	[264]	$^3P_2$	61.17	2014	Estimated via correlation with $R_{\max}(np_{3/2})$
		[5]	$--$	67 ± 10	2019	recommended
117	Ts	[264]	$^2P_{3/2}$	52.24	2014	Estimated via correlation with $R_{\max}(np_{3/2})$
		[265]	$^2P_{3/2}$	76.3	2017	empirical estimate
		[5]	$--$	76 ± 15	2019	recommended
118	Og	[244]	$^1S_0$	52.4	2005	R, SOPP, CCSD(T)
		[251]	$^1S_0$	46.33	2008	R, Dirac, CCSD(T)
		[153]	$^1S_0$	59.0/57.2	2016	R, RPA, PolPot
		[153]	$^1S_0$	57 ± 3	2016	R, RPA, PolPot
		[266]	$^1S_0$	57.98	2018	R, Dirac + Gaunt, CCSD(T)
		[5]	$--$	58 ± 6	2019	recommended
		[236]	$^1S_0$	56.5 ± 1.8	2021	PRCC(T)+Breit+QED
119	Uue	[17]	^2S	169	1999	R, Dirac, CCSD(T)
		[104]	^2S	163.7	2005	R, DK, CCSD(T), ARPP
		[104]	^2S	166.0	2005	R, DK, CCSD(T), AE

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Z	Atom	Refs.	State	α	Year	Comments
		[193]	$^2S_{1/2}$	169.7	2013	R, Dirac, CCSD(T)
		[5]	$--$	169 ± 4	2019	recommended
120	Ubn	[196]	$^1S_0$	162.6	2013	R, Dirac + Gaunt, CCSD(T)
		[153]	$^1S_0$	147	2016	R, RPA, PolPot
		[153]	$^1S_0$	159 ± 10	2016	R, RPA, PolPot
		[5]	$--$	159 ± 10	2019	recommended

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