2018 Table of Polarizabilities

Lit.: P. Schwerdtfeger, J. K. Nagle, "2018 Table of Static Dipole Polarizabilities of the Neutral Elements in the Periodic Table", ***Mol. Phys.*** (**2019**): https://doi.org/10.1080/00268976.2018.1535143

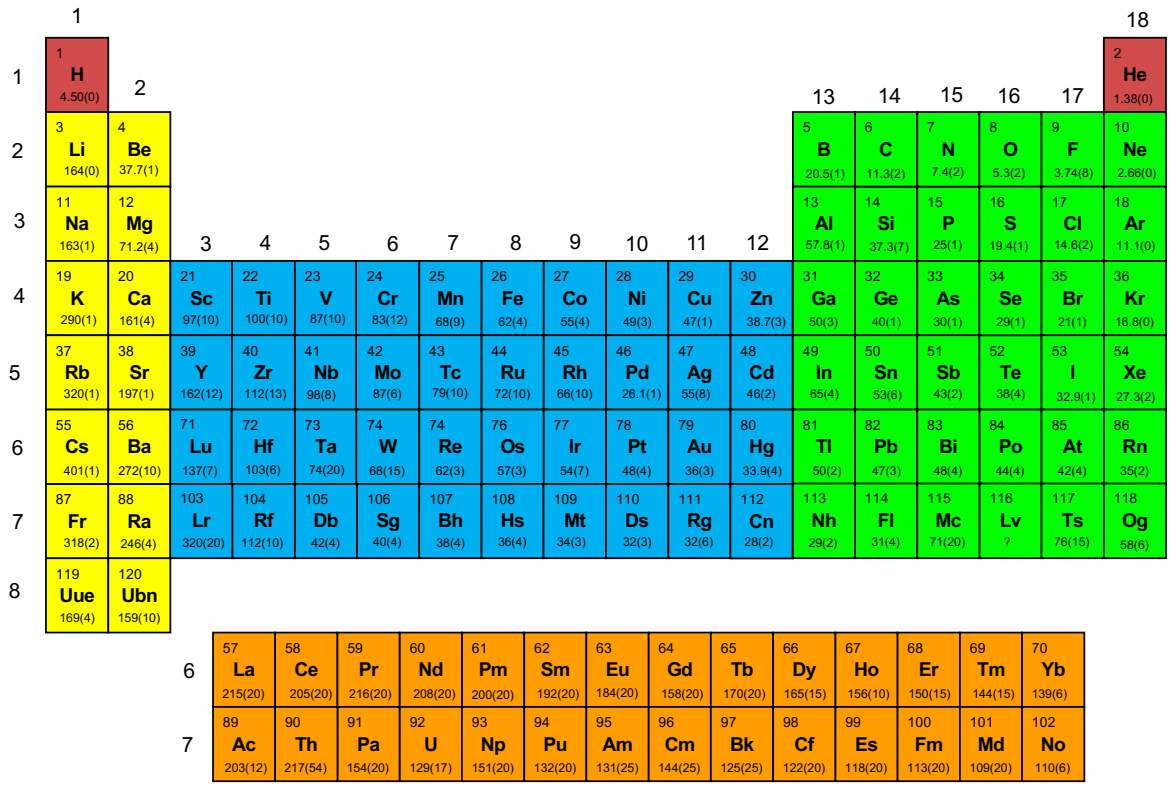

Figure 1. Recommended values from Table 1 for the atomic polarizabilities (atomic units; estimated uncertainties in parentheses) of elements Z = 1-120. The various blocks of elements are color-coded: *s*-block, yellow; *p*-block, green; *d*-block, blue; *f*-block, orange.

Acknowledgment

PS thanks Ivan Lim and Nicola Gaston (Auckland), Uwe Hohm (Braunschweig), Antonio Rizzo (Pisa), Jürgen Hinze (Bielefeld), Gary Doolen (Los Alamos National Laboratory), Dirk Andrae (Bielefeld), Vitaly Kresin (Los Angeles), Timo Fleig (Düsseldorf), Ajit Thakkar (Fredericton), Pekka Pyykkö (Helsinki), Zong-Chao Yan, (Brunswick), Juha Tiihonen (Helsinki) and Keith Bonin (Winston-Salem) for helpful discussions. Financial support from Marsden funding (17-MAU-021) by the Royal Society of New Zealand is gratefully acknowledged. JN thanks Bowdoin College for sabbatical leave support.

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]	$^2S_{1/2}$	4.504654245	R, Dirac (as above), but with finite mass correction added for the ^{1}H isotope
			$^2S_{1/2}$	**4.50465(3)**	**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	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
		[123]	$^1S_0$	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	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)
		[123]	^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, $3d^1$	142±21	NR, MCPF
		[90]	^2D, $3d^1$	115.46	DFT
		[91]	$^2D_{3/2}$, $3d^1$	121±12	R, DK, MRCI
		[92]	^2D, $3d^1$	105.88	TD-DFT
		[93]	^2D, $3d^1$	114.00	Interacting-induced-dipoles polarization model
		[94]	^2D, $3d^1$	123	TD-DFT (LEXX)
		[66,95]	$^2D_{3/2}$, $3d^1$	106.0	SIC-DFT (RXH)
		[95]	^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
		[89]	^3F, $3d^2$	114±17	NR, MCPF
		[91]	$^3F_2$, $3d^2$	102±10	R, DK, MRCI
		[92]	^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
		[89]	^4F, $3d^3$	97±15	NR, MCPF
		[91]	$^4F_{3/2}$, $3d^3$	87.3±8.7	R, DK, MRCI
		[66]	^4F, $3d^3$	72.8	SIC-DFT
		[52]	$^4F_{3/2}$, $3d^3$	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
		[89]	^7S, $3d^5$	95±15	NR, MCPF
		[96]	$^7S_3$, $3d^5$	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
		[89]	^6S, $3d^5$	76±11	NR, MCPF
		[96]	$^6S_{5/2}$, $3d^5$	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
		[89]	^5D, $3d^6$	63.93	NR, MCPF
		[97]	^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
		[89]	^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
		[89]	^3F, $3d^8$	51.10	NR, MCPF
		[91]	$^3F_4$, $3d^8$	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
		[89]	^2S, $3d^{10}$	53.44	NR, MCPF
		[98]	$^2S_{1/2}$, $3d^{10}$	45.0	R, PP, QCISD(T)
		[21,99]	$^2S_{1/2}$, $3d^{10}$	46.50±0.35	R, DK, CCSD(T)
		[96]	$^2S_{1/2}$, $3d^{10}$	40.7±4.1	R, DK, CASPT2
		[91]	$^2S_{1/2}$, $3d^{10}$	43.7±4.4	R, DK, MRCI
		[100]	^2S, $3d^{10}$	51.8	semi-empirical
		[101]	$^2S_{1/2}$, $3d^{10}$	46.98	R, DK, CCSD(T)
		[66]	$^2S_{1/2}$, $3d^{10}$	39.5	SIC-DFT
		[102,103]	$^2S_{1/2}$, $3d^{10}$	41.65	CICP
		[104]	$^2S_{1/2}$, $3d^{10}$	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
		[105]	^1S, $3d^{10}$	39.2±0.8	NR, CCSD(T), MP2 basis correction
		[106]	^1S, $3d^{10}$	38.01	R, PP, CCSD(T)
		[107]	^1S, $3d^{10}$	37.6	R, MVD, CCSD(T)
		[96]	^1S, $3d^{10}$	38.4	R, DK, CASPT2
		[108]	$^1S_0$, $3d^{10}$	38.666±0.096	R, Dirac, CCSDT
		[21,107]	$^1S_0$, $3d^{10}$	38.35±0.29	R, MVD, CCSD(T)
		[109]	$^1S_0$, $3d^{10}$	38.75	R, PRCC(T)
		[66]	$^1S_0$, $3d^{10}$	37.7	SIC-DFT
		[110]	$^1S_0$, $3d^{10}$	39.12	R, MRCI, pseudo-potential
		[109,111]	$^1S_0$, $3d^{10}$	38.92	exp.
		[105]	$^1S_0$, $3d^{10}$	38.8±0.8	exp.
				38.67±0.30	**recommended**
31	Ga	[112]	^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.
		[113]	$^2P_{1/2}/^2P_{3/2}$	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)
		[114]	^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	[112]	^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	[112]	^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
		[115]	$^3P_2$	28.9±1.0	exp.
				28.9±1.0	**recommended**
35	Br	[116]	$^2P_{1/2}$	21.9	R, DK, SO-CI
		[116]	$^2P_{3/2}$	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
		[117]	$^1S_0$	16.012	R, Dirac, CCSD/T
		[118]	$^1S_0$	16.47	R, RPA, PolPot
		[119]	$^1S_0$	16.79	DOSD (constrained dipole oscillator strength distribution)
		[146]	$^1S_0$	16.736	R, DK3, CCSD(T)
		[120]	$^1S_0$	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
		[56,121]	$^1S_0$	197.2±3.6	R, Dirac, CI+MBPT+ experimental data
		[122]	$^1S_0$	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
		[123]	$^1S_0$	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
		[124]	$^2D_{3/2}$, $4d^1$	140.94	DFT, ECP
		[59,125]	$^2D_{3/2}$, $4d^1$	139±28	TD-DFT
		[95]	$^2D_{3/2}$, $4d^1$	134.9	SIC-DFT (RXH)
		[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
		[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
		[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
		[59,96]	^7S, $4d^5$	73±11	R, DK, CASPT2
		[36]	$^7S_3$, $4d^5$	84	R, CCSD(T)
		[36]	$^7S_3$, $4d^5$	79	MRCI
		[52]	$^7S_3$, $4d^5$	87.1±6.1	exp.
		[126]	$^7S_3$, $4d^5$	61±10	exp.
				87±6	**recommended**
43	Tc	[85,86]	$^6S_{5/2}$, $4d^5$	77±20	R, Dirac, LDA
		[59,96]	^6S, $4d^5$	80±12	R, DK, CASPT2
		[94]	$^6S_{5/2}$, $4d^5$	79.6	TD-DFT (LEXX)
		[36]	$^6S_{5/2}$, $4d^5$	78.6	R, CCSD(T)
				79±10	**recommended**
44	Ru	[85,86]	$^5F_5$, $4d^7$	65±16	R, Dirac, LDA
		[94]	$^5F_5$, $4d^7$	72.3	TD-DFT (LEXX)
				72±10	**recommended**

Z	Atom	Refs.	State	α_D	Comments
45	Rh	[85,86]	$^4F_{9/2}$, $4d^8$	58±15	R, Dirac, LDA
		[94]	$^4F_{9/2}$, $4d^8$	66.4	TD-DFT (LEXX)
		[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
		[127]	$^1S_0$, $4d^{10}$	26.14±0.10	CCSDTQP, DKH2+Gaunt, CBS
		[128]	^1S, $4d^{10}$	26.612	NR, ECP, CCSD(T)
		[129]	$^1S_0$, $4d^{10}$	24.581	R, DK
				26.14±0.10	**recommended**
47	Ag	[98,101]	^2S, $4d^{10}$	52.2	R, PP, QCISD(T)
		[21,99]	^2S, $4d^{10}$	52.46±0.52	R, DK, CCSD(T)
		[96]	^2S, $4d^{10}$	36.7	R, DK, CCSD(T)
		[100]	^2S, $4d^{10}$	55.2	Semi-empirical
		[99]	$^2S_{1/2}$, $4d^{10}$	55.3±0.5	R, DK, CCSD(T)
		[130]	$^2S_{1/2}$, $4d^{10}$	46.17	CICP
		[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**
48	Cd	[106]	^1S, $4d^{10}$	46.25	R, PP, CCSD(T)
		[107]	^1S, $4d^{10}$	46.8	R, MVD, CCSD(T)
		[96]	^1S, $4d^{10}$	46.9	R, DK, CASPT2
		[131]	$^1S_0$, $4d^{10}$	46.02±0.50	R, DHF, CCSD(T)
		[21,107]	$^1S_0$, $4d^{10}$	47.55±0.48	R, MVD, CCSD(T)
		[132]	$^1S_0$, $4d^{10}$	44.63	R, DHF, CPMP
		[108]	$^1S_0$, $4d^{10}$	45.86±0.15	R, DF, CCSD(T), MBPT3
		[133]	$^1S_0$, $4d^{10}$	49.7±1.6	exp.
		[134,135]	$^1S_0$, $4d^{10}$	45.3±1.4	exp.
		[135]	$^1S_0$, $4d^{10}$	48.2 ±1.1	exp.
				46±2	**recommended**

Z	Atom	Refs.	State	α_D	Comments
49	In	[136]	$^2P_{1/2}$	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.
		[113]	$^2P_{1/2}/^2P_{3/2}$	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)
		[137]	$^2P_{1/2}$	62.4	R, Dirac+Breit, CI+all-order
		[114]	$^2P_{1/2}$	68.67±0.69	R, DK, CCSD(T)
		[30,113]	$^2P_{1/2}$	61.5	CCSD(T)
		[67]	$^2P_{1/2}$	66.4±5.0/74.4±8.0	SI-SOCI, M_J res.
		[138]	$^2P_{1/2}/^2P_{3/2}$	68.7±8.1	exp.
		[52]	$^2P_{1/2}$	62.1±6.1	exp.
				65±4	**recommended**
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)
		[139]	$^3P_0$	54.48	R, PP, DFT, BP386
		[66]	^3P	57.5	SIC-DFT
		[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
		[140]	^4S	42.55	NR, CCSD(T)
		[36]	^4S	43.03	ECP, CCSD(T)
		[66]	^4S	47.07	SIC-DFT
				43±2	**recommended**

Z	Atom	Refs.	State	α_D	Comments
52	Te	[85,86]	^3P	37±4	R, LDA
		[21,141]	^3P	38.1±3.8	QR, MVD-HF, GTO basis set
		[66]	^3P	40.06	SIC-DFT
				38±4	**recommended**
53	I	[116]	$^2P_{1/2}$	35.1	R, DK, SO-CI
		[116]	$^2P_{3/2}$	34.6	R, DK, SO-CI, M_J res.
		[21,116,141]	$^2P_{3/2}$	33.0±1.7	R, DK, SO-CI
		[66]	^2P	33.6	SIC-DFT
		[142]	$^2P_{3/2}$	32.9±1.3	exp.
		[143]	$^2P_{3/2}$	33.4	exp.
				32.9±1.3	**recommended**
54	Xe	[41]	^1S	27.06±0.27	R, DK3, CCSD(T)
		[144]	$^1S_0$	27.36	R, SOPP, CCSD(T) + MP2 basis set correction
		[119]	$^1S_0$	27.16	DOSD (constrained dipole oscillator strength distribution)
		[33]	^1S	26.7	R, DK, CASPT2
		[117]	$^1S_0$	25.297	R, Dirac, CCSD/T
		[145]	$^1S_0$	27.42	R, DK3, CCSD(T)
		[118]	$^1S_0$	26.7	R, RPA, PolPot
		[146]	$^1S_0$	26.432	R, DK3, CCSD
		[44]	$^1S_0$	27.2937±0.0003	CCSD(T), ECP
		[147]	$^1S_0$	28.4±0.5	R, CCSD(T)
		[148]	$^1S_0$	27.508	R, CCSD(T)
		[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
		[149]	$^2S_{1/2}$	399.0	R, Dirac, CCSD(T)
		[150]	$^2S_{1/2}$	399.5±0.8	R, Dirac, RCC-SD
		[77]	$^2S_{1/2}$	399.8	Combination of theoretical and experimental data
		[151]	$^2S_{1/2}$	398.2±0.9	R, Dirac, SDpT
		[152]	$^2S_{1/2}$	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
		[153]	$^2S_{1/2}$	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
		[154]	$^1S_0$	272.7	R, Dirac+Gaunt, CCSD(T)
		[57]	$^1S_0$	274.68	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[118]	$^1S_0$	251	R, RPA, PolPot
		[27]	$^1S_0$	261.2	Model potential
		[155]	$^1S_0$	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
		[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
		[156]	$^2D_{3/2}$, $5d^1$	213.7	R, Dirac, CI+MBPT+CP(RPA); (α_D = 218.7 for the $5d^26s^1$ configuration)
		[125]	$^2D_{3/2}$, $5d^1$	201±40	TD-DFT
		[59,157]	$^2D_{3/2}$, $5d^1$	220±22	R, CASSCF, ECP
		[157]	$^2D_{3/2}$, $5d^1$	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
		[156]	$4f^15d^1$	204.7	R, Dirac, CI+MBPT+CP(RPA); (α_D = 223.4 for the $4f^2$ configuration)
		[125]	$4f^15d^1$	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
		[156]	$4f^3$	215.8	R, Dirac, CI+MBPT+CP(RPA); (α_D = 195.7 for the $4f^25d^1$ configuration)
		[125]	$4f^3$	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
		[156]	$4f^4$	208.4	R, Dirac, CI+MBPT+CP(RPA); (α_D = 187.5 for the $4f^35d^1$ configuration)
		[125]	$4f^4$	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
		[156]	$4f^5$	200.2	R, Dirac, CI+MBPT+CP(RPA); (α_D = 179.3 for the $4f^45d^1$ configuration)
		[125]	$4f^5$	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
		[156]	$4f^6$	192.1	R, Dirac, CI+MBPT+CP(RPA); (α_D = 171.7 for the $4f^5 5d^1$ configuration)
		[125]	$4f^6$	200±40	TD-DFT
		[157]	$4f^6$	196.8	R, CASSCF, ECP
		[59,157]	$4f^6$	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
		[156]	$4f^7$	184.2	R, Dirac, CI+MBPT+CP(RPA); (α_D = 164.7 for the $4f^6 5d^1$ configuration)
		[125]	$4f^7$	194±39	TD-DFT
		[157]	$4f^7$	189.4	R, CASSCF, ECP
		[59,157]	$4f^7$	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
		[156]	$4f^7 5d^1$	158.3	R, Dirac, CI+MBPT+CP(RPA); (α_D = 194.5 for the $4f^7 5d^2 6s^1$ configuration)
		[125]	$4f^7 5d^1$	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
		[156]	$4f^9$	169.5	R, Dirac, CI+MBPT+CP(RPA); (α_D = 152.4 for the $4f^8 5d^1$ configuration)
		[125]	$4f^9$	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
		[156]	$4f^{10}$	162.7	R, Dirac, CI+MBPT+CP(RPA); (α_D = 148.3 for the $4f^9 5d^1$ configuration)
		[156]	$4f^{10}$	165	R, RPA, PolPot
		[118]	$4f^{10}$	168	R, RPA, PolPot
		[125]	$4f^{10}$	175±35	TD-DFT
		[158]	$^5I_8$, $4f^{10}$	164	exp.
		[52]	$^5I_8$, $4f^{10}$	157±11	exp.
				163±15	**recommended**
67	Ho	[85,86]	$4f^{11}$	159±40	R, Dirac, LDA
		[156]	$4f^{11}$	156.3	R, Dirac, CI+MBPT+CP(RPA); (α_D = 142.9 for the $4f^{10}5d^1$ configuration)
		[118]	$4f^{11}$	161	R, RPA, PolPot
		[125]	$4f^{11}$	170±34	TD-DFT
		[158]	$^4I_{15/2}$, $4f^{11}$	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
		[156]	$4f^{12}$	150.2	R, Dirac, CI+MBPT+CP(RPA); (α_D = 139.4 for the $4f^{11}5d^1$ configuration)
		[156]	$4f^{12}$	169	R, RPA, PolPot
		[118]	$4f^{12}$	154	R, RPA, PolPot
		[125]	$4f^{12}$	166±33	TD-DFT
		[159]	$4f^{12}$	141±7	R, HF, Darwin, SO
		[160]	$4f^{12}$	149	R, HF, Darwin, SO
		[160]	$^3H_6$, $4f^{12}$	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
		[156]	$4f^{13}$	144.3	R, Dirac, CI+MBPT+CP(RPA); (α_D = 137.8 for the $4f^{12}5d^1$ configuration)
		[118]	$4f^{13}$	147	R, RPA, PolPot
		[125]	$4f^{13}$	161±32	TD-DFT
		[59,161]	$4f^{13}$	152±15	R, MR-ACQQ, ECP
		[157]	$4f^{13}$	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
		[162]	$^1S_0$, $4f^{14}$	140.7±7.0	R, Dirac+Gaunt, CCSD(T)
		[163]	$^1S_0$, $4f^{14}$	141±6	R, Dirac, CI+MBPT+ experimental data, see also ref 170 for error estimates
		[164]	$^1S_0$, $4f^{14}$	142.6	ECP, CCSD(T)
		[156]	$^1S_0$, $4f^{14}$	138.9	R, Dirac, CI+MBPT+CP(RPA); (α_D = 312.2 for the $4f^{14}6s^16p^1$ configuration)
		[118]	$^1S_0$, $4f^{14}$	142	R, RPA, PolPot
		[165]	$^1S_0$, $4f^{14}$	144	R, CCSD, PolPot
		[166]	$^1S_0$, $4f^{14}$	141±2	R, CI+MBPT+RPA
		[167]	$^1S_0$, $4f^{14}$	141±4	R, DHF+Breit+QED, PP
		[59,161]	$^1S_0$, $4f^{14}$	145.3±4.4	R, Dirac, CCSD(T)
		[168]	$^1S_0$, $4f^{14}$	135.73	R, DFT, CAM-B3LYP, 2c-NESC
		[168]	$^1S_0$, $4f^{14}$	147.26	R, DFT, PBE0, 2c-NESC
		[162]	$^1S_0$, $4f^{14}$	140.44	R, Dirac, CCSD(T)
		[161]	$^1S_0$, $4f^{14}$	152.9	R, Dirac, CCSD(T)
		[169]	$^1S_0$, $4f^{14}$	143	R, DCHF, CCSD(T), ECP
		[125]	$^1S_0$, $4f^{14}$	157.3	TD-DFT
		[157]	$^1S_0$, $4f^{14}$	151.0	R, CASSCF, ECP
		[147]	$^1S_0$, $4f^{14}$	136±5	R, CCSD(T)
		[52]	$^1S_0$, $4f^{14}$	147±20	exp.
		[170]	$^1S_0$, $4f^{14}$	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
		[156]	$^2D_{3/2}$, $5d^1$	137±7	R, Dirac, CI+MBPT+CP(RPA); (α_D = 61.3 for the $4f^{14}6s^26p^1$ configuration)
		[171]	$^2D_{3/2}$, $5d^1$	145	R, DF, CI+all-order+Breit+QED
		[125]	$^2D_{3/2}$, $5d^1$	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
		[171]	$^3F_2$, $5d^2$	97	R, DF, CI+all-order+Breit+QED
		[156,171]	$^3F_2$, $5d^2$	103±5	R, DF, CI+MBPT+Breit+QED
		[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
		[118]	$5d^3$	73.7	R, RPA, PolPot
		[94]	$^4F_{3/2}$, $5d^3$	73.9	TD-DFT (LEXX)
		[52]	$^4F_{3/2}$, $5d^3$	58±12	exp.
		[172]	$^4F_{3/2}$, $5d^3$	128±20	exp.
		[126]	$^4F_{3/2}$, $5d^3$	115±20	exp.
		[172]	$^4F_{3/2}$, $5d^3$	108±20	exp.
				74±20	**recommended**
74	W	[85,86]	$^5D_0$, $5d^4$	75±19	R, Dirac, LDA
		[118]	$5d^4$	68.1	R, RPA, PolPot
		[94]	$^5D_0$, $5d^4$	65.8	TD-DFT (LEXX)
		[126]	$^5D_0$, $5d^4$	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
		[96]	^6S, $5d^5$	61.1	DK, CASPT2
		[118]	$5d^5$	65.6	R, RPA, PolPot
		[94]	$^6S_{5/2}$, $5d^5$	60.2	TD-DFT (LEXX)
		[36]	$^6S_{5/2}$, $5d^5$	61.9	R, CCSD(T)
				62±3	**recommended**
76	Os	[85,86]	$^5D_4$, $5d^6$	57	R, Dirac, LDA
		[118]	$5d^6$	57.8	R, RPA, PolPot
		[94]	$^5D_4$, $5d^6$	55.3	TD-DFT (LEXX)
				57±3	**recommended**
77	Ir	[85,86]	$^4F_{9/2}$, $5d^7$	51±13	R, Dirac, LDA
		[118]	$5d^7$	51.7	R, RPA, PolPot
		[94]	$^4F_{9/2}$, $5d^7$	51.3	TD-DFT (LEXX)
		[172,173]	$^4F_{9/2}$, $5d^7$	54.0±6.7	exp.
				54±7	**recommended**
78	Pt	[85,86]	$^3D_3$, $5d^9$	44±11	R, Dirac, LDA
		[94]	$^3D_3$, $5d^9$	48.0	TD-DFT (LEXX)
				48±4	**recommended**
79	Au	[98,101,174]	^2S, $5d^{10}$	35.1	R, PP, QCISD(T)
		[21,99]	^2S, $5d^{10}$	36.06±0.54	R, DK, CCSD(T)
		[59,96]	^2S, $5d^{10}$	27.9±4.2	R, DK, CASPT2
		[175]	^2S, $5d^{10}$	34.9	R, DK, CCSD(T)
		[94]	$^2S_{1/2}$, $5d^{10}$	45.4	TD-DFT (LEXX)
		[176]	$^2S_{1/2}$, $5d^{10}$	30±4	R, HFR, HS, CI, CACP
		[59,71]	$^2S_{1/2}$, $5d^{10}$	49.1±4.1	exp.
		[96]	$^2S_{1/2}$, $5d^{10}$	39.1±9.8	exp.
				36±3	**recommended**

Z	Atom	Refs.	State	α_D	Comments
80	Hg	[106]	^1S, $5d^{10}$	34.42	R, PP, CCSD(T)
		[107]	^1S, $5d^{10}$	31.24	R, MVD, CCSD(T)
		[100]	^1S, $5d^{10}$	32.9	semi-empirical
		[96]	^1S, $5d^{10}$	33.3	R, DK, CASPT2
		[177]	$^1S_0$, $5d^{10}$	34.15	R, Dirac, CCSD(T)
		[178]	$^1S_0$, $5d^{10}$	34.27	R, Dirac, CCSDT+QED
		[118]	$^1S_0$, $5d^{10}$	39.1	R, RPA, PolPot
		[21,179]	$^1S_0$, $5d^{10}$	34.73±0.52	R, DK, CCSD(T)
		[180]	$^1S_0$, $5d^{10}$	34.1	R, Dirac, CCSD(T)
		[109]	$^1S_0$, $5d^{10}$	33.59	R, PRCC(T)
		[181]	$^1S_0$, $5d^{10}$	34.2±0.5	R, CCSD(T)+Breit
		[147]	$^1S_0$, $5d^{10}$	34.5±0.8	R, CCSD(T)
		[107,111,182]	$^1S_0$, $5d^{10}$	33.75	exp.
		[183]	$^1S_0$, $5d^{10}$	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.
		[184]	$^2P_{1/2}$	52.3	R, Dirac, FS-CCSD
		[113]	$^2P_{1/2}/^2P_{3/2}$	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)
		[59,114]	^2P	71.7±1.1	R, DK, CCSD(T)
		[180,184]	^2P	51.3	R, Dirac, FS-CCSD
		[185,186]	^2P	49.2	RCI + MBPT
		[187]	^2P	48.81	R, Dirac, CI+MBPT
		[188]	^2P	47.78	R, Dirac+Breit+QED, SD+CI, RPA
		[189]	^2P	50.0±3.0	R, CC
		[189]	^2P	50.7	R, CI + all-order
		[113]	^2P	52.1±1.6	R, Dirac, FSCC
		[190]	^2P	50.4	R, DHF, SD, MBPT all-order
		[114]	^2P	50.48	R, DK, CCSD(T)
		[114]	^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.
		[86]	$^2P_{1/2}$	51.3±5.4	exp.
				50±2	**recommended**
82	Pb	[85]	^3P	46±11	R, Dirac, LDA
		[191]	$^3P_0$	51.0	R, SOPP, CCSD(T)
		[32]	$^3P_0$	47.70	R, Dirac+Gaunt, CCSD(T)
		[177]	$^3P_0$	46.96	R, Dirac, CCSD(T)
		[32]	$^3P_0$	47.3±0.9	R, Dirac+Gaunt, CCSD(T)
		[180]	$^3P_0$	47.0	R, Dirac, FS-CCSD
		[188]	$^3P_0$	44.04	R, Dirac+Breit+QED, SD+CI, RPA
		[192]	$^3P_0$	46.5	R, CI + all-order, RPA
		[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
		[193]	^4S	52.85	R, Cowan-Griffin, HF only
		[36]	^4S	48.75	ECP, CCSD(T)
		[188]	^4S	44.62	R, Dirac+Breit+QED, SD+CI, RPA
		[52]	$^4S_{3/2}$	55±11	exp.
				48±4	**recommended**
84	Po	[85,86]	$^3P_2$	46	R, R, Dirac, LDA
		[193]	$^3P_2$	46.8	R, Cowan-Griffin, HF only, M_L res.
		[21,59,193]	$^3P_2$	43.6±4.4	R, Cowan-Griffin, HF only
				44±4	**recommended**
85	At	[116]	$^2P_{1/2}$	45.6	R, DK, SO-CI
		[116]	$^2P_{3/2}$	43.0	R, DK, SO-CI, M_J res.
		[21,59,193]	$^2P_{3/2}$	40.7±2.0	R, Cowan-Griffin, HF only
				42±4	**recommended**

Z	Atom	Refs.	State	α_D	Comments
86	Rn	[41]	^1S	33.18	R, DK3, CCSD(T)
		[144]	$^1S_0$	34.33	R, SOPP, CCSD(T) + MP2 basis set correction
		[191]	$^1S_0$	28.6	R, SOPP, CCSD(T)
		[33]	^1S	32.6	R, DK, CASPT2
		[118]	$^1S_0$	34.2	R, RPA, PolPot
		[175,194]	$^1S_0$	35.77	R, DK, CCSD(T)
		[194]	$^1S_0$	35.47	CCSD, ECP
		[146]	$^1S_0$	35.391	R, RPA, PolPot
		[180]	$^1S_0$	35.0	R, Dirac, CCSD(T)
		[85,86]	$^1S_0$	36±5	R, Dirac, LDA
		[195]	$^1S_0$	35.87	R, DFT, DC, PBE38
		[196]	$^1S_0$	34.89	R, DKH2, B3LYP, SARC
		[196]	$^1S_0$	34.70	R, DKH2, B3LYP, UGBS
		[144]	$^1S_0$	34.60	R, SOPP, CCSD(T) + MP2 basis set correction
		[195]	$^1S_0$	33.62	R, DFT, sfDC, PBE38
		[44]	$^1S_0$	34.4374±0.0001	CCSD(T), ECP
		[59,197]	$^1S_0$	35.04±1.8	R, Dirac, CCSD(T)
		[147]	$^1S_0$	37.0±0.5	R, CCSD(T)
		[198]	$^1S_0$	35.3	R, Dirac-Gaunt, CCSD(T)
				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
		[149]	$^2S_{1/2}$	311.5	R, Dirac, CCSD(T)
		[199]	$^2S_{1/2}$	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)
		[154]	$^1S_0$	242.8	R, Dirac+Gaunt, CCSD(T)
		[57]	$^1S_0$	242.42	R, Dirac+Breit, perturbed relativistic coupled-cluster theory (PRCC)
		[118]	$^1S_0$	232	R, RPA, PolPot
		[83]	$^1S_0$	248.56	R, DK+SO, CCSD(T)
		[147]	$^1S_0$	236±15	R, CCSD(T)
				246±4	**recommended**
89	Ac	[85,86]	$^2D_{3/2}$, $6d^1$	217±44	R, Dirac, LDA
		[156]	$^2D_{3/2}$, $6d^1$	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
		[156]	$5f^26d^1$	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
		[156]	$5f^36d^1$	127.8	R, Dirac, CI+MBPT+CP(RPA); (α_D = 153.2 for the $5f^4$ configuration)
		[200]	$^5L_6$, $5f^36d^1$	137±9	exp.
				129±17	**recommended**
93	Np	[85,86]	$5f^46d^1$	167±42	R, Dirac, LDA
		[156]	$5f^46d^1$	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
		[156]	$5f^6$	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
		[201]	$5f^7$	116±29	R, DK, CASPT2
		[156]	$5f^7$	131.2	R, Dirac, CI+MBPT+CP(RPA); (α_D = 144.7 for the $5f^6 6d^1$ configuration)
		[202]	$5f^7$	122.4	R, DFT, DKH, B3LYP
				131±25	**recommended**
96	Cm	[85,86]	$5f^7 6d^1$	155±39	R, Dirac, LDA
		[156]	$5f^7 6d^1$	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
		[156]	$5f^9$	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
		[156]	$5f^{10}$	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
		[156]	$5f^{11}$	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
		[156]	$5f^{12}$	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
		[156]	$5f^{13}$	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
		[162]	$^1S_0$, $5f^{14}$	110.8±5.5	R, Dirac+Gaunt, CCSD(T)
		[156]	$^1S_0$, $5f^{14}$	105.4	R, Dirac, CI+MBPT+CP(RPA); (α_D = 267.8 for the $5f^{14}7s^17p^1$ configuration)
		[118]	$^1S_0$, $5f^{14}$	114	R, RPA, PolPot
		[156,171]	$^1S_0$, $5f^{14}$	112±6	R, DF, CI+MBPT+Breit+QED
		[156,171]	$^1S_0$, $5f^{14}$	110±8	R, DF, CI+all-order+Breit+QED
		[168]	$^1S_0$, $5f^{14}$	107.77	R, DFT, CAM-B3LYP, 2c-NESC
		[162]	$^1S_0$, $5f^{14}$	115.64	R, DK, CCSD(T)
		[202]	$^1S_0$, $5f^{14}$	115.6	R, DFT, DKH, B3LYP
				110±6	**recommended**
103	Lr	[171]	$7p^1$	323±80	R, DF, CI+all-order+Breit+QED
		[171]	$7p^1$	320±80	R, DF, CI+MBPT+Breit+QED
		[203]	$7p^1$	225.2	R, DK, DFT, CAM-B3LYP
				320±20	**recommended**
104	Rf	[171]	$6d^2$	107±5	R, DF, CI+MBPT+Breit+QED
		[171]	$6d^2$	115±13	R, DF, CI+all-order+Breit+QED
				112±10	**recommended**
105	Db	[118]	$6d^3$	42.5	R, RPA, PolPot
		[118]	$6d^3$	42±4	R, RPA, PolPot (value recommended by authors)
				42±4	**recommended**
106	Sg	[118]	$6d^4$	40.7	R, RPA, PolPot
		[118]	$6d^4$	40±4	R, RPA, PolPot (value recommended by authors)
				40±4	**recommended**
107	Bh	[118]	$6d^5$	38.4	R, RPA, PolPot
		[118]	$6d^5$	38±4	R, RPA, PolPot (value recommended by authors)
				38±4	**recommended**
108	Hs	[118]	$6d^6$	36.2	R, RPA, PolPot
		[118]	$6d^6$	36±4	R, RPA, PolPot (value recommended by authors)
				36±4	**recommended**

Z	Atom	Refs.	State	α_D	Comments
109	Mt	[118]	$6d^7$	34.2	R, RPA, PolPot
		[118]	$6d^7$	34±3	R, RPA, PolPot (value recommended by authors)
				34±3	**recommended**
110	Ds	[118]	$6d^8$	32.3	R, RPA, PolPot
		[118]	$6d^8$	32±3	R, RPA, PolPot (recommended value by authors)
				32±3	**recommended**
111	Rg	[118]	$6d^9$	30.6	R, RPA, PolPot
		[118]	$6d^9$	30±3	R, RPA, PolPot (value recommended by authors)
		[204]	$6d^9$	31.6	ARPP CCSD(T)
				32±6	**recommended**
112	Cn	[106]	$^1S_0$, $6d^{10}$	25.82	R, PP, CCSD(T)
		[191]	$^1S_0$, $6d^{10}$	28.68	R, SOPP, CCSD(T)
		[177]	$^1S_0$, $6d^{10}$	27.64	R, Dirac, CCSD(T)
		[118]	$^1S_0$, $6d^{10}$	28.2	R, RPA, PolPot
		[177]	$^1S_0$, $6d^{10}$	27.40	R, Dirac, CCSD(T)
		[118]	$^1S_0$, $6d^{10}$	28±4	R, RPA, PolPot (value recommended by authors)
				28±2	**recommended**
113	Nh	[184]	$^2P_{1/2}$	29.85	R, Dirac, FS-CCSD
		[188]	$^2P_{1/2}$	28.8	R, Dirac+Breit+QED, SD+CI, RPA
				29±2	**recommended**
114	Fl	[191]	$^3P_0$	34.35	R, SOPP, CCSD(T)
		[32]	$^3P_0$	31.98	R, Dirac+Gaunt, CCSD(T)
		[177]	$^3P_0$	30.59	R, Dirac, CCSD(T)
		[177]	$^3P_0$	29.52	estimate
		[188]	$^3P_0$	31.4	R, Dirac+Breit+QED, SD+CI, RPA
		[32]	$^3P_0$	31.0	R, Dirac+Gaunt, CCSD(T)
				31±4	**recommended**

115	Mc	[188]	$^4S_{3/2}$	70.5 **71±20**	R, Dirac+Breit+QED, SD+CI, RPA **recommended**
116	Lv		$^3P_2$	-	No value currently available
117	Ts	[205]	$^2P_{3/2}$	76.3 **76±15**	empirical estimate **recommended**
118	Og	[191] [197] [118] [206] [118]	$^1S_0$ $^1S_0$ $^1S_0$ $^1S_0$ $^1S_0$	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] [149] [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	[154] [118] [118]	$^1S_0$ $^1S_0$ $^1S_0$	162.6 147 159±10 **159±10**	R, Dirac+Gaunt, CCSD(T) R, RPA, PolPot R, RPA, PolPot **recommended**

References

1. J. P. Desclaux, Relativistic Dirac-Fock expectation values for atoms with $Z = 1$ to $Z = 120$, *Atomic Data Nucl. Data Tabl.* **12**, 311-406 (1973).
2. S. P. Goldman, Gauge-invariance method for accurate atomic-physics calculations: Application to relativistic polarizabilities, *Phys. Rev. A* **39**, 976-980 (1989).
3. Li-Yan Tang, Yong-Hui Zhang, Xian-Zhou Zhang, Jun Jiang, and J. Mitroy, Computational investigation of static multipole polarizabilities and sum rules for ground-state hydrogenlike ions, *Phys. Rev. A* **86**, 012505-1-10 (2012).
4. L. Filippin, M. Godefroid, and D. Baye, Relativistic polarizabilities with the Lagrange-mesh method, *Phys. Rev. A* **90**, 052520-1-12 (2014).
5. K. Pachucki and J. Sapirstein, Relativistic and QED corrections to the polarizability of helium, *Phys. Rev. A* **63**, 012504-1-3 (2001).
6. G. Łach, B. Jeziorski, and K. Szalewicz, Radiative corrections to the polarizability of helium, *Phys. Rev. Lett.* **92**, 233001-1-4 (2004).
7. M. Puchalski, K. Piszczatowski, J. Komasa, B. Jeziorski, and K. Szalewicz, Theoretical determination of the polarizability dispersion and the refractive index of helium, *Phys. Rev A* **93**, 032515-1-14 (2016).
8. A. C. Newell and R. D. Baird, Absolute determination of refractive indices of gases at 47.7 gigahertz, *J. Appl. Phys.* **36**, 3751-3759 (1965).
9. K. Grohman and H. Luther, *Temperature—Its Measurement and Control in Science and Industry,* AIP, New York, 1992, Vol. 6, p 21.
10. J. W. Schmidt, R. M. Gavioso, E. F. May, and M. R. Moldover Polarizability of helium and gas metrology**,** *Phys. Rev. Lett.* **98**, 254504 (2007).
11. J. Komasa, Dipole and quadrupole polarizabilities and shielding factors of beryllium from exponentially correlated Gaussian functions, *Phys. Rev. A* **65**, 012506-1-11 (2002).
12. I. S. Lim, M. Pernpointner, M. Seth, J. K. Laerdahl, P. Schwerdtfeger, P. Neogrady, and M. Urban, Accurate relativistic coupled cluster static dipole polarizabilities of the alkali metals from Li to element 119, *Phys. Rev. A* **60**, 2822-2828 (1999).
13. W. R. Johnson, U. I. Safronova, A. Derevianko, and M. S. Safronova, Relativistic many-body calculation of energies, lifetimes, hyperfine constants, and polarizabilities in ^{7}Li, *Phys. Rev. A* **77**, 022510-1-9 (2008).
14. M. Puchalski, D. Kędziera, and K. Pachucki, Lithium electric dipole polarizability, *Phys. Rev. A* **84**, 052518-1-5 (2011); Erratum *Phys. Rev. A* **85**, 019910E (2012).
15. J.-Y. Zhang, J. Mitroy, and M. W. J. Bromley, Dispersion coefficients of the excited states of lithium atoms *Phys. Rev. A* **75**, 042509 (2007).

16. R. W. Molof, H. L. Schwartz, T. M. Miller, and B. Bederson, Measurements of electric dipole polarizabilities of the alkali-metal atoms and the metastable noble-gas atoms, *Phys. Rev. A* **10**, 1131-1140 (1974).
17. A. Miffre, M. Jacquey, M Büchner, G. Trénec, and J. Vigué, Measurement of the electric polarizability of lithium by atom interferometry, *Phys. Rev. A* **73**, 011603-1-4 (2006).
18. K. Singer, The Use of Gaussian (Exponential Quadratic) Wave functions in molecular problems. I. General formulae for the evaluation of integrals, *Proc. R. Soc. London Ser. A* **258**, 412-420 (1960).
19. B. K. Sahoo and B. P. Das, Relativistic coupled-cluster studies of dipole polarizabilities in closed-shell atoms, *Phys. Rev. A* **77**, 062516-1-5 (2008).
20. S. G. Porsev and A. Derevianko, High-accuracy calculations of dipole, quadrupole, and octupole electric dynamic polarizabilities and van der Waals coefficients C_6, C_8, and C_{10} for alkaline-earth dimers, *J. Exp. Theor. Phys. (JETP)* **102**, 195–205 (2006).
21. A. J. Thakkar and C. Lupinetti, "Atomic polarizabilities and hyperpolarizabilities: a critical compilation", in *Theoretical Approaches to the Calculation of Electric Polarizability: Atoms, Molecules and Clusters in Electric Fields,* ed. G. Maroulis, Imperial College Press, London, 2006; pp 505-529.
22. Y. Singh, B. K. Sahoo, and B. P. Das, Correlation trends in the ground-state static electric dipole polarizabilities of closed-shell atoms and ions, *Phys. Rev.* A **88**, 062504-1-11 (2013).
23. D. Tunega, J. Noga, and W. Klopper, Dipole and quadrupole polarizabilities and shielding factors of beryllium from exponentially correlated Gaussian functions, *Chem. Phys. Lett*. **269**, 435-440 (1997).
24. G. L. Bendazzoli, and A. Monari, A Davidson technique for the computation of dispersion constants: Full CI results for Be and LiH, *Chem. Phys.* **306**, 153-161 (2004).
25. J. Mitroy and M. W. J. Bromley, Semiempirical calculation of van der Waals coefficients for alkali-metal and alkaline-earth-metal atoms, *Phys. Rev. A* **68**, 052714-1-16 (2003).
26. W, Müller, J. Flesch, and W. Meyer, Treatment of intershell correlation effects in *ab initio* calculations by use of core polarization potentials. Method and application to alkali and alkaline earth atoms, *J. Chem. Phys.* **80**, 3297-3310 (1984).
27. S. H. Patil, A simple model potential description of the alkaline earth isoelectronic sequences, *Eur. Phys. J. D* **10**, 341–347 (2000).
28. H.-J. Werner and W. Meyer, Finite perturbation calculations for the static dipole polarizabilities of the first-row atoms, *Phys. Rev. A* **13**, 13- 16 (1976).
29. A. K. Das and A. J. Thakkar, Static response properties of second-period atoms: coupled cluster calculations, *J. Phys. B, At. Mol. Opt. Phys.* **31**, 2215-2223 (1998).
30. T. Fleig, Spin-orbit-resolved static polarizabilities of group-13 atoms: Four-component relativistic configuration interaction and coupled cluster calculations, *Phys. Rev. A* **72**, 052506 (2005).
31. K. Anderson and A. J. Sadlej, Electric dipole polarizabilities of atomic valence states, *Phys. Rev. A* **46**, 2356-2362 (1992).

32. C. Thierfelder, B. Assadollahzadeh, P. Schwerdtfeger, S. Schäfer, and R. Schäfer, Relativistic and electron correlation effects in static dipole polarizabilities for the group 14 elements from carbon to element 114, *Phys. Rev. A* **78**, 052506-1-7 (2008).
33. B. O. Roos, R. Lindh, P.-A. Malmqvist, V. Veryazov, and P.-O. Widmark, Main group atoms and dimers studied with a new relativistic ANO basis set, *J. Phys. Chem. A* **108**, 2851-2858 (2004).
34. R. D. Alpher and D. R. White, Optical refractivity of high-temperature gases. I. Effects resulting from dissociation of diatomic gases, *Phys. Fluids* **2**, 153-161 (1959).
35. G. D. Zeissj, and W. J. Meath, Dispersion energy constants C_6(A, B), dipole oscillator strength sums and refractivities for Li, N, O, H_2, N_2, O_2, NH_3, H_2O, NO and N_2O, *Mol. Phys.* **33**, 1155-1176 (1977).
36. A. A. Buchachenko, Anisotropy of the static dipole polarizability induced by the spin−orbit interaction: The *S*-state atoms N−Bi, Cr, Mo and Re, *Proc. R. Soc. A* **467**, 1310-1328 (2011).
37. M. Medved, P. W. Fowler, and J. M. Hutson, Anisotropic dipole polarizabilities and quadrupole moments of open-shell atoms and ions: O, F, S, Cl, Se, Br and isoelectronic systems, *Mol. Phys.* **7**, 453-463 (2000).
38. J. E. Rice, G. E. Scuseria, T. J. Lee, P. R. Taylor, and J. Almlöf, Connected triple excitations in coupled-cluster calculations of hyperpolarizabilities: neon, *Chem. Phys. Lett.* **191**, 23-26 (1992).
39. K. Hald, F. Pawlowski, P. Jørgensen, and C. Hättig, Calculation of frequency-dependent polarizabilities using the approximate coupled-cluster triples model CC3, *J. Chem. Phys.* **118**, 1292-1300 (2003).
40. H. Larsen, J. Olsen, C. Hättig, P. Jørgensen, O. Christiansen, and J. Gauss, Polarizabilities and first hyperpolarizabilities of HF, Ne, and BH from full configuration interaction and coupled cluster calculations, *J. Chem. Phys.* **111**, 1917-1925 (1999).
41. T. Nakajima and K. Hirao, Relativistic effects for polarizabilities and hyperpolarizabilities of rare gas atoms, *Chem. Lett. (Jpn.)* 766-767 (2001).
42. S. Chattopadhyay, B. K. Mani, and D. Angom, Electric dipole polarizability from perturbed relativistic coupled-cluster theory: Application to neon *Phys. Rev. A* **86**, 022522-1-6 (2012).
43. R. H. Orcutt, and R. H. Cole, Dielectric constants of imperfect gases. III. Atomic gases, hydrogen, and nitrogen, *J. Chem. Phys.* **46**, 697-702 (1967).
44. P. Soldán, E. P. F. Lee, and T. G. Wright, Static dipole polarizabilities (α) and static second hyperpolarizabilities (γ) of the rare gas atoms (He– Rn), *Phys. Chem. Chem. Phys*. **3**, 4661-4666 (2001).
45. A. Dalgarno and A. E. Kingston, The refractive indices and Verdet constants of the inert gases, *Proc. Roy. Soc. A* **259,** 424-431 (1960).
46. J. Huot and T. K. Bose, Experimental determination of the dielectric virial coefficients of atomic gases as a function of temperature, *J. Chem. Phys.* **95**, 2683-2687 (1991).
47. C. Gaiser and B. Fellmuth, Experimental benchmark value for the molar polarizability of neon, *Eur. Phys. Lett.* **90**, 63002-1-5 (2010).

48. A. Derevianko, W. R. Johnson, M. S. Safronova, and J. F. Babb, High-precision calculations of dispersion coefficients, static dipole polarizabilities, and atom-wall interaction constants for alkali-metal atoms, *Phys. Rev. Lett.* **82**, 3589-3592 (1999).
49. A. J. Thakkar and C. Lupinetti, The polarizability of sodium: theory and experiment reconciled, *Chem. Phys. Lett.* **402**, 270-273 (2005).
50. C. R. Ekstrom, J. Schmiedmayer, M. S. Chapman, T. D. Hammond, and D. E. Pritchard, Measurement of the electric polarizability of sodium with an atom interferometer, *Phys. Rev. A* **51**, 3883-3888 (1995).
51. W. F. Holmgren, M. C. Revelle, V. P. A. Lonij, and A. D. Cronin, Absolute and ratio measurements of the polarizability of Na, K, and Rb with an atom interferometer, *Phys. Rev. A* **81**, 053608-1-7 (2010).
52. L. Ma, J. Indergaard, B. Zhang, I. Larkin, R. Moro, and W. A. de Heer, Measured atomic ground-state polarizabilities of 35 metallic elements, *Phys. Rev. A* **91**, 010501(R)-1-5 (2015).
53. E. F. Archibong and A. J. Thakkar, Finite-field many-body-perturbation-theory calculation of the static hyperpolarizabilities and polarizabilities of Mg, Al^+, and Ca, *Phys. Rev. A* **44**, 5478-5484 (1991).
54. A. Sadlej and M. Urban, Medium-size polarized basis sets for high-level-correlated calculations of molecular electric properties: III. Alkali (Li, Na, K, Rb) and alkaline-earth (Be, Mg, Ca, Sr) atoms, *J. Mol. Struct. (Theochem)* **234**, 147-171 (1991).
55. B. O. Roos, V. Veryazov, and P.-O. Widmark, Relativistic atomic natural orbital type basis sets for the alkaline and alkaline-earth atoms applied to the ground-state potentials for the corresponding dimers, *Theor. Chem. Acc.* **111**, 345-351 (2004).
56. S. G. Porsev and A. Derevianko, Multipolar theory of blackbody radiation shift of atomic energy levels and its implications for optical lattice clocks, *Phys. Rev. A* **74**, 020502-1-4(R) (2006).
57. S. Chattopadhyay, B. K. Mani, and D. Angom, Electric dipole polarizability of alkaline-earth-metal atoms from perturbed relativistic coupled- cluster theory with triples, *Phys. Rev. A* **89**, 022506-1-12 (2014).
58. F. Maeder and W. Kutzelnigg, Natural states of interacting systems and their use for the calculation of intermolecular forces. IV. Calculation of van der Waals coefficients between one- and two-valence-electron atoms in their ground states, as well as of polarizabilities, oscillator strength sums and related quantities, including correlation effects, *Chem. Phys.* **42**, 95-112 (1979).
59. U. Hohm and A. J. Thakkar, New Relationships connecting the dipole polarizability, radius, and second ionization potential for atoms, *J. Phys. Chem. A* **116**, 697-703 (2012).
60. W. C. Stwalley, Polarizability and long-range interactions of magnesium atoms, *J. Chem. Phys.* **54**, 4517-4518 (1971).
61. J. Stiehler and J. Hinze, Calculation of static polarizabilities and hyperpolarizabilities for the atoms He through Kr with a numerical RHF method, *J. Phys. B* **28**, 4055-4071 (1995).
62. L. London, B. Engman, J. Hilke, and I. Martinson, Lifetime measurements in Mg I – Mg IV, *Phy. Scr.* **8**, 274-278 (1973).
63. E. A. Reinsch and W. Meyer, Finite perturbation calculation for the static dipole polarizabilities of the atoms Na through Ca, *Phys. Rev. A* **14**, 915-918 (1976).

64. C. Lupinetti and A. J. Thakkar, Polarizabilities and hyperpolarizabilities for the atoms Al, Si, P, S, Cl, and Ar: Coupled cluster calculations, *J. Chem. Phys.* **122**, 044301-1-7 (2005).
65. A. Hibbert, Atomic polarisabilities and polarized pseudostates in the multiconfigurational approach III. Second-row atoms and ions, *J. Phys. B, Atom. Mol. Phys*. **13**, 3725-3731 (1980).
66. X. Chu and A. Dalgarno, Linear response time-dependent density functional theory for van der Waals coefficients, *J. Chem. Phys.* **121**, 4083-4088 (2004).
67. A. A. Buchachenko, State interacting spin orbit configuration interaction method for *J*-resolved anisotropic static dipole polarizabilities: application to Al, Ga, In, and Tl atoms, *Russ. J. Phys. Chem.* **84**, 2325-2333 (2010).
68 P. Fuentealba, The static dipole polarizability of aluminium atom: discrepancy between theory and experiment, *Chem. Phys. Lett.* **397**, 459-461 (2004).
69. P. Milani, I. Moullet, and W. A. de Heer, Experimental and theoretical electric dipole polarizabilities of Al and Al_2, *Phys. Rev. A* **42**, 5150- 5154 (1990).
70. All theoretical values yield significantly larger values compared to the experimental results of ref. 69, which casts some doubts on the accuracy of this experiment.
71. G. S. Sarkisov, I. L. Beigman, B. P. Shevelko, and K. W. Struve, Interferometric measurements of dynamic polarizabilities for metal atoms using electrically exploding wires in vacuum, *Phys. Rev. A* **73**, 042501-1-8 (2006).
72. G. Maroulis and C. Pouchan, Static dipole (hyper)polarizability of the silicon atom, *J. Phys. B, At. Mol. Opt. Phys.* **36**, 2011-2017 (2003).
73. U. Hohm and K. Kerl, Interferometric measurements of the dipole polarizability α of molecules between 300 K and 1100 K. I. Monochromatic measurements at $\lambda = 632.99$ nm for the noble gases and H_2, N_2, O_2, and CH_4, *Mol. Phys.* **69**, 803-817 (1990); *ibid.* Interferometric measurements of the dipole polarizability of atoms and molecules between 300 K and 1100 K. II. A new method for measuring the dispersion of the polarizability and its application to Ar, H_2, and O_2, *Mol. Phys.* **69**, 819-831 (1990).
74. D. R. Johnston, G. J. Oudemans, and R. H. Cole, Dielectric constants of imperfect gases. I. Helium, argon, nitrogen, and methane, *J. Chem. Phys.* **46**, 697-702 (1966).
75. P. W. Langhoff and M. Karplus, Padé summation of the Cauchy dispersion equation, *J. Opt. Soc. Am.* **59**, 863-871 (1969).
76. I. Lim, P. Schwerdtfeger, B. Metz and H. Stoll, Relativistic small-core energy-consistent pseudopotentials for the group 1 elements from K to element 119, *J. Chem. Phys.* **122**, 104103-1-12 (2005).
77. A. Derevianko, S. G. Porsev, and J. F. Babb, Electric dipole polarizabilities at imaginary frequencies for hydrogen, the alkali–metal, alkaline–earth, and noble gas atoms, *Atom. Dat. Nucl. Dat. Tabl.* **96**, 323-331 (2010).
78. J. Jiang and J. Mitroy, Hyperfine effects on potassium tune-out wavelengths and polarizabilities, *Phys. Rev. A* **88**, 032505-1-7 (2013).

79. M. D. Gregoire, I. Hromada, W. F. Holmgren, R. Trubko, and A. D. Cronin, Measurements of the ground-state polarizabilities of Cs, Rb, and K using atom interferometry, *Phys. Rev. A* **92**, 052513-1-14 (2015).
80. M. D. Gregoire, N. Brooks, R. Trubko, and A. D. Cronin, Analysis of polarizability measurements made with atom interferometry, *Atoms* **4**, 21-1-23 (2016).
81. S. Porsev and A. Derevianko, High-accuracy relativistic many-body calculations of van der Waals coefficients C_6 for alkaline-earth-metal atoms, *Phys. Rev. A* **65**, 02701(R)-1-4 (2002).
82. A. J. Sadlej, M. Urban, and O. Gropen, Relativistic and electron-correlation contributions to the dipole polarizability of the alkalineearth- metal atoms Ca, Sr, and Ba, *Phys. Rev. A* **44**, 5547-5557 (1991).
83. I. Lim and P. Schwerdtfeger, Four-component and scalar relativistic Douglas-Kroll calculations for static dipole polarizabilities of the alkaline- earth elements and their ions from Ca^n to Ra^n (n = 0, +1, +2), *Phys. Rev. A* **70**, 062501-1-13 (2004).
84. H. L. Schwartz, T. M. Miller, and B. Bederson, Measurement of the static electric dipole polarizabilities of barium and strontium, *Phys. Rev. A* **10**, 1924-1926 (1974).
85. G. Doolen, personal communication August 2003 and values taken from ref 86. The calculations are relativistic LDA in linear response theory. The method is described in: G. Doolen and D. A. Liberman, Calculations of photoabsorption by atoms using a linear response method, *Phys. Scr.* **36**, 77-79 (1987). See also: D.A. Liberman, J. T. Waber, and D. T. Cromer, Self-consistent-field Dirac-Slater wave functions for atoms and ions. I. Comparison with previous calculations, *Phys. Rev.* **137**, A27-A34 (1965). The program used is described in: D. A. Liberman and D. T. Cromer, J. T. Waber, Relativistic self-consistent field program for atoms and ions, *Comput. Phys. Comm.* **2**, 107-113 (1971).
86. T. M. Miller, in *CRC Handbook of Chemistry and Physics*, Ed. D. R. Lide (CRC Press New York, 2002).
87. G. S. Chandler and R. Glass, Evaluation of atomic polarisabilities using the variational perturbation approach: the first transition series, *J. Phys. B* **20**, 1-10 (1987).
88. R. Glass and G. S. Chandler, The mean static dipole polarisability of scandium, *J. Phys. B* **16**, 2931-2936 (1983).
89. R. Pou-Amérigo, M. Merchán, I. Nebot-Gil, P-O.Widmark, and B. O. Roos, Density matrix averaged atomic natural orbital (ANO) basis sets for correlated molecular wave functions. III. First row transition metal atoms *Theor. Chim. Acta* **92**, 149-181 (1995).
90. X.-B Li, H.-Y. Wang, J.-S. Luo, Y.-D. Guo, W.-D. Wu, and Y.-J. Tang, Static dipole polarizabilities of Sc_n ($n \leq 15$ clusters, *Chin. Phys. B* **18**, 3414-3418 (2009).
91. J. Kłos, Anisotropic dipole polarizability of transition metal atoms: Sc(^2D), Ti(^3F, ^3P), V(^4F, ^4P, ^4D), Ni(^3F) and ions: Sc^{2+}(^2D), Ti^{2+}(^3F, ^3P), *J. Chem. Phys.* **123**, 024308-1-7 (2005).
92. X. Chu, A. Dalgarno, and G. C. Groenenboom, Polarizabilities of Sc and Ti atoms and dispersion coefficients for their interaction with helium atoms, *Phys. Rev. A* **72**, 032703-1-5 (2005).
93. F. Torrens, Molecular polarizability of Sc_n, C_n and endohedral $Sc_n@C_m$ clusters, *Nanotechnol.* **13**, 433-438 (2002).

94. T. Gould and T. Bucko, C_6 coefficients and dipole polarizabilities for all atoms and many ions in rows 1−6 of the periodic table, *J. Chem. Theor. Comput.* **12**, 3603-3613 (2016).
95. T. Gould, How polarizabilities and C_6 coefficients actually vary with atomic volume, *J. Chem. Phys.* **145**, 084308-1-8 (2016).
96. B. O. Roos, R. Lindh, P-Å. Malmqvist, V. Veryazov, and P-O. Widmark, New relativistic ANO basis sets for transition metal atoms, *J. Phys. Chem. A* **109**, 6575-6579 (2005).
97. P. Calaminici, Polarizability of Fe$_n$ ($n \leq 4$) clusters: an all-electron density functional study, *Chem. Phys. Lett.* **387**, 253-257 (2004).
98. P. Schwerdtfeger and G. A. Bowmaker, Relativistic effects in gold chemistry. V. Group 11 Dipole-polarizabilities and weak bonding in monocarbonyl compounds, *J. Chem. Phys.* **100**, 4487-4497 (1994).
99. P. Neogrady, V. Kellö, M. Urban, and A. J. Sadlej, Ionization potentials and electron affinities of Cu, Ag, and Au: Electron correlation and relativistic effects, *Int. J. Quant. Chem.* **63**, 557-565 (1997).
100. A. M. Dyugaev and E. V. Lebedeva, New qualitative results of the atomic theory *JETP Lett.* **104**, 639-644 (2016).
101. P. Schwerdtfeger and M. Lein, Theoretical chemistry of gold—From atoms to molecules, clusters, surfaces and the solid state, in *Gold Chemistry: Applications and Future Directions in the Life Sciences*, F. Mohr, Ed. Wiley, Weinheim, pp 183-247 (2010).
102. J. Mitroy, M. S. Safronova, and C. W, Clark, Theory and applications of atomic and ionic polarizabilities, *J. Phys. B: At. Mol. Opt. Phys.* **43**, 202001-1-38 (2010).
103. J. Y. Zhang, J. Mitroy, H. R. Sadeghpour, and M. W. J. Bromley, Long-range interactions of copper and silver atoms with hydrogen, helium, and rare-gas atoms, *Phys. Rev. A* **78**, 062710-1-6 (2008).
104. M. Ernst, L. H. R. Dos Santos, and P. Macchi, Optical properties of metal–organic networks from distributed atomic polarizabilities, *CrystEngComm* **18**, 7339 (2016).
105. D. Goebel, U. Hohm, and G. Maroulis, Theoretical and experimental determination of the polarizabilities of the zinc $^1S_0$ state, *Phys. Rev. A* **54**, 1973-1978 (1996).
106. M. Seth, P. Schwerdtfeger, and M. Dolg, The chemistry of the superheavy elements I. Pseudopotentials for 111 and 112 and relativistic coupled cluster calculations for (112)H^+, (112)F_2 and (112)F_4, *J. Chem. Phys*. **106**, 3623-3632 (1997).
107. V. Kellö and A. J. Sadlej, Polarized basis sets for high-level-correlated calculations of molecular electric properties VIII. Elements of the group IIb: Zn, Cd, Hg, *Theor. Chim. Acta* **91**, 353-371 (1995).
108. Y. Singh and B. K. Sahoo, Correlation trends in the polarizabilities of atoms and ions in the boron, carbon, and zinc homologous sequences of elements, *Phys. Rev. A* **90**, 022511-1-8 (2014).
109. S. Chattopadhyay, B. K. Mani, and D. Angom, Triple excitations in perturbed relativistic coupled-cluster theory and electric dipole polarizability of group-IIB elements, *Phys. Rev. A* **91**, 052504-1-14 (2015).

110. K. Ellingsen, M. Mérawa, M. Rérat, C. Pouchan, and O. Gropen, Dynamic dipole polarizabilities for the ground 4 ^{1}S and the low-lying 4 ^{1,3}P and 5 ^{1,3}S excited states of Zn. Calculation of long-range coefficients of Zn_2, *J. Phys. B, Atom. Mol. Opt. Phys.* **34**, 2313-2323 (2001).
111. L. W. Qiao, P. Li, and K. T. Tang, Dynamic polarizabilities of Zn and Cd and dispersion coefficients involving group 12 atoms, *J. Chem. Phys.* **137**, 084309-1-13 (2012).
112. E. A. Reinsch and W. Meyer, published in ref. [60].
113. A. Borschevsky, T. Zelovich, E. Eliav, and U. Kaldor, Precision of calculated static polarizabilities: Ga, In and Tl atoms, *Chem. Phys.* **395**, 104-107 (2012).
114. I. Cernusak, V. Kellö, and A. J. Sadlej, Standard medium-size basis set for calculations of molecular electric properties: group IIIA, *Collect. Czech. Chem. Comm.* **68**, 211-239 (2003).
115. C. Cuthbertson and E. P. Metcalfe, On the refractive indices of gaseous potassium, zinc, cadmium, mercury, arsenic, selenium and tellurium, *Trans. Roy. Soc. Lond. A* **207**, 135-148 (1907).
116. T. Fleig and A. J. Sadlej, Electric dipole polarizabilities of the halogen atoms in $^{2}P_{1/2}$ and $^{2}P_{3/2}$ states: Scalar relativistic and two-component configuration-interaction calculations *Phys. Rev. A* **65**, 032506-1-8 (2002).
117. B. K. Mani, K. V. P. Latha, and D. Angom, Relativistic coupled-cluster calculations of ^{20}Ne, ^{40}Ar, ^{84}Kr, and ^{129}Xe: Correlation energies and dipole polarizabilities, *Phys. Rev. A* **80**, 062505-1-10 (2009).
118. V. A. Dzuba, Ionization potentials and polarizabilities of superheavy elements from Db to Cn (Z=105 to 112), *Phys. Rev. A* **93**, 032519-1-5 (2016).
119. A. J. Thakkar, H. Hettema, and P. E. S. Wormer, Ab initio dispersion coefficients for interactions involving rare-gas atoms, *J. Chem. Phys.* **97**, 3252-3257 (1992).
120. J. Huot and T. K. Bose, Experimental determination of the dielectric virial coefficients of atomic gases as a function of temperature, *J. Chem. Phys.* **95**, 2683-2687 (1991).
121. S. G. Porsev, A. D. Ludlow, M. M. Boyd, and J. Ye, Determination of Sr properties for a high-accuracy optical clock, *Phys. Rev. A* **78**, 032508-1-9 (2008).
122. J. Mitroy and J. Y. Zhang, Dispersion and polarization interactions of the strontium atom, *Mol. Phys.* **108**, 1999–2006 (2010).
123. M. W. J. Bromley and J. Mitroy, Configuration-interaction calculations of positron binding to group-II elements, *Phys. Rev. A* **65**, 062505- 1-10 (2002).
124. X. B. Li, H.-Y. Wang, R. Lv, W.-D. Yu, J.-S. Luo, and Y.-J. Tang, Correlations of the stability, static dipole polarizabilities, and electronic properties of yttrium clusters, *J. Phys. Chem. A* **113**, 10335-10342 (2009).
125. X. Chu, A. Dalgarno, and G. C. Groenenboom, Dynamic polarizabilities of rare-earth-metal atoms and dispersion coefficients for their interaction with helium atoms, *Phys. Rev. A* **75**, 032723-1-4 (2007).

126. H. Liepack and M. Drechsler, Messung der polarisierbarkeiten von metallatomen mit dem feldelektronenmlkroskop, *Naturwiss.*, **43**, 52-53 (1956).
127. P. Jerabek, P. Schwerdtfeger, and J. K. Nagle, The static dipole polarizability of palladium from relativistic coupled cluster theory, *Phys. Rev. A Phys. Rev. A* **98**, 012508-1-5 (2018).
128. R. Bast, A. Heßelmann, P. Sałek, T. Helgaker, and T. Saue, Static and frequency-dependent dipole–dipole polarizabilities of all closed-shell atoms up to radium: a four-component relativistic DFT study, *ChemPhysChem* **9**, 445-453 (2008).
129. J. Granatier, P. Lazar, M. Otyepka, and P. Hobza, The nature of the binding of Au, Ag, and Pd to benzene, coronene, and graphene: from benchmark CCSD(T) calculations to plane-wave DFT calculations, *J. Chem. Theory Comput.* **7**, 3743-3755 (2011).
130. J. Y. Zhang, J. Mitroy, H. R. Sadeghpour, and M. W. J. Bromley, Long-range interactions of copper and silver atoms with hydrogen, helium, and rare-gas atoms, *Phys. Rev. A* **78**, 062710-1-6 (2008).
131. B. K. Sahoo and Y.-M. Yu, Dipole polarizability calculation of Cd Atom: Inconsistency with experiment, *Phys. Rev. A* **98**, 012513-1-9 (2018).
132. A. Ye and G. Wang, Dipole polarizabilities of $ns^2\ ^1S_0$ and $nsnp\ ^3P_0$ states and relevant magic wavelengths of group-IIB atoms, *Phys. Rev. A* **78**, 014502-1-4 (2008).
133. D. Goebel and U. Hohm, Dispersion of the refractive index of cadmium vapor and the dipole polarizability of the atomic cadmium $^1S_0$ state, *Phys. Rev. A* **52**, 3691-3694 (1995).
134. M. W. J. Bromley and J. Mitroy, Configuration-interaction calculations of positron binding to zinc and cadmium, *Phys. Rev. A* **65**, 062506-1-10 (2002).
135. D. Goebel, U. Hohm, and K. Kerl, Dispersive Fourier transform spectroscopy in the visible of absorbing gases and vapours, *J. Mol. Struct.* **349**, 253-256 (1995).
136. D. A. Liberman and A. Zangwill, theoretical value published as a personal communication in ref. 138.
137. M. S. Safronova, U. I. Safronova, and S. G. Porsev, Polarizabilities, Stark shifts, and lifetimes of the In atom, *Phys. Rev. A* **87**, 032513-1-7 (2013).
138. T. P. Guella, T. M. Miller, and B. Bederson, J. A. D. Stockdale, and B. Jaduszliwer, Polarizability of $5s^25p(^2P_{1/2})$ atomic indium, *Phys. Rev. A* **29**, 2977-2980 (1984).
139. B. Assadollahzadeh, S. Schäfer, and P. Schwerdtfeger, Electronic properties for small tin clusters Sn_n ($n \leq 20$) from density functional theory and the convergence toward the solid state, *J. Comput. Chem.* **31**, 929-937 (2010).
140 G. Maroulis, Cluster size effect on the electric polarizability and hyperpolarizability in small antimony clusters Sb_n, n = 1, 2 and 4, *Chem. Phys. Lett.* **444**, 44-47 (2007).
141. A. J. Sadlej, Medium-size polarized basis sets for high-level-correlated calculations of molecular electric properties - V. Fourth-row atoms: Sn through I, *Theor. Chim. Acta* **81**, 339-354 (1992).

142. G. Maroulis, C. Makris, U. Hohm, and D. Goebel, Electrooptical properties and molecular polarization of iodine, I_2, *J. Phys. Chem. A* **101**, 953- 956 (1997).
143. P. Hölemann and A. Braun, Über die adsorption von molekularem und atomarem jod an quarzglas (The adsorption of molecular and atomic iodine on quartz), *Z. Physik. Chem.* **B34**, 381-395 (1936).
144. N. Runeberg and P. Pyykkö, Relativistic pseudopotential calculations on Xe_2, RnXe, and Rn_2: The van der Waals properties of radon, *Int. J. Quantum Chem.* **66**, 131-140 (1998).
145. V. G. Bezchasnov, M. Pernpointner, P. Schmelcher, and L. S. Cederbaum, Nonadditivity and anisotropy of the polarizability of clusters: Relativistic finite-field calculations for the Xe dimer, *Phys. Rev. A* **81**, 062507-1-8 (2010).
146. S. Chattopadhyay, B. K. Mani, and D. Angom, Perturbed coupled-cluster theory to calculate dipole polarizabilities of closed-shellsystems: Application to Ar, Kr, Xe, and Rn, *Phys. Rev. A* **86**, 062508-1-6 (2012).
147. B. K. Sahoo and B. P. Das, The role of relativistic many-body theory in probing new physics beyond the standard model via the electric dipole moments of diamagnetic atoms, *J. Phys.*: *Conf. Ser.* **1041**, 012014-1-14 (2018).
148. A. Sakurai, B. K. Sahoo, and B. P. Das, Electric dipole polarizability of ^{129}Xe using the relativistic coupled-clusterand the normal coupled-cluster methods, *Phys. Rev. A* **97**, 062510-1-6 (2018).
149. A. Borschevsky, V. Pershina, E. Eliav, and U. Kaldor, *Ab initio* studies of atomic properties and experimental behavior of element 119 and its lighter homologs, *J. Chem. Phys.* **138**, 124302-1-5 (2013).
150. S. Singh, K. Kaur, B. K. Sahoo, and B. Arora, Comparing magic wavelengths for the $6s^2\ S_{1/2}$ — $6p^2\ P_{1/2;3/2}$ transitions of Cs using circularly and linearly polarized light, *J. Phys. B At. Mol. Opt. Phys.* **49**, 145005-1-10 (2016).
151. M. S. Safronova and C. W. Clark, Inconsistencies between lifetime and polarizability measurements in Cs, *Phys. Rev. A* **69**, 040501(R)-1-4 (2004).
152. E. Iskrenova-Tchoukova, M. S. Safronova, and U. I. Safronova, High-precision study of Cs polarizabilities, *J. Comput. Meth. Sci. Eng.* **7**, 521-540 (2007).
153. J. M. Amini and H. Gould, High Precision measurement of the static dipole polarizability of cesium, *Phys. Rev. Lett.* **91**, 153001-1-4 (2003).
154. A. Borschevsky, V. Pershina, E. Eliav, and U. Kaldor, Ab initio predictions of atomic properties of element 120 and its lighter group-2 homologues, *Phys. Rev. A* **87**, 022502-1-8 (2013).
155. S. Schäfer, M. Mehring, R. Schäfer, and P. Schwerdtfeger, Polarizabilities of Ba and Ba_2: Comparison of molecular beam experiments with relativistic quantum chemistry, *Phys. Rev. A* **76**, 052515-1-5 (2007).
156. V. A. Dzuba, A. Kozlov, and V. V. Flambaum, Scalar static polarizabilities of lanthanides and actinides, *Phys. Rev. A* **89**, 042507-1-8 (2014).

157. A. A. Buchachenko, G. Chałasinski, and M. M. Szczesniak, Diffuse basis functions for small-core relativistic pseudopotential basis setsand static dipole polarizabilities of selected lanthanides La, Sm, Eu, Tm and Yb, *Struct. Chem.* **18**, 769-772 (2007).
158. H. Li, J.-F. Wyart, O. Dulieu, S. Nascimbène, and M. Lepers, Optical trapping of ultracold dysprosium atoms: transition probabilities, dynamic dipole polarizabilities and van der Waals C_6 coefficients, *J. Phys. B: At. Mol. Opt. Phys.*, **50**, 014005-1-15 (2017).
159. M. Lepers, J.-F. Wyart, and O. Dulieu, Anisotropic optical trapping of ultracold erbium atoms, *Phys. Rev. A* **89**, 022505-1-13 (2014).
160. J. H. Becher, S. Baier, K. Aikawa, M. Lepers, J.-F. Wyart, O. Dulieu, and F. Ferlaino, Anisotropic polarizability of erbium atoms, *Phys. Rev. A* **97**, 012509-1-7 (2018).
161. A. A. Buchachenko, M. M. Szcześniak, and G. Chałasiński, van der Waals interactions and dipole polarizabilities of lanthanides: Tm(^{2}F–He and Yb(^{1}S–He potentials, *J. Chem. Phys.* **124**, 114301-1-8 (2006).
162. C. Thierfelder and P. Schwerdtfeger, Effect of relativity and electron correlation in static dipole polarizabilities of ytterbium and nobelium, *Phys. Rev. A* **79**, 032512-1-4 (2009).
163. V. A. Dzuba and A. Derevianko, Dynamic polarizabilities and related properties of clock states of the ytterbium atom, *J. Phys. B: At. Mol. Opt. Phys.* **43**, 074011-1-8 (2010).
164. A. A. Buchachenko, Ab initio dipole polarizabilities and quadrupole moments of the lowest excited states of atomic Yb, *Eur. Phys. J. D* **61**, 291-296 (2011).
165. P. Zhang, A. Dalgarno, and R. Côté, Scattering of Yb and Yb^+, *Phys. Rev. A* **80**, 030703(R)-1-4 (2009).
166. M. S. Safronova, S. G. Porsev, and C. W. Clark, Ytterbium in quantum gases and atomic clocks: van der Waals interactions and blackbody shifts, *Phys. Rev. Lett.* **109**, 230802-1-5 (2012).
167. Y. Wang and M. Dolg, Pseudopotential study of the ground and excited states of Yb_2, *Theor. Chem. Acc.* **100**, 124-133 (1998).
168. T. Yoshizawa, W. Zou, and D. Cremer, Calculations of electric dipole moments and static dipole polarizabilities based on the two-component normalized elimination of the small component method, *J. Chem. Phys.* **145**, 184104-1-14 (2016).
169. P. Zhang and A. Dalgarno, Static dipole polarizability of ytterbium, *J. Phys. Chem. A* **2007**, 12471-12476 (2007).
170. K. Beloy, Experimental constraints on the polarizabilities of the $6s^2\ ^1S_0$ and 6s6p $^3P_0$ states of Yb, *Phys. Rev. A* **86**, 022521-1-6 (2012).
171. V. A. Dzuba, M. S. Safronova, and U. I. Safronova, Atomic properties of superheavy elements No, Lr, and Rf, *Phys. Rev. A* **90**, 012504-1-9 (2014).
172. M. W. Cole and J. Bardon, van der Waals interaction between a tungsten surface and iridium and tantalum atoms, *Phys. Rev. B* **33**, 2812-2813 (1986).

173. J. Bardon and M. Audiffren, The polarizability of iridium neutral atoms and their van der Waals interaction with a tungsten surface measured by F.I.M, *J. Phys. (Paris) Colloq.* **45**, 245-249 (1984).
174. P. Schwerdtfeger, J. R. Brown, J. K. Laerdahl, and H. Stoll, The accuracy of the pseudopotential approximation. III. A comparison between pseudopotential and all-electron methods for Au and AuH, *J. Chem. Phys.* **113**, 7110-7118 (2000).
175. R. Wesendrup and P. Schwerdtfeger, Extremely strong s^2–s^2 closed-shell interactions, *Angew. Chem., Intl. Ed. Engl.* **39**, 907-910 (2000).
176. M. Henderson, L. J. Curtis, R. Matulioniene, D. G. Ellis, and C. E. Theodosiou, Lifetime measurements in Tl III and the determination of the ground-state dipole polarizabilities for Au I–Bi V, *Phys. Rev. A* **56**, 1872-1878 (1997).
177. V. Pershina, A. Borschevsky, E. Eliav, and U. Kaldor, Prediction of the adsorption behavior of elements 112 and 114 on inert surfaces from ab initio Dirac-Coulomb atomic calculations, *J. Chem. Phys.* **128**, 024707-1-9 (2008).
178. Y. Singh and B. K. Sahoo, Rigorous limits on the hadronic and semileptonic *CP*-violating coupling constants from the electric dipole moment of ^{199}Hg, *Phys. Rev. A* **91**, 030501(R)-1-5 (2015).
179. V. Kellö and A. J. Sadlej, Standardized basis sets for high-level-correlated relativistic calculations of atomic and molecular electric properties in the spin-averaged Douglas-Kroll (no-pair) approximation I. Groups Ib and IIb, *Theor. Chim. Acta* **94**, 93-104 (1996).
180. A. Borschevsky, H. Yakobi, E. Elias, and U. Kaldor, High-accuracy coupled cluster calculations of atomic properties, *Proc. Intl. Conf. Comput. Meth. Sci. Eng. 2010* (AIP Conf. Proc. 1642), 209-212 (2015).
181. B. K. Sahoo and B. P. Das, Relativistic normal coupled-cluster theory for accurate determination of electric dipole moments of atoms: First application to the ^{199}Hg atom, *Phys. Rev. A* **120**, 203001-1-6 (2018).
182. K. T. Tang and J. P. Toennies, The dynamical polarizability and van der Waals dimer potential of mercury, *Mol. Phys.* **106**, 1645-1653 (2008).
183. D. Goebel and U. Hohm, Dipole polarizability, Cauchy moments, and related properties of Hg, *J. Phys. Chem.* **100**, 7710-7712 (1996).
184. V. Pershina, A. Borschevsky, E. Eliav, and U. Kaldor, Atomic properties of element 113 and its adsorption on inert surfaces from *Ab Initio* Dirac-Coulomb calculations, *J. Phys. Chem. A* **112**, 13712-13716 (2008).
185. J. Mitroy, M. S. Safronova, and C. W, Clark, Theory and applications of atomic and ionic polarizabilities, *J. Phys. B: At. Mol. Opt. Phys.* **43**, 202001-1-38 (2010).
186. M. G. Kozlov, S. G. Porsev, and W. R. Johnson, Parity nonconservation in thallium, *Phys. Rev. A* **64**, 052107-1-7 (2001).
187. V. A. Dzuba and V. V. Flambaum, Calculation of the (*T*, *P*)-odd electric dipole moment of thallium and cesium, *Phys. Rev. A* **80**, 062509- 1-5 (2009).
188. V. A. Dzuba and V. V. Flambaum, Electron structure of superheavy elements Uut, Fl and Uup (Z = 113 to 115), *Hyperfine Interact.* **237**, 160: 1-17 (2016).

189. M. S. Safranova and P. K. Majumder, Thallium 7*p* lifetimes derived from experimental data and *ab initio* calculations of scalar polarizabilities, *Phys. Rev. A* **87**, 042502-1-5 (2013).
190. M. S. Safronova, W. R. Johnson, U. I. Safronova, and T. E. Cowan, Relativistic many-body calculations of the Stark-induced amplitude of the $^6P_{1/2}$-$^7P_{1/2}$ transition in thallium, *Phys. Rev. A* **74**, 022504-1-5 (2006).
191. C. S. Nash, Atomic and molecular properties of elements 112, 114, and 118, *J. Phys. Chem. A* **109**, 3493-3500 (2005).
192. S. G. Porsev, M. G. Kozlov, M. S. Safronova, and I. I. Tupitsyn, Development of the configuration-interaction + all-order method and application to the parity-nonconserving amplitude and other properties of Pb, *Phys. Rev. A*. **93**, 012510-1-10 (2016).
193. V. Kellö and A. J. Sadlej, Medium-size polarized basis sets for high-level-correlated calculations of molecular electric properties. VI. Fifth- row atoms: Pb through At, *Theor. Chim. Acta* **83**, 351-366 (1992).
194 N. P. Labello, A. M. Ferreira, and H. A. Kurtz, An Augmented effective core potential basis set for the calculation of molecular polarizabilities, *J. Comput. Chem.* **26**, 1464-1471 (2005).
195. D. Sulzer, P. Norman, and T. Saue, Atomic C_6 dispersion coefficients: a four-component relativistic Kohn–Sham study, *Mol. Phys.* **110**, 2535-2541 (2012).
196. D. A. Pantazis and F. Neese, All-electron scalar relativistic basis sets for the 6*p* elements, *Theor. Chem. Acc.* **131**, 1292-1-7 (2012).
197. V. Pershina, A. Borschevsky, E. Eliav, and U. Kaldor, Adsorption of inert gases including element 118 on noble metal and inert surfaces from *ab initio* Dirac–Coulomb atomic calculations, *J. Chem. Phys*. **129**, 144106-1-9 (2008).
198. O. Smits, P. Jerabek, E. Pahl, P. Schwerdtfeger, A hundred-year-old experiment re-evaluated: accurate ab-initio Monte-Carlo simulations of the melting of radon, *Angew. Chem. Int. Ed.* **57**, 9961-9964 (2018).
199. S. Singh, B. K. Sahoo, and B. Arora, Determination of magic wavelengths for the $7s\ ^2S_{1/2}$–$7p\ ^2P_{3/2,1/2}$ transitions in Fr, *Phys. Rev. A* **94**, 023418-1-10 (2016).
200. M. A. Kadar-Kallen and K. D. Bonin, Uranium polarizability measured by light-force technique, *Phys. Rev. Lett.* **72**, 828-831 (1994).
201. B. O. Roos, R. Lindh, P-Å. Malmqvist, V. Veryazov, and P.-O. Widmark, New relativistic ANO basis sets for actinide atoms, *Chem. Phys. Lett.* **409**, 295-299 (2005).
202. L. S. C. Martins, F. E. Jorge, M. L. Franco, and I. B. Ferreira, All-electron Gaussian basis sets of double zeta quality for the actinides, *J. Chem. Phys.* **145**, 244113-1-6 (2016).
203. A. K. Srivastava, S. K. Pandey, and N. Misra, Encapsulation of lawrencium into C_{60} fullerene: Lr@C_{60} versus Li@C_{60}, *Mater. Chem. Phys.* **177**, 437-441 (2016).
204. M. Seth, P. Schwerdtfeger, M. Dolg, K. Faegri, B. A. Hess, and U. Kaldor, Large relativistic effects in molecular properties of the hydride of superheavy element 111, *Chem. Phys. Lett.* **250**, 461-465 (1996).

205. R. F. de Farias, Estimation of some physical properties for tennessine and tennessine hydride (TsH), *Chem. Phys. Lett.* **667**, 1-3 (2016).
206. P. Jerabek, B. Schuetrumpf, P. Schwerdtfeger, and W. Nazarewicz, Electron and nucleon localization functions of oganesson: Approaching the Thomas-Fermi limit, *Phys. Rev. Lett.* **120**, 053001-1-5 (2018).