Relativistic many-body calculation of energies, oscillator strengths, transition rates, and lifetimes of Sc III ion

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A systematic study of Sc III atomic properties is carried out using a high-precision relativistic all-order method where all single, double, and partial-triple excitations of the Dirac-Fock wave functions are included to all orders of perturbation theory. Reduced matrix elements, oscillator strengths, transition rates, and lifetimes are determined for the ns, np_j, nd_j, nf_j, and ng_j levels with $n \leqslant 7$. Recommended values and estimates of their uncertainties are provided for a large number of electric-dipole transitions. Electric-quadrupole and magnetic-dipole matrix elements are evaluated to determine lifetimes of the $3d_{5/2}$ and $4s$ metastable levels. These calculations provide recommended values critically evaluated for their accuracy for a number of Sc III atomic properties for use in theoretical modeling as well as planning and analysis of various experiments. We hope that the present study will stimulate further exploration of Sc III for various applications owing to its interesting structure of different low-lying metastable levels.

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I. INTRODUCTION

We report results of *ab initio* calculations of excitation energies, oscillator strengths, transition rates, and lifetimes in K-like scandium. K and K-like ions are excellent systems for tests of high-precision theories and benchmark comparisons with experiments owing to their relatively simple electronic structure. High-accuracy calculation of energies, lifetimes, hyperfine constants, and multipole polarizabilities of neutral K was reported in Ref. [1]. In 2011, a systematic study of K-like Ca^+ atomic properties was carried out [2] using a high-precision relativistic all-order method where all single, double, and partial-triple excitations of the Dirac-Fock wave functions are included to all orders of perturbation theory. Ca^+ ions have been used for a number of quantum-information processing experiments (see Refs. [3–5] and references therein). Prospects of an optical frequency standard based on the metastable $4s$-$3d_{5/2}$ transition in Ca^+ ion have been studied in [6–8]. Properties of Ca^+ are also of interest in astrophysics as the absorption spectrum of the Ca^+ ion is used to explore the structure and properties of interstellar dust clouds [9,10]. Both K and K-like Ca II have an [Ar]$4s$ ground state, where $[\mathrm{Ar}] = 1s^2 2s^2 2p^6 3s^2 3p^6$. We omit [Ar] from the electronic configurations below. The first excited configuration of K is $4p$, while the first excited configuration of Ca^+ is $3d$. Availability of low-lying metastable $3d$ levels in Ca^+ led to the numerous applications mentioned above. The level scheme of K-like Sc III is different from both K and K-like Ca II: the ground state is $3d_{3/2}$, and the first two excited states are $3d_{5/2}$ and $4s$. The next configuration is $4p$. Therefore, two different types of low-lying metastable states are available. The $3d$ fine-structure splitting is large, 198 cm^{-1}, and the lifetime of the $3d_{5/2}$ level is very long, 3.3 h. The $4s$ level is also metastable, with a 0.05 s lifetime. Metastable levels of ions are of interest in astrophysics and plasma diagnostics.

It would also be interesting to explore the possibility of using $3d_{3/2}$-$3d_{5/2}$ states for quantum memory owing to a very long lifetime of the $3d_{5/2}$ level. Quantum information can be encoded in the ground state and a metastable energy state of an ion [11] since they represent sufficiently isolated two-level systems that can be used as a quantum bit (qubit). In the Ca^+ ion, where all building blocks for quantum-information processing have been successfully demonstrated, the ground $4s$ and $3d_{5/2}$ excited states represent a qubit, i.e., basis set states $|0\rangle$ and $|1\rangle$. One of the decoherence sources with such a scheme is a 1 s lifetime of the $3d_{5/2}$ state. As an alternative to such a scheme, two ground $4s$ hyperfine states of $^{43}Ca^+$ can be used as a qubit. The energy splitting between the hyperfine states is 3.2 GHz. Both of these approaches are described in detail in Ref. [3] and references therein. In Sc III, there is an alternative possibility of using $3d_{3/2}$ and $3d_{5/2}$ fine structure states as a qubit instead. It would be interesting to explore if much higher separation of the fine-structure states (198 cm^{-1}) may be advantageous in comparison with using the hyperfine states. While quantum-information processing experiments so far have been conducted with singly charged ions, the Th IV ion has been successfully laser cooled as a step toward developing a superprecise frequency standard with this system [12]. A possible disadvantage of multiply charged ions is substantially lower wavelengths of the transitions that can be used for cooling, detection, and one-qubit rotations. For example, the $3d_{3/2}$-$4p_{1/2}$ transition wavelength is in the UV range, 161 nm.

Recently, theoretical calculations of the lowest metastable state lifetimes in Sc III were reported by Sahoo *et al.* [13]. Lifetimes of the $3d_{5/2}$ and $4s$ levels were determined using the relativistic coupled-cluster theory [13]. In 2011, transition properties such as oscillator strengths, transition rates, branching ratios, and lifetimes of many low-lying states in Sc III were calculated using the same approach by Nandy *et al.* [14]. The weakest bound electron potential model (WBEPM) theory was used in Ref. [15] to calculate transition probabilities and oscillator strengths for a number of Sc III transitions.

The Sc III ion has been studied in a number of earlier experimental [16–19] and theoretical [20–35] papers. More than 40 years ago, Weiss [20] reported transition rates for the

$4s$-$4p$ and $3d$-$4p$ transitions in K I, Ca II, and Sc III. Analytical approximations to Hartree-Fock wave functions were used for the $4s$, $4p$, and $3d$ states of these ions. Multiplet strengths for the $4s$-$4p$ and $4p$-$3d$ transitions were also computed [20]. Warner [21] calculated dipole integrals from radial wave functions using the scaled Thomas-Fermi method. Oscillator strengths were reported for the $4p$-$5s$, $4p$-$4d$, and $4p$-$5d$ transitions in Sc III. Buchta *et al.* [16] studied the spectra of scandium (600–6000 Å) with the beam-foil method. Lifetimes of the $4p$, $4d$, $4f$, $5s$, $5p$, $5d$, and $5f$ levels were reported. The spectrum of doubly ionized scandium was studied by Holmström [17] by using a sliding spark in vacuum. About 30 new lines were observed in the region 9000 to 2000 Å. One year later, a vacuum sliding spark at 250-A peak current was used by Cornelius *et al.* [18] to investigate the Sc III spectrum in the region 550–9400 Å. All these data were used in the NIST compilation published in 1975 by Wiese and Fuhr [23]. The next NIST compilation published in 1988 by Martin *et al.* [30] included recommended values for transition rates, oscillator strengths, and line strengths in Sc III based on results published by Weiss [20], Kurucz and Peytremann [22], and Biémont [24]. Hartree-Fock wave functions were used by Bièmont [24] to calculate oscillator strengths for dipole transitions between the nl ($n = 4$–8, $l = s$, p, and d) configurations in Sc III.

Electric-quadrupole and magnetic-dipole transition probabilities between the $4s$ and the $3d_j$ levels of Sc III and other ions of the potassium isoelectronic sequence were calculated by Ali and Kim [31] using the (relativistic) Dirac-Fock single-configuration approximation implemented by the Desclaux [36] code. $M1$ and $E2$ transition probabilities between the $4s$ and $3d_j$ levels in K-like ions with $Z = 19$ to 24 were studied by Zeippen [33] using the SUPERSTRUCTURE code of Eissner *et al.* [37]. None of the previous studies listed above, except the recent calculations of [13,14], were carried out to high-precision.

In the present work, a relativistic high-precision all-order (linearized coupled-cluster) method is used to calculate atomic properties of doubly ionized scandium for the ns, np_j, nd_j, nf_j, and ng_j states with $n \leqslant 7$. Excitation energies and lifetimes are calculated for the first 36 excited states. The reduced electric-dipole matrix elements, line strengths, oscillator strengths, and transition rates are determined for allowed transitions between these levels. The $M1$ $3d_{3/2}$-$3d_{5/2}$ and $3d_{3/2}$-$4s$ and the $E2$ $3d_{3/2}$-$3d_{5/2}$ and $3d_j$-$4s$ matrix elements are evaluated and used to calculate lifetimes of the metastable $3d_{5/2}$ and $4s$ levels. The uncertainties of the final values are estimated for all properties.

The main motivation for this work is to provide recommended values critically evaluated for their accuracy for a number of atomic properties via a systematic high-precision study for use in theoretical modeling as well as planning and analysis of various experiments that may utilize the interesting structure of Sc III levels.

II. THIRD-ORDER AND ALL-ORDER CALCULATIONS OF ENERGIES

Energies of nl_j states in Sc III are evaluated for $n \leqslant 7$ and $l \leqslant 3$ using both third-order relativistic many-body perturbation theory (RMBPT) and the single-double (SD) all-order method discussed in Refs. [1,2]. The B splines [39] are used to generate a complete set of Dirac-Fock (DF) basis orbitals for use in the evaluation of all atomic properties. The present calculation of the transition rates and lifetimes required accurate representation of rather highly excited states, such as $7lj$, leading to the use of the large R = 110 a.u. cavity for the generation of the finite basis set and higher number ($N = 70$) of splines to produce high-accuracy single-particle orbitals. Results of our energy calculations are summarized in Table I. Columns 2–8 of Table I give the lowest-order DF energies $E^{(0)}$, second-order and third-order Coulomb correlation energies $E^{(2)}$ and $E^{(3)}$, first-order and second-order Breit corrections $B^{(1)}$ and $B^{(2)}$, and an estimated Lamb shift contribution, $E^{(\mathrm{LS})}$. The Lamb shift $E^{(\mathrm{LS})}$ is calculated as the sum of the one-electron self-energy and the first-order vacuum-polarization energy. The vacuum-polarization contribution is calculated from the Uehling potential using the results of Fullerton and Rinker [40]. The self-energy contribution is estimated for the s, $p_{1/2}$, and $p_{3/2}$ orbitals by interpolating among the values obtained by Mohr [41–43] using Coulomb wave functions. For this purpose, an effective nuclear charge Z_{eff} is obtained by finding the value of Z_{eff} required to give a Coulomb orbital with the same average $\langle r \rangle$ as the DF orbital. It should be noted that the values of $E^{(\mathrm{LS})}$ are very small. For states with $l > 0$, the Lamb shift is estimated to be smaller than 0.1 cm^{-1} using scaled Coulomb values and is ignored. We list the all-order SD energies in the column labeled E^{SD} and list the part of the third-order energies missing from E^{SD} in the column labeled $E^{(3)}_{\mathrm{extra}}$. The sum of the six terms $E^{(0)}$, E^{SD}, $E^{(3)}_{\mathrm{extra}}$, $B^{(1)}$, $B^{(2)}$, and $E^{(\mathrm{LS})}$ is our final all-order result $E^{\mathrm{SD}}_{\mathrm{tot}}$, listed in the 11th column of Table I. Recommended energies from the National Institute of Standards and Technology (NIST) database [44] are given in the column labeled E_{NIST}. Differences between our third-order and all-order calculations and experimental data, $\delta E^{(3)} = E^{(3)}_{\mathrm{tot}} - E_{\mathrm{NIST}}$ and $\delta E^{\mathrm{SD}} = E^{\mathrm{SD}}_{\mathrm{tot}} - E_{\mathrm{NIST}}$, are given in the two final columns of Table I, respectively.

As expected, the largest correlation contribution to the valence energy comes from the second-order term $E^{(2)}$. Therefore, we calculate $E^{(2)}$ with higher numerical accuracy. The second-order energy includes partial waves up to $l_{\max} = 8$ and is extrapolated to account for contributions from higher partial waves (see, for example, Refs. [45,46] for details of the extrapolation procedure). As an example of the convergence of $E^{(2)}$ with the number of partial waves l, consider the $3d_{3/2}$ state. Calculations of $E^{(2)}$ with $l_{\max} = 6$ and 8 yield $E^{(2)}(3d_{1/2}) = -15280.3$ and -15476.3 cm^{-1}, respectively. Extrapolation of these calculations yields -15546.6 and -15554.9 cm^{-1}, respectively. Thus, in this particular case, we have a numerical uncertainty in $E^{(2)}(3d_{3/2})$ of 8.3 cm^{-1}. The same value of numerical uncertainty is found for $E^{(2)}(3d_{5/2})$. It should be noted that this is the largest uncertainty among all states considered in Table I; smaller uncertainties (about 0.8–1.6 cm^{-1}) are obtained for the $4s$, $4p$, and $4d$ states and much smaller uncertainties (0.3–0.5 cm^{-1}) are obtained for the $n = 5$ states owing to much smaller contributions of higher partial waves.

Owing to numerical complexity, we restrict $l \leqslant l_{\max} = 6$ in the E^{SD} calculation. As noted above, the second-order contribution dominates E^{SD}; therefore, we can use the extrapolated value of the $E^{(2)}$ described above to account for the

TABLE I. Zeroth-order (DF), second-, and third-order Coulomb correlation energies $E^{(n)}$, single-double Coulomb energies $E^{\rm SD}$, $E^{(3)}_{\rm extra}$, and first-order Breit and second-order Coulomb-Breit corrections $B^{(n)}$ to the energies of Sc III. The total removal energies ($E^{(3)}_{\rm tot} = E^{(0)} + E^{(2)} + E^{(3)} + B^{(1)} + B^{(2)} + E^{(\rm LS)}$, $E^{\rm SD}_{\rm tot} = E^{(0)} + E^{\rm SD} + E^{(3)}_{\rm extra} + B^{(1)} + B^{(2)} + E^{(\rm LS)}$) are compared with recommended NIST energies $E_{\rm NIST}$ [38], $\delta E = E_{\rm tot} - E_{\rm NIST}$. Units: cm^{-1}.

nlj	$E^{(0)}$	$E^{(2)}$	$E^{(3)}$	$B^{(1)}$	$B^{(2)}$	$E^{(\rm LS)}$	$E^{(3)}_{\rm tot}$	$E^{\rm SD}$	$E^{(3)}_{\rm extra}$	$E^{\rm SD}_{\rm tot}$	$E_{\rm NIST}$	$\delta E^{(3)}$	$\delta E^{\rm SD}$
$3d_{3/2}$	−186245	−15554.9	2953.0	84.9	−196.8	0.0	−198959	−14392.3	1444.8	−199305	−199677	718	373
$3d_{5/2}$	−186081	−15478.1	2938.5	52.9	−194.0	0.0	−198761	−14320.4	1435.1	−199107	−199480	718	373
$4s_{1/2}$	−168598	−6321.8	1155.9	43.8	−36.7	7.6	−173749	−6038.5	687.1	−173934	−174138	389	204
$4p_{1/2}$	−133665	−4254.6	672.3	43.3	−23.9	−0.1	−137228	−4244.5	429.3	−137461	−137573	345	112
$4p_{3/2}$	−133221	−4203.3	662.7	31.2	−25.7	0.1	−136756	−4195.3	423.5	−136988	−137099	343	112
$4d_{3/2}$	−84672	−2952.2	423.6	13.7	−27.6	0.0	−87214	−2889.9	278.1	−87297	−87420	206	122
$4d_{5/2}$	−84626	−2947.2	423.4	8.7	−27.7	0.0	−87168	−2884.7	277.4	−87252	−87374	206	123
$4f_{5/2}$	−62027	−775.1	84.1	0.1	−0.6	0.0	−62718	−831.9	78.2	−62781	−62804	85	22
$4f_{7/2}$	−62028	−774.5	84.1	0.0	−0.5	0.0	−62718	−831.0	78.1	−62781	−62803	85	22
$5s_{1/2}$	−83126	−1944.3	359.0	14.9	−12.2	1.5	−84707	−1821.8	214.0	−84730	−84815	108	85
$5p_{1/2}$	−70200	−1499.5	240.2	16.8	−9.3	0.0	−71452	−1471.7	153.1	−71511	−71570	118	59
$5p_{3/2}$	−70030	−1485.7	237.5	12.1	−9.9	0.0	−71276	−1459.0	151.5	−71336	−71394	118	58
$5d_{3/2}$	−50316	−1302.3	174.9	5.9	−11.6	0.0	−51449	−1291.9	123.3	−51490	−51547	98	57
$5d_{5/2}$	−50295	−1300.7	174.9	3.8	−11.6	0.0	−51429	−1289.9	123.1	−51470	−51527	98	57
$5f_{5/2}$	−39741	−450.7	47.8	0.1	−0.5	0.0	−40144	−495.1	45.5	−40191	−40205	61	14
$5f_{7/2}$	−39742	−450.2	47.8	0.0	−0.4	0.0	−40144	−494.2	45.4	−40191	−40205	61	14
$5g_{7/2}$	−39509	−102.8	10.3	0.0	0.0	0.0	−39601	−104.9	10.7	−39603	−39605	4	2
$5g_{9/2}$	−39508	−102.8	10.3	0.0	0.0	0.0	−39601	−104.8	10.7	−39603	−39605	4	3
$6s_{1/2}$	−49733	−867.0	160.5	6.9	−5.6	0.4	−50438	−806.2	95.7	−50442	−50483	46	42
$6p_{1/2}$	−43532	−717.4	114.8	8.3	−4.6	0.0	−44131	−701.0	66.4	−44163	−44188	56	25
$6p_{3/2}$	−43449	−711.8	113.7	5.9	−4.9	0.0	−44046	−695.8	73.6	−44070	−44102	56	32
$6d_{3/2}$	−33419	−699.0	90.6	3.2	−6.1	0.0	−34030	−697.5	72.9	−34047	−34085	55	38
$6d_{5/2}$	−33408	−698.2	90.7	2.0	−6.1	0.0	−34020	−696.5	66.3	−34042	−34074	55	32
$6f_{5/2}$	−27598	−277.8	28.5	0.1	−0.3	0.0	−27847	−311.0	28.1	−27881	−27890	43	9
$6f_{7/2}$	−27598	−277.4	28.5	0.0	−0.3	0.0	−27847	−310.3	28.0	−27881	−27890	43	9
$6g_{7/2}$	−27438	−66.6	6.8	0.0	0.0	0.0	−27497	−67.8	6.8	−27499	−27500	3	1
$6g_{9/2}$	−27437	−66.5	6.8	0.0	0.0	0.0	−27497	−67.8	6.8	−27498	−27500	3	2
$7s_{1/2}$	−33119	−464.4	85.9	3.8	−3.0	0.2	−33497	−427.7	51.3	−33495	−33520	23	25
$7p_{1/2}$	−29673	−400.6	64.0	4.7	−2.6	0.0	−30007	−391.1	41.2	−30021	−30039	32	19
$7p_{3/2}$	−29626	−397.7	63.4	3.4	−2.8	0.0	−29960	−388.5	40.8	−29973	−29991	32	19
$7d_{3/2}$	−23819	−419.6	53.3	1.9	−3.6	0.0	−24187	−420.1	39.9	−24201	−24220	33	19
$7d_{5/2}$	−23812	−419.2	53.3	1.2	−3.6	0.0	−24181	−419.5	39.9	−24195	−24214	33	19
$7f_{5/2}$	−20269	−181.3	18.1	0.0	−0.2	0.0	−20432	−205.8	18.3	−20457	−20463	30	6
$7f_{7/2}$	−20269	−181.0	18.1	0.0	−0.2	0.0	−20432	−205.2	18.3	−20456	−20463	30	6
$7g_{7/2}$	−20159	−44.6	4.6	0.0	0.0	0.0	−20199	−45.4	4.6	−20199	−20200	2	1
$7g_{9/2}$	−20158	−44.6	4.6	0.0	0.0	0.0	−20198	−45.4	4.6	−20199	−20200	2	1

contributions of the higher partial waves. Six partial waves are also used in the calculation of $E^{(3)}$.

We note that the contributions of higher partial waves to removal energies are very large for the $3d$ states: $l > 6$ contribution is 266 cm^{-1}. Therefore, they must be included in a high-precision calculation. Restricting basis sets in coupled-cluster calculations to only a few first partial waves will lead to a significant loss of numerical accuracy.

The column labeled $\delta E^{\rm SD}$ in Table I gives the differences between our *ab initio* results and the available experimental values [44]. The all-order values for removal energies are in excellent agreement with experimental data. The ionization potential agrees with experiment to 0.2%. The SD results agree better with NIST values than do the third-order MBPT results (the ratio of $\delta E^{(3)}/\delta E^{\rm SD}$ is about 2–3 for some cases), illustrating the importance of fourth- and higher-order correlation corrections. It should be noted that we find remarkable agreement of our value for $3d_{3/2}$-$3d_{5/2}$ splitting and the NIST result [44]. The energy difference between the $3d_{3/2}$ and $3d_{5/2}$ levels ($E^{(3)}_{\rm tot} = 197.79$ cm^{-1} and $E^{(3)}_{\rm SD} = 197.58$ cm^{-1}) is in perfect agreement with $E_{\rm NIST} = 197.64$ cm^{-1}.

III. ELECTRIC-DIPOLE MATRIX ELEMENTS, OSCILLATOR STRENGTHS, TRANSITION RATES, AND LIFETIMES IN Sc III

A. Electric-dipole matrix elements

In Table II, we list our recommended values for 57 $E1$ ns-$n'p$, nd-$n'p$, nd-$n'f$, and ng-$n'f$ transitions. The absolute values in atomic units ($a_0 e$) are given in all cases. We note that we have calculated about 200 $E1$ matrix elements to consider all dipole transitions between the ns, np_j, nd_j, nf_j, and ng_j states with $n \leqslant 7$. We refer to these values as the recommended

TABLE II. Recommended values of the reduced electric-dipole matrix elements in Sc III in atomic units. The first-order, second-order, third-order MBPT, and all-order SD and SDpT values are listed; the label "sc" indicates the scaled values. Final recommended values and their uncertainties are given in the $Z^{\rm final}$ column. The last column gives relative uncertainties of the final values in %. Absolute values are given.

Transition		$Z^{\rm DF}$	$Z^{\rm (DF+2)}$	$Z^{\rm (DF+2+3)}$	$Z^{\rm SD}$	$Z^{\rm (SD)}_{\rm sc}$	$Z^{\rm SDpT}$	$Z^{\rm SDpT}_{\rm sc}$	$Z^{\rm final}$	Unc. (%)
$4s_{1/2}$	$4p_{1/2}$	2.5819	2.3804	2.3187	2.3325	2.3379	2.3412	2.3379	2.332(9)	0.37
$4s_{1/2}$	$4p_{3/2}$	3.6520	3.3682	3.2807	3.3004	3.3079	3.3126	3.3079	3.300(12)	0.37
$4s_{1/2}$	$5p_{1/2}$	0.1119	0.1973	0.1878	0.1883	0.1890	0.1879	0.1882	0.1883(7)	0.37
$4s_{1/2}$	$6p_{1/2}$	0.0847	0.1388	0.1338	0.1329	0.1331	0.1325	0.1330	0.1329(4)	0.30
$4s_{1/2}$	$6p_{3/2}$	0.1117	0.1887	0.1811	0.1799	0.1805	0.1794	0.1803	0.1799(6)	0.33
$4s_{1/2}$	$7p_{1/2}$	0.0616	0.1006	0.0975	0.0964	0.0965	0.0961	0.0965	0.0964(3)	0.31
$4s_{1/2}$	$7p_{3/2}$	0.0820	0.1375	0.1328	0.1313	0.1317	0.1309	0.1317	0.1313(4)	0.31
$5s_{1/2}$	$4p_{1/2}$	1.4581	1.5000	1.4521	1.4452	1.4488	1.4472	1.4477	1.445(5)	0.35
$5s_{1/2}$	$4p_{3/2}$	2.0910	2.1485	2.0825	2.0726	2.0769	2.0753	2.0753	2.073(6)	0.29
$5s_{1/2}$	$5p_{1/2}$	4.9692	4.8948	4.7955	4.8098	4.8157	4.8203	4.8151	4.816(8)	0.17
$5s_{1/2}$	$5p_{3/2}$	7.0208	6.9163	6.7755	6.7959	6.8045	6.8108	6.8036	6.804(12)	0.18
$6s_{1/2}$	$5p_{1/2}$	2.9468	2.9728	2.9029	2.8935	2.8986	2.8980	2.8968	2.899(5)	0.18
$6s_{1/2}$	$5p_{3/2}$	4.2190	4.2538	4.1578	4.1442	4.1497	4.1504	4.1472	4.150(5)	0.13
$6s_{1/2}$	$6p_{1/2}$	8.0750	8.0400	7.9121	7.9305	7.9378	7.9439	7.9365	7.938(7)	0.09
$6s_{1/2}$	$6p_{3/2}$	11.4022	11.3536	11.1718	11.1982	11.2090	11.2172	11.2073	11.209(11)	0.10
$7s_{1/2}$	$5p_{1/2}$	0.8050	0.8207	0.8036	0.8025	0.8030	0.8036	0.8035	0.8030(8)	0.11
$7s_{1/2}$	$5p_{3/2}$	1.1442	1.1659	1.1422	1.1406	1.1412	1.1422	1.1419	1.141(1)	0.12
$7s_{1/2}$	$6p_{1/2}$	4.8684	4.8856	4.7936	4.7765	4.7846	4.7847	4.7820	4.785(3)	0.06
$7s_{1/2}$	$6p_{3/2}$	6.9647	6.9866	6.8609	6.8361	6.8450	6.8474	6.8413	6.845(4)	0.05
$7s_{1/2}$	$7p_{1/2}$	11.9058	11.8868	11.7347	11.7589	11.7662	11.7737	11.7643	11.766(8)	0.06
$7s_{1/2}$	$7p_{3/2}$	16.8055	16.7797	16.5630	16.5979	16.6091	16.6189	16.6064	16.609(10)	0.06
$3d_{3/2}$	$5p_{3/2}$	0.1307	0.1151	0.1144	0.1135	0.1138	0.1141	0.1140	0.1135(4)	0.38
$4d_{3/2}$	$4f_{5/2}$	7.9569	7.8263	7.5436	7.5425	7.5543	7.5708	7.5519	7.554(16)	0.22
$4d_{3/2}$	$5p_{3/2}$	2.0321	2.0324	1.9088	1.9172	1.9199	1.9269	1.9184	1.9120(7)	0.36
$4d_{3/2}$	$7p_{3/2}$	0.1039	0.1042	0.1086	0.1080	0.1079	0.1076	0.1083	0.1079(3)	0.32
$4d_{5/2}$	$4f_{5/2}$	2.1276	2.0927	2.0173	2.0170	2.0200	2.0246	2.0194	2.020(45)	0.22
$4d_{5/2}$	$4f_{7/2}$	9.5151	9.3587	9.0218	9.0205	9.0340	9.0543	9.0311	9.034(20)	0.22
$5d_{3/2}$	$4f_{5/2}$	5.2832	5.3098	5.4587	5.4139	5.4180	5.4053	5.4161	5.418(13)	0.24
$5d_{3/2}$	$5f_{5/2}$	13.5653	13.5070	13.0080	13.0302	13.0456	13.0750	13.0416	13.046(29)	0.23
$5d_{3/2}$	$6p_{1/2}$	8.4834	8.4869	8.0942	8.1049	8.1130	8.1394	8.1083	8.113(26)	0.33
$5d_{3/2}$	$6p_{3/2}$	3.7769	3.7791	3.6022	3.6071	3.6113	3.6227	3.6092	3.611(11)	0.31
$5d_{5/2}$	$4f_{5/2}$	1.4100	1.4173	1.4569	1.4449	1.4462	1.4426	1.4457	1.446(4)	0.25
$5d_{5/2}$	$4f_{7/2}$	6.3052	6.3379	6.5152	6.4618	6.4677	6.4515	6.4653	6.468(16)	0.25
$5d_{5/2}$	$5f_{5/2}$	3.6282	3.6123	3.4794	3.4854	3.4891	3.4973	3.4881	3.489(8)	0.23
$5d_{5/2}$	$5f_{7/2}$	16.2258	16.1549	15.5605	15.5870	15.6041	15.6405	15.5993	15.604(36)	0.23
$5d_{5/2}$	$6p_{3/2}$	11.3462	11.3512	10.8225	10.8376	10.8482	10.8840	10.8419	10.848(36)	0.33
$6d_{3/2}$	$5f_{5/2}$	10.3105	10.3261	10.5991	10.5158	10.5228	10.5035	10.5182	10.523(19)	0.18
$6d_{3/2}$	$6f_{5/2}$	20.1506	20.1224	19.3957	19.4440	19.4632	19.5053	19.4569	19.463(42)	0.22
$6d_{3/2}$	$6p_{1/2}$	10.2222	10.2020	10.2676	10.2670	10.2785	10.2627	10.2753	10.278(16)	0.15
$6d_{3/2}$	$6p_{3/2}$	4.6039	4.5939	4.6244	4.6239	4.6279	4.6219	4.6265	4.628(6)	0.13
$6d_{3/2}$	$7p_{1/2}$	13.3816	13.3841	12.8566	12.8613	12.8718	12.9097	12.8655	12.872(38)	0.29
$6d_{3/2}$	$7p_{3/2}$	5.9584	5.9603	5.7222	5.7246	5.7301	5.7464	5.7273	5.730(16)	0.28
$6d_{5/2}$	$5f_{5/2}$	2.7518	2.7564	2.8290	2.8067	2.8089	2.8034	2.8077	2.809(6)	0.20
$6d_{5/2}$	$5f_{7/2}$	12.3056	12.3260	12.6514	12.5523	12.5619	12.5374	12.5564	12.562(24)	0.20
$6d_{5/2}$	$6f_{5/2}$	5.3900	5.3820	5.1886	5.2016	5.2061	5.2179	5.2044	5.206(12)	0.23
$6d_{5/2}$	$6f_{7/2}$	24.1055	24.0698	23.2042	23.2617	23.2826	23.3349	23.2819	23.283(52)	0.22
$6d_{5/2}$	$6p_{3/2}$	13.7972	13.7686	13.8588	13.8570	13.8708	13.8512	13.8666	13.871(20)	0.14
$6d_{5/2}$	$7p_{3/2}$	17.8970	17.9006	17.1893	17.1969	17.2109	17.2620	17.2023	17.211(51)	0.30
$7d_{3/2}$	$6f_{5/2}$	16.4127	16.4198	16.8441	16.7084	16.7174	16.6925	16.7103	16.717(25)	0.15
$7d_{3/2}$	$7f_{5/2}$	27.7977	27.7852	26.8016	26.8897	26.9133	26.9679	26.9035	26.913(54)	0.20
$7d_{3/2}$	$7p_{1/2}$	14.3502	14.3430	14.4954	14.5024	14.5158	14.4899	14.5111	14.516(26)	0.18
$7d_{3/2}$	$7p_{3/2}$	6.4648	6.4602	6.5302	6.5330	6.5374	6.5273	6.5351	6.537(10)	0.15
$7d_{5/2}$	$6f_{5/2}$	4.3807	4.3832	4.4960	4.4596	4.4626	4.4554	4.4605	4.463(7)	0.16
$7d_{5/2}$	$6f_{7/2}$	19.5895	19.6005	20.1067	19.9451	19.9571	19.9257	19.9479	19.957(31)	0.16
$7d_{5/2}$	$7f_{5/2}$	7.4360	7.4320	7.1702	7.1939	7.1995	7.2147	7.1971	7.199(15)	0.21
$7d_{5/2}$	$7f_{7/2}$	33.2561	33.2380	32.0665	32.1711	32.1973	32.2647	32.1864	32.197(67)	0.21
$7d_{5/2}$	$7p_{3/2}$	19.3722	19.3607	19.5684	19.5763	19.5917	19.5595	19.5848	19.593(32)	0.16

matrix elements. We only list the matrix elements that give significant contributions to the atomic properties calculated in the other sections. To evaluate the uncertainties of these values, we carried out several calculations by several different methods of increasing accuracy: lowest-order DF, second-order relativistic many-body perturbation theory (RMBPT), third-order RMBPT, and all-order methods. The many-body perturbation theory (MBPT) calculations are carried out following the method described in Ref. [47]. The third-order RMBPT includes random-phase-approximation (RPA) terms iterated to all orders, Brueckner orbital (BO) corrections, the structural radiation, and normalization terms (see [47] for definition of these terms). Comparisons of the values obtained in different approximations allows us to evaluated the size of the second-, third-, and higher-order correlation corrections.

We list the lowest-order Dirac-Fock $Z^{\rm DF}$, second-order $Z^{\rm (DF+2)}$, and third-order $Z^{\rm (DF+2+3)}$ values in the first three numerical columns of Table II. The values $Z^{\rm (DF+2)}$ are obtained as the sum of the second-order correlation correction $Z^{(2)}$ and the DF matrix elements $Z^{\rm DF}$. The second-order Breit corrections $B^{(2)}$ are very small in comparison with the second-order Coulomb corrections $Z^{(2)}$ (the ratio of $B^{(2)}$ to $Z^{(2)}$ are about 1–2%). The third-order matrix elements $Z^{\rm (DF+2+3)}$ include the DF values, the second-order $Z^{(2)}$ results, and the third-order $Z^{(3)}$ correlation correction.

The next four columns contain results of four different all-order calculations: *ab initio* single-double (SD) and single-double partial-triple (SDpT) calculations, and the corresponding scaled SD and SDpT calculations. Below, we briefly describe the differences in these calculations. In the SD all-order method, the wave function is described by

$$|\Psi_v\rangle = \left[1 + \sum_{ma} \rho_{ma} a_m^\dagger a_a + \frac{1}{2}\sum_{mnab} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a + \sum_{m\neq v} \rho_{mv} a_m^\dagger a_v + \sum_{mna} \rho_{mnva} a_m^\dagger a_n^\dagger a_a a_v\right]\left|\Psi_v^{(0)}\right\rangle, \quad (1)$$

where $|\Psi_v^{(0)}\rangle$ is the lowest-order atomic state vector. In Eq. (1), the indices m and n range over all possible virtual states while indices a and b range over all occupied core states. The quantities ρ_{ma}, ρ_{mv} are single-excitation coefficients for core and valence electrons, and ρ_{mnab} and ρ_{mnva} are double-excitation coefficients for core and valence electrons, respectively.

The matrix elements of any one-body operator $Z = \sum_{ij} z_{ij}\ a_i^\dagger a_j$ are obtained within the framework of the SD all-order method as

$$Z_{wv} = \frac{\langle\Psi_w|Z|\Psi_v\rangle}{\sqrt{\langle\Psi_v|\Psi_v\rangle\langle\Psi_w|\Psi_w\rangle}}, \quad (2)$$

where the numerator consists of the sum of the DF matrix element z_{wv} and 20 other terms that are linear or quadratic functions of the excitation coefficients. The all-order method yielded results for the properties of alkali-metal atoms and many other monovalent systems [2,48–51] in excellent agreement with experiment.

Generally, only two out of twenty terms give dominant correlation contributions to transition matrix elements

$$Z^{(a)} = \sum_{ma}(z_{am}\tilde{\rho}_{wmva} + z_{ma}\tilde{\rho}^*_{vmwa}), \quad (3)$$

or

$$Z^{(c)} = \sum_{m}(z_{wm}\rho_{mv} + z_{mv}\rho^*_{mw}), \quad (4)$$

where $\tilde{\rho}_{mnab} = \rho_{mnab} - \rho_{nmab}$ and z_{wv} are lowest-order matrix elements of the electric-dipole (or other) operator. For most of the transitions considered in this work, $Z^{(c)}$ is the dominant term. In many cases, it is overwhelmingly dominant (by a factor of 3 or more). Its accuracy can be improved using the SDpT approach.

In the SDpT calculation, an additional triple valence term

$$\frac{1}{6}\sum_{mnrab} \rho_{mnrvab} a_m^\dagger a_n^\dagger a_r^\dagger a_b a_a a_v \left|\Psi_v^{(0)}\right\rangle \quad (5)$$

is added to the wave function. Then, the equations for the correlation energy and valence excitation coefficients ρ_{mv} are modified perturbatively to include the effects of the triple term described by the Eq. (5). These triple corrections are important for many of the nd–$n'p$ matrix elements and have to be included.

Ab initio electric-dipole matrix elements evaluated in the all-order SD and SDpT approximations [48] are given in the columns labeled $Z^{\rm SD}$ and $Z^{\rm SDpT}$ of Table II. The SD and SDpT matrix elements $Z^{\rm SD}$ and $Z^{\rm SDpT}$ include $Z^{(3)}$ completely, along with important fourth- and higher-order corrections. The fourth-order corrections omitted from the SD matrix elements were discussed by Derevianko and Emmons [52]. The difference between the $Z^{\rm SD}$ and $Z^{\rm SDpT}$ values is about 0.2–0.4% for most of the transitions.

The term $Z^{(c)}$ given by Eq. (4) is dominant for a large fraction of the transitions considered in this work. We can evaluate missing corrections to this term by correcting the valence single-excitation coefficients ρ_{mv} via the scaling procedure [53]. These excitation coefficients are closely related to the correlation energy δE_v. Therefore, the part of the omitted correlation correction can be estimated by adjusting the single-excitation coefficients ρ_{mv} to the experimentally known value of the valence correlation energy, and then recalculating the matrix elements using Eq. (2) with the modified coefficients [53].

We have developed [2] some general criteria to establish the final values for all transitions and evaluate uncertainties owing to the need to analyze a very large number of transitions. The scaling procedure and evaluation of the uncertainties are described in detail in [2]. We note that it is a rather complicated procedure that involves complete recalculation of the matrix elements with new values of the valence excitation coefficients. The scaling factors depend on the correlation energy given by the particular calculation and are different for the SD and SDpT calculations, and these values have to be scaled separately. The corresponding results are listed in Table II with subscript "sc".

We establish the recommended set of values and their uncertainties based on the ratio $R = Z^{(c)}/Z^{(a)}$ since term a is not corrected by the scaling procedure. We take the final value to be SD scaled if $R > 1$. Otherwise, we use SD as the final

value. If $0.5 < R < 1.5$, we evaluate the uncertainty in term $Z^{(c)}$ as the maximum difference of the final value and the other three all-order values from the SD, SDpT, SDsc, and SDpTsc set. Then, we assume that the uncertainty of all the other terms does not exceed this value and add two uncertainties in quadrature. If $1.5 < R < 3$, we evaluate the final uncertainty as the max(SDsc-SD, SDsc-SDpT, SDsc-SDpTsc). If the term $Z^{(c)}$ strongly dominates and $R > 3$, we evaluate the final uncertainty as max(SDsc-SDpT, SDsc-SDpTsc). We note that we have conducted numerous comparisons of all available data on various properties of many different monovalent systems with different types of experiments in many other works (see [2,48,49,53–65], and references therein) and found that such procedures do not underestimate the uncertainties.

The last column of Table II gives relative uncertainties of the final values $Z^{\rm final}$ in %. We find that the uncertainties are 0.1–0.3% for most of the transitions. Larger uncertainties (0.5–0.7%) occur for some of the transitions such as $3d_j$-$nf_{j'}$. Our final results and their uncertainties are used to calculate the recommended values of the transition rates, oscillator strengths, and lifetimes as well as evaluate the uncertainties of these results.

Comparison of the present reduced electric-dipole matrix elements with coupled-cluster calculations of Ref. [14] in Sc III (a.u.) is given in Table III. Absolute values are given for convenience. To illustrate initial starting points of both calculations, we also list lowest-order Dirac-Fock data for both present calculations and Ref. [14]. Our final data are listed in column Final. The final data from Ref. [14] are listed in the column CCSDpT. The method used in Ref. [14], i.e., relativistic coupled-cluster (CC) theory, is similar to the one used in the present work, but the implementations are different. The present calculations are based on the linearized version of the coupled-cluster approach (LCC), and are carried out with very large numerically complete basis sets generated in a large cavity. Numerical completeness of the basis sets was tested by performing calculations with different size basis sets to ensure that an increase in the basis set size will not change the calculated observables well within the estimated final accuracy. The nonlinear terms, which are omitted in the present work, were demonstrated [66] to significantly cancel with nonperturbative triple excitations (omitted in both this work and Ref. [14]). As a result, the *ab initio* LCCSDpT approach used in this work may prove to provide more accurate recommended values than CCSDpT used in Ref. [14]. The scaling procedure carried out in the present work estimates parts of both nonlinear and nonperturbative triple terms (see [53] for detailed discussion of this issue).

The differences between our final values and Ref. [14] are small (less than 1%) for the first 12 transitions that include the $3d$, $4s$, $5s$, and $5p$ one-electron states. It is expected owing to the similarity of the high-precision approaches used here and in Ref. [14]. The difference between the present and Ref. [14] values increases up to 3% for transitions involving the $5d$, $6s$, and $6p$ states. We note that this difference appears already at the DF level, which was not observed for the previous low-lying levels. As we have noted, we carry out all calculations with a very large basis set ($N = 70$ orbitals for each partial wave) for the specific purpose of accurately calculating the properties of higher excited states. Large basis sets are required to describe these states. In Ref. [14], the initial basis set used to generate DF orbitals is smaller ($N = 32$), and it further truncated to $N = 12$–15 for the coupled-cluster part of the calculations. Only partial waves up to $l_{\rm max} = 4$ are used in [14], while $l_{\rm max} = 6$ is used in all present calculations. Higher partial waves give significant contributions to the properties of the nd states as was studied in detail in Ref. [53]. The codes used in the present work were optimized for efficiency to allow the inclusion of higher partial waves and very large number of orbitals. While the basis set of Ref. [14] was probably optimized in some way to generate good accuracy data for low-lying states, it appears to lead to reduced accuracy for higher states. The largest disagreement, 5–20%, is observed for the three last transitions with small matrix elements that are particularly sensitive to both differences in the treatment of the correlation correction and incompleteness of the basis set.

TABLE III. Comparison of the present reduced electric-dipole matrix elements with coupled-cluster calculations of Ref. [14] in Sc III (a.u.). Absolute values are given for convenience. To illustrate initial starting points of both calculations, we also list lowest-order Dirac-Fock data for both present calculations and Ref. [14]. Our final data are listed in column Final. The final data from Ref. [14] are listed in the column CCSDpT.

Transition		Present work		Ref. [14]	
		DF	Final	DF	CCSDpT
$4s_{1/2}$	$4p_{1/2}$	2.5819	2.332(9)	2.584	2.345
$4s_{1/2}$	$4p_{3/2}$	3.6520	3.300(12)	3.650	3.318
$4d_{5/2}$	$4f_{5/2}$	2.1276	2.020(45)	2.130	2.025
$4d_{5/2}$	$4f_{7/2}$	9.5151	9.034(20)	9.526	9.055
$5s_{1/2}$	$4p_{1/2}$	1.4581	1.445(5)	1.453	1.442
$5s_{1/2}$	$4p_{3/2}$	2.0910	2.073(6)	2.083	2.068
$5s_{1/2}$	$5p_{1/2}$	4.9692	4.816(8)	4.949	4.849
$5s_{1/2}$	$5p_{3/2}$	7.0208	6.804(12)	7.063	6.851
$3d_{3/2}$	$5p_{3/2}$	0.1307	0.1135(4)	0.130	0.113
$4d_{3/2}$	$5p_{1/2}$	4.5654	4.314(16)	4.578	4.330
$4d_{3/2}$	$5p_{3/2}$	2.0321	1.9120(7)	2.037	1.936
$4d_{5/2}$	$5p_{3/2}$	6.1065	5.769(22)	6.124	5.793
$5d_{3/2}$	$4f_{5/2}$	5.2832	5.418(13)	5.348	5.500
$5d_{5/2}$	$4f_{5/2}$	1.4100	1.446(4)	1.427	1.468
$5d_{5/2}$	$4f_{7/2}$	6.3052	6.468(16)	6.382	6.564
$6s_{1/2}$	$5p_{1/2}$	2.9468	2.899(5)	2.922	2.862
$6s_{1/2}$	$5p_{3/2}$	4.2190	4.150(5)	4.182	4.100
$6s_{1/2}$	$6p_{1/2}$	8.0750	7.938(7)	8.268	8.160
$6s_{1/2}$	$6p_{3/2}$	11.4022	11.209(11)	11.676	11.522
$5d_{3/2}$	$6p_{1/2}$	8.4834	8.113(26)	8.600	8.168
$5d_{3/2}$	$6p_{3/2}$	3.7769	3.611(11)	3.830	3.636
$5d_{5/2}$	$6p_{3/2}$	11.3462	10.848(36)	11.506	10.928
$4s_{1/2}$	$5p_{1/2}$	0.1119	0.1883(7)	0.106	0.179
$4s_{1/2}$	$6p_{1/2}$	0.0847	0.1329(4)	0.068	0.115
$4s_{1/2}$	$6p_{3/2}$	0.1117	0.1799(6)	0.088	0.155

B. Transition rates, oscillator strengths, and line strengths

We combine recommended NIST energies [38] and our final values of the matrix elements listed in Table II to calculate transition rates A_r and oscillator strengths f. The transition

rates are calculated using

$$A_{ab} = \frac{2.02613 \times 10^{18}}{\lambda^3} \frac{S}{2j_a + 1} \mathrm{s}^{-1}, \quad (6)$$

where the wavelength λ is in Å and the line strength $S = d^2$ is in atomic units.

Transition rates A (s^{-1}) for the 150 allowed electric-dipole transitions between ns, np_j, nd_j, nf_j, and ng_j states with $n \leqslant 7$ in Sc III are summarized in Table IV. Vacuum wavelengths obtained from NIST energies are also listed for reference. The transitions are ordered by the value of the wavelength. The relative uncertainties of the transition rates are twice the corresponding matrix element uncertainties since these properties are proportional to the squares of the matrix elements. The uncertainties in percent are listed in the column labeled "Unc." The largest uncertainties (about 1%) are for the $3d_j$-$nf_{j'}$ and $3d_j$-$np_{j'}$ transitions, while the smallest ones (about 0.1–0.3%) are for the nf_j-$ng_{j'}$ transitions. The larger uncertainties generally result from the larger relative size of the correlation corrections.

In Table V, we compare the line strengths S for transitions in Sc III calculated using our recommended values of reduced electric-dipole matrix elements with S values recommended by NIST compilation [38]. Our all-order values are listed in the column labeled "Final". The relative uncertainties of the final values are listed in column "Unc." in %. NIST wavelengths λ are listed for convenience. We already mentioned that line strengths S, oscillator strengths f, and transition rates A_r in NIST compilation [38] were based on results obtained using analytical approximations to Hartree-Fock wave functions [20], semiempirical approximation [22], and Hartree-Fock approximation [24]. Therefore, we also list our lowest-order DF data in column "DF" for the purposes of this comparison and to illustrate the size of the correlation corrections estimated as the difference of our final and DF values. The data recommended by NIST compilation [38] are generally in better agreement with lowest-order DF results than with our final values. This may be expected since the calculations used in NIST compilations largely omitted correlation corrections. For convenience of comparison, we order the transitions by the size of the correlation correction. The transitions within the groups are ordered by their wavelengths. The left column of Table V includes transitions with small contribution of correlation effects, with the difference $[S^{\mathrm{final}} - S^{\mathrm{DF}}]$ being about 10%. The right column of Table V includes transitions with large contribution of correlation effects, 30–50%.

In Table VI, we present oscillator strengths f for transitions in Sc III calculated using our recommended values of reduced electric-dipole matrix elements f^{final} and their uncertainties. The relative uncertainties are listed in column "Unc." in %. We also list the lowest-order DF values to illustrate the size of the correlation correction. Recommended NIST wavelengths λ [38] are listed for reference. We sort the transitions by the size of the correlation correction. The left column of Table VI includes transitions with small contribution of correlation effects, when the difference $[f^{\mathrm{final}} - f^{\mathrm{DF}}]$ is about 10%. In column "WBEPM", we list f values calculated by the WBEPM method [15], which is a nonrelativistic semiempirical method that uses parameters obtained by fitting of the experimental energy data. The WBEPM values are in reasonably good agreement with our final data for the cases where correlation correction is small, as expected. Otherwise, we did not find any regularity in the f^{WBEPM} values, as the differences between our values and WBEPM vary. This outcome may be expected, because the fitting into the energy levels carried out in [15] may produce better approximation for some levels but worse approximation for the other levels. Our calculations include the correlation corrections in a rather complete way and are expected to be more accurate, in particular for the stronger transitions.

C. Lifetimes in Sc III

We calculated lifetimes of the ns ($n = 5$–7), np_j ($n = 4$–7), nd_j ($n = 4$–7), nf_j ($n = 4$–7), and ng_j ($n = 5$–7) states in Sc III using our final values of the transition rates listed in Table IV. The lifetimes of the metastable $3d_{5/2}$ and $4s$ states are discussed in the next section. The uncertainties in the lifetime values are obtained from the uncertainties in the transition rates listed in Table IV. We also included the lowest-order DF lifetimes to illustrate the size of the correlation effects. The recommended NIST energies [38] are given in column 'Energy' for reference. The present values are compared with experimental measurements by Buchta *et al.* [16] and by Andersen *et al.* [19]. The beam-foil method was used in both papers. We did not include results from [16] for the $4f$ and $5f$ states with $\tau^{\mathrm{expt}}(4f) = 3.5$ ns and $\tau^{\mathrm{expt}}(5f) = 2.7$ ns. Our $\tau^{\mathrm{final}}(4f_{5/2}) = 0.645(7)$ and $\tau^{\mathrm{final}}(5f_{5/2}) = 1.145(10)$ differ from results in [16] by a factor of 5.4 and 2.4, respectively. Wiese and Fuhr [23] criticized these measurements and included comparisons with theoretical values $\tau(4f) = 0.59$ ns and $\tau(5f) = 0.99$ ns, obtained by the scaled Thomas-Fermi method [21]. Our values are compared with CCSDpT calculations of Ref. [14]. As expected from the comparison of the matrix elements given in Table III and discussed at the end of Sec. III A, our values are in excellent agreement with Ref. [14] for $4p$, $4d$, $5s$, and $5p$ states. Differences for higher states follow from the corresponding differences in the matrix elements discussed in Sec. III A.

IV. ELECTRIC-QUADRUPOLE AND MAGNETIC-DIPOLE MATRIX ELEMENTS

The $M1$ $3d_{3/2}$-$3d_{5/2}$ and $3d_{3/2}$-$4s$, and the $E2$ $3d_{3/2} - 3d_{5/2}$ and $3d_j$-$4s$ matrix elements are evaluated using the same approach as for the $E1$ matrix elements [see Eq. (2)]. In Table VIII, we list results for the magnetic-dipole ($M1$) and electric-quadrupole ($E2$) matrix elements calculated in different approximations: lowest-order DF, second-order RMBPT, third-order RMBPT, and all-order method with and without the triple excitations. The label "sc" indicates the scaled values. Final recommended values and their uncertainties are given in the Z^{final} column. The Unc. column gives relative uncertainties of the final values in %. The final value of the $M1$ $3d_{3/2}$-$3d_{5/2}$ matrix element is the same as the lowest-order DF result. The $M1$ matrix element for the $3d_{3/2}$-$3d_{5/2}$ transition changes substantially with the inclusion of the correlation. The value of the $M1$ $3d_{3/2}$-$4s$ matrix element is not zero due to relativistic effects; it is smaller than the value of the $M1$ $3d_{3/2}$-$3d_{5/2}$ matrix element by five orders of magnitude. The breakdown of the correlation correction for this $M1$ transition is different

TABLE IV. Transition rates A_r (s^{-1}) in Sc III calculated using our recommended values of reduced electric-dipole matrix elements. The relative uncertainties of the final values are listed in column "Unc." in %. Lowest-order DF values are listed in column "DF". The vacuum wavelengths λ in Å from NIST compilation [38] are listed for reference. Numbers in brackets represent powers of 10.

Transition		λ	A_r	Unc.	Transition		λ	A_r	Unc.	Transition		λ	A_r	Unc.
Lower	Upper	(Å)	(s^{-1})	(%)	Lower	Upper	(Å)	(s^{-1})	(%)	Lower	Upper	(Å)	(s^{-1})	(%)
$3d_{3/2}$	$7f_{5/2}$	557.99	2.85[8]	1.3	$4f_{7/2}$	$7g_{7/2}$	2347.25	2.08[6]	0.40	$5f_{7/2}$	$6g_{7/2}$	7870.8	3.20[6]	0.6
$3d_{5/2}$	$7f_{5/2}$	558.61	2.04[7]	1.4	$4f_{7/2}$	$7g_{9/2}$	2347.25	5.83[7]	0.40	$5f_{7/2}$	$6g_{9/2}$	7870.8	8.96[7]	0.6
$3d_{5/2}$	$7f_{7/2}$	558.61	3.07[8]	1.3	$4f_{5/2}$	$7d_{5/2}$	2591.37	1.60[5]	1.34	$5d_{3/2}$	$5f_{5/2}$	8816.6	8.39[7]	0.5
$3d_{5/2}$	$6f_{5/2}$	582.78	3.20[7]	1.3	$4f_{7/2}$	$7d_{5/2}$	2591.38	3.19[6]	1.34	$5d_{5/2}$	$5f_{5/2}$	8832.3	5.97[6]	0.5
$3d_{5/2}$	$6f_{7/2}$	582.78	4.80[8]	1.3	$4f_{5/2}$	$7d_{3/2}$	2591.80	3.34[6]	1.32	$5d_{5/2}$	$5f_{7/2}$	8832.3	8.95[7]	0.5
$3d_{3/2}$	$7p_{3/2}$	589.32	3.71[6]	1.1	$5p_{1/2}$	$7s_{1/2}$	2628.12	3.60[7]	0.22	$4f_{5/2}$	$5d_{5/2}$	8868.2	1.01[6]	0.5
$3d_{3/2}$	$7p_{1/2}$	589.49	3.62[7]	1.1	$5p_{3/2}$	$7s_{1/2}$	2640.33	7.17[7]	0.24	$4f_{7/2}$	$5d_{5/2}$	8868.4	2.03[7]	0.5
$3d_{5/2}$	$7p_{3/2}$	590.01	3.35[7]	1.0	$5p_{1/2}$	$6d_{3/2}$	2667.70	4.27[7]	1.48	$4f_{5/2}$	$5d_{3/2}$	8884.0	2.12[7]	0.5
$3d_{3/2}$	$5f_{5/2}$	627.07	7.31[8]	1.1	$5p_{3/2}$	$6d_{5/2}$	2679.52	4.98[7]	1.48	$6p_{1/2}$	$7s_{1/2}$	9374.4	2.82[7]	0.1
$3d_{5/2}$	$5f_{5/2}$	627.85	5.24[7]	1.1	$5p_{3/2}$	$6d_{3/2}$	2680.29	8.25[6]	1.44	$6p_{3/2}$	$7s_{1/2}$	9450.0	5.62[7]	0.1
$3d_{5/2}$	$5f_{7/2}$	627.85	7.86[8]	1.0	$4s_{1/2}$	$4p_{3/2}$	2699.87	2.80[8]	0.74	$6p_{1/2}$	$6d_{3/2}$	9898.3	5.52[7]	0.3
$3d_{3/2}$	$6p_{3/2}$	642.78	6.66[6]	0.9	$4s_{1/2}$	$4p_{1/2}$	2734.86	2.69[8]	0.74	$6p_{3/2}$	$6d_{5/2}$	9972.0	6.55[7]	0.3
$3d_{3/2}$	$6p_{1/2}$	643.13	6.50[7]	1.0	$4f_{5/2}$	$6g_{7/2}$	2832.58	1.17[8]	0.18	$6p_{3/2}$	$6d_{3/2}$	9982.7	1.09[7]	0.3
$3d_{5/2}$	$6p_{3/2}$	643.59	6.00[7]	0.9	$4f_{7/2}$	$6g_{7/2}$	2832.60	4.33[6]	0.20	$6f_{5/2}$	$7g_{7/2}$	13005	2.83[7]	0.9
$4s_{1/2}$	$7p_{3/2}$	693.74	2.62[7]	0.6	$4f_{7/2}$	$6g_{9/2}$	2832.60	1.21[8]	0.18	$6f_{7/2}$	$7g_{7/2}$	13005	1.05[6]	0.9
$4s_{1/2}$	$7p_{1/2}$	693.97	2.82[7]	0.6	$4f_{5/2}$	$6d_{5/2}$	3480.75	3.08[5]	1.22	$6f_{7/2}$	$7g_{9/2}$	13005	2.93[7]	0.9
$3d_{3/2}$	$4f_{5/2}$	730.60	1.16[9]	1.4	$4f_{7/2}$	$6d_{5/2}$	3480.78	6.16[6]	1.22	$5d_{3/2}$	$6p_{3/2}$	13432	2.73[6]	0.6
$3d_{5/2}$	$4f_{7/2}$	731.65	1.25[9]	1.3	$4f_{5/2}$	$6d_{3/2}$	3482.05	6.44[6]	1.20	$5d_{5/2}$	$6p_{3/2}$	13468	2.44[7]	0.7
$3d_{5/2}$	$4f_{5/2}$	731.66	8.33[7]	1.3	$4d_{3/2}$	$4f_{5/2}$	4062.36	2.87[8]	0.44	$5d_{3/2}$	$6p_{1/2}$	13587	2.66[7]	0.7
$4s_{1/2}$	$6p_{3/2}$	769.02	3.60[7]	0.7	$4d_{5/2}$	$4f_{7/2}$	4069.81	3.07[8]	0.44	$6s_{1/2}$	$6p_{3/2}$	15671	1.65[7]	0.2
$4s_{1/2}$	$6p_{1/2}$	769.52	3.93[7]	0.6	$4d_{5/2}$	$4f_{5/2}$	4069.85	2.04[7]	0.44	$6s_{1/2}$	$6p_{1/2}$	15884	1.59[7]	0.2
$3d_{3/2}$	$5p_{3/2}$	779.53	1.38[7]	0.8	$4f_{5/2}$	$5g_{7/2}$	4310.66	3.44[8]	0.30	$6d_{3/2}$	$6f_{5/2}$	16142	3.04[7]	0.4
$3d_{3/2}$	$5p_{1/2}$	780.60	1.35[8]	0.9	$4f_{7/2}$	$5g_{7/2}$	4310.71	1.27[7]	0.30	$6d_{5/2}$	$6f_{5/2}$	16170	2.16[6]	0.5
$3d_{5/2}$	$5p_{3/2}$	780.73	1.24[8]	0.8	$4f_{7/2}$	$5g_{9/2}$	4310.71	3.56[8]	0.30	$6d_{5/2}$	$6f_{7/2}$	16170	3.25[7]	0.4
$4p_{1/2}$	$7s_{1/2}$	961.05	6.78[7]	0.2	$5d_{3/2}$	$7p_{3/2}$	4639.11	6.99[5]	0.90	$5f_{5/2}$	$6d_{5/2}$	16310	6.14[5]	0.4
$4p_{3/2}$	$7s_{1/2}$	965.45	1.35[8]	0.1	$5d_{5/2}$	$7p_{3/2}$	4643.44	6.23[6]	0.90	$5f_{7/2}$	$6d_{5/2}$	16310	1.23[7]	0.4
$4s_{1/2}$	$5p_{3/2}$	973.29	3.42[7]	1.2	$5d_{3/2}$	$7p_{1/2}$	4649.45	6.66[6]	0.94	$5f_{5/2}$	$6d_{3/2}$	16339	1.29[7]	0.4
$4s_{1/2}$	$5p_{1/2}$	974.96	3.88[7]	0.7	$5p_{1/2}$	$6s_{1/2}$	4742.28	7.98[7]	0.36	$7p_{1/2}$	$7d_{3/2}$	17185	2.10[7]	0.4
$4p_{1/2}$	$6s_{1/2}$	1148.24	1.28[8]	0.2	$5p_{3/2}$	$6s_{1/2}$	4782.20	1.60[8]	0.26	$7p_{3/2}$	$7d_{5/2}$	17308	2.50[7]	0.3
$4p_{3/2}$	$6s_{1/2}$	1154.52	2.56[8]	0.2	$5p_{1/2}$	$5d_{3/2}$	4994.28	1.82[8]	0.28	$7p_{3/2}$	$7d_{3/2}$	17328	4.16[6]	0.3
$4d_{3/2}$	$7f_{5/2}$	1493.49	9.85[6]	1.3	$5f_{5/2}$	$7g_{7/2}$	4998.75	4.58[7]	0.14	$6d_{3/2}$	$7p_{3/2}$	24430	1.14[6]	0.6
$4d_{5/2}$	$7f_{5/2}$	1494.51	7.14[5]	1.5	$5f_{7/2}$	$7g_{7/2}$	4998.75	1.70[6]	0.14	$6d_{5/2}$	$7p_{3/2}$	24494	1.02[7]	0.6
$4d_{5/2}$	$7f_{7/2}$	1494.51	1.07[7]	1.4	$5f_{7/2}$	$7g_{9/2}$	4998.75	4.75[7]	0.14	$6d_{3/2}$	$7p_{1/2}$	24719	1.11[7]	0.6
$3d_{3/2}$	$4p_{3/2}$	1598.00	4.29[7]	1.1	$6p_{1/2}$	$7d_{3/2}$	5008.20	1.67[7]	1.10	$7d_{3/2}$	$7f_{5/2}$	26612	1.30[7]	0.4
$3d_{5/2}$	$4p_{3/2}$	1603.06	3.85[8]	1.0	$6p_{3/2}$	$7d_{5/2}$	5028.07	1.96[7]	1.10	$7d_{5/2}$	$7f_{5/2}$	26659	9.24[5]	0.4
$3d_{3/2}$	$4p_{1/2}$	1610.19	4.23[8]	1.1	$6p_{3/2}$	$7d_{3/2}$	5029.72	3.25[6]	1.08	$7d_{5/2}$	$7f_{7/2}$	26659	1.39[7]	0.4
$4d_{3/2}$	$7p_{3/2}$	1741.30	1.12[6]	0.6	$5p_{3/2}$	$5d_{5/2}$	5033.48	2.16[8]	0.26	$6f_{5/2}$	$7d_{5/2}$	27204	3.34[5]	0.3
$4d_{5/2}$	$7p_{3/2}$	1742.68	9.98[6]	0.7	$5p_{3/2}$	$5d_{3/2}$	5038.58	3.59[7]	0.24	$6f_{7/2}$	$7d_{5/2}$	27204	6.68[6]	0.3
$4d_{3/2}$	$7p_{1/2}$	1742.76	1.07[7]	0.8	$4d_{3/2}$	$5p_{3/2}$	6240.04	7.68[6]	0.72	$6f_{5/2}$	$7d_{3/2}$	27253	6.99[6]	0.3
$5s_{1/2}$	$7p_{3/2}$	1824.04	2.90[6]	1.2	$5f_{5/2}$	$7d_{5/2}$	6253.39	2.08[5]	1.12	$7s_{1/2}$	$7p_{3/2}$	28339	6.14[6]	0.1
$5s_{1/2}$	$7p_{1/2}$	1825.63	3.34[6]	0.4	$5f_{7/2}$	$7d_{5/2}$	6253.39	4.16[6]	1.10	$7s_{1/2}$	$7p_{1/2}$	28729	5.91[6]	0.1
$4p_{1/2}$	$5s_{1/2}$	1895.44	3.11[8]	0.7	$5f_{5/2}$	$7d_{3/2}$	6255.95	4.35[6]	1.10	$5f_{5/2}$	$5g_{7/2}$	166683	1.08[4]	0.1
$4p_{3/2}$	$5s_{1/2}$	1912.62	6.22[8]	0.6	$4d_{5/2}$	$5p_{3/2}$	6257.74	6.88[7]	0.76	$5f_{7/2}$	$5g_{7/2}$	166683	4.01[2]	0.1
$4p_{1/2}$	$4d_{3/2}$	1993.89	8.78[8]	0.4	$4d_{3/2}$	$5p_{1/2}$	6309.35	7.51[7]	0.74	$5f_{7/2}$	$5g_{9/2}$	166683	1.12[4]	0.1
$4p_{3/2}$	$4d_{5/2}$	2011.07	1.04[9]	0.4	$6d_{3/2}$	$7f_{5/2}$	7340.99	3.26[6]	1.14	$6f_{5/2}$	$6g_{7/2}$	256562	9.48[3]	0.1
$4p_{3/2}$	$4d_{3/2}$	2012.91	1.73[8]	0.4	$6d_{5/2}$	$7f_{5/2}$	7346.78	2.29[5]	1.30	$6f_{7/2}$	$6g_{7/2}$	256562	3.51[2]	0.1
$4d_{3/2}$	$6p_{3/2}$	2308.53	2.08[6]	1.3	$6d_{5/2}$	$7f_{7/2}$	7346.78	3.44[6]	1.26	$6f_{7/2}$	$6g_{9/2}$	256562	9.83[3]	0.1
$4d_{5/2}$	$6p_{3/2}$	2310.95	1.86[7]	1.4	$5s_{1/2}$	$5p_{3/2}$	7451.19	5.67[7]	0.36	$7f_{5/2}$	$7g_{7/2}$	380894	6.49[3]	0.1
$4d_{3/2}$	$6p_{1/2}$	2313.09	2.00[7]	1.2	$5s_{1/2}$	$5p_{1/2}$	7550.22	5.46[7]	0.34	$7f_{7/2}$	$7g_{7/2}$	380894	2.40[2]	0.1
$4f_{5/2}$	$7g_{7/2}$	2347.23	5.62[7]	0.4	$5f_{5/2}$	$6g_{7/2}$	7870.81	8.64[7]	0.62	$7f_{7/2}$	$7g_{9/2}$	380894	6.73[3]	0.1

from the breakdown for $E1$ transitions. Terms $Z^{(a)}$ and $Z^{(c)}$ described by Eqs. (3) and (4) are an order of magnitude smaller than a number of other terms. Therefore, our procedure for estimating the uncertainty described in Sec. III A can not be applied. The contribution of this transition to the $4s$ lifetime is negligible. For all three $E2$ transitions considered here, the term $Z^{(c)}$ strongly dominates. Therefore, we can use the uncertainty estimate procedure described in Sec. III A.

TABLE V. Line strengths S (a.u.) in Sc III calculated using our recommended values of reduced electric-dipole matrix elements are compared with data from the NIST compilation [38]. The relative uncertainties of the final values are listed in column "Unc." in %. Lowest-order DF values are listed in column "DF". The vacuum wavelengths λ in Å from the NIST compilation [38] are listed for reference. Numbers in brackets represent powers of 10.

Transition		λ	Line strengths (a.u.)			Unc.	Transition		λ	Line strengths (a.u.)			Unc.
Lower	Upper	NIST	Final	DF	NIST	(%)	Lower	Upper	NIST	Final	DF	NIST	(%)
$4p_{1/2}$	$7s_{1/2}$	961.05	5.94[−2]	5.56[−2]	5.3[−2]	0.2	$4s_{1/2}$	$7p_{3/2}$	693.74	1.72[−2]	6.70[−3]	7.9[−3]	0.6
$4p_{3/2}$	$7s_{1/2}$	965.45	1.20[−1]	1.13[−1]	1.1[−1]	0.1	$4s_{1/2}$	$7p_{1/2}$	693.97	9.30[−3]	3.80[−3]	4.0[−3]	0.6
$4p_{1/2}$	$6s_{1/2}$	1148.24	1.92[−1]	1.84[−1]	1.6[−1]	0.2	$4s_{1/2}$	$6p_{3/2}$	769.02	3.24[−2]	1.25[−2]	1.4[−2]	0.7
$4p_{3/2}$	$6s_{1/2}$	1154.52	3.89[−1]	3.74[−1]	3.5[−1]	0.2	$4s_{1/2}$	$6p_{1/2}$	769.52	1.77[−2]	7.20[−3]	7.2[−3]	0.6
$4p_{1/2}$	$5s_{1/2}$	1895.44	2.09[0]	2.13[0]	2.0[0]	0.7	$4p_{1/2}$	$6d_{3/2}$	966.29	5.74[−2]	1.15[−1]	1.0[−1]	6.2
$4p_{3/2}$	$5s_{1/2}$	1912.62	4.30[0]	4.37[0]	4.0[0]	0.6	$4p_{3/2}$	$6d_{5/2}$	970.64	9.93[−2]	2.02[−1]	1.8[−1]	6.3
$4p_{1/2}$	$4d_{3/2}$	1993.89	1.37[1]	1.53[1]	1.5[1]	0.4	$4p_{3/2}$	$6d_{3/2}$	970.74	1.09[−2]	2.23[−2]	2.0[−2]	6.2
$4p_{3/2}$	$4d_{5/2}$	2011.07	2.50[1]	2.77[1]	2.6[1]	0.4	$4s_{1/2}$	$5p_{3/2}$	973.29	6.22[−2]	2.00[−2]	3.1[−2]	1.2
$4p_{3/2}$	$4d_{3/2}$	2012.91	2.78[0]	3.09[0]	2.9[0]	0.4	$4s_{1/2}$	$5p_{1/2}$	974.96	3.55[−2]	1.25[−2]	1.5[−2]	0.7
$4d_{3/2}$	$6p_{3/2}$	2308.53	5.06[−2]	4.72[−2]	4.1[−2]	1.3	$4p_{1/2}$	$5d_{3/2}$	1162.44	3.54[−1]	5.54[−1]	5.0[−1]	3.9
$4d_{5/2}$	$6p_{3/2}$	2310.95	4.53[−1]	4.22[−1]	3.9[−1]	1.4	$4p_{3/2}$	$5d_{5/2}$	1168.61	6.24[−1]	9.82[−1]	9.0[−1]	3.9
$4d_{3/2}$	$6p_{1/2}$	2313.09	2.44[−1]	2.27[−1]	2.1[−1]	1.2	$4p_{3/2}$	$5d_{3/2}$	1168.88	6.86[−2]	1.08[−1]	1.0[−1]	3.8
$5p_{1/2}$	$7s_{1/2}$	2628.11	6.45[−1]	6.48[−1]	6.3[−1]	0.2	$5p_{1/2}$	$7d_{3/2}$	2111.94	3.21[−1]	4.22[−1]	3.9[−1]	2.2
$5p_{3/2}$	$7s_{1/2}$	2640.33	1.30[0]	1.31[0]	1.3[0]	0.2	$5p_{3/2}$	$7d_{5/2}$	2119.52	5.63[−1]	7.44[−1]	6.8[−1]	2.2
$4f_{5/2}$	$6d_{5/2}$	3480.75	3.85[−2]	4.26[−2]	3.1[−2]	1.2	$5p_{3/2}$	$7d_{3/2}$	2119.82	6.21[−2]	8.21[−2]	7.7[−2]	2.1
$4f_{7/2}$	$6d_{5/2}$	3480.78	7.69[−1]	8.53[−1]	6.2[−1]	1.2	$5s_{1/2}$	$6p_{1/2}$	2461.40	2.56[−2]	1.33[−2]	1.5[−2]	2.7
$4f_{5/2}$	$6d_{3/2}$	3482.05	5.37[−1]	5.96[−1]	4.4[−1]	1.2	$5p_{1/2}$	$6d_{3/2}$	2667.71	1.60[0]	1.92[0]	1.8[0]	1.5
$4d_{3/2}$	$4f_{5/2}$	4062.35	5.71[1]	6.33[1]	5.8[1]	0.4	$5p_{3/2}$	$6d_{5/2}$	2679.52	2.84[0]	3.42[0]	3.2[0]	1.5
$4d_{5/2}$	$4f_{7/2}$	4069.81	8.16[1]	9.05[1]	8.3[1]	0.4	$5p_{3/2}$	$6d_{3/2}$	2680.29	3.14[−1]	3.78[−1]	3.6[−1]	1.4
$4d_{5/2}$	$4f_{5/2}$	4069.85	4.08[0]	4.53[0]	4.2[0]	0.4	$4s_{1/2}$	$4p_{3/2}$	2699.86	1.09[1]	1.33[1]	1.33[1]	0.7
$5d_{3/2}$	$7p_{3/2}$	4639.10	1.38[−1]	1.21[−1]	1.1[−1]	0.9	$4s_{1/2}$	$4p_{1/2}$	2734.86	5.44[0]	6.67[0]	6.7[0]	0.7
$5d_{5/2}$	$7p_{3/2}$	4643.43	1.23[0]	1.08[0]	1.0[0]	0.9							
$5d_{3/2}$	$7p_{1/2}$	4649.45	6.61[−1]	5.79[−1]	5.7[−1]	0.9	$3d_{3/2}$	$5f_{5/2}$	627.07	5.33[−1]	8.02[−1]	5.8[−1]	1.1
$5p_{1/2}$	$6s_{1/2}$	4742.28	8.40[0]	8.68[0]	8.4[0]	0.4	$3d_{5/2}$	$5f_{5/2}$	627.85	3.84[−2]	5.76[−2]	4.3[−2]	1.0
$5p_{3/2}$	$6s_{1/2}$	4782.19	1.72[1]	1.78[1]	1.6[1]	0.3	$3d_{5/2}$	$5f_{7/2}$	627.85	7.68[−1]	1.15[0]	8.4[−1]	1.0
$5p_{1/2}$	$5d_{3/2}$	4994.28	4.48[1]	4.55[1]	4.5[1]	0.3	$3d_{3/2}$	$4f_{5/2}$	730.60	1.34[0]	1.97[0]	1.4[0]	1.4
$6p_{1/2}$	$7d_{3/2}$	5008.21	4.15[0]	4.67[0]	4.5[0]	1.1	$3d_{5/2}$	$4f_{5/2}$	731.66	9.67[−2]	1.42[−1]	1.0[−1]	1.3
$6p_{3/2}$	$7d_{5/2}$	5028.06	7.38[0]	8.32[0]	7.9[0]	1.1	$3d_{5/2}$	$4f_{7/2}$	731.65	1.93[0]	2.84[0]	2.0[0]	1.3
$6p_{3/2}$	$7d_{3/2}$	5029.73	8.17[−1]	9.21[−1]	8.8[−1]	1.1	$3d_{3/2}$	$5p_{3/2}$	779.53	1.29[−2]	1.71[−2]	1.3[−2]	0.8
$5p_{3/2}$	$5d_{5/2}$	5033.47	8.15[1]	8.28[1]	7.9[1]	0.3	$3d_{3/2}$	$5p_{1/2}$	780.60	6.33[−2]	8.44[−2]	6.6[−2]	0.9
$5p_{3/2}$	$5d_{3/2}$	5038.57	9.07[0]	9.22[0]	9.1[0]	0.2	$3d_{5/2}$	$5p_{3/2}$	780.73	1.16[−1]	1.54[−1]	1.2[−1]	0.8
$4d_{3/2}$	$5p_{3/2}$	6240.05	3.69[0]	4.13[0]	3.6[0]	0.7	$4d_{3/2}$	$7f_{5/2}$	1493.49	9.72[−2]	1.15[−1]	9.2[−2]	1.3
$5f_{5/2}$	$7d_{5/2}$	6253.40	1.51[−1]	1.68[−1]	1.5[−1]	1.1	$4d_{5/2}$	$7f_{5/2}$	1494.50	7.10[−3]	8.30[−3]	6.6[−3]	1.5
$5f_{7/2}$	$7d_{5/2}$	6253.40	3.01[0]	3.36[0]	3.0[0]	1.1	$4d_{5/2}$	$7f_{7/2}$	1494.50	1.41[−1]	1.67[−1]	1.3[−1]	1.4
$5f_{5/2}$	$7d_{3/2}$	6255.94	2.10[0]	2.34[0]	2.1[0]	1.1	$3d_{3/2}$	$4p_{3/2}$	1598.00	3.45[−1]	4.66[−1]	3.7[−1]	1.1
$4d_{5/2}$	$5p_{3/2}$	6257.74	3.33[1]	3.73[1]	3.2[1]	0.8	$3d_{5/2}$	$4p_{3/2}$	1603.07	3.13[0]	4.22[0]	3.3[0]	1.0
$4d_{3/2}$	$5p_{1/2}$	6309.35	1.86[1]	2.08[1]	1.8[1]	0.7	$3d_{3/2}$	$4p_{1/2}$	1610.19	1.74[0]	2.36[0]	1.8[0]	1.1
$5s_{1/2}$	$5p_{3/2}$	7451.18	4.63[1]	4.93[1]	4.7[1]	0.4	$4d_{3/2}$	$6f_{5/2}$	1679.83	1.07[−1]	1.40[−1]	8.8[−2]	2.3
$5s_{1/2}$	$5p_{1/2}$	7550.25	2.32[1]	2.47[1]	2.3[1]	0.3	$4d_{5/2}$	$6f_{5/2}$	1681.10	7.80[−3]	1.02[−2]	6.3[−3]	2.5
$5d_{3/2}$	$5f_{5/2}$	8816.63	1.70[2]	1.84[2]	1.7[2]	0.5	$4d_{5/2}$	$6f_{7/2}$	1681.10	1.56[−1]	2.05[−1]	1.3[−1]	2.5
$5d_{5/2}$	$5f_{5/2}$	8832.28	1.22[1]	1.32[1]	1.2[1]	0.5	$5s_{1/2}$	$6p_{3/2}$	2456.24	3.86[−2]	1.80[−2]	2.9[−2]	3.7
$5d_{5/2}$	$5f_{7/2}$	8832.28	2.43[2]	2.63[2]	2.4[2]	0.5	$5d_{3/2}$	$6f_{5/2}$	4226.97	8.43[−1]	5.85[−1]	9.6[−1]	2.2
$4f_{5/2}$	$5d_{5/2}$	8868.16	2.09[0]	1.99[0]	2.0[0]	0.5	$5d_{5/2}$	$6f_{5/2}$	4230.57	5.79[−2]	4.07[−2]	7.0[−2]	3.4
$4f_{7/2}$	$5d_{5/2}$	8868.39	4.18[1]	3.98[1]	4.1[1]	0.5	$6d_{3/2}$	$7f_{5/2}$	7340.96	3.81[0]	3.06[0]	4.0[0]	1.1
$4f_{5/2}$	$5d_{3/2}$	8883.99	2.94[1]	2.79[1]	2.8[1]	0.5	$6d_{5/2}$	$7f_{5/2}$	7346.78	2.70[−1]	2.15[−1]	2.8[−1]	1.3
$6p_{1/2}$	$7s_{1/2}$	9374.36	2.29[1]	2.37[1]	2.3[1]	0.1	$6d_{5/2}$	$7f_{7/2}$	7346.78	5.39[0]	4.30[0]	5.6[0]	1.3
$6p_{3/2}$	$7s_{1/2}$	9450.01	4.69[1]	4.85[1]	4.6[1]	0.1							

The present values are compared with CCSDpT calculations of Ref. [14]. Our values for the electric-quadrupole matrix elements are in agreement with the results of Ref. [14].

We combine recommended NIST energies [38] and our final values of the matrix elements listed in Table VIII to calculate transition rates A_r as

$$A(M1) = \frac{2.69735 \times 10^{13}}{(2J+1)\lambda^3} S(M1),$$
$$A(E2) = \frac{1.11995 \times 10^{18}}{(2J+1)\lambda^5} S(E2), \quad (7)$$

TABLE VI. Oscillator strengths f in Sc III calculated using our recommended values of reduced electric-dipole matrix elements are compared with WBEPM semiempirical results [15]. The relative uncertainties of the final values are listed in column "Unc." in %. Lowest-order DF values are listed in column "DF". The vacuum wavelengths λ in Å from the NIST compilation [38] are listed for reference. Numbers in brackets represent powers of 10.

Transition		λ	Oscillator strengths			Unc.	Transition		λ	Oscillator strengths			Unc.
Lower	Upper	NIST	Final	DF	WBEPM	(%)	Lower	Upper	NIST	Final	DF	WBEPM	(%)
$4p_{1/2}$	$7s_{1/2}$	961.05	9.39[−3]	8.79[−3]	9.40[−3]	0.2	$4p_{1/2}$	$5s_{1/2}$	1895.44	1.67[−1]	1.70[−1]	1.25[−1]	0.7
$4p_{3/2}$	$7s_{1/2}$	965.45	9.45[−3]	8.85[−3]	9.51[−3]	0.1	$4p_{3/2}$	$5s_{1/2}$	1912.62	1.71[−1]	1.74[−1]	1.28[−1]	0.6
$4p_{1/2}$	$6s_{1/2}$	1148.24	2.54[−2]	2.44[−2]	2.36[−2]	0.2	$4p_{1/2}$	$4d_{3/2}$	1993.89	1.05[0]	1.16[0]	9.29[−1]	0.4
$4p_{3/2}$	$6s_{1/2}$	1154.52	2.56[−2]	2.46[−2]	2.40[−2]	0.2	$4p_{3/2}$	$4d_{5/2}$	2011.07	9.44[−1]	1.05[0]	8.40[−1]	0.4
$4f_{5/2}$	$7g_{7/2}$	2347.23	6.19[−2]	6.19[−2]	6.54[−2]	0.4	$4p_{3/2}$	$4d_{3/2}$	2012.91	1.05[−1]	1.16[−1]	9.33[−2]	0.4
$4f_{7/2}$	$7g_{7/2}$	2347.25	1.72[−3]	1.72[−3]	1.82[−3]	0.4	$4d_{3/2}$	$6p_{3/2}$	2308.53	1.66[−3]	1.55[−3]	2.15[−3]	1.3
$4f_{7/2}$	$7g_{9/2}$	2347.25	6.02[−2]	6.02[−2]	6.35[−2]	0.4	$4d_{5/2}$	$6p_{3/2}$	2310.95	9.91[−3]	9.25[−3]	1.29[−2]	1.4
$5p_{1/2}$	$7s_{1/2}$	2628.11	3.73[−2]	3.74[−2]	4.01[−2]	0.2	$4d_{3/2}$	$6p_{1/2}$	2313.09	8.01[−3]	7.46[−3]	1.05[−2]	1.2
$5p_{3/2}$	$7s_{1/2}$	2640.33	3.75[−2]	3.77[−2]	4.02[−2]	0.2	$4f_{5/2}$	$6d_{5/2}$	3480.75	5.59[−4]	6.20[−4]	3.78[−4]	1.2
$4f_{5/2}$	$6g_{7/2}$	2832.58	1.88[−1]	1.90[−1]	1.96[−1]	0.2	$4f_{7/2}$	$6d_{5/2}$	3480.78	8.39[−3]	9.30[−3]	5.67[−3]	1.2
$4f_{7/2}$	$6g_{7/2}$	2832.60	5.21[−3]	5.29[−3]	5.45[−3]	0.2	$4f_{5/2}$	$6d_{3/2}$	3482.05	7.80[−3]	8.66[−3]	5.26[−3]	1.2
$4f_{7/2}$	$6g_{9/2}$	2832.60	1.82[−1]	1.85[−1]	1.91[−1]	0.2	$5d_{3/2}$	$7p_{3/2}$	4639.10	2.26[−3]	1.99[−3]	2.78[−3]	0.9
$4d_{3/2}$	$4f_{5/2}$	4062.35	1.07[0]	1.18[0]	1.06[0]	0.4	$5d_{5/2}$	$7p_{3/2}$	4643.43	1.34[−2]	1.18[−2]	1.66[−2]	0.9
$4d_{5/2}$	$4f_{7/2}$	4069.81	1.02[0]	1.13[0]	1.01[0]	0.4	$5d_{3/2}$	$7p_{1/2}$	4649.45	1.08[−2]	9.45[−3]	1.34[−2]	0.9
$4d_{5/2}$	$4f_{5/2}$	4069.85	5.08[−2]	5.63[−2]	5.06[−2]	0.4	$5f_{5/2}$	$7d_{5/2}$	6253.40	1.22[−3]	1.36[−3]	9.16[−4]	1.1
$4f_{5/2}$	$5g_{7/2}$	4310.66	1.28[0]	1.37[0]	1.32[0]	0.3	$5f_{7/2}$	$7d_{5/2}$	6253.40	1.83[−2]	2.04[−2]	1.37[−2]	1.1
$4f_{7/2}$	$5g_{7/2}$	4310.71	3.55[−2]	3.80[−2]	3.66[−2]	0.3	$5f_{5/2}$	$7d_{3/2}$	6255.94	1.70[−2]	1.90[−2]	1.28[−2]	1.1
$4f_{7/2}$	$5g_{9/2}$	4310.71	1.24[0]	1.33[0]	1.28[0]	0.3							
$5p_{1/2}$	$6s_{1/2}$	4742.28	2.69[−1]	2.78[−1]	2.34[−1]	0.4	$4p_{1/2}$	$6d_{3/2}$	966.29	9.02[−3]	1.81[−2]	1.94[−2]	6.2
$5p_{3/2}$	$6s_{1/2}$	4782.19	2.73[−1]	2.83[−1]	2.39[−1]	0.3	$4p_{3/2}$	$6d_{5/2}$	970.64	7.77[−3]	1.58[−2]	1.71[−2]	6.3
$5p_{1/2}$	$5d_{3/2}$	4994.28	1.36[0]	1.38[0]	1.27[0]	0.3	$4p_{3/2}$	$6d_{3/2}$	970.74	8.51[−4]	1.74[−3]	1.89[−3]	6.2
$5f_{5/2}$	$7g_{7/2}$	4998.75	2.29[−1]	2.35[−1]	2.35[−1]	0.1	$4s_{1/2}$	$5p_{3/2}$	973.29	9.71[−3]	3.12[−3]	5.20[−3]	1.2
$5f_{7/2}$	$7g_{7/2}$	4998.75	6.35[−3]	6.53[−3]	6.54[−3]	0.1	$4s_{1/2}$	$5p_{1/2}$	974.96	5.52[−3]	1.95[−3]	3.05[−3]	0.7
$5f_{7/2}$	$7g_{9/2}$	4998.75	2.22[−1]	2.29[−1]	2.29[−1]	0.1	$4p_{1/2}$	$5d_{3/2}$	1162.44	4.63[−2]	7.24[−2]	6.04[−2]	3.9
$6p_{1/2}$	$7d_{3/2}$	5008.21	1.26[−1]	1.42[−1]	1.19[−1]	1.1	$4p_{3/2}$	$5d_{5/2}$	1168.61	4.05[−2]	6.38[−2]	5.35[−2]	3.9
$6p_{3/2}$	$7d_{5/2}$	5028.06	1.11[−1]	1.26[−1]	1.06[−1]	1.1	$4p_{3/2}$	$5d_{3/2}$	1168.88	4.46[−3]	7.05[−3]	5.91[−3]	3.8
$6p_{3/2}$	$7d_{3/2}$	5029.73	1.23[−2]	1.39[−2]	1.17[−2]	1.1	$4d_{3/2}$	$7f_{5/2}$	1493.49	4.94[−3]	5.84[−3]	4.18[−3]	1.3
$5p_{3/2}$	$5d_{5/2}$	5033.47	1.23[0]	1.25[0]	1.15[0]	0.3	$4d_{5/2}$	$7f_{5/2}$	1494.50	2.39[−4]	2.82[−4]	2.03[−4]	1.5
$5p_{3/2}$	$5d_{3/2}$	5038.57	1.37[−1]	1.39[−1]	1.27[−1]	0.2	$4d_{5/2}$	$7f_{7/2}$	1494.50	4.78[−3]	5.65[−3]	4.05[−3]	1.4
$4d_{3/2}$	$5p_{3/2}$	6240.05	4.49[−2]	5.03[−2]	4.49[−2]	0.7	$4d_{3/2}$	$6f_{5/2}$	1679.83	4.83[−3]	6.32[−3]	3.19[−3]	2.3
$4d_{5/2}$	$5p_{3/2}$	6257.74	2.69[−1]	3.02[−1]	2.69[−1]	0.8	$4d_{5/2}$	$6f_{5/2}$	1681.10	2.35[−4]	3.08[−4]	1.56[−4]	2.5
$4d_{3/2}$	$5p_{1/2}$	6309.35	2.24[−1]	2.51[−1]	2.24[−1]	0.7	$4d_{5/2}$	$6f_{7/2}$	1681.10	4.70[−3]	6.16[−3]	3.13[−3]	2.5
$5s_{1/2}$	$5p_{3/2}$	7451.18	9.44[−1]	1.00[0]	9.49[−1]	0.4	$5p_{1/2}$	$7d_{3/2}$	2111.94	2.31[−2]	3.03[−2]	2.73[−2]	2.2
$5s_{1/2}$	$5p_{1/2}$	7550.25	4.67[−1]	4.97[−1]	4.69[−1]	0.3	$5p_{3/2}$	$7d_{5/2}$	2119.52	2.02[−2]	2.67[−2]	2.41[−2]	2.2
$5f_{5/2}$	$6g_{7/2}$	7870.81	1.07[0]	1.18[0]	1.08[0]	0.6	$5p_{3/2}$	$7d_{3/2}$	2119.82	2.22[−3]	2.94[−3]	2.66[−3]	2.1
$5f_{7/2}$	$6g_{7/2}$	7870.81	2.97[−2]	3.27[−2]	3.01[−2]	0.6	$5p_{1/2}$	$6d_{3/2}$	2667.71	9.11[−2]	1.09[−1]	8.97[−2]	1.5
$5f_{7/2}$	$6g_{9/2}$	7870.81	1.04[0]	1.14[0]	1.05[0]	0.6	$5p_{3/2}$	$6d_{5/2}$	2679.52	8.04[−2]	9.69[−2]	7.95[−2]	1.5
$5d_{3/2}$	$5f_{5/2}$	8816.63	1.47[0]	1.58[0]	1.45[0]	0.5	$5p_{3/2}$	$6d_{3/2}$	2680.29	8.89[−3]	1.07[−2]	8.80[−3]	1.4
$5d_{5/2}$	$5f_{5/2}$	8832.28	6.98[−2]	7.55[−2]	6.90[−2]	0.5	$4s_{1/2}$	$4p_{3/2}$	2699.86	6.13[−1]	7.50[−1]	6.56[−1]	0.7
$5d_{5/2}$	$5f_{7/2}$	8832.28	1.40[0]	1.51[0]	1.38[0]	0.5	$4s_{1/2}$	$4p_{1/2}$	2734.86	3.02[−1]	3.70[−1]	3.24[−1]	0.7
$4f_{5/2}$	$5d_{5/2}$	8868.16	1.19[−2]	1.13[−2]	1.21[−2]	0.5							
$4f_{7/2}$	$5d_{5/2}$	8868.39	1.79[−1]	1.70[−1]	1.81[−1]	0.5	$5d_{3/2}$	$6f_{5/2}$	4226.97	1.51[−2]	1.05[−2]	2.51[−2]	2.2
$4f_{5/2}$	$5d_{3/2}$	8883.99	1.67[−1]	1.59[−1]	1.69[−1]	0.5	$5d_{5/2}$	$6f_{5/2}$	4230.57	6.93[−4]	4.87[−4]	1.18[−3]	3.4
$6p_{1/2}$	$7s_{1/2}$	9374.36	3.71[−1]	3.84[−1]	3.40[−1]	0.1	$5d_{5/2}$	$6f_{7/2}$	4230.57	1.41[−2]	9.73[−3]	2.35[−2]	2.4
$6p_{3/2}$	$7s_{1/2}$	9450.01	3.77[−1]	3.90[−1]	3.45[−1]	0.1	$6d_{3/2}$	$7f_{5/2}$	7340.96	3.95[−2]	3.16[−2]	5.35[−2]	1.1
$6f_{5/2}$	$7g_{7/2}$	13004.6	9.55[−1]	1.08[0]	9.60[−1]	0.9	$6d_{5/2}$	$7f_{5/2}$	7346.78	1.86[−3]	1.48[−3]	2.52[−3]	1.3
$6f_{7/2}$	$7g_{7/2}$	13004.6	2.65[−2]	3.00[−2]	2.67[−2]	0.9	$6d_{5/2}$	$7f_{7/2}$	7346.78	3.71[−2]	2.96[−2]	5.04[−2]	1.3
$6f_{7/2}$	$7g_{9/2}$	13004.6	9.28[−1]	1.05[0]	9.33[−1]	0.9							

where the wavelength λ is in Å and the line strength $S = d^2$ is in atomic units. Transition rates A_r (in s^{-1}) for the $M1$ $3d_{3/2}$-$3d_{5/2}$ and $3d_{3/2}$-$4s_{1/2}$ transitions and the $E2$ $3d_{3/2}$-$3d_{5/2}$, $3d_{3/2}$-$4s_{1/2}$, and $3d_{5/2}$-$4s_{1/2}$ transitions in Sc III are summarized in Table IX. Final lifetimes of the $3d_{5/2}$ and $4s$ levels are also given (in s). Uncertainties are given in parentheses.

Our transition rate and lifetime values are compared with CCSDpT results presented by Nandy *et al.* [14]. The only substantial difference between our final results and

TABLE VII. Lifetimes ($\tau^{\rm final}$ in ns) of nl_j states in Sc III. Uncertainties are given in parentheses. Recommended NIST energies are given in $\rm cm^{-1}$. The values of lifetimes evaluated in the DF approximation are given in column $\tau^{\rm DF}$ to illustrate the correlation contribution. The present values are compared with CCSDpT calculations of Ref. [14]. Experimental values from Refs. [19] (superscript *a*) and [16] (*b*) are listed in the last column.

Level	Energy	$\tau^{\rm DF}$	$\tau^{\rm final}$	Ref. [14]	$\tau^{\rm expt}$
$4p_{1/2}$	62104.3	1.109	1.445(10)	1.43(2)	1.7(2)[a]
$4p_{3/2}$	62578.2	1.087	1.413(9)	1.40(3)	1.7(2)[a]
$4d_{3/2}$	112258	0.857	0.951(3)	0.95(1)	1.2[b]
$4d_{5/2}$	112303	0.870	0.962(4)	0.96(3)	1.2[b]
$5s_{1/2}$	114863	1.054	1.072(5)	1.08(2)	1.4
$5p_{1/2}$	128107	2.977	3.295(15)	3.32(2)	3.6[b]
$5p_{3/2}$	128283	2.946	3.277(13)	3.31(3)	3.6[b]
$4f_{5/2}$	136874	0.460	0.645(7)	0.61(1)	
$4f_{7/2}$	136874	0.459	0.642(7)	0.63(2)	
$5d_{3/2}$	148130	2.197	2.667(32)	2.56(1)	2.4[b]
$5d_{5/2}$	148150	2.236	2.708(38)	2.63(1)	2.4[b]
$6s_{1/2}$	149194	1.622	1.603(02)	1.66(1)	
$6p_{1/2}$	155490	5.794	5.933(27)	6.32(9)	
$6p_{3/2}$	155575	5.773	5.942(24)	6.33(8)	
$5f_{5/2}$	159472	0.784	1.145(10)		
$5f_{7/2}$	159472	0.783	1.142(11)		
$5g_{7/2}$	160072	2.620	2.803(8)		
$5g_{9/2}$	160072	2.625	2.809(8)		
$6d_{3/2}$	165593	4.480	5.727(70)		
$6d_{5/2}$	165603	4.565	5.835(83)		
$7s_{1/2}$	166157	2.590	2.532(2)		
$7p_{1/2}$	169638	9.949	9.779(43)		
$7p_{3/2}$	169686	9.953	9.813(39)		
$6f_{5/2}$	171788	1.263	1.908(85)		
$6f_{7/2}$	171788	1.265	1.911(24)		
$6g_{7/2}$	172177	4.504	4.741(13)		
$6g_{9/2}$	172177	4.512	4.748(13)		
$7d_{3/2}$	175457	7.900	10.467(23)		
$7d_{5/2}$	175464	8.068	10.669(45)		
$7f_{5/2}$	179215	1.923	2.981(33)		
$7f_{7/2}$	179215	1.932	3.003(37)		
$7g_{7/2}$	179477	7.132	7.400(19)		
$7g_{9/2}$	179477	7.132	7.402(20)		

the CCSDpT results is for the $M1$ $3d_{3/2}$-$4s_{1/2}$ transition rate. For this transition, correlation correction is actually larger than the DF value. Therefore, this value is extremely sensitive to the treatment of the correlation correction which differs between our approach and that of Ref. [14]. As we noted above, the contribution of the $M1$ $3d_{3/2}$-$4s_{1/2}$ transition to the $4s$ lifetime is negligible and this difference really does not affect the lifetime value. Our values of

TABLE VIII. $E2$ and $M1$ reduced matrix elements in Sc III in atomic units calculated in different approximations. The lowest-order DF, second-order, third-order MBPT, and all-order SD and SDpT values are listed; the label "sc" indicates the scaled values. Final recommended values and their uncertainties are given in the $Z^{\rm final}$ column. The Unc. column gives relative uncertainties of the final values in %. The present values are compared with CCSDpT calculations of Ref. [14]. Absolute values are given.

Transition		$Z^{\rm DF}$	$Z^{\rm (DF+2)}$	$Z^{\rm (DF+2+3)}$	$Z^{\rm SD}$	$Z^{\rm (SD)}_{\rm sc}$	$Z^{\rm SDpT}$	$Z^{\rm SDpT}_{\rm sc}$	$Z^{\rm final}$	Unc. (%)	Ref. [14]
Magnetic-dipole transitions											
$3d_{3/2}$	$3d_{5/2}$	1.5490	1.5490	1.5423	1.5490	1.5490	1.5490	1.5490	1.5490(0)	0	1.541
$3d_{3/2}$	$4s_{1/2}$	5.11[−6]	7.25[−6]	2.52[−3]	1.31[−5]	1.30[−5]	1.29[−5]	1.30[−5]	1.30[−5]		0.001
Electric-quadrupole transitions											
$3d_{3/2}$	$3d_{5/2}$	1.9341	1.8660	1.5887	1.6278	1.6368	1.6444	1.6325	1.637(9)	0.55%	1.649
$3d_{3/2}$	$4s_{1/2}$	4.0500	4.0281	3.4572	3.5499	3.5722	3.5895	3.5627	3.57(2)	0.48%	3.589
$3d_{5/2}$	$4s_{1/2}$	4.9737	4.9464	4.2489	4.3621	4.3882	4.4106	4.3765	4.39(2)	0.51%	4.414

TABLE IX. $M1$ and $E2$ transition rates A_r (in s^{-1}) and $4s$ and $3d_{5/2}$ lifetimes τ (in s) in Sc III. Uncertainties are given in parentheses. Our values are compared with theoretical results from Ref. [14].

	Transition		Present	Ref. [14]
$A(E2)$	$3d_{3/2}$	$3d_{5/2}$	1.51(2)[−11]	1.53[−11]
$A(M1)$	$3d_{3/2}$	$3d_{5/2}$	8.3275[−5]	8.33[−5]
Lifetime (in s)	$3d_{5/2}$		12008	12135(100)
$A(E2)$	$3d_{3/2}$	$4s_{1/2}$	7.76(7)	7.83
$A(M1)$	$3d_{3/2}$	$4s_{1/2}$	3.8(1)[−8]	1.95[−4]
$A(E2)$	$3d_{5/2}$	$4s_{1/2}$	11.27(11)	11.40
Lifetime (in s)	$4s_{1/2}$		0.0525(4)	0.05(1)

the $4s$ and $3d_{5/2}$ lifetimes are in agreement with Ref. [14] results.

V. CONCLUSION

A systematic study of Sc III atomic properties is carried out using a high-precision relativistic all-order method where all single, double, and partial-triple excitations of the Dirac-Fock wave function are included to all orders of perturbation theory. Energies, $E1$, $E2$, $M1$, matrix elements, line strengths, oscillator strengths, transition rates, and lifetimes of the $3d_{5/2}$, $4s$, ns ($n = 5$–7), np_j ($n = 4$–7), nd_j ($n = 4$–7), nf_j ($n = 4$–7), and ng_j ($n = 5$–7) states are calculated. The uncertainties of our calculations are evaluated for most of the values listed in this work. These calculations provide recommended values critically evaluated for their accuracy for a number of Sr III atomic properties useful for a variety of applications.

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