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Blackbody radiation shift, multipole polarizabilities, oscillator strengths, lifetimes, hyperfine constants, and excitation energies in Hg^+

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Excitation energies of the $[Xe]4f^{14}5d^{10}ns$, $[Xe]4f^{14}5d^{10}np_j$, $[Xe]4f^{14}5d^{10}nd_j$, $[Xe]4f^{14}5d^{10}n'f_j$, and $[Xe]4f^{14}5d^{10}n'g_j$ states in Hg^+ are evaluated ($n \leqslant 10$, $n' \leqslant 9$, and $[Xe] = 1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10} 4s^2 4p^6 4d^{10} 5s^2 5p^6$). First-, second-, third-, and all-order Coulomb energies and first- and second-order Coulomb-Breit energies are calculated. Reduced matrix elements, oscillator strengths, and transition rates are determined for electric-dipole transitions, including the ns ($n = 6$–11), np ($n = 6$–10), nd ($n = 6$–10), nf ($n = 5$–9), and ng ($n = 5$–9) states. Lifetime values are determined for all above-mentioned states. The ground state $E1$, $E2$, and $E3$ polarizabilities are evaluated. The hyperfine structure in $^{199}Hg^+$ and $^{201}Hg^+$ ions is investigated. The hyperfine A and B values are determined for the first low-lying levels up to $n = 7$. The quadratic Stark effect on hyperfine structure levels of $^{199}Hg^+$ and $^{201}Hg^+$ ground states is investigated. The calculated shift for the $^{199}Hg^+$ $(F = 1, M = 0) \leftrightarrow (F = 0, M = 0)$ transition is $-0.0597(2)$ Hz/(kV/cm)^2, in agreement with previous theoretical result $-0.060(3)$ Hz/(kV/cm)^2. These calculations provide a theoretical benchmark for comparison with experiment and theory and provide values of blackbody radiation shifts for microwave frequency standards with $^{199}Hg^+$ and $^{201}Hg^+$ ions.

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I. INTRODUCTION

Mercury is among the most frequently used elements in spectral sources; therefore, investigation of atomic properties of the mercury ion could help to explain the properties of these sources, as well as continuous wave and pulsed mercury lasers [1]. Measurements of the lifetimes for the $7p_{1/2}$ and $7p_{3/2}$ levels in Hg^+ were carried out using beam-foil excitation [2]. Maniak *et al.* [2] noted that it is important to obtain the accurate values of the $7p_J$ lifetimes. The intrashell transitions to the $7s$ level give rise to the well-known He-Hg laser lines at 7944 Å and 6149 Å, and a knowledge of their transition rates and lifetimes would be useful in the study of this and other light sources that employ the mercury ion spectrum [2]. Hg^+ properties are also needed for applications to stellar atmosphere modeling [3].

Both microwave and optical frequency standards based on laser-cooled Hg^+ ions were discussed by Berkeland *et al.* [4]. The ground-state hyperfine interval was measured to be 40 507 347 996.841 59(14)(41) Hz [4], where the first number in parentheses was the uncertainty due to statistics and systematic errors, and the second was the uncertainty in the frequency of the time scale to which the standard was compared. The frequency ratio of the Al^+ and $^{199}Hg^+$ optical atomic clocks with a fractional uncertainty of 5.2×10^{-17} was reported in Ref. [5]. High-resolution spectroscopy has been performed on the ground-state hyperfine transitions in trapped $^{201}Hg^+$ ions in Ref. [6] as part of a program to investigate the viability of $^{201}Hg^+$ for clock applications. The differences between the two isotopes and how they can be exploited for fieldable clock applications, particularly those in space, was examined [6]. While present implementations of the $^{199}Hg^+$ clock were done at cryogenic temperatures, suppressing the blackbody radiation (BBR) shift [7] of the clock transition, accurate calculations of the BBR shift will be needed if clock is implemented at room temperature. Designing clocks with both isotopes may improve the limits on variations of the fine-structure constant [6]. Frequency shift of hyperfine transitions due to blackbody radiation in $^{199}Hg^+$ was investigated by Angstmann *et al.* [8] by performing calculations of the size of the frequency shift induced by a static electric field. These calculations were carried out for the clock transition frequencies of the hyperfine splitting of Yb^+, Rb, Cs, Ba^+, and Hg^+, but the uncertainty of Hg^+ value was not estimated.

The Hg^+ ion has been studied in a number of experimental [1,2,9–21] and theoretical [3,22–27] papers. The beam-foil technique was used by Andersen and Sørensen [9] to determine the radiative lifetimes of the $7s$, $9s$, $6p$, $6d$, $8d$, $9d$, and $5f$ states in Hg^+. The zero-field level-crossing technique was used by Andersen *et al.* [12] to measure the $6p_{3/2}$-$6d_{5/2}$, $6d_{3/2}$-$5f_{5/2}$, and $6d_{5/2}$-$5f_{7/2}$ transition rates in Hg^+. Lifetime measurements of the $6p_j$ and $6d_j$ levels in Hg^+ were reported by Eriksen and Poulsen in Ref. [13]. The technique of beam foil spectroscopy was applied by Pinnington *et al.* [19] to obtain measurements of the radiative lifetimes of the $6p_J$, $6d_J$, and $7s$ levels in Hg^+. The multichannel delayed-coincidence method was used by Blagoev *et al.* in Ref. [1] to determine the radiative lifetimes of the $9s$, $10s$, $7p_j$, $7d_j$, $8d_j$, $9d_{3/2}$, $5f_j$, $6g$, $7g$, $8g$, and $9g$ states.

Sansonetti and Reader [21] studied the Hg^+ spectrum and energy levels, obtaining about 500 lines classified as transitions between 114 levels. Many of the observed configurations were theoretically interpreted by means of Hartree-Fock calculations and least-squares fits of energy parameters. The fitted parameters were then used to calculate oscillator strengths for most of the classified lines [21].

Theoretical oscillator strengths in Hg^+ ion reported by Migdalek in Ref. [22] were obtained using a semiempirical approach that determined nonrelativistic and relativistic wave functions and oscillator strengths, including exchange effects. Some years later, Migdalek and Baylis [23] presented theoretical oscillator strengths in Hg$^+$ calculated by relativistic, single-configuration Hartree-Fock method that included core polarization effects. Numerical values of oscillator strengths were given in Ref. [23] for the $6s$-$6p_j$, $6p_j$-$6d_{j'}$, and $6p_j$-$7s$ transitions. The same transitions were considered by Migdalek and Garmulewicz [26] using the relativistic *ab initio* model potential. Relativistic many-body perturbation theory calculations through third order were performed by Chou and Johnson [24] to study amplitudes of the $6s$-$6p_j$ transitions in Hg$^+$. Theoretical oscillator strengths and hyperfine structure in Hg$^+$ were presented by Brage *et al.* [3]. The fully relativistic multiconfiguration Dirac-Fock methods (GRASP code) was used to calculate oscillator strengths for the $6s$-$6p_j$ and $6p_j$-$6p_{j'}$ transitions. A larger number of transitions were treated with a more flexible, but less accurate, version of the method. Authors utilized a highly systematic restricted active space approach and predicted gf values and hyperfine structure constants to an accuracy of a few percentage points. The results were used in stellar atmosphere models, assuming local thermodynamic equilibrium (LTE), where a line-by-line investigation was important [3]. Multiconfiguration Dirac-Fock method (MCDF) was employed by Yu *et al.* [27] to calculate excitation energies, ionization potentials, and oscillator strengths for all neutral and up to 5 times ionized species of element Uub, as well as the homolog elements Zn, Cd, and Hg. Numerical values for oscillator strengths in Hg$^+$ were given only for the $6s$-$6p_j$ transitions [27].

The infinite-order regular approximation (IORA) and IORA with modified metric (IORAmm) was used by Filatov and Cremer [28] to develop an algorithm for calculating relativistically corrected isotropic hyperfine structure (HFS) constants. The numerical value of the HFS constant was given for the Hg$^+$ $6s$ ground state.

Recently, Glowacki and Migdalek [29] presented calculations of relativistic configuration-interaction oscillator strengths for lowest $E1$ transitions in the gold isoelectronic sequence. Numerical results for Hg$^+$ ion were listed only for the $6s$-$6p_j$ transitions. Relativistic corrections to transition frequencies of Ag I, Dy I, Ho I, Yb II, Yb III, Au I, and Hg$^+$ ions were investigated recently by Dzuba and Flambaum [30] due to the search for variation of the fine-structure constant. Relativistic many-body perturbation theory was used by Safronova and Johnson [31] to evaluate excitation energies, oscillator strengths, and lifetimes of levels along the gold isoelectronic sequence. Numerical results for Hg$^+$ ion were presented for the ns ($n = 6$–9), np_j ($n = 6$–8), nd_j ($n = 6$–7), and $5f_j$ states for excitation energies and oscillator strengths between those states.

In this article, we carry out a systematic study of atomic properties of singly ionized mercury. First-, second-, third-, and all-order Coulomb energies and first- and second-order Coulomb-Breit energies are calculated for the $6s$-$11s$, $6p$-$10p$, $6d$-$10d$, $5f$-$9f$, and $5g$-$9g$ levels. The electric-dipole reduced matrix elements, oscillator strengths, and transition rates are determined for allowed transitions between these states. Additionally, lifetime values are determined for all above-mentioned states. Electric-dipole ($6s$-np_j, $n = 6$–26) matrix elements are calculated to obtain the ground-state $E1$ polarizabilities. We investigate the hyperfine structure in ^{199}Hg$^+$ and ^{201}Hg$^+$ ions. The hyperfine A and B values are determined for the first low-lying levels up to $n = 7$. Finally, the quadratic Stark effect on hyperfine structure levels of the ground state is also investigated to evaluate the relevant blackbody radiation shift in the microwave frequency standards with ^{199}Hg$^+$ and ^{201}Hg$^+$ ions.

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

Energies of nl_j states in Hg$^+$ are evaluated for the $6s$-$11s$, $6p$-$10p$, $6d$-$10d$, $5f$-$9f$, and $5g$-$9g$ states using both third-order relativistic many-body perturbation theory (RMBPT) and the single-double (SD) all-order method discussed in Refs. [32–34], in which single and double excitations of Dirac-Fock (DF) wave functions are iterated to all orders.

We use B splines [35] to generate a complete set of DF basis orbitals for use in the evaluation of all atomic properties. The present calculation of the polarizabilities required accurate representation of rather highly excited states, such as $6l_j$-$13l_j$, leading to the use of the large $R = 220$ a.u. cavity for the generation of the finite basis set and higher number of splines to produce high-accuracy single-particle orbitals.

Results of our energy calculations are summarized in Table I. Columns 2–6 give the lowest-order DF energies $E^{(0)}$, second-order and third-order Coulomb correlation energies $E^{(2)}$ and $E^{(3)}$, second-order Breit corrections $B^{(2)}$, 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 [36]. 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 [37–39] 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.

We list the all-order SD energies in the column labeled E^{SD} and list that part of the third-order energies missing from E^{SD} in the column labeled $E^{(3)}_{\mathrm{extra}}$. The sum of the five terms $E^{(0)}$, E^{SD}, $E^{(3)}_{\mathrm{extra}}$, $B^{(2)}$, and $E^{(\mathrm{LS})}$ is our final all-order result $E^{\mathrm{SD}}_{\mathrm{tot}}$, listed in the tenth column of Table I. Recommended energies from the National Institute of Standards and Technology (NIST) database [40] 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. We include both Coulomb and Breit contributions to the Breit-Dirac-Fock potential and then treat the residual Breit and Coulomb interactions perturbatively. As a result, the first-order Breit correction $B^{(1)}$ was already included in the lowest-order DF energies $E^{(0)}$ and omitted from Table I.

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 $l_{\max} = 8$

TABLE I. The total all-order $E^{\mathrm{SD}}_{\mathrm{tot}}$ and third-order $E^{(3)}_{\mathrm{tot}}$ Hg^+ energies [$E^{(3)}_{\mathrm{tot}} = E^{(0)} + E^{(2)} + E^{(3)} + B^{(2)}$, $E^{\mathrm{SD}}_{\mathrm{tot}} = E^{(0)} + E^{\mathrm{SD}} + E^{(3)}_{\mathrm{extra}} + B^{(2)}$] for Hg^+ are compared with experimental energies E_{NIST} [40], $\delta E = E_{\mathrm{tot}} - E_{\mathrm{NIST}}$. $E^{(n)}$ is zeroth-order (DF), second-, and third-order Coulomb correlation energies, E^{SD} is single-double all-order Coulomb energies, and $E^{(3)}_{\mathrm{extra}}$ is the third-order energies missing from E^{SD}. Last, $B^{(2)}$ is the second-order Coulomb-Breit corrections. All units are in cm^{-1}.

nlj	$E^{(0)}$	$E^{(2)}$	$E^{(3)}$	$B^{(2)}$	$E^{\mathrm{LS)}}$	$E^{(3)}_{\mathrm{tot}}$	E^{SD}	$E^{(3)}_{\mathrm{extra}}$	$E^{\mathrm{SD}}_{\mathrm{tot}}$	E_{NIST}	$\delta E^{(3)}$	δE^{SD}
$6s_{1/2}$	−136333.2	−18387.3	5622.5	−756.0	78.9	−149775	−15827.1	1665.4	−151172	−151284	1509	112
$6p_{1/2}$	−89541.3	−11017.7	2811.1	−375.1	−1.7	−98125	−10548.2	877.7	−99589	−99798	1674	210
$6p_{3/2}$	−81958.6	−8889.9	2201.0	−272.0	0.5	−88919	−8861.0	740.0	−90351	−90676	1757	325
$6d_{3/2}$	−44301.7	−1985.3	410.4	−57.7	0.0	−45934	−2094.2	183.1	−46271	−46300	366	30
$6d_{5/2}$	−43867.1	−1870.6	367.7	−59.6	0.0	−45430	−1967.6	168.0	−45726	−45740	311	14
$7s_{1/2}$	−52800.2	−3313.7	1009.3	−129.1	7.2	−55226	−2901.0	343.3	−55480	−55570	344	90
$7p_{1/2}$	−40851.3	−2479.4	624.4	−90.3	−0.3	−42797	−2327.9	210.6	−43059	−42986	189	−73
$7p_{3/2}$	−38711.5	−2208.4	527.8	−74.5	0.0	−40467	−2092.3	189.0	−40689	−39313	−1154	1376
$5f_{5/2}$	−27610.6	−574.8	117.5	−2.8	0.0	−28071	−605.3	62.8	−28156	−27873	−198	−283
$5f_{7/2}$	−27625.6	−574.9	115.2	−2.8	0.0	−28088	−619.3	61.9	−28186	−28131	43	−55
$7d_{3/2}$	−25170.4	−781.9	150.6	−27.1	0.0	−25829	−808.3	67.4	−25938	−25959	130	20
$7d_{5/2}$	−24966.3	−744.5	117.5	−27.9	0.0	−25621	−761.6	62.1	−25694	−25705	84	11
$8s_{1/2}$	−28828.4	−1241.1	381.1	−49.7	1.7	−29736	−1077.0	130.7	−29823	−29868	131	45
$8p_{1/2}$	−23776.2	−1020.2	253.7	−38.2	−0.1	−24581	−986.0	88.0	−24713	−24343	−238	−370
$8p_{3/2}$	−22834.5	−934.5	216.0	−32.5	0.0	−23586	−1017.1	80.6	−23804	−23489	−97	−315
$9s_{1/2}$	−18208.7	−605.9	186.4	−24.6	0.6	−18652	−526.6	64.2	−18695	−18724	72	29
$6f_{5/2}$	−17700.8	−334.4	64.6	−2.3	0.0	−17973	−370.9	34.1	−18040	−18015	42	−25
$6f_{7/2}$	−17712.3	−334.2	62.7	−2.4	0.0	−17986	−371.1	33.3	−18052	−18001	14	−52
$5g_{7/2}$	−17559.1	−75.0	16.5	0.0	0.0	−17618	−74.8	9.7	−17624	−17630	12	5
$5g_{9/2}$	−17559.2	−75.0	16.5	0.0	0.0	−17618	−74.8	9.7	−17624	−17629	12	5
$8d_{3/2}$	−16309.7	−399.1	71.2	−14.6	0.0	−16652	−413.4	33.5	−16704	−16722	69	17
$8d_{5/2}$	−16199.6	−383.7	36.3	−15.0	0.0	−16562	−372.2	31.1	−16559	−16585	23	26
$9p_{1/2}$	−15595.9	−526.2	129.5	−19.9	−0.1	−16013	−525.2	45.7	−16095			
$9p_{3/2}$	−15095.8	−489.1	110.2	−17.2	0.0	−15492	−576.9	42.3	−15648	−15474	−18	−174
$10s_{1/2}$	−12550.8	−342.4	105.4	−14.0	0.3	−12801	−298.5	36.4	−12827	−12850	48	23
$7f_{5/2}$	−12293.6	−205.7	38.2	−1.6	0.0	−12463	−233.8	20.2	−12509	−12489	26	−20
$7f_{7/2}$	−12301.5	−205.5	36.8	−1.7	0.0	−12472	−233.5	19.7	−12517	−12471	−1	−46
$6g_{7/2}$	−12194.3	−48.6	10.7	0.0	0.0	−12232	−48.6	6.2	−12237	−12240	8	3
$6g_{9/2}$	−12194.3	−48.6	10.6	0.0	0.0	−12232	−48.6	6.2	−12237	−12240	8	3
$9d_{3/2}$	−11441.2	−232.8	38.6	−8.7	0.0	−11644	−241.8	19.3	−11672	−11657	13	−15
$9d_{5/2}$	−11375.4	−225.8	1.6	−9.0	0.0	−11609	−238.9	17.9	−11605	−11596	−13	−9
$10p_{1/2}$	−11025.0	−308.5	75.5	−11.7	0.0	−11270	−286.0	26.9	−11296			
$10p_{3/2}$	−10727.4	−289.1	64.3	−10.3	0.0	−10962	−296.9	25.1	−11010			
$8f_{5/2}$	−9028.5	−134.1	24.5	−1.2	0.0	−9139	−155.2	12.9	−9172	−9156	17	−16
$8f_{7/2}$	−9033.9	−133.8	23.4	−1.2	0.0	−9146	−154.7	12.5	−9177	−9150	5	−27
$7g_{7/2}$	−8959.2	−32.6	7.2	0.0	0.0	−8985	−32.6	4.1	−8988	−8990	5	2
$7g_{9/2}$	−8959.2	−32.6	7.2	0.0	0.0	−8985	−32.6	4.1	−8988	−8990	5	2
$10d_{3/2}$	−8472.9	−147.9	23.0	−5.6	0.0	−8603	−155.0	12.2	−8621	−8624	21	3
$10d_{5/2}$	−8430.5	−144.7	−11.6	−5.8	0.0	−8593	−147.8	11.3	−8573	−8572	−20	−1
$9f_{5/2}$	−6908.8	−91.9	14.4	−0.8	0.0	−6987	−107.6	8.7	−7009			
$9f_{7/2}$	−6912.7	−91.7	13.4	−0.8	0.0	−6992	−107.1	8.4	−7012			
$8g_{7/2}$	−6859.4	−22.7	6.1	0.0	0.0	−6876	−22.8	2.8	−6879	−6881	5	2
$8g_{9/2}$	−6859.4	−22.7	6.1	0.0	0.0	−6876	−22.8	2.8	−6879	−6881	4	1
$9g_{7/2}$	−5419.8	−17.7	4.6	0.0	0.0	−5433	−16.4	2.0	−5434	−5435	2	1
$9g_{9/2}$	−5419.8	−17.7	4.6	0.0	0.0	−5433	−16.4	2.0	−5434	−5435	2	1

and is extrapolated to account for contributions from higher partial waves (for details of the extrapolation procedure, see Refs. [41,42]). As an example of the convergence of $E^{(2)}$ with the number of partial waves l, consider the $6s$ state. Calculations of $E^{(2)}$ with $l_{\max} = 6$ and 8 yield $E^{(2)}(6s_{1/2}) = -18\,158.0$ and $-18\,351.4$ cm^{-1}, respectively. Extrapolation of these calculations yields $-18\,387.3$ and $-18\,381.3$ cm^{-1}, respectively. Thus, in this particular case, we have a numerical uncertainty in $E^{(2)}(6s)$ of 6.0 cm^{-1}. It should be noted that the 193.34 cm^{-1} contribution from partial waves with $l > 6$ for the $6s$ state is the largest among all states considered in Table I; smaller (about 16–17 cm^{-1}) contributions are obtained for the $6d_{3/2}$ and $6d_{5/2}$ states and much smaller contributions (2–3 cm^{-1}) are obtained for $n = 7$ states.

Due to computational 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 contributions of the higher partial waves. Additionally, six partial waves are used in the calculation of $E^{(3)}$. Since the asymptotic l dependence of the second- and third-order energies are similar (both fall off as l^{-4}), we use the second-order remainder as a guide to estimate the remainder in the third-order contribution. The term $E^{(3)}_{\text{extra}}$ in Table I, which accounts for that part of the third-order MBPT energy missing from the SD energy, is smaller than $E^{(3)}$ by an order of magnitude for the states considered here.

The column labeled δE^{SD} in Table I gives differences between our *ab initio* results and the available experimental values [40]. The SD results are in substantially better agreement with recommended NIST values than the third-order MBPT results (the ratio of $\delta E^{(3)}/\delta E^{\text{SD}}$ is about three for some cases) as expected, illustrating the importance of fourth- and higher-order correlation corrections.

III. ELECTRIC-DIPOLE MATRIX ELEMENTS, OSCILLATOR STRENGTHS, TRANSITION RATES, AND LIFETIMES IN THE Hg$^+$ ION

A. Electric-dipole matrix elements

The calculation of the transition matrix elements provides another test for both the quality of atomic-structure calculations and the size of correlation corrections. Reduced electric-dipole matrix elements between low-lying states of Hg$^+$ calculated in various approximations are presented in Table II.

In Table II, we list our recommended values for 50 $E1$ ns-$n'p$, nd-$n'p$, and nd-$n'f$ transitions. While we have calculated over 500 $E1$ matrix elements to evaluate lifetimes and polarizabilities presented in this work, only matrix elements that give significant contributions to the atomic properties calculated in the other sections are listed. To evaluate the uncertainties of these values, several calculations were carried out in different approximations. We list the lowest-order DF Z^{DF}, second-order $Z^{(\text{DF}+2)}$, and third-order $Z^{(\text{DF}+2+3)}$ values in the first three numerical columns of Table II to demonstrate the size of the second-, third-, and higher-order correlation corrections. The absolute values of the reduced matrix elements in atomic units (a_0e) are given in all cases. The MBPT calculations are carried out following the method described in Ref. [43]. The values $Z^{(\text{DF}+2)}$ are obtained as the sum of the second-order correlation correction $Z^{(2)}$ and the DF matrix elements Z^{DF}. The third-order matrix elements $Z^{(\text{DF}+2+3)}$ include the DF values, the second-order $Z^{(2)}$ results, and the third-order $Z^{(3)}$ correlation correction. $Z^{(3)}$ includes random-phase-approximation terms (RPA) iterated to all orders, Brueckner orbital (BO) corrections, the structural radiation, and normalization terms (see Ref. [43] for definition of these terms).

Our calculations of the reduced matrix elements in the lowest, second, and third orders were carried out following the pattern described in Refs. [43–45]. The lowest-order DF values for transitions between valence v and w states (labelled as $Z^{(\text{DF})}_{vw}$) are given in the third column of Table II. The values $Z^{(\text{DF}+2)}_{vw}$ are obtained as the sum of the second-order correlation correction $Z^{(2)}_{vw}$ and the DF matrix elements $Z^{(\text{DF})}_{vw}$. It should be noted that the second-order Breit corrections $B^{(2)}_{vw}$ are rather small in comparison with the second-order Coulomb corrections $Z^{(2)}_{vw}$ (the relative ratio of $B^{(2)}_{vw}$ to $Z^{(2)}_{vw}$ is about 1–3%).

The third-order matrix elements $Z^{(\text{DF}+2+3)}_{vw}$ include the DF values, the second-order $Z^{(2)}_{vw}$ results, and the third-order $Z^{(3)}_{vw}$ correlation correction. It should be noted that the third-order matrix elements $Z^{(\text{DF}+2+3)}_{vw}$ are divided in the following way:

$$Z^{(\text{DF}+2+3)}_{vw} = Z^{(\text{DF})}_{vw} + Z^{(\text{RPA})}_{vw} + Z^{(\text{BO})}_{vw} + Z^{(\text{SR})}_{vw} + Z^{(\text{NORM})}_{vw}. \tag{1}$$

We include the corresponding set of the high-order contributions using the well-known random-phase approximation in $Z^{(\text{RPA})}$ term using the procedure described in Ref. [43]. The subscript BO stands for Brueckner orbitals. The last two terms in Eq. (1) describe structural radiation, $Z^{(\text{SR})}_{vw}$, and normalization, $Z^{(\text{NORM})}_{vw}$.

The terms $Z^{(\text{RPA})}_{vw}$ and $Z^{(\text{BO})}_{vw}$ give the largest contributions to $Z^{(\text{DF}+2+3)}_{vw}$. The sum of terms $Z^{(\text{RPA})}_{vw}$ and $Z^{(\text{BO})}_{vw}$ is about 20% of the $Z^{(\text{DF})}_{vw}$ term and has different sign for the $6s$-$6p$, $6p$-$6d$, $6p$-$7s$, and $6p$-$7d$ transitions. That decreases the $Z^{(\text{DF}+2+3)}$ values in comparison with the $Z^{(\text{DF})}_{vw}$ values.

The value of $Z^{(\text{BO})}_{vw}$ becomes the largest contribution for the $6p$-$7s$ transitions. The ratios of values $Z^{(\text{RPA})}_{vw}$ and $Z^{(\text{DF})}_{vw}$ are equal to -1.9 and -0.8 for the $6s$-$7p_{1/2}$ and $6s$-$7p_{3/2}$ transitions, respectively. As a result, the value of $Z^{(\text{DF}+2+3)}$ decreases by a factor of 28 in comparison with the $Z^{(\text{DF})}$ term for the $6s$-$7p_{3/2}$ transition, while value of $Z^{(\text{DF}+2+3)}$ increases by a factor of 1.5 and changes sign in comparison with the $Z^{(\text{DF})}$ term for the $6s$-$7p_{1/2}$ transition (see Table II).

The structural radiation $Z^{(\text{SR})}_{vw}$ and normalization $Z^{(\text{NORM})}_{vw}$ terms give a small contribution to $Z^{(\text{DF}+2+3)}$ values (about 0.3–3.3%). All the results given in Table II are obtained using length form of the matrix elements.

The next four columns of Table II contain four different all-order calculations. *Ab initio* electric-dipole matrix elements evaluated in the all-order SD (single-double) and SDpT approximations (single-double all-order method including partial triple excitations [46]) are given in columns labeled Z^{SD} and Z^{SDpT}. Differences between the Z^{SD} and Z^{SDpT} values are generally 0.5–2.0% for the transitions listed in Table II. The SD and SDpT matrix elements Z^{SD} 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 [47].

Recently, we have developed some general criteria to establish the final values for all transitions and evaluate uncertainties due to the need to analyze a very large number of transitions [48]. To evaluate the uncertainties of our matrix elements and to provide recommended values, we carried out semiempirical evaluation of the missing correlation corrections using the scaling procedure. The uncertainty evaluation was discussed in detail in Ref. [48], and we briefly summarize it below.

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

$$Z_{wv} = \frac{\langle \Psi_w | Z | \Psi_v \rangle}{\sqrt{\langle \Psi_v | \Psi_v \rangle \langle \Psi_w | \Psi_w \rangle}}. \tag{2}$$

TABLE II. Recommended values of the reduced electric-dipole matrix elements 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 are given in the Z^{final} column. Absolute values are given. The last column gives relative uncertainties of the final values in percentage points. These are estimated uncertainties associated with the present all-order approach. These uncertainties do not account for the mixing of the one-particle and one-hole–two-particle configurations.

Transition		Z^{DF}	$Z^{(\text{DF}+2)}$	$Z^{(\text{DF}+2+3)}$	Z^{SD}	$Z^{(\text{SD})}_{\text{sc}}$	Z^{SDpT}	$Z^{\text{SDpT}}_{\text{sc}}$	Z^{final}	Unc. (%)
$6s_{1/2}$	$6p_{1/2}$	2.2892	1.8185	1.6883	1.6600	1.6646	1.6651	1.6627	1.6646	0.28
$6s_{1/2}$	$6p_{3/2}$	3.1845	2.5661	2.4026	2.3510	2.3586	2.3585	2.3563	2.3586	0.32
$7s_{1/2}$	$6p_{1/2}$	1.7106	1.7093	1.5335	1.5187	1.5214	1.5234	1.5163	1.5214	0.34
$7s_{1/2}$	$6p_{3/2}$	3.1029	3.0528	2.7920	2.7348	2.7292	2.7444	2.7258	2.7292	0.56
$7s_{1/2}$	$7p_{1/2}$	5.2298	5.0803	4.8460	4.8600	4.8615	4.8759	4.8610	4.8600	0.42
$8s_{1/2}$	$6p_{1/2}$	0.4843	0.4802	0.4668	0.4664	0.4665	0.4678	0.4676	0.4665	0.28
$8s_{1/2}$	$6p_{3/2}$	0.7328	0.7027	0.6979	0.6956	0.6964	0.6983	0.6993	0.6964	0.41
$9s_{1/2}$	$6p_{1/2}$	0.2673	0.2634	0.2627	0.2668	0.2668	0.2682	0.2681	0.2668	0.52
$9s_{1/2}$	$6p_{3/2}$	0.3912	0.3696	0.3759	0.3787	0.3791	0.3806	0.3811	0.3791	0.53
$9s_{1/2}$	$7p_{1/2}$	0.9608	0.9740	0.9386	0.9381	0.9379	0.9400	0.9402	0.9379	0.24
$9s_{1/2}$	$8p_{3/2}$	11.7655	11.7758	11.2408	11.0845	11.1985	11.2353	11.2498	11.1985	0.46
$9s_{1/2}$	$9p_{3/2}$	18.5382	18.5035	18.0569	18.2017	18.1870	18.1752	18.1364	18.1870	0.28
$6d_{3/2}$	$6p_{1/2}$	3.6118	3.2841	2.9607	2.9225	2.9246	2.9326	2.9205	2.9225	0.39
$6d_{3/2}$	$6p_{3/2}$	1.8788	1.7262	1.5778	1.5532	1.5524	1.5591	1.5504	1.5532	0.61
$6d_{3/2}$	$7p_{1/2}$	6.5612	6.4793	6.2220	6.2073	6.2074	6.2307	6.2054	6.2074	0.38
$6d_{5/2}$	$6p_{3/2}$	5.5647	5.1199	4.6680	4.5908	4.5881	4.6089	4.5818	4.5908	0.64
$6d_{5/2}$	$5f_{7/2}$	11.8444	11.5388	10.9887	10.9418	10.9462	10.9814	10.9398	10.9462	0.32
$7d_{3/2}$	$8p_{3/2}$	5.5199	5.5125	5.4149	5.4037	5.3877	5.3868	5.3692	5.3877	0.34
$7d_{5/2}$	$8p_{3/2}$	16.9078	16.8812	16.6001	16.5812	16.5415	16.5280	16.4879	16.5415	0.32
$8d_{3/2}$	$7p_{1/2}$	2.0426	1.9983	1.9201	1.9112	1.9133	1.9150	1.9164	1.9133	0.16
$8d_{3/2}$	$8p_{3/2}$	4.9838	4.9721	4.6360	4.6499	4.7154	4.7208	4.7396	4.7154	0.51
$8d_{3/2}$	$9p_{3/2}$	8.9750	8.9714	8.8663	8.8284	8.8088	8.8202	8.7900	8.8088	0.21
$8d_{5/2}$	$8p_{3/2}$	16.9078	16.8812	16.6001	13.4127	13.6648	13.6913	13.7342	13.6648	0.51
$8d_{5/2}$	$9p_{3/2}$	27.4180	27.4046	27.0938	27.1020	26.9877	26.9981	26.9261	26.9877	0.23
$9d_{3/2}$	$7p_{1/2}$	1.1405	1.1049	1.0801	1.0664	1.0669	1.0714	1.0694	1.0669	0.42
$9d_{3/2}$	$8p_{3/2}$	1.4304	1.4199	1.3886	1.3785	1.3779	1.3828	1.3829	1.3779	0.37
$9d_{3/2}$	$7f_{5/2}$	31.9963	32.0084	31.6460	31.4671	31.6525	31.4337	31.6650	31.6525	0.69
$9d_{5/2}$	$8p_{3/2}$	4.3106	4.2820	4.1738	4.1927	4.1893	4.2179	4.2177	4.1893	0.68
$9d_{5/2}$	$7f_{5/2}$	8.4295	8.4330	8.3313	8.2170	8.2833	8.2275	8.2749	8.2833	0.67
$5g_{7/2}$	$5f_{7/2}$	3.0937	3.0702	2.9425	2.9253	2.9531	2.9369	2.9527	2.9531	0.55
$5g_{7/2}$	$6f_{5/2}$	21.0220	21.0198	21.1035	21.2291	21.1740	21.2137	21.1694	21.1740	0.19
$5g_{7/2}$	$6f_{7/2}$	4.0488	4.0483	4.0650	4.0895	4.0723	4.0868	4.0714	4.0723	0.36
$5g_{9/2}$	$5f_{7/2}$	18.3030	18.1639	17.4095	17.3067	17.4711	17.3751	17.4688	17.4711	0.55
$5g_{9/2}$	$6f_{7/2}$	23.9522	23.9495	24.0485	24.1931	24.0917	24.1773	24.0865	24.0917	0.36
$6g_{7/2}$	$5f_{7/2}$	0.9450	0.9282	0.9419	0.9406	0.9361	0.9399	0.9363	0.9406	0.67
$6g_{7/2}$	$7f_{5/2}$	37.5965	37.5946	37.7237	37.8647	37.7895	37.8491	37.7820	37.7895	0.16
$6g_{7/2}$	$7f_{7/2}$	7.2404	7.2401	7.2656	7.2937	7.2657	7.2912	7.2643	7.2657	0.35
$6g_{9/2}$	$5f_{7/2}$	5.5904	5.4912	5.5732	5.5646	5.5384	5.5605	5.5393	5.5646	0.67
$6g_{9/2}$	$7f_{7/2}$	42.8340	42.8317	42.9827	43.1490	42.9843	43.1344	42.9758	42.9843	0.35
$7g_{7/2}$	$6f_{5/2}$	7.2143	7.1742	7.0891	7.0408	7.0576	7.0528	7.0600	7.0576	0.07
$7g_{7/2}$	$6f_{7/2}$	1.3877	1.3800	1.3632	1.3541	1.3590	1.3564	1.3594	1.3590	0.20
$7g_{7/2}$	$8f_{5/2}$	56.3033	56.3019	56.4640	56.5957	56.5101	56.5833	56.5000	56.5101	0.13
$7g_{7/2}$	$8f_{7/2}$	10.8421	10.8418	10.8735	10.9004	10.8749	10.8987	10.8729	10.8749	0.22
$7g_{9/2}$	$6f_{7/2}$	8.2100	8.1644	8.0652	8.0114	8.0403	8.0245	8.0427	8.0403	0.20
$7g_{9/2}$	$8f_{7/2}$	64.1414	64.1396	64.3272	64.4861	64.3369	64.4764	64.3251	64.3369	0.22
$8g_{7/2}$	$6f_{5/2}$	3.9919	3.9578	4.0045	3.9875	3.9777	3.9868	3.9791	3.9875	0.35
$8g_{7/2}$	$6f_{7/2}$	0.7688	0.7623	0.7709	0.7678	0.7649	0.7677	0.7651	0.7678	0.53
$8g_{7/2}$	$7f_{5/2}$	9.3593	9.3397	9.0473	8.9485	9.0165	8.9789	9.0211	9.0165	0.42
$8g_{9/2}$	$6f_{7/2}$	4.5483	4.5095	4.5610	4.5425	4.5263	4.5420	4.5275	4.5425	0.51
$9g_{7/2}$	$6f_{5/2}$	2.6491	2.6201	2.6860	2.6788	2.6656	2.6756	2.6664	2.6656	0.50
$9g_{7/2}$	$7f_{5/2}$	5.3193	5.3014	5.2597	5.2166	5.2282	5.2247	5.2308	5.2282	0.07
$9g_{7/2}$	$7f_{7/2}$	1.0234	1.0199	1.0114	1.0033	1.0073	1.0048	1.0077	1.0073	0.24
$9g_{7/2}$	$8f_{5/2}$	11.5547	11.5443	11.0136	10.8574	10.9924	10.9075	10.9993	10.9924	0.77
$9g_{9/2}$	$7f_{7/2}$	6.0544	6.0341	5.9838	5.9360	5.9592	5.9447	5.9618	5.9592	0.24

In the SD approximation, the $|\Psi_v\rangle$ and $|\Psi_w\rangle$ are given by the expansions

$$|\Psi_v\rangle = \Big[1 + \sum_{ma} \rho_{ma} a_m^\dagger a_a + \frac{1}{2} \sum_{mnab} \rho_{mnab} a_m^\dagger a_n^\dagger a_b a_a + \sum_{m\neq v} \rho_{mv} a_m^\dagger a_v + \sum_{mna} \rho_{mnva} a_m^\dagger a_n^\dagger a_a a_v \Big] |\Psi_v^{(0)}\rangle, \quad (3)$$

where $|\Psi_v^{(0)}\rangle$ is the lowest-order atomic state vector. In Eq. (3), 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}, ρ_{mnab}, and ρ_{mnva} are single-excitation coefficients for core and valence electrons and double-excitation coefficients for core and valence electrons, respectively. In the SD approximation, the resulting expression for the numerator of Eq. (2) 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.

From these 20 terms, only two terms give dominant contributions for all transition matrix elements considered in this work:

$$Z^{(a)} = \sum_{ma} (z_{am} \tilde{\rho}_{wmva} + z_{ma} \tilde{\rho}^*_{vmwa}) \quad (4)$$

or

$$Z^{(c)} = \sum_{m} (z_{wm} \rho_{mv} + z_{mv} \rho^*_{mw}), \quad (5)$$

where $\tilde{\rho}_{mnab} = \rho_{mnab} - \rho_{nmab}$ and z_{wv} are lowest-order matrix elements of the corresponding one-body operator. For most of the transitions considered in this work, term $Z^{(c)}$ is the dominant term. To evaluate missing corrections to this term, we need to improve the values of the valence single-excitation coefficients ρ_{mv} [49]. These excitation coefficients are closely related to the correlation energy δE_v. 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 [49]

$$\rho'_{mv} = \rho_{mv} \frac{\delta E_v^{\text{expt}}}{\delta E_v^{\text{theory}}}. \quad (6)$$

The δE_v^{expt} is defined as the experimental energy [40] minus the lowest-order DF energy ϵ_v. Since the scaling factors depend on the correlation energy given by the particular calculation, they differ for the SD and SDpT calculations, and these values have to be scaled separately. This is a rather complicated procedure that involves complete recalculation of the matrix elements with new values of the valence excitation coefficients. The corresponding results are listed in Table II with the subscript "sc." The scaled SD and SDpT values are close together, as expected.

The term $Z^{(a)}$ is not corrected by the scaling procedure. However, it is dominant for very few transitions that give significant contributions to the atomic properties considered in this work, and we consider such cases separately. Therefore, the recommended set of values and their uncertainties can be established based on the ratio $R = Z^{(c)}/Z^{(a)}$. We take the SD scaled result as the final value if $R > 1$. Otherwise, we use SD result 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, SD$_{\text{sc}}$, and SDpT$_{\text{sc}}$ set. 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(SD$_{\text{sc}}-$SD, SD$_{\text{sc}}-$SDpT, SD$_{\text{sc}}-$SDpT$_{\text{sc}}$). If the term $Z^{(c)}$ strongly dominates and $R > 3$, we evaluate the final uncertainty as max(SD$_{\text{sc}}-$SDpT, SD$_{\text{sc}}-$SDpT$_{\text{sc}}$). 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 Refs. [44,46,48–57] and references therein) and found that such procedures do not underestimate the uncertainties in monovalent systems but may somewhat overestimate them in some cases. The case of Hg$^+$ is more complicated due to the presence of the low-lying one-hole–two-particle configurations. The procedure described above is expected to estimate only the uncertainties that are associated with the present approach; it cannot estimate full uncertainties due to mixing of the one-particle configurations considered in this work with the one-hole–two-particle configurations. Such uncertainties cannot be fully estimated within the framework of the present approach.

The last column of Table II gives relative uncertainties in the final values Z^{final} in percentage points estimated as described above. Our final results and their uncertainties are used to calculate the recommended values of the transition rates, oscillator strengths, lifetimes, and polarizabilities as well as evaluate the uncertainties of these results.

B. Transition rates and oscillator strengths

We combine recommended NIST energies [40] and our final values of the matrix elements listed in Table II to calculate transition rates A and oscillator strengths f. The transition rates are calculated using

$$A_{ab} = \frac{2.02613 \times 10^{18}}{\lambda^3} \frac{S}{2j_a + 1} \text{s}^{-1}, \quad (7)$$

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

Wavelengths and transition rates A_r in the first-order (DF), second-order (RPA), and third-order RMBPT approximation are given in Table III for the limited number of transitions in Hg$^+$. We chose transitions that can be compared with data presented on the NIST Web site [40] as recommended NIST data. We note that NIST data for these transition rates mainly come from the theoretical calculations, generally obtained by using standard atomic codes which may not accurately take into account the correlation corrections. The higher-order contributions are generally omitted in such calculations. Therefore, it is instructive to compare NIST data with the first-, second-, and third-order MBPT calculations. In Table III, our transition rates calculated in the first-, second-, and third-order approximations ($A_r^{(i)}$) are compared with NIST transition rates, $A^{(\text{NIST})}$. This table shows some $A^{(\text{NIST})}$ values agree better with A_r values obtained from each approximation, and a substantial part of the $A^{(\text{NIST})}$ values disagree with all of our results. In the left column of Table III, we list the 39 transitions when the $A^{(\mathrm{NIST})}$ values are in the better agreement with our $A_r^{(1)}$ values obtained in the DF approximation. Disagreement between the $A^{(\mathrm{NIST})}$ and $A_r^{(1)}$ values is about 2–20%. The first 12 transitions given in the right column of Table III are transitions when the $A^{(\mathrm{NIST})}$ values are in the better agreement with our $A_r^{(2)}$ values obtained in the RPA approximation. The next six lines present transitions when the $A^{(\mathrm{NIST})}$ values are in better agreement with our $A_r^{(3)}$ values obtained in the third-order RMBPT approximation. Disagreement between the $A^{(\mathrm{NIST})}$ and $A_r^{(i)}$ values in both cases with $i = 2$ and 3 is about 2–20%. The last 21 transitions given in the right column of Table III present transitions when the $A^{(\mathrm{NIST})}$ values disagree with our $A_r^{(i)}$ values by a factor of 1.3–20. These 21 transitions represent cases that illustrate the importance of correlation contributions. The difference in $A_r^{(1)}$, $A_r^{(2)}$, and $A_r^{(3)}$ values is about 10–50% for the most of these cases.

Our final values of the transition rates A (s^{-1}) and oscillator strengths (f) for the ns-$n'p$, np-$n's$, np-$n'd$, nd-$n'p$, and nd-$n'f$ transitions in Hg^+ are summarized in Table IV. Vacuum wavelengths obtained from NIST energies are also listed for reference. The relative uncertainties in percentage points are listed in the column labeled "Unc.." The relative uncertainties of the transition rates and oscillator strengths are twice of the corresponding matrix element uncertainties since

TABLE III. Transition rates (A_r in 1/s) for transitions in Hg^+ calculated in lowest- (DF approximation) $A_r^{(1)}$, second- $A_r^{(2)}$ and third-order $A_r^{(3)}$ RMBPT are compared with recommended NIST values $A_r^{(\mathrm{NIST})}$ [40].

nl_j-$n'l'_{j'}$		$\lambda^{(\mathrm{NIST})}$	$A^{(\mathrm{NIST})}$	$A_r^{(1)}$	$A_r^{(2)}$	$A_r^{(3)}$	nl_j-$n'l'_{j'}$		$\lambda^{(\mathrm{NIST})}$	$A^{(\mathrm{NIST})}$	$A_r^{(1)}$	$A_r^{(2)}$	$A_r^{(3)}$
$6s_{1/2}$	$6p_{1/2}$	1942.3	7.5[8]	7.25[8]	4.57[8]	3.94[8]	$6p_{3/2}$	$6d_{3/2}$	2253.5	1.2[8]	1.56[8]	1.32[8]	1.10[8]
$6s_{1/2}$	$6p_{3/2}$	1649.9	1.2[9]	1.14[9]	7.43[8]	6.51[8]	$6p_{3/2}$	$6d_{5/2}$	2225.4	7.5[8]	9.49[8]	8.03[8]	6.68[8]
$6p_{1/2}$	$6d_{3/2}$	1869.2	1.0[9]	1.01[9]	8.37[8]	6.80[8]	$6p_{1/2}$	$7d_{3/2}$	1354.3	2.1[8]	2.84[8]	1.96[8]	1.85[8]
$6d_{3/2}$	$6f_{5/2}$	3535.4	3.0[7]	3.25[7]	2.76[7]	2.73[7]	$6p_{3/2}$	$7d_{5/2}$	1539.1	1.8[8]	2.27[8]	1.58[8]	1.57[8]
$6d_{5/2}$	$6f_{7/2}$	3604.9	3.0[7]	3.00[7]	2.53[7]	2.49[7]	$7s_{1/2}$	$7p_{1/2}$	7946.7	4.3[7]	5.52[7]	5.21[7]	4.74[7]
$6d_{5/2}$	$6f_{5/2}$	3606.8	2.0[6]	2.02[6]	1.71[6]	1.67[6]	$6s_{1/2}$	$8p_{3/2}$	782.5	1.0[7]	3.32[7]	9.44[6]	1.11[7]
$6p_{1/2}$	$7s_{1/2}$	2261.0	3.0[8]	2.57[8]	2.56[8]	2.06[8]	$6p_{1/2}$	$8d_{3/2}$	1203.7	9.0[7]	1.28[8]	7.91[7]	7.91[7]
$6p_{3/2}$	$7d_{3/2}$	1545.2	3.0[7]	3.56[7]	2.44[7]	2.42[7]	$6p_{1/2}$	$10d_{3/2}$	1096.8	2.1[7]	4.28[7]	2.35[7]	2.46[7]
$6d_{3/2}$	$7f_{5/2}$	2957.6	9.5[6]	1.05[7]	7.95[6]	7.95[6]	$7s_{1/2}$	$8p_{3/2}$	3117.1	8.8[6]	1.15[7]	8.87[6]	7.46[6]
$6d_{5/2}$	$7f_{7/2}$	3005.7	9.5[6]	9.02[6]	6.72[6]	6.59[6]	$7s_{1/2}$	$9p_{3/2}$	2499.5	2.4[6]	4.00[6]	2.56[6]	2.09[6]
$6d_{5/2}$	$7f_{5/2}$	3007.4	6.3[5]	6.14[5]	4.59[5]	4.49[5]	$7p_{1/2}$	$10d_{3/2}$	2910.2	9.0[6]	1.21[7]	1.12[7]	1.09[7]
$6d_{5/2}$	$5f_{7/2}$	5678.7	1.8[8]	1.94[8]	1.84[8]	1.67[8]	$5f_{5/2}$	$6g_{7/2}$	6396.7	1.8[7]	2.33[7]	2.25[7]	2.32[7]
$7d_{3/2}$	$7f_{5/2}$	7423.9	1.1[7]	1.16[7]	1.11[7]	1.09[7]							
$7d_{5/2}$	$7f_{7/2}$	7556.2	1.1[7]	1.11[7]	1.07[7]	1.04[7]	$6p_{3/2}$	$7s_{1/2}$	2848.5	3.0[8]	4.22[8]	4.09[8]	3.42[8]
$6p_{1/2}$	$8s_{1/2}$	1430.0	8.5[7]	8.13[7]	7.99[7]	7.55[7]	$7p_{3/2}$	$7d_{5/2}$	7348.5	5.3[7]	7.84[7]	7.68[7]	6.54[7]
$6p_{3/2}$	$8s_{1/2}$	1644.5	1.1[8]	1.22[8]	1.13[8]	1.11[8]	$6s_{1/2}$	$8p_{1/2}$	787.8	3.1[7]	1.15[6]	2.03[7]	3.31[7]
$6p_{3/2}$	$8d_{3/2}$	1352.2	1.5[7]	1.50[7]	8.95[6]	9.48[6]	$7p_{1/2}$	$9d_{3/2}$	3191.9	1.5[7]	2.03[7]	1.90[7]	1.82[7]
$6p_{3/2}$	$8d_{5/2}$	1349.7	8.8[7]	9.71[7]	5.96[7]	6.36[7]	$8s_{1/2}$	$9p_{3/2}$	6990.0	2.2[6]	3.13[6]	2.93[6]	2.58[6]
$6d_{3/2}$	$8p_{3/2}$	4383.8	8.5[4]	8.13[4]	7.02[4]	3.19[4]	$6d_{3/2}$	$5f_{5/2}$	5426.8	1.4[8]	2.00[8]	1.90[8]	1.71[8]
$6d_{3/2}$	$8f_{5/2}$	2692.2	3.8[6]	4.57[6]	3.13[6]	3.11[6]							
$6d_{5/2}$	$8f_{7/2}$	2733.0	3.8[6]	3.71[6]	2.45[6]	2.36[6]	$6s_{1/2}$	$7p_{1/2}$	923.4	6.5[8]	1.24[7]	1.08[7]	1.65[7]
$6p_{1/2}$	$9s_{1/2}$	1233.4	4.6[7]	3.86[7]	3.74[7]	3.73[7]	$6s_{1/2}$	$7p_{3/2}$	893.1	5.8[7]	1.11[8]	5.21[6]	2.70[6]
$6p_{3/2}$	$9d_{5/2}$	1264.5	4.3[7]	5.19[7]	2.94[7]	3.27[7]	$6d_{5/2}$	$8p_{3/2}$	4494.1	7.5[5]	4.17[5]	3.37[5]	8.05[4]
$6p_{3/2}$	$10s_{1/2}$	1284.9	3.4[7]	3.23[7]	2.83[7]	3.00[7]	$6p_{3/2}$	$9s_{1/2}$	1389.8	7.0[7]	5.78[7]	5.16[7]	5.33[7]
$7p_{1/2}$	$7d_{3/2}$	5872.9	1.0[8]	9.40[7]	9.24[7]	7.72[7]	$6p_{1/2}$	$11s_{1/2}$	1105.9	3.8[7]	1.33[7]	1.27[7]	1.32[7]
$7p_{1/2}$	$8s_{1/2}$	7622.9	4.0[7]	3.58[7]	3.63[7]	3.14[7]	$7s_{1/2}$	$7p_{3/2}$	6151.2	6.2[7]	1.09[8]	1.04[8]	9.48[7]
$7p_{1/2}$	$8d_{3/2}$	3807.4	3.2[7]	3.83[7]	3.67[7]	3.38[7]	$7p_{3/2}$	$7d_{3/2}$	7488.4	8.5[6]	1.29[7]	1.27[7]	1.09[7]
$7d_{3/2}$	$8f_{5/2}$	5951.3	4.5[6]	4.99[6]	4.66[6]	4.64[6]	$7s_{1/2}$	$8p_{1/2}$	3202.3	1.0[7]	1.98[6]	9.36[5]	5.37[5]
$7d_{5/2}$	$8f_{7/2}$	6040.6	4.5[6]	4.58[6]	4.27[6]	4.22[6]	$7p_{3/2}$	$8d_{3/2}$	4426.5	1.3[6]	5.02[6]	4.74[6]	4.55[6]
$7p_{1/2}$	$9s_{1/2}$	4121.6	1.2[7]	1.34[7]	1.37[7]	1.28[7]	$7p_{3/2}$	$8d_{5/2}$	4399.9	9.0[6]	3.13[7]	2.97[7]	2.84[7]
$8p_{1/2}$	$9d_{3/2}$	7883.2	9.5[6]	9.82[6]	9.73[6]	8.97[6]	$7p_{3/2}$	$9s_{1/2}$	4856.9	2.2[6]	1.63[7]	1.64[7]	1.56[7]
$8p_{3/2}$	$9d_{5/2}$	8408.4	9.8[6]	1.06[7]	1.04[7]	9.90[6]	$7p_{3/2}$	$9d_{3/2}$	3615.9	8.5[5]	2.57[6]	2.36[6]	2.36[6]
$8p_{1/2}$	$10d_{3/2}$	6362.0	4.8[6]	5.79[6]	5.71[6]	5.42[6]	$7p_{3/2}$	$9d_{5/2}$	3607.9	5.7[6]	1.63[7]	1.51[7]	1.50[7]
$8p_{3/2}$	$10d_{5/2}$	6703.9	5.3[6]	5.95[6]	5.82[6]	5.72[6]	$7p_{1/2}$	$10s_{1/2}$	3318.2	5.5[6]	7.04[6]	7.29[6]	6.91[6]
$5f_{7/2}$	$5g_{9/2}$	9522.8	7.2[7]	7.86[7]	7.74[7]	7.11[7]	$7p_{3/2}$	$10s_{1/2}$	3778.8	2.7[6]	8.84[6]	8.88[6]	8.65[6]
$5f_{7/2}$	$6g_{9/2}$	6293.0	2.6[7]	2.54[7]	2.45[7]	2.53[7]	$7p_{1/2}$	$10s_{1/2}$	3318.2	5.5[6]	7.04[6]	7.29[6]	6.91[6]
$5f_{7/2}$	$7g_{9/2}$	5224.4	1.3[7]	1.21[7]	1.15[7]	1.24[7]	$7p_{3/2}$	$10d_{5/2}$	3253.0	2.5[6]	9.68[6]	8.80[6]	8.91[6]
$5f_{7/2}$	$8g_{9/2}$	4705.9	6.7[6]	6.86[6]	6.43[6]	7.12[6]	$7p_{1/2}$	$11s_{1/2}$	2974.9	8.0[6]	4.23[6]	4.40[6]	4.21[6]
$5f_{7/2}$	$9g_{9/2}$	4406.1	4.5[6]	4.33[6]	4.02[6]	4.53[6]	$7p_{3/2}$	$11s_{1/2}$	3339.9	2.6[4]	5.40[6]	5.41[6]	5.33[6]
							$6d_{5/2}$	$5f_{5/2}$	5596.8	8.8[6]	1.35[7]	1.28[7]	1.16[7]
							$5f_{5/2}$	$5g_{7/2}$	9762.3	5.1[7]	7.06[7]	6.95[7]	6.38[7]

TABLE IV. Wavelengths λ (Å), transition rates A (s^{-1}), and oscillator strengths (f) for transitions in Hg^+ calculated using our recommended values of reduced electric-dipole matrix elements Z^{final} and their uncertainties. The relative uncertainties in the values of transition rates and oscillator strengths are the same, listed in column "Unc." in percentage points. These are estimated uncertainties associated with the present all-order approach. These uncertainties do not account for the mixing of the one-particle and one-hole–two-particle configurations. Numbers in brackets represent powers of 10.

Transition		λ	A	f	Unc.(%)	Transition		λ	A	f	Unc.(%)
$6s_{1/2}$	$6p_{1/2}$	1942.3	3.83[8]	2.17[-1]	0.56	$6d_{3/2}$	$5f_{5/2}$	5426.8	1.68[8]	1.11[0]	1.80
$6s_{1/2}$	$6p_{3/2}$	1649.9	6.27[8]	5.12[-1]	0.64	$6d_{5/2}$	$5f_{5/2}$	5596.8	1.14[7]	5.36[-2]	1.58
$6s_{1/2}$	$7p_{1/2}$	923.4	3.50[7]	4.47[-3]	2.00	$6d_{5/2}$	$5f_{7/2}$	5678.7	1.66[8]	1.07[0]	0.64
$6s_{1/2}$	$7p_{3/2}$	893.1	1.73[5]	4.14[-5]	2.00	$6d_{3/2}$	$7f_{5/2}$	2957.6	7.74[6]	1.52[-2]	2.00
$8s_{1/2}$	$8p_{1/2}$	18 098.8	1.36[7]	6.66[-1]	2.00	$6d_{5/2}$	$7f_{5/2}$	3007.4	4.30[5]	5.82[-4]	2.00
$8s_{1/2}$	$8p_{3/2}$	15 676.8	1.84[7]	1.35[0]	0.72	$6d_{5/2}$	$7f_{7/2}$	3005.7	6.32[6]	1.14[-2]	2.00
$9s_{1/2}$	$9p_{1/2}$	36 908.7	3.82[6]	7.80[-1]	0.50	$6d_{3/2}$	$8f_{5/2}$	2692.2	3.01[6]	4.91[-3]	2.00
$9s_{1/2}$	$9p_{3/2}$	30 769.4	5.75[6]	1.63[0]	0.56	$6d_{5/2}$	$8f_{5/2}$	2733.4	1.53[5]	1.71[-4]	2.00
						$6d_{5/2}$	$8f_{7/2}$	2733.0	2.22[6]	3.32[-3]	2.00
$6p_{1/2}$	$7s_{1/2}$	2261.0	2.03[8]	1.55[-1]	0.68	$7d_{3/2}$	$6f_{5/2}$	12 588.1	3.59[7]	1.28[0]	1.74
$6p_{3/2}$	$7s_{1/2}$	2848.5	3.26[8]	1.99[-1]	1.12	$7d_{5/2}$	$6f_{5/2}$	13 004.1	2.47[6]	6.27[-2]	1.46
$6p_{1/2}$	$8s_{1/2}$	1430.0	7.54[7]	2.31[-2]	0.56	$7d_{5/2}$	$6f_{7/2}$	12 980.0	3.72[7]	1.25[0]	2.18
$6p_{3/2}$	$8s_{1/2}$	1644.5	1.10[8]	2.24[-2]	0.82	$8d_{3/2}$	$7f_{5/2}$	23 625.4	1.14[7]	1.43[0]	2.80
$6p_{1/2}$	$9s_{1/2}$	1233.4	3.84[7]	8.76[-3]	1.04	$8d_{5/2}$	$7f_{5/2}$	24 413.3	7.93[5]	7.08[-2]	2.42
$6p_{3/2}$	$9s_{1/2}$	1389.8	5.42[7]	7.85[-3]	1.06	$8d_{5/2}$	$7f_{7/2}$	24 305.7	1.19[7]	1.41[0]	3.98
$6p_{1/2}$	$10s_{1/2}$	1150.1	2.30[7]	4.56[-3]	1.82	$8d_{3/2}$	$8f_{5/2}$	13 217.7	4.51[6]	1.77[-1]	1.74
$6p_{3/2}$	$10s_{1/2}$	1284.9	3.12[7]	3.86[-3]	1.18	$8d_{5/2}$	$8f_{5/2}$	13 460.7	2.95[5]	8.00[-3]	2.06
$8p_{1/2}$	$10s_{1/2}$	8701.1	3.63[6]	4.13[-2]	0.60	$8d_{5/2}$	$8f_{7/2}$	13 450.5	4.45[6]	1.61[-1]	3.20
$8p_{3/2}$	$10s_{1/2}$	9399.2	5.51[6]	3.65[-2]	0.48	$9d_{3/2}$	$8f_{5/2}$	39 977.0	4.47[6]	1.60[0]	2.28
$9p_{1/2}$	$10s_{1/2}$	31 598.1	3.29[6]	4.93[-1]	2.92	$9d_{5/2}$	$8f_{5/2}$	40 980.7	3.16[5]	7.95[-2]	1.64
$9p_{3/2}$	$10s_{1/2}$	38 107.3	5.41[6]	5.89[-1]	1.44	$9d_{5/2}$	$8f_{7/2}$	40 885.7	4.75[6]	1.59[0]	2.82
$6p_{1/2}$	$6d_{3/2}$	1869.2	6.62[8]	6.94[-1]	0.78	$6f_{5/2}$	$8d_{3/2}$	77 319.5	4.49[5]	2.68[-1]	1.70
$6p_{3/2}$	$6d_{3/2}$	2253.5	1.07[8]	8.13[-2]	1.22	$6f_{5/2}$	$8d_{5/2}$	69 932.8	2.80[4]	2.05[-2]	1.78
$6p_{3/2}$	$6d_{5/2}$	2225.4	6.46[8]	7.19[-1]	1.28	$6f_{7/2}$	$8d_{5/2}$	70 638.9	5.46[5]	3.06[-1]	2.78
$6p_{1/2}$	$7d_{3/2}$	1354.3	1.66[8]	9.12[-2]	2.00						
$6p_{3/2}$	$7d_{3/2}$	1545.2	2.22[7]	7.94[-3]	2.00	$6f_{5/2}$	$9g_{7/2}$	7949.3	3.58[6]	4.53[-2]	1.00
$6p_{3/2}$	$7d_{5/2}$	1539.1	1.43[8]	7.64[-2]	2.00	$6f_{7/2}$	$9g_{7/2}$	7958.3	1.32[5]	1.25[-3]	1.54
$6p_{1/2}$	$8d_{3/2}$	1203.7	6.69[7]	2.91[-2]	2.00	$6f_{7/2}$	$9g_{9/2}$	7958.1	3.69[6]	4.38[-2]	1.48
$6p_{3/2}$	$8d_{3/2}$	1352.2	8.46[6]	2.32[-3]	2.00	$6f_{5/2}$	$8g_{7/2}$	8981.5	5.56[6]	8.96[-2]	0.70
$6p_{3/2}$	$8d_{5/2}$	1349.7	5.75[7]	2.36[-2]	2.00	$6f_{7/2}$	$8g_{7/2}$	8993.1	2.05[5]	2.49[-3]	1.06
$6p_{1/2}$	$9d_{3/2}$	1134.5	3.32[7]	1.28[-2]	2.00	$6f_{7/2}$	$8g_{9/2}$	8992.8	5.75[6]	8.71[-2]	1.02
$6p_{3/2}$	$9d_{3/2}$	1265.5	4.13[6]	9.91[-4]	2.00	$6f_{5/2}$	$7g_{7/2}$	11 080.0	9.27[6]	2.28[-1]	0.14
$6p_{3/2}$	$9d_{5/2}$	1264.5	3.55[7]	1.28[-2]	2.00	$6f_{7/2}$	$7g_{7/2}$	11 097.6	3.42[5]	6.32[-3]	0.40
$6p_{1/2}$	$10d_{3/2}$	1096.8	1.86[7]	6.70[-3]	2.00	$6f_{7/2}$	$7g_{9/2}$	11 097.5	9.58[6]	2.21[-1]	0.40
$6p_{3/2}$	$10d_{3/2}$	1218.7	2.33[6]	5.18[-4]	2.00	$7f_{5/2}$	$9g_{7/2}$	14 176.9	2.43[6]	9.76[-2]	0.14
$6p_{3/2}$	$10d_{5/2}$	1218.0	1.78[7]	5.94[-3]	2.00	$7f_{7/2}$	$9g_{7/2}$	14 213.5	8.95[4]	2.71[-3]	0.48
$8p_{1/2}$	$10d_{3/2}$	6362.0	5.32[6]	6.45[-2]	0.44	$7f_{7/2}$	$9g_{9/2}$	14 212.8	2.51[6]	9.49[-2]	0.48
$8p_{3/2}$	$10d_{3/2}$	6727.3	8.83[5]	5.99[-3]	1.40	$7f_{5/2}$	$8g_{7/2}$	17 831.9	3.63[6]	2.31[-1]	0.84
$8p_{3/2}$	$10d_{5/2}$	6703.9	7.27[6]	7.34[-2]	2.62	$7f_{7/2}$	$8g_{7/2}$	17 889.8	1.34[5]	6.44[-3]	2.02
$9p_{1/2}$	$9d_{3/2}$	22 951.0	6.04[6]	9.54[-1]	5.76	$7f_{7/2}$	$8g_{9/2}$	17 888.6	3.76[6]	2.25[-1]	1.98
$9p_{3/2}$	$9d_{3/2}$	26 201.8	1.23[6]	1.26[-1]	1.60	$8f_{5/2}$	$9g_{7/2}$	26 875.8	1.58[6]	2.28[-1]	1.54
$9p_{3/2}$	$9d_{5/2}$	257 87.9	7.04[6]	1.05[0]	2.08	$8f_{7/2}$	$9g_{7/2}$	26 916.8	5.84[4]	6.35[-3]	2.72
$9p_{1/2}$	$10d_{3/2}$	135 31.2	3.49[6]	1.91[-1]	2.14	$8f_{7/2}$	$9g_{9/2}$	26 914.4	1.64[6]	2.22[-1]	2.64
$9p_{3/2}$	$10d_{3/2}$	14 599.1	6.29[5]	2.01[-2]	0.76	$6f_{5/2}$	$5g_{7/2}$	25 9501.0	6.50[3]	8.75[-2]	0.38
$9p_{3/2}$	$10d_{5/2}$	14 489.2	5.16[6]	2.43[-1]	2.68	$6f_{7/2}$	$5g_{7/2}$	269 498.3	2.15[2]	2.34[-3]	0.72
						$6f_{7/2}$	$5g_{9/2}$	269 469.7	6.01[3]	8.18[-2]	0.72
$8d_{3/2}$	$9p_{1/2}$	141 425.5	1.52[5]	2.27[-1]	0.84	$7f_{5/2}$	$6g_{7/2}$	401 690.2	5.58[3]	1.80[-1]	0.32
$8d_{3/2}$	$9p_{3/2}$	80 149.1	7.63[4]	7.35[-2]	0.42	$7f_{7/2}$	$6g_{7/2}$	433 260.4	1.64[2]	4.63[-3]	0.70
$8d_{5/2}$	$9p_{3/2}$	90 003.9	5.06[5]	4.10[-1]	0.46	$7f_{7/2}$	$6g_{9/2}$	433 259.8	4.60[3]	1.62[-1]	0.70
						$8f_{5/2}$	$7g_{7/2}$	601 311.0	3.72[3]	2.69[-1]	0.26
						$8f_{7/2}$	$7g_{7/2}$	622 543.7	1.24[2]	7.21[-3]	0.44
						$8f_{7/2}$	$7g_{9/2}$	622 387.1	3.48[3]	2.53[-1]	0.44

TABLE V. Comparison of our final values for the oscillator strengths with theoretical values given by Glowacki and Migdalek [29], Migdalek and Garmulewicz [26], and by Migdalek [22]. Uncertainties associated with the present all-order approach are given in parenthesis. These uncertainties do not account for the mixing of the one-particle and one-hole–two-particle configurations. References are given in square brackets.

Transitions		Present	Other
$6s_{1/2}$	$6p_{1/2}$	0.217(1)	0.200 [29]
$6s_{1/2}$	$6p_{3/2}$	0.512(3)	0.493 [29]
$6p_{1/2}$	$7s_{1/2}$	0.155(1)	0.164 [26]
$6p_{3/2}$	$7s_{1/2}$	0.199(2)	0.208 [26]
$6p_{1/2}$	$8s_{1/2}$	0.0231(1)	0.0212 [22]
$6p_{3/2}$	$8s_{1/2}$	0.0224(2)	0.0229 [22]
$6p_{1/2}$	$6d_{3/2}$	0.694(5)	0.684 [26]
$6p_{3/2}$	$6d_{3/2}$	0.081(1)	0.0791 [26]
$6p_{3/2}$	$6d_{5/2}$	0.719(9)	0.706 [26]
$6p_{1/2}$	$7d_{3/2}$	0.091(2)	0.137 [22]
$6p_{3/2}$	$7d_{3/2}$	0.0079(2)	0.0118 [22]
$6p_{3/2}$	$7d_{5/2}$	0.0764(15)	0.112 [22]
$6p_{1/2}$	$8d_{3/2}$	0.0291(6)	0.0498 [22]
$6p_{3/2}$	$8d_{3/2}$	0.0023(0)	0.003 89 [22]
$6p_{3/2}$	$8d_{5/2}$	0.0236(5)	0.0379 [22]
$7s_{1/2}$	$7p_{1/2}$	0.451(4)	0.446 [22]
$7s_{1/2}$	$7p_{3/2}$	1.08(12)	1.063 [22]
$7p_{1/2}$	$8s_{1/2}$	0.275(5)	0.268 [22]
$7p_{3/2}$	$8s_{1/2}$	0.36(8)	0.361 [22]

these properties are proportional to the squares of the matrix elements.

Comparison of the oscillator strengths given by Glowacki and Migdalek [29], Migdalek and Garmulewicz [26], and by Migdalek [22] with our theoretical values is illustrated by Table V. Uncertainties are given in parenthesis. Relativistic configuration-interaction approximation was used in Ref. [29] to evaluate oscillator strengths for the $6s$-$6p$ transitions. These two values are in a better agreement (7–10% difference) with our $f^{(\mathrm{DF}+2+3)}$ values. However, the theoretical oscillator strengths presented by Migdalek in Ref. [22] are in better agreement with our $f^{(\mathrm{DF})}$ values. It should be noted that we evaluate the $f^{(\mathrm{DF})}$ values with the Dirac-Fock energies, while the $f^{(\mathrm{DF}+2)}$ and $f^{(\mathrm{DF}+2+3)}$ values are calculated with recommended NIST energies [40].

There is small difference (1–5%) between our oscillator strength values and the $f^{(3)}$ values given in Ref. [31]. The approach used here differs from Ref. [31] by the treatments of the Breit interaction. In Ref. [31], Breit contributions to the Dirac-Fock potential was omitted and Breit corrections were included perturbatively in second-order MBPT. In the approach used in the present article, we include both Coulomb and Breit contributions to the Breit-Dirac-Fock potential and then treat the residual Breit and Coulomb interactions perturbatively. In the present work, we increase number of basis set orbitals up to 70 instead of 40 used in Ref. [31].

TABLE VI. Comparison of the Hg^+ lifetimes (in ns) with experiment. Uncertainties associated with the present all-order approach are given in parenthesis. These uncertainties do not account for the mixing of the one-particle and one-hole–two particle configurations. References are given in square brackets. Only decay channels via the one-particle states are considered. We note that some of the experimental values give the lifetimes due to only a single decay channel.

Level	Present	Expt.
$7s_{1/2}$	1.889(14)	1.99(10) [19]
$8s_{1/2}$	3.85(14)	
$9s_{1/2}$	7.10(12)	7.5(4) [1]
$10s_{1/2}$	11.62(24)	3.8(4) [1]
$6p_{1/2}$	2.610(15)	2.91(11) [19]
$6p_{3/2}$	1.594(10)	1.80(8) [19]
$7p_{1/2}$	11.89(11)	18.8(12) [1]
$7p_{3/2}$	9.56(96)	3.1(2) [1]
$8p_{1/2}$	63.9(6.0)	
$8p_{3/2}$	32.8(2.9)	
$9p_{1/2}$	134(63)	
$9p_{3/2}$	92.0(2.7)	
$6d_{3/2}$	1.300(9)	1.15(10) [19]
$6d_{5/2}$	1.548(20)	1.56(10) [19]
$7d_{3/2}$	3.535(58)	5.0(6) [1]
$7d_{5/2}$	4.44(18)	6.7(5) [1]
$8d_{3/2}$	7.44(15)	10.6(6) [1]
$8d_{5/2}$	9.52(17)	10.7(5) [1]
$9d_{3/2}$	13.31(17)	11.3(6) [1]
$9d_{5/2}$	14.55(62)	
$10d_{3/2}$	23.17(40)	18.9(17) [1]
$10d_{5/2}$	24.5(1.6)	
$5f_{5/2}$	5.58(9)	3.2(2) [1]
$5f_{7/2}$	6.04(4)	8.6(9) [1]
$6f_{5/2}$	14.96(36)	
$6f_{7/2}$	16.27(69)	
$7f_{5/2}$	30.79(43)	
$7f_{7/2}$	34.02(87)	
$8f_{5/2}$	54.6(1.2)	
$8f_{7/2}$	61.2(2.2)	
$5g_{7/2}$	14.37(71)	
$5g_{9/2}$	13.96(15)	
$6g_{7/2}$	23.32(35)	26.8(20) [1]
$6g_{9/2}$	23.99(69)	
$7g_{7/2}$	38.0(1.7)	
$7g_{9/2}$	36.43(65)	40.7(24) [1]
$8g_{7/2}$	55.6(2.7)	
$8g_{9/2}$	53.49(90)	
$9g_{7/2}$	84.8(4.6)	90(7) [1]
$9g_{9/2}$	81.5(1.3)	

IV. LIFETIMES IN Hg^+

We calculate lifetimes of the $ns_{1/2}$ ($n = 7$–11), np_j ($n = 6$–10), nd_j ($n = 6$–10), nf_j ($n = 5$–9), and ng_j ($n = 5$–9) states in Hg^+ using our final values of the dipole matrix elements and NIST data [40] for energies and then compare the values with available experimental data [1,19] in Table VI. The uncertainties in the lifetime values are obtained from the uncertainties in the matrix elements listed in Table II.

Our lifetime values for the $7s_{1/2}$ and $6d_j$ states agree with experimental measurements performed by Pinnington *et al.* [19] when experimental uncertainties are taken into account. There is a small difference (10–15%) between our τ values and Pinnington's measurements for the $6p_j$ states, but disagreement between our results and the measurements can be explained by considering only one channel for decay in Ref. [1]. For example, there are five channels for decay from the $7d_{3/2}$ level ($7d_{3/2} \rightarrow 6p_{1/2}, 7d_{3/2} \rightarrow 6p_{3/2}, 7d_{3/2} \rightarrow 7p_{1/2}$, $7d_{3/2} \rightarrow 7p_{3/2}$, and $7d_{3/2} \rightarrow 5f_{5/2}$). If we take into account only the $7d_{3/2} \rightarrow 6p_{1/2}$ channel with largest transition rate, we find $\tau^{(2)} = 5.105$ ns and $\tau^{(3)} = 5.450$ ns, which agrees perfectly with the experimental lifetime for the $7d_{3/2}$ state (5.0 ± 0.6 ns, see Table VI).

The theoretical and experimental studies of the $7p_j$ lifetime were presented by Maniak *et al.* in Ref. [2], who underlined very large differences in transition rates A_r for $6s_{1/2}$-$7p_j$. The ratio of transition rates obtained in different approximations was about 700 and 30 for the $6s_{1/2}$-$7p_{1/2}$ and $6s_{1/2}$-$7p_{3/2}$ transitions, respectively. As a result, the ratio of calculated lifetimes was equal to 11 for the $7p_{1/2}$ level and about two for the $7p_{3/2}$ level. It was underlined in Ref. [2] that there is a large contribution to the $7p_{3/2}$ lifetime from the $7p_{3/2} \rightarrow 5d^{-1}6s^2\ ^2D_{5/2}$ channel; however, we did not consider this channel in the present study. Regardless, experimental measurement for the lifetime of $7p_{1/2}$ level (14.5 ± 1.0 ns) is in good agreement with our $\tau^{(2)} = 15.52$ ns and $\tau^{(3)} = 15.31$ ns lifetimes.

V. STATIC MULTIPOLE POLARIZABILITIES OF THE 6*s* GROUND STATE OF Hg$^+$

The static multipole polarizabilities α^{Ek} of Hg$^+$ in its $6s$ ground state can be separated into two terms: a dominant first term from intermediate valence-excited states and a polarizability of the ionic core, which is evaluated in the RPA [58]. The accuracy of the RPA core value for the $E1$ polarizability is expected to be better than 5% [7]. There are no available comparisons of the RPA ionic core values for the $E2$ and $E3$ polarizabilities with accurate theoretical or experimental data, so we have no direct way to assign uncertainties to these values. We assign 5% uncertainties for the core $E2$ and $E3$ values as in the case of $E1$ polarizabilities. The ionic core polarizability has to be corrected for the presence of the valence electron. This small valence-core (vc) term is also calculated in the RPA. We assign 5% uncertainties to these values as in the case of the ionic core contributions.

The dominant valence contribution is calculated using the sum-over-state approach

$$\alpha_v^{Ek} = \frac{1}{2k+1} \sum_n \frac{|\langle nl_j \| r^k C_{kq} \| 6s \rangle|^2}{E_{nlj} - E_{6s}}, \qquad (8)$$

where $C_{kq}(\hat{r})$ is a normalized spherical harmonic and where nl_j is np_j, nd_j, and nf_j for k = 1, 2, and 3, respectively [59]. The reduced matrix elements in the above sum are evaluated using out final values of the reduced matrix elements and NIST energies [40]. The uncertainties in the lifetime values are obtained from the uncertainties in the matrix elements listed in Table II. We evaluate the final values together with uncertainties for the quadrupole and octupole matrix elements using procedure that was described above for the dipole matrix elements.

Contributions to dipole, quadrupole, and octupole polarizabilities of the $6s$ ground state are presented in Table VII.

TABLE VII. Contributions to multipole polarizabilities of the $6s$ state of Hg$^+$ in a_0^3. Uncertainties associated with the present all-order approach are given in parenthesis. These uncertainties do not account for the mixing of the one-particle and one-hole–two-particle configurations. The final results are compared with other theory [61].

Contr.	α^{E1}
$6p_{1/2}$	3.937(22)
$6p_{3/2}$	6.715(43)
(7–26)p_j	0.938(0)
Tail	0.004
Core	7.37(37)
vc	−0.040
Total	18.93(37)
α_{th}^{E1} [61]	19.49
Contr.	α^{E2}
$6d_{3/2}$	16.89(6)
(7–12)$d_{3/2}$	3.59(2)
(13–26)$d_{3/2}$	0.23(0)
$6d_{5/2}$	23.84(9)
(7–12)$d_{5/2}$	5.07(4)
(13–26)$d_{5/2}$	6.61(0)
Tail	2.6(0.8)
Core	37.1(1.9)
vc	−5.1(3)
Total	90.8(2.1)
Contr.	α^{E3}
$5f_{5/2}$	116.0(7.5)
$6f_{5/2}$	44.8(0.4)
$7f_{5/2}$	20.9(0.1)
$8f_{5/2}$	11.6(0)
(9–12)$f_{5/2}$	17.3
(13–18)$f_{5/2}$	7.4
(19–26)$f_{5/2}$	73.3
$5f_{7/2}$	159.6(2.5)
$6f_{7/2}$	56.6(0.7)
$7f_{7/2}$	25.7 (0.2)
$8f_{7/2}$	13.8 (0)
(9–12)$f_{7/2}$	19.8
(13–18)$f_{7/2}$	8.1
(19–26)$f_{7/2}$	39.2
Tail	13.7(4.1)
Core	171.5(8.6)
vc	0
Total	799(12)

The first two terms in the sum-over states for α^{E1}, α^{E2}, and α^{E3} contribute 92, 72, and 45%, respectively, of the totals. The remaining 28% of α^{E2} contribution from the (5–26)nd_j is divided in two parts, from (7–12)nd_j and (13–26)nd_j. The remaining 55% of α^{E3} contribution from the (6–26)nf_j states is divided into six parts: $6f_j$, $7f_j$, $8f_j$, (9–12)n_j, (13–18)nd_j, and (19–26)nd_j.

The rapid convergence of the sum-over states for α^{E1} has been emphasized in many publications (for example, Refs. [46,60]). We use recommended energies from NIST [40] and values of "final" matrix elements to evaluate terms in the sum with $n \leqslant 13$, and we use theoretical SD energies and wave functions to evaluate terms with $13 \leqslant n \leqslant 26$. The remaining contributions to α^{Ek} from basis functions with $27 \leqslant n \leqslant 70$ are evaluated in the DF approximation. These remainder tail contributions are assigned 30% uncertainties. As one can see from Table VII, sums over n for $n \leqslant 26$ in α^{E2} and α^{E3} essentially reproduce the final results, since the contributions from $27 \leqslant n \leqslant 70$ are rather small (0.2, 3, and 2% for the $E1$, $E2$, and $E3$ polarizabilities, respectively). The final result for the $E1$ polarizability of the ground state Hg$^+$ is compared in Table VII with the theoretical result from Ref. [61].

Static dipole polarizability α_{6s} of Hg$^+$ was calculated by Iliaš and Neogrády [61] using the relativistic one-component spin-averaged Douglas-Kroll (DK) no-pair approximation combined with the coupled cluster with single- and double-excitation amplitudes (CCSD) treatment of the electron correlation. Different values for α_{6s} were obtained by use of different approaches, for example, the α_{6s} is equal to 22.59 a.u. and 19.49 a.u. in the DK approach and CCSD approaches, respectively. Our value (18.93) is 3% smaller than the CCSD value.

VI. HYPERFINE CONSTANTS FOR ^{199}Hg$^+$ AND ^{201}Hg$^+$

Calculations of hyperfine constants follow the pattern described earlier for calculations of transition matrix elements. In Table VIII, we list hyperfine constants A for ^{199}Hg$^+$ and ^{201}Hg$^+$ and compare our values with available theoretical and experimental results from Ref. [3].

In this table, we present the lowest-order $A^{(\mathrm{DF})}$, all-order $A^{(\mathrm{SD})}$, and $A^{(\mathrm{SDpT})}$ values for the ns, np, and nd levels up to $n = 7$. It should be noted that the values of $A^{(\mathrm{SDpT})}$ are obtained by using single-double all-order method, including partial triple excitations. The difference between $A^{(\mathrm{SD})}$ and $A^{(\mathrm{SDpT})}$ is about 0.1–2%, while the ratios of $A^{(\mathrm{SD})}$ and $A^{(\mathrm{DF})}$ are equal to 0.6–1.6 for some cases. We compare our $A^{(\mathrm{SD})}$ and $A^{(\mathrm{SDpT})}$ values with the $A^{(\mathrm{DF+2+3})}$ values evaluated in the third-order RMBPT (see also Ref. [31]). The difference between the $A^{(\mathrm{SD})}$ and $A^{(\mathrm{DF+2+3})}$ gives the contributions of the fourth-order and other high-order RMBPT. The largest difference between $A^{(\mathrm{SD})}$ and $A^{(\mathrm{DF+2+3})}$ (about 30 and 40%) occurred for the $6d_{3/2}$ and $6d_{5/2}$ levels. The smallest difference (about 0.4–0.6%) is for the $7s_{1/2}$ and $6p_{1/2}$ levels. For other levels given in Table VIII, the difference between $A^{(\mathrm{SD})}$ and $A^{(\mathrm{DF+2+3})}$ is about 3–7%.

TABLE VIII. Hyperfine constants A (in MHz) in Hg$^+$. The SD and SDpT (single-double all-order method including partial triple excitations) data are compared with experimental results.

Level	$A^{(\mathrm{DF})}$	$A^{(\mathrm{SD})}$	$A^{(\mathrm{SDpT})}$	$A^{(\mathrm{theor.})}$	$A^{(\mathrm{expt.})}$
		Hg$^+$, $I = 1/2$, $\mu = 0.505\,885\,2$ [64]			
$6s_{1/2}$	34002	41909	41477	42366[a]	40460[a]
$7s_{1/2}$	6470	7506	7422	6730[a]	
$6p_{1/2}$	5482	7063	6984	7116[a]	6970[a]
$6p_{3/2}$	454	651	642	659[a]	
$6d_{3/2}$	55.0	96.2	94.4	92.2[a]	
$6d_{5/2}$	22.4	36.8	36.2	45.3[a]	
$7p_{1/2}$	1433	1578	1562		
$7p_{3/2}$	132	196	195		
$7d_{3/2}$	25.8	42.3	41.7		
$7d_{5/2}$	10.5	16.8	16.6		
		^{201}Hg$^+$, $I = 3/2$, $\mu = -0.560\,225$ [64]			
$6s_{1/2}$	−12551	−15470	−15311	−15527[a]	−14960[a]
$7s_{1/2}$	−2388	−2771	−2740	−2466[a]	
$6p_{1/2}$	−2023	−2607	−2578	−2608[a]	−2610[a]
$6p_{3/2}$	−167	−240	−237	−241[a]	
$6d_{3/2}$	−20.3	−35.5	−34.8	−33.8[a]	
$6d_{5/2}$	−8.27	−13.60	−13.35	−16.6[a]	
$7p_{1/2}$	−529	−582	−577		
$7p_{3/2}$	−48.9	−72.3	−71.9		
$7d_{3/2}$	−9.54	−15.60	−15.38		
$7d_{5/2}$	−3.87	−6.21	−6.13		

[a]The data are compared with theoretical and experimental results from Ref. [3].

TABLE IX. Hyperfine constants B (in MHz) in ^{201}Hg$^+$. Nuclear quadrupole moment Q is taken to be 0.455b in barns ($1\mathrm{b} = 10^{-24}$ cm^2) [3]. The SD and SDpT (single-double all-order method including partial triple excitations) data are compared with other theoretical results [3].

Level	$\frac{B^{(\mathrm{DF})}}{Q}$	$\frac{B^{(\mathrm{SD})}}{Q}$	$\frac{B^{(\mathrm{SDpT})}}{Q}$	$B^{(\mathrm{DF})}$	$B^{(\mathrm{SD})}$	$B^{(\mathrm{SDpT})}$	$B^{(\mathrm{th})}$
$6p\ ^2P_{3/2}$	927	1451	1434	422	660	652	659
$7p\ ^2P_{3/2}$	270	357	355	123	163	161	
$6d\ ^2D_{3/2}$	38.0	127	126	17.3	57.9	57.1	28.7
$7d\ ^2D_{3/2}$	17.9	50.3	49.8	8.14	22.9	22.7	
$6d\ ^2D_{5/2}$	46.6	165	163	21.2	75.1	74.1	34.1
$7d\ ^2D_{5/2}$	21.8	65.3	64.7	9.92	29.7	29.5	

Our results for the hyperfine constants B in ^{201}Hg$^+$ are compared with theoretical values from Ref. [3] in Table IX. The nuclear quadrupole moment Q in ^{201}Hg$^+$ was taken to be 0.455 b ($1\mathrm{b} = 10^{-24}$ cm^2) [3]. The first three columns of Table IX list the $B^{(\mathrm{DF})}$, $B^{(\mathrm{SD})}$, and $B^{(\mathrm{SDpT})}$ values divided by nuclear quadrupole moment Q. The next three columns list the $B^{(\mathrm{DF})}$, $B^{(\mathrm{SD})}$, and $B^{(\mathrm{SDpT})}$ values. The ratios $B^{(\mathrm{SD})}$ and $B^{(\mathrm{DF})}$ are equal to 1.5–2.7 for some cases. In the last column of Table IX, we show few available theoretical values of B constants.

VII. HYPERFINE-INDUCED TRANSITION POLARIZABILITY OF THE ^{199}Hg II AND ^{201}Hg II GROUND STATES

We now turn to the calculation of the quadratic Stark shifts of the ground-state hyperfine interval ($F = 1 - F = 0$) in ^{199}Hg$^+$ and the ground-state hyperfine interval ($F = 2 - F = 1$) in ^{201}Hg$^+$. The quadratic Stark shift is closely related to the blackbody radiation shift discussed, for example, in Refs. [32,33,62,63]. Our calculation follows the methodology outlined in those works. The dominant second-order contribution to the polarizability cancels between the two hyperfine components of the $6s$ state so the Stark shift of the hyperfine interval is governed by the the third-order F-dependent polarizability $\alpha_F^{(3)}(0)$. The expression for the $\alpha_F^{(3)}(0)$ is [32]:

$$\alpha_F^{(3)}(0) = \frac{1}{3}\sqrt{(2I)(2I+1)(2I+2)} \begin{Bmatrix} j_v & I & F \\ I & j_v & 1 \end{Bmatrix} \times g_I \mu_n (-1)^{F+I+j_v} (2T + C + R), \tag{9}$$

where g_I is the nuclear gyromagnetic ratio, μ_n is the nuclear magneton equal to 0.505 885 2 [64] for $^{199}\mathrm{Hg}^+$, I is the nuclear spin, and $j_v = 1/2$ is the total angular momentum of the atomic ground state. The formulas for the F-independent terms T, C, and R are given in Ref. [62]. These terms are similar to the polarizability sum-over-state expression but are more complicated.

We note, first, that in the DF approximation the values of T, C, and R in atomic units for $^{199}\mathrm{Hg}^+$ are

$$\begin{gathered}2T^{\mathrm{DF}} = 5.8545\times10^{-4},\quad C^{\mathrm{DF}} = 1.4482\times10^{-5},\\ R^{\mathrm{DF}} = 8.8095\times10^{-4}.\end{gathered}\tag{10}$$

Since the value of C^{DF} is smaller than the T^{DF} and R^{DF} by almost two orders of magnitude, we do not recalculate the C term in the SD approximation.

The expression for R is similar to that for α^{E1} [32]. The difference is an additional factor of the diagonal hyperfine matrix element:

$$\begin{aligned}{}^{199}\langle 6s_{1/2}\|\mathcal{T}\|6s_{1/2}\rangle^{(\mathrm{SD})} &= 7.4523\times10^{-6}\ \text{a.u.}\\ {}^{201}\langle 6s_{1/2}\|\mathcal{T}\|6s_{1/2}\rangle^{(\mathrm{SD})} &= -3.8797\times10^{-5}\ \text{a.u.}\end{aligned}$$

We use our all-order recommended values for the reduced electric-dipole matrix elements described in Sec. III A and their uncertainties to calculate the main terms in the T and R sums. We refer to these values as the "best set" values. Available recommended NIST energies [40] are used for $nl = 6s$-$10s$, $6p$-$8p$, and SD energies are used for the other states up to $n = 26$. The sum of terms for $n \leqslant 26$ is $R_{n\leqslant 26} = 4.728(20)\times10^{-4}$ for $^{199}\mathrm{Hg}^+$. The remainder of the sum, evaluated in the Dirac-Hartree-Fock (DHF) approximation, $R_{n>26} = 1.4\times10^{-7}$ that gives $R^{\mathrm{final}} = 4.729(20)\times10^{-4}$.

Term T contains two sums, over ns and over mp_j. We evaluate main contributions that include $n \leqslant 26$ and $m \leqslant 26$ using all-order matrix elements and NIST or all-order energies as described above. We find that the remaining contributions with $n > 26$ and $m > 26$ are very small. We break down each mp term as

$$\sum_{mp}\left(\sum_{7s}^{26s}[\ldots] + \sum_{27s}^{70s}[\ldots]\right).$$

Each term inside the square brackets is given by

$$A_T\frac{\langle 6s\|D\|mp_j\rangle\langle mp_j\|D\|ns\rangle\langle ns\|\mathcal{T}\|6s\rangle}{(E_{mp}-E_{6s})(E_{ns}-E_{6s})},\tag{11}$$

where A_T is an angular factor. Our final value for this term is $2T^{\mathrm{final}} = 3.838(22)\times10^{-4}$ for $^{199}\mathrm{Hg}^+$. Combining these contributions, we obtain for $^{199}\mathrm{Hg}^+$

$$2T^{\mathrm{final}} + C^{\mathrm{DF}} + R^{\mathrm{final}} = 8.712(30)\times10^{-3}\ \text{a.u.}.\tag{12}$$

The F-dependent factor [see Eq. (9)]

$$\begin{aligned}A(F) = {}&\frac{g_I\mu_n}{3I}\sqrt{(2I)(2I+1)(2I+2)}\\ &\times\begin{Bmatrix} j_v & I & F\\ I & j_v & 1\end{Bmatrix}(-1)^{F+I+j_v}\end{aligned}$$

is equal to $-0.413\,053\,5$ for $F = 0$ and $0.137\,684\,5$ for $F = 1$ in the case of $^{199}\mathrm{Hg}^+$ isotope and is equal to $0.254\,123\,2$ for $F = 1$ and $-0.152\,473\,9$ for $F = 2$ in the case of $^{201}\mathrm{Hg}^+$ isotope. Using these values and the result from Eq. (12), we obtain for two isotopes

$$\begin{aligned}{}^{199}\alpha^{(3)}_{F=1}(0) - \alpha^{(3)}_{F=0}(0) &= 4.798(16)\times10^{-4}\ \text{a.u.}\\ {}^{201}\alpha^{(3)}_{F=2}(0) - \alpha^{(3)}_{F=1}(0) &= -3.452(12)\times10^{-4}\ \text{a.u.}.\end{aligned}$$

The Stark shift coefficient k defined as $\Delta\nu = kE^2$ is $k = -\frac{1}{2}[\alpha^{(3)}_{F=1}(0) - \alpha^{(3)}_{F=0}(0)]$ for $^{199}\mathrm{Hg}^+$ and $k = -\frac{1}{2}[\alpha^{(3)}_{F=2}(0) - \alpha^{(3)}_{F=1}(0)]$ for $^{201}\mathrm{Hg}^+$. Converting from atomic units, we obtain

$$\begin{aligned}{}^{199}k^{(\mathrm{SD})} &= -2.399(8)\times10^{-4}\text{a.u.} = -5.969(20)\\ &\quad\times10^{-12}\ \mathrm{Hz/(V/m)^2},\\ {}^{201}k^{(\mathrm{SD})} &= 1.726(6)\times10^{-4}\text{a.u.} = 4.295(15)\\ &\quad\times10^{-12}\ \mathrm{Hz/(V/m)^2}.\end{aligned}$$

In the lowest-order DF approximation [Eq. (10)], we find $k^{(\mathrm{DF})} = -10.147\times10^{-12}\mathrm{Hz/(V/m)^2}$ in the case of the $^{199}\mathrm{Hg}^+$ isotope.

The relative blackbody radiative shift β is defined as

$$\beta = -\frac{2}{15}\frac{1}{\nu_{\mathrm{hf}}}(\alpha\pi)^3\,T^4\alpha_{\mathrm{hf}}(6s_{1/2}),\tag{13}$$

where ν_{hf} is the $^{199}\mathrm{Hg}^+$ hyperfine ($F = 1$ and $F = 0$) splitting equal to 40507.347997 MHz [4] and the $^{201}\mathrm{Hg}^+$ hyperfine ($F = 2$ and $F = 1$) splitting equal to 29920 MHz [3]. T is a temperature that we take to be 300 K. Using those factors, we can rewrite Eq. (13) as

$$^{199}\beta = -2.1258\times10^{-13}\alpha^{199}_{\mathrm{hf}}(6s_{1/2}),\tag{14}$$

$$^{201}\beta = 2.8781\times10^{-13}\alpha^{201}_{\mathrm{hf}}(6s_{1/2}).\tag{15}$$

Using the final value for $\alpha^{199}_{\mathrm{hf}}(6s_{1/2}) = 4.798(16)\times10^{-4}$ a.u. and $\alpha^{201}_{\mathrm{hf}}(6s_{1/2}) = -3.452(12)\times10^{-4}$ a.u, we obtain, finally,

$$^{199}\beta^{(\mathrm{final})} = -1.020(3)\times10^{-16},\tag{16}$$

$$^{201}\beta^{(\mathrm{final})} = -0.994(3)\times10^{-16},\tag{17}$$

Our result for $^{199}\mathrm{Hg}^+$ isotope is in an excellent agreement with result $-1.02(5)\times10^{-16}$ from Ref. [65]. Such an excellent agreement between results obtained by use of different methods is very important when correlation contributions are so large.

VIII. CONCLUSION

In summary, a systematic all-order study of the properties of the $ns_{1/2}$, np_j, nd_j, $n'f_j$, and $n'g_j$, ($n \leqslant 10$, $n' \leqslant 9$) states in singly ionized mercury is presented. The energy values are in excellent agreement with existing experimental data. Reduced matrix elements, oscillator strengths, and transition rates for electric-dipole transitions, including the $6s$-$11s$, $6p$-$10p$, $6d$-$10d$, $5f$-$9f$, and $5g$-$9g$ states, are calculated. Lifetime values are determined for all above-mentioned states, and electric-dipole ($6s_{1/2}$-np_j, $n = 6$–12) matrix elements are calculated to obtain the ground-state $E1$ polarizability. We evaluate the uncertainties of our calculations for most of the values listed in this work. Hyperfine A and B values for the $^{199}\mathrm{Hg}^+$ and $^{201}\mathrm{Hg}^+$ ions are presented for the first low-lying levels up to $n = 7$. The quadratic Stark shifts of the ground-state hyperfine intervals in ^{199}Hg$^+$ and ^{201}Hg$^+$ and corresponding values of the BBR shifts are also evaluated. These calculations provide a theoretical benchmark for comparison with experiment and theory.

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