All-electron Dirac-Coulomb and RECP calculations of excitation energies for mercury atom with combined CI/MBPT2 method.

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Abstract

Calculations of transition energies between low-lying states of mercury atom are performed in the frame of combined CI/MBPT2 method. Results of all-electron relativistic calculations (using the Dirac-Coulomb Hamiltonian) are compared with experimental data and results of other four-component calculations. The results of the RECP calculations are compared with the corresponding all-electron results in order to estimate accuracy of different RECPs. Contributions from correlations in different shells to the calculated excitation energies as well as effects of basis set truncation at different orbital angular momenta, nuclear models, errors in gaussian approximation of the GRECP components are reported. Analysis of the obtained results shows that at least 34 external electrons of mercury atom should be correlated and the one-electron basis set should contain up to $l$ angular momentum functions in order to reach a reliable agreement with experimental data within 200 cm$^{-1}$. It is concluded that correlations of the 4$f$ electrons can be efficiently taken into account for 20 electron GRECP at the generation stage.

SHORT NAME: CI/MBPT2 calculations of mercury.

KEYWORDS FOR INDEXING: Configuration Interaction, Many Body Perturbation Theory, correlation structure (electronic structure), excitation energies (transition energies), Relativistic Effective Core Potential (pseudopotential), four-component calculations, mercury, heavy atoms.
I. INTRODUCTION

During the last few years, a considerable number of papers devoted to electronic structure calculations of heavy atoms have been published (e.g., see [1–3]) that is not only due to experimental requirements but because they are good test systems to check or estimate accuracy of different approximations before using them in more expensive molecular calculations.

In paper [4], Generalized Relativistic Effective Core Potentials (GRECPs) were tabulated for atoms Hg through Rn and were tested in numerical Hartree-Fock (HF) calculations by comparison with the all-electron Dirac-Fock (DF) and other RECP ones. However, the question of quality of the GRECPs for description of correlation effects was not clarified yet. Whereas paper [5] contains an answer on this question from theoretical point of view, the present paper is devoted to our correlation structure calculations for mercury atom. For this atom, the RECPs were generated by other groups [6,7] where the same number of electrons (20) was explicitly included into calculations as in the case of the GRECP [4]. Therefore, one should expect about the same computational expenses in calculations with all these RECPs and the comparison of their accuracy appears to be of practical interest.

II. METHODS AND BASIS SETS

The GRECP method was described in details in papers [3,4]. The main distinguishing features of this method are presence of non-local terms with the projectors on the outercore (OC) pseudospinors together with the standard semi-local ones in the effective potential operator and generation of the effective potential components for smoothed pseudospinors which may have nodes [9].

Theory of the CI/MBPT2 method is presented in papers [2]. In this method, the correlations in the valence (V) region of an atom which are the most important ones are treated by the Configuration Interaction (CI) method (which is able to provide excellent results for the small number of correlated electrons) whereas the relatively small contributions to the considered low excitation energies from the large number of the core-valence correlations are taken into account with the help of less expensive second order Many Body Perturbation Theory (MBPT2).

The program (in the $jj$-coupling scheme) for all-electron relativistic four-component CI/MBPT2 calculations (using the Dirac-Coulomb Hamiltonian) was modified to make possible two-component RECP calculations (with the nonrelativistic kinetic energy operator and relativistic $j$-dependent potentials). This program allows one to use two different basis sets of numerical spinors at the CI and MBPT2 calculation stages for description of the correlations taking into account a space separation of the core and valence regions. Basis functions for the present calculations were obtained from numerical SCF (DF or HF) calculations of the corresponding spinors for positive ion states. For example, the $[4,4,3,2,1]$ basis set for the 2 electron valence CI (2e-CI) was derived from the calculations for the following nonrelativistically averaged configurations of Hg: $5d^{10}6s^2$, $[5d^8]7s^1$, $[5d^8]8s^1$, $[5d^9]9s^1$, $[5d^{10}]$. 

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al. in the RECPs \[6,7\]; see \[8,5\] for details).

(first of all, due to the neglect of the difference between the outer core and valence potentials about 30 times more accurate than the 20 electron energy-adjusted PseudoPotential (PP) \[7\].

GRECP is about 8 times more accurate than the 20 electron RECP of Ross.

correlations and that the RECP errors are rather stable in respect to the basis set size but for the small ones as well. In fact, the calculated RECP errors depend only slightly on the size of such basis sets.

III. RESULTS AND DISCUSSION

Series of the correlation structure calculations were performed for the number of correlated electrons varied from 2 to 34 and one-electron basis sets truncated at the orbital quantum numbers from 2 to 5. The all-electron relativistic calculations were implemented for two nuclear models: a point nucleus and an uniformly charged ball with $1.334 \cdot 10^{-4}$ a.u. radius. The GRECP calculations were made with both the numerical GRECP components and their gaussian expansions from [4]. Moreover, 34 electron GRECP variant (where the outercore $4f, 5s, 5p, 5d$ and valence $6s, 6p$ shells of mercury atom are explicitly treated in calculations) was generated and tested in these calculations.

The results of the 2e-CI calculations (where all the possible excitations of 2 valence electrons were considered and the core 1s$_{1/2}$–5d$_{5/2}$ spinors were frozen from the SCF calculations of the ground state with the 6s$^2$ configuration) are presented in tables [4] and [11] for [8, 8, 7, 6, 5, 4] and [4, 4, 3, 2, 1] basis sets. One can see from these tables that the use of the [4, 4, 3, 2, 1] basis set allows one to describe adequately the V-V correlations and that the RECP errors are rather stable in respect to the basis set size variation. Whereas the correlations only in the valence region are considered, the 20 electron GRECP is about 8 times more accurate than the 20 electron RECP of Ross et al. [3] and about 30 times more accurate than the 20 electron energy-adjusted PseudoPotential (PP) [6] (first of all, due to the neglect of the difference between the outercore and valence potentials in the RECPs [3, 4]; see [8, 9] for details).

From tables III and IV in [4] one can see that the errors of the energy-adjusted PP, Ross et al.’s RECP, and the GRECP for the excitations from the 6s$^2$ ground state to the 6s$_{1/2}$d$^2$$(J = 0)$...
and $6s_{1/2}^1 6p_{3/2}^1 (J = 2)$ states are -667 and +347 cm$^{-1}$, +182 and +224 cm$^{-1}$, -9 and -9 cm$^{-1}$, correspondingly. They are in agreement with the errors from tables I and II here with an exception of the GRECP errors (because the main contribution to the GRECP errors is due to errors of reproducing the two-electron integrals rather than drawbacks of the effective potential operator).

In tables I–V, results of both the all-electron relativistic and 20 electron GRECP calculations are presented for different numbers of correlated electrons using the equivalent basis sets. One can see that the 2e-CI (table II) gives only rough description of the correlation structure of mercury atom, the errors in energies of excitations from the ground state are 3000–6000 cm$^{-1}$ in respect to the experimental data or the most elaborated calculations in table V. Such a large deviation is mainly due to neglect of the OC-V correlations involving the 5d shell. Their consideration (in the 12e-CI/MBPT2, table III) reduces these errors to a level of about 1000 cm$^{-1}$. The contributions from the correlations with the 5p and 5s shells (the 18e-CI/MBPT2 and 20e-CI/MBPT2, tables III and V) to the excitation energies are 400–600 cm$^{-1}$ and about -300 cm$^{-1}$, correspondingly. However, these contributions are mainly compensated and the total contribution from the correlations with both these shells is only 100–300 cm$^{-1}$. The correlations with the 4f shell (the 34e-CI/MBPT2, table V) give an essential contribution that is 600–700 cm$^{-1}$. Our final all-electron results for transitions between the first four states are within 200 cm$^{-1}$ with the experimental data and the Relativistic Coupled Cluster (RCC) calculation results of Eliav et al. A relatively large deviation for the last state is rather due to the MBPT2 approximation than due to basis set incompleteness or correlations in more inner shells. Our estimates show that the contribution from the correlations with the 4d shell to the excitation energies is of order of 100 cm$^{-1}$.

When only the V-V correlations are considered (tables I and II), the GRECP errors in reproducing the all-electron results are within 30 cm$^{-1}$. This is a good confirmation to our previous estimates that the GRECP describes the electronic structure in the valence region with a high accuracy. However, the consideration of the correlations in the outercore region (tables III and IV) leads to an increase of these errors (due to a rather large smoothing region for the nodeless outercore 5s, 5p, 5d pseudospinors) up to 200 cm$^{-1}$. These results are in a good agreement with that from table III in paper where a significant increase in the GRECP errors can be observed for the case of excitations from the 5d shell. One should expect that the contribution from the correlations

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1 Analysis for the case of the $6s_{1/2}^1 6p_{3/2}^1 (J = 1)$ and $6s_{1/2}^1 6p_{3/2}^1 (J = 1)$ SCF states is more complicated because they are strongly mixed in the CI calculations.

2 Electrons are included in the calculations in the following order: 6p, 6s; 5d; 5p; 5s; 4f; ...

3 We suggest that these GRECP errors can be seriously reduced due to more artificial generator configuration selection and smoothing procedure and with the help of corrections to the GRECP operator (see [6], subsection 4.5) because these errors arise from electronic structure reorganization in the outercore region.
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the outercore region to low excitation energies and GRECP errors in their reproducing
will be reduced when passing from Hg toward Rn.

The errors of different RECPs for the case of 20 correlated electrons are presented in
Table I. The errors of the GRECP are only about 4 times less than that of Ross et al.’s
RECP $^6$ and about 7
times less than that of the energy-adjusted PP $^7$ for the same number of electrons
explicitly included in calculations. This is also in agreement with the results from Table III
in paper $^4$ where the ratio between GRECP errors and errors of the other RECPs was
reduced from one order of magnitude (when excitations only for the valence electrons were
under consideration) to 1.5–2 times (for the case of excitations from the outercore shells
described by nodeless pseudospinors). In fact, additional changes in the RECP errors when
the OC-V correlations are taken into account (Tables I and II) are within 200 cm$^{-1}$ for the
used GRECP variants and within 400 cm$^{-1}$ for the other RECPs. The main reason is the
spinor smoothing which has similar features for all these RECPs.

The data from the MRCI calculations with the energy-adjusted PP using the CIPSO
method for the transitions between the first four states from Table 6 in paper $^7$ are within
100 cm$^{-1}$ with the experimental data but the 20 electron PP does not take into account
contributions from the correlations with the 4f shell (which are up to
700 cm$^{-1}$) and the used basis set does not contain functions with $h$ orbital momentum
(their contributions are up to 300 cm$^{-1}$). Therefore, these data are results from cancelation
of a few contributions: PP errors (e.g., the $6s_{1/2}6p_{1/2}^1(J = 0)–6s_{1/2}6p_{3/2}^1(J = 2)$ splitting is
overestimated about 1000 cm$^{-1}$ by the energy-adjusted PP because of the features of the
spin-orbit simulation in the $LS$-based variant of the energy-adjusted scheme), a neglect of
the correlations with the 4f shell, a basis set incompleteness, etc. The estimation of error
for these data within 5% $^8$ appears to be correct. The data in paper $^10$ were obtained
with the 12 electron RECP of Ross et al. which differs from the used here 20 electron RECP.

One can see from Tables I, II, and IV that the errors of the 20 and 34 electron GRECPs
are of the same order of magnitude because the main distinctions between these GRECP
variants are

inclusion of the 4f electrons in calculations with the 34 electron GRECP and smoothing
the 5f spinors for the 20 electron GRECP. However, the 34 electron GRECP allows one to
take into account explicitly the correlations with the 4f shell which are important for an
agreement with the experimental data within 200 cm$^{-1}$. As one can see from Table V, the
34 electron GRECP errors are within 200 cm$^{-1}$ in this case.

The basis set truncation effect at different orbital quantum numbers on energies of exci-
tations from the ground state can be observed in Tables III and IV for the 34e-CI/MBPT2
calculations. It is clear that ($spd$) correlation basis set$^6$ does not allow one to take into
account the correlations with the 5d shell properly. This leads to the excitation energies
(table IV) rather close to that from the 2e-CI calculations. Addition of functions

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$^4$ The [12, 12, 11, 1] basis set contains only such functions with $f$ orbital momentum which corre-
 respond to the 4f$_{5/2}$ and 4f$_{7/2}$ spinors.
with \(f\) orbital momentum is crucial for description of these correlations and leads to an increase in the excitation energies on 2000–4000 cm\(^{-1}\). The excitation energies for the \((spdf)\) basis set are within 900 cm\(^{-1}\) from that for the \((spdfgh)\) basis set (tables \(V\) and \(VI\)). In turn, \((spdf)\) basis set is inadequate for description of the correlations with the \(4f\) shell. The results for this basis set are rather close to that from the 20e-CI/MBPT2 calculations in table \(V\). Addition of functions with \(g\) orbital momentum is necessary for the correct description of these correlations and gives the contribution 300–600 cm\(^{-1}\) to the excitation energies (table \(VII\)) whereas addition of \(h\) functions contributes about 300 cm\(^{-1}\) (table \(V\)). Our test calculations showed that the contribution from functions with \(i\) orbital momentum is of order 50 cm\(^{-1}\).

One can see from comparison between the 6 and 7 columns in tables \(I\), \(II\), and \(IV\) that the errors due to the gaussian approximation of the GRECP components are approximately one order of magnitude less than the errors of the numerical GRECP. As one can see from tables \(I\), \(II\), \(IV\), and \(V\) the effects of different nuclear models may be neglected for accuracy within 200 cm\(^{-1}\).

### IV. CONCLUSIONS

The GRECP allows one to reproduce the electronic structure in the valence and outercore regions essentially better than the other tested RECPs for the same number of explicitly treated electrons.

At least 34 external electrons (occupying the \(4f, 5s, 5p, 5d, 6s, 6p\) shells) of mercury atom should be correlated and the one-electron basis set should contain up to \(h\) angular momentum functions in order to obtain a reliable agreement with experimental data for low excitation energies within 200 cm\(^{-1}\) whereas the errors of the gaussian approximation of the GRECP components and the effects of different nuclear models are negligible for this accuracy. However, our test calculations show that the main contribution from the correlations with the \(4f\) shell is due to the one-electron correction from the self-energy diagrams \(2\), therefore, this contribution can be taken into account for 20 electron GRECP with the help of the technique proposed in \(I\) (subsection 5.2).

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TABLE I. All-electron and RECP correlation energies\textsuperscript{a}, all-electron transition energies (TE) and absolute errors (AE) of different RECPs in their reproducing from the 2 electron valence CI calculations of low-lying states of Hg for the [8, 8, 7, 6, 5, 4] basis set (in cm\textsuperscript{-1}).

| Symmetry | Leading configuration | All-el. symmetry | 20 el. RECP energy | 20 el. RECP energy |
|----------|----------------------|------------------|--------------------|--------------------|
|          |                      | finite point nucl. | GreCP num.       | GreCP num. gaus. et al. |
|          |                      | 34 el. nucl. |                   |                   |
|          |                      | 20 el.        |                   |                   |
| 0\textsubscript{g} | 6s\textsubscript{1/2}       | -5991 | -6019 | -6023 | -6024 | -6006 | -5990 |
| 0\textsubscript{u} | 6s\textsubscript{1/2}6p\textsubscript{1/2} | -922  | -927  | -927  | -927  | -926  | -933  |
| 1\textsubscript{u} | 6s\textsubscript{1/2}6p\textsubscript{1/2}       | -6919 | -6936 | -6937 | -6937 | -6923 | -6735 |
| 2\textsubscript{u} | 6s\textsubscript{1/2}6p\textsubscript{3/2} | -1108 | -1111 | -1112 | -1112 | -1111 | -1116 |
| 1\textsubscript{u} | 6s\textsubscript{1/2}6p\textsubscript{3/2}       | 171   | 164   | 163   | 163   | 171   | 17    |
|           |                      | 0\textsubscript{g} | -5987 | -6023 | -6024 | -6006 | -5990 |
|           |                      | 0\textsubscript{u} | -922  | -927  | -927  | -926  | -933  |
|           |                      | 1\textsubscript{u} | -6916 | -6937 | -6937 | -6923 | -6735 |
|           |                      | 2\textsubscript{u} | -1108 | -1111 | -1112 | -1111 | -1116 |
|           |                      | 1\textsubscript{u} | 172   | 163   | 163   | 171   | 17    |

\textsuperscript{a}The correlation energies were calculated as a difference between the total energies from the above mentioned CI calculations and the numerical SCF calculations with the frozen core 1s\textsubscript{1/2}–5d\textsubscript{5/2} spinors for the corresponding terms.

\textsuperscript{b}The 6s\textsubscript{1/2}6p\textsubscript{1/2} and 6s\textsubscript{1/2}6p\textsubscript{3/2} configurations are strongly mixed for these terms in the CI calculations.

\textsuperscript{c}The RECP from Ref. [6].

\textsuperscript{d}The PP from Ref. [7] with the corrected \( V_{so} \) by the factors \((2l + 1)/2\) (M. Dolg, private communication).
TABLE II. All-electron and RECP correlation energies$^a$, all-electron transition energies (TE) and absolute errors (AE) of different RECPs in their reproducing from the 2 electron valence CI calculations of low-lying states of Hg for the \([4, 4, 3, 2, 1]\) basis set (in \(\text{cm}^{-1}\)).

| Symmetry \((J_{parity})\) | Leading \((J_{parity})\) | All-el. \(34\) el. | 20 el. RECP of Ross | 20 el. energy-adjusted RECP et al.$^c$ | 20 el. PP$^d$ |
|---------------------------|----------------------|------------------|-------------------|---------------------------|----------------|
|                           | conf.                | finite point nucl. | GRECP num. | GRECP num. gaus. | GRECP num. gaus. | GRECP num. gaus. |
| \(0_g\)                   | \(6s_{1/2}^2\)       | -5927 \(-5923\) | -5954 \(-5964\) | -5965 \(-5941\) | -5924 \(-5941\) |
| \(0_u\)                   | \(6s_{1/2}^1 6p_{1/2}^1\) | -909 \(-910\) | -914 \(-915\) | -915 \(-913\) | -919 \(-919\) |
| \(1_u\)                   | \(6s_{1/2}^1 6p_{1/2}^1\) | -6903 \(-6900\) | -6920 \(-6922\) | -6923 \(-6907\) | -6718 \(-6718\) |
| \(2_u\)                   | \(6s_{1/2}^1 6p_{3/2}^1\) | -1097 \(-1097\) | -1100 \(-1101\) | -1101 \(-1100\) | -1106 \(-1106\) |
| \(1_u\)                   | \(6s_{1/2}^1 6p_{3/2}^1\) | 237 \(238\) | 227 \(221\) | 221 \(235\) | 79 \(79\) |

|                     | Correlation energies$^a$ | TE | TE | AE | AE | AE | AE |
|---------------------|-------------------------|----|----|----|----|----|----|
| \(0_g\)             | \(6s_{1/2}^2\)         | 0  | 0  | 0  | 0  | 0  | 0  |
| \(0_u\)             | \(6s_{1/2}^1 6p_{1/2}^1\) | 31780 \(31839\) | -1 | 22 | 21 | 202 | -687 |
| \(1_u\)             | \(6s_{1/2}^1 6p_{1/2}^1\) | 33655 \(33716\) | -4 | 21 | 21 | 214 | -438 |
| \(2_u\)             | \(6s_{1/2}^1 6p_{3/2}^1\) | 38020 \(38083\) | -9 | 22 | 21 | 247 | 358 |
| \(1_u\)             | \(6s_{1/2}^1 6p_{3/2}^1\) | 50109 \(50164\) | 3  | 31 | 31 | 241 | -73 |

$^a$The correlation energies were calculated as a difference between the total energies from the above mentioned CI calculations and the numerical SCF calculations with the frozen core \(1s_{1/2}^1 5d_{5/2}^5\) spinors for the corresponding terms.

$^b$The \(6s_{1/2}^1 6p_{1/2}^1\) and \(6s_{1/2}^1 6p_{3/2}^1\) configurations are strongly mixed for these terms in the CI calculations.

$^c$The RECP from Ref. [6].

$^d$The PP from Ref. [7] with the corrected \(V_{so}\) by the factors \((2l + 1)/2\) (M. Dolg, private communication).
TABLE III. All-electron transition energies (TE) and absolute errors (AE) of the 20 electron GRECP in their reproducing from the 12 and 18 electron CI/MBPT2 calculations of low-lying states of Hg for the \([4,4,3,2,1]\) CI, \([11,11,11,9,8,7]\) and \([11,12,11,9,8,7]\) MBPT basis sets (in \(\text{cm}^{-1}\)).

| Symmetry \((J_{\text{parity}})\) | Leading conf. | All-el. point | 20 el. GRECP nucl. | All-el. point | 20 el. GRECP gaus. |
|----------------------------------|---------------|---------------|-------------------|---------------|-------------------|
| Number of correlated electrons: 12 | 12 | 18 | 18 |
| \(0_g\) | \(6s_{1/2}^2\) | 0 | 0 | 0 | 0 |
| \(0_u\) | \(6s_{1/2}^1p_{1/2}^1\) | 36753 | -194 | 37264 | -211 |
| \(1_u\) | \(6s_{1/2}^1p_{1/2}^1\) | 38526 | -178 | 39049 | -192 |
| \(2_u\) | \(6s_{1/2}^1p_{3/2}^1\) | 43149 | -167 | 43751 | -172 |
| \(1_u\) | \(6s_{1/2}^1p_{3/2}^1\) | 52919 | -30 | 53325 | -24 |

TABLE IV. All-electron transition energies (TE) and absolute errors (AE) of different RECPs in their reproducing from the 20 electron CI/MBPT2 calculations of low-lying states of Hg for the \([4,4,3,2,1]\) CI and \([12,12,11,9,8,7]\) MBPT basis sets (in \(\text{cm}^{-1}\)).

| Symmetry \((J_{\text{parity}})\) | Leading conf. | All-el. finite point | 34 el. GRECP nucl. | 20 el. RECP energy of Ross adjusted et al.\(^a\) PP\(^b\) |
|----------------------------------|---------------|-------------------|-------------------|------------------|------------------|
| Number of correlated electrons: \(20\) | 20 | 20 | 20 |
| \(0_g\) | \(6s_{1/2}^2\) | 0 | 0 | 0 | 0 | 0 | 0 |
| \(0_u\) | \(6s_{1/2}^1p_{1/2}^1\) | 36900 | 36963 | -137 | -135 | -130 | 570 | -468 |
| \(1_u\) | \(6s_{1/2}^1p_{1/2}^1\) | 38690 | 38754 | -128 | -115 | -111 | 581 | -233 |
| \(2_u\) | \(6s_{1/2}^1p_{3/2}^1\) | 43415 | 43481 | -127 | -94 | -90 | 656 | 795 |
| \(1_u\) | \(6s_{1/2}^1p_{3/2}^1\) | 53004 | 53062 | -22 | 50 | 52 | 545 | 303 |

\(^a\)The RECP from Ref. [6].

\(^b\)The PP from Ref. [7] with the corrected \(V_{so}\) by the factors \((2l + 1)/2\) (M. Dolg, private communication).
TABLE V. All-electron transition energies (TE) and absolute errors (AE) of the 34 electron GRECP in their reproducing from the 34 electron CI/MBPT2 calculations of low-lying states of Hg for the [4, 4, 3, 2, 1] CI and [12, 12, 11, 10, 8, 7] MBPT basis sets in comparison with experimental data and results of RCC calculations (in cm$^{-1}$).

| Symmetry (J$_{parity}$) | Leading conf. | Exper. data$^a$ | RCC$^b$ (all-el., finite nucl.) | All-el. finite nucl. | 34 el. point nucl. GRECP | 34 el. num. |
|-------------------------|---------------|----------------|--------------------------|------------------|------------------|---------|
|                         |               |                | TE                       | TE               | TE               | AE      |
| 0$_g$                   | 6s$^2$$_{1/2}$| 37645          | 37569                    | 37634            | 153              |
| 0$_u$                   | 6s$^1$$_{1/2}$6p$_{1/2}^1$ | 39412          | 39361                    | 39426            | 169              |
| 1$_u$                   | 6s$^1$$_{1/2}$6p$_{3/2}^1$ | 44043          | 44157                    | 44224            | 225              |
| 1$_u$                   | 6s$^1$$_{1/2}$6p$_{3/2}^1$ | 54069          | 53553                    | 53612            | 224              |

$^a$The data from Ref. [10].
$^b$The results from Ref. [3] for the [27, 23, 21, 16, 10, 6] basis set (in the notations of the present paper) and 34 correlated electrons.

TABLE VI. All-electron transition energies (TE) from the 34 electron CI/MBPT2 calculations of low-lying states of Hg for different basis sets (in cm$^{-1}$).

| Symmetry (J$_{parity}$) | Leading conf. | All-el. point conf. | All-el. point conf. | All-el. point conf. |
|-------------------------|---------------|---------------------|---------------------|---------------------|
| CI basis:               |               | [4, 4, 3, 2, 1]     | [4, 4, 3, 2]        | [4, 4, 3]           |
| MBPT basis:             |               | [12, 12, 11, 9, 8]  | [12, 12, 11, 9]     | [12, 12, 11, 1]     |
|                         |               | TE                  | TE                  | TE                  |
| 0$_g$                   | 6s$^2$$_{1/2}$| 37370               | 37068               | 32680               |
| 0$_u$                   | 6s$^1$$_{1/2}$6p$_{1/2}^1$ | 39151          | 38798               | 34530               |
| 1$_u$                   | 6s$^1$$_{1/2}$6p$_{1/2}^1$ | 43906          | 43296               | 38847               |
| 1$_u$                   | 6s$^1$$_{1/2}$6p$_{3/2}^1$ | 53272          | 52726               | 50604               |