Uncertainty evaluation of the isotope shift factors for $2s2p\ ^{3,1}P^o_1$–$2s^2\ ^1S_0$ transitions in B II*

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Accurate isotope shift factors of the $2s2p\ ^{3,1}P_1$–$2s2\ ^1S_0$ transitions in B II, obtained with the multi-configuration Dirac–Hartree–Fock and the relativistic configuration interaction methods, are reported. We found a linear correlation relation between the mass shift factors and the energies for the transitions concerned, considering all-order electron correlations. This relation is important for estimating the uncertainty in the calculation of isotope shift factors. These atomic data can be used to extract the nuclear mean-square charge radii of the boron isotopes with halo structures or to resolve the high precise spectroscopy of B II in astronomical observation.

Keywords: isotope shifts, B II, halo state, MCDHF method

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1. Introduction

The halo nucleus, in which an individual nucleon resides far away from the nuclear core, has extended charge or matter distribution. This exotic characteristic attracts a great deal of attention for understanding the interactions in the nucleus.[1,2] The laser spectroscopy technique to measure isotope shifts (IS) plays an important role in extracting the nuclear charge radius.[3–8] Compared with the electron scattering experiments or x-ray measurements in muonic atoms,[9] this method provides nuclear-model-independent data if accurate isotope shift factors are available.

The kinds of halo nuclei include neutron halo and proton halo, while the latter is rarer than the former because of the Coulomb repulsion. So far, it was found that ^{8}B has the one-proton halo structure in the ground state,[10] which triggers some collision experiments for its large nuclear charge distribution later.[11,12] In addition, the neutron halo structure has been discovered in the neutron-rich isotope ^{17}B.[13] Therefore, one is interested in investigating the evolution of nuclear mean-square radius along the boron isotopes. In astrophysics, the isotope shifts of the transitions in boron can be applied to study the change of the isotopic content in cosmic production, like the composition of ^{10}B and ^{11}B[14,15] for understanding the nuclear spallation reactions. Data for the isotope shift of Be-like B $2s2p\ ^1P_1$–$2s^2\ ^1S_0$ transition, obtained from laboratory and astronomical observations, were reported in Refs. [14] and [15]. However, the large uncertainty in the laboratory measurements and telescope observation result in less accurate isotope shifts. Turning to theory, King *et al.* presented the ground-state isotope shift factors of Be-like Boron in the non-relativistic theoretical framework by a standard Hylleraas approach involving Slater-type basis functions.[16] The results by King *et al.* agree well with the non-relativistic results of Komasa *et al.* by exponentially correlated Gaussian functions[17] and Gálvez *et al.* by a production of a symmetric correlation factor.[18] Litzén *et al.*[14] also calculated the isotope shift factors of $2s2p\ ^{3,1}P_1$–$2s^2\ ^1S_0$ transition using the multi-configuration Hartree–Fock (MCHF) method, which agreed well with the experimental values. Similar calculations were performed by Jönsson *et al.*[19,20] taking into account electron correlations more adequately. All these results are consistent with each other. Recently, Nazé *et al.* gave the relativistic mass shift factors in the framework of the multi-configuration Dirac–Hartree–Fock (MCDHF) method, in which the Breit interaction and the quantum electrodynamic (QED) effects and the relativistic recoil corrections were considered.[21] Nevertheless, all the theoretical works mentioned above did not give an uncertainty estimation. In particular, Korol *et al.* presented results with an error bar in the configuration-interaction + many-body perturbation theory (CI+MBPT),[22] and had small differences with the non-relativistic results in Refs. [14], [19], and [20].

Due to the large influence of electron correlations on isotope shift factors,[23] a method to estimate the uncertainty of

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the calculated factors is needed. References [24]–[26] have reported that the convergence of the mass shift factors is linearly correlated to the convergence of the energies in the complex atomic system taking into account part of the electron correlation effects. However, the evaluation of the mass shift uncertainty by the transition energies may not be correct if the higher-order electron correlation effects are neglected. Therefore, this linear correlation should be checked by including all-order electron correlations.

In this work, we calculated the isotope shift factors for the $2s2p\ ^{3,1}P_1$–$2s^2\ ^1S_0$ transitions of B II in the framework of the multi-configuration Dirac–Hartree–Fock (MCDHF) method. The convergence relation between the mass shift factors and the energies for the transitions concerned were investigated in order to evaluate the uncertainty in the calculation.

2. Theory

2.1. Isotope shift

The isotope shift is composed of the mass shift (MS) and the field shift (FS). The former is caused by the motion of nucleus with the finite mass and the latter by the nuclear charge distribution.

In the approximation of first-order perturbation theory, the MS Hamiltonian including the relativistic nuclear recoil corrections is given by[27]

$$H_{\rm MS} = \frac{1}{2M}\sum_{i,j}\left[\boldsymbol{P}_i\cdot\boldsymbol{P}_j - \frac{\alpha Z}{r_i}\left(\boldsymbol{\alpha}_i + \frac{(\boldsymbol{\alpha}_i\cdot\boldsymbol{r}_i)\boldsymbol{r}_i}{r_i^2}\right)\cdot\boldsymbol{P}_j\right], \quad (1)$$

where $\boldsymbol{\alpha}_i$ is a vector incorporating the Dirac matrices, and α is the fine structure constant. The operator can be divided into the one-body and two-body terms, referred to as the normal mass shift (NMS) and the specific mass shift (SMS), respectively. For an atomic state Ψ_i, the mass shift factor K_i is defined as[28]

$$\frac{K_i}{M} = \langle\Psi_i|H_{\rm MS}|\Psi_i\rangle. \quad (2)$$

Furthermore, the mass shift between two isotopes A and A' for a transition k can be written as

$$\delta\nu_{k,\rm MS}^{A,A'} = \left(\frac{M'-M}{MM'}\right)\frac{\Delta K_{\rm MS}}{h} = \left(\frac{M'-M}{MM'}\right)\Delta\tilde{K}_{\rm MS}, \quad (3)$$

where $\Delta K_{\rm MS} = K_{u,\rm MS} - K_{l,\rm MS}$ is defined as the difference of K parameter between upper (u) and lower (l) for the transition.

The field shift between isotopes A and A' for the i atomic state, neglecting the higher-order nuclear charge moment, is written as[29,30]

$$\delta E_{i,\rm FS}^{A,A'} = F_i\delta\langle r^2\rangle^{A,A'}. \quad (4)$$

Here, F_i is the electronic factor proportional to the total probability density at the origin $|\Psi_i(0)|^2$

$$F_i = \frac{2\pi}{3}Z|\Psi(0)|_i^2. \quad (5)$$

The field shift for the transitions is given by

$$\delta\nu_{k,FS}^{A,A'} = \Delta\tilde{F}_k\delta\langle r^2\rangle^{A,A'} = \frac{2\pi}{3h}Z\Delta|\Psi(0)|^2\delta\langle r^2\rangle^{A,A'} \quad (6)$$

with $\Delta|\Psi(0)|^2 = |\Psi(0)|_u^2 - |\Psi(0)|_l^2$.

2.2. MCDHF method

In the multi-configuration Dirac–Hartree–Fock method, an atomic state wave function (ASF) is composed of configuration state wave functions (CSFs) with the same parity P, the total angular momentum J and its component along the z direction M_J,

$$\Psi(\gamma PJM_J) = \sum_{i=1}^{\rm NCSF} c_i\Phi(\gamma_i PJM_J), \quad (7)$$

where NCSF is the number of CSFs, c_i the mixing coefficients, and γ_i is the additional quantum number specifying each CSF. The CSF is built from the one-electron Dirac orbitals. Applying the variation principle, one can optimize the one-electron Dirac orbitals and the mixing coefficient in the self-consistent field (SCF) procedure for minimizing the energy eigenvalue. The Breit interaction in the low-frequency approximation[31]

$$B_{ij} = -\frac{1}{2r_{ij}}\left[\boldsymbol{\alpha}_i\cdot\boldsymbol{\alpha}_j + \frac{(\boldsymbol{\alpha}_i\cdot\boldsymbol{r}_{ij})(\boldsymbol{\alpha}_i\cdot\boldsymbol{r}_{ij})}{r_{ij}^2}\right] \quad (8)$$

is taken into account in the relativistic configuration interaction (RCI) computations.

3. Results and discussion

3.1. Computational model

The active space (AS) approach is applied to capture the electron correlation effects. According to the perturbation theory,[32] the CSFs obtained by single (S), double (D), triple (T), and quadruple (Q) substitutions from the occupied in the reference configuration to the active set can be regarded as the first-order and the higher-order set, respectively. Furthermore, the first-order correlation wave function can be classified into several particular pair correlations, i.e., valence–valence (VV), core–valence (CV), and core–core (CC) correlations. In this work, the reference configurations are $\{1s^22s^2\}$ and $\{1s^22s2p\}$ for the ground state and the excited state, respectively. The 1s orbital is treated as the core, and the others are valence orbitals. At the first step, the configuration space is expanded by the single and restricted double (SrD) substitutions from the reference configuration for taking into account the CV and VV correlations. The restricted double excitation means that only one electron in the 1s core can be

excited to the active set. The active set is enlarged layer by layer up to $n = 10$ and $l = 5$ to monitor the convergence of the calculated energies and mass shift factors. Each correlation layer is label as nSrD. The calculation starts from the Dirac–Hartree–Fock (DHF) approximation, and the orbitals in the reference configuration are treated as spectroscopic. The virtual orbitals in the active set are optimized as correlation orbitals. Subsequently, CC and higher-order correlations, labeled as "CInSD" and "CInTQ", respectively, and the Breit interaction, are considered in the RCI computation. All calculations are performed by using the GRASP2K package.[33,34] The isotope shift factors are calculated by the RIS module.[35]

3.2. Results and discussion

The isotope shift factors of the 2s2p ^{3,1}P$_1$–2s^2 ^{1}S$_0$ transitions in B II are shown in Fig. 1 as the functions of the computational model. It can be seen from this figure that the mass shift factors are sensitive to core–valence and valence–valence correlations. The core–core and higher-order correlations are also important, especially for the specific mass shift factors.[23] For the field shift factors it is more stable. We also made a comparison for the mass and the field shift factors of the ground state. The present results, displayed in Table 1, are in excellent agreement with other theoretical values.

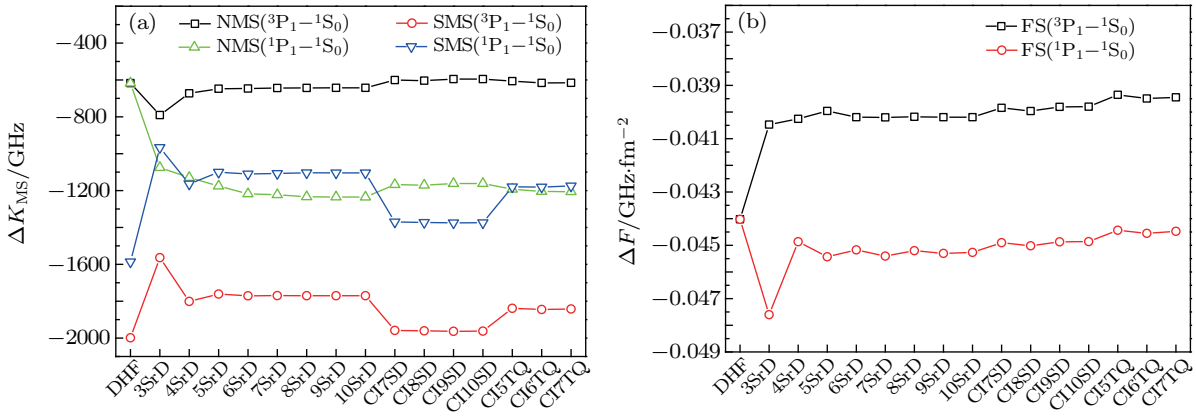


Fig. 1. (color online) NMS factor $\tilde{K}_{\rm NMS}$ (in unit GHz), SMS factor $\tilde{K}_{\rm SMS}$ (in unit GHz), and FS factor F (in units GHz·fm^{-2}) of the 2s2p ^{3,1}P$_1$–2s^2 ^{1}S$_0$ transitions for B II as functions of the computational models. (a) NMS and SMS factors; (b) FS factors. The unit 1 fm = 10^{-15} m.

Table 1. IS factors (in unit a.u.) of the ground state 2s^2 ^{1}S$_0$ and other results obtained with the non-relativistic theories.

	$K_{\rm NMS}$	$K_{\rm SMS}$	$\rho^{\rm e}(0)$
This work	24.3467	0.5968	73.22
Other methods	24.3488[16]	0.59554(40),[16] 0.59514[17]	72.517(30),[16] 71.9(2)[18]

The mass shift factor and the field shift factor for the 2s2p ^{3,1}P$_1$–2s^2 ^{1}S$_0$ transitions and the energy eigenvalues for the ^{3,1}P$_1$ and ^{1}S$_0$ states are given in Table 2. We found that the contribution of the relativistic correction of the mass shift factor is less than 1%. The effect of the Breit interaction is less than 0.5%. The normal mass shift factors can be estimated from the scaling law

$$\Delta\tilde{K}_{\rm NMS} = -\nu/1823\ {\rm GHz}$$

in the nonrelativistic frame, where ν is the transition frequency.[36] Results from the scaling law are consistent with our results since the relativistic correction is small in such a light atomic system. In Table 3, we display the calculated mass and the field shift factors for the 2s2p ^{1}P$_1$–2s^2 ^{1}S$_0$ transition in B II between ^{11}B and ^{10}B as well as other theoretical and experimental values available. As can be seen from this table, all results are in excellent agreement.

Table 2. MS factors (in unit GHz), FS factors (in units MHz·fm^{-2}), and energy eigenvalues (in unit Hartree) of the 2s2p ^{3,1}P$_1$–2s^2 ^{1}S$_0$ transitions in B II with and without Breit interaction, compared with results from other calculations. For $\Delta\tilde{K}_{\rm NMS}$ results from the scaling law are also given.

	^{1}S$_0$	^{3}P$_1$	^{1}P$_1$	^{3}P$_1$–^{1}S$_0$			^{1}P$_1$–^{1}S$_0$		
	E/a.u.			$\Delta\tilde{K}_{\rm NMS}$	$\Delta\tilde{K}_{\rm SMS}$	ΔF	$\Delta\tilde{K}_{\rm NMS}$	$\Delta\tilde{K}_{\rm SMS}$	ΔF
DF	–24.24516	–24.12704	–23.91541	–61.69	–1998.5	–44.03	–61.70	–1586.6	–44.03
This work	–24.35567	–24.18563	–24.02099	–615.53	–1842.56	–39.453	–1206.10	–1174.90	–44.479
+Breit	–24.35450	–24.18445	–24.01983	–615.65	–1842.63	–39.442	–1205.97	–1175.20	–44.467
Ref. [21]	–24.35345	–24.18360	–24.01858	–613.49	–1840.16	–39.490	–1183.04	–1174.99	–44.427
Scaling law				–614.08			–1207.01		

Table 3. MS factors for the 2s2p $^1P_1$ - 2s^2 $^1S_0$ for ^{10,11}B.

	$\delta\sigma_{IS}$/cm^{-1} in experiment	$\delta\sigma_{MS}$/cm^{-1} in this work	$\delta\sigma_{MS}$/cm^{-1} in other theories
$^1P_1$–$^1S_0$	0.70(3)[14] 0.74(19)[15]	0.7179[a] 0.718(2)[b]	0.711,[21] 0.7145[14] 0.7146,[19] 0.7165,[20] 0.7106(22)[22]

[a]Breit results in this work, [b]for uncertainty estimation, see text.

Furthermore, we investigated the relation between the energies and the MS factors as expansion of the configuration space. The results are illustrated in Fig. 2. For convenience, the results obtained from the RCI computation are shown in the large figure. $\delta\tilde{K}^k_{MS}$ and δE^k is defined as $\delta\tilde{K}^k_{MS} = \left|\tilde{K}_{MS}(\alpha) - \tilde{K}_{MS}(\zeta)\right|$ and $\delta E^k = |E(\alpha) - E(\zeta)|$ for the state, respectively. α and ζ represents the configuration space used in each computational step and the largest configuration space "CI7TQ" for two states, respectively. One can see from Fig. 2 that $\delta\tilde{K}_{MS}$ and δE for these two states approximate to a linear correlation. A similar relation can also be found for the 2s2p $^1P_1$ - 2s^2 $^1S_0$ transition as shown in Fig. 3. It is worth noting that the linear correlation only occurs in the large-scale calculation. In addition, the linear correlations between the MS factors and the energies for the transition are not as good as those for the level since the transition MS factors are too small and thus sensitive to the electron correlations.

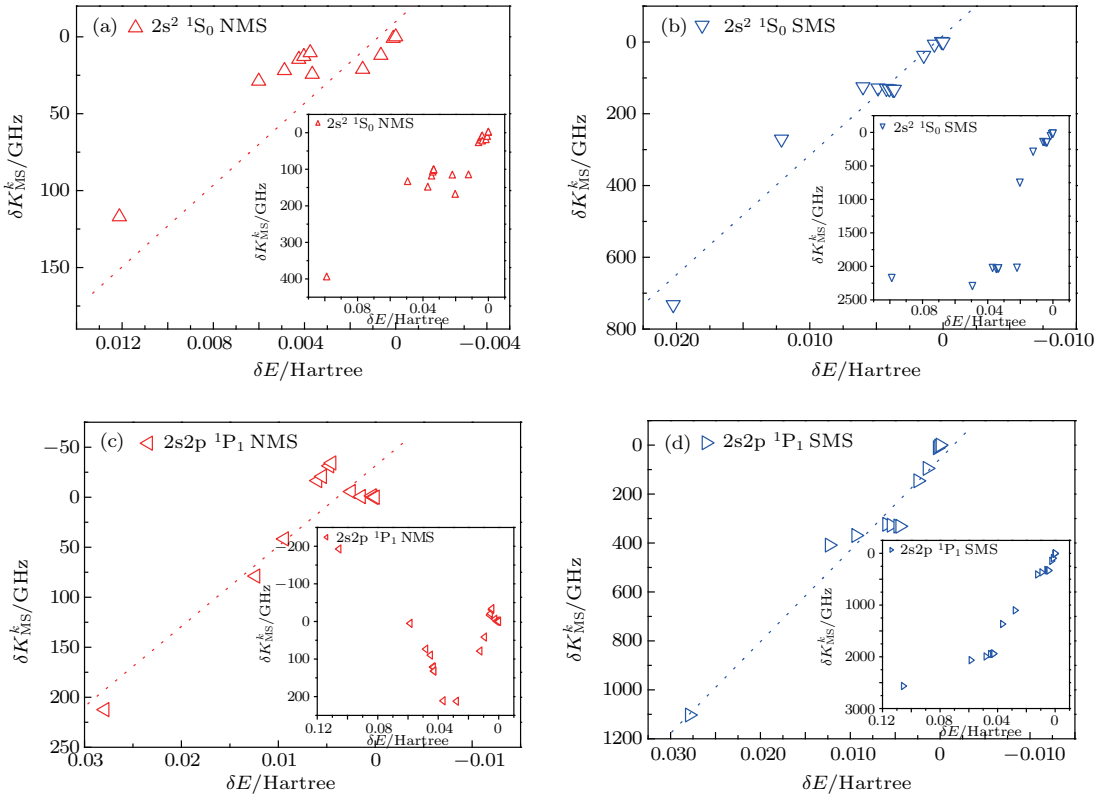


Fig. 2. (color online) The convergence of the NMS and SMS factor (in unit GHz) versus the corresponding energy eigenvalues (in unit Hartree). (a) 2s^2 $^1S_0$ NMS; (b) 2s^2 $^1S_0$ SMS; (c) 2s2p $^1P_1$ NMS; (d) 2s2p $^1P_1$ SMS.

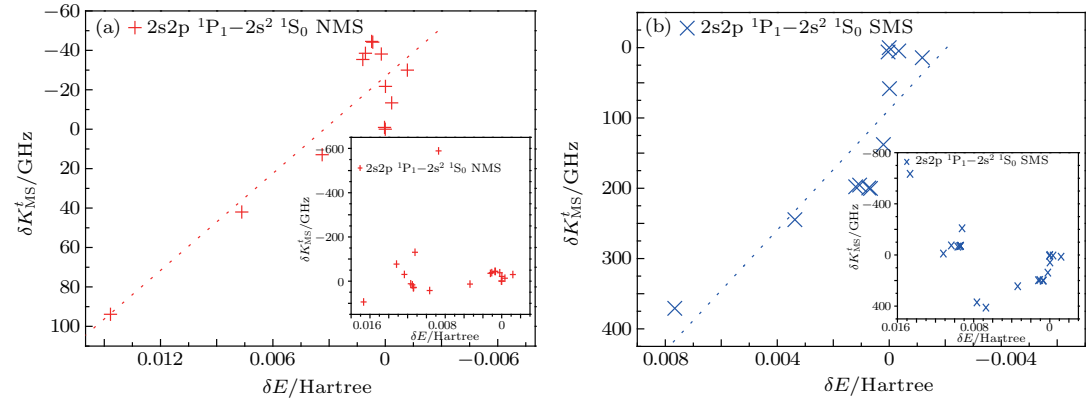


Fig. 3. (color online) The convergence of the NMS and SMS factors (in unit GHz) in 2s2p $^1P_1$–2s^2 $^1S_0$ transition versus the corresponding transition energy (in unit Hartree). (a) NMS; (b) SMS.

Based on the discussion above, we evaluated the uncertainties in the MS factors. Two methods were used for this purpose. From the linear correlation between the transition energies and the MS factors, the uncertainty of the MS factors with the experiment transition energies of the NIST database can be estimated. The advantage of this method is to evaluate the uncertainty of the unknown and sensitive MS factors based on the known and exact experimental transition energy with the linear correlation. In our work, the results of MS factors are 8 GHz and 36 GHz for the $^3P_1$–$^1S_0$ transition and the $^1P_1$–$^1S_0$ transition, respectively. On the other hand, we can also estimate the uncertainty through the convergence trend of the MS factors by the difference of the result obtained with the "CI7TQ″ and the "CI6TQ″ model. Because the all-order electron correlation effects were considered in the model, the uncertainties mainly come from the truncation error reflecting on the convergence trend as the expansion of the computational model. The corresponding uncertainties of the MS factors are 3 GHz and 6 GHz, which are quite a bit smaller than the ones obtained with the former method. It can be seen that the uncertainties in the former method estimated by these two methods have a positive relation. Therefore, we can say that the uncertainty estimation of the MS factor based on the linear correlation is possible. However, due to the relation being worse between the MS factors and the energies for the transition, we use the latter method to present the final results. The reason for this relation being worse is that the transition MS factors are so tiny as to be sensitive to the electron correlations.

4. Conclusion

In this paper, the mass and the field shift factors for $2s^2$ $^1S_0$, $2s2p$ $^{3,1}P_1$ of B II are calculated. We analyzed its convergence trend based on a large-scale calculation including all-order electron correlations in the framework of the multi-configuration Dirac–Hartree–Fock method. The final results with the uncertainties estimated through the convergence trend are consistent with the experimental results. The linear correlation between the transition energies and the mass shift factors was found as an expansion of the configuration space. We confirmed that the linear correlation can provide the uncertainty estimation of the MS factors. It would be interesting to study the relation in more complex atomic systems.

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References

[1] Tanihata I, Hamagaki H, Hashimoto O, Shida Y, Yoshikawa N, Sugimoto K, Yamakawa O, Kobayashi T and Takahashi N 1985 *Phys. Rev. Lett.* **55** 2676
[2] Nörtershäuser W, Tiedemann D, Žáková M, *et al.* 2009 *Phys. Rev. Lett.* **102** 062503
[3] Orts R S, Harman Z, Crespo Lóez-Urrutia J R, *et al.* 2006 *Phys. Rev. Lett.* **97** 103002
[4] Yan Z C, Nörtershäuser W and Drake G W F 2008 *Phys. Rev. Lett.* **100** 243002
[5] Pálffy A 2010 *Contemp. Phys.* **51** 471
[6] Cheal B an6d Flanagan K T 2010 *J. Phys. G: Nucl. Part. Phys.* **27** 113101
[7] Lee J, Chen J and Leanhardt A E 2013 *J. Phys. B: At. Mol. Opt. Phys.* **46** 075003
[8] Charlwood F C, Billowesa J, Campbella P, *et al.* 2010 *Phys. Lett. B* **690** 346
[9] Kluge H 2010 *Hyper. Interact.* **196** 295
[10] Minamisono T, Ohtsubo T, Minami I, *et al.* 1992 *Phys. Rev. Lett.* **69** (14) 2058
[11] Aguilera E F, Martinez-Quiroz E, Lizcano D, *et al.* 2009 *Phys. Rev. C* **79** 021601
[12] Negoita F, Borcea C, Carstoiu F, *et al.* 1996 *Phys. Rev. C* **54** 1787
[13] Tanihata I 1988 *Nucl. Phys. A* **488** 113
[14] Litzén U, Zethson T, Jösson P *et al.* 1998 *Phys. Rev. A* **57** 2477
[15] Federman S R, Lambert D L, Cardelli J A and Sheffer Y 1996 *Nature* **381** 764
[16] King F W, Quicker D and Langer J 2011 *J. Chem. Phys.* **134** 124114
[17] Komasa J, Rychlewski J and Jankowski K 2002 *Phys. Rev. A* **65** 042507
[18] Gálvez F J, Buendia E and Sarsa A 1999 *J. Chem. Phys.* **111** 10903
[19] Jönsson P, Fischer C F and Godefroid M 1999 *J. Phys. B: At. Mol. Opt. Phys.* **32** 1233
[20] Jönsson P, Johansson S G and Fischer C F 1994 *Astrophys. J. Lett.* **429** L45-L48
[21] Nazé C, Verdebouta S, Rynkun P, *et al.* 2014 *At. Data Nucl. Data Tables* **100** 1197
[22] Korol V A and Kozlov M G 2007 *Phys. Rev. A* **76** 022103
[23] Godefroid M, Jönsson P and Fischer C F 1998 *Phys. Scr.* **T78** 33
[24] Carette T and Godefroid M 2011 *Phys. Rev. A* **83** 062505
[25] Carette T, Drag C, Scharf O, *et al.* 2010 *Phys. Rev. A* **81** 042522
[26] Carette T and Godefroid M 2016 arXiv: 1602.06574p
[27] Tupitsyn I I, Shabaev V M, Crespo Lóez-Urrutia J R, *et al.* 2003 *Phys. Rev. A* **68** 022511
[28] Gaidamauskas E, Nazé C, Rynkun P, *et al.* 2011 *J. Phys. B: At. Mol. Opt. Phys.* **44** 175003
[29] Torbohm G, Fricke B and Rosén A 1985 *Phys. Rev. A* **31** 2038
[30] Blundell S A, Baird P E G, Palmer C W P, Stacey D N and Woodgate G K 1987 *J. Phys. B: At. Mol. Phys.* **20** 3663
[31] Li J G, Jösson P, Godefroid M, *et al.* 2012 *Phys. Rev. A* 86 052523
[32] Fischer C F, Brage T and Jösson P 1997 *Computational Atomic Structure: An MCHF Approach* (Bristol and Philadelphia: Institute of Physics Publishing)
[33] Jönsson P, He X, Fischer C F and Grant I 2007 *Comput. Phys. Commun.* **177** 597
[34] Jönsson P, Gaigalas G, Bierón J, Fischer C F and Grant I 2013 *Comput. Phys. Commun.* **184** 2197
[35] Nazé C, Gaidamauskas E, Gaigalas G, Godefroid M and Jönsson P 2013 *Comput. Phys. Commun.* **184** 2187
[36] Godefroid M, Fischer C F and Jönsson P 2001 *J. Phys. B: At. Mol. Opt. Phys.* **34** 1079