Advanced computational approach in electron-collisional spectroscopy of atoms and multicharged ions in plasmas

IOP Conf. Series: Journal of Physics: Conf. Series **1136** (2018) 012011 doi:10.1088/1742-6596/1136/1/012011

Advanced computational approach in electron-collisional spectroscopy of atoms and multicharged ions in plasmas

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Abstract. An advanced computational approach to determination of the electron-collisional strengths and cross-sections for atomic ions in the Debye plasmas is presented and used to calculate effective collision strengths of the Kr^{26+} Ne-like ion excitation states for temperature $T=5\times10^6$K and density $n_e==10^{14}cm^{-3}$. The obtained results are compared with the R-matrix data by Griffin et al and other theoretical estimates. The approach is based on the generalized relativistic energy formalism and relativistic many-body perturbation theory with the Debye shielding model Hamiltonian for electron-nuclear and electron-electron systems. The optimized one-electron representation in the perturbation theory zeroth approximation is constructed by means of the correct treating the gauge dependent multielectron contribution of the lowest perturbation theory corrections to the radiation widths of atomic levels.

1. Introduction

The properties of laboratory and astrophysical plasmas have drawn considerable attention over the last decades [1-6]. It is known that multicharged ions play an important role in the diagnostics of a wide variety of plasmas. Similar interest is also stimulated by importance of this information for correct determination of the characteristics for plasma in thermonuclear (tokamak) reactors, searching new mediums for X-ray range lasers. The electron-ion collisions play a major role in the energy balance of plasmas. For this reason, modelers and diagnosticians require absolute cross sections for these processes. The cross sections for electron-impact excitation of ions are needed to interpret spectroscopic measurements and for simulations of plasmas using collisional-radiative models. Such well-known atomic methods such as multi-configuration Dirac–Fock, relativistic distorted-wave method, R-matrix and others approaches [4-18] have been intensively applied to problems considered. At present time a considerable interest has been encapsulated to studying elementary atomic processes in plasmas environments (for example, see [1-54] and Refs. therein) because of the plasmas screening effect on the plasmas-embedded atomic systems. In many papers the calculations of various atomic and ionic systems embedded in the Debye plasmas have been performed [4-10, 16-20]; it is well-known that the Debye model is justified only in the limit of high temperature and low density. However, a development of the advanced computational quantum-mechanical models for the further accurate computing oscillator strengths, electron-collisional strengths and cross-sections for the atomic ions in plasmas, including the Debye plasmas, remained very actual and difficult problem.

In this paper we develop and apply an advanced computational approach to determination of the electron-collisional strengths and cross-sections for the atomic ions in the Debye plasmas. The

approach is based on the generalized relativistic energy formalism and relativistic many-body perturbation theory (PT) with the Debye shielding model Hamiltonian for electron-nuclear and electron-electron systems [17-25]. The PT formalism is constructed on the base of the same fundamental points as the well-known PT approach with the model potential zeroth approximation by Ivanov-Ivanova et al [1-3,26-32]. However there are a few fundamental differences. For example, in our case the PT zeroth approximation [18-20] is in fact the Dirac-Debye-Hückel one. In order to compute the radiative and collisional parameters an advanced version of a relativistic energy approach is used [47,55-64]. It is important to remind that a model relativistic energy approach in a case of a multielectron atom has been developed by Ivanov-Ivanova *et al* [26-30]. A generalized gauge-invariant version of relativistic energy approach in a case of the multielectron atomic systems has been developed by Glushkov-Ivanov-Ivanova (see Refs. [30,33-36]). Earlier this approach has been successfully applied to many actual problems of modern atomic, nuclear, mesonuclear, molecular optics and spectroscopy etc (look Refs. [37-52,55-68]). The method [33] is used to construct the optimized one-electron representation in the PT zeroth approximation by means of the correct treating the gauge dependent multielectron contribution of the lowest PT corrections to the radiation widths of atomic levels. The presented approach has been used to calculate effective collision strengths of the Kr^{26+} Ne-like ion excitation states for temperature $T=5\times10^6$K and density $n_e==10^{14}cm^{-3}$. The obtained results are compared with the R-matrix data by Griffin et al and model potential data [5,20]. All computing was performed with using the modified PC code "Superatom-ISAN" (version 93). Other details can be found in Refs. [17-22].

2. Generalized energy approach in scattering theory

In the theory of the non-relativistic atom a convenient field procedure is known for calculating the energy shifts ΔE of degenerate states. This procedure is connected with the secular matrix M diagonalization [26-32]. In constructing M, the Gell-Mann and Low adiabatic formula for ΔE is used. A similar approach, using the Gell-Mann and Low formula with the QED scattering matrix, is applicable in the relativistic atom theory. The secular matrix elements are already complex in the PT second order and their imaginary parts are connected with the radiation decay possibility. The total energy shift of the state is presented in the form:

$$\Delta E = \mathrm{Re}\Delta E + \mathrm{i}\ \mathrm{Im}\Delta E,$$
$$\mathrm{Im}\ \Delta E = -\Gamma/2, \qquad (1)$$

where Γ is interpreted as the level width. The whole calculation of the energies and decay probabilities of a non-degenerate excited state is reduced to calculation and diagonalization of the complex matrix M and definition of matrix of the coefficients with eigen-state vectors $B^{IK}_{ie,iv}$ [27-31]. To calculate all necessary matrix elements one must use the basis's of the 1QP relativistic functions. In ref. [33] it has been proposed "ab initio" optimization principle for construction of cited basis's. There is used the minimization of the gauge dependent multielectron contribution of the lowest QED PT corrections to the radiation widths of atomic levels. In the fourth order of QED PT there appear diagrams, whose contribution into the ImδE accounts for the polarization effects. This contribution describes collective effects and it is dependent upon the electromagnetic potentials gauge (the gauge non-invariant contribution ΔE_{ninv}). The minimization of the functional $Im\ \Delta E_{ninv}$ leads to the integral differential equation, that is numerically solved [33].

The Dirac-Debye shielding model Hamiltonian for electron-nuclear and electron-electron subsystems is as follows (atomic units are used) [18-20]:

$$H = \sum_i [\alpha cp - \beta mc^2 - Z\exp(-\mu r_i)/r_i] + \sum_{i>j} \frac{(1-\alpha_i\alpha_j)}{r_{ij}} \exp(-\mu r_{ij}) , \quad (2)$$

where c is the velocity of light and Z is a charge of the atomic ion nucleus, ω_{ij} is the transition frequency; α_i , α_j are the Dirac matrices. The plasmas environment effect is modelled by the shielding parameter μ , which describes a shape of the long-rang potential. The parameter μ is connected with the plasmas parameters such as temperature T and the charge density n as follows:

$$\mu \sim \sqrt{e^2 n / k_B T} . \quad (3a)$$

Here e is the electron charge and k_B is the Boltzman constant. The density n is given as a sum of the electron density N_e and the ion density N_k of the k-th ion species with the nuclear charge q_k :

$$n = N_e + \sum_k q_k^2 N_k \cdot \quad (3b)$$

It is very useful to remind the simple estimates for the shielding parameter. For example, under typical laser plasmas conditions of T~ 1keV and n~ 10^{22} cm^{-3} the parameter μ is of the order of 0.1 in atomic units; in the EBIT plasmas T~ 0.05keV, n~10^{18} cm^{-3} and μ~10^{-3}. We are interested in studying the spectral parameters of ions in plasmas with the temperature T~ 0.1-1keV (10^6-10^7K) and n~10^{14}-10^{26} cm^{-3} (μ~10^{-5}-10^0). It should be noted that indeed the Debye screening for the atomic electrons in the Coulomb field of nuclear charge is well understood due to the presence of the surrounding plasma electrons with high mobility. On the other hand, the contribution due to the Debye screening between electrons would be orders of magnitude smaller. Majority of the previous works on the spectroscopy study have considered the screening effect only in the electron-nucleus potential where the electron-electron interaction potential is truncated at its first term of the standard exponential expansion for its dominant contribution [5-10,18,19]. However, as the authors [8] note, it is also important to take into account the screening in the electron- electron interactions for large plasma strengths to achieve more realistic results in the search for stability of the atomic structure in the plasma environment.

In the PT zeroth approximation we use the mean-field potential, which includes the Yukawa-type potential (insist of the pure Coulomb one) plus exchange Kohn-Sham potential [54,55] and additionally the modified Lundqvist-Gunnarsson correlation potential (with the optimization parameter b) as in Refs. [18,19,55-58]. The most complicated problem of the relativistic PT computing the radiative and collisional characteristics of the multielectron atomic systems is in an accurate, precise accounting for the exchange-correlation effects (including polarization and screening effects, a continuum pressure etc) as the effects of the PT second and higher orders . Using the standard Feynman diagrammatic technique one should consider two kinds of diagrams (the polarization and ladder ones), which describe the polarization and screening exchange-correlation effects. The polarization diagrams take into account the quasiparticle (external electrons or vacancies) interaction through the polarizable core, and the ladder diagrams account for the immediate quasiparticle interaction. The detailed description of the polarization diagrams and the corresponding analytical expressions for matrix elements of the polarization quasiparticles interaction (through the polarizable core) potential are presented in Refs. [6-8,31,59-65].

An effective approach to accounting of the polarization diagrams contributions is in adding the effective two-quasiparticle polarizable operator into the PT first order matrix elements. In Ref. [31] the corresponding non-relativistic polarization functional has been derived. More correct relativistic expression has been presented in the Refs. [55, 59] and used in our work. According to Ref. [59], the polarization potential is as follows:

$$V_{pol}^{d}(r_1 r_2) = X\left\{\int \frac{dr'\left(\rho_c^{(0)}(r')\right)^{1/3}\theta(r')}{|r_1 - r'|\cdot|r' - r_2|} - \int \frac{dr'\left(\rho_c^{(0)}(r')\right)^{1/3}\theta(r')}{|r_1 - r'|}\int \frac{dr''\left(\rho_c^{(0)}(r'')\right)^{1/3}\theta(r'')}{|r'' - r_2|}\right/\left\langle\left(\rho_c^{(0)}\right)^{1/3}\right\rangle,$$

$$\left\langle\left(\rho_c^{(0)}\right)^{1/3}\right\rangle = \int dr\left(\rho_c^{(0)}(r)\right)^{1/3}\theta(r),$$

$$\theta(r) = \left\{1 + \left[3\pi^2\cdot\rho_c^{(0)}(r)\right]^{2/3}/c^2\right\}^{1/2} \qquad (4)$$

where X is the numerical coefficient.

The justification of the energy approach in the scattering problem is in details described in Refs. [18-20,27-30]. The scattered part of energy shift *Im ΔE* appears first in the second order of the atomic perturbation theory. For example, the collisional de-excitation cross section is defined as follows:

$$\sigma(IK \to 0) = 2\pi\sum_{j_{in}, j_{sc}}(2j_{sc}+1)\{\sum_{j_{ie}, j_{iv}} < 0 \mid j_{in}, j_{sc} \mid j_{ie}, j_{iv}, J_i > B_{ie,iv}^{IK}\}^2 \qquad (5)$$

$$< 0 \mid j_{in}, j_{sc} \mid j_{ie}, j_{iv}, J_i >= \sqrt{(2j_{ie}+1)(2j_{iv}+1)}(-1)^{j_{ie}+1/2}\times\sum_{\lambda}(-1)^{\lambda+J_i}\times$$

$$\times\{\delta_{\lambda,J_i}/(2J_i+1)Q_\lambda(sc,ie;iv,in) + \begin{bmatrix} j_{in}\ldots j_{sc}\ldots J_i \\ j_{ie}\ldots j_{iv}\ldots\ldots\lambda \end{bmatrix} Q_\lambda(ie;in;iv,sc)\}, \qquad (6)$$

where $Q_\lambda = Q_\lambda^{\mathrm{Qul}} + Q_\lambda^{\mathrm{Br}}$ is the sum of the Coulomb and Breit matrix elements. For example, the Coulomb part Q_λ^{Qul} contains the radial R_λ and angular S_λ integrals as follows see details in Refs.[17-19, 27-31]):

$$Q_\lambda^{\text{Coul-Yuk}} = \{R_\lambda(1243)S_\lambda(1243) + R_\lambda(\tilde{1}24\tilde{3})S_\lambda(\tilde{1}24\tilde{3}) + R_\lambda(1\tilde{2}\tilde{4}3)S_\lambda(1\tilde{2}\tilde{4}3) + R_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3})S_\lambda(\tilde{1}\tilde{2}\tilde{4}\tilde{3})\}. \qquad (7)$$

Here the tilde designates that the large radial Dirac component f must be replaced by the small Dirac component g, and instead of l_i, $l_i'=l_i$-1 should be taken for $j_i < l_i$ and $l_i'=l_i$+1 for $j_i > l_i$. The plasmas shielding model is incorporated and based on introducing the Yukawa - type electron-nuclear attraction and electron-electron repulsion potentials. The relativistic wave functions are calculated by solution of the Dirac-Kohn-Sham equation with the optimized one-parameter exchange-correlation potential. The calibration of the single model potential parameter has been performed on the basis of the special ab initio procedure within [33] (see also [30,55]).

3. Results and conclusions

In table 1 we present the theoretical data on the effective collision strengths of the Kr^{26+} Ne-like ion excitation states for the temperature $T=5\cdot10^6$ K and the electron density $n_e=10^{14}$ cm^{-3}. The R-matrix data by DF Griffin et al (RM) [5] and model potential (MP) data [20] are listed for comparison too. It should be noted that strong compensation of different PT terms is a characteristic feature of the states with vacancies in the core. This is one of the main reasons for the fact that the accuracy of conventional a priori calculations of such states does not always satisfy the requirements arising in

many applications. Summation over j_{in},j_{sc} in (18) spreads over the range 1/2-23/2. For some levels the corrections due the correlation effects change the results by a factor of 2-3,5.

Table 1. The effective collision strengths of the Kr^{26+} Ne-like ion excitation states for the temperature $T=5\cdot10^6$ K and electron density $n_e=10^{14}$ cm^{-3} (see text).

Term	RM	MP	Our paper
$2p^53s\ (3/2,1/2)_2$	8.29(-3)	8.13(-3)	8.17(-3)
$2p^53s\ (3/2,l/2)_1$	9.36(-3)	9.19(-3)	9.23(-3)
$2p^53p\ (3/2,l/2)_1$	3.49(-3)	3.38(-3)	3.41(-3)
$2p^53p\ (3/2,1/2)_2$	4.30(-3)	4.18(-3)	4.24(-3)
$2p^53s\ (1/2,l/2)_0$	1.32(-3)	1.21(-3)	1.26(-3)
$2p^53s\ (1/2,l/2)_1$	7.69(-3)	7.56(-3)	7.60(-3)
$2p^53p\ (3/2,3/2)_3$	4.03(-3)	3.89(-3)	3.94(-3)
$2p^53p\ (3/2,3/2)_1$	3.14(-3)	3.01(-3)	3.06(-3)
$2p^53p\ (3/2,3/2)_2$	3.36(-3)	3.12(-3)	3.16(-3)
$2p^53p\ (3/2,3/2)_0$	8.67(-3)	8.49(-3)	8.55(-3)
$2p^53p\ (1/2,1/2)_1$	2.69(-3)	2.54(-3)	2.59(-3)
$2p^53p\ (1/2,3/2)_1$	2.80(-3)	2.72(-3)	2.75(-3)
$2p^53p\ (1/2,3/2)_2$	3.27(-3)	3.16(-3)	3.21(-3)
$2p^53d\ (3/2,3/2)_0$	1.24(-3)	1.13(-3)	1.18(-3)
$2p^53p\ (1/2.1/2)_0$	1.71(-2)	1.58(-2)	1.63(-2)
$2p^53d\ (3/2,3/2)_1$	3.45(-3)	3.31(-3)	3.36(-3)
$2p^53d\ (3/2,3/2)_3$	3.80(-3)	3.67(-3)	3.74(-3)
$2p^53d\ (3/2,5/2)_2$	4.13(-3)	3.96(-3)	4.01(-3)

Using of the shielding approach and an account for the highly-lying excited states is quantitatively important for the adequate description of the collision strengths.

To conclude, let us note that in any case our calculation encourages us to believe that using relativistic energy approach with the optimal Dirac-Kohn-Sham one-electron PT basis and shielding model block is quite consistent and effective one from the point of view of the theory correctness and results exactness. This fact was surely confirmed by calculations of the oscillator strengths, radiative widths in atoms and multicharged ions (c.f. [3,18-30,66-70]).

Acknowledgements

The authors would like to thank the organizers of the CCP-2017 (Paris) for invitation to make contributions. The useful comments of the anonymous referees are very much acknowledged too.

References

[1] Ivanova E P and Grant I P 1998 *J. Phys.B: At. Mol. Opt. Phys.* **31** 2871
[2] Ivanova E P 2011 *Phys. Rev. A.* **84** 043829
[3] Ivanova E P and Zinoviev N A 2001 *Phys. Lett. A* **274** 239
[4] Nakamura N, Kavanagh A P, Watanabe H, Sakaue H A, Li Y, Kato D, Curell F J and Ohtani S 2007 *Journ. Phys. Conf. Ser.* **88** 012066
[5] Griffin D C, Balance C P, Mitnik D M, Berengut J C 2008 *J. Phys. B* **41** 21520
[6] Bielińska-Wąż D, Karwowski J, Saha B and Mukherjee P K 2004 *Phys. Rev. E* **69** 016404
[7] Kar S and Ho Y K 2006 *Phys. Rev. A* **73** 032502
[8] Madhulita Das M, Sahoo B K and Pal S 2014 *J. Phys. B: At. Mol. Opt. Phys.* **47** 175701
[9] Li Y, Wu J, Hou Y and Yuan J 2008 J. *Phys. B: At. Mol. Opt. Phys*. **41** 145002
[10] Chen Z B, Dong C Z, Jiang J and Xie L Y 2015 *J. Phys. B: At. Mol. Opt. Phys.* **48** 144030
[11] Grant I P 1984 *Int. J. Quant. Chem.* **25** 23

[12] Bartschat K, Hudson E T, Scott M P, Burke P G, and Burke V M 1996 *J. Phys. B: At. Mol. Opt. Phys.* **29** 115
[13] Descouvemont P, Tursunov E M and Baye D 2006 *Nucl. Phys. A* **765** 370
[14] Dyall K G, Grant I P, Johnson C T, Parpia F A and Plummer E P 1989 *Comput. Phys. Commun.* **55** 425
[15] Zhang H, Sampson D H, Clark R E H and Mann J B 1987 *At.Data Nucl. Data Tabl.* **37** 17
[16] Khetselius O Yu 2008 *Hyperfine structure of atomic Spectra* (Odessa: Astroprint)
[17] Glushkov A V 2008 *Relativistic Quantum theory. Quantum mechanics of atomic systems* (Odessa: Astroprint)
[18] Glushkov A V, Khetselius O Yu, Loboda A V, Ignatenko A, Svinarenko A , Korchevsky D, Lovett L 2008 *AIP Conf. Proc.* **1058** 175
[19] Glushkov A V, Malinovskaya S V, Loboda A V, Shpinareva I M, Gurnitskaya E P, Korchevsky D A 2005 *J. Phys.: Conf. Ser.* **11** 188
[20] Glushkov A V 1990 *Sov. Phys. Journ.* **33**(9) 754
[21] Glushkov A V, Kondratenko P A, Lepikh Y I, Fedchuk A P, Lovett L, Svinarenko A A 2009 *Int. Journ. Quant. Chem*. **109**(14) 3473
[22] Malinovskaya S V, Glushkov A V, Khetselius O Yu, Svinarenko A A, Mischenko E V and Florko T A 2009 *Int. J. Quant. Chem.* **109** 3325
[23] Glushkov A V, Khetselius O Yu and Svinarenko A A 2013 *Phys. Scr.* **T153** 014029
[24] Glushkov A V, Loboda A, Gurnitskaya E and Svinarenko A 2009 *Phys. Scr.* **T135** 014022
[25] Glushkov A V, Khetselius O Yu, Lopatkin Yu M, Florko T A, Kovalenko O A, Mansarliysky V F 2014 *J. Phys.: Conf. Ser.* **548** 012026
[26] Ivanova E P and Ivanov L N 1979 *Atom. Data. Nucl. Data. Tabl*. **24** 95
[27] Ivanov L N, Ivanova E P and Knight L 1993 *Phys. Rev. A* **48** 4365
[28] Driker M N, Ivanova E P, Ivanov L N and Shestakov A F 1982 *J. Quant. Spectr. Rad. Transfer*. **28** 531
[29] Ivanov L N, Ivanova E P and Aglitsky E V 1988 *Phys. Rep.* **166** 315
[30] Glushkov A V, Ivanov L N and Ivanova E P 1986 *Autoionization Phenomena in Atoms*, (Moscow: Moscow State University) p 58
[31] Ivanova E P, Ivanov L N, Glushkov A V and Kramida A E 1985 *Phys. Scr.* **32** 513
[32] Ivanova E P and Glushkov A V 1986 *J. Quant. Spectr. Rad. Transfer*. **36** 127
[33] Glushkov A V, Ivanov L N 1992 *Phys. Lett. A.* **170** 33
[34] Glushkov A V 1992 *JETP. Lett.* **55** 97
[35] Glushkov A and Ivanov L N 1993 *J. Phys. B: At. Mol. Opt. Phys*. **26** L379
[36] Glushkov A V 2012 Quantum Systems in Chemistry and Physics, Series: Progress in Theoretical Chemistry and Physics (Dordrecht: Springer) **26** pp 231-252
[37] Glushkov A V 2012 *J. Phys.: Conf. Ser*. **397** 012011
[38] Glushkov A V 2014 *J. Phys.: Conf. Ser*. **548** 012020
[39] Khetselius O Yu 2009 *Phys. Scripta.* **T135** 014023
[40] Khetselius O Yu 2010 *AIP Conf. Proc.* **1290** 29
[41] Khetselius O Yu 2008 *AIP Conf. Proc.* **1058** 363
[42] Glushkov A V, Ambrosov S V, Ignatenko A V, Korchevsky D A 2004 *Int. J. Quant.Chem*. **99** 936
[43] Glushkov A V, Malinovskaya S V, Khetselius O Yu, Loboda A V, Sukharev D E and Lovett L 2009 *Int. J. Quant. Chem.* **109** 1717
[44] Glushkov A V, Malinovskaya S V, Prepelitsa G P and Ignatenko V M 2005 *J. Phys.: Conf. Ser*. **11** 199
[45] Glushkov A V, Khetselius O Yu and Malinovskaya S V 2008 *Europ. Phys. J. ST* **160** 195
[46] Glushkov A V, Khetselius O Yu and Malinovskaya S V 2008 *Molec. Phys.* **106** 1257
[47] Malinovskaya S V, Glushkov A V, Dubrovskaya Y V, Vitavetskaya L A 2006 *Recent Advances in the Theory of Chemical and Physical Systems, Ser.: Progress in Theoretical*

Chem. and Phys. (Dordrecht: Springer) **15** pp 301-307
[48] Glushkov A V 2012 *Quantum Systems in Chemistry and Physics. Ser.: Progress in Theoretical Chem. and Phys.* (Dordrecht: Springer) **26** pp 231-252
[49] Glushkov A V, Khetselius O Y and Lovett L 2009 *Advances in the Theory of Atomic and Molecular Systems. Ser.: Progress in Theoretical Chem. and Phys.* (Dordrecht: Springer) **20** pp 125-152
[50] Glushkov A V, Lovett L, Khetselius O Yu, Gurnitskaya E P, Dubrovskaya Yu V and Loboda A V 2009 *Int. Journ. Modern Phys. A* **24** 611
[51] Glushkov A V, Malinovskaya S V, Gurnitskaya E P, Khetselius O Yu and Dubrovskaya Yu V 2006 *J. Phys.: Conf. Ser.* **35** 425
[52] Khetselius O Y 2012 *Quantum Systems in Chemistry and Physics. Ser.: Progress in Theoretical Chem. and Phys.* (Dordrecht: Springer) **26** pp 217-229
[53] Kohn J W and Sham L J 1964 *Phys. Rev. A*. **140** 1133
[54] Gross E G and Kohn W 2005 *Exchange-Correlation Functionals in Density Functional Theory* (New York: Plenum)
[55] Glushkov A V 2006 *Relativistic and correlation effects in spectra of atomic systems* (Odessa: Astroprint).
[56] Khetselius O Y 2012 *J. Phys.: Conf. Ser*. **397** 012012
[57] Glushkov A V, Mansarliysky V F, Khetselius O Yu, Ignatenko A V, Smirnov A V, Prepelitsa G P 2017 *J. Phys.: Conf. Ser.* **810** 012034
[58] Glushkov A V, Ambrosov S V, Loboda A V, Gurnitskaya E P and Prepelitsa G P 2005 *Int. Journ. Quant.Chem*. **104** 562
[59] Glushkov A V 1990 *Soviet Phys. J.* **33**(1) 1
[60] Glushkov A V 1990 *J. Struct. Chem.* **31**(4) 529
[61] Glushkov A V 2005 *AIP Conference Proc*. **796** 206
[62] Glushkov A V and Loboda A V 2007 *J. Applied. Spectr.* **74**(2) 305
[63] Malinovskaya S V, Dubrovskaya Yu V, Vitavetskaya L A 2005 *AIP Conference Proc.* **796** 201
[64] Glushkov A V, Malinovskii A V, Efimov V A, Kivganov A F, Khokhlov V N, Vitavetskaya L A, Borovskaya G A 1998 *J. Struct. Chem.* **39**(2) 179
[65] Glushkov A V, Efimov V A, Gopchenko E D, Dan'kov S V, Polishchyuk V N, Goloshchak O P 1998 *Opt. and Spectr.* **84**(5) 670
[66] Khetselius O Yu 2009 *Int. J. Quant. Chem.* **109** 3330
[67] Glushkov A V, Khetselius O Yu, Svinarenko A A, Prepelitsa G P, Mischenko E V 2010 *AIP Conference Proc*. **1290** 263
[68] Glushkov A V, Khetselius O Yu, Svinarenko A A, Prepelitsa G P, Shakhman A N 2010 *AIP Conference Proc*. **1290** 269
[69] Svinarenko A A 2014 *J. Phys.: Conf. Ser*. **548** 012039
[70] Khetselius O Yu, Glushkov A V, Gurskaya M Yu, Kuznetsova A A, Dubrovskaya Yu V, Serga I N, Vitavetskaya L A 2017 *J. Phys.: Conf. Ser.* **905** 012029