

## CALCULATION OF THE SPECTROSCOPIC CHARACTERISTICS OF THE DIMERS OF ALKALI ELEMENTS ON THE BASIS OF A MODEL PERTURBATION THEORY

A. V. Glushkov,\* V. N. Polishchuk, V. A. Efimov, A. N. Polevoi,  
A. F. Kivganov, V. N. Khokhlov, G. A. Borovskaya, and S. V. Dan'kov

UDC 539.186

*Based on a pseudopotential approach within the model, formally accurate perturbation theory of the Rayleigh–Schrödinger type with a zero-approximation priming potential, a problem of calculation of some alkaline diatomic molecules is considered in homo- and heteronuclear variants of Na<sub>2</sub> and RbM (M = Na, Li, K, Rb, Cs). The results of calculation of the energy parameters, in particular, the dissociation energies, are given; some of the data were obtained for the first time. The results of the calculation for the energies of Rydberg states  $n^1\Sigma_g^+$  ( $n = 4-6$ ) and spectroscopic constants of the Na dimer are given. The calculation demonstrated the important role, in attainment of acceptable accuracy, of two basic 2nd order effects in the theory of perturbations, i.e., the effect of polarization interaction of valence particles through the core and the effect of their screening by one another. For Rydberg states, the contribution of core excitations turns out to be important.*

**Key words:** *pseudopotential, perturbation theory, polarization of the core, Rydberg state, dimer of an alkali element.*

**Introduction.** Calculation of the spectroscopic parameters of diatomic molecules is as before, an urgent problem due to the importance of the corresponding information for a number of optical applications. In particular, information on the spectroscopic characteristics of alkaline dimers are of special interest for laser spectroscopy, creation of laser sources of continuous radiation, etc. [1-4]. This problem is of current interest also from the viewpoint of further development of modern computational methods for diatomic molecules [5]. The very common methods of model potential and pseudopotential (PP) were used intensively in calculations of light alkaline dimers [6-13]. All the same, the rich background of experience acquired in applying PP in molecular calculations showed that PP methods are capable of reproducing, sometimes with high enough accuracy, the results of correct *ab initio* total multielectron calculations, in particular, as far as the molecules containing the atoms of the first two periods of the periodic table and transition metals are concerned [1-10]. A comparison of the results of PP-calculations with the best calculations by the configuration interaction method shows that PP methods give a calculation error in computation of the effects of electron correlation on average of about 10% and greater. It seems that the most suitable objects for applying the PP methods are single-quasi-particle (i.e., one electron above a core of filled electron shells) molecular alkaline ions of the form  $M_2^+$ , M = Li, Na, K, Rb, Cs [5, 8]. If a system has several outer electrons (quasi particles), the problem of accurately accounting for interelectron correlation acquires very great importance, and without the use of correct methods for its solution, PP methods may fail to give a high accuracy of calculation [2, 3, 5]. One of the well-known methods of accounting for exchange-polarization effects is provided by density functional theory, but in many cases the accuracy of calculation is far from the spectroscopic accuracy. In a number of works [9, 12], the effects of exchange and correlation were taken into account by adding a model

---

Odessa Hydrometeorological Institute, 108 Odessa-9, 270009, Ukraine. Translated from Zhurnal Prikladnoi Spektroskopii, Vol. 65, No. 3, pp. 333-339, May-June, 1998. Original article submitted february 28, 1997.

PP (MPP) with potentials that depend on the dipole  $\alpha_d$  and quadrupole  $\alpha_q$  polarizabilities of the core. The drawbacks of the method comprise the necessity of preliminary determination of  $\alpha_d$  and  $\alpha_q$  (as a rule, the accuracy of their calculation is not great) and incompletely accounting for the most important exchange–correlation effects. In our opinion, a very effective and successive procedure is to construct MPP within the framework of Rayleigh–Schrödinger perturbation theory (PT) with effective consideration of exchange–correlation effects as higher–order effects and with a priming PP of zero approximation (ZA). At least, such a technique has been realized with success in the theory of calculation of atoms, ions as well as molecules [13–31].

In the present work, on the basis of the PP method within the framework of the PT model, a problem of calculation of alkaline diatomic molecules is considered in homo- and heteronuclear variants of RbM ( $M = \text{Li, Na, K, Rb, Cs}$ ). The model Hamiltonian of the system was constructed within the framework of Rayleigh–Schrödinger PT with priming PP of ZA [13, 15]. As a model Hamiltonian, a local Hellman-type model potential was used [6]. To take into account the two basic 2nd-order effects of PT (polarization interaction of valence particles through the core and their screening by each other), original procedures were used. The use of empirical information about simpler corresponding ions for calculating alkaline molecules in the zero approximation of PT with PP of ZA made it possible to increase the accuracy of calculation without additional computations.

Within the framework of the PP-approach, the problem of calculation of RbM-type molecules can be reduced to the problem of calculation of a system consisting of two outer electrons (quasi particles) moving in the field of ions of the type of the atoms of noble gases  $M^+ - M^+$  that form the core [13, 15]. The main state of the system (the state with two quasi particles above the core in the representation of secondary quantization) has the form

$$\Phi = \sum_{\xi\eta} c_{\xi\eta} a_{\xi}^{\dagger} a_{\eta}^{\dagger} \Phi_0,$$

where  $a^{\dagger}$  is the creation operator for a particle above the core;  $\Phi_0$  is the state of the core;  $c$  is the coefficient that takes into account the angular symmetry. The electron Hamiltonian of the system has the form

$$H = \sum_i \varepsilon_i a_i^{\dagger} a_i + \sum_{ij} F_{ij} a_i^{\dagger} a_j^{\dagger} + \sum_{ijkl} F_{ijkl} a_i^{\dagger} a_j^{\dagger} a_k a_l,$$

where  $\varepsilon_i$  are the single-quasi-particle energies;

$$F_{ij} = - \sum_{\sigma=a,b} \int d^3r \varphi_i(r_1) V_M(r_{i\sigma}) \varphi_j(r_2);$$

$$F_{ijkl} = \int \int d^3r_1 d^3r_2 \varphi_i(r_1) \varphi_j(r_2) r_{12}^{-1} \varphi_k(r_2) \varphi_l(r_1).$$

Here  $V_M(r_{i\sigma})$  is the single particle MPP that imitates the potential of the core in which quasi particles move. The interaction energy  $E_0$  of the  $M^+$  ions of the core is defined in the form

$$E_0 = z_a^c z_b^c / R,$$

where  $R$  is the internuclear distance;  $z_a^c$  and  $z_b^c$  are the effective charges [32–35]. The procedure for correct determination of  $z^c$  is given, for example, in [32]. As the model potential  $V_M$  the following Hellman-type potential was used [5, 8]:

$$V_M = -\frac{1}{r} + \frac{A}{r} \exp(-2kr), \quad (1)$$

where  $A$  and  $k$  are the parameters of the potential usually calibrated against the experimental energies of the basic state of alkaline atoms (see Table 1). The correct molecular MPP is presented in the form of the sum

TABLE 1. Parameters of the Priming Model Potential  $V_M$  (a.e.) and Experimental Ionization Energies  $E$  of Alkaline Atoms (eV)

Atom	$A$	$k$	$-E$
Li	1.287	0.422	5.39
Na	1.826	0.536	5.14
K	1.989	0.449	4.32
Rb	1.640	0.358	4.18
Cs	1.672	0.333	3.88

$$V_M = V_M(r_a, \theta_a, \varphi_a) + V_M(r_b, \theta_b, \varphi_b). \quad (2)$$

For successive implementation of the developed method of the PT with ZA PP, the eigenfunctions of the well-known problem of two centers of quantum mechanics with potential  $V_M$  should be used as ZA functions [35]. Below this will be realized for an  $Rb_2$  molecule as one of the variants of the calculation. The solution of a two-center problem was considered earlier [13, 18, 33]. The Rayleigh–Ritz variational principle is used as an alternative variant, whereas as a test wave function the following function was used [8]:

$$\Psi(\lambda, \mu) = (R\lambda)^n e^{-(\alpha R\lambda + \beta R\mu)}, \quad (3)$$

where  $\lambda$  and  $\mu$  are the ordinary elliptic coordinates ( $\lambda = (r_a + r_b)/R$ ,  $1 \leq \lambda \leq \infty$ ;  $\mu = (r_a - r_b)/R$ ,  $-1 \leq \mu \leq 1$ );  $\alpha$  and  $\beta$  are the variational parameters determined by minimization of the energy of the ground state;  $n$  is an integer selected to obtain the best energy (for details see [8]). The third variant of the calculation virtually coincides with the second one, except for the fact that parameters  $\alpha$ ,  $\beta$ , and  $n$  are selected from the condition of reproduction of the experimental dissociation energy of the corresponding ion  $M_2^+$ . The calculation of system  $M_2$  under investigation is divided into two stages: construction of the zero-order model approximation using empirical information for determining the PP parameters; calculation of corrections of various order with Rayleigh–Schrödinger PT with effective consideration of exchange–correlation effects as higher-order PT effects by using corresponding single- and multiparticle PP. As a perturbation operator, an operator of the form

$$H_{PT} = \sum_{\sigma} \sum_{ij} \left[ r_{ij}^{-1} - V_M(r_{i\sigma}) \right], \quad (4)$$

is used, in which  $\sigma$ ,  $i$ , and  $j$  are the summation suffixes over nuclei and electrons.

In [13, 18] a PT series was constructed for the matrix of a secular operator and techniques of summation of diagrams for the secular matrix were considered. The terms of such a series were presented in the form of Feynman diagrams contributions which were classified by the number of end lines. According to this classification, matrix element  $M$  of the secular operator was represented in the form:

$$M_{\xi\eta} = M_{\xi\eta}^{(0)} + M_{\xi\eta}^{(1)} + \dots + M_{\xi\eta}^{(i)},$$

where  $i$  is the total number of quasi particles,  $M^{(0)}$  is the contribution of vacuum diagrams (without end lines);  $M^{(1)}$  is the contribution of single-quasi-particle diagrams (one pair of end lines);  $M^{(2)}$  is the contribution of two-quasi-particle diagrams (two pairs of end lines), and so on. The contribution of  $M^{(0)}$  determines the energy of the core. The contribution of  $M^{(1)}$  is equal to the sum of single-quasi-particle states  $\varepsilon_i$ . In the first order of PT, one should calculate only the contribution of two-quasi-particle diagrams of the 1st order that take into account the direct Coulomb interaction of quasi particles. The 1st order correction sought is equal to the interaction energy of quasi particles  $\Delta E^{(1)}$  and is expressed in terms of ordinary matrix elements on ZA wave functions. For operator  $r_{12}^{-1}$ , one uses, as usual, the Neumann expansion in associated Legendre polynomials of the 1st and 2nd kind and in spherical harmonics [35]. We note that in the 1st order of PT, two-particle diagrams with the compensating term  $-V_M$  are absent in  $H_{PT}$ , but such diagrams appear in the 2nd order, even though their contribution is

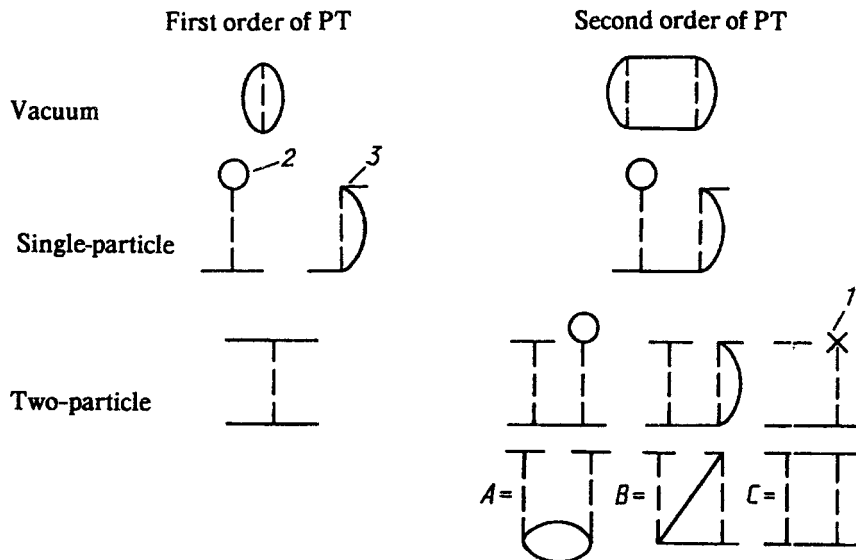


Fig. 1. Basic Feynman diagrams of PT with model ZA potential; the diagram corresponding to  $V_M$  (vertex 1) is almost completely compensated by the diagrams with Hartree–Fock insets (2, 3) in all PT orders; A, B are the straight and exchange polarization diagrams, C is the ladder diagram.

substantially compensated by the contribution of diagrams with strictly energy insertions [22–24]. Then the 2nd-order diagrams A, B, C are considered (Fig. 1) for which the calculation is to be carried out. In the theory of multielectron systems, correlations are usually taken into account by the superposition of additional configurations, i.e., by expansion of a secular matrix. The additional configurations can be subdivided into two groups:

1: states with excitation of electrons from the core (states with one vacancy in the core and three electrons above the core); the superposition of these states accounts for the polarization interaction of quasi particles with one another through the polarizable core (2nd order diagrams, Fig. 1, A, B); 2) states corresponding to excitation of one of the outer quasi particles, with the number of outer particles remaining unchanged; the superposition of these states describes the effect of outer screening of outer particles by one another (the 2nd-order diagram, Fig. 1, C). These two types of states give the correction of the 2nd order of PT:

$$\Delta E^{(2)} = \Delta E_{\text{pol}}^{(2)} + \Delta E_{\text{scr}}^{(2)}.$$

Note that such an additive subdivision is possible only in the 2nd order of the PT; in the higher orders terms appear that describe the interference of these effects. The superposition of states of the second type would have led to calculation of very cumbersome matrix elements. In principle, the 2nd type states can be taken into account in a secular matrix by the expression of  $\Delta E^{(1)}$  for the matrix element. However, it may turn out that a whole continuum of higher states must be taken into account to achieve the desired accuracy. An effective means for taking into account the states of both the 1st and 2nd type without increasing the dimensions of the secular matrix (and without additional computations) was suggested in [24–28] (see also [15–19]). It consists in supplementing the Coulomb interparticle interaction operator with a polarization operator which describes the interaction of outer particles through a polarizable core. The matrix elements of the polarization operator, which has the form [13, 26]

$$F_{\text{pol}}(r_1, r_2) = X \left\{ \int d^3r \rho_c^{1/3}(r) / |r_1 - r| |r - r_2| - \right. \\ \left. - \left[ \int d^3r \rho_c^{1/3}(r) / |r_1 - r| \int d^3r \rho_c^{1/3}(r) / |r - r_2| \right] / \int d^3r \rho_c^{1/3}(r) \right\}, \quad (5)$$

TABLE 2. Values of Parameters  $\alpha$ ,  $\beta$ ,  $n$ ,  $\theta$ , and  $N$  of Equilibrium Distances  $R_e$ , and Dissociation Energies of Ions  $D_e$

Ion	$\alpha$	$\beta$	$n$	$D_e$	$R_e$	$N$	$\theta$
LiRb <sub>2</sub> <sup>+</sup>	0.5548	0.0603	3	-	7.20	0.1108	0.7523
Na <sub>2</sub> <sup>+</sup>	0.5865	0	3	1.13	6.48	0.3777	0.7318
NaRb <sub>2</sub> <sup>+</sup>	0.5249	0.0576	3	0.60	7.53	0.1149	0.7752
KRb <sub>2</sub> <sup>+</sup>	0.4836	0.0538	3	-	8.20	0.1216	0.8012
Rb <sub>2</sub> <sup>+</sup>	0.4731	0	3	0.86	8.40	0.1270	0.8149
CsRb <sub>2</sub> <sup>+</sup>	0.4624	0.0516	3	-	8.62	0.1214	0.8233

Note:  $N$  is the normalization constant; the values of  $D_e$  are given in eV; the values of the remaining quantities are in a.u.

are the contributions from the polarization diagrams (see Fig. 1). Here  $X$  is a numerical coefficient (the procedure for its determination is described in detail in [26]);  $\rho_c$  is the electron density of the core without consideration of outer quasi particles. In calculation of the polarization correction for the value of  $\rho_c$ , the relation  $\rho_c = \rho_a + \rho_b$  was used, and thereafter the densities  $\rho_{a,b}$  were defined by expressions in the same way as in [43]. The general computational procedure for  $\Delta E_{\text{pol}}^{(2)}$  is described in [26, 27]. Note that the corner portions of the matrix elements  $r_{12}^{-1}$  and  $F_{\text{pol}}(r_1, r_2)$  coincide, therefore accounting for the correction  $\Delta E^{(2)}$  is reduced only to modification of the radial integrals that enter into the expression for  $\Delta E^{(1)}$ . The introduction of  $F_{\text{pol}}$  made it possible to reduce the problem to one concerning two particles that interact via the potential  $[r_{12}^{-1} + F_{\text{pol}}(r_1, r_2)]$ , accurate to within the second order of PT. Accounting for the effect of screening of the outer particles by each other can be done by supplementing the potential of the interaction between an outer electron and all the core electrons in the ZA Hamiltonian with an additional screening potential  $W_{\text{scr}}$  owing its origin to the presence of the second particle. The unknown potential  $W_{\text{scr}}$  is selected so that  $\langle | \sum_{\sigma} \frac{\theta}{r_{i\sigma}} | \rangle = \langle | r_{12}^{-1} | \rangle$ , where  $\theta$  is the parameter of the potential (see below). The matrix elements are calculated on ZA wave functions with the priming model potential. Other variants of accounting for the screening effect are also possible [32-35]. The inclusion of  $W_{\text{scr}}$  in the zero order allows one to take into effective account the ladder-type diagram in all orders of PT (Fig. 1).

We shall give the results of the calculation on the basis of the developed Rayleigh-Schrödinger method of PT with a priming model ZA potential of dissociation energies  $D_e$ , and equilibrium distances  $R_e$  of a number of diatomic dimers of alkaline atoms RbM. The values of parameters  $A$ ,  $k$  of potential (!), which were calibrated by the empirical energies of the ground state of the alkaline atoms [1, 13], are presented in Table 1. Table 2 gives the priming values of parameters  $\alpha$ ,  $\beta$ ,  $n$  and  $N$  of the ZA wave function that were found variationally for corresponding molecular ions  $M_2^+$  proceeding from the energy minimization procedure. It is natural that  $\beta = 0$  in the homonuclear variant and  $\beta \neq 0$  in the heteronuclear one. Table 2 also contains the values of parameter  $\theta$  of the screening potential  $W_{\text{scr}}$ . The results of calculation of the dissociation energy for dimer Rb in the three variants are listed in Table 3: 1) the ZA was found by solving the problem of two centers in quantum mechanics; 2) as the ZA wave function, a trial function with variationally determined parameters was used (see Table 2); 3) as the ZA wave function a trial function, was used with parameter  $\alpha$  selected from the condition of reproduction of the experimental value for the dissociation energy of Rb<sub>2</sub><sup>+</sup>. In all of the variants, the exchange-correlation effects are taken into account identically following the procedure described above. Table 3 also contains the calculated results for the dissociation energies of other alkaline diatomic molecules. For comparison, Table 3 lists the literature data on the energies of some of the indicated molecules calculated by other methods: within the framework of different versions of the PP approach [1-11, 34, 35]. We note the good agreement between our calculated data and the available empirical results. For a number of molecules, the energies sought were obtained for the first time. A most

TABLE 3. Dissociation Energies (eV) of Alkaline Dimers  $M_2$  Calculated in the Present Work by the PT Method as Well as Within the Framework of Other Approximations, and Available Experimental Data

	$M_2$					
	RbLi	Na <sub>2</sub>	RbNa	RbK	Rb <sub>2</sub>	RbCs
Experimental data		0.74	0.58		0.49	
Gaussian PP and model wave functions		1.33	0.79		0.49	
Hellman potential and Gaussian model wave functions		0.25	0.09		0.02	
Hellman potential and Heitler–London ansatz with Sleigher orbitals		0.23				
Hartree–Fock potential + Phillips–Kleinman point PP and Heitler–London ansatz with Slater orbitals; polarization of the core in the form of the effective potential is taken into account		0.25				
Model PP and 13-configuration wave function		0.59				
Model PP and configuration interaction approximation with the use of approximate natural orbitals						
Present work:						
1 variant of calculation;	0.66	0.74	0.58	0.52	0.48	0.45
2 variant of calculation;	0.61	0.68	0.51	0.48	0.40	0.39
3 variant of calculation (see the text)		0.74	0.57		0.46	
Semi-empirical PT (with fitting $D_e$ to the experiment)		0.71				
Local density approximation in density functional theory		0.75				

TABLE 4. Spectroscopic Constants of the Rydberg States Calculated in the Present Work and Also Within the Framework of Other Approaches and Experimental Data for the Excitation Energy  $T_e$ , for the Rotational,  $B_e$ , and Vibrational,  $\omega_e$ , Constants

State		$4^1\Sigma_g^+$	$5^1\Sigma_g^+$	$6^1\Sigma_g^+$
$T_e, 10^2 \text{ cm}^{-1}$	a	283.26	317.72	325.62
	b	285	319	328
	c	286	319	327
	d	285	320	326
$B_e, \text{ cm}^{-1}$	a	0.0899	0.1136	0.1059
	b	0.0838	0.107	0.101
	c	0.088	0.110	0.110
	d	0.093	0.109	0.107
$\omega_e, \text{ cm}^{-1}$	a	108.74	109.41	123.67
	b	107	110	119
	c	105	113	123
	d	106	110	123

Note: a) experimental data [11]; b) Hartree–Fock *ab initio* PP polarization of the core [14]; c) empirical PP + polarization of the core [12]; d) present work.

important feature of this calculation is accurately accounting for the effect of the polarization interaction of outer quasi particles through the core and mutual screening of these particles, so that our results exceed in accuracy the calculations performed earlier. The analysis of calculation of the Rb<sub>2</sub> dimer in three variants shows that use of the eigenfunctions of the two-centers problem as wave functions in ZA leads to more accurate results than with use of model wave functions with variational parameters  $\alpha, \beta$ . Fitting of parameter  $\alpha$  of the wave function in the 3rd calculation variant by using the experimental value of the dissociation energy of Rb<sub>2</sub><sup>+</sup> leads to a more accurate value of  $D_e$  for Rb<sub>2</sub> than in the case of variational determination of  $\alpha$ . Obviously, this is explained by the well-known

fact from the theory of calculations of atoms and ions within the framework of a similar approach (see [23-28]) – the fact which is associated with the use of empirical information about a simpler related system in the ZA of PT. Diagrammatically this means fuller consideration of the corresponding correlation diagrams. The results of calculating the potential curves and spectroscopic constants for the Rydberg states  $n^1\Sigma_g^+$  ( $n = 4-6$ )  $\text{Na}_2$  are presented in Table 4, which also lists the results of similar PP calculations on the basis of the *ab initio* PP method with calibration of the ground state into the Hartree–Fock wave function and calculations using empirical PP and with consideration of the polarization of the core by means of the Dalgarno PP, as well as the experimental data in [11, 12, 14]. As seen from Table 4, the calculated data are in good agreement with the experiment. It is very important to emphasize the fundamental role of accounting for the effects of polarization of the core and screening in obtaining high accuracy. Inclusion of the screening potential also improves the convergence of the PT.

In conclusion, we will emphasize that the computational scheme of our approach includes the possibility of use of the *ab initio* PP in the PT ZA as was done earlier for atomic systems [22-26]. This makes it possible to use our method for calculating diatomic systems for which there are no experimental data on the structure and spectrum.

The work is carried out with partial support from the International Soros Support Educational Program (ISSEP), grant No. SPU 061016 (A, C, D).

## REFERENCES

1. K.-P. Hewber and G. Herzberg, Constants of Diatomic Molecules [Russian translation], Moscow (1984).
2. E. E. Nikitin and S. Ya. Umanskii, Semiempirical Methods for Calculating the Interaction Potentials of Atoms. Outcomes of Science and Technology. VINITI, Series Structure of Molecules and Chemical Bonding, Issue 4 (1980).
3. H. Haberland, Y. T. Lee, and P. E. Siska, Excited States in Chem. Phys., Vol. 2, ed. J. W. McGowan, Adv. Chem. Phys., 45, 457-478 (1981).
4. W.-T. Luh, J. T. Bahns, et al., J. Chem. Phys., 88, 2235-2241 (1988).
5. Ph. Durand and J. P. Malrieu, Ab initio Methods of Quantum Chemistry, ed. K. P. Lawley, Chichester, et al., New York (1987).
6. P. Gombas, Pseudopotentials, Berlin (1967).
7. M. Frauss and W. Stevens, J. Chem. Phys., 93, 4236-4242 (1990).
8. L. Bellomonte, F. Cavaliere, and G. Ferrante, J. Chem. Phys., 61, 3225-3234 (1974).
9. C. Bottcher and A. Dalgarno. Proc. Roy. Soc. London A, 340, 187-196 (1974).
10. A. V. Nemukhin and N. F. Stepanov, Vestn. MGU, Ser. 2, Khim., 18, 282-286 (1977).
11. A. J. Taylor, K. M. Jones, and A. L. Schawlow, Opt. Commun., 39, 47-50 (1981).
12. A. Henriot and F. Masnou-Secuws, J. Phys. B: At. Mol. Opt. Phys., 21, L339-346 (1988).
13. A. V. Glushkov, Zh. Strukt. Khim., 34, No. 5, 3-10 (1993).
14. G. H. Jeung, Phys. Rev. A, 35, 26-35 (1987); J. Phys. B: At. Mol. Opt. Phys., 16, 4289-4297 (1983).
15. A. V. Glushkov, Zh. Strukt. Khim., 29, No. 4, 3-10 (1988); 30, No. 6, 3-6 (1989); 31, No. 1, 11-14 (1990); 30, No. 4, 11-16 (1990).
16. A. V. Glushkov, N. N. Dudnik, and S. V. Malinovskaya, Zh. Strukt. Khim., 29, No. 1, 165-167 (1988).
17. A. V. Glushkov and S. V. Malinovskaya, Zh. Fiz. Khim., 62, 100-105 (1988); 65, 2970-2977 (1991); 66, 1259-1268 (1992).
18. A. V. Glushkov, Zh. Fiz. Khim., 66, 589-595 (1992).
19. A. V. Glushkov, Opt. Spektrosk., 76, 885-890 (1994); 77, 5-10 (1994).
20. A. V. Glushkov, Izv. VUZov, Fiz., 33, No. 10, 41-46 (1990); 35, No. 10, 3-9 (1992); No. 6, 41-48 (1994).
21. A. V. Glushkov, S. V. Ambrosov, T. V. Buidzhi, et al., Zh. Prikl. Spektrosk., 64, 256-259 (1997).
22. V. V. Tolmachev, Adv. Chem. Phys., 14, 421-482 (1969).
23. L. V. Tolmachev, L. N. Ivanov, and E. P. Ivanova, Izv. VUZov, Fiz., 12, 84-89 (1969).
24. A. V. Glushkov, L. N. Ivanov, and E. P. Ivanova, In: Autoionization Phenomena in Atoms [in Russian], Moscow (1986).

25. V. S. Letochov and L. N. Ivanov, *Com. At. Mol. Phys. D*, **14**, 169-192 (1985).
26. E. P. Ivanova, L. N. Ivanov, A. V. Glushkov, and A. E. Kramida, *Phys. Scripta*, **32**, 512-524 (1985).
27. A. V. Glushkov and E. P. Ivanova, *J. Quant. Spectr. Rad. Transf.*, **36**, 127-145 (1986).
28. A. V. Glushkov and L. N. Ivanov, *Phys. Lett. A.*, **170**, 33-36 (1992).
29. A. V. Glushkov, *Pis'ma Zh. Éksp. Teor. Fiz.*, **55**, No. 2, 104-107 (1992).
30. A. V. Glushkov and L. N. Ivanov, *J. Phys. B: At. Mol. Opt. Phys.*, **26**, No. 16, L379-386 (1993).
31. A. V. Glushkov, S. V. Ambrosov, V. E. Orlova, et al., *Proc. 5-th Atomic Spectra & Oscillator Strengths for Astrophysical and Laboratory Plasma Conf. (5-th ASOSALP)*, Paris–Meudon (1995).
32. M. D. Dolgushin, *Zh. Fiz. Khim.*, **64**, 3250-3256 (1990).
33. A. V. Glushkov, *Zh. Prikl. Spektrosk.*, **49**, 840-843 (1988).
34. J. Harris and R. O. Jones, *J. Chem. Phys.*, **68**, 1190-1198 (1978).
35. K. Miller and A. E. S. Green, *J. Chem. Phys.*, **60**, 2426-2432 (1974).