[1)] The symbol σ_N is used to designate the cross section for multiphoton ionization of an atom.

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Excitation mechanisms in the systems $Na^+ + Ne$ and $O^+ + Ne$

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On the assumption of definite molecular excitation mechanisms, a calculation has been made of the relative intensities and polarizations of radiation from the multiplets $Ne^*(2p^5 3p)$ and $X^*(3p)$ for $X = Na$ and O, excited in collisions of X^+ with neon at high incident-ion energies ($E \gtrsim 10$ keV). The mechanism assumed excitation to the lowest Σ term (with the least spin) of the X^+Ne^+ ionic cores with possible σ or π molecular states of the excited electron. The calculation enables us to understand a number of correlations of experimental data on polarization. Comparison of the theoretical intensity distribution with experimental values shows that excitation of the $3p$ states of X and Ne occurs both through σ and through π terms of the outer electron, but the oscillatory structure of the total cross sections is due to interference of π states.

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INTRODUCTION

Measurements made by various workers[1–6] of the excitation function of optical lines in the systems Na^+Ne and others and recent systematic studies of the excitation processes

$$X^+ + \mathrm{Ne}(2p^6) \to \begin{cases} \mathrm{Ne}^+(2p^5)+X^* \\ \mathrm{Ne}(2p^5 3p)+X^+, \end{cases} \qquad \Delta E \sim 18\ \mathrm{eV} \tag{1}$$

for $X^+ = Na^+$, O^+, Mg^+, and N^+ have shown[7] a regular oscillating structure of the cross sections due to interference of energetically close channels of direct excitation and charge exchange,[3,8] and also a strong polarization of the excited lines. In addition to the phase of the oscillations, which characterizes the relative arrangement of the molecular terms taking part in the interference,[3,8] measurements have also been made of the distribution of intensities of the various components of the $3p - 3s$ transitions of $Ne^*(2p^5 3p)$ and $X^*(3p)$ and their polarization. On the basis of these data, possible molecular excitation mechanisms have been discussed.

In the present work, in order to clarify the excitation mechanism at higher collision energies ($E \geqslant 10$ keV), we have calculated the relative intensities and polarizations of the components of $3p - 3s$ transitions of Ne^* and X^* in reaction (1) for $X^+ = Na^+(^1S)$ and $O^+(^4S)$. Only at such high energies, when only the main components of the molecular interactions can have a substantial influence on the evolution of the excited states arising, is it possible to calculate with relative simplicity the probabilities of population of individual components of the multiplets in such multilevel systems as Ne^*Na^+ and Ne^*O^+. Calculations carried out for two possible mechanisms (σ and π) permit an understanding of a number of correlations of the experimental data and enable us to conclude what is the role of each of the excitation mechanisms at high energies.

DISCUSSION OF EXCITATION MECHANISMS

The processes considered have a low excitation threshold (80 and 220 eV for $X^+ = O^+$ and Na^+),[7] which at energies $E > 10$ keV corresponds to scattering at small angles $\theta < 2U_0/E \approx 3\times 10^{-2}$ with an impact parameter ρ close to the radius $R_1 \approx 1$ atomic unit of crossing of the ground-state term with the lowest excited terms (smaller impact parameters correspond to higher ionization-energy loss, two-electron excitation, and so forth). Therefore in calculation of the polarizations we will assume that in process (1) the trajectories of the nuclei are straight lines and that the impact parameter is $\rho \sim R_1$.

The ionization potential of the ions Na^+ and O^+ (47 and 35 eV) is significantly greater than the ionization potential of Ne. Therefore the behavior of the terms $U^*(R)$ which are correlated with singly excited states (1) is determined for $R \gtrsim R_1$ in the first approximation by the interaction potential of the ionic cores Ne^+X^+, to which must be added the energy of the molecular orbit (MO) $\varepsilon_m(R)$ of the outer electron (with angular-momentum projection m on the molecular axis):

$$U_m{}^{\varkappa}(R) = U^{i}_{\mathrm{core}}(R) + \varepsilon_m{}^{\varkappa}(R). \tag{2}$$

The ionic core terms $U^{i}_{\mathrm{core}}(R) = U_{\mathrm{core}}(S_{12}, M_{12}, R)$ depend on the total spin $S_{12} = S_1 + S_2$ of the ions X^+ and Ne^+ and on the projection of the electronic angular momentum M of the ionic cores X^+Ne^+. In this case for $X^+ = Na^+\,(^1S)$ and $O^+\,(^4S)$ we have respectively $S_1 = 0$, $S_2 = 1/2$ and $S_1 = 3/2$, $S_2 = 1/2$, while $M = 0$, 1 coincide with the angular momentum projections of $Ne^+(2p^5, 2P)$.

At small distances $R_1 < R < R_2 \sim 5$ atomic units the terms U^{i}_{core} are strongly split, so that within the boundary of the combined atom $\Delta U_{\mathrm{core}} \sim 1$ atomic unit (see the scheme of MO levels given by Andersen *et al.*[6]). Therefore we can assume that the group of $3p$ states (1) is populated only through terms (2) corresponding to the lower core state $U^{0}_{\mathrm{core}}(R)$: $^2\Sigma$ is the term for Na^+Ne^+ and $^3\Sigma$ is for O^+Ne^+. Actually the ground-state term crosses a large number of excited terms (higher excitations, ionization, and so forth) before it crosses the terms (2) with $i \neq 0$.

The MO of the external electron levels $\varepsilon^{\varkappa}_m$ for process (1) have projections $m = 0$ (the σ orbit) and $m = \pm 1$ (π orbit) and for the point of resonance excitations (1) are characterized by an approximate parity ($\varkappa = g$ or u):

$$\Psi^{u(g)}(m) = [\Psi_1(m) \pm \Psi_2(m)]/\sqrt{2}, \tag{3}$$

where Ψ_1 and Ψ_2 are functions localized respectively in X and Ne.

From the estimate of the resonance interaction and also the MO scheme of the levels for the Na^+Ne system given by Andersen *et al.*,[6] it is evident that transition of molecular states to atomic states occurs at distances $R_3 \sim 15-20$ atomic units and the corresponding Massey parameter of the transition is $\xi \sim 0.1$ for $E = 10$ keV and an average resonance defect $\Delta E \sim 1500$ cm^{-1}. The smallness of the Massey parameter indicates that in calculation of the probabilities of atomic states in the transition from MO it is possible to use the sudden approximation, i.e., projection of the initial molecular state on the atomic states in the transition region $R \sim R_3$.

The approximation (2) does not take into account:

1) spin-orbit interaction V_{I} in the Ne^+ ion with a constant $B = -520$ cm^{-1};

2) the exchange interaction V_{II} of the external electron with each core (more accurately, the fraction of it which characterizes the splitting of the multiplet in Ne^* and the relative location of the levels of X^*), which has the order 1000 cm^{-1};

3) the rotational coupling $V_{\mathrm{rot}} \sim \hbar\dot{\varphi} = \hbar v\rho/R^2$, which for $E = 10$ keV has a magnitude ~ 3 eV at $R \sim R_1 \sim 1$ atomic unit and which mixes the σ and π states in the transition region $R \sim R_1$.

The interaction V_{rot} at the same time is insufficiently large to shift the Σ and Π states of the X^+Ne^+ cores at $R \sim R_1$, where the $\Sigma-\Pi$ splitting is of the order of 1 atomic unit; however, it can shift them at $R \gtrsim R_2$, where the Σ and Π states are degenerate in the principal exchange interaction of the X^+ and Ne^+ ions. The maximum admixture of the Π state to the initial Σ state (for the condition of complete $\Sigma-\Pi$ degeneracy) of Ne^+ is determined by the angle of rotation θ of the molecular axis in the portion of the trajectory $R_2 < R < R_3$ with impact parameter $\rho \sim R_1$ and is equal to $\sin[(\pi - \theta)/2] \sim R_1/R_2 \lesssim 0.25$.

In the region $R \sim R_1$ of the transition from the ground-state term to the excited states, for the condition of the Σ states of X^+Ne^+ as most probable, population of the $\sigma^{u(g)}$ MO is possible and if the rotational coupling is taken into account also of the π orbits lying in the collision plane:

$$\pi^+ = (\pi_{+1} - \pi_{-1})/\sqrt{2}. \tag{4}$$

Then, at the moment of the transition we can consider the total spin of the system $S^0 = S_1 + S_2 + S_3$ conserved, where S_1, S_2, and S_3 are respectively the spins of X^+, Ne^+, and the electron. Thus, an excited molecular state arising at $R \sim R_1$ can be represented as a superposition of states:

$$\Psi(S_z{}^0) = \Psi^{(\sigma)}(S_z{}^0) + \Psi^{(\pi)}(S_z{}^0)$$

or

$$\Psi(S_z{}^0, R) = \sum_{m=0,1}\sum_{\varkappa=g,u} A(m, \varkappa, R)\,\Phi_{M=0}(m, \varkappa, S_z{}^0), \tag{5}$$

where $\Psi^{\sigma(\pi)}(S^0_z)$ is the contribution of terms with $m = 0$ ($m = 1$) to the sum (5) and

$$\Phi_M(m, \varkappa, S_z{}^0) = \chi(S_1, S_2\,[S_{12}]S_3, S^0, S_z{}^0)\,\Psi_{\mathrm{core}}(M)\,\Psi^{\varkappa}(|m|). \tag{6}$$

Here χ is the spin function of the system with total spin S^0 and its projection S^0_z equal to the spin and projection of the incident ion X^+; S_1, $S_2 = 1/2$, and $S_3 = 1/2$ are the spins of X^+, Ne^+, and the external electron; $S_{12} = S_1 + S_2$ has a minimal value; $\Psi_{\mathrm{core}}(M = 0)$ corresponds to the Σ

state of the core and $\Psi^{\varkappa}(|m|)$ is the MO of the external electron.

On separation of the atoms to distances $R \sim R_3$ the states forming the function (5) are developed adiabatically from the terms (2), so that (omitting the phase which is common for Ψ):

$$A^{\varkappa}(m)=A(m,\varkappa,R_3)=A^0(m,\varkappa)\exp\left\{-i\int\limits_{R_1}^{R_3}\frac{\varepsilon_m{}^{\varkappa}(R)\,dR}{\hbar v}\right\}. \tag{7}$$

Actually, at high energies the spin-orbit interaction is not able to change the total spin of the system in the region $R_1 < R < R_3$, since

$$\int\limits_{R_1}^{R_3}\frac{V_1 dR}{\hbar v}\sim\frac{BR_3}{\hbar v}\ll 1.$$

Similarly, a change of the molecular state (4) under the influence of the exchange interaction V_{II} reduces to addition of small phases in (6), i.e., to small shifts $\varepsilon_m^{\varkappa}(R)$, since the part of the interaction V_{II} which is non-diagonal in the states (6) has a magnitude ~ 600 cm$^{-1} \sim V_I$. As a result, in the region $R \sim R_3$ on the atomic states $|\gamma J, M_J\rangle$ of the atoms Ne$^*(3p)$ or X$^*(3p)$ (with the states of X$^+$ or Ne$^+$ corresponding to them) there is projected a superposition of the states (6) with the phases (7), which depend on energy, which also gives an oscillatory structure of the cross sections. Here in the amplitudes of the states $|\gamma J, M_J\rangle$ of the atoms Ne* and X* only two σ or two π states can interfere, but not σ and π states between themselves, since for the Σ state of the core they lead to different projections M_J.

Consequently, we can speak individually of the contributions of σ or π mechanisms to the probability of excitation and evaluate them by comparing experimental data with the calculated intensities and polarization, which differ strongly for the two mechanisms. Here, for each of the mechanisms the probabilities P_i corresponding to atomic states $|\gamma J, M_J\rangle$ for the charge-exchange channel ($i=1$) and for direct excitation ($i=2$) in Eq. (1) turn out to be proportional to the weight of the corresponding atomic orbit

$$T_i={}^1/_2|A^u(m)+(-1)^iA^g(m)|^2, \tag{8}$$

where $m=0$ and 1 for the σ and π mechanisms. Thus, the distribution of intensities $I_q(\lambda)$ with polarizations q in each channel i is completely determined by the weights T_i^σ and T_i^π:

$$I_q{}^i=I_q{}^\sigma T_i{}^\sigma+I_q{}^\pi T_i{}^\pi, \tag{9}$$

and $I_q^{\sigma(\pi)}$ can be calculated simply, for example, by setting the coefficients in Eq. (5) equal to

$$A^u(1)=A^g(1)=A^u(0)=0,\ A^g(0)=1 \quad \text{for the } \sigma \text{ mechanism}, \tag{10a}$$

$$A^g(0)=A^u(0)=A^u(1)=0,\ A^g(1)=1 \quad \text{for the } \pi \text{ mechanism}. \tag{10b}$$

At high collision energies the energy dependence of the intensities (9) of the excited radiation is determined only by the factors $T_i^{\sigma(\pi)}$. Consequently, if we were dealing only with one (σ or π) excitation mechanism and not with a combination of them, the intensities of all lines of Ne* or X* would change identically with energy with preservation of the relative splitting inside the multiplet.

PROJECTION FORMULAS

The total intensity I of a line $\gamma J \to \gamma' J'$ of the $3p \to 3s$ transition in reaction (1), averaged over the projections S_{1z} of the incident-ion spin, for each of the mechanisms (σ or π) is calculated from the formula[9]

$$I^{\sigma(\pi)}=\sum_{q=0;\pm1}I_q=K\sum_q\langle\hat{D}_q\rangle^2, \tag{11}$$

where $K=(\lambda/\lambda_0)^{-3}K_0$, λ is the wavelength of the transition, K_0 is the constant for the multiplet and is expressed in terms of the excitation cross section, $\lambda_0 = 6402$ Å,

$$\langle\hat{D}_q\rangle=\frac{1}{2S_1+1}\sum_{\substack{S_{1z}M,M'\\J^+,M^+}}|\langle\Phi^{\sigma(\pi)}(S_{1z})|\Psi(\gamma J,M)\Psi(J^+,M^+)\rangle \times\langle\Psi(\gamma J,M)|\hat{D}_q|\Psi(\gamma' J',M')\rangle, \tag{12}$$

$\hat{D}(q)$ is the corresponding component of the dipole-moment operator, $\Psi(\gamma J, M)$ and $\Psi(J^+, M^+)$ are the wave functions of the excited atom and ion in Eq. (1), and $\Phi^{\sigma(\pi)}$ is the molecular function in Eq. (5) with coefficients (9) or (10).

The degree of polarization of the light in a direction normal to the beam is calculated in terms of the components $I_\parallel = I_{q=0}$ and $I_\perp = (I_{q=1}+I_{q=-1})/2$ with polarizations parallel and perpendicular to the beam axis and is equal to

$$\Pi=\frac{I_\parallel-I_\perp}{I_\parallel+I_\perp}=\frac{3I_{q=0}-I}{I_{q=0}+I}. \tag{13}$$

For convenience in the calculations we go over to the LS basis for the excited atom and ion:

$$\Psi(\gamma J,M)\Psi(J^+,M^+)=\sum_{\substack{L,S,L^+,S^+\\M_L,M_S,M_{L^+},M_{S^+}}}\Psi(L,M_L,S,M_S)\Psi(L^+,M_{L^+},S^+,M_{S^+}) \times C_{LS}{}^{\gamma J}\langle LSM_LM_S|JM\rangle\langle L^+S^+M_{L^+}M_{S^+}|J^+M^+\rangle. \tag{14}$$

Here for X* = Na* and O*, in which LS coupling exists and $\gamma = L, S$, we have the coefficients $C_{LS}^{\gamma J} = \delta_{LL(\gamma)}\delta_{SS(\gamma)}$, and for Ne$^*(3p)$ with an intermediate type of coupling the coefficients $C_{LS}^{\gamma J}$ are given in the Appendix.

As a result in Eq. (12) we have the amplitudes of the states of the LS basis in the functions $\Phi^{\sigma(\pi)}$ (with coefficients (9) for the σ mechanism and (10) for the π mechanism):

$$\langle\Phi^{\sigma(\pi)}|\Psi(L,M_L,S,M_S)\Psi(L^+,M_{L^+},S^+,M_{S^+})\rangle =\sum_S\alpha_i(S)\langle SS^+M_SM_{S^+}|S^0S_z{}^0\rangle\langle L_i,l=1,M_{L_i},m|L,M_L\rangle, \tag{15}$$

where $m=0$ for the σ mechanism and $m=1$ for the π mechanism; L_i is the angular momentum of the core of the excited atom in each channel, $M_{L_i}=0$ is its projection on the molecular axis, $L_1=0$ for X$^+$, $L_2=1$ for Ne$^+$, Intensities of lines of Ne($2p^5 3p$) for the σ and π mechanisms, normalized to the experimental dependence of the p_6 lines.

Level	J	Na++Ne			O++Ne		
		I^σ	I^π	$I_{\exp}$ [7]	I^σ	I^π	$I_{\exp}$ [7]
p_1	0	120	0	13	105	~0	7
p_2	1	0	69	46	~0	67	46
p_3	0	~0	0	4	~0	29	11
p_4	2	51	52	53	60	67	68
p_5	1	0	88	41	21	63	46
p_6	2	77	77	77	74	74	74
p_7	1	0	31	27	35	39	40
p_8	2	33	33	44	82	49	71
p_9	3	0	0	25	105	57	100
p_{10}	1	0	~0	14	82	0	38

and α_i are equal to

$$\alpha_i(S)=\begin{cases}(S_1S_2[S_{12}],S_3S_0|S_1S_2S_3[S_{23}=S],S_0), & i=1,\\ (S_1S_2[S_{12}],S_3S_0|S_1S_3[S_{13}=S],S_2S_0), & i=2,\end{cases}\qquad (16)$$

where S_1, $S_2=1/2$, and $S_3=1/2$ are respectively the spins of X$^+$, Ne$^+$, and e. From the assumptions of the model we find

$$S_{12}=|S_1-S_2|,\quad S_0=S_1.\qquad (17)$$

Substituting Eqs. (14)–(16) into (11) and (12) and carrying out the summation over q, J^+, M^+, S^+, M_{S^+}, and S_z^0, we obtain for the total intensities and for the parallel component for the σ and π mechanisms the following expressions. In the charge-exchange channel ($i=1$) (the transition X*($3p$, SJ) → X*($3s$, SJ')

$$I=I^{(\sigma)}=I^{(\pi)}=\frac{(l=1,S,J\|D\|l=0,S,J')^2}{3}\frac{\alpha_1^2(S)}{2S+1}\left(\frac{\lambda}{\lambda_0}\right)^{-3},\qquad (18)$$

λ is the wavelength of the transition,

$$I_\|^\sigma=IQ,\quad I_\|^\pi={}^1/_2 I(1-Q),\qquad (19)$$
$$Q=3(2J+1)\sum_M\begin{pmatrix}J & 1 & J'\\ -M & 0 & M\end{pmatrix}^2\begin{pmatrix}S & 1 & J\\ M & 0 & -M\end{pmatrix}^2;$$

in the Ne* ($2p^5 3p$) excitation channel (the transition Ne*($2p^5 3p\gamma J$) → Ne*($2p^5 3s\gamma' J'$)

$$I^{\sigma(\pi)}=(\gamma J\|D\|\gamma' J')^2\left(\frac{\lambda}{\lambda_0}\right)^{-3}\sum_{L,S}\frac{\alpha_2^2(S)}{2S+1}(C_{LS}^{\gamma J})^2\begin{pmatrix}1 & 1 & L\\ 0 & -m & m\end{pmatrix}^2,\qquad (20)$$

$$I_\|^{\sigma(\pi)}=\left(\frac{\lambda}{\lambda_0}\right)^{-3}(\gamma J\|D\|\gamma' J')^2(2J+1)\sum_{M,S}\frac{\alpha_2^2(S)}{2S+1}\begin{pmatrix}J & 1 & J'\\ -M & 0 & M\end{pmatrix}^2$$
$$\times\left|\sum_L(2L+1)^{1/2}(-1)^L\begin{pmatrix}1 & 1 & L\\ 0 & m & -m\end{pmatrix}\begin{pmatrix}L & S & J\\ m & M-m & -M\end{pmatrix}C_{LS}^{\gamma J}\right|^2,\qquad (21)$$

where $m=0$ and 1 for the σ and π mechanisms.

Calculation of the intensities and polarizations for the two mechanisms in the systems Na$^+$Ne and O$^+$Ne was carried out on the basis of Eqs. (18)–(21) and (13) with the coefficients $C_{LS}^{\gamma J}$ given in the Appendix and with the line strengths ($J\|D\|J'$) of Ne*, Na*, and O* taken from Ref. 10.

DISCUSSION OF RESULTS

1. The system Na$^+$Ne

The ground state of the quasimolecule Na$^+$Ne is a singlet, so that the intensities (20) and (21) of the lines from the states γJ of the atom Ne($3p$) turn out to be proportional to the weights $(C_{L=J,S=0}^{\gamma J})^2$ of the singlet structures in the atomic systes γJ. This means, in particular, that in our approximation the triplet states p_3, p_9, and p_{10} are not excited. The experimental values of the intensities of radiation from the p_3 and p_{10} levels are actually small[7] (see the table). However, the observed excitation probability of the p_9 state in the Na$^+$Ne system, when the ratio of the line strengths is taken into account, amounts to ~20% of the excitation probability of the singlet states, which also provides an estimate of the accuracy of our approximation. For comparison we note that for other systems X$^+$Ne (X = O, N, Mg) where there is no forbiddenness of excitation of triplet states, the p_9 level has an excitation probability which is the greatest of all of the states p_1–p_{10}.

Calculation of the polarization shows that for the transitions $\gamma J \to \gamma' J'$ of the Ne* atom from states with $J=1$ the value of $\Pi(J=1,\ J')$ does not depend on the mechanism and for $J'=0$, 1, and 2 we have respectively $\Pi=-1$, 0.33, and -0.077. In complete correspondence with experiment, the lines $J=1\to J'=0$ have perpendicular polarization. This fact, like the independence of Π from the mechanism of the process for all transitions from states with $J=1$, can be understood from considerations of symmetry of the complete Hamiltonian on reflection in the collision plane. Actually, on such a reflection $\Psi(\gamma JM)$ Ne* goes over to $(-1)^{J-M}\Psi(\gamma,\ J,\ -M)$. Therefore only the state $[\Psi(\gamma,\ 1,\ 1)-\Psi(\gamma,\ 1,\ -1)]/\sqrt{2}$ turns out to be allowed when the parity of the initial state of the Na$^+$Ne system is taken into account for $J=1$, while the state with $M=0$, which is responsible for the parallel component of the transition $J=1\to J'=0$, turns out to be forbidden. However, for the transition $J=3/2\to J'=1/2$ of the atom Na* and the transition $J=2\to J'=1$ and 2 of the Ne* atom the values of Π are sensitive to the mechanism (σ and π) and are respectively equal to

$$\begin{gathered}\Pi^\sigma({}^3/_2\to{}^1/_2)=0.6;\quad \Pi^\sigma(2\to1)=0.6;\quad \Pi^\sigma(2\to2)=-1;\\ \Pi^\pi({}^3/_2\to{}^1/_2)=-0.43;\quad \Pi^\pi(2\to1)=0.33;\quad \Pi^\pi(2\to2)=-0.43.\end{gathered}\qquad (22)^{1)}$$

The erroneous value given previously[11] $\Pi^\sigma(3/2\to1/2)=0.33$ must be replaced by the value 0.6. The small difference in residual polarizations (22) from those given in Ref. 11 is due to the fact that in the latter case the small admixture of the Π state to the initial Σ state of the core was taken into account.

The two excitation mechanisms differ substantially also in the distribution of intensities within the multiplets Ne($3p$) and Na($3p$). For the σ mechanism the line $\lambda=5852$ Å from the p_1($J=0$) level has the maximal intensity and the lines from the levels p_2, p_5, and p_7 with $J=1$ have zero intensities. On taking into account the mixing of Σ and Π states of the core by the Coriolis interaction the intensities of radiation from these levels for the σ mechanism (just as for $I^\pi(p_1)$) will be nonzero. However, as shown by the calculations previously carried out[11] for the system Na$^+$Ne with the maximum Σ–Π mixing parameter equal to $\sin[(\pi-\theta)/2]=0.25$, these intensities as before are small and the general pattern of the distribution of intensities and polarizations is preserved (see the table of the present work and the table in Ref. 11). For the π mechanism there is an inverse relation in the population of the states p_1 and p_2, p_5, p_7.

In the table we have given the distribution of the combined relative intensities I^σ/N_σ and I^π/N_π of the lines $\mathrm{Ne}^*(3p)$, which have been reduced by means of the normalization coefficients

$$N_\sigma=\frac{I^\sigma(p_6)}{I_{\exp}(p_6)}=2.46\cdot10^{-2},\quad N_\pi=\frac{I^\pi(p_6)}{I_{\exp}(p_6)}=1.85\cdot10^{-2} \tag{23}$$

to the common experimental value of the combined intensity of radiation from the p_6 level.

For the present system $N_\sigma/N_\pi=1.33$. In the same relative units the total intensities $I(J\to J')$ of the lines of the $3p\to3s$ transition of Na are

$$\begin{gathered}I^\sigma(^3/_2\to{}^1/_2)/N_\sigma=170,\quad I^\sigma(^1/_2\to{}^1/_2)/N_\sigma=85,\\ I^\pi(^3/_2\to{}^1/_2)/N_\pi=226,\quad I^\pi(^1/_2\to{}^1/_2)/N_\pi=113.\end{gathered} \tag{24}$$

The dependence of the Na^* intensities on the mechanism appears only as the result of the difference in the normalization factors. In the table we have also given the experimental values of the total intensities of the lines from the levels p_1–p_{10} of Ne^*.

From comparison of the theoretical results with experiment we can conclude that both mechanisms contribute to the excitation reaction. This is indicated also by the the small experimental value of the polarization of the radiation from the $\mathrm{Na}(3p_{3/2})$ level. However, the π mechanism makes a large contribution to the cross section for excitation of $3p$ states and it must be considered responsible for the oscillatory structure. Actually, a regular oscillatory structure exists in the lines $\lambda=6030$ and 6266 Å from the states p_2 and p_5 with $J=1$, excitation of which occurs according to the π mechanism, and is absent in the line $\lambda=5852$ Å from the state p_1, which is due to the σ mechanism. Similarly, only the π channel is responsible for the parallel component $I_\parallel(2\to2)$ of the radiation for the transition $J=2\to J'=2$, so that in the energy dependence of $I_\parallel(2\to2)$ we can expect the same oscillatory structure.

2. The system $\mathrm{O^+\,Ne}$

The initial spin of the system $\mathrm{O}^+(^4S_{3/2})+\mathrm{Ne}(^1S_0)$ is $S_0=3/2$, and therefore the selection rules based on symmetry which exist in the $\mathrm{Na^+Ne}$ system do not operate here and we cannot expect such a strong polarization of the $\mathrm{Ne}(3p)$ lines as in the $\mathrm{Na^+Ne}$ system. Further, the condition of preservation of the total spin of the $\mathrm{O^+Ne}$ system does not forbid the appearance of the $\mathrm{Ne}(3p)$ triplet states, since the Ne^* spin can change simultaneously with the change of direction of the O^+ spin, which is different from zero. This explains the substantial increase in the relative intensities of radiation from the triplet levels p_3, p_9, and p_{10} for the $\mathrm{O^+Ne}$ system in comparison with $\mathrm{Na^+Ne}$ (Ref. 7) (see also the table).

The results of a calculation in accordance with Eq. (20) of the combined intensities I^σ and I^π of the $3p\to3s$ lines of Ne^*, normalized by means of the coefficients (23), are given in the table. In the same relative units the intensities (18) of the transitions $3pJ\to3sJ'$ of the lines $\mathrm{O}^*(^{2S+1}P_J)$, summed over angular momenta J and J', are:

$$\begin{gathered}I^\sigma(^3P)/N_\sigma=5.4,\quad I^\sigma(^5P)/N_\sigma=98,\\ I^\pi(^3P)/N_\pi=7.5,\quad I^\pi(^5P)/N_\pi=137.\end{gathered} \tag{25}$$

As in Eq. (24), the dependence of the O^* intensities on the mechanism is only the result of the difference between N_σ and N_π (for $\mathrm{O^+Ne}$ the ratio N_σ/N_π is 1.4). The ratio of the intensities of excitation of the ^5P and ^3P states with spin $S=2$ and $S=1$ is

$$I(^5P)/I(^3P)\approx18, \tag{26}$$

which corresponds to the experimental fact[7] of a large value of $I(^5P)$ in comparison with $I(^3P)$. Admixture of another spin mechanism of the process (for example, participation in the excitation of the terms of the cores $\mathrm{O^+Ne}$ with spin $S_{12}>|S_1-S_2|$) would substantially change the ratio (26).

The polarizations $\Pi^{\sigma(\pi)}$ calculated from Eqs. (13) and (18)–(21) for the transitions $J=1\to J'$ from the levels p_2, p_5, p_7, and p_{10} are respectively

$$\begin{gathered}\Pi^\sigma(1\to0)=0.0;\ 0.60;\ 0.60;\ 0.0;\ \Pi^\sigma(1\to1)=0.0;\ -0.43;\ -0.43;\ 0.0;\\ \Pi^\pi(1\to0)=-0.17;\ -0.99;\ 0.33;\ -0.18;\ \Pi^\pi(1\to1)=0.7;\ 0.35;\ 0.22;\ 0.09;\\ \Pi^\sigma(1\to2)=0.0;\ 0.08;\ 0.08;\ 0.0;\ \Pi^\pi(1\to2)=0.0;\ -0.06;\ 0.59;\ 0.03.\end{gathered} \tag{27}$$

Similarly for the transitions $J=2\to J'$ from the levels p_4, p_6, and p_8 we have respectively

$$\begin{gathered}\Pi^\sigma(2\to1)=0.48;\ 0.58;\ 0.41;\ \Pi^\sigma(2\to2)=-0.84;\ -0.96;\ -0.64;\\ \Pi^\pi(2\to1)=0.30;\ -0.04;\ 0.06;\ \Pi^\pi(2\to2)=-0.31;\ 0.14;\ -0.12.\end{gathered} \tag{28}$$

Finally, for the transition $3\to2$ from the level p_9 and for the transitions $^3P\to{}^3S$, $^5P\to{}^5S$ we have

$$\begin{gathered}\Pi^\sigma(3\to2)=0.40;\quad \Pi^\sigma(^3P\to{}^3S)=0.3;\quad \Pi^\sigma(^5P\to{}^5S)=0.22;\\ \Pi^\pi(3\to2)=0.23;\ \Pi^\pi(^3P\to{}^3S)=-0.22;\ \Pi^\pi(^5P\to{}^5S)=0.1.\end{gathered} \tag{29}$$

As in the $\mathrm{Na^+Ne}$ system from comparison of the calculated intensity distribution and the experimental values it follows that both channels (σ and π) make a contribution of the same order to excitation of $3p$ states. Comparison of the polarizations (26)–(28) with the available experimental values confirms this conclusion. In particular, if we proceed from the polarizations (27) and (28) and the intensities, we can understand why the polarization of the Ne line $\lambda=6266$ Å for the $1\to0$ transition from the p_5 level has a maximal value $\Pi(\lambda=6266\ \text{Å})\approx-0.4$.[7]

3. Other systems

Extension of a similar calculation to the pairs $\mathrm{Mg^+Ne}$ and $\mathrm{N^+Ne}$ in the series Na^+, O^+, Mg^+, and N^+ studied by Andersen *et al.*[7] is not possible, because of the substantially more complicated term diagram of these systems. Thus, for the Mg^+ ion (with ionization potential ~15.0 eV) we can expect effective excitation of Mg^+ ions together with excitation of Ne. For the $\mathrm{N}^+(^3P)+\mathrm{Ne}$ system there are two terms (Σ and Π) which are correlated with the ground state. In addition, the large (~1.5 eV) exchange splitting of the $3p$ levels of N* and Mg* can substantially distort the terms and the dynamics of the system at medium and large distances.

In the limit of high energies the method considered can be applied to calculation of polarizations also in other simpler systems, for example, in the system Li⁺He, for which on the basis of data on the differential scattering a definite excitation mechanism has been proposed.[12] Thus, the radiation He($1s2p$, ^1P) → He($1s2s$, ^1S) from the state excited in accordance with the correlation diagram[12] for the Π term, will be polarized perpendicular to the beam axis. Similarly, the degree of polarization of the radiation (normal to the beam) $2p \rightarrow 2s$ of Li* from the state Li($1s^22p$, ^2P), excited according to Ref. 12 also on the basis of the Π term, is $\Pi = -0.43$ for the allowed component $j = 3/2$ of the Li(^2P) doublet and $\Pi = -0.2$ in the case when the doublet is not allowed.

Thus, at high energies from the pattern of polarizations and intensities it is possible to deduce the mechanisms of population of the excited states at close distances. At lower energies to describe the excitation of the X⁺Ne pairs which have been discussed a detailed calculation of the dynamics of the multilevel system up to the distances of the transition of the molecular states into atomic states would be necessary. This is possible, obviously, only for simpler systems. Examples of calculations for simple systems of the characteristics of optical radiation excited in collisions of low energy can be found in the review of Alber *et al.*[13]

APPENDIX

To find the structure of the atomic states Ne*($3p$) we used the Hamiltonian

$$\hat{H}=A_0+a(L,\ S)+B_1\mathbf{l}_1\mathbf{S}_1+B_2\mathbf{l}_2\mathbf{S}_2, \tag{A.1}$$

where L and S are the total orbital angular momentum and spin of Ne*($3p$), $l_1 = 1$, $S_1 = 1/2$ and $l_2 = 1$, $S_2 = 1/2$ are the orbital angular momentum and spin of the outer electron and the Ne⁺($2p^5$, $2P$) core. The term $a(L, S)$ corresponds to exchange interaction of the Ne⁺ core and external electron, and the second and third terms describe the spin-orbit interaction of the Ne⁺ ion. The spin-orbit interaction $B_1\mathbf{l}_1\mathbf{S}_1$ of the outer electrons were neglected ($B_1 < 10$ cm^{-1}). The parameters $a(L, S)$ and B_2 were chosen from the condition of agreement of the calculated energy values with the experimental levels[14] of Ne*($3p$). For choice of A_0 equal to the energy of the p_9 ($J = 3$) level, the values of $a(L, S)$ and B_2 in cm^{-1} are:

$$\begin{gathered}a(0.0)=3246,\ a(0.1)=-1355;\ a(1.0)=1070;\ a(1.1)=1068;\\ a(2.0)=700;\ a(2.1)=0;\ B_2=520;\ B_1=0.\end{gathered} \tag{A.2}$$

The Hamiltonian (1) is similar to that proposed previously,[15] from which follow the similar parameter values:

$$\begin{gathered}a(0.0)=3252,\ a(0.1)=-1364;\ a(1.0)=1072;\ a(1.1)=1072;\\ a(2.0)=707;\ a(2.1)=0;\ B_2=518;\ B_1=7.8.\end{gathered}$$

As a result of diagonalization of the Hamiltonian (A.1) we obtain the following expressions for the atomic states p_i of Ne($3p$) in terms of the states of LS basis:

$$\begin{gathered}p_1=0.983(^1S_0)+0.182(^3P_0);\\ p_2=0.807(^3P_1)-0.574(^1P_1)+0.133(^3S_1);\\ p_3=0.983(^3P_0)+0.182(^1S_0);\\ p_4=0.415(^3D_2)-0.536(^1D_2)+0.735(^3P_2);\\ p_5=0.526(^2D_1)+0.493(^3P_1)+0.692(^1P_1);\\ p_6=-0.276(^3D_2)+0.696(^1D_2)+0.663(^3P_2);\\ p_7=0.85(^3D_1)-0.34(^3P_1)-0.430(^1P_1);\\ p_8=0.867(^3D_2)+0.479(^1D_2)-0.41(^3P_2);\\ p_9=(^3D_3);\ p_{10}=-0.109(^3P_1)+0.077(^1P_1)+0.991(^3S_1).\end{gathered} \tag{A.3}$$

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1)*Note added in proof.* The polarizations $\Pi^\sigma(3/2 \rightarrow 1/2) = 0.6$ and $\Pi^\pi(3/2 \rightarrow 1/2) = -0.43$ given in (22) for Na($^2P_{3/2}$) were calculated without allowance for the hyperfine interaction. If the latter is taken into account, the values are $\Pi^\sigma(3/2 \rightarrow 1/2) = 0.21$ and $\Pi^\pi)3/2 \rightarrow 1/2) = -0.10$. They can be easily calculated by using formulas (15), (17) and (37) of the paper by U. Fano and J. Macek, Rev. Mod. Phys. 45, 533 (1973). The obtained polarizations agree with the results of N. V. Talk, J. C. Tully, C. W. White, J. Kraus, A. A. Monge, D. L. Simms, M. F. Robbins, S. H. Neff, and W. Lichten, Phys. Rev. A13, 965 (1976).

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