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Near-LTE Linear Response Calculations with a Collisional-Radiative Model for He-like Al Ions

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Near-LTE linear response calculations with a collisional-radiative model for He-like Al ions

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ABSTRACT

We investigate non-equilibrium atomic kinetics using a collisional-radiative model modified to include line absorption. Steady-state emission is calculated for He-like aluminum immersed in a specified radiation field having fixed deviations from a Planck spectrum. The calculated net emission is presented as a NLTE response matrix. In agreement with a rigorous general rule of non-equilibrium thermodynamics, the linear response is symmetric. We compute the response matrix for 1% and ± 50% changes in the photon temperature and find linear response over a surprisingly large range.

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The calculations describe He-like aluminum. The Maxwellian free electrons have a fixed density $N_e = 10^{20}$ cm^{-3} and temperature $T_e = 150$ eV.

The CR model [4] includes 65 He-like levels up to n=22, with n,l,S-splitting up to n = 4 and n,S-splitting up to n=8, but does not include autoionizing doubly-excited levels. Li-like ions and Li-like satellite levels are omitted.

Electron collisional rates for excitation and de-excitation obey detailed balance and we do not change the collisional rates. Electron collisional ionization to and 3-body recombination from the hydrogen-like ion are included. Ionization from excited states is included. Solution of the collisional-radiative model determines steady-state populations of He-like excited states. The CR model [4] also includes radiative and dielectronic recombination but for simplicity these processes have been suppressed.

Because hydrogenlike ions are coupled through collisional ionization and recombination, it is necessary to use the appropriate ratio of helium-like and hydrogen-like ions. This is done by finding the steady state solution of the rate equations, i.e., by using the excited state populations to determine effective ionization and recombination rate coefficients which determine the ratio of He-like and H-like ions.

The isotropic radiation field has a spectrum I_ν characterized by the number of photons per mode, n_ν. In complete equilibrium n_ν is the blackbody function,

$$n_\nu^0 = [\exp(h\nu/kT_e) - 1]^{-1} \qquad (1a)$$

Non-LTE populations will be induced by a difference $(n_\nu - n_\nu^0)$. In order to generate the response matrix, a non equilibrium radiation spectrum is defined by altering n_ν for one line at a time, using

$$n_\nu = [\exp(h\nu/k\{T_e + \delta T_\nu\}) - 1]^{-1} \qquad (1b)$$

$T_e + \delta T_\nu$ is the effective photon temperature (brightness temperature) for the selected line.

While radiative properties of dense plasmas such as stellar interiors are usually studied using LTE (local thermodynamic equilibrium) methods, low-density plasmas such as tokomak plasmas or the solar corona require NLTE (non-equilibrium) kinetic models. Intermediate plasmas including laser-produced plasmas, laser hohlraums, Z-pinches and divertor plasmas combine high density, a significant radiation environment, and non-LTE populations.

This paper examines non-LTE atomic kinetics using methods of non equilibrium thermodynamics.[1,2,3] We adapt an existing collisional-radiative (CR) model of Fujimoto and Kato[4] to near-LTE conditions and verify the application of non equilibrium thermodynamics by finding a symmetric linear-response matrix.

We consider an ion interacting with radiation which is approximately a blackbody field at the temperature of the free electrons. The difference between the actual radiation and the black-body field causes non equilibrium populations of excited states and leads to a net difference of emission and absorption rates. The difference of emission and absorption at frequency ν is a function of the deviation from the black-body spectrum at frequency ν' and can be described by a response matrix $R_{\nu,\nu'}$.

According to non equilibrium thermodynamics, the steady-state near LTE is constrained by rigorous general requirements of energy conservation, by the principle of minimum entropy production, and by symmetry relations (Onsager relations) which require that the linear response function $R_{\nu,\nu'}$ should be symmetric. This symmetry can be used as a consistency test for a NLTE model.

At densities high enough so that electron rates greatly exceed radiative rates, the deviations from LTE should be small, as shown in previous general studies of NLTE kinetics by Klapisch[5], Salzmann[6] and Fujimoto[7]. Recently the effect of radiation on NLTE populations has begun to attract interest.[8,9] In the present work we consider a moderate density and study the effect of coupling to near-equilibrium radiation, which can induce non-LTE populations in a controlled manner.

The CR model includes spontaneous emission, described by the rate of radiative transitions $i \to j$, (i is the upper level, j is the lower level), (dN_i/dt). This is the rate for transitions $i \to j$, but the initial or final states are also connected to other states (k, l, etc.). We <u>extend</u> the CR model by adding stimulated emission and absorption for each transition,

$$(dN_i/dt) = - A_{ij} N_i (n_\nu + 1) + A_{ji} N_j n_\nu + C_i \qquad (2)$$

The new terms are absorption = $A_{ji} N_j n_\nu$ and stimulated emission = $A_{ij} N_i n_\nu$. In Eq. (2), C_i denotes the net collisional rate. In Eq. (2) the absorption coefficient is determined by detailed balance (Einstein relation),

$$A_{ji} = (g_i/g_j) A_{ij} \qquad (3)$$

Here g_i, g_j are the degeneracies of upper and lower levels.

We have verified that when $n_\nu = n_\nu^0$ for all transitions, the computed population ratios are Boltzmann ratios, so the LTE solution of the extended model can differ from true LTE only in the overall normalization of the populations.

To construct a 5x5 response matrix we perform 5 different NLTE calculations. For each calculation we vary $n_{\nu'}$ for one specific line ν' (Table I). The variation is induced by a photon temperature change $\delta T_{\nu'}$ applied to that one line. All other lines still couple to the black-body spectrum n_ν^0. For each line, in NLTE there is a net radiated power,

$$dE_{ij}/dt = h\nu \; [A_{ij} N_i (n_\nu + 1) - A_{ji} N_j n_\nu] \qquad (4)$$

This rate can be positive (emission) or negative (absorption). The net power in Eq. (4) is zero in LTE (when $n_\nu = n_\nu^0$ and $N_{i,j} = N_{i,j}^0$) and should be proportional to $\delta T_{\nu'}$ for small perturbations. In NLTE there is emission or absorption for many lines (see Figures 1, 2). If we examine the same lines we perturbed, we obtain a square response matrix. The linear response matrix is defined by

$$R_{\nu,\nu'} = h\nu \, [A_{ij} N_i (n_\nu + 1) - A_{ji} N_j n_\nu] \, / \, \delta T_{\nu'} \qquad (5)$$

Then $R_{\nu,\nu'}$ is the net emission from line ν ($i \rightarrow j$) induced by a temperature change $\delta T_{\nu'}$ applied to the line ($i' \rightarrow j'$) denoted ν'. According to non equilibrium thermodynamics, if $R_{\nu,\nu'}$ is defined in precisely this way, it should be a symmetric matrix.

Linear response means a response function independent of $\delta T_{\nu'}$. For large perturbations $\delta T_{\nu'}$, the photon population $n_{\nu'}$ changes in a nonlinear way, especially for lines with $h\nu' \gg kT_e$. Therefore we consider the modified matrix,

$$RL_{\nu,\nu'} = R_{\nu,\nu'} \; ([\partial n_{\nu'}{}^0/\partial T] \cdot \delta T_{\nu'}/[n_{\nu'} - n_{\nu'}{}^0])$$

$$= h\nu \, [A_{ij} N_i (n_\nu + 1) - A_{ji} N_j n_\nu][\partial n_{\nu'}{}^0/\partial T]/[n_{\nu'} - n_{\nu'}{}^0] \qquad (6)$$

The extra factor in Eq. (6) is unity for small perturbations so the modified response matrix is still symmetric in that case. However $RL_{\nu,\nu'}$ remains constant for larger perturbations.

Table I defines the 5 transitions studied in Tables II, III. The transitions are in the singlet spectrum but the calculation includes coupling to triplet states. Table II gives the linear-response matrix calculated as the average of $RL_{\nu,\nu'}$ for small radiation temperature changes of +1% and -1%. Table III gives the response matrix $RL_{\nu,\nu'}$ for radiation temperature perturbations of ± 50%.

The linear-response matrix in Table II is accurately symmetric. Table III shows the range of linear response. For the Heβ transition a 50% increase in photon temperature raises the photon flux by a factor sixty, while a 50% decrease reduces n_ν by a factor 10^{-5}.

These large changes produce only small changes in the response function $RL_{\nu,\nu'}$. The range of linear response is surprisingly large.

This is the response to a perturbation affecting only one line and we can expect nonlinear response for sufficiently strong perturbations affecting several lines.

To interpret the response function, we consider perturbation of the He_α line (see Figure 1 and the first row in Table II). In this case $n_{\nu'}$ is increased relative to the black-body function for the transition from the $1s^2$ ground state to the 1s2p ^1P excited state. Absorption of this extra radiation produces a negative diagonal matrix-element. The absorption decreases the ground state population and increases the (1s2p ^1P) population.

Since the ground state population is reduced with respect to LTE, there is net emission for the line 1s3p ^1P -> $1s^2$. However the population of 1s2p ^1P is higher than LTE, so there is net absorption for transitions 1s2p ^1P -> 1s3s ^1S and 1s2p ^1P -> 1s3d ^1D. There is evidently enough collisional transfer 1s2p ^1P -> 1s2s ^1S to overpopulate the 1s2s ^1S state and for that reason there is also weak absorption for the transition 1s2s ^1S -> 1s3p^1P. This simple reasoning explains the first row of the response matrix. From Figure 1 it is seen that the (1s2p ^3P - $1s^2$ ^1S) inter combination line has net emission and the transitions from n=4 to n=2 are absorptions. At higher magnification many weak emitting and absorbing transitions can be seen.(Figure 1c)

When the radiation is enhanced in the He_β ($1s^2$ ^1S -> 1s3p ^1P) line, the ground state population is reduced and the 1s3p ^1P population is raised relative to LTE.(See Figure 2) The second row of the response matrix in Table II has all signs reversed. There is weak emission on the 3 -> 2 transitions, principally because of collisional transfer between the n=3 levels, which distributes the enhanced population of the 1s3p ^1P state. The 1s2p ^1P population increases by cascade and there is net emission on the resonance transition (1s2p ^1P -> $1s^2$ ^1S). (The rest of the matrix is easily understood by similar reasoning.)

In this discussion we do not speak of emission or absorption lines because $R_{\nu,\nu'}$ involves one-atom rates. It is a separate question of radiative transfer to decide whether a line would appear light or dark against its background as seen from outside the plasma.

We have performed calculations for the same density-temperature conditions using a NLTE screened-hydrogenic average-atom model.[10] The calculations will be reported in detail elsewhere, but give qualitatively similar results for the response matrix. (see Fig. 3). In this case the response function is averaged over frequency groups for perturbed and emitting parts of the spectrum, and has units of Watts/[gram-keV^3]. With appropriate conversion of units the numerical values agree roughly with the CR model.

This approximate agreement is interesting because the average-atom model does not have singlet-triplet splitting but includes photo ionization, radiative recombination and an approximate treatment of other ion charge states. The average-atom response function is less accurately symmetric than the CR results shown in Table II.

The work of this paper could be extended in several directions. If one examined response within the line profiles, the ion temperature would enter the discussion. If the electron distribution were slightly non-Maxwellian, there would be an analogous response function defining response to perturbations of the electron distribution. In addition there are many questions about nonlinear response and the combination of the rate-equation description with more fundamental theory of multi-photon processes.

Symmetry of the response matrix is a test of the NLTE model, especially sensitive to detailed balance. The numerical values of the response coefficients test the entire set of rates in the calculation and give an excellent way to compare different atomic models.

The linear-response method considered here is limited to a special class of NLTE states. The system must be in a steady state and must be "near" LTE, although in these calculations we have found a surprising large range of linear response. We believe this response function can be used to simplify calculation of NLTE atomic kinetics in plasma simulation calculations.

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Table I. He-like aluminum transitions analyzed in Tables II, III.

transition 1	:	$1s^2\ ^1S$ - $1s2p\ ^1P$	1.600 keV
transition 2	:	$1s^2\ ^1S$ - $1s3p\ ^1P$	1.870 keV
transition 3	:	$1s2s\ ^1S$ - $1s3p\ ^1P$	0.276 keV
transition 4	:	$1s2p\ ^1P$ - $1s3s\ ^1S$	0.268 keV
transition 5	:	$1s2p\ ^1P$ - $1s3d\ ^1D$	0.270 keV

TABLE II

Linear-response coefficients (Watts/atom-eV) for He-like aluminum plasma at electron density $n_e = 10^{20}$ cm^{-3} and temperature T_e = 150 eV. The matrix is obtained by averaging NLTE calculations with +1% and -1% perturbations in lines identified in Table I. The matrix is accurately symmetric.

	1	2	3	4	5
1	$-5.234\ 10^{-10}$	$3.564\ 10^{-10}$	$-9.317\ 10^{-12}$	$-1.662\ 10^{-12}$	$-4.333\ 10^{-11}$
2	$3.564\ 10^{-10}$	$-6.221\ 10^{-10}$	$1.068\ 10^{-11}$	$1.590\ 10^{-12}$	$3.538\ 10^{-11}$
3	$-9.317\ 10^{-12}$	$1.068\ 10^{-11}$	$-2.344\ 10^{-12}$	$1.178\ 10^{-14}$	$2.449\ 10^{-13}$
4	$-1.662\ 10^{-12}$	$1.590\ 10^{-12}$	$1.177\ 10^{-14}$	$-3.601\ 10^{-13}$	$4.507\ 10^{-14}$
5	$-4.333\ 10^{-11}$	$3.538\ 10^{-11}$	$2.449\ 10^{-13}$	$4.506\ 10^{-14}$	$-8.827\ 10^{-12}$

Table IIIa

Response coefficient $RL_{u,v}$ (Watts/atom-eV) for He-like aluminum plasma at electron density $n_e = 10^{20}$ cm^{-3}, temperature $T_e = 150$ eV. The perturbations are 50% of Te. While the matrix is not much different from Table II the symmetry is no longer perfect.

	1	2	3	4	5
1	$-5.230\ 10^{-10}$	$3.561\ 10^{-10}$	$-9.309\ 10^{-12}$	$-1.661\ 10^{-12}$	$-4.329\ 10^{-11}$
2	$3.563\ 10^{-10}$	$-6.220\ 10^{-10}$	$1.068\ 10^{-11}$	$1.589\ 10^{-12}$	$3.537\ 10^{-11}$
3	$-7.335\ 10^{-12}$	$8.407\ 10^{-12}$	$-1.845\ 10^{-12}$	$9.269\ 10^{-15}$	$1.928\ 10^{-13}$
4	$-1.651\ 10^{-12}$	$1.579\ 10^{-12}$	$1.170\ 10^{-14}$	$-3.577\ 10^{-13}$	$4.477\ 10^{-14}$
5	$-3.993\ 10^{-11}$	$3.260\ 10^{-11}$	$2.257\ 10^{-13}$	$4.153\ 10^{-14}$	$-8.135\ 10^{-12}$

Table IIIb

Response coefficient $RL_{u,v}$ (Watts/atom-eV) for He-like aluminum plasma at electron density $n_e = 10^{20}$ cm^{-3} and temperature $T_e =$ 150 eV. The perturbation is -50% of Te. It is emphasized in the text that this is a large perturbation. The matrix is not much different from Table II.

	1	2	3	4	5
1	$-5.234\ 10^{-10}$	$3.564\ 10^{-10}$	$-9.317\ 10^{-12}$	$-1.662\ 10^{-12}$	$-4.333\ 10^{-11}$
2	$3.564\ 10^{-10}$	$-6.222\ 10^{-10}$	$1.068\ 10^{-11}$	$1.590\ 10^{-12}$	$3.538\ 10^{-11}$
3	$-1.156\ 10^{-11}$	$1.326\ 10^{-11}$	$-2.908\ 10^{-12}$	$1.461\ 10^{-14}$	$3.040\ 10^{-13}$
4	$-1.670\ 10^{-12}$	$1.597\ 10^{-12}$	$1.183\ 10^{-14}$	$-3.618\ 10^{-13}$	$4.528\ 10^{-14}$
5	$-4.619\ 10^{-11}$	$3.772\ 10^{-11}$	$2.611\ 10^{-13}$	$4.804\ 10^{-14}$	$-9.410\ 10^{-12}$

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Figure 1.) (a) Basic term-diagram for He-like aluminum. When extra radiation is applied to the He$_\alpha$ transition, the n=2 excited states are populated more strongly than in LTE and the 2→3 transitions have a net absorption. (b) The response matrix (eV/atom-sec) for this case shows absorption (negative R values) for the 2→3 transitions. (c) At higher magnification, many other transitions show small responses. The plasma conditions are given in Tables II, III.

Figure 2.) (a) In this case, the perturbation is applied to the He$_\beta$ transition. Now the 2→3 transitions have net emission, as does the He$_\alpha$ line. (b) The signs of 2→3 response coefficients at 280 eV have become positive. (c) At higher magnification, many other transitions show small responses.

Figure 3.) Calculations from the NLTE screened-hydrogenic average-atom model for aluminum plasma at the conditions described in Table II. The response matrix, shown here as a histogram, is normalized by frequency group-widths for emitting and perturbed portions of the radiation spectrum and has units of Watts/[gram-keV^3]. For perturbations of He$_\alpha$ (Fig 3a) and He$_\beta$ (Fig 3b) lines, the signs of the response coefficients agree with results from the CR model.

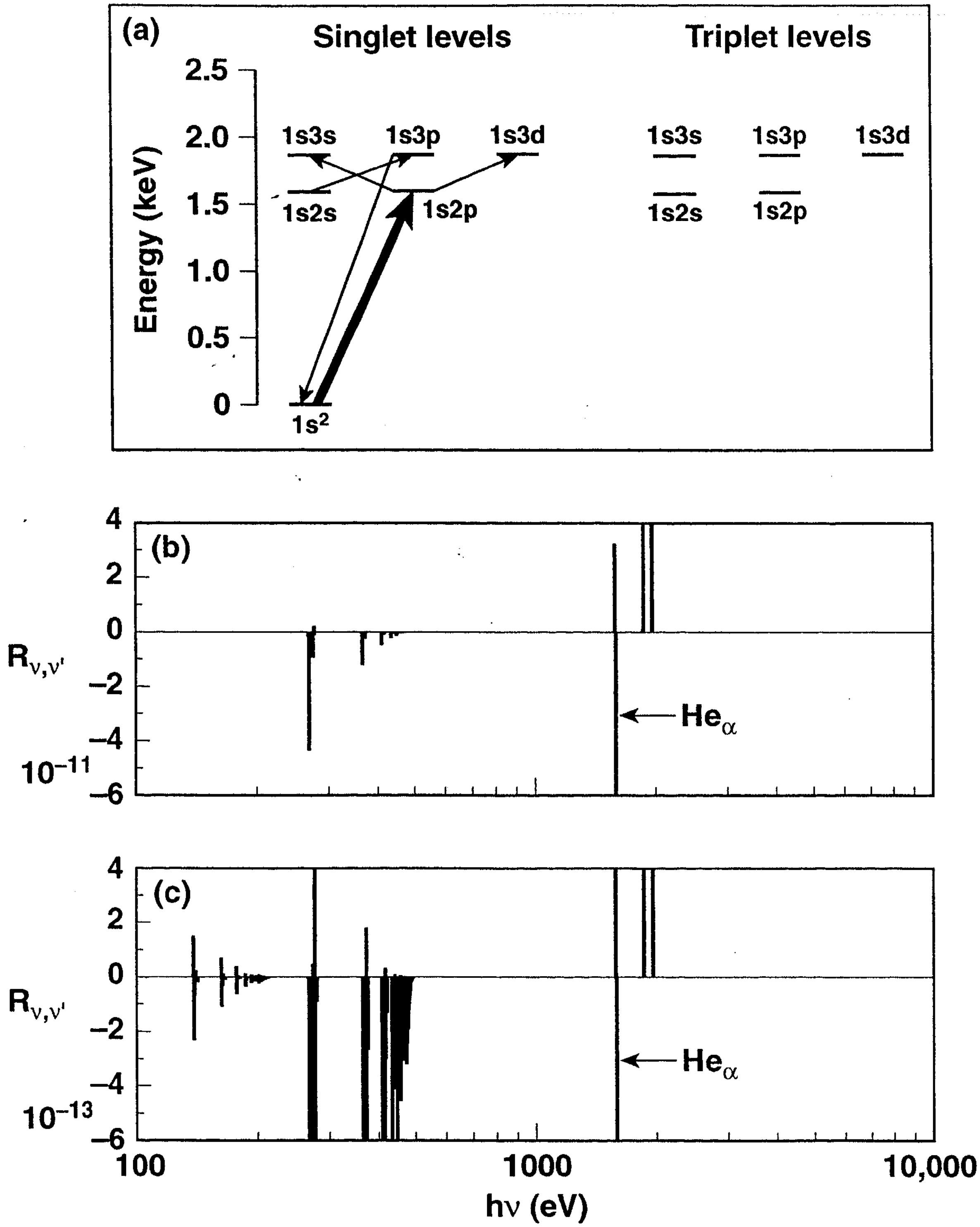
(a)
Singlet levels
Triplet levels
Energy (keV)
2.5
2.0
1.5
1.0
0.5
0
1s3s
1s3p
1s3d
1s2s
1s2p
1s²
(b)
(c)
$R_{\nu,\nu'}$
10^{-11}
10^{-13}
4
2
0
−2
−4
−6
He_α
100
1000
10,000
hν (eV)

Figure 1.

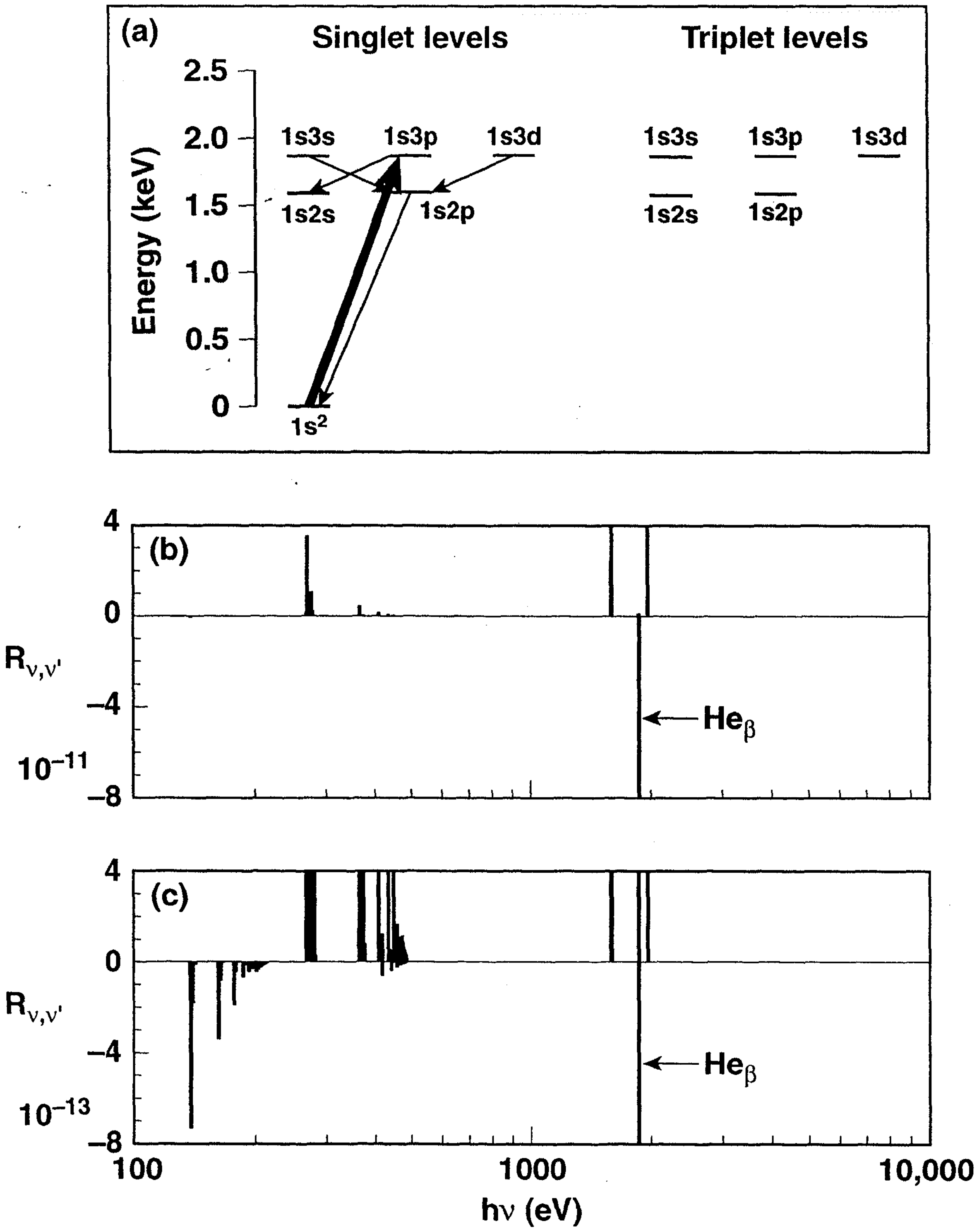

Figure 2.

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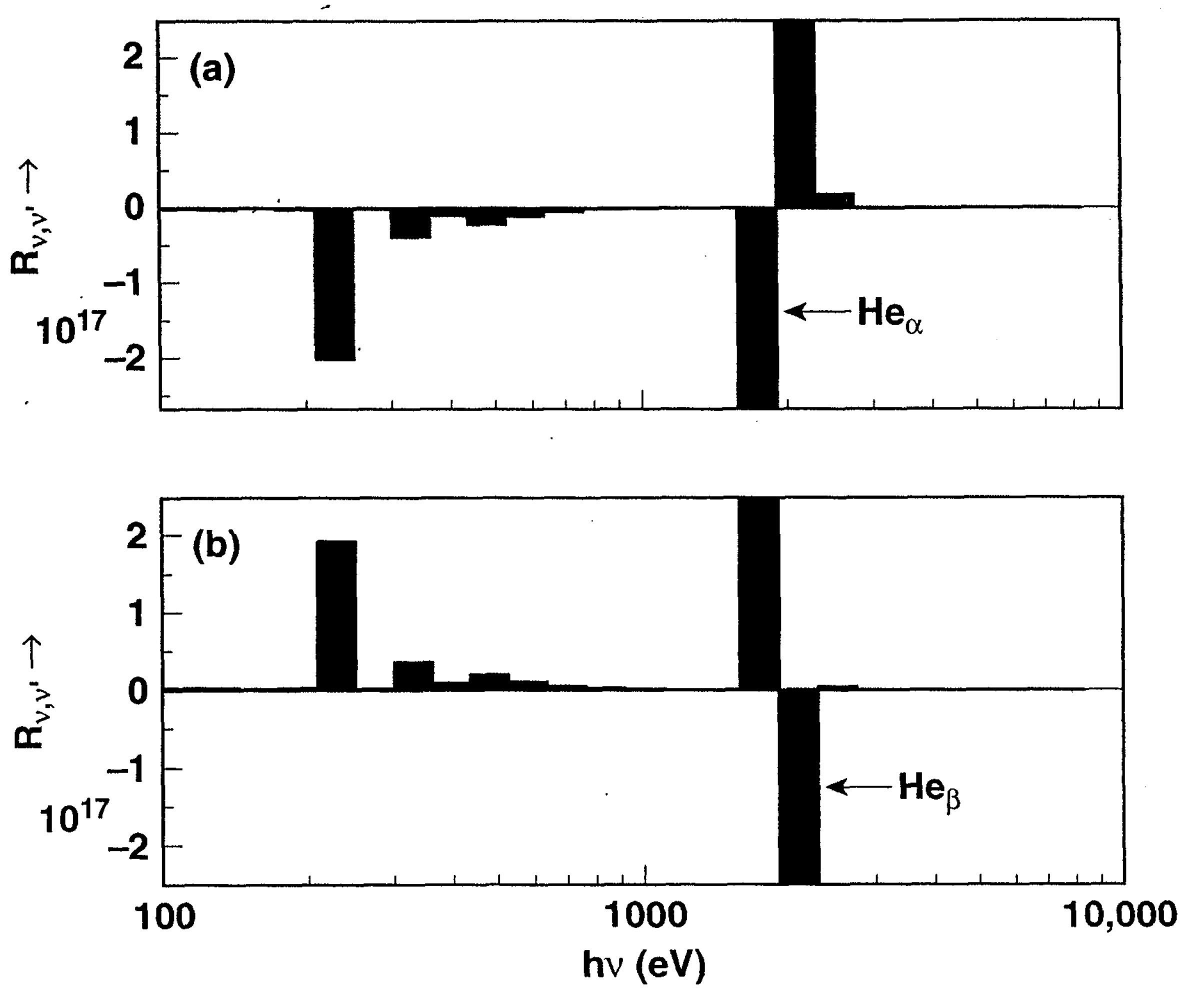

Figure 3.

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