Shifts and asymmetry parameters of hydrogen Balmer lines in dense plasmas

Sibylle Günter and Axel Könies
Universität Rostock, Fachbereich Physik, Universitätsplatz 1, 18051 Rostock, Germany

(Received 28 November 1995; revised manuscript received 9 August 1996)

Shifts and asymmetry parameters of hydrogen Balmer lines have been calculated and compared with experimental data. In order to determine these theoretical values, shifted and asymmetric line profiles have been calculated. This way it is possible to employ the same definitions for shifts and asymmetry parameters as it has been done in corresponding experiments. The resulting theoretical values are in excellent agreement with experimental results. [S1063-651X(97)01501-8]

PACS number(s): 52.25.Rv, 32.70.Jz

I. INTRODUCTION

Spectral lines emitted from dense plasmas are broadened, shifted, and asymmetric due to the interaction between the radiator and the plasma environment. Numerous theories have been developed in order to calculate the width of hydrogen spectral lines. By inclusion of the effects of ion dynamics via computer simulations, excellent agreement between theoretical and experimental linewidths has been reached [1–4].

Up to now, the deviations between theoretical and experimental results are larger for the line shifts and especially for the asymmetry parameters. Considering previous theoretical approaches to shift and asymmetry of hydrogen lines, one finds at least two causes of important uncertainties of the theoretical results.

One of them is the treatment of strong electron-radiator collision contributions to the shift. Most of the shift calculations apply the theory developed by Griem [5,6]. Since this theory is based on a Born approximation for the radiator-perturber interaction, it is restricted to weak collisions only. Therefore (and to avoid divergences that occur within the applied semiclassical approach), a cutoff procedure has been applied at a minimal impact parameter. Unfortunately, the resulting shifts depend strongly on the choice of this parameter. Applying Baranger's relation between the electronic shift contributions and the phase shifts for elastic scattering of the perturbing electrons at excited atomic states, in principle, this problem does not occur. Using this theoretical approach, calculations have been carried out for hydrogen lines by Unnikrishnan and Callaway [7,8]. Since they included explicitly only the states $1s$, $2s$, $2p$, $3s$, $3p$, and $3d$ in the corresponding close-coupling equations, the resulting shifts are too small, except for the L_α line.

The second problem concerning line-shift calculations is the inclusion of the ionic contributions to the shift [5,6,9]. Often the theoretical shift simply is regarded as a superposition of electronic and ionic contributions to the line shift [10,5]. To be correct, however, all contributions to shift and asymmetry should be included in the line-profile calculations in such a way that shifted and asymmetric line profiles result.

The aim of this paper is to calculate such line profiles that allow the determination of shifts and asymmetry parameters in the same manner as from experimental data. Therefore, a theoretical approach based on a Green's-function technique has been applied, which has been developed in a number of earlier papers [11–15]. This approach treats the perturbing electrons quantum mechanically. Strong collision contributions for collisions between radiator and perturbing electrons have been calculated via partial summation of the corresponding T matrix as described in [14,15]. The influence of the perturbing ions on the line profile is described via the well-known model microfield method (MMM) [16–18]. The MMM has been applied successfully to the calculation of hydrogen spectral line profiles for the moderate plasma densities that are considered in this paper. It has been found, however, that the MMM underestimates ion dynamic effects especially for low electron densities. As it will be shown in Sec. III, the influence of ion dynamics on the investigated shifts and asymmetry parameters is rather small. Therefore, these shortcomings of the MMM will not have a measurable influence on the final results.

The time development operator for a constant ionic microfield strength $U(\Delta\omega|\vec{E})$ has been modified in order to account for shift and asymmetry. Thereby, the shift due to inhomogeneities of the ionic microfield has been included as proposed by Halenka in [9]. Besides the ion quadrupole effect, further contributions to the asymmetry of spectral lines such as the trivial asymmetry, the asymmetry due to the different electronic shifts of the various Stark components, and the asymmetry due to the frequency dependence of electronic width and shift [20,21] are included. Additionally, the quadratic Stark effect approximately has been taken into account.

II. THEORY

In previous papers [11–15] a Green's-function approach to spectral line profiles has been developed. Decoupling the ionic and the electronic subsystems and applying the quasistatic approximation for the perturbing ions, the theory comes out with the following formula for the line profile:

$$L(\Delta\omega)\sim\sum_{i,f,i',f'} I_{if}^{i'f'}(\Delta\omega)\int_0^\infty d\beta\, W_\rho(\beta)\times\left\langle i\left|\left\langle f\left|\frac{1}{\Delta\omega-\Sigma(\Delta\omega,\beta)+\Gamma^v}\right|i'\right\rangle\right|f'\right\rangle. \quad (1)$$

Here $W_\rho(\beta)$ is the microfield distribution function according to Hooper and

$$I_{if}^{i'f'}(\Delta\omega)=\langle i|\vec{r}|f\rangle\langle i'|\vec{r}|f'\rangle\left(1+\frac{\Delta\omega}{\omega_0}\right)^4\exp\left(-\frac{\hbar\Delta\omega}{k_BT}\right) \quad (2)$$

is the intensity of the transition $i\rightarrow f$ including the trivial asymmetry. Within our Green's-function approach the radiator is considered as a quasiparticle. All interactions between the radiator and the plasma environment are contained in the self-energy Σ and the vertex term Γ^v, which corresponds to the well-known upper-lower interference term.

The self-energy can be written as the sum of ionic and electronic contributions

$$\Sigma_{ii}(\Delta\omega,\beta)=\Sigma_{ii}^{\text{ion}}(\beta)+\Sigma_{ii}^{\text{el}}(\Delta\omega,\beta),$$
$$\Sigma_{ii'}(\beta)=\Sigma_{ii'}^{\text{ion}}(\beta)+\Sigma_{ii'}^{\text{el}}, \quad i\neq i'. \quad (3)$$

Thereby, the self-energy caused by the interaction between the radiator and the plasma ions depends only on the normalized microfield strength β. The electronic contributions, however, are frequency dependent. Therefore, they depend on both the detuning $\Delta\omega$ and the shift of the energy levels due to the ionic microfield. Since the main contributions to widths and shifts arise from the upper level of the radiating transition, only the frequency dependence for that level has been taken into account. The same is true for the vertex contribution Γ^v.

In order to determine the electronic contributions to the self-energy, a quantum-mechanical many-particle theory has been applied [14,15], which leads to

$$\Sigma(E_n^0+\Delta\omega)$$
$$=-\frac{2}{e^2}\sum_\alpha\int\frac{d\vec{q}}{(2\pi)^3}\int\frac{d\vec{p}}{(2\pi)^3}V^2(q)f_e(E_p)\times\frac{|M_{n\alpha}(\vec{q})|^2}{E_\alpha(\beta)-E_n^0-\Delta\omega+E_{\vec{p}-\vec{q}}-E_p}\,\frac{1}{1+iA(n,\alpha,\vec{p},\vec{q})}, \quad (4)$$

with

$$A(n,\alpha,\vec{p},\vec{q})=\frac{1}{e}\sum_{\alpha''}\int\frac{d\vec{q}''}{(2\pi)^3}\times\frac{M_{n\alpha''}^{(0)}(-\vec{q}'')M_{\alpha''\alpha}^{(0)}(\vec{q}''-\vec{q})}{M_{n\alpha}^{(0)}(-\vec{q})}\,\frac{V(q'')V(\vec{q}''-\vec{q})}{V(q)}\times\frac{1}{E_n+E_p-E_{\vec{p}-\vec{q}''}-E_{\alpha''}}. \quad (5)$$

Via partial summation of the three-particle T matrix for the perturber-radiator-interaction strong collisions between the radiator and a perturbing electron also have been included in a systematic manner. The term A, which leads to corrections of the Born approximation result due to strong collisions, has been given in detail in [14,15].

Taking into account the ionic contributions to the self-energy, besides the well-known linear Stark effect, the quadrupole interaction between the radiator and inhomogeneities of the ionic microfield also has been considered. Within parabolic states for the resulting ion quadrupole shift one finds

$$\Sigma_{ii'}^{q}(\beta)=\begin{cases}\frac{\pi}{3}a_0^2e^2n_e(n^i)^2\sqrt{n_1^i(n^i-n_1^i)(n_2^i+1)(n^i-n_2^i-1)}B_\rho(\beta), & n_1^i=n_1^{i'}-1,\quad n_2^i=n_2^{i'}+1\\ \frac{\pi}{3}a_0^2e^2n_e(n^i)^2[(n^i)^2-1-6(n_1^i-n_2^i)^2]B_\rho(\beta), & i=i'\\ \frac{\pi}{3}a_0^2e^2n_e(n^i)^2\sqrt{(n_1^i+1)(n^i-n_1^i-1)n_2^i(n^i-n_2^i)}B_\rho(\beta), & n_1^i=n_1^{i'}+1,\quad n_2^i=n_2^{i'}-1.\end{cases} \quad (6)$$

The function $B_\rho(\beta)$ has been given by Halenka [9]. It is a generalization of the Chandrasekhar–von Neumann function $B(\beta)$ [22] introduced by Demura and Sholin [23] into line broadening theory. It is different because it takes into account the screening of the ionic microfield by the plasma electrons as well as ion pair correlations.

Further, the quadratic Stark effect has been included approximately using the well-known formula [24]

$$\Sigma_{ii}^{k}(\beta)=-\frac{1}{16}(n^i)^4[17(n^i)^2-3(n_1^i-n_2^i)^2-9(m^i)^2+19]\beta^2E_0^2. \quad (7)$$

Accounting for ion dynamics by applying the model microfield method, the line profile is described by the time development operator (see [17])

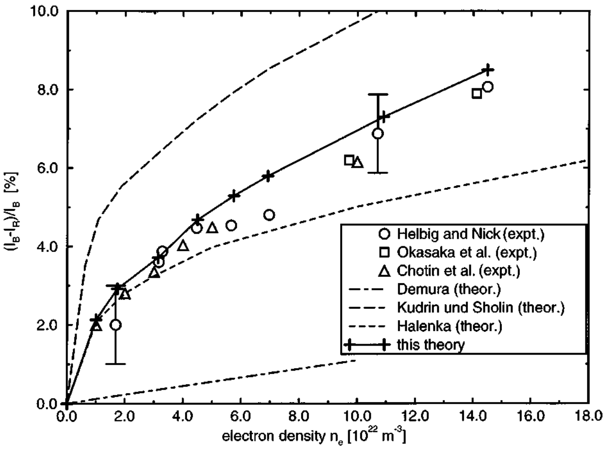

FIG. 1. Asymmetry parameter of the hydrogen H_β line. The experimental data refer to [27,35,36]. The theoretical data have been taken from [28,29,9].

$$\langle U(\Delta\omega)\rangle_{\mathrm{KP}}=\langle U(\Delta\omega|\vec{E})\rangle_s+\langle\Omega(E)U(\Delta\omega|\vec{E})\rangle_s \times[\langle\Omega(E)\rangle_s-\langle\Omega^2(E)U(\Delta\omega|\vec{E})\rangle_s]^{-1} \times\langle\Omega(E)U(\Delta\omega|\vec{E})\rangle_s \tag{8}$$

if, as usual, a ''kangaroo process'' is chosen to describe the stochastic variation of the ionic microfield strength. The average has to be carried out with the ionic microfield distribution function as given by Hooper [19], i.e.,

$$\langle\,\rangle_s=\int d\vec{E}W_\rho(E)\cdots. \tag{9}$$

The time development operator for a constant ionic microfield as given in [17] has to be modified, however, in order to evaluate shifted and asymmetric line profiles

$$U(\Delta\omega|\vec{E})=\left[\Delta\omega-\frac{\vec{P}\vec{k}}{M}-\frac{k^2}{2M}-\mathrm{Re}\{\Sigma(\Delta\omega,E)\}+i\Omega(E) +i\mathrm{Im}\{\Sigma(\Delta\omega,E)\}+i\Gamma^v\right]^{-1}. \tag{10}$$

$\Omega(E)$ is the jumping frequency, which is determined by the field autocorrelation function [25]. The self-energy Σ has been given above.

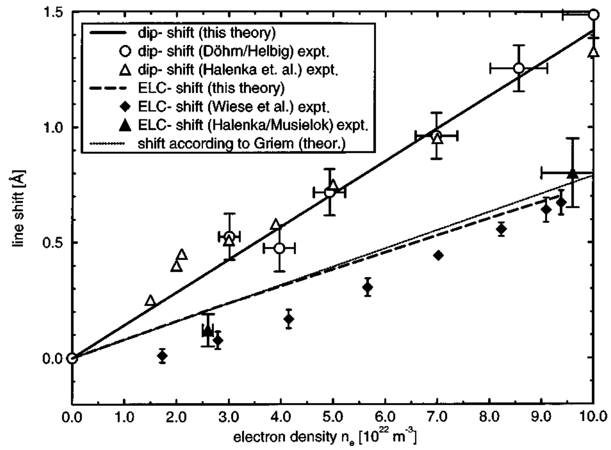

FIG. 2. Shift of the hydrogen H_β line according to different definitions. The dip shifts have been measured by Döhrn [31] and Halenka *et al.* [37]. The ELC shifts stem from [26,38]. For the theoretical values of Griem, see Ref. [5].

III. RESULTS

Within the theory developed in Sec. II, shifted and asymmetric profiles of the first Balmer lines (H_α, H_β, and H_γ) have been calculated. From these profiles, it is possible to evaluate the asymmetry parameter of the H_β line

$$A=\frac{I^{\mathrm{blue}}-I^{\mathrm{red}}}{I^{\mathrm{blue}}} \tag{11}$$

(where I^{red} and I^{blue} are the peak intensities of the line) as well as the line shift.

In order to determine the shifts of spectral lines from experimental profiles, various definitions have been applied, among them the maximum shift (for lines with a central Stark component) and the dip shift (for lines without a central component), respectively. Wiese introduced the shift of the estimated line center (ELC) [26]. Further, sometimes the center-of-mass shift

$$\Delta=\int_{-\Delta s}^{\Delta s}P(\Delta\lambda)d(\Delta\lambda) \tag{12}$$

is applied. Due to the asymmetry of the spectral lines, the resulting shifts depend strongly on the applied shift definition. Therefore, for comparison with experimental results we use the same shift definitions as the experimentalists have done.

TABLE I. Shifts of the H_α line for different experimental conditions and shift definitions.

Shift	n_e (10^{16} cm^{-3})	T (K)	$\Delta\lambda_{\mathrm{theor}}$ (Å)	$\Delta\lambda_{\mathrm{expt}}$ (Å)	Reference
Maximum	9	12600	0.44	0.41 ± 0.06	[30]
	10	12 000	0.48	0.43	[31]
	61	16 500	3.30	1.80 ± 0.2	[32]
	100	62 700	5.35	5.33 ± 0.3	[33]
Half maximum	8.8	13 000	0.38	0.38 ± 0.4	[34]
ELC	9	12 600	0.41	0.47 ± 0.08	[30]
	9.21	13 000	0.42	0.52	[26]

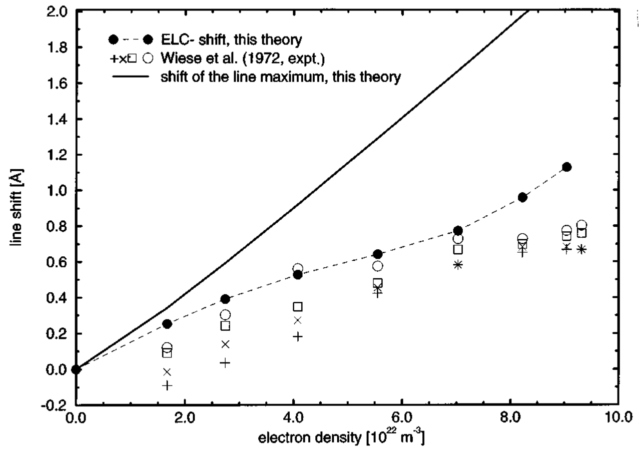

FIG. 3. ELC and maximum shifts of the hydrogen H_γ line. The experimental ELC shifts are from Ref. [26].

In Fig. 1, the theoretical asymmetry parameters A of the H_β line are compared to experimental and former theoretical results. Of course, there are many experimental data that could be used for comparison. For clarity, however, only a few results are included in Fig. 1. The concrete evaluations have been carried out for exactly the same plasma conditions as those in the experiment of Helbig and Nick [27]. It can be stated that the agreement between the theoretical and the corresponding experimental results is excellent. Former theoretical results by Kudrin and Sholin [28] and Demura *et al.* [29], however, strongly differ from any experimental results. For lower electron densities the theoretical results given by Halenka [9] also agree very well with the experimental data.

Considering Eqs. (1)–(7), it becomes obvious that several effects lead to an asymmetry of the resulting spectral line: (i) the trivial asymmetry [see Eq. (2)], (ii) the ion quadrupole effect [see Eq. (6)], (iii) the different electronic shifts of the various Stark components, (iv) the quadratic Stark effect [see Eq. (7)], (v) the frequency dependence of the electronic width and shift (see [20]), and (vi) the fine structure splitting. The fine structure splitting is not relevant for the plasma parameters considered and therefore has not been accounted for. The influence of effects (i)–(v) on the asymmetry parameter of the H_β line has been investigated in detail for an electron density of 9.9×10^{16} cm^{-3} and a temperature of 12 000 K. Taking into account each time only one of the effects (i)–(v), one finds for the asymmetry parameter the values (i) 0.47%, (ii) 2.50%, (iii) 0.98%, (iv) 3.81%, and (v) -0.18%. The asymmetry parameter determined from a shifted and asymmetric theoretical line profile has been found to be 7.07%. The inclusion of ion dynamics diminishes the asymmetry parameter to 6.81%. The sum of the several contributions (i)–(v) to the asymmetry parameter gives 7.59%. Obviously, one has to calculate shifted and asymmetric line profiles including all the effects (i)–(v) in order to reach an agreement with experimental results.

Considering the shift of the H_β line in Fig. 2, our calculations yield clearly distinct results for different shift definitions. For the dip shift one finds from experimental as well as theoretical results a linear dependence on the electron density. Since the dip shift, in principle, is given by the sum of the electronic shift contributions (proportional to n_e) and the ion quadrupole shift (proportional to n_i) of the two inner Stark components, a linear behavior of the shift results. For the ELC shift, however, the different shifts of the outer Stark components become important. They cause a nonlinear behavior with respect to the electron density.

Whereas the theoretical dip shift agrees excellently with corresponding experimental results, the theoretical ELC shifts are larger than the experimental ones for lower electron densities. As it has to be expected, the theory gives no ELC shift for vanishing electron density. Assuming, however, a nearly linear behavior of the ELC shift for low densities, from experimental values a negative shift for $n_e\rightarrow0$ results.

The shift given by Griem [10,5] agrees very well with our theoretical ELC shift. However, Griem did not calculate a shift from a complete shifted and asymmetric profile. He obtained his values by a superposition of the electronic contributions to the shift and the shift caused by the ionic microfield at a quarter of the maximum intensity. This purely theoretical shift definition considers the line asymmetry and appears to be a good approximation for the ELC shift.

Due to the central component, the H_α line is much less asymmetric than the H_β line. Therefore, the influence of the various shift definitions is less important. In Table I we compare our theoretical shifts with various experimental results. The agreement with the experimental shifts of the line center is excellent, whereas the ELC shift appears to be somewhat to small.

The ELC and the maximum shift of the H_γ line are given in Fig. 3. The theoretical ELC shift agrees very well with the measurement [26]. Unfortunately, there are no experimental data for the maximum shift up to now.

Since the motion of the plasma ions is relevant only in the line center, it does have a small influence on the ELC shift and the asymmetry parameter defined in Eq. (11). Only the dip and the maximum shift are slightly sensitive to ion dynamic effects. The dip shift of the H_β line, e.g., becomes somewhat larger (+4%) if ion dynamics are included. Thus the influence of ion dynamics on the shift and asymmetry parameters seems an almost immeasureable effect. This is not necessarily true for the Lyman lines which are influenced much more by the motion of the plasma ions.

IV. CONCLUSION

Asymmetric and shifted line profiles for the first three Balmer lines of hydrogen have been calculated including ion dynamics. Besides the electronic shift, the ion quadrupole shift as well as the quadratic Stark effect have been accounted for. The frequency-dependent electronic widths and shifts have been calculated using a Green's-function technique. Strong collision contributions have been included via partial summation of the corresponding perturbation series.

For comparison with experimental results, the asymmetry parameter and the line shift have been determined from theoretical profiles according to the same definitions as has been done in the corresponding experiments. For the shifts of all lines investigated, good agreement between experimental and theoretical data has been achieved. The agreement is even excellent for the H_β asymmetry. The theory sucessfully reproduces the difference between the ELC and the dip shift.

ACKNOWLEDGMENTS

This work has been supported by the Deutsche Forschungsgemeinschaft (Contract No. Ro 905/8-1). The authors gratefully acknowledge a grant by the GermanAcademic Exchange Service (DAAD). In addition, they wish to thank the National Institute of Standards and Technology, Gaithersburg and the University of Maryland for the kind hospitality.

[1] R. Stamm and E. Smith, Phys. Rev. A **30**, 450 (1984).
[2] R. Stamm, B. Talin, E. Pollock, and C. Iglesias, Phys. Rev. A **34**, 4144 (1986).
[3] V. Cardenoso and M. Gigosos, Phys. Rev. A **39**, 5258 (1989).
[4] J. Seidel, Phys. Rev. Lett. **57**, 2154 (1986).
[5] H. Griem, Phys. Rev. A **38**, 2943 (1988).
[6] H. Griem, *Spectral Line Broadening in Plasmas* (Academic, New York, 1974).
[7] K. Unnikrishnan and J. Callaway, Phys. Rev. A **43**, 3619 (1991).
[8] K. Unnikrishnan and J. Callaway, Phys. Rev. A **44**, 3001 (1991).
[9] J. Halenka, Z. Phys. D **16**, 1 (1990).
[10] H. Griem, Phys. Rev. A **28**, 1596 (1983).
[11] G. Röpke, T. Seifert, and K. Kilimann, Ann. Phys. (Leipzig) **38**, 381 (1981).
[12] L. Hitzschke and G. Röpke, Phys. Rev. A **37**, 4991 (1988).
[13] S. Günter, L. Hitzschke, and G. Röpke, Phys. Rev. A **44**, 6834 (1991).
[14] S. Günter, Phys. Rev. E **48**, 500 (1993).
[15] A. Könies and S. Günter, Phys. Rev. E **52**, 6658 (1995).
[16] A. Brissaud, C. Goldbach, L. Leorat, and A. Mazure, J. Phys. B **9**, 1147 (1976).
[17] J. Seidel, Z. Naturforsch. Teil A **32**, 1195 (1977).
[18] J. Seidel, Z. Naturforsch. Teil A **35**, 679 (1980).
[19] C. Hooper, Phys. Rev. **165**, 215 (1968).
[20] S. Günter and A. Könies, J. Quant. Spectrosc. Radiat. Transfer **52**, 819 (1994).
[21] A. Könies and S. Günter, J. Quant. Spectrosc. Radiat. Transfer **52**, 825 (1994).
[22] S. Chandrasekhar and J. von Neumann, Astrophys. J. **97**, 1 (1943).
[23] A. Demura and G. Sholin, J. Quant. Spectrosc. Radiat. Transfer **15**, 881 (1975).
[24] L. Landau and E. Lifshitz, *Lehrbuch der theoretischen Physik. Band 3* (Akademie-Verlag, Berlin, 1986).
[25] A. Brissaud, C. Goldbach, L. Leorat, A. Mazure, and G. Nollez, J. Phys. B **9**, 1129 (1976).
[26] W. Wiese, D. Kelleher, and D. Paquette, Phys. Rev. A **6**, 1132 (1972).
[27] V. Helbig and K. Nick, J. Phys. B **14**, 3573 (1981).
[28] L. Kudrin and G. Sholin, Dokl. Akad. Nauk SSSR **147**, 342 (1963) [Sov. Phys. Dokl. **7**, 1015 (1963)].
[29] A. Demura, V. Pleschakov, and G. Sholin (unpublished).
[30] J. Halenka, in *Proceedings of the XVIIth International Conference on the Physics of Ionized Gases*, edited by J. S. Bakos and Z. Sörlei (Budapest, 1985), pp. 993–995.
[31] A. Döhrn, Ph.D. thesis, Universität Kiel, 1995 (unpublished).
[32] Y. Vitel, J. Phys. B **20**, 2327 (1987).
[33] S. Böddeker *et al.*, Phys. Rev. E **47**, 2785 (1993).
[34] D. Kelleher, N. Konjevic, and W. Wiese, Phys. Rev. A **20**, 1195 (1979).
[35] R. Okasaka, M. Nagashima, and K. Fukuda, J. Phys. Soc. Jpn. **42**, 1339 (1977).
[36] J. Chotin, J. Lemaire, J. Marque, and F. Rostas, J. Phys. B **11**, 371 (1978).
[37] J. Halenka, B. Vujičić, and S. Durić, J. Quant. Spectrosc. Radiat. Transfer **42**, 571 (1989).
[38] J. Halenka and J. Musielok, J. Quant. Spectrosc. Radiat. Transfer **36**, 233 (1986).