J. Phys. Chem. A **2008,** *112,* 3816−3822

Resonant Vibrational Excitation and De-Excitation of $N_2(v)$ by Low-Energy Electrons

G. B. Poparić,*,† M. Ristić,‡ and D. S. Belić†

Faculty of Physics, University of Belgrade, Studentski trg 12, P.O. Box 368, 11000 Belgrade, Serbia, and
Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12, P.O. Box 137,
11000 Belgrade, Serbia

Received: November 7, 2007; In Final Form: February 5, 2008

We have calculated cross sections and rate coefficients for low-energy electron impact excitation of the nitrogen molecule from vibrationally excited levels $N_2(v)$ 1−8. Calculations are performed in the $^2\Pi_g$ shape resonance energy region, from 0 to 5 eV. The cross sections are determined by using our recent integral cross section measurements of the ground level vibrational excitation and the most recent cross sections for elastic electron scattering, applying the principle of detailed balance. The rate coefficient calculations are performed for the Maxwellian electron energy distribution. By using extended Monte Carlo simulations, the electron energy distribution functions (EEDF) and the rate coefficients are also determined for the nonequilibrium conditions, in the presence of the homogeneous external electric field for the typical, moderate values of the electric field over gas number density ratios, E/N.

1. Introduction

Nitrogen molecules play an important role as the most abundant in the Earths atmosphere. Electron−nitrogen molecule collision processes are important in upper atmosphere,[1] but also in any plasma and discharge technology, in plasma etching industry, diffuse discharge switches, ionized gases in flames, chemical detectors and in laser devices.[2−4] For modeling all of these phenomena, one needs to know the cross sections and rate coefficients for the various involved processes. At the low electron energies vibrational excitation is dominant in electron energy transfer and it is necessary to have accurate absolute differential cross sections, both for elastic scattering and for vibrational excitation and de-excitation as a function of energy[5] as well as their angular distributions.

Vibrational excitation of the nitrogen molecule by electron impact, via the $^2\Pi_g$ resonance, was the first experimental evidence of resonant electron−molecule scattering.[6,7]The unusual behavior of the excitation cross sections, in particular the shifts and widths of the quasi-vibrational resonant structures as a function of excitation channel, was described by the boomerang model, Herzenberg[8] and Birtwistle and Herzenberg.[9] Excitation from the ground level, $v = 0$ of N_2 has been experimentally studied by Ehrhardt and Willmann,[10] Boness and Schulz,[11] Wong and Dube,[12] Jung et al.[13] and more recently by Allan,[14] Brunger et al.,[15] Brennan et al.,[16] and Vićić et al.[17,18] It has also become a touchstone for the theories of resonant coupling of the electronic and vibrational motion and it remains of current interest, as is shown by numerous studies, Schneider et al.,[19] Dube and Herzenberg,[20] Cederbaum and Domcke,[21] Berman et al.,[22] Domcke et al.,[23] Nestman and Peyerimhoff,[24] and Huo et al.[25] The field has been recently reviewed by Brunger and Buckman.[26] On the basis of this review, Brunger et al.[27] constructed a set of recommended integral cross sections for the 0 → 1, 0 → 2 and 0 → 3 vibrational excitation processes in N_2.

Due to the experimental difficulties, angular distributions of electron−molecule collision processes usually are incomplete, i.e., are measured for a limited angular range. Only recently absolute differential elastic and vibrational excitation cross sections have been measured for N_2 in the scattering angle starting between 0° and 20° and extending to 180°. These measurements of Allan[28] have been performed by use of the “magnetic angle changer” (MAC) technique. They confirmed d-partial wave character of the $^2\Pi_g$ resonance, by observing angular distribution in a whole range from 0° to 180° degrees for the first time. We have used the results of Allan[28] to renormalize our differential cross sections measurements[17] of N_2 and to obtain corresponding integral cross sections, Ristić et al.[29]

Integral cross sections (ICS) for vibrational excitation and de-excitation processes for 3, 2, 1 → 0 transitions have been calculated by the “boomerang model” with exchange for the resonant electron-molecule scattering by Dube and Herzenberg.[18] Integral excitation and de-excitation cross sections from $v = 1$, 2, 3, ..., 8 have also been calculated by using the principle of detailed balance by Mihajlov et al.[30] and by Campbell et al.[5] They used these ICS to calculate corresponding rate coefficients and electron energy transfer rates for vibrational excitation of N_2, as a function of electron temperature.

The aim of this paper is to complete a new set of accurate integral cross sections data and to obtain partial and total rate coefficients for vibrational excitation of $N_2(v)$ below and in the $^2\Pi_g$ resonance region. Our high-resolution vibrational excitation relative cross section measurements for the first 10 vibrational levels are renormalized and by using the principle of detailed balance, excitation and de-excitation cross sections are calculated for $N_2(v)$. Obtained ICSs are used as the starting data set for modeling electron transport processes in nitrogen. The rate coefficients for the Maxwellian electron energy distribution function are determined. By using extended Monte Carlo simulations, the electron energy distribution functions (EEDF) and the rate coefficients are determined for the nonequilibrium conditions, in a presence of the homogeneous external electric

---

* Corresponding author. E-mail address: Goran_Poparic@ff.bg.ac.yu.
† Faculty of Physics.
‡ Faculty of Physical Chemistry.

10.1021/jp710667n CCC: $40.75

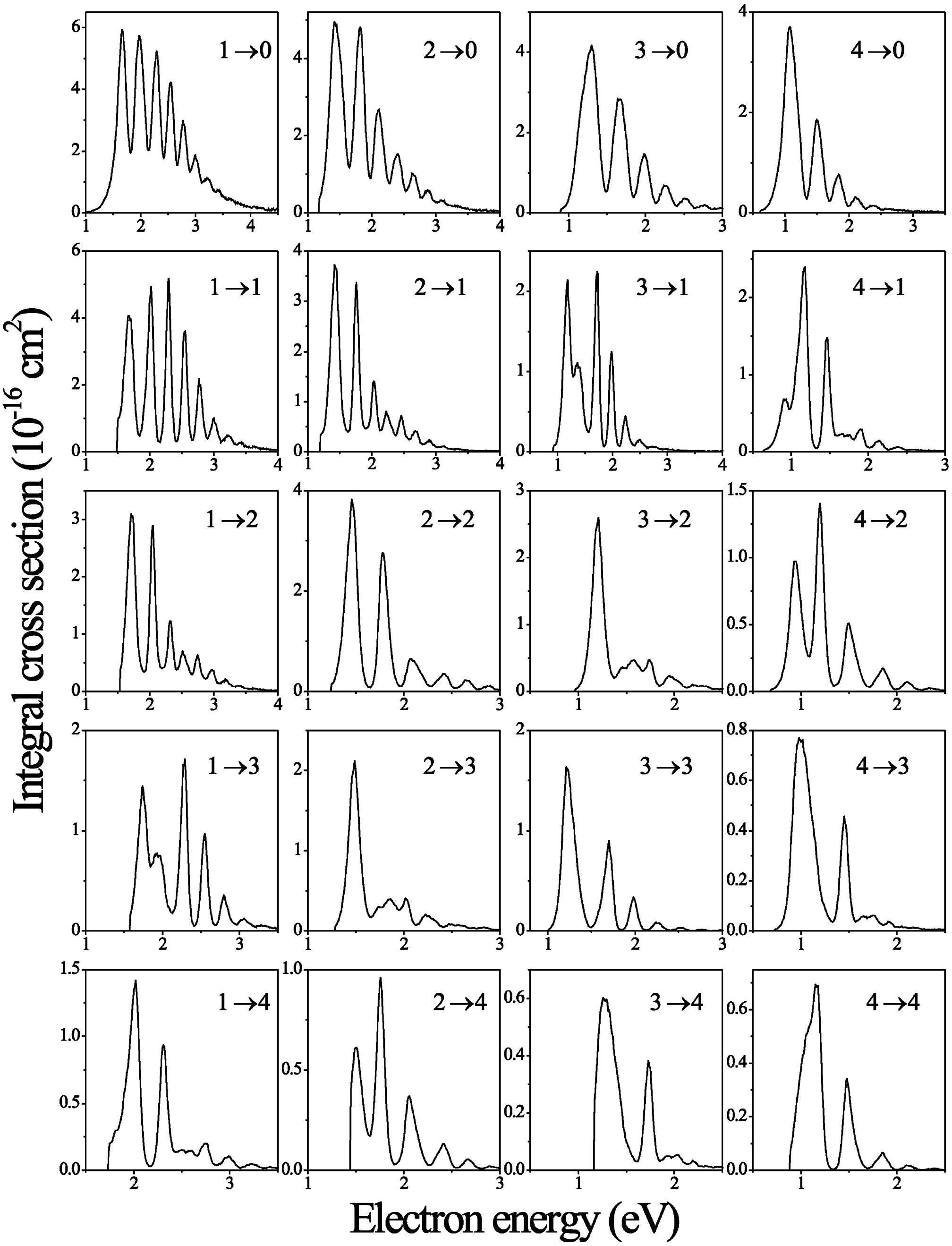

Figure 1. Integral cross sections for vibrational excitation and de-excitation of $N_2(v)$ for v, $k \leq 4$.

field for the typical, moderate values of the electric field over gas number density ratios, E/N, ranging from 1 to 220 Td.

2. Vibrational Excitation Cross Sections of $N_2(v)$

In our previous publications the low-energy electron impact vibrational excitation cross sections of N_2 are reported.[17,29] The measurements are performed by use of the crossed-beams double trochoidal electron spectrometer; see Vićić et al.[18] and Poparić et al.[31,32] We have focused our attention to measure the excitation functions from $v = 0$ of N_2 ground state to the first 10 vibrationally excited states ($v = 1-10$) via the $^2\Pi_g$ resonance, with the high-energy resolution.

To normalize our results, we have used absolute cross section value of 4.64×10^{16} cm^2 at 1.988 eV in the $v = 1$ excitation channel, obtained by the most recent measurements of Allan.[28] Our result for $v = 1$ excitation channel is normalized, and other results are scaled relative to the $v = 1$ by using the number of counts for each particular vibrational channel under the same experimental conditions. The results for vibrational excitation of the first ten levels are published by Ristić et al.[29]

Corresponding ICSs for excitation from vibrationally excited levels $N_2(v)$ and for de-excitation processes to lower vibrational levels can be obtained from the measured data set by using the principle of detailed balance (Fowler 1936;[33] Mihajlov et al. 1999;[30] Campbell et al. 2004[5]). For this purpose we have used our ICSs[29] for vibrational excitation from the ground level and the elastic cross sections of Allan.[28]

The cross section for electron impact transitions from the initial level v to the final level k is given by[30]

$$\sigma_{vk}(\epsilon) = \frac{(\epsilon + \epsilon_v)}{\epsilon}\,\frac{\sigma_{0v}(\epsilon + \epsilon_v)\,\sigma_{0k}(\epsilon + \epsilon_v)}{\sigma_{00}(\epsilon + \epsilon_v)} \qquad (1)$$

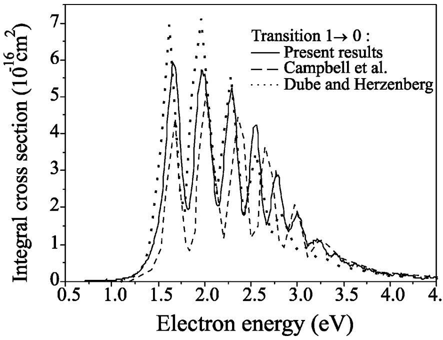

Figure 2. Integral cross sections for $v = 1 \rightarrow 0$ transition. Solid line shows present results, dashed lines are from Campbell et al.[5] and the dotted line is from Dube and Herzenberg.[20]

Here, σ_{00} is the resonant part of the ground level elastic cross section, σ_{0v} and σ_{0k} are the inelastic cross sections for vibrational excitation of the levels v and k from the ground state and ϵ and ϵ_v are the electron energy and the energy of the initial level v, respectively.

We have determined ICSs for inelastic, elastic and superelastic transitions between all levels with $v, k \leq 8$. Representative results are shown in Figure 1. The ICSs for transitions between lower levels, v and $k \leq 4$, are selected because they have larger cross sections and have dominant rate coefficient values. For each cross section corresponding transition $v \rightarrow k$ is indicated in the figure. With $v = k$ elastic processes are indicated, with $v < k$ inelastic and with $v > k$ superelastic processes are shown. It can be noted that the vertical scale is not the same for all transitions and that the cross sections decrease rapidly with increasing v or k, or both of them.

Obtained ICSs are compared to the results of Dube and Herzenberg,[20] Mihajlov et al.[30] and Campbell et al.[5] for a selected transitions. In Figure 2, the comparison is made for $1 \rightarrow 0$ transition and the agreement is satisfactory. ICSs of Campbell et al.[5] and Dube and Herzenberg[20] for this superelastic transition agree with the present results within 15%. In general, the agreement is relatively good for the transitions between low vibrational levels and is not so good for higher levels. In some cases the difference amounts up to an order of magnitude. It obviously depends on the set of cross sections for the ground level excitation as well as on the elastic cross sections used to generate all other transitions.

In performing the cross sections and the rate coefficients calculations, important role have the threshold energies for corresponding transitions. Great care has been dedicated to this issue. The thresholds are determined as a difference between the incident level energy and the beginning of the resonance. The last one is determined accurately from our experimental results for ground level excitation functions, Vićić et al.,[17] for all vibrational levels. Determined threshold energies are listed in Table 1. For each transition between initial level v and final level k the threshold energy is indicated in the table. The results for the elastic and inelastic transitions are compared with the data given by Mihajlov et al.,[30] which are cited in parentheses.

3. Results and Discussion

The rate coefficients for the vibrational excitation and de-excitation of $N_2(v)$ are determined by using our set of integral cross sections introduced in section 2. Calculations are performed for both Maxwellian and nonequilibrium electron energy distribution functions (EEDF). For the Maxwellian EEDF, rate coefficients are determined for a number of mean electron energy values in the range from 0 to 5 eV, which is of interest for atmospheric modeling studies. Vibrational rate coefficients in the nonequilibrium case, in a presence of homogeneous external electric field, for typical values of fields strength and gas number density ratios, are determined by using the extended Monte Carlo simulation technique, developed in our laboratory.

TABLE 1: Threshold Energies for Vibrational Transitions (Values in Parentheses from Mihajlov et al.[30])

v	$k = 0$	$k = 1$	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$	$k = 7$	$k = 8$
0	1.75 (1.8)	1.77 (1.80)	1.82 (1.80)	1.86 (1.91)	2.02 (2.08)	2.08 (2.10)	2.27 (2.30)	2.47 (2.40)	2.56 (2.59)
1	1.46	1.48 (1.51)	1.53 (1.51)	1.57 (1.62)	1.73 (1.79)	1.79 (1.81)	1.98 (2.01)	2.18 (2.11)	2.27 (2.30)
2	1.18	1.20	1.25 (1.21)	1.29 (1.32)	1.45 (1.49)	1.51 (1.51)	1.70 (1.71)	1.90 (1.81)	1.99 (2.00)
3	0.89	0.91	0.96	1.00 (1.03)	1.16 (1.20)	1.22 (1.22)	1.41 (1.42)	1.61 (1.52)	1.70 (1.71)
4	0.62	0.64	0.69	0.73	0.89 (0.91)	0.95 (0.93)	1.14 (1.13)	1.34 (1.23)	1.43 (1.42)
5	0.34	0.36	0.41	0.45	0.61	0.67 (0.63)	0.86 (0.83)	1.06 (0.93)	1.15 (1.13)
6	0.07	0.09	0.14	0.18	0.34	0.40	0.59 (0.54)	0.79 (0.64)	0.88 (0.84)
7					0.07	0.13	0.32	0.52 (0.34)	0.61 (0.53)
8							0.06	0.26	0.35 (0.24)

3.1. Maxwellian EEDF Rate Coefficients. The rate coefficient for vibrational excitation is given by

$$K(\bar{E}_{\mathrm{el}}) = \sqrt{2/m_{\mathrm{e}}} \int_{\epsilon_{\mathrm{thres}}}^{+\infty} \sigma_v(\epsilon) \sqrt{(\epsilon)}\, f_{\mathrm{e}}(\bar{E}_{\mathrm{el}},\epsilon)\, \mathrm{d}\epsilon \qquad (2)$$

where $\bar{E}_{\mathrm{el}}$ is the mean electron energy, $\sigma_v(\epsilon)$ is the vibrational excitation cross section and $f_{\mathrm{e}}(\bar{E}_{\mathrm{el}},\epsilon)$ is the normalized electron energy distribution function:[34,35]

$$\int_0^{+\infty} f_{\mathrm{e}}(\bar{E}_{\mathrm{el}},\epsilon)\, \mathrm{d}\epsilon = 1 \qquad (3)$$

For the equilibrium case, the electron energy distribution function is given by the Maxwellian equation:

$$f_{\mathrm{e}}(\bar{E}_{\mathrm{el}},\epsilon) = 2\pi^{-1/2}(3/2\bar{E}_{\mathrm{el}})^{+3/2}\sqrt{\epsilon}\, \exp(-3\epsilon/2\bar{E}_{\mathrm{el}}) \qquad (4)$$

For this case, the rate coefficients are determined by the direct numerical integration of the product of the integral cross sections and the Maxwellian electron energy distribution function. The rate coefficients are calculated for all vibrational transitions between vibrational levels $v > 0$; $v,k \leq 8$ including inelastic, elastic and superelastic processes. The results are shown in Figure 3 for the mean electron energies up to 5 eV.

The rate coefficients are arranged by the initial vibrational level. For each transition initial level v and final level k are indicated in the figure, $v - k$. The maxima of the rate coefficients range from 10^{-8} to 10^{-11} cm^3 s^{-1} and most of them are situated at the mean electron energies between 1 and 2 eV. To illustrate relative magnitudes of the coefficients, we have shown corresponding values near maxima for all transitions with $v, k \leq 8$ in a 3D plot in Figure 4. The rate coefficients for mean electron energy of 1.6 eV are plotted versus initial and final vibrational quantum numbers which define corresponding vibrational transitions. As it can be noted, the vertical axis is logarithmic and thus the rate coefficients decrease very rapidly with increasing vibrational quantum numbers.

We have compared our results for excitation rates with the data of Mihajlov et al.[30] for inelastic transitions from non-ground vibrational levels. Comparison is made in the energy range from 0.1 to 4 eV and for selected rates with high magnitude which

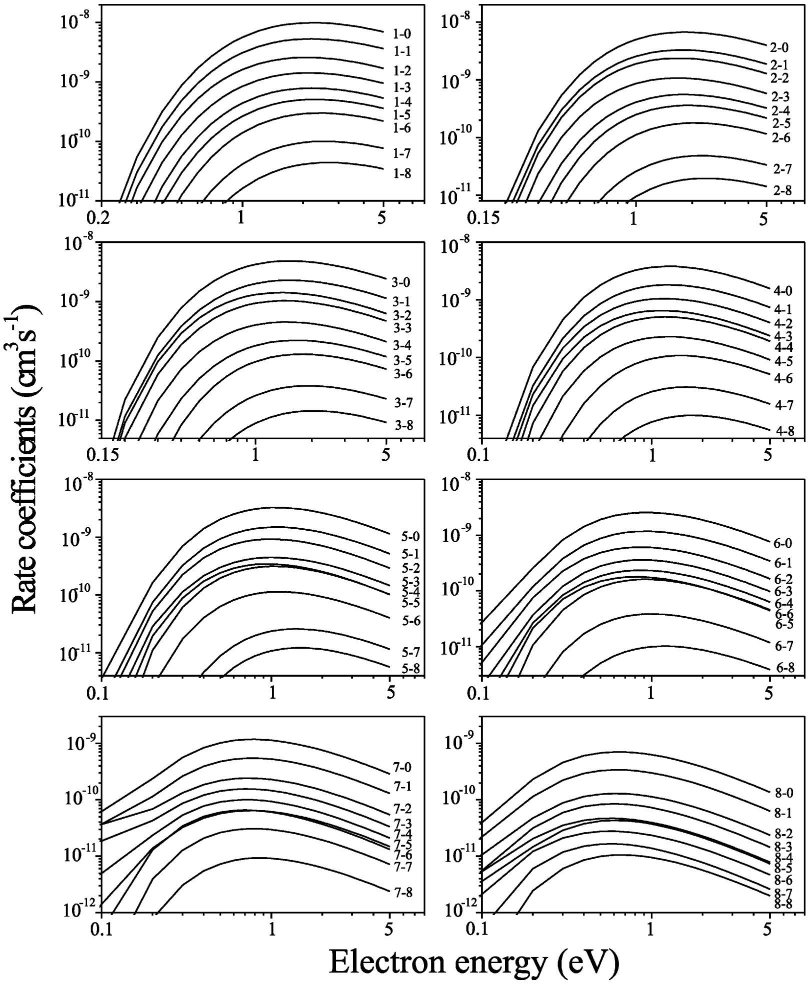

Figure 3. Vibrational excitation rate coefficients of $N_2(v)$ for Maxwellian EEDF. Initial and final states for each transition are indicated.

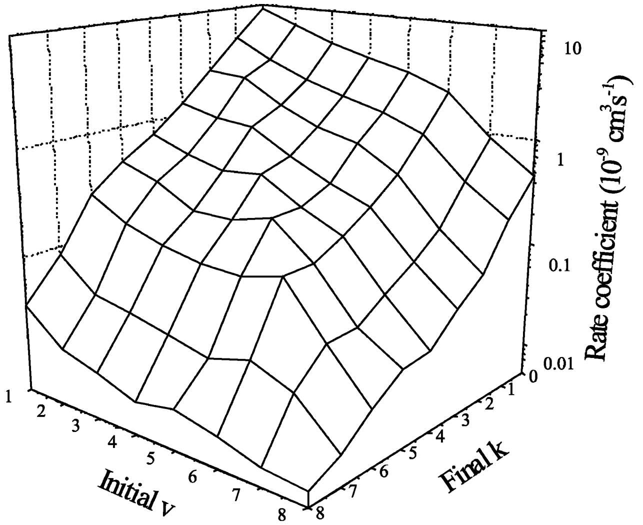

Figure 4. Vibrational excitation rate coefficients of $N_2(v)$ for Maxwellian EEDF at electron energy of 1.6 eV.

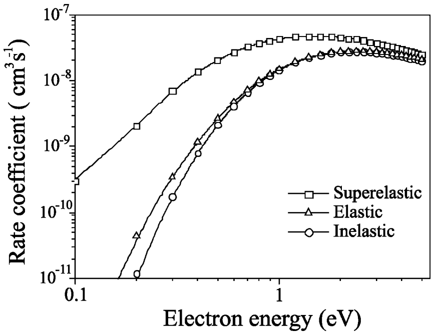

Figure 5. Comparison of total rate coefficients for superelastic (squares), elastic (triangles) and inelastic (circles) processes for equilibrium conditions.

is of interest for atmospheric modeling studies. Our results are somewhat higher in the whole energy region. The differences at the maximum are of the order of 15% . This is expected having in mind ICS values used to obtain these two sets of data; see section 2.

Valuable information can be drown by comparing the total rate coefficients for various processes regarding their classification from the point of view of transfer of energy between the electron and the target molecule in its excited states. In Figure 5, the total rate coefficients for superelastic, elastic and inelastic processes are shown. They represent the sum of rates for transitions in which electrons gain energy, do not exchange energy or transfer a part of their kinetic energy to the excitation of the molecule to higher vibrational level, respectively. The rate coefficients for superelastic transitions are significantly higher in the whole energy region and they extend to lower electron energies. This is an efficient mechanism of cooling molecules and increasing electron temperature of the discharge. The reason the total superelastic rate coefficients are higher from both elastic and inelastic processes can be explained by the results of Figure 1. Integral cross sections for superelastic excitation are in general higher than for inelastic excitation, and also are shifted toward lower electron energies where Max-

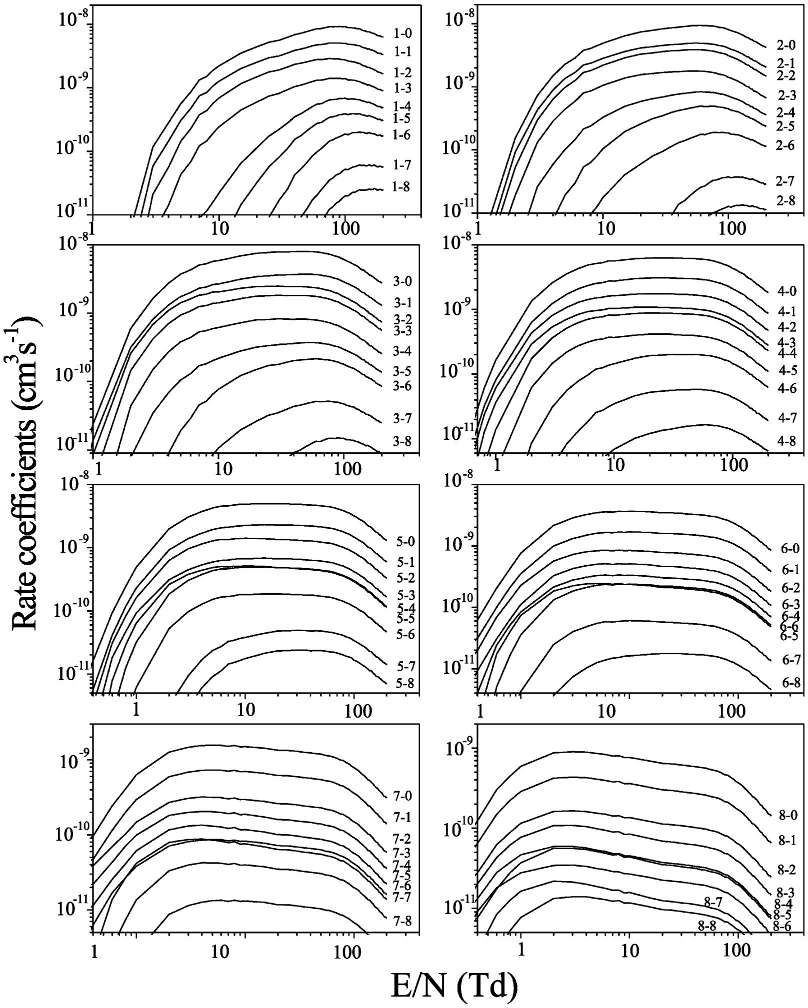

Figure 6. Nonequilibrium vibrational excitation rate coefficients for $N_2(v)$.

wellian EEDFs are narrower and thus higher. The cross sections for elastic collisions are in general higher than for others, for the same vibrational levels (initial or final one), but the number of other two processes is larger what results in the situation shown in Figure 5.

3.2. Nonequilibrium EEDF Rate Coefficients. To determine the rate coefficients in the case of nonequilibrium conditions, we have developed an extended Monte Carlo simulation technique.[29,36] We have simulated the movement of electrons through N_2 gas in the presence of the uniform external electric field. All relevant scattering processes, both elastic and inelastic are included in this modeling by using experimentally measured data of integral cross sections as a function of energy. The probability for possible elastic scattering or vibrational excitation, electronic excitation or ionization is proportional to the value of the corresponding integral cross sections. The decision of which possible processes will happen in each collision event is left to the pseudo-random generated numbers. The scattering angle of electrons after the collision is determined by using experimentally measured data of differential cross sections, i.e., corresponding angular distributions. In that way, the scattering angle is also determined by using pseudo-random numbers, but weighted by real differential cross sections. Because the sets of integral and differential cross sections are measured for the discrete values of energy, we have dynamically interpolated all cross section data for the actual values of electron energy during its motion. This type of simulation is similar to the simulations developed earlier by White et al.[37] and by Stojanović et al.,[38,39] To test our algorithm, we have used the Reid ramp model gas[40] simulation tests. We have obtained the same results (within statistical error bars) for the mean electron energy and for the diffusion coefficients as White et al.[37] in their benchmark simulations.

For modeling electron diffusion through the nitrogen gas, we have used the data for elastic scattering from several sources. In the energy range from 0 to 5.5 eV we have used the most recent data of Allan.[28] For higher electron energies, from 6 to 10 eV, we have used the data of Sun et al.[41] In the energy region from 10 to 70 eV we have used the data of Gote and Ehrhardt,[42] and in the high-energy region from 70 to 90 eV we used the data of Nickel et al.[43] Actually, only a small number of electrons reach energies higher than 20 eV in the case where the mean electron energy is in the range from 0 to 5 eV, as is in our case. In modeling inelastic electron collision processes we used our integral cross section data for vibrational excitation, given in section 2. All other excitation processes of the valence and Rydberg levels of the nitrogen molecule have significantly lower cross sections and lie above 6 eV. Their contribution to the electron scattering in the low-energy region is estimated to be less than 5% . However, these processes are also included in the modeling. For the integral cross sections for electron impact excitation of singlet electronic states of N_2 for $a'^1\Sigma_u^-$, $w^1\Delta_u$, $a''^1\Sigma_g^+$ and $a^1\Pi_g$ levels included are recommended values from Itikawa,[44] for $b^1\Pi_u$ from James et al.[45] and for $c'^4\Sigma_u^{1+}$ and b'^1 Σ_u^+ from Ajello et al.[46] For triplet electronic states we have

TABLE 2: Rate Coefficients Maxima for $v-k$ Transitions for Maxwellian (Upper) and Nonequilibrium (Lower Numbers) in 10^{-9}cm^3 s^{-1}

v	$k = 0$	$k = 1$	$k = 2$	$k = 3$	$k = 4$	$k = 5$	$k = 6$	$k = 7$	$k = 8$
0	19.14	8.25	4.40	2.48	1.43	0.94	0.56	0.18	0.08
	12.57	5.65	3.11	1.72	0.93	0.57	0.32	0.10	0.05
1	9.93	5.30	2.58	1.42	0.79	0.51	0.30	0.10	0.04
	9.18	5.07	2.89	1.41	0.69	0.39	0.20	0.06	0.03
2	6.69	3.28	2.36	1.07	0.56	0.36	0.18	0.05	0.02
	9.36	4.91	3.88	1.78	0.83	0.50	0.19	0.04	0.01
3	4.83	2.29	1.42	1.03	0.45	0.22	0.13	0.04	0.01
	7.98	3.70	2.49	1.83	0.83	0.37	0.22	0.05	0.02
4	3.81	1.82	1.06	0.65	0.51	0.23	0.11	0.03	0.01
	6.26	3.07	1.75	1.08	0.89	0.42	0.20	0.06	0.02
5	3.25	1.49	0.92	0.45	0.34	0.31	0.11	0.03	0.01
	5.01	2.31	1.41	0.68	0.51	0.50	0.18	0.05	0.02
6	2.55	1.17	0.61	0.36	0.23	0.18	0.16	0.04	0.01
	3.67	1.70	0.86	0.52	0.34	0.24	0.24	0.06	0.02
7	1.17	0.55	0.24	0.16	0.10	0.06	0.06	0.03	0.01
	1.56	0.73	0.32	0.20	0.14	0.09	0.09	0.04	0.01
8	0.70	0.34	0.13	0.08	0.05	0.04	0.03	0.02	0.01
	0.90	0.43	0.16	0.11	0.06	0.05	0.03	0.02	0.01

included $A^3\Sigma_u^+$, $B^3\Pi_g$, $W^3\Delta_u$, $B'^3\Sigma_u^-$, $C^3\Pi_u$ and $E^3\Sigma_g^+$ levels from Itikawa.[44] Also, the recommended values of the integral cross sections for electron impact ionization of N_2[44] are included in the modeling.

For the purpose of the nonequilibrium case calculations, by using Monte Carlo simulations for transport of electrons in the nitrogen gas, we have generated electron energy distribution functions for different values of E/N or different mean values of electron energy. They are in a very good agreement with the data obtained by numerically solving Boltzmann equation based on the two term Legendre expansion of the velocity distribution function (Bolsig v1.05[47,48]). These EEDFs are used together with the vibrational excitation cross sections to calculate corresponding rate coefficients. Obtained results for the partial vibrational excitation rate coefficients are shown in Figure 6.

The nonequilibrium rate coefficients also range from 10^{-8} to 10^{-11} cm^3 s^{-1}. They are arranged in the figure by the initial vibrational level. For each transition initial level v and final level k are indicated in the figure, $v - k$. Relative magnitudes of the nonequilibrium coefficients decrease rapidly with the vibrational quantum numbers, same as for Maxwellian case illustrated in Figure 4.

We have compared our results for excitation rates for the Maxwellian and for the nonequilibrium electron energy distributions, for inelastic transitions from non-ground vibrational levels, in Table 2. The results from the ground vibrational levels, by Ristić et al.,[29] are also included in the table. The comparison is made for the rate coefficients maxima, for E/N values in the nonequilibrium distribution which correspond to the same mean electron energy value in the Maxwellian distribution. The Maxwellian rates are presented with the top values and nonequilibrium with the bottom values. Maxwellian rates are higher for transitions from ground and from $v = 1$ vibrational level. For all other transitions from excited vibrational levels the nonequilibrium rates are significantly higher. This situation is expected having in mind different EEDFs used to obtain these two sets of data.

The total rate coefficients for various processes, regarding their classification from the point of view of the transfer of energy between the electron and the target molecule in its excited states, are compared also for nonequilibrium conditions. In Figure 7, the total rate coefficients for superelastic, elastic and inelastic processes are shown. The rate coefficients for the superelastic transitions are significantly higher in the whole energy region and they extend to lower electron energies. The reason why the total superelastic rate coefficients are higher from both elastic and inelastic rates can be explained by the results of Figure 1, same as in the case of the Maxwellian distribution. The integral cross sections for superelastic excitation are in general higher than for inelastic excitations and are shifted toward lower electron energies. Rate coefficients for the elastic collisions are in general higher than for the others, for the same vibrational levels (initial or final one), but the number of other two processes is larger.

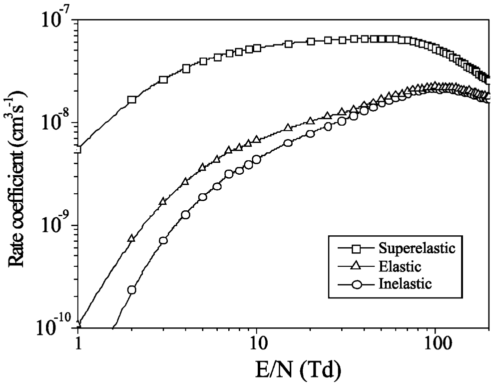

Figure 7. Comparison of total rate coefficients for superelastic (squares), elastic (triangles) and inelastic (circles) processes for nonequilibrium conditions.

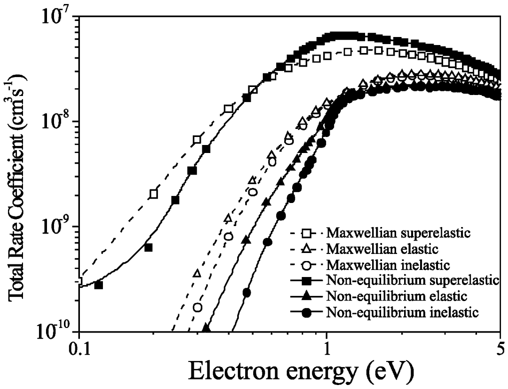

Figure 8. Total vibrational excitation rates for $N_2(v)$ for Maxwellian (dashed lines) and nonequilibrium (solid lines) EEDFs.

In Figure 8, we have compared the total rate coefficients for Maxwellian and nonequilibrium conditions. Compared are the total rates for superelastic, elastic and inelastic excitations, as presented in Figures 5 and 7. At the low electron energies the Maxwellian coefficients are significantly higher. However, above 0.5 eV the nonequilibrium rates for superelastic transitions are higher, and elastic and inelastic rates approach the Maxwellian. The explanation for such a behavior lies on one hand in the EEDF shape and on the other hand in the different energy locations of particular cross sections for corresponding vibrational transitions.

Obtained results and conclusions are in good general agreement with our previous calculations[29] and with the conclusions drown out by Mihajlov et al.[30] and by Campbell et al.[5]

4. Conclusions

Electron impact vibrational excitation of the N_2 molecule, in the low-energy region, via the $^2\Pi_g$ shape resonance, has been investigated. The cross sections for ground vibrational level excitation are renormalized and, by applying the principle of detailed balance, are used to obtain the integral cross sections for excitation from vibrationally excited levels $N_2(v)$, for elastic collisions and for de-excitation processes to lower vibrational levels. All the ICSs for inelastic, elastic and superelastic transitions between vibrational levels lower than 8 are determined. The rate coefficients for vibrational transitions are determined in equilibrium conditions with the Maxwellian electron energy distribution functions. The nonequilibrium electron energy distribution functions and rate coefficients are determined in the presence of homogeneous electric field for the moderate values of the field strength over gas number density ratios. The two sets of rate coefficients are compared with each other.

Acknowledgment. This work was supported in part by the Ministry of Science of the Republic of Serbia by the Project No. 141015.

References and Notes

(1) Dalgarno, A. *Can. J. Chem.* **1969**, *47*, 1723.
(2) Pearson, G. N.; Hall, D. R. *J. Phys. D: Appl. Phys.* **1989**, *22*, 1102.
(3) Adamovich, I. V.; Reich, J. W. *J. Phys. D: Appl. Phys.* **1997**, *30*, 1741.
(4) Markushev, D. D.; Jovanović-Kurepa, J.; Terzić, M. *Rev. Sci. Instrum.* **2003**, *74*, 303.
(5) Campbell, L.; Brunger, M. J.; Cartwright, D. C.; Teubner, P. J. O. *Planet. Space Sci.* **2004**, *52*, 815.
(6) Haas, R. *Z. Phys.* **1957**, *148*, 177.
(7) Schulz, G. J. *Phys. Rev.* **1964**, *135*, A988.
(8) Herzenberg, A. *J. Phys. B* **1968**, *1*, 548.
(9) Birtwistle, D. T.; Herzenberg, A. *J. Phys. B: At. Mol. Phys.* **1971**, *4*, 53.
(10) Ehrhardt, H.; Willmann, K. *Z. Phys.* **1967**, *204*, 462.
(11) Boness, M. J. W.; Schulz, G. J. *Phys. Rev. A* **1973**, *8*, 2883.
(12) Wong, S. F.; Dube, L. *Phys. Rev. A* **1978**, *17*, 570.
(13) Jung, K.; Antoni, T.; Muller, R.; Kochem, K.-H.; Ehrhardt, H. *J. Phys. B: At. Mol. Phys.* **1982**, *15*, 3535.
(14) Allan, M. J. *Electron Spectrosc.* **1989**, *48*, 219.
(15) Brunger, M. J.; Teubner, P. J. O.; WeigoldA. M.; Buckman, S. J. *J. Phys. B: At. Mol. Opt. Phys.* **1989**, *22*, 1443.2
(16) Brennan, M. J.; Alle, D. T.; Euripides, P.; Buckman, S. J.; Brunger, M. J. *J. Phys. B: At. Mol. Opt. Phys.* **1992**, *25*, 2669.
(17) Vićić, M.; Poparić; G.; Belić, D. S. *J. Phys. B: At. Mol. Phys.* **1996**, *29*, 1273.
(18) Vićić, M.; Poparić, G.; Belić, D. S. *Rev. Sci. Instrum.* **1998**, *69*, 1996.
(19) Schneider, B. I.; Le Dourneuf, M.; Vo Ky Lan, *Phys. Rev. Lett.* **1979**, *43*, 1926.
(20) Dube, L.; Herzenberg, A. *Phys. Rev. A* **1979**, *20*, 194.
(21) Cederbaum, L. S.; Domcke, W. *J. Phys. B: At. Mol. Phys.* **1981**, *14*, 4665.
(22) Berman, M.; Estrada, H.; Cederbaum, L. S.; Domcke, W. *Phys. Rev. A* **1983**, *28*, 1363.
(23) Domcke, W.; Berman, N.; Estrada, H.; Mundel, C.; Cederbaum, L. S. *J. Phys. Chem.* **1984**, *88*, 4862.
(24) Nestman, B. M.; Peyerimhof, S. D. *J. Phys. B: At. Mol. Phys.* **1985**, *18*, 4309.
(25) Huo, W. M.; Gibson, T. L.; Lima, M. A. P.; McKoy, V. *Phys. Rev. A* **1987**, *36*, 1632.
(26) Brunger, M. J.; Buckman, S. J. *Phys. Rep.* **2002**, *357*, 215.
(27) Brunger, M. J.; Buckman, S. J.; Elford, M. T. In *Electron Collisions with Molecules: Scattering and Excitation*; Itikawa, Y., Landolt-Bornstein, Eds.; Springer: Berlin, 2003; Vol. I/17C, Chapter 6.4.
(28) Allan, M. *J. Phys. B: At. Mol. Phys.* **2005**, *38*, 3655.
(29) Ristić, M.; Poparić, G. B.; Belić, D. S. *Chem. Phys.* **2007**, *331*, 410.
(30) Mihajlov, A. A.; Stojanović, V. D.; Petrović, Z. Lj. *J. Phys. D: Appl. Phys.* **1999**, *32*, 2620.
(31) Poparić, G. B.; Galijas, S. M. D.; Belić, D. S. *Phys. Rev. A.* **2004**, *70*, 024701.
(32) Poparić, G. B.; Vićić, M. D.; Belić, D. S. *Phys. Rev. A.* **2002**, *66*, 022711.
(33) Fowler, R. H. *Statistical Mechanics. The Theory of the Properties of Matter in Equilibrium*; The University Press: Cambridge, 1936.
(34) Chantry, P. Final Technical Report ARPA, Order No 3342 (1978).
(35) Belić, D. S. *Chem. Phys.* **1989**, *130*, 141.
(36) Ristić, M.; Poparić, G. B.; Belić, D. S. *Chem. Phys.* **2007**, *336*, 58.
(37) White, R. D.; Brennan, M. J.; Ness, K. F. *J. Phys. D: Appl. Phys.* **1997**, *30*, 810.
(38) Stojanović, V. D.; Jelenković, B.; Petrović, Z. Lj. *J. Appl. Phys.* **1997**, *81*, 1601.
(39) Stojanović, V. D.; Petrović, Z. Lj. *J. Phys. D: Appl. Phys.* **1998**, *31*, 834.
(40) Reid, I. D. *Aust. J. Phys.* **1979**, *32*, 231.
(41) Sun, W.; Morrison, M. A.; Isaacs, W. A.; Trail, W. K.; Alle, D. T.; Gulley, R. J.; Brennan, M. J.; Buckman, S. J. *Phys. Rev. A* **1995**, *52*, 1229.
(42) Gote, M.; Ehrhardt, H. *J. Phys. B: At. Mol. Phys.* **1995**, *28*, 3957.
(43) Nickel, J. C.; Mott, C.; Kanik, I.; McCollum, D. C. *J. Phys. B: At. Mol. Phys.* **1988**, *21*, 1867.
(44) Itikawa, Y. J. *Phys. Chem. Ref. Data* **2006**, *35*, No. 1.
(45) James, G. K.; Ajello, J. M.; Franklin, B.; Shemansky, D. E. *J. Phys. B* **1990**, *23*, 2055.
(46) Ajello, J. M.; James, G. K.; Franklin, B. O.; Shemansky, D. E. *Phys. Rev. A* **1989**, *40*, 3524.
(47) Pitchford, L. C.; Oneil, S. V.; Rumble, J. R. *Phys. Rev. A* **1981**, *23*, 294.
(48) Pitchford, L. C.; Boeuf, J.-P.; Morgan, W. L. *BOLSIG: Electron Boltzmann Equation*; CPAT, France and Kinema Software, 1996.