

ELECTRON IMPACT VIBRATIONAL EXCITATION RATES OF CO_2 MOLECULE

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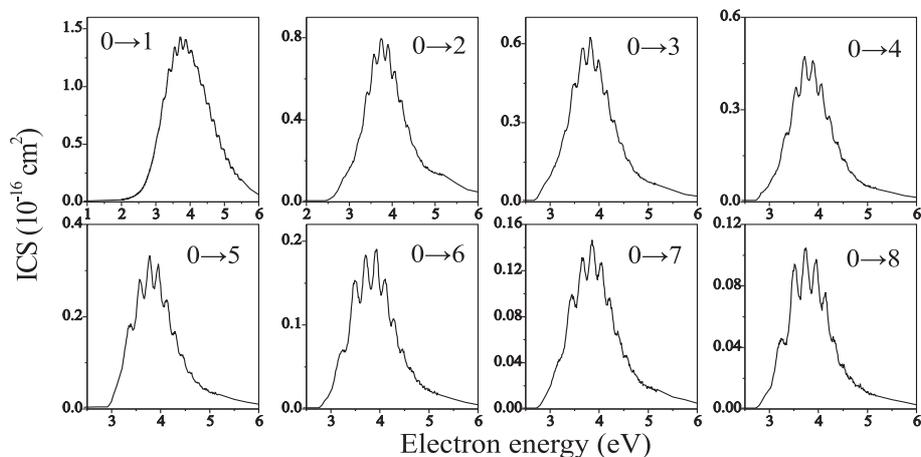
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Abstract. Integral cross sections (ICS) for electron impact vibrational excitation of CO_2 molecule have been used to calculate electron energy transfer rate coefficients for the equilibrium electron energy distribution conditions. Symmetric stretch vibrational excitation cross sections are measured by using our high resolution trochoidal electron spectrometer. ICS for bending and asymmetric vibration of CO_2 have been adopted from previous results. Total and partial electron energy transfer rate coefficients for vibrational excitations are calculated by use of the Maxwellian electron energy distribution function (EEDF) and by direct numerical integration of experimental cross sections. These preliminary calculations have been compared with the previous results.

1. INTRODUCTION

Electron collision processes with the carbon-dioxide molecules are important in many naturally occurring phenomena and also in plasma devices and laser technology. In particular, CO_2 has been intensively studied as a dominant constituent of the Earth's atmosphere responsible for the greenhouse effects. For modeling all of these phenomena, one needs to know cross sections and rate coefficients for various involved processes. At low electron energies vibrational excitation is dominating process of energy transfer. In order to determine rate coefficients for these processes it is necessary to have accurate absolute integral cross sections for vibrational excitation.

Vibrational excitation of the CO_2 molecule has two significant resonant contributions at low energy: $^2\Pi_u$ shape resonance (Bonnes and Schulz, 1974) with the maximum between 3 and 4 eV and a virtual state below 2 eV (Morrison 1982, Herzenberg 1984, Kochem et al. 1985, Estrada and Domcke 1985, Morgan 1998, Rescigno et al. 1999, Mazevet et al. 2001, Field et al. 2001) which causes ICSs for (100) and (020) vibrational transitions to rise steeply above threshold energy.

Figure 1: ICS for symmetric stretch vibrational excitation of CO_2 .

2. VIBRATIONAL EXCITATION CROSS SECTIONS OF CO_2

Low energy electron impact vibrational excitation cross sections of CO_2 are measured by use of a high resolution crossed-beams double trochoidal electron spectrometer. Experimental procedure has been described in detail by Vičić *et al.* 1998 and only a brief outlook will be given here. The electron beam is prepared by using a trochoidal electron monochromator (TEM), and is crossed at right angles with the gas beam, introduced by one-dimensional capillary array, aligned along the electron beam trajectory, in the collision region. After the collision, inelastically scattered electrons are analyzed by use of a double TEM device. Selected electrons are detected by use of a channel electron multiplier, counted and the results are stored in an on line-computer.

We have focused our attention to measure the excitation functions from the ground level of the CO_2 molecule to the first 8 vibrationally excited symmetric stretch levels via the $^2\Pi_u$ shape resonance. In order to normalize our results to the absolute scale, we have used absolute ICS value of $1.33 \times 10^{-16} cm^2$ at 3.8 eV in the $v = 1$ excitation channel, obtained by the recent measurements of Kitajima *et al.* 2001. Our result for $v = 1$ excitation channel is normalized, and other results are scaled relative to the $v = 1$ by using number of counts for each particular vibrational channel under the same experimental conditions. This normalization is performed under the assumption of the angular distributions being the same for all vibrational levels and independent of the electron energy, that is of constant ratios of differential and integral cross sections. Our normalized results for the symmetric stretch vibrational excitation of the first eight levels are shown in figure 1.

ICSs for bending mode and asymmetric stretch have been determined from differential cross sections published by Kitajima *et al.* 2001. For bending mode, only (010) and (020) ICSs have been determined because ICSs for higher levels are much lower. For the same reason, only (001) ICS is determined for asymmetric stretch. A contribution of the virtual state resonance below 2 eV to all ICSs is taken into account separately, using the experimental data of Morgan *et al.* 1997.

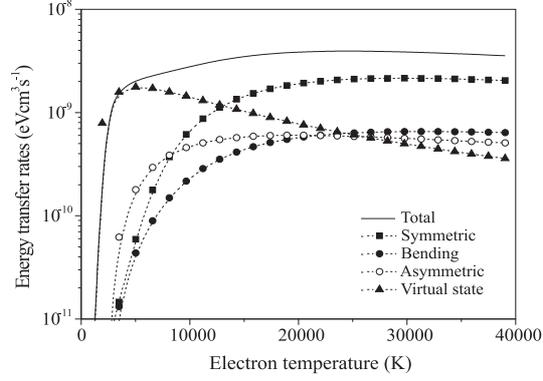


Figure 2: Electron energy transfer rate coefficients for bending, symmetric, asymmetric vibrations and virtual state contributions.

3. RATE COEFFICIENTS CALCULATION

The energy transfer rate coefficient, K , for vibrational excitation is given by Campbell et al. 2004:

$$K(\bar{E}_{el}) = \epsilon_{thres.} \sqrt{2/m_e} \int_{\epsilon_{thres.}}^{+\infty} \sigma_v(\epsilon) \sqrt{\epsilon} f_e(\bar{E}_{el}, \epsilon) d\epsilon \quad (1)$$

where \bar{E}_{el} is the mean electron energy, $\sigma_v(\epsilon)$ is the vibrational excitation cross section, $\epsilon_{thres.}$ is the threshold energy for vibrational excitation and $f_e(\bar{E}_{el}, \epsilon)$ is the normalized electron energy distribution function (Chantry P., 1987, Belić D. S., 1989):

$$\int_0^{+\infty} f_e(\bar{E}_{el}, \epsilon) d\epsilon = 1. \quad (2)$$

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

$$f_e(\bar{E}_{el}, \epsilon) = 2\pi^{-1/2} (3/2\bar{E}_{el})^{+3/2} \sqrt{\epsilon} \exp(-3\epsilon/2\bar{E}_{el}) \quad (3)$$

For this case the energy transfer rate coefficients are determined by the direct numerical integration of integral cross sections multiplied by the Maxwellian electron energy distribution function, for a wide electron energy range. The energy transfer rate coefficients are calculated for each vibrational mode and separately for contribution of the virtual state below 2 eV to all ICSs. Calculations are performed for the mean electron energies up to 5 eV, which correspond to the mean electron temperatures up to 40000 K. Obtained results are shown in figure 2.

4. RESULTS AND DISCUSSION

As it can be seen from figure 2, the maxima of the partial energy transfer rates range from 0.3 to $1 \times 10^{-9} eVcm^3s^{-1}$, for excitation of bending, over symmetric, asymmetric

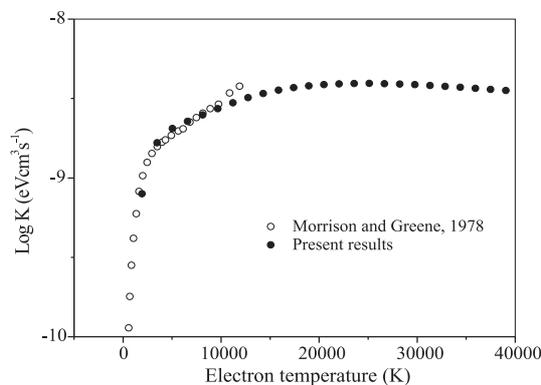


Figure 3: Comparison of our total electron energy transfer rate coefficients with the data of Morrison and Greene, 1978.

vibrations and virtual state contributions, respectively. At low electron temperatures, contribution of virtual state resonance is dominant. The higher contribution in the region from 1 to 5 eV (10000-40000 K) is that of symmetric vibration via the ${}^2\Pi_u$ resonance.

Our results are compared with the previous results published by Morrison and Greene, 1978. Comparison is shown in figure 3. and as it can be seen, our results are in very good agreement with these data.

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