

## Electron-impact excitation of acetylene above 12 eV

A. C. de A. e Souza and G. G. B. de Souza

*Instituto de Química, Universidade Federal do Rio de Janeiro, Cidade Universitária, 21910 Rio de Janeiro, Rio de Janeiro, Brazil*

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Electron-energy-loss spectra have been measured for the acetylene molecule ( $X^1\Sigma_g^+$ ) in the angular range of  $1^\circ$ – $7^\circ$ . The incident energy was 1 keV, the excitation energy range was 0–50 eV, and the energy resolution was 0.6 eV full width at half maximum. Special attention has been given to the broad and intense structures appearing at 13.3 and 15.7 eV, which have been recently studied by photoionization techniques. The generalized oscillator strengths for these transitions have been determined and extrapolated to the optical oscillator strengths. Their values are  $0.21 \pm 0.03$  and  $0.54 \pm 0.08$ , respectively. A new electronic transition has also been observed at 18.7 eV.

### I. INTRODUCTION

We present in this paper the electronic excitation spectrum for the acetylene molecule as determined by the variable-angle ( $1^\circ$ – $7^\circ$ ) low-resolution (0.6 eV), high-incident-energy (1 keV) electron-energy-loss technique. The measured spectra covered the excitation-energy range of 0 to 50 eV. Considering the availability in the literature of several photoabsorption and electron-energy-loss spectra for this molecule in the energy range of 5 to 12 eV and considering also our limited energy resolution, we address our attention here mainly to the energy-loss range above 12 eV. Little experimental and theoretical work has been done in this range and very broad (1 eV FWHM) and intense structures have been reported, as discussed below. Working at a high incident energy and small scattering-angle range, we were able to obtain the generalized oscillator strengths for these structures and to search for quadrupole-allowed electronic transitions. As a result, a previously unreported quadrupole transition has been observed at 18.7 eV.

The ground state of acetylene,  $C_2H_2$ , has a linear geometry, belonging to the  $D_{\infty h}$  symmetry point group, with configuration  $(1\sigma_g)^2(1\sigma_u)^2(2\sigma_g)^4(3\sigma_g)^2(1\pi_u)^4$ ,  $X^1\Sigma_g^+$ .<sup>1</sup>

The photoabsorption spectrum of this molecule has been extensively studied, both experimentally and theoretically, in the energy range of 5 to 12 eV (2500–1000 Å), and the results have been reviewed by Hezberg<sup>2</sup> and Robin.<sup>3</sup> An update on the previous work can also be found in Peric, Buekner, and Peyermanhoff,<sup>4</sup> who also did detailed calculations on the singlet excited states found in this energy range. Quite recently, Lischka and Karpfen<sup>5</sup> published configuration-interaction (CI) calculations on the singlet and triplet excited states lying below 8 eV. For the spectral range above 12 eV, the only known photoabsorption measurements were made in 1955 by Walker and Weissler,<sup>6</sup> who measured the absorption cross section between 11.3 and 18 eV, and by Metzger and Cook<sup>7</sup> who in 1964 did the same kind of measurements for the energy range of 12.4 to 21.4 eV. In both cases the authors observed intense and large bands

at about 13.2 and 15.3 eV, but no assignment was proposed for them.

The electron-energy-loss technique has also been used several times to characterize the electronic excitation spectrum of  $C_2H_2$ . Working at low incident energy (50 and 40 eV) Lassetre *et al.*<sup>8</sup> measured the excitation spectrum for this molecule at  $\theta=0^\circ$  and  $\theta=10^\circ$  in the energy-loss range of approximately 5 to 15 eV. These spectra, measured on a relative intensity scale, showed general good agreement with the photoabsorption results in the energy range of 8 to 12 eV. A very weak structure was also observed between 6.2 and 8.0 eV, but the high-energy bands observed in the photoabsorption spectra above 12 eV were not present in these electron-impact measurements.

Low-incident-energy, large-scattering-angle electron-impact studies for this molecule were also made by Trajmar, Rice, and Kuppermann,<sup>9</sup> Dance and Walker,<sup>10</sup> and Van Veen and Plantenga,<sup>11</sup> resulting in the discovery of singlet-triplet transitions at 5.2 and 6.1 eV. Wilden, Hicks, and Comer<sup>12</sup> demonstrated, through a detailed analysis of the vibrational structure of these bands, that their final states can be associated to a *trans*-bent geometry. They also observed several new singlet-triplet transitions in the spectra measured at low incident energies (2–10 eV) and large scattering angles ( $40^\circ$ – $60^\circ$ ).

Working at 100 eV incident electron energy and a very small scattering angle ( $\theta=0.5^\circ$ ), Wilson, Comer, and Taylor<sup>13</sup> also obtained a high-resolution electron-energy-spectrum in the energy range between 8 and 11.5 eV, obtaining very good agreement with available optical data. At the same incident energy, spectra were measured in the energy range from 9.0 to 10 eV at  $\theta=5^\circ$  and  $10^\circ$ . As a result, three new quadrupole-allowed transitions were observed and assigned.

In one of the very few known high-energy electron-impact studies of polyatomic molecules, Lee<sup>14</sup> working at 24 keV incident energy, reported the presence of significant oscillator strength in the region of 18 to 40 eV in a large number of molecules, including acetylene, but was unable to see any individual peaks because of his poor energy resolution (2.5 eV). Lee's paper and the

present work, as will be seen later on, do emphasize the outstanding capability of high-energy, variable-angle electron-energy-loss spectroscopy to lead to the observation of quadrupole features above 15 eV.

Quite recently, Hammond *et al.*<sup>15</sup> measured the threshold electron-impact spectrum of acetylene but no structure was observed above 12 eV.

Summarizing the work done up to the present time with respect to the electronic excitation of the acetylene molecule, one can say that between 5 and 12 eV an impressive amount of work has been done, both by photoabsorption and electron-energy-loss techniques. Both experimental and theoretical work has been devoted to the determination of the excitation energies and to the assignment of the electronic states participating in the observed transition.

Above 12 eV very few results are found in the literature and most of our knowledge about the electronic excitation in this energy-range comes from photoionization studies, as will be discussed later on.

As a whole, only a limited effort has been directed to the task of calculating and/or measuring absolute cross sections and optical and generalized oscillator strengths for the electronic transitions observed in the acetylene molecule.

## II. EXPERIMENTAL

The apparatus used for the present measurements has been described before.<sup>16</sup> It consists basically of a rotatable electron gun, a neutral-gas beam, and a Mollenstedt velocity analyzer<sup>17</sup> fixed on the vacuum chamber wall. A crossed-beam geometry is used for the electron-gas collision. The electron beam, produced by a triode-type electron gun, is used without prior energy selection. A typical beam current is 10  $\mu$ A and the beam diameter, measured at the scattering region, is approximately 0.5 mm. The gas beam is produced by the expansion of a given sample inside the scattering chamber through a hypodermic needle with a 0.2-mm internal diameter and aspect ratio (length to diameter) of 50.

The scattered electrons are velocity-analyzed by the Mollenstedt analyzer and detected by an electron multiplier (Spiraltron, Galileo Electro Optics). The energy resolution of this system was set to 0.6 eV, as determined by the full width at half maximum (FWHM) of the elastic peak.

The analyzer viewing cone is determined by two parallel, circular apertures of 200 and 50  $\mu$ m diameter, located, respectively, at 120 and 150 mm from the scattering center. The apertures have been selected so that the acceptance cone includes as little in excess of the scattering volume as possible.

The stray magnetic fields in the plane of the measurements have been reduced to less than 10 mG in all directions by three pairs of square, orthogonal, Helmholtz coils.

The energy-loss spectra were measured in a signal-average mode, using an 8-bit microcomputer, which scanned a digitally programmable power supply (Bertan,

model 205-01R) and stored the acquired data.<sup>18</sup> The scattering zero angle was determined by measuring the scattering distribution over a 15° range on both the right-hand and left-hand side of the primary beam. A very precise positioning mechanism allows the determination of the scattered angle with an accuracy of 0.02°. The angular resolution, defined by the entrance apertures of the Mollenstedt analyzer, was 0.2°. The vacuum was  $1 \times 10^{-6}$  Torr without a gas beam and  $4.5 \times 10^{-5}$  Torr (maximum) when the gas sample was injected. The residual gas contribution to the energy-loss spectrum was always limited to less than 2% of the scattering signal. The observed count rate was never allowed to exceed 20 kHz, in order to eliminate the need for dead-time correction.

A further correction was necessary owing to the field-sweeping mode of the analyzer; the intensity of the spectrum was multiplied by  $E_0/(E_0 - E)$ , where  $E_0$  is the primary beam intensity and  $E$  is the excitation energy.<sup>19</sup> A correction of 1% was needed at the highest energy losses corresponding to the broad structures whose generalized oscillator strengths have been determined in the present work.

Gaukler<sup>20</sup> has demonstrated that the energy resolution of a Mollenstedt analyzer has a dependence on the electron energy that goes with the power  $\frac{2}{3}$ , in the energy range of 5 to 30 keV; accordingly, the multiplicative factor should be affected by the same power. Our preliminary study of the energy dependence of resolution of the Mollenstedt analyzer in the 500–2000-eV range has shown that the Gaukler dependence may not be applicable to this lower energy range, and we have decided to keep the multiplicative factor as mentioned earlier. The energy calibration was checked by measuring the energy-loss spectrum for helium. An excitation energy of 21.22 eV was found for the  $1s-2p$  line, in good agreement with the known value.

The uncertainties are estimated in the following manner: The maximum statistical uncertainty was 1.5% as at least 4500 counts were accumulated at the maximum of the inelastic profile for each scattering angle. Fluctuations in the primary beam current and in the sample pressure were of the order of 1% and 0.5%, respectively. The main source of errors in the determination of the scattering intensity was the limited angular resolution (0.2°) which contributes with an uncertainty of approximately 20% below 4° and 10% above it due to the strong angular dependence of the cross section. The area of the two peaks located at 13.3 and 15.7 eV, determined by a Gaussian fitting, is subject to an uncertainty which we estimate to be of the order of 20% for all scattering angles.

An additional source of errors comes from the quoted uncertainty in the absolute elastic cross section (6%) which was used in the normalization procedure, described in Sec. III.<sup>21</sup>

The overall uncertainty  $\delta$  is defined as

$$\delta = \left[ \sum_i \delta_i^2 \right]^{1/2}$$

and is equal to approximately 30% below 4.0° and 25% above this angle.

### III. RESULTS

Energy-loss spectra, including the elastic line, have been measured for acetylene, up to 50-eV energy loss, for  $\theta=1.5^\circ, 2.0^\circ, 2.5^\circ, 3.0^\circ, 4.0^\circ, 5.0^\circ,$  and  $7.0^\circ$ . Some of these spectra are shown in Fig. 1 (spectra measured at 2.0, 2.5, and 4.0 were omitted for the sake of clarity).

Several peaks can be observed between 5 and 25 eV; an enlargement of this spectral range is presented in Fig. 2 for  $\theta=5.0^\circ$ . The inelastic intensities were normalized to the absolute elastic cross sections of Fink, Jost, and Herrmann.<sup>21</sup> In order to obtain the experimental areas, the peaks were fitted using Gaussian curves plus exponential tails.

For the structures observed above the first ionization potential, located at 11.41 eV (Ref. 22), we made the crude approximation that they did not interact with the underlying continuum. A parabolic background was then subtracted from the main peaks in the fitting procedure. A typical result of the fitting procedure can be seen in Fig. 3, in which the spectra obtained at  $3.0^\circ$  and  $5.0^\circ$  are shown. As the angle increases, the Bethe ridge<sup>23</sup> becomes prominent; a similar fitting procedure was used in order to obtain the area of the peaks for each angle.

Within the theoretical framework of the first Born approximation (Mott and Massey,<sup>24</sup> and Inokuti,<sup>23</sup> and Bonham and Fink,<sup>25</sup>) the differential inelastic cross section ( $d\sigma_{0n}/d\Omega$ ) can be related to a more general quantity, the generalized oscillator strength (GOS) by the formula

$$f_{0n} = \frac{W}{2} \frac{K_0}{K_n} K^2 (d\sigma_{0n}/d\Omega), \quad (1)$$

where  $f_{0n}$  is the GOS for the electronic transition from

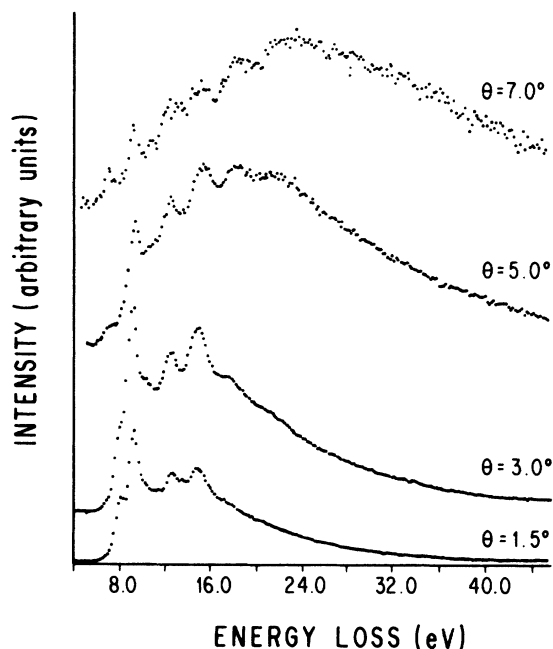


FIG. 1. Energy-loss spectra for  $C_2H_2$  measured at  $\theta=1.5^\circ, 3.0^\circ, 5.0^\circ,$  and  $7.0^\circ$  in the energy-loss range of 4 to 50 eV.

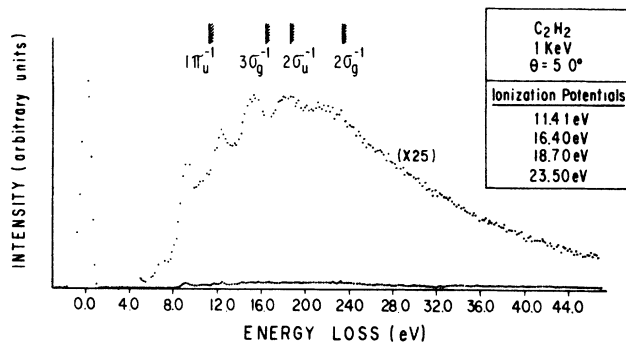


FIG. 2. Energy-loss spectra for  $C_2H_2$  measured at  $\theta=5.0^\circ$  in the energy-loss range of 0 to 50 eV.

the initial state 0 to the final state  $n$ ;  $W$  is the excitation energy in atomic units;  $K_0$  and  $K_n$  are, respectively, the initial and final momenta of the scattered electron; and  $K$  is the magnitude of the momentum transfer  $K$ .

Among the important properties of the GOS we emphasize that as its values are independent of the incident electron energy, and the fact that the limit as  $K^2 \rightarrow 0$  of  $f_{0n}$  approaches the optical oscillator strength  $f_0$ . These properties have been extensively confirmed by Lassetre and collaborators in a series of very interesting papers

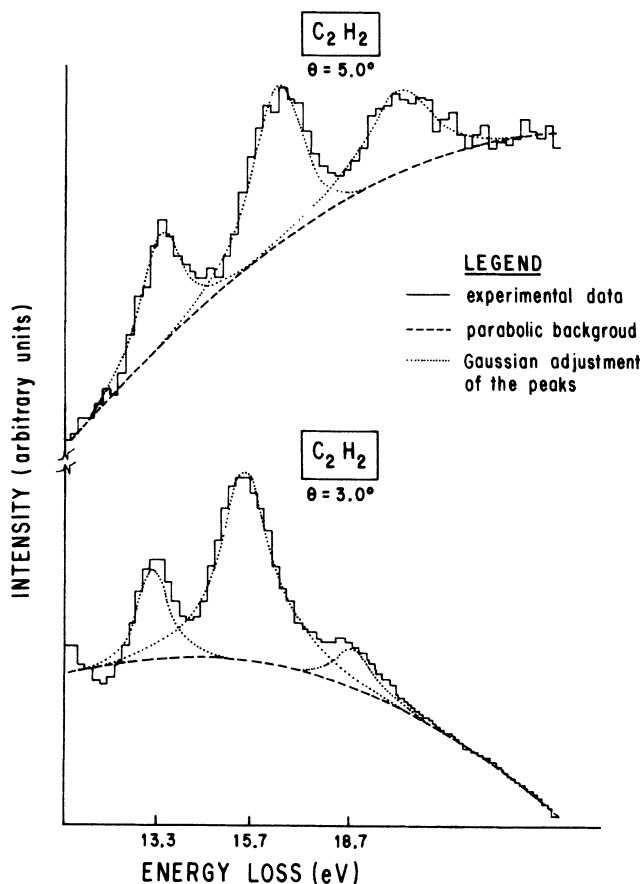


FIG. 3. Typical adjusted spectra obtained at  $3.0^\circ$  and  $5.0^\circ$ .

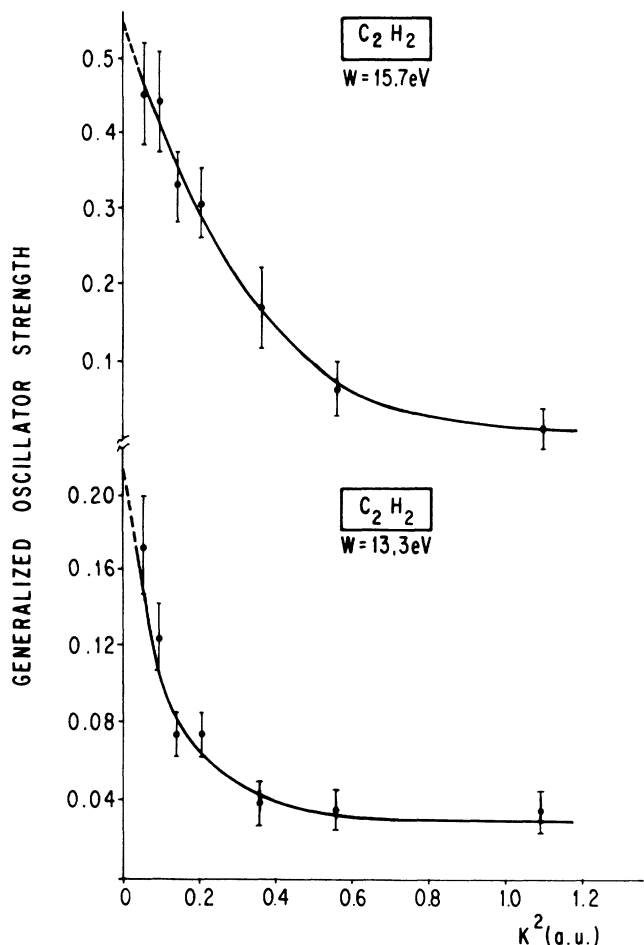


FIG. 4. GOS as a function of  $K^2$  for the 13.3- and 15.7-eV energy loss.

which have been reviewed by Lassette.<sup>26</sup>

Lassette showed, for instance, that even when the first Born approximation does not hold one can still define an apparent generalized oscillator strength,  $f'_{0n}$ , by an equation entirely similar to (1) (Ref. 27) and that it will also approach the optical oscillator strength for very small values of the square of the momentum transfer.

In the present work, considering that our incident energy is at least 20 times the largest studied energy loss, we assume as entirely valid the first Born approximation and we have accordingly generated the GOS from Eq. (1).

We present in Fig. 4 the GOS as a function of  $K^2$  for  $W=13.3$  and  $15.7$  eV. The optical oscillator strengths for each transition were obtained through an extrapolation procedure suggested by Lassette<sup>26</sup> and are shown to be  $0.21 \pm 0.03$  and  $0.54 \pm 0.08$ , respectively.

#### IV. DISCUSSION

As mentioned before, the spectral region between 8 and 12 eV has been thoroughly studied before and will not be discussed in the present work; it suffices to say that the main lines which we observe in our small-angle spectrum are in good agreement with previous observations in photoabsorption and electron-energy-loss studies.

The discussion concerning the spectral region above 12 eV will be divided in our discussion into two parts: first, we analyze the intense structures observed between 12 and 17 eV and then we will comment on the electronic transition observed at 18.7 eV.

The only known photoabsorption measurements in the energy range from 12 to 17 eV were made by Walker and Weissler<sup>6</sup> and by Metzger and Cook<sup>7</sup> who observed the intense structures at 13.2 and 15.3 eV but did not assign them to any specific electronic transition.

These structures have also been observed in the photoionization efficiency curves for  $C_2H_2$  as measured by Botter *et al.*<sup>28</sup> and Hayashishi *et al.*<sup>29</sup> The latter authors have also performed *ab initio* calculations and assigned the structures to the  $3\sigma_u(\sigma^*) \leftarrow 3\sigma_g$  and  $1\pi_g(\pi^*) \leftarrow 2\sigma_u$  transitions at 13.2 and 15.3 eV, respectively. They also assumed that the broadness of the bands originates from a molecular geometry change in the final states.

Recently, a large number of theoretical and experimental works appeared in the literature concerning the "double bump" structure observed in the photoionization cross section for the  $(1\pi_u^{-1})X^2\Pi_u$  ionic state in the energy range from 13 to 16 eV. These results have been carefully reviewed by Dehmer, Parr, and Southworth.<sup>30</sup>

The picture that emerges from these photoionization studies is the following.

(i) The intense peak at 13.3 eV is due to a  $3p\pi_u \leftarrow 3\sigma_g$  shape resonance. Its oscillator strength was calculated by Langhoff *et al.*<sup>31</sup> to be  $f_0=0.1480$ . Hayaishi *et al.*<sup>29</sup> obtained a calculated value of 0.1632.

(ii) The peak at 15.7 eV corresponds, according to the calculations of Langhoff *et al.*<sup>31</sup> to a  $1\pi_g(\pi^*) \leftarrow 2\sigma_u$  transition, with an oscillator strength  $f_0=0.8036$ . Hayaishi *et al.*<sup>29</sup> found  $f=0.4290$  for the same peak, which was assigned to  $1\sigma_g \leftarrow 2\sigma_u$  transition. Parr *et al.*<sup>32</sup> suggested that the final states proposed by Langhoff *et al.*<sup>31</sup> and Hayaishi *et al.*<sup>29</sup> are possibly the same, the difference in assignment being due only to a terminology problem. Dehmer and co-workers<sup>30</sup> though, based on the precise calculations of Levine and Soven,<sup>33</sup> considered that this peak owes half of its intensity to the  $1\pi_g \leftarrow 2\sigma_u$  autoionization profile and the other half to a local maximum in the  $\epsilon\pi_g \leftarrow 1\pi_u$  continuum. A minor contribution from the  $3\sigma_u \leftarrow 3\sigma_g$  transition might exist for this peak according to Dehmer and co-workers.<sup>30</sup> So one can infer that the question concerning the assignment of this peak is far from settled.

Particularly striking is the disagreement between the calculated  $f_0$  values for the  $1\pi \leftarrow 2\sigma$  transition. Besides, as pointed out by Lynch *et al.*,<sup>34</sup> a similar discrepancy (100%) exists between the experimental cross-section values for this transition, as determined by Walker and Weissler<sup>6</sup> and Metzger and Cook.<sup>7</sup> As to the theoretical calculations, the cross-sections values calculated by Lynch *et al.*<sup>34</sup> in the dipole-length and dipole-velocity forms also differ by a factor of approximately 2 at 15 eV.

In Table I we present the assignments and optical oscillator strengths for these transitions. Both calculations show that the transition observed at 15.7 eV should be much more intense than the transition observed at 13.3 eV, a trend that is confirmed by our experimental results.

TABLE I. Assignments and oscillator strengths for the autoionizing structures at 13.3 and 15.7 eV.

Energy (eV)	Assignment	Langhoff <i>et al.</i> (Ref. 30)	Hayaishi <i>et al.</i> (Ref. 28)	This work
13.3	$3p\pi_u \leftarrow 3\sigma_g$	0.1480	0.1632	$0.21 \pm 0.03$
15.7	$1\pi_g \leftarrow 2\sigma_u$	0.8036	0.4290	$0.54 \pm 0.08$

Within error bars, our results seem to confirm the CI calculations of Hayaishi *et al.*<sup>29</sup>

The calculated optical oscillator strength for the  $1\pi_g \leftarrow 2\sigma_u$  transition, 0.4290, is in good agreement with our measured value ( $0.54 \pm 0.08$ ) and only a slight discrepancy is observed between our result ( $0.21 \pm 0.03$ ) and the calculated oscillator strength for the  $3p\pi_u \leftarrow 3\sigma_g$  transition, 0.1623.

The results of Langhoff *et al.*,<sup>31</sup> based on calculations performed employing Franck-Condon and static-exchange approximations, disagree with our results for the oscillator strength for the electronic transition at 15.7 eV; their result for the electronic transition observed at 13.3 eV, on the other hand is in reasonable agreement with the results of Hayaishi *et al.*<sup>29</sup> and with the present results.

We now comment on the structure observed in our spectra at 18.7 eV for scattering angles equal or larger than  $3.0^\circ$ . Both Hayaishi *et al.* and Langhoff *et al.* predict the existence of very weak dipole-allowed transitions in this excitation energy range. Hayaishi *et al.* place the minimum of the potential energy curve for a  $B_3$  state  $4s\sigma_g \leftarrow 2\sigma_u$  configuration at approximately 17.3 eV. The  $f$  value for this transition is calculated to be 0.0027. According to Langhoff *et al.*,<sup>31</sup> a number of Rydberg transitions should appear between 17 and 19 eV, one of them with a moderately high value  $4s\sigma_g(\sigma^*) \leftarrow 2\sigma_u$   $f=0.1551$ , and all the others with  $f$  values smaller than 0.04.

Robin,<sup>3</sup> on the other hand, suggests that the broad maximum observed at about 18 eV by Metzger and Cook<sup>7</sup> could be related to the  $3s \leftarrow 2\sigma_g$  dipole-allowed Rydberg transition.

Although limited by poor resolution, our high-incident-energy, small-angle variation work is ideally suited to the observation of contributions from symmetric-forbidden, spin-allowed transitions.

Our small-angle spectrum seems to rule out the existence of an even moderately intense dipole-allowed transition around 18.7 eV. As the scattering angle in-

creases, on the other hand, a well-defined peak, with a full width at full maximum (FWFM) of approximately 1.0 eV, can be clearly observed. The behavior of the intensity ratio between this peak and the allowed band at 9.2 eV shows that the peak at 18.7 eV can be associated to a symmetry-forbidden, quadrupole-allowed transition. The final state could be either of  $^1\Sigma_g^+$ ,  $^1\Pi_g$ , or  $^1\Delta_g$  symmetry, if one assumes that the molecule keeps its linear geometry in the excited state. Theoretical calculations concerning the transitions to symmetry-forbidden electronic states in acetylene are necessary to clearly identify this state. We remind the reader that quadrupole-allowed transitions have also been observed in acetylene, below 12 eV, by Wilden *et al.*<sup>13</sup> and that a similar type of transition has been previously observed in the isoelectronic molecule  $N_2$  at 31.2 eV by Lee, Wong, and Bonham.<sup>35</sup>

## V. CONCLUSIONS

The electronic excitation of the acetylene molecule above 12 eV has been studied by variable-angle, low-resolution, high-energy electron, energy-loss techniques. The generalized oscillator strengths have been determined for the intense structures observed at 13.3 and 15.7 eV. The extrapolated optical oscillator strengths were  $0.21 \pm 0.03$  and  $0.54 \pm 0.08$ , respectively. A new electronic transition, to which a quadrupole-allowed character was associated, has been observed at 18.7 eV.

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