PHYSICAL REVIEW A VOLUME 31, NUMBER 1 JANUARY 1985

Recalibration of the *KLL* Auger spectrum of carbon

Reinhard Bruch
Department of Physics, University of Nevada, Reno, Nevada 89557

Kwong T. Chung
Department of Physics, North Carolina State University, Raleigh, North Carolina 27695-8202

William L. Luken
Department of Chemistry, Mississippi State University, Mississippi State, Mississippi 39762

John C. Culberson
Quantum Theory Project, University of Florida, Gainesville, Florida 32611

(Received 29 May 1984)

Numerous *KLL* Auger transition energies for C II, C III, and C IV have been calculated using the saddle-point variational method and the unrestricted Hartree-Fock self-consistent-field technique. For Li-like C IV resonances, relativistic corrections are made. The theoretical energy for the C IV $(1s2s2p)^4P^o$ state is calculated to high accuracy by means of a multiconfiguration-interaction wave function and by taking relativistic and mass polarization effects into account. The $^4P^o$ channel energy is then used as a calibration point of the high-resolution carbon Auger spectra reported by Rødbro, Bruch, and Bisgaard. Generally, excellent agreement is found between our theoretical results and experimental data. A number of carbon Auger lines have been identified for the first time.

I. INTRODUCTION

KLL Auger spectra of various carbon ionic states play an important role in ion-atom collision processes. They are of importance in surface diagnostic studies using electron- and ion-impact excitation as well as synchrotron radiation. Core-excited carbon ions are also of theoretical interest for studies of electron correlation and relativistic interactions in few-electron atomic systems. Despite this fundamental importance it was only recently that Rødbro *et al.*[1] reported the first high-resolution free-atom Auger spectra of carbon by means of beam-gas electron spectroscopy.[2] In this work a large number of well-resolved Auger peaks arising mainly from Li-, Be-, and B-like states were observed. However, due to the kinematic transformation from the laboratory to the source-particle frame the entire experimental transition energies were determined with rather large error bars. Other projectile Auger-electron measurements of carbon suffered from the same difficulty.[3,4]

The $(1s\,2s\,2p)^4P^0$ state may be used to calibrate the projectile Auger spectrum of carbon. This state is metastable with respect to Coulomb autoionization and decays to the adjacent doublet continuum via relativistic interactions.

TABLE I. The energy for the C IV resonances, H_0 nonrelativistic Hamiltonian, H_1+H_2 mass correction and Darwin term, H_3 contact term, H_4 mass polarization term, H_5 retardation term. For explicit expressions of these operators, see Refs. 8, 12, and 32.

Resonance	$\langle H_0 \rangle$	$\langle H_1+H_2 \rangle$ (10^2)	$\langle H_3 \rangle$ (10^4)	$\langle H_4 \rangle$[a] (10^4)	$\langle H_5 \rangle$ (10^4)	E_{tot}[b]
$(1s\,2s^2)^2S$	−24.059 445	−1.1491	1.827	−0.043	0.083	−24.070 849
$(1s\,2s\,2p)^4P^0$	−23.969 309	−1.0821	0	−0.761	1.692	−23.980 037
$[1s\,(2s\,2p)^3P]^2P^0$	−23.752 280	−1.0552	1.257	0.599	−1.101	−23.762 757
$[1s\,(2s\,2p)^1P]^2P^0$	−23.623 455	−1.0413	0.754	−0.588	1.233	−23.634 229
$[1s\,2p^2]^2D$	−23.513 251	−0.9613	0.279	−0.791	1.421	−23.522 774
$[1s\,2p^2]^2S$	−23.286 599	−0.9764	0.5078	−0.5841	1.778	−23.296 188
$[(1s\,2s)^3S\,3s]^2S$	−22.452 745	−1.0742	0.307	−0.049	0.077	−22.463 453
$[(1s\,2s)^3S\,3p]^2P^0$	−22.414 518	−1.0507	0.132	0.050	0.027	−22.425 004
$[(1s\,2s)^3S\,3d]^2D$	−22.328 130	−1.0476	0.049	0.006	0.019	−22.338 599
$[(1s\,2s)^1S\,3s]^2S$	−22.304 035	−1.0038	1.790	0.121	−0.230	−22.313 905
$[(1s\,2s)^1S\,3d]^2D$	−22.162 831	−0.9753	1.262	0.164	−0.132	−22.172 454

[a] The $_6C^{12}$ isotope is used for mass polarization computation.
[b] $E_{\text{tot}} = \langle H_0 \rangle + \langle H_1+H_2 \rangle + \langle H_3 \rangle + \langle H_4 \rangle + \langle H_5 \rangle$.

By using correlated wave functions and including relativistic effects the $(1s2s2p)^4P^0$ term energy of C IV has been determined in this work with much higher accuracy than before. An estimate of the accuracy of the theoretical energy may be gained by studying the C IV $(1s2p^2)^4P \rightarrow (1s2s2p)^4P^0$ photon transition. Thus Chung[5] predicted the transition wavelength to be 1344.22 Å. This value coincides with the experimental result of 1344.2±0.3 Å.[6] From this excellent agreement and from the accuracy obtained for the $^4P^0$ state of other Li-like ions,[5,7] we conclude that our C IV $^4P^0$ energy should be correct within a few meV. Hence it provides a very precise calibration point of the measured carbon projectile Auger spectra. Recently a similar procedure has been adopted to recalibrate the projectile electron spectrum of boron.[8]

It has been demonstrated quite recently that the saddle-point technique provides a very effective and accurate method to calculate resonance energies and widths[9–11] of two- and three-electron atomic systems. In this work it is applied to compute resonance energies of ten singly-core-excited C IV doublet states. These results and additional C III and C II Auger energies calculated by the unrestricted Hartree-Fock self-consistent-field (UHF-SCF) method are used to identify the observed carbon Auger spectra. The theoretical procedure is outlined in Secs. II and III and a comparison of experimental and theoretical results is given in Sec. IV.

II. C IV AUGER ENERGIES

To determine the nonrelativistic wave functions and energies of the C IV doublet states, the saddle-point technique is applied.[2] The theoretical calculation of these resonances is very similar to the work of Davis and Chung.[10] For a detailed discussion of this technique the reader is referred to Ref. 10. The relativistic effects considered here are mass polarization, Darwin term, and retardation term due to the Breit-Pauli operator derived by Bethe and Salpeter[12] for two-electron atoms. The corresponding expressions for three-electron states are given by Chung and Bruch.[8] We note that for B III (see Ref. 8) the retardation potential, i.e., the orbit-orbit interaction was neglected. However, since this potential increases rapidly with nuclear charge Z, it is expected to contribute up to 9.3 meV (Ref. 5) to the total energy for some $Z=6$ states. Hence, this effect is also considered for the C IV resonance energies. The expectation values of the relativistic operators are then calculated with the wave functions obtained by the saddle-point method. We note that relativistic effects and mass polarization were evaluated using first-order perturbation theory.

Ten doublets were investigated, namely, four ^2S, three $^2P^0$ and ^2D states, respectively. The theoretical results for these doublets are listed in Table I. In this table we have also tabulated the corresponding result for the C*IV*$(1s2s2p)^4P^0$ quartet state. The nonrelativistic energy of $-23.969\,309$ a.u. was derived by using a 12-partial-wave, 80-linear-parameter wave function. We note that our value is slightly lower than the $-23.969\,19$ a.u. result of Larsson *et al.*[13] who used r_{ij} coordinates explicitly and a 97-parameter wave function. Lunnell and Beebe[14] calculated the $^4P^0(1)$ energy to be -23.9683 a.u. With the relativistic corrections taken into account (see Table I) our result for the $^4P^0(1)$ term is $-23.980\,037$ a.u. Finally, by adopting an energy value of $-32.419\,028$ a.u. (Ref. 15) for the C V $(1s^2)^1S$ ground state, we obtained a transition energy of 229.639 eV for the C IV $(1s2s2p)^4P^0 \rightarrow 1s^2+\epsilon p$ or ϵf) decay process.

TABLE II. C II *KLL* Auger energies (eV).

C$^+$	C^{2+}	UHF-SCF	UHF-SCF + Corr
$(1s2s2p^3)^4D^0$	$(1s^22s^2)^1S$	268.65	269.21
	$(1s^22s2p)^3P^0$	263.95	262.79
	$(1s^22s2p)^1P^0$	256.48	256.24
	$(1s^22p^2)^3P$	253.27	251.95
	$(1s^22p^2)^1D$	250.12	250.13
	$(1s^22p^2)^1S$	248.08	246.12
$(1s2p^4)^4P$	$(1s^22s^2)^1S$	280.78	
	$(1s^22s2p)^3P^0$	276.08	
	$(1s^22s2p)^1P^0$	268.61	
	$(1s^22p^2)^3P$	265.40	
	$(1s^22p^2)^1D$	262.25	
	$(1s^22p^2)^1S$	260.21	
$(1s2p^4)^2D$	$(1s^22s^2)^1S$	285.13	
	$(1s^22s2p)^3P^0$	280.43	
	$(1s^22s2p)^1P^0$	272.96	
	$(1s^22p^2)^3P$	269.75	
	$(1s^22p^2)^1D$	266.61	
	$(1s^22p^2)^1S$	264.56	
$(1s2s^22p^2)^4P$	$(1s^22s^2)^1S$	260.23	260.60
	$(1s^22s2p)^3P^0$	255.53	254.17
	$(1s^22s2p)^1P^0$	248.06	247.62
	$(1s^22p^2)^3P$	244.85	243.33
	$(1s^22p^2)^1D$	241.71	241.52
	$(1s^22p^2)^1S$	239.66	237.50
$(1s2s^22p^2)^2D$	$(1s^22s^2)^1S$	264.93	264.95
	$(1s^22s2p)^3P^0$	260.23	258.52
	$(1s^22s2p)^1P^0$	252.76	251.97
	$(1s^22p^2)^3P$	249.55	247.68
	$(1s^22p^2)^1D$	246.40	245.87
	$(1s^22p^2)^1S$	244.36	241.85
$(1s2s2p^3)^6S$	$(1s^22s^2)^1S$	259.39	262.04
	$(1s^22s2p)^3P^0$	254.69	255.62
	$(1s^22s2p)^1P^0$	247.22	249.07
	$(1s^22p^2)^3P$	244.02	244.78
	$(1s^22p^2)^1D$	240.87	242.97
	$(1s^22p^2)^1S$	238.82	238.95

III. C II AND C III AUGER ENERGIES

Theoretical energies for the C II and C III Auger spectra presented in Tables II and III were calculated by the method previously used to calculate Auger energies of B II and B III.[16] These results are based on variational wave functions determined by the UHF-SCF method.[17] The

TABLE III. C III *KLL* Auger energies (eV).

C^{2+}	C^{3+}	UHF-SCF	UHF-SCF + Corr
$(1s2s^22p)^3P^0$	$1s^22s\ ^2S$	244.91	243.48
	$1s^22p\ ^2P^0$	236.85	235.43
$(1s2s2p^2)^5P$	$1s^22s\ ^2S$	244.40	245.16
	$1s^22p\ ^2P^0$	236.33	237.11
$(1s2s2p^2)^3D$	$1s^22s\ ^2S$	253.52	252.61
	$1s^22p\ ^2P^0$	245.46	244.56
$(1s2p^3)^5S^0$	$1s^22s\ ^2S$	256.89	257.85
	$1s^22p\ ^2P^0$	248.83	249.80
$(1s2p^3)^3D^0$	$1s^22s\ ^2S$	263.00	261.82
	$1s^22p\ ^2P^0$	254.94	253.77

UHF-SCF method is a special case of the saddle-point variational method[18] for a wave function with a vacancy in the most tightly bound orbital.[19]

As noted below, the UHF-SCF wave functions are not as accurate as those determined by previous applications of the saddle-point variational method.[20] The UHF-SCF method, however, has the advantage of being easily applied to electronic states with four or more electrons. The UHF-SCF method has recently been used to calculate variational wave functions for a polyatomic molecule (formaldehyde) with an inner-shell vacancy on the oxygen atom.[21]

Unlike previous calculations based on the saddle-point variational method,[20] the variational wave functions determined by the UHF-SCF method are not exact eigenfunctions of L^2 and S^2. The calculations reported here have been limited to electronic states for which exact eigenfunctions of L^2 and S^2 may be formed from a single Slater determinant. These states generally possess the maximum values of L and or S possible for their electronic configuration. The expectation values of S^2 determined by the UHF-SCF wave functions calculated here each differed from the exact values, $S(S+1)$, by less than 1%.

The UHF-SCF wave functions also neglect the effects of electron correlation.[22] The effects of electron correlation on the energy of each electronic state may introduce errors as large as 1–2 eV in the resulting Auger energies. Consequently, it is necessary to include corrections for the

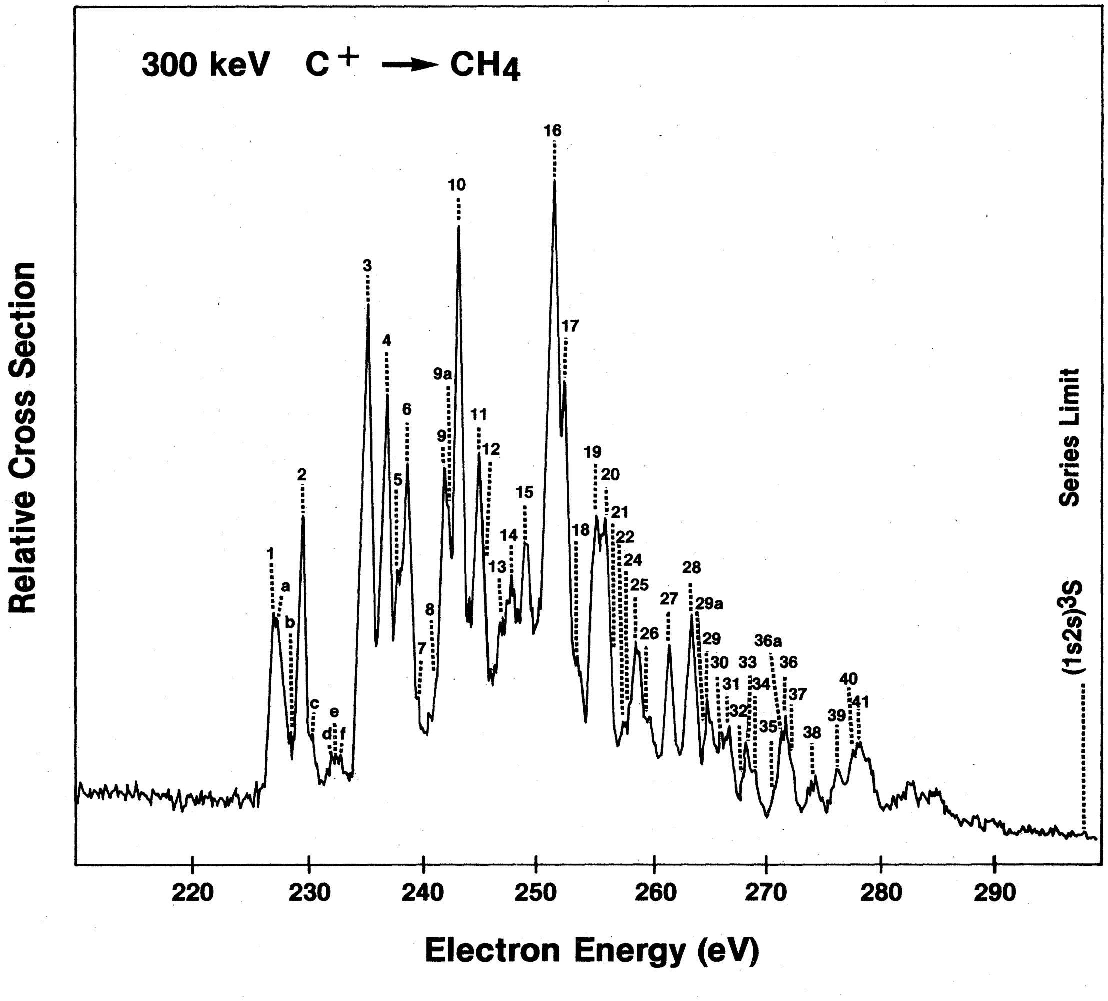

FIG. 1. High-resolution *KLL* Auger spectrum of carbon produced by 300-keV $C^+ \rightarrow CH_4$ impact under single-collision conditions. Electron observation angle θ is 6.4° with respect to the beam axis.

TABLE IV. Recalibrated transition energies (eV) of carbon *KLL* Auger spectra in comparison with theoretical predictions.

Line number	Line identification		Theory	Report data[e]	Uncalibrated data	Recalibrated data[f]
	Initial state	Final state				
1	$(1s\,2s^2)^2S$	$(1s^2)^1S$	227.17[a]	227.6	226.90	227.23±0.3
2	$(1s\,2s\,2p)^4P^0$	$(1s^2)^1S$	229.64[a]	229.7	229.31	229.64[a]
3	$(1s\,2s^2 2p)^3P^0$	$(1s^2 2p)^2P^0$	235.43[b]	235.5	235.11	235.44±0.2
	$[1s\,(2s\,2p)^3P^0]^2P^0$	$(1s^2)^1S$	235.55[a]			
4	$(1s\,2s\,2p^2)^5P$	$(1s^2 2p)^2P^0$	237.11[b]	237.1	236.72	237.05±0.2
	$(1s\,2s^2 2p^2)^4P$	$(1s^2 2p^2)^1S$	237.50[b]			
5	$(1s\,2s^2 2p)^1P^0$	$(1s^2 2p)^2P^0$	238.50[c]	283.3	237.88	238.21
6	$[(1s\,(2s\,2p)^1P^0]^2P^0$	$(1s^2)^1S$	238.78[a]	238.9	238.53	238.86±0.2
7				239.8	239.43	239.76
8	$(1s\,2s^2 2p^2)^4P$	$(1s^2 2p^2)^1D$	241.52[b]	241.6	241.18	241.51
	$(1s\,2s^2 2p^2)^2D$	$(1s^2 2p^2)^1S$	241.85[b]			
9	$(1s\,2p^2)^2D$	$(1s^2)^1S$	242.08[a]	242.2	241.82	242.15±0.2
10	$(1s\,2s^2 2p^2)^4P$	$(1s^2 2p^2)^3P$	243.33[b]	243.4	243.05	243.38±0.2
	$(1s\,2s^2 2p)^3P^0$	$(1s^2 2s)^2S$	243.48[b]			
11	$(1s\,2s\,2p^2)^5P$	$(1s^2 2s)^2S$	245.16[b]	245.1	244.73	245.06±0.2
12	$(1s\,2s^2 2p^2)^2D$	$(1s^2 2p^2)^1D$	245.87[b]	245.7	245.32	245.65
13	$(1s\,2s^2 2p^2)^4P$	$(1s^2 2s\,2p)^1P^0$	247.62[b]	247.3	246.87	247.20
14	$(1s\,2p^2)^2S$	$(1s^2)^1S$	248.25[a]	248.1	247.71	248.04
15	$(1s\,2s\,2p^3)^6S$	$(1s^2 2s\,2p)^1P^0$	249.07[b]	249.3	248.88	249.21
	$(1s\,2s\,2p^3)^4D^0$	$(1s^2 2p^2)^1D$	250.13[b]			
16	$(1s\,2s\,2p^3)^4D^0$	$(1s^2 2p^2)^3P$	251.95[b]	251.5	251.15	151.48±0.2
	$(1s\,2s^2 2p^2)^2D$	$(1s^2 2s\,2p)^1P^0$	251.97[b]			
17	$(1s\,2s\,2p^2)^3D$	$(1s^2 2s)^2S$	252.61[b]	252.6	252.25	252.58±0.2
18	$(1s\,2p^3)^3D^0$	$(1s^2 2p)^2P^0$	253.77[b]	253.8	253.36	253.69
	$(1s\,2s^2 2p^2)^4P$	$(1s\,2s\,2p)^3P^0$	254.17[b]			
19	$(1s\,2s\,2p^3)^6S$	$(1s^2 2s\,2p)^3P^0$	255.62[b]	255.4	254.98	255.31±0.4
20	$(1s\,2s\,2p^3)^4D^0$	$(1s^2 2s\,2p)^1P^0$	256.24[b]	256.2	255.76	256.09
22	$(1s\,2p^3)^5S^0$	$(1s^2 2s)^2S$	257.85[b]	257.8	257.45	257.78
24	$(1s\,2s^2 2p^2)^2D$	$(1s^2 2s\,2p)^3P^0$	258.52[b]	258.6	258.23	258.56
25				259.1	258.69	259.02
26	$(1s\,2s^2 2p^2)^4P$	$(1s^2 2s^2)^1S$	260.60[b]	260.1	259.66	259.99
27	$(1s\,2p^3)^3D^0$	$(1s^2 2s)^2S$	261.82[b]	261.9	261.49	261.82±0.2
28				263.8	263.38	263.71
29a	$(1s\,2s^2 2p^2)^2D$	$(1s^2 2s^2)^1S$	264.95[b]			264.9
29						265.3±0.5
30	$(1s\,2p^4)^2D$	$(1s^2 2p^2)^1D$				266.6
31						267.5
32	$(1s\,2p^4)^4P$	$(1s^2 2s\,2p)^1P^0$				268.8
33	$(1s\,2s\,2p^3)^4D^0$	$(1s^2 2s^2)^1S$	269.21[b]			269.4
34						270.0
35	$[(1s\,2s)^3S\,3p]^2P^0$	$(1s^2)^1S$	271.95[a]			272.1
36a						272.9
36						273.4
37	$[(1s\,2s)^3S\,3d]^2D$	$(1s^2)^1S$	274.31[a]			274.1
38						276.2
39	$[(1s\,2s)^1S\,3d]^2D$	$(1s^2)^1S$	278.85[a]			278.7
40						280.4
41						280.9
Series limit	$(1s\,2s)^3S\,\infty l$	$(1s^2)^1S$	298.96[d]			

[a] Relativistic configuration-interaction calculation, this work.

[b] Unrestricted Hartree-Fock plus electron pair correlation energies, this work.

[c] Safronova and Kharitanova (Ref. 30).

[d] Bashkin and Stoner (Ref. 31)

[e] Rødbro *et al.* (Ref. 1).

[f] Recalibrated data, this work.

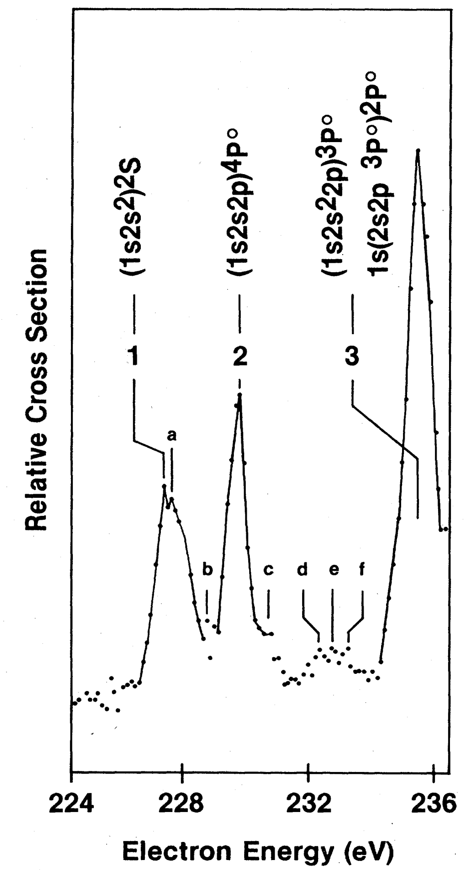

FIG. 2. Segment of the *KLL* Auger spectrum in the vicinity of the C IV $(1s2s^2)^2S \rightarrow (1s^2\epsilon s)^2S$ transition.

correlation energies of each state in order to obtain accurate values of Auger energies.

The UHF-SCF wave functions for the electronic states of C II, C III, and C IV were calculated using basis sets consisting of five Slater-type orbitals (STO's) of *s* symmetry, and four sets of *p*-symmetry STO's. The STO exponential factors were taken from those of the restricted Hartree-Fock (RHF) wave function for the C II ground state.[23] For electronic states with an inner-shell vacancy (the upper states in the Auger transitions), the largest exponential factor was changed to 6.0.

The effects of electron correlation were treated using the nonclosed-shell many-electron theory (NCMET) of Sinanoğlu.[24] The correlation energy of each state was calculated as the sum of internal, polarization plus semi-internal, and all-external contributions,

$$E_{\text{corr}} = E_{\text{int}} + E_F + E_U \ .$$

The internal contributions E_{int}, and the polarization plus semi-internal contributions E_F, of each state were taken from the NCMET charge wave function of the electronic state with the same $2s$ and $2p$ configuration.[25,26] The contributions of core-valence correlation to the internal and polarization plus semi-internal energies were neglected.

The all-external contributions E_U were each calculated as a sum of irreducible external pair correlation energies. Pair energy set II of Oksuz and Sinanoğlu[27] was used for these calculations. Electronic energies calculated in this manner are usually accurate to within approximately 0.1 eV.[16,27]

The UHF-SCF calculations reported here were performed by the electronic structure program MOLECI developed by Luken and collaborators.[16,21]

IV. RESULTS AND DISCUSSION

A typical high-resolution carbon Auger spectrum for $C^+ \rightarrow CH_4$ impact is shown in Fig. 1. To minimize line broadening due to the kinematic transformation[2] from the laboratory to the source-particle frame, an observation angle close to 0° with respect to the beam axis was chosen. Although some Auger lines were tentatively assigned by Rødbro *et al.*,[1] many features remained unclassified due to the lack of accurate theoretical transition energies. The Auger spectrum shown in Fig. 1 is calibrated using a theoretical energy value of 229.64 eV for the decay of $(1s2s2p)^4P^0$. The low-energy group of lines (predominantly three-electron systems) is indicated in more detail in Fig. 2. A remarkable feature seen from this figure are the satellite structures labeled *a*—*f*. Rødbro *et al.* assumed that these structures might originate from four-electron states in C III, characterized by a three-electron core and a loosely attached "spectator" electron. On the other hand, these satellites may also originate from the formation of core-excited neutral C I or even C^- states. Very recently Beck and Nicolaides[28,29] predicted such highly excited bound states for Li^- and B^-.

Table IV summarizes our recalibrated observed peak energies together with the theoretical results. Generally experimental energy values are in excellent agreement with those derived by the saddle-point technique and the UHF-SCF method. The lowest-energy feature of the carbon spectrum (see Fig. 2) was identified as the C IV $(1s2s^2)^2S \rightarrow (1s^2\epsilon s)^2S$ transition by Rødbro *et al.*[1] However, the centroid energy of this structure deviates significantly from the theoretical value predicted at 227.17 eV. A careful analysis shows that this peak may be composed of two structures, i.e., the $(1s2s^2)^2S$ line and the peak labeled *a*, where peak *a* cannot be classified so far. This feature may arise from the Auger decay of C I $(1s2s^22p^3)$ or C^- $(1s2s^22p^4)$. We also note that the structures labeled *b*—*f* cannot be identified in terms of our C IV, C III, and C II Auger transition energies. Similar satellite structures were observed in the boron case.[1] For the $(1s2s^2)^2S$ initial state we extracted a transition energy of 227.23±03 eV. This value is in good agreement with our theoretical prediction of 227.17 eV (see Table IV). We also found excellent agreement between the C IV $[1s(2s2p)^3P^0]^2P^0$, $[1s(2s2p)^1P^0]^2P^0$, and $(1s2p^2)^2D$ recalibrated Auger positions and those calculated by the saddle-point method. We also note that peak 14 may be assigned as the C IV $(1s2p^2)^2S \rightarrow (1s^2\epsilon s)^2S$ transition. The energy difference of about 0.2 eV between theory and experiment may be caused by overlapping Auger features arising from C II and C III states. Three additional C IV resonances appearing at 272.1, 274.1, and 278.7 eV were identified as

C IV $[(1s2s)^3S3p]^2P^0$, C IV $[(1s2s)^3P^03d]^2D^0$, and C IV $[(1s2s)^1S3d]^2D$ initial states. Several other prominent peaks indicated in Fig. 1 can be attributed to C II and C III *KLL* Auger lines. For example, the structures labeled 4 and 11 are mainly due to the metastable autoionizing C III $(1s2s2p^2)^5P$ states decaying to the C IV $(1s^22p)^2P^0$ and $(1s^22s)^2S$ final states. Another prominent peak, labeled 10, may be composed of two lines, arising from the C II $(1s2s^22p^2)^4P$ and C III $(1s2s^22p)^3P^0$ initial states (see Table IV). Furthermore, peak 16 should be associated with the C II $(1s2s2p^3)^4D^0$ and $(1s2s^22p^2)^2D$ levels. Another prominent line, labeled 17, is assigned due to the C III $(1s2s2p^2)^3D$ Auger decay.

V. CONCLUSION

In this study the *KLL* Auger energies of carbon were recalibrated by means of the C IV $(1s2s2p)^4P^0$ metastable autoionizing state. The calculated transition energies enabled us to make several new identifications in the high-resolution carbon Auger spectra. Some striking features in the low-energy region close to the C IV $(1s2s^2)^2S$, $(1s2s2p)^4P^0$, and $[1s(2s2p)^3P^0]^2P^0$ resonances still remain to be classified. These structures may originate from core-excited neutral C I or even negative C^- states.

ACKNOWLEDGMENTS

This work was supported by the National Science Foundation Grant No. PHY-82-06490. The authors also acknowledge the Donors of the Petroleum Research Fund, administered by the American Chemical Society, for support of this research. One of us (R.B.) wishes to thank Professor P. Winkler for stimulating discussions on negative ions.

---

[1] M. Rødbro, R. Bruch, and P. Bisgaard, J. Phys. B **12**, 2413 (1979).

[2] R. Bruch and K. T. Chung, Comments At. Mol. Phys. **14**, 117 (1984).

[3] D. Schneider, R. Bruch, W. H. E. Schwarz, and T. C. Chang, Phys. Rev. A **15**, 926 (1977).

[4] D. Schneider, R. Bruch, W. Butscher, and W. H. E. Schwarz, Phys. Rev. A **24**, 1223 (1981).

[5] K. T. Chung, Phys. Rev. A **29**, 682 (1984).

[6] A. E. Livingston and H. G. Berry, Phys. Rev. A **17**, 1966 (1978).

[7] K. T. Chung, Phys. Rev. A **29**, 439 (1984).

[8] K. T. Chung and R. Bruch, Phys. Rev. A **28**, 1418 (1983).

[9] K. T. Chung, Phys. Rev. A **23**, 2957 (1981); **24**, 1350 (1981); **25**, 1596 (1982); **23**, 1079 (1981).

[10] B. F. Davis and K. T. Chung, J. Phys. B **15**, 3113 (1982); K. T. Chung and B. F. Davis, Phys. Rev. A **26**, 3278 (1982).

[11] B. F. Davis and K. T. Chung, Phys. Rev. A **29**, 1878 (1984).

[12] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One and Two Electron Atoms*, (Springer, Berlin, 1957).

[13] S. Larsson, R. Crossley, and T. Ahlenius, J. Phys. (Paris) Colloq. **40**, C1-6 (1979).

[14] S. Lunell and W. H. F. Beebe, Phys. Scr. **15**, 268 (1977).

[15] C. L. Pekeris, Phys. Rev. **112**, 1649 (1958).

[16] W. L. Luken and J. M. Leonard, Phys. Rev. A **28**, 532 (1983).

[17] J. A. Pople and R. K. Nesbet, J. Chem. Phys. **22**, 571 (1954).

[18] K. T. Chung, Phys. Rev. A **20**, 1743 (1979).

[19] W. L. Luken, J. M. Leonard, and J. C. Culberson, Int. J. Quantum Chem. Symp. **17**, 401 (1983).

[20] K. T. Chung and B. F. Davis, Phys. Rev. A **22**, 835 (1980); K. T. Chung, *ibid.* **22**, 1341 (1980); **23**, 1079 (1981).

[21] W. L. Luken, J. M. Leonard, and J. C. Culberson, J. Chem. Phys. (to be published).

[22] P.-O. Löwdin, Adv. Chem. Phys. **2**, 207 (1959).

[23] E. Clementi and C. Roetti, At. Data Nucl. Data Tables **14**, 177 (1974).

[24] H. J. Silverstone and O. Sinanoğlu, J. Chem. Phys. **44**, 1899 (1966); **44**, 3608 (1966).

[25] W. L. Luken and O. Sinanoğlu, Phys. Rev. A **13**, 1293 (1976).

[26] W. L. Luken and O. Sinanoğlu, At. Data Nucl. Data Tables **18**, 525 (1976).

[27] I. Oksuz and O. Sinanoğlu, Phys. Rev. **181**, 42 (1969); **181**, 54 (1969).

[28] D. R. Beck, Phys. Rev. A **27**, 1197 (1983).

[29] D. R. Beck and C. A. Nicolaides, Phys. Rev. A **28**, 3112 (1983).

[30] U. I. Safronova and V. N. Kharitonova, Opt. Spectrosc. **27**, 300 (1969).

[31] S. Bashkin and Y. O. Stoner, *Atomic Energy Levels and Grotrian Diagrams* (North-Holland, Amsterdam, 1975).

[32] R. Bruch, K. T. Chung, E. Träbert, P. H. Heckmann, B. Raith, and H. R. Müller, J. Phys. B **17**, 333 (1984).