Spectra Induced by Proton Impact on Helium*

J. G. Dodd† AND R. H. Hughes

Department of Physics, University of Arkansas, Fayetteville, Arkansas

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Spectra induced by proton impact on helium have been studied in the energy range of 20 keV to 130 keV. Absolute cross sections have been measured for helium emissions from $n\,^1S \to 2\,^1P\,(n=3,4,5)$, $3\,^1P \to 2\,^1S$, and He II$(4 \to 3)$ transitions. From these measurements cross sections have been estimated for excitation into the $3\,^1P$, $3\,^1S$, $4\,^1S$, and $5\,^1S$ states, and for simultaneous ionization (including charge transfer) and excitation of helium into the $n=4$ state of He$^+$.

I. APPARATUS

MAGNETICALLY analyzed protons from the 140-keV accelerator in the University of Arkansas Department of Physics were allowed to enter a differentially pumped helium-filled collision chamber where the beam was observed by a JA-82 000 Ebert-type scanning spectrometer coupled to an EMI 6095B photomultiplier. A more complete description of the apparatus can be found in a previous paper.[1]

To insure the highest gas purity, helium was introduced through a well out-gassed, liquid-air-cooled charcoal trap. A liquid-air-cooled finger extended into the collision chamber and was struck by the beam. In the absence of this additional trapping, the chamber "background" was equivalent to a few microns of hydrogen as determined from the residual H_α and H_β spectra. With a cooled target the background was below detectability.

The spectrometer, photomultiplier, and lens were the same equipment used in an earlier study and were recalibrated by a previously described procedure.[2] However, it was necessary to extrapolate the standard lamp calibration curve beyond the 6500 Å Yerkes Observatory calibration limit to permit absolute intensity measurements of the $2\,^1P - 3\,^1S$ ($\lambda 7281$ Å) line. This was done by plotting $\log_e \lambda^5 E_\lambda$ versus $1/\lambda$ (the short-wavelength approximation to the Planck law) as a straight line through the calibration points and then simply extrapolating this line into the desired region. The calibration curve of the spectrometer photomultiplier system was checked at $\lambda 7281$ Å to make certain that radiation from the standard lamp was not appearing in the second order. This was done by interposing a yellow filter and noting the ratios of the filtered to the unfiltered intensity for both the standard-lamp light source and the $\lambda 7281$ Å line where there was no second-order contribution. The ratios were found to be the same within experimental error.

II. MEASUREMENT PROCEDURE

Runs were taken at constant pressure, varying the energy. Normally the spectrum was not scanned. The spectrometer was set manually on a line and the recorder chart allowed to run long enough to obtain a good average reading over a period of stable current. Pressures from 5 to 25 μ(Hg) were employed.

The uncertainties of our measurements are difficult to assess as we have previously noted.[2] Accidental errors might result from uncertainties in the gas temperature, current, pressure, energy, optical calibration, and noise fluctuations in the photomultiplier output. Run-to-run reproducibility from these errors was within 5%. Individual runs were self-consistent to within 2%. The possibility of systematic errors makes our absolute measurements good to within an estimated 40% although our relative measurements are, of course, much better.

III. $n\,^1S \to 2\,^1P$ TRANSITIONS

The $4\,^1S \to 2\,^1P$ ($\lambda 5047$ Å) and the $5\,^1S \to 2\,^1P$ ($\lambda 4437$ Å) transitions were linear with pressure up to
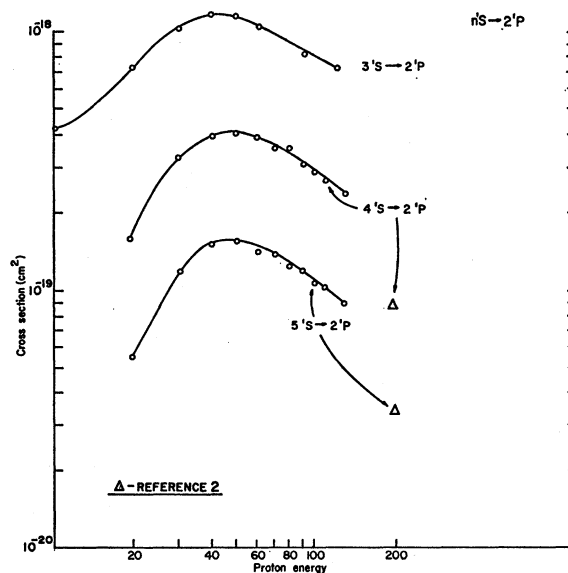
Fig. 1. Cross sections for the production of $n\,^1S \to 2\,^1P$ radiation for $n=3$, 4 and 5.

[1] R. H. Hughes, Sabrina Lin, and L. L. Hatfield, Phys. Rev. 130, 2318 (1963).

[2] R. H. Hughes, R. C. Waring, and C. Y. Fan, Phys. Rev. 122, 525, (1961).

the highest pressure used. The $3\,^1S \rightarrow 2\,^1P$ ($\lambda7281$ Å) line departed very slightly from linearity with pressure but the cross section at zero pressure was easily obtained by extrapolation. An assumed pressure dependence of the form $\sigma = \sigma_0 + bp$ was used where σ is the apparent cross section, σ_0 is the cross section at zero pressure, b is a constant (at a given proton energy), and p is the pressure. The apparent line cross section increased at a linear rate of about 1×10^{-20} cm^2/μ(Hg) at 40 keV. Since studies extended only from 5 μ(Hg) to 25 μ(Hg), the maximum variation we could observe was only about 5%. Run-to-run reproducibility was no better than this, thus, while precise form of the pressure relationship may be in some doubt, the existence of the pressure dependence is not in doubt. Presumably the pressure dependence is due to cascade from higher $n\,^1P$ levels whose population is pressure sensitive since they optically connect to the ground state and are subject to imprisonment of resonance radiation.

Figure 1 displays the measured line cross sections. Cross sections for populating the $n\,^1S$ levels are displayed in Fig. 2. Branching ratios were determined, using the transition probabilities tabulated by Gabriel and Heddle.[3] Cascade from higher levels has been neglected.

No theoretical work is available with which to compare these cross sections but Van Eck et al.[4] obtained cross sections experimentally for the $4\,^1S$ and $5\,^1S$ levels in an energy range which overlaps ours. Their measurements are also displayed in Fig. 2. Their values appear lower than ours. Previous results[2] at 200 keV are shown and also seem low if our present measurements were extrapolated to the higher energy. The possibility that the 200-keV points are low has been pointed out by Šternberg and Tomaš.[5] We offer no explanation for such a discrepancy.

The cross sections at given energies were plotted as log-log graphs versus the square root of the term value expressed in Rydberg units. Above 30 keV, the slopes of a straight line connecting the points were close to 3, indicating $\sigma \propto (n^*)^{-3}$ where n^* is the effective principal quantum number. Gabriel and Heddle[3] have shown the expected n^{*-3} dependence for electron excitation of helium.

IV. EXCITATION OF THE $3\,^1P \rightarrow 2\,^1S$ ($\lambda5015$ Å) LINE

The apparent cross section for this line is greatly amplified by imprisonment of resonance radiation. Phelps[6] has treated the imprisonment problem rather completely, and Gabriel and Heddle have applied his analysis to this line (excited by electron bombardment)
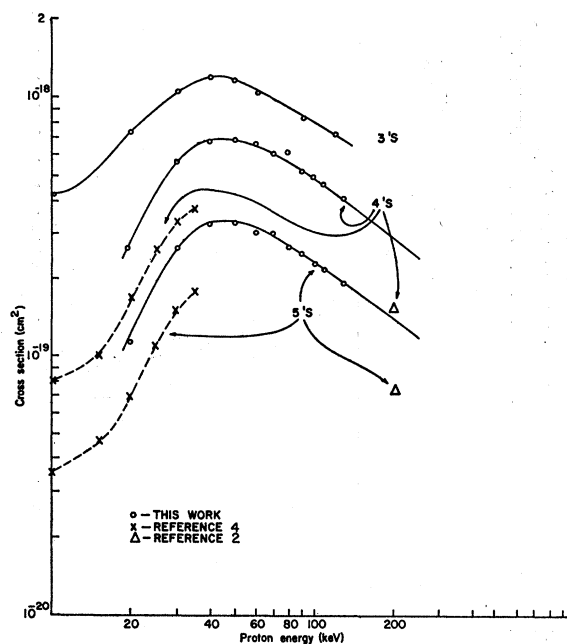

FIG. 2. Cross sections for populating $n\,^1S$ levels for $n=3$, 4 and 5.

to obtain the absolute $3\,^1P$ excitation. It can be shown that to a good approximation $\sigma_3\,^1P = \sigma_a[1 + 42.7g(\rho)]$ where σ_a is the apparent cross section for the $3\,^1P \rightarrow 2\,^1S$ line at a given pressure, $g(\rho)$ is a determined function of the pressure p and of the effective chamber radius ρ for resonance radiation (neglecting cascade from higher levels). By plotting trial $\sigma_3\,^1P$ from the above equation against ρ as a variable for various pressures at constant energy (in our case, 90 keV was chosen), one finds that value ρ_0 of the effective chamber radius necessary to yield a consistent value of $\sigma_3\,^1P$. The results of such a determination are shown in Fig. 3. Our chamber "radius" ρ_0 seems to be about 0.6 cm. This is much smaller than the geometrical radius (about 1 in.), presumably because the narrow spectrometer slit ($\frac{1}{16}$ in.) acts as the field stop, limiting the amount of resonance radiation accepted by the system. ρ_0 may be less well known than the triple intersection in Fig. 3 would lead one to believe. Our data fix ρ_0 at 0.6±0.1 cm.

Using 0.6 cm for ρ, we calculated the $\sigma_3\,^1P$ excitation function shown in Fig. 4. The peak appears to lie near 130 keV. Bell's theoretical values[7] (curve without experimental points) seem in agreement with our results, especially considering how sensitive $3\,^1P$ is to the assumed value of ρ_0.

At this point perhaps it would be of interest to compare the excitation by H$^+$ impact with electron impact. Extrapolating our present results to 200 keV will allow us to compare H$^+$ excitation with 108-eV electron excitation.[3] This is a comparison of excitation of the

[3] A. H. Gabriel and W. O. Heddle, Proc. Roy. Soc. (London) A258, 124 (1960).
[4] J. Van Eck, F. de Heer, and J. Kistemaker, Physica 28, 1184 (1962).
[5] Z. Šternberg and P. Tomaš, Phys. Rev. 124, 810 (1961).
[6] A. V. Phelps, Phys. Rev. 110, 1362 (1958).

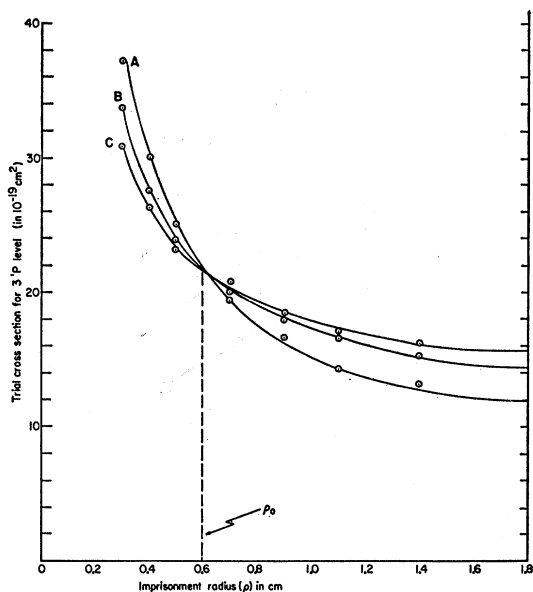[7] R. G. Bell, Proc. Phys. Soc. (London) 78, 903 (1961).

FIG. 3. Determination of the effective chamber radius for the imprisonment of resonance radiation $3\,^1P \rightarrow 1\,^1S$. Curves A, B, and C are trial $3\,^1P$ cross sections versus trial imprisonment radii at 10, 18.5, and 25 μ pressure, respectively.

FIG. 5. Cross section for the production of He II $(4 \rightarrow 3)$ radiation along with estimates of the population of the $n=4$ level of He^+. Theory estimate includes both charge transfer and simultaneous ionization and excitation mechanisms (from Mapleton, Refs. 8 and 9).

two particles at the same velocity. It appears that H^+ impact is one-half as effective as electron impact in exciting the $3\,^1P$ state. At this velocity the excitation is fairly near maximum in both cases. On the other hand, our present data on ^1S excitation would indicate that H^+ impact is about twice as effective in exciting ^1S states than is electron impact. However, the experimental uncertainties are large.

V. EXCITATION OF THE He_{II} $(4 \rightarrow 3)$ $(\lambda 4686\ \text{Å})$ LINE

The excitation function for the He II $(4 \rightarrow 3)$ $(\lambda 4686\ \text{Å})$ line is shown in Fig. 5. This radiation results
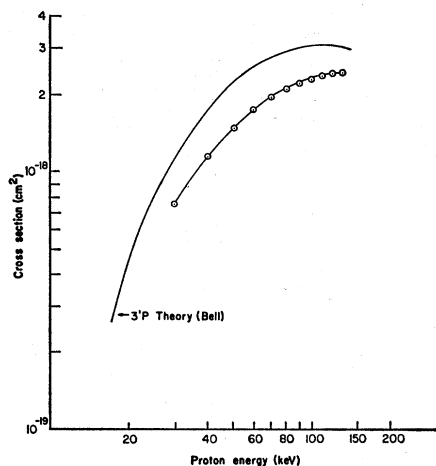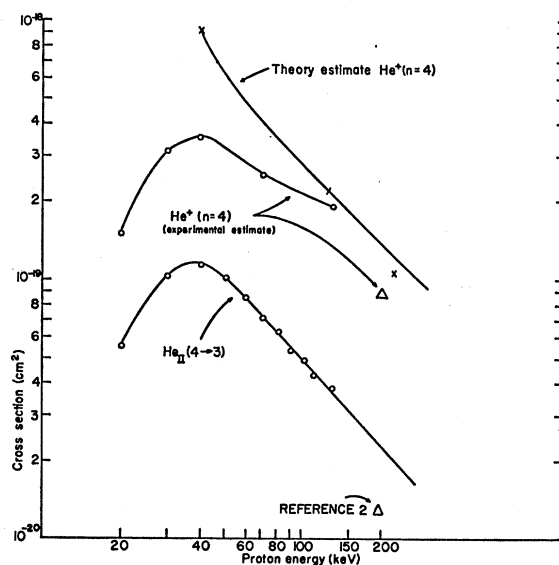
from the decay of the excited He^+ ion. Two mechanisms are competing here. Charge transfer is dominant at the lower energies while simultaneous ionization and excitation becomes dominant at the higher energies. The maximum cross section occurs at about 40 keV. At this energy, charge transfer is most probably dominant. The population of the $n=4$ level of He^+ can be estimated by using Mapleton's theoretical work (Born approximation) on charge transfer[8] and simultaneous ionization and excitation[9] in helium to obtain cross-section ratios for the various angular momentum states which can be placed in the formula used by Hughes and Weaver[10] to estimate population of the $n=4$ He^+ level by electron impact. Unfortunately, Mapleton's charge transfer work includes only the excitation to the $n=2$ He^+ level and his ionization work includes excitation
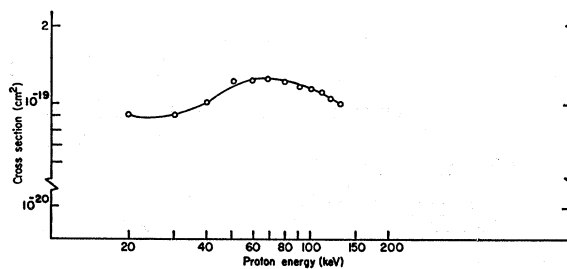

FIG. 4. Cross sections for populating the $3\,^1P$ level in comparison with the calculations of Bell (Ref. 7).

FIG. 6. Excitation function of the $4\,^1D \rightarrow 2\,^1P$ radiation at 4 μ pressure.

[8] R. A. Mapleton, Phys. Rev. **122**, 528 (1961).
[9] R. A. Mapleton, Phys. Rev. **109**, 1166 (1958).
[10] R. H. Hughes and L. D. Weaver, Phys. Rev. **132**, 710 (1963).

only up to the $n=3$ He$^+$ level. We used an n^{-3} law in extrapolating to $n=4$. Also shown in Fig. 5 are our results in transforming the line cross sections into $n=4$ cross sections.

It would seem that fair agreement is being reached at the higher energies where the Born approximation is expected to hold. Both estimates are rough, however.

VI. EXCITATION OF THE $4\,^1D \to 2\,^1P$ ($\lambda 4922$Å) LINE

This line is pressure-dependent with the apparent cross section increasing with pressure. Population mechanisms include collisional transfer, $n\,^1P \to n\,^1F$ with subsequent $n\,^1F$ ($n>4$) cascade to $4\,^1D$, and also $4\,^1P \to 4\,^1D$ collisional transfer. Figure 6 is an excitation curve to this line at $4\,\mu$ pressure.

Validity of the Concept of the Core Polarization Effect in Hyperfine Structure

E. A. BURKE

St. John's University, Jamaica, New York

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The core polarization effect in hyperfine structure is discussed by a semiempirical evaluation of 16 recently calculated values of the Fermi contact term for the ground state of lithium. The analysis proceeds by an investigation of the manner in which the various wave functions approximate eigenfunctions of S^2, in conjunction with an examination of the one-electron orbitals employed. The concept of core polarization by non-s electrons is shown to be valid, while if the polarizing electron is an s electron, no definite conclusion concerning core polarization can be made. Finally, it is proposed that for all cases of a single polarizing electron, the following many-electron, approximate unrestricted Hartree-Fock wave function may be used:

$$\phi = A_p\{B_1[\prod_i U_{n(i)l(i)}\alpha U_{n'(i)l(i)}\beta]U_{N,L}\alpha + B_2[U_{N,L}\alpha \prod_i U_{n(i)l(i)}\beta U_{n'(i)l(i)}\alpha]\},$$

where N, L are the quantum numbers of the polarizing electron and $B_1 = -B_2$ if $L=0$. Two tests of the validity of this wave-function approximation are proposed.

INTRODUCTION

RECENTLY, many approximate wave functions of the ground state of lithium have been reported.[1-9] For all of these, the Fermi[10] contact term in hyperfine structure has also been calculated. The calculation of the contact term is of interest since it has been predicted by Pratt[11] that one should expect a contribution to the contact term from the core, $1s$ electrons in an open-shell configuration due to the spin polarization of the core, in this case by the outer, unpaired $2s$ electron. This effect is called the core polarization effect and has been applied[12] to cases for which the polarizing electron is not an s electron. The hyperfine fields thereby calculated are at least of the same order as those observed experimentally and have not been predicted by any other theory.

[1] J. B. Martin and A. W. Weiss, J. Chem. Phys. **39**, 1618 (1963).

[2] R. P. Hurst, J. D. Gray, G. H. Brigman, and F. A. Matsen, Mol. Phys. **1**, 189 (1958). Hyperfine structure calculations are reported in Ref. 1.

[3] Lester M. Sachs, Phys. Rev. **117**, 1504 (1960).

[4] This result was reported as a private communication from J. N. Silverman in Ref. 1.

[5] K. F. Berggren and R. F. Wood, Phys. Rev. **130**, 198 (1963).

[6] J. Kerwin and E. A. Burke, J. Chem. Phys. **36**, 2987 (1962).

[7] Z. W. Ritter, R. Pauncz, and K. Appel, J. Chem. Phys. **35**, 571 (1961). Hyperfine structure calculations are reported in Ref. 1.

[8] E. A. Burke, Phys. Rev. **130**, 1871 (1963).

[9] R. K. Nesbet, Phys. Rev. **118**, 681 (1960).

[10] E. Fermi, Z. Physik, **60**, 320 (1930).

[11] G. W. Pratt, Jr., Phys. Rev. **102**, 1303 (1956).

[12] R. E. Watson and A. J. Freeman, Phys. Rev. **123**, 2027 (1961).

The lithium atom in its ground state represents the simplest test of the validity of the core polarization hypothesis. One expects for hyperfine structure a large contribution from the $2s$ valence orbitals and a smaller contribution from the core orbitals provided that the latter orbitals are represented by an open-shell configuration.[11] Recent hyperfine structure calculations,[1-9] however, show several inconsistencies. In the first place, there seems to be little correlation between the "goodness" (as determined by calculated total energy) of a wave function and the "goodness" (as determined by deviation of experimental and calculated values) of the contact term. Of greater significance are the results using nearly exact wave functions which show that the value of the contact term with and without open-shell orbitals changes only slightly. This result has been interpreted[5] as casting serious doubt on the physically simple and highly useful concept of core polarization.

It is the purpose of this paper to investigate these inconsistencies. For the energy versus contact term correlation it will be shown that the energy value (known to be a poor criterion of "goodness") must be considered in conjunction with the structure of the wave function before any comparisons with hyperfine structure calculations can be made. By this analysis one is able to show a correlation between the ground state energy and the contact term. Furthermore, one may then predict the best form of a wave function for more complicated physical situations. On the question of core