CALIBRATION OF THE H\textsc{ii} REGION ABUNDANCE SEQUENCE
AND ABUNDANCES IN SEYFERT GALAXIES

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A thesis submitted for the degree of
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To my parents, whose love, support, and encouragement have made this work possible.
Contribution of Candidate

This thesis consists of five papers, each of which has either been published, or is currently in press, or has been submitted for publication. The contributions of the candidate to the content of these papers is described below. All sections not specifically mentioned are the work of the candidate alone.

**Paper 1** The description of the radiative transfer in section IIIb was largely taken from Binette (1982, Ph.D thesis, Australian National University). Dr. Dopita made constructive suggestions regarding the content of this paper.

**Paper 2** The theoretical fit to the observed emission-line sequence and the recalibration of the abundance diagnostics were the work of the candidate alone, subject to suggestions by Dr. Dopita. Both the candidate and Dr. Dopita contributed equally to the remaining content of the paper.

**Paper 3** The paper is the work of the candidate alone.

**Paper 4** The observations were carried out by the candidate and Dr. Dopita. Dr. Dopita made constructive suggestions with respect to the text of the paper.

**Paper 5** The observations were carried out by the candidate and Dr. Dopita. The candidate and Dr. Dopita both contributed to the modeling of the high-excitation gas.

Ian N. Evans
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Being before the time, the astronomers are to be killed without respite;
and being behind the time, they are to be slain without reprieve

Shu Ching, before 250 B.C.
ABSTRACT

An extensive, homogeneous grid of theoretical photoionization models with conditions appropriate to observed H II regions is computed. This grid is used to develop a comprehensive set of theoretical diagnostic diagrams for H II regions which employ ratios of prominent emission lines to determine the ionization parameter within the nebula, and the ionization temperature of its exciting star(s). It is also possible to estimate the element-averaged metallicity in the nebula and stars from these diagnostics. Theoretical loci for H II regions on the principal excitation diagrams of Baldwin, Phillips, and Terlevich (1981) are constructed and confirm that the theoretical models overlie the observed distribution of H II regions on these diagrams. Comparison of current observational data with the theoretical models on these and other diagrams implies the existence of a correlation between element-averaged metallicity and mean ionization parameter. The data also suggest that the ionization temperature of the exciting star(s) in the ionizing OB associations of H II regions is approximately constant and independent of metallicity and ionization parameter for the range of conditions considered here.

A multiline fit to the observed emission-line spectral sequence of extragalactic H II regions is generated. It is possible to produce an excellent fit between the (rather narrow) emission-line ratio sequences that are observed and the theoretical sequences, provided that the average ionization parameter is strongly coupled with metallicity, and provided that nitrogen is a product of secondary nucleosynthesis. Using this theoretical sequence of H II region models, the semiempirical abundance diagnostic ratios used by Alloin et al. (1979), Pagel et al. (1979), and McCall, Rybski, and Shields (1985)
are recalibrated and new abundance diagnostic ratios formulated. The correlation between ionization parameter and abundance is found to have the effect of changing the previous abundance calibration toward lower abundances, particularly for the most metal-rich H II regions. A new technique to derive abundances from H II region spectra is suggested.

Oxygen and other heavy element abundances in a selection of well observed H II regions in M101 are determined from the theoretical abundance sequence calibration. Comparison of abundances derived from the sequence with abundances derived from "exact" photoionization modeling demonstrate that the accuracy with which H II region abundances may be derived from the sequence is ~ 0.15 dex. The data are employed to measure radial abundance gradients and heavy element yields for oxygen, nitrogen, and sulfur in M101. The combined abundance gradient and heavy element yield data suggest that the production of elements by massive stars (oxygen, neon) is enhanced in the inner regions of the disk of M101, whilst the production of heavy elements (S, Ar, Ca, Fe) by low and intermediate mass stars is enhanced in the outer disk. A simple model for galaxy disk formation is suggested which is at least qualitatively capable of explaining these observations.

The theoretical abundance sequence calibration is also applied to optical spectrophotometry of 23 H II regions located in the inner disk regions of two Seyfert 1 and two Seyfert 2 galaxies, including the prototype Seyfert 2, NGC 1068, in order to determine oxygen, nitrogen, and sulfur abundances. The mean oxygen abundance derived for each galaxy is shown to range between solar abundance and twice solar abundance. There is no evidence for abnormal N/O or S/O abundance ratios in any of the H II regions observed.
The observations suggest that the abundances derived for the H\textsc{ii} regions may be adopted as nuclear abundances and employed to constrain theoretical models of the Seyfert nucleus. The observations then place limits on the influence which the active nucleus can have on chemical enrichment of the local interstellar medium.

Observations of the candidate near-nuclear H\textsc{ii} regions in the disk of NGC 1068 also indicate the presence of high-excitation extra-nuclear emission. The optical spectra appear to be very similar to ordinary H\textsc{ii} region spectra with the addition of strong lines of [Ne\textsc{v}]\(\lambda\lambda3346,3426\) and He\textsc{ii}\(\lambda4686\). This is interpreted as the superposition of an H\textsc{ii} region spectrum with the high-excitation emission, and theoretical nebular models are presented which suggest that the high-excitation gas is most likely photoionized by a power-law spectrum, probably from the nearby Seyfert nucleus.
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1

INTRODUCTION

An outstanding goal in the study of active galactic nuclei is the construction of accurate photoionization models which can be employed to derive the shape of the ionizing spectrum emitted by the central photon source, and hence deduce constraints on the physical conditions in the nucleus and the physical processes giving rise to the nuclear emission. One approach to this problem is to combine observations with conceptual theoretical models for the geometrical- and density-structure of, and physical processes occuring in, the nucleus in order to constrain photoionization and shock model parameters. Such models are then computed in an attempt to establish the shape of the input ionizing spectrum, which, provided that the observations and conceptual models furnish sufficient constraints, should (hopefully) be the only remaining variable parameter. To apply this procedure, one first considers only the narrow-line region, and then proceeds inward to the broad-line region after having established the input ionizing spectrum to the narrow-line region. Finally the ionizing spectrum emitted by the central source may be deduced. A multistage process such as this ought to yield a realistic and self-consistent model for the active nucleus.

To minimize the number of free parameters in the models it is necessary in the first instance to have accurate estimates of the elemental abundances in the nuclear region. Since the measurement of abundances directly from observations of the active nucleus itself is fraught with difficulties arising from unknown physical processes and conditions, and uncertain reddening corrections, the abundances employed in the models are frequently assumed a priori to be solar or approximately so. Such unjustified assumptions are a cause for concern, particularly in the light of evidence which suggests that in some
cases abundances may be considerably higher than solar (e.g., Ford et al. 1985; Wills, Netzer, and Wills 1985). Possibly the most accurate method of deriving nuclear abundances is from studies of near-nuclear H II regions and extrapolation of radial abundance gradients into the nucleus. The observational data indicate that abundances are high enough that methods which rely on estimating the electron temperature in the gas from measurements of the intensity of weak auroral lines such as [O III] \( \lambda 4363 \) to compute abundances (e.g., the semiempirical ionization correction factor technique of Peimbert and Costero 1969) cannot be employed. Instead, a calibration of H II region abundance versus some intensity ratio involving only prominent emission lines is required. Such calibrations have been performed by Pagel et al. (1979) and McCall (1982), but photoionization models employing recent atomic data (e.g., Mendoza 1983) and including additional atomic processes such as low-temperature dielectronic recombination (Nussbaumer and Storey 1983) are incompatible with the earlier calibrations except at low metal abundances. A recalibration of the H II region abundance sequence using theoretical photoionization models and state-of-the-art atomic data is clearly required.

The aim of this dissertation is to provide an modern calibration of the H II region abundance sequence from theoretical photoionization modeling, and to apply this calibration to beginning studies of abundances in near-nuclear H II regions in Seyfert galaxies. It is anticipated that further studies of the narrow- and broad-line nuclear regions can be built upon these foundations, as suggested above, in order to derive self-consistent models for active galactic nuclei.
This thesis is organized into five papers, each of which has either been published, or is currently in press, or has been submitted for publication. The first paper applies systematic modeling techniques employing the latest atomic data to develop a very large set of homogeneous photoionization models for H II regions, covering a wide range of physical conditions. The models are used to construct theoretical diagnostic diagrams from which the ionization parameter and element-averaged metallicity of an observed H II region, and also the ionization temperature of the exciting star or stars, may be determined. Correlations found between the fundamental model parameters in real H II regions are studied in greater detail in the second paper, which attempts to fit simultaneously all the important emission-line ratios observed in extragalactic H II regions. With the aid of additional photoionization models, a new absolute calibration of the H II region abundance sequence is constructed and new abundance sequencing ratios which may be useful from an observational viewpoint are suggested. In the third paper, the abundance sequence calibration is employed to derive oxygen abundances for a number of H II regions in the spiral galaxy M101. Theoretical photoionization models are computed for a subset of the H II regions in order to assess the accuracy with which oxygen abundances can be derived from the abundance sequence calibration. These data are combined to derive the O, N, S, Ne, and Ar abundance gradients in M101, and the implications of these results for galaxy evolution and chemical enrichment models are considered. Oxygen, nitrogen, and sulfur abundances are derived for 23 near-nuclear H II regions in a sample of two Seyfert 1 and two Seyfert 2 galaxies in the fourth paper. The oxygen abundance gradients in the inner regions of NGC 1068 and other Seyfert and active galaxies are considered in the light of theoretical models for disk evolution (e.g., Su and Simkin 1980) which have been proposed for
Seyfert galaxies on the basis of morphological features. The implications of the data for theoretical models of Seyfert nuclei and the influence which the active nucleus can have on the chemical enrichment of the local interstellar medium are discussed. Finally, the fifth paper presents spectrophotometry which demonstrates the existence of high-excitation extra-nuclear emission in NGC 1068. Theoretical nebular models for the data suggest that the observed emission is a superposition of an ordinary H II region spectrum and emission from a region photoionized by the power-law spectrum emanating from the nearby Seyfert nucleus.
REFERENCES


THEORETICAL MODELS FOR H II REGIONS.

I. DIAGNOSTIC DIAGRAMS

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ABSTRACT

We have computed an extensive, homogeneous grid of theoretical photoionization models with conditions appropriate to observed H II regions. This grid has been used to develop a comprehensive set of theoretical diagnostic diagrams for H II regions, which employ ratios of prominent emission lines to determine the ionization parameter within the nebula, and the ionization temperature of its exciting star(s). It is also possible to estimate the element-averaged metallicity in the nebula and stars from these diagnostics.

We construct theoretical loci for H II regions on the principal excitation diagrams of Baldwin, Phillips, and Terlevich (1981) and confirm that the theoretical models overlie the observed distribution of H II regions on these diagrams. Comparison of current observational data with the theoretical models on these and other diagrams implies the existence of a correlation between element-averaged metallicity and mean ionization parameter. The data also suggest that the ionization temperature of the exciting star(s) in the ionizing OB associations of H II regions is approximately constant and independent of metallicity and ionization parameter for the range of conditions considered here.

Subject headings: nebulae: abundances — nebulae: H II regions
I. INTRODUCTION

Improvements in observational technique during the past decade have resulted in a significant expansion of the available spectrophotometric data concerning H II regions. Interpretation of such data in terms of elemental abundances is of fundamental importance to our understanding of the chemical evolution of galaxies (see, e.g., Talbot and Arnett 1975; Jensen, Strom, and Strom 1976; Alloin et al. 1979), whilst an understanding of the characteristics of the ionizing stars is useful in testing theories of star formation, and in evolution studies of O, B stars (Shields and Tinsley 1976).

Until relatively recently, determinations of elemental abundances in H II regions have employed the semiempirical ionization correction factor technique first applied to galactic H II regions by Peimbert and Costero (1969). In this approach the ionization corrections for various observable ions are estimated from a comparison of the observed O$^0$/O$^+$/O$^{++}$ ratios and the ionization potentials. In normal O stars, the atmospheric blanketing above the He II ionization potential is so heavy that negligibly few photons with energy above 54.4 eV find their way into the H II region. Thus all helium is either in the ionization stages He I or He II, and the oxygen (which is the major coolant) is in the ionization stages O I, O II, or O III. In the transition zone at the ionization front, the O and H ionization are coupled by the charge exchange process H$^+$ + O$^0$ $\rightarrow$ H$^0$ + O$^+$, and, because the O II ionization potential lies above the He I ionization potential, the oxygen is entirely in the form O$^+$ in the zone where hydrogen is ionized and helium is neutral. To derive an accurate oxygen abundance, the temperature of the O$^{++}$ zone must be estimated from the temperature-sensitive $[\text{O III}]\lambda4363/\lambda5007$ ratio, and, provided that the density is known (usually obtained from the
[S ii] $\lambda 6716/\lambda 6731$ ratio), the temperature in the O II zone can be extracted from the temperature- and density-sensitive [O ii] $\lambda\lambda 3726, 3729/\lambda\lambda 7320, 7330$ ratio. If, owing to systematic stratification or the presence of dense clumps in which the ionization state of the gas is depressed or in which collisional de-excitation occurs, the temperature in an H II region is nonuniform, corrections need to be applied to the temperature derived from forbidden-line ratios. They are biased toward regions of higher than average temperature. Peimbert (1967) quantified this effect in terms of the relative variance, $t^2 = \langle (T - T_0)^2 \rangle / T_0^2$, where $T_0$ is the emission measure-weighted electron temperature. As $t^2$ increases, so does the derived value of the oxygen abundance. A value for $t^2$ of 0.035 typically increases the "observed" abundance of oxygen by 0.2 dex. Observational estimates of $t^2$ are obtained by comparison of forbidden-line temperatures with recombination-line temperatures or gas kinetic temperatures. Having estimated the total oxygen abundance and the fractional abundance in each ionization stage, the abundance of the other elements is estimated from the fraction of each observable stage of ionization that is coextensive with the various ionization zones of oxygen. This technique has been applied with success to the determination of H II region abundances in the LMC and SMC by Dufour (1975, 1977).

Although measurement of the temperature-sensitive line ratio [O III] $\lambda 4363/\lambda 5007$ is possible in the case of low metal abundance H II regions which may be observed in the outer regions of late-type spiral and irregular galaxies, the [O III] $\lambda 4363$ line is far too weak to be observed in H II regions with high metal abundances common toward the nuclei of early-type spirals and also in Seyfert galaxies (Evans and Dopita 1986). Accordingly, considerable effort has been directed in recent years toward calibrating the abundances of H II regions on the basis of ratios of prominent emission lines.
common to all H II regions, following the suggestion of Searle (1971) that radial abundance gradients are responsible for the observed gradients in the line ratios [O III] $\lambda\lambda$ 4959, 5007/$\beta$ and [N II] $\lambda\lambda$ 6548, 6584/$\alpha$ measured for giant H II regions in late-type spirals. Pagel et al. (1979) proposed, on empirical grounds, a calibration of oxygen abundance using the line ratio ([O II] $\lambda$ 3727 + [O III] $\lambda\lambda$ 4959, 5007)/$\beta$ and have extended this work (Pagel, Edmunds, and Smith 1980; Edmunds and Pagel 1984) following theoretical calculations of Dufour et al. (1980). Binette (1982) has studied the effect of taking a weighted sum of the [O II] $\lambda$ 3727 and [O III] $\lambda\lambda$ 4959, 5007 lines (([O II] $\lambda$ 3727 + $\alpha$ [O III] $\lambda\lambda$ 4959, 5007)/$\beta$ in order to minimize the dispersion in the relationship caused by variations in the ionization temperature of the central star(s), $T_{\text{ion}}$, and finds from theoretical photoionization models that the dispersion is minimized for the value $\alpha = 0.27$. The calibration of $\text{[O/H]}$ versus ([O II] $\lambda$ 3727 + [O III] $\lambda\lambda$ 4959, 5007)/$\beta$ has also been considered in detail by McCall (1982; see also McCall, Rybski, and Shields 1985), who has employed a large, homogeneous observational data set and photoionization modeling in order to recalibrate the sequence. An alternative calibration has been proposed by Alloin et al. (1979), who suggested using the ratio [O III] $\lambda\lambda$ 4959, 5007/[N II] $\lambda\lambda$ 6548, 6584 in order to determine the electron temperature when the [O III] $\lambda$ 4363 line is not observable. The accuracy with which abundances can be estimated using the empirical calibrations of both Alloin et al. (1979) and Pagel et al. (1979) has been studied by Stasińska et al. (1981), who also compare the relative merits of the two approaches.

In this paper, we apply systematic modeling techniques employing the latest atomic data to compute a comprehensive grid of model H II regions, covering a wide range of physical conditions, comprising a total of 211 independent models. We use the models to construct theoretical diagnostic
diagrams for H II regions and show that these diagrams can be employed to
determine the metallicity and ionization parameter of an observed H II re-
gion, and also the ionization temperature of the exciting star or stars. As a
check on the modeling procedure, we also generate theoretical loci for H II
regions on the three principal excitation diagrams of Baldwin, Phillips, and
Terlevich (1981, hereafter BPT) and demonstrate that the theoretical mod-
els agree with the observed positions of H II regions on these diagrams. In a
later paper (Dopita and Evans 1986, Paper II) we shall employ our models
to construct theoretical abundance calibrations and compare these with the
empirical calibrations of Pagel et al. (1979) and Alloin et al. (1979).

II. THE OBSERVATIONAL DATA BASE

In order to compare our model calculations with published spectropho-
tometry of H II regions, we have gathered together from the literature a
substantial set of observational data covering objects with a wide range of
observed line strengths and line ratios, and hence (presumably) covering a
range of physical conditions. To minimize the effects of possible systematic
differences between observations reported separately, it is preferable to use,
where possible, large sets of internally consistent data. For this reason, we
have employed the set of H II region data referred to by BPT, augmented
by the spectrophotometry of McCall (1982). To ensure that all observations
were treated equally, line intensity ratios were dereddened using the redden-
ing law of Schild (1977) to determine line flux ratios, and in each case the
correction was applied using an assumed mean nebular electron temperature
of 8000 K. Generally, the data referred to above cover most of the visible
spectrum, extending from [O II] \( \lambda 3727 \) to at least [S II] \( \lambda \lambda 6716,6731 \). In prin-
ciple, therefore, it is possible to model the observed spectrum of each object
individually to deduce absolute abundances of the elements N, O, Ne, and S, and also to determine values for the ionization parameter and ionization temperature, and this has been done in some cases (see, e.g., Shields and Searle 1978; Pagel et al. 1979; Dufour, Shields, and Talbot 1982). However, for those people without access to a photoionization modeling code, this is not a viable option. What is needed are diagnostic diagrams and generalized techniques whereby such data can be analyzed with sufficient accuracy. Diagnostic diagrams are also of general interest because they often reveal correlations between quantities and provide insight into physical conditions and processes which do not become manifest from single-observation modeling. A set of such diagnostic diagrams, applicable to observations of supernova remnants, has recently been published by Dopita et al. (1984). Since the same modeling code was used, a direct comparison of SNR and H II region abundances now becomes possible.

In the following sections we develop a number of diagnostic diagrams which may be employed to deduce the ionization parameter, ionization temperature, and element-averaged metallicity in the H II regions. The use of these diagnostics enables some conclusions to be drawn which are of general applicability to H II regions.

III. THE THEORETICAL MODELS

Our general-purpose modeling code MAPPINGS was used to compute all of the H II region models described below. This code is intended for use in modeling not only H II regions but also shocks and galactic nuclei ionized by "nonthermal" continua, both in the steady-state and in the time-dependent ionization cases. Except for the inclusion of more recent atomic
data (see below), the code used for these computations is identical to an earlier version described in detail by Binette (1982). The major features of the code (specifically the determination of thermal balance, recombination and ionization rates, the solution of the time-dependent ionization balance, and radiation transfer) are also discussed by Binette, Dopita, and Tuohy (1985) and will not be repeated in detail here, although we briefly review our treatment of radiative transfer in § IIIb to aid comparison with the recent work of Rubin (1985).

a) New Atomic Data

Radiative transition rates and collision strengths employed in calculating forbidden-line intensities and associated cooling are taken from a recent paper by Mendoza (1983) and references cited therein. Each of the ions O i, O ii, O iii, N i, N ii, S ii, S iii, Ne iii, Ne iv, Ne v, Ar iii, Ar iv, Ar v, Cl ii, Cl iii, and Cl iv is treated as a five-level system and the forbidden-line intensities and cooling are computed by solving for statistical equilibrium between the metastable states. Variations of collision strength with temperature are included for O i and N i.

In addition to radiative and dielectronic recombination at high electron temperatures for the heavy elements calculated using the formulation of Aldrovandi and Péquignot (1973, 1976), we now also treat dielectronic recombination at low electron temperatures for ions of C, N, and O according to the prescription of Nussbaumer and Storey (1983). This contribution to the total recombination rate becomes important under nebular conditions when the mean kinetic energy of the free electron gas is much lower than the
ionization energy of the emitting ions. Such conditions can occur in high-metallicity H II regions ionized by low ionization temperature stars because the efficiency of collisional cooling and the relative lack of high-energy UV ionizing photons both conspire to keep the electron temperature low throughout the line-emitting region. For example, at 3000 K the low-temperature dielectronic recombination coefficient for the ion C II is roughly twice the radiative recombination coefficient and so will have a noticeable effect on the calculated line strengths.

Twenty-four charge-transfer reactions with H or He have been included in the computations. The rates result mainly from the compilations of Butler and Dalgarno (1980) and Butler, Heil, and Dalgarno (1980), supplemented by the data of Field and Steigman (1971), Butler and Dalgarno (1979), and Dalgarno, Heil, and Butler (1981). The specific charge exchange reactions included in the code are described in detail by Binette (1982).

b) Radiative Transfer

The transfer of ionizing ultraviolet and soft X-ray radiation is computed by dividing the energy spectrum into 230 contiguous bins covering the range from 7.6 eV to 5 keV. Edges of the bins coincide with all the photoionization thresholds of the ionic species treated by the modeling code. Additional bins are placed just above the ionization thresholds of H, He, C, N, O, Ne, and S, and where strong UV lines are expected. At any radius \( r \) in the nebula, the mean intensity of the direct radiation from the ionizing source in energy bin \( k \) is given by

\[
J_k(r) = w(r) I_k(R_*) \exp(-\tau_k),
\]
where \( w(r) \) is the geometrical dilution factor for the radius \( r \), \( I_k(R_\odot) \) is the specific intensity of radiation in the energy bin \( k \) evaluated at the surface of the source, and \( \tau_k \) is the integrated optical depth from the source to the radius \( r \) in energy bin \( k \). For each space step and energy bin, the continuous and (in the appropriate energy bins) line opacities for every ionic species are calculated from the photoionization cross section for that species. The opacity of the heavy elements is included since they become important absorbers at X-ray energies and may significantly alter the ionization balance in H\ II regions (as emphasized by Rubin 1985).

In calculating the contribution of the diffuse radiation field arising from photons generated in the plasma itself, we consider photons resulting from recombinations to the ground state of all ionic species (and also to the \( n = 2 \) level of He\ II) if their energies exceeded 7.6 eV, secondary photons resulting from line emission of resonance and intercombination lines, collisionally excited resonance and intercombination lines with photon energies greater than 7.6 eV, free-free (bremsstrahlung) emission, and two-photon emission for the species H\ I, He\ I, and He\ II. To simplify calculations the spatial integration of the continuous component of the diffuse field was calculated using the "outward only" approximation, unlike Rubin (1985), who employed an iterative technique to "exactly" solve for the diffuse field emission, but this approximation should result in an error of only a few percent relative to an exact calculation, with a considerable saving in computation time. The ultraviolet resonance lines, on the other hand, are the object of a separate solution to the radiative-transfer equation, and their intensities are kept in a distinct source vector. The main effect of the resonance scattering of line photons is to decrease their penetrating power, and this is taken into account by assuming that the mean travel length of a resonant photon across a slab
is increased by a factor which is the inverse of the mean escape probability from that slab, and consequently that the probability of absorption inside the slab is increased by the same factor. The mean escape probability for a photon is derived from the escape probability formulation of Capriotti (1965; see also Netzer 1975).

For our models, the spatial integration was commenced at the outer edge of the empty zone (see § IIIc) and proceeded outward until $N_{H^+}/N_H < 1\%$. The integration was carried out in steps of 0.01 in the mean optical depth of the ionizing radiation, in order to ensure that fine detail in the ionization structure (particularly near the important metal edges in the nebula) was not lost through too coarse a gridding. We do not consider the presence of dust in the nebula, nor its effect in absorbing the radiation field, although earlier papers (Sarazin 1976, 1977; Dufour et al. 1980; Stasińska 1980) suggest that dusty models would resemble dust-free models of lower $T_{\text{ion}}$.

c) The Models

We modeled the H II regions as steady-state spherically symmetric nebulae with uniform density, unity filling factor, and an empty zone surrounding the ionizing photon source. In the case of giant extragalactic H II regions, the ionizing OB association is likely to consist of a distribution of stars with differing ionization temperatures, $T_{\text{ion}}$. Assuming that these stars cluster near the center of the H II region, it is possible to construct a composite ionizing spectrum using some initial mass function for the stars. In order to minimize the number of free parameters we replace the cluster by a single ionizing star of temperature $\langle T_{\text{ion}} \rangle$ yielding the cluster average photon density. The adopted ionization temperature will correspond to an effective
temperature, $T_{\text{eff}}$, close to $T_{\text{max}}$, the temperature of the hottest stars in the cluster, since, as shown by Searle (1971), the number of photons increases very rapidly with $T_{\text{max}}$ and consequently the energy distribution of the ionizing photons will depend mainly on $T_{\text{max}}$ rather than the slope of the initial mass function. Since the redistribution of flux across the metal edges in a stellar atmosphere is a function of metal abundance, it is important to be self-consistent in assuring that the metallicity in the stellar atmosphere matches the nebular value. This is emphasized by Balick and Sneden (1976; but see also Borsenberger and Stasińska 1982). Accordingly, we employ the $\log g = 4.0$ models of Hummer and Mihalas (1970) since these models cover a range of abundance which is adequate for our purpose. The stellar atmosphere fluxes were parameterized so as to be continuous functions of $T_{\text{ion}}$ and $Z$ in a manner similar to that of Shields and Searle (1978).

The choice of geometry and density behavior for the models was necessarily a compromise. Observations indicate that H II regions have rather low densities ($N_H \lesssim 10^3 \text{ cm}^{-3}$) and often have complicated geometrical structure. For many objects, density-sensitive line ratios indicate variations larger than a factor of 10 within the same object (Danks and Meaburn 1971; Danks and Manfroid 1976; Deharveng, Israel, and Maucherat 1976). Although it is possible to construct models with complicated geometries and density behavior that would apply to individual nebulae, the necessary spatial information is available for only a few objects. Furthermore, most of the data relating to many extragalactic H II regions consists only of the brightest emission lines from the core of each object. In general, it is more useful to reproduce only the broad characteristics of the geometry and spatial density distribution. For example, Stasińska (1980, 1982) computed a grid of models in which she assumed a simple two-zone spherical geometry with the outer zone 10 times
denser than the inner zone. This was intended to represent the particular case of H II regions on the edge of dense clouds where a systematic density gradient is observed between the star and the parent cloud (Tenorio-Tagle, Yorke, and Bodenheimer 1979). From inspection of Stasińska's models, it is apparent that the effect on the spectrum of using two zones is maximized when the outer zone is the main contributor to the total emission. This is because the inner low-emissivity zone has the single effect of increasing the geometrical dilution for the ionizing flux in the high-density zone, and therefore, replacing the inner zone by an empty zone of the same size would result in qualitatively the same spectrum whilst significantly reducing the total time required for computation. In our models, the number density of hydrogen atoms plus ions, $N_H$, in the outer zone was fixed at 10 cm$^{-3}$. The actual value chosen for $N_H$ is not critical, but should clearly be in the low-density limit since observations of the density-sensitive line ratio $[^{[S\,ii]}]_{\lambda 6716}/\lambda 6731$ indicate that the majority of H II regions are in or near this limit (McCall 1982). Provided that the total number density of atoms and ions (including helium and the heavy elements), $N$, remains in the low-density limit, the effect on the spectrum of changing $N$ by a factor $\lambda$ is equivalent to changing the mean ionization parameter $\overline{Q}(H)$ by a factor $1/\lambda$, and so models with densities differing from 10 cm$^{-3}$ can be found by scaling $\overline{Q}(H)$ accordingly.

We define the ionization parameter at any radius, $Q(H,r)$, by the expression

$$Q(H,r) = \frac{L_c}{4\pi r^2 N},$$

where $L_c$ is the number of photons that can ionize $H^0$ emitted per unit time from the central source, and $r$ is the radius at which the ionization parameter is calculated. The mean ionization parameter, $\overline{Q}(H)$, is defined
by $\bar{Q}(H) = Q(H, \bar{r})$, where the mean radius $\bar{r}$ is given by $\bar{r} = \frac{1}{2} (r_{\text{empty}} + R_2)$. The radius $R_2$ is the effective Strömgren radius of the nebula, including the effect of the empty zone, and can be found from the defining equation

$$L_C = \frac{4\pi}{3} R_2^3 N^2 \epsilon \alpha_B \left[ 1 + \left( \frac{r_{\text{empty}}}{R_1} \right)^3 \right]^{-1},$$

where $\epsilon$ is the volume filling factor (unity in our case), $\alpha_B$ is the case B recombination coefficient for hydrogen calculated at $T = 10^4$ K, and $R_1$ is the Strömgren radius of the nebula excluding the effect of the empty zone [$L_C = (4\pi/3) R_1^3 N^2 \epsilon \alpha_B$]. In our models we take $r_{\text{empty}} = \frac{1}{2} R_1$; such a choice has the advantage that the geometrical dilution of the ionizing flux at any radius in the nebula does not differ greatly from the “mean” geometrical dilution, and so $Q(H, r)$ is a relatively slowly varying function of $r$, and hence the choice of geometry does not critically affect the resulting spectrum. If, on the other hand, we had taken $r_{\text{empty}} = 0$, then density fluctuations and the geometrical distribution of the ionized gas near the central photon source would dominate, since $Q(H, r)$ is much larger at small radii and is changing rapidly there.

We can relate $\bar{Q}(H)$ to the commonly used ionization parameter, $U$, defined by

$$U = \left( N_H \epsilon^2 L_C \right)^{1/3},$$

according to the relationship

$$U \approx \left\{ 4\pi \bar{r}^2 \left[ 1 + Z(\text{He}) \right] N_H^2 \epsilon^2 \bar{Q}(H) \right\}^{1/3},$$

where $Z(\text{He})$ is the relative abundance of helium by number with respect to hydrogen, and we have assumed helium to be singly ionized. For $T_{\text{ion}} \gtrsim 40,000$ K, this approximation should not be in error by more than about 2%. 
To ensure that our diagnostic diagrams cover a sufficiently large range of physical conditions to be generally useful, we have developed five grids of models, each of which demonstrates a particular aspect of a diagnostic diagram. First, we have computed a "solar" grid, which illustrates in detail the effect of changing $\bar{Q}(H)$ and $T_{\text{ion}}$ on models with solar abundances. Five values of $\bar{Q}(H)$ are modeled for each of six values of $T_{\text{ion}}$ from 37,000 K to 56,000 K, giving a total of 30 models. We then have an "abundance" grid, which demonstrates the results of changing metal abundances for models with fixed $\bar{Q}(H)$ and $T_{\text{ion}}$. For this grid, the ratios of all the metal abundances are kept fixed at the solar value, and the absolute abundances are changed in both the nebula and its exciting stars. Whenever abundances are changed, the H/He ratio is kept constant at its solar value. Six values of the metal abundance, from $\frac{1}{4}$ solar to 2 times solar, are calculated for each of three values of $\bar{Q}(H)$ and three values of $T_{\text{ion}}$ (54 models). The range of values of $\bar{Q}(H)$, $T_{\text{ion}}$, and $Z$ to be modeled was selected on the basis of comparison of the theoretical models with the observational data set on the excitation diagrams of BPT, in order to envelop the observed points. Finally, there are three "depletion/enhancement" grids, which illustrate the effect of changing the elemental abundance ratios for some of the metals at specific $\bar{Q}(H)$, $T_{\text{ion}}$, and $Z$. The first such grid considers the result of refractory grains locking up the elements C, Mg, and Si, and consists of models with varying C/O ratio but fixed C/Mg/Si ratios. In this case models were computed for no depletion, depletion by a factor 2, and depletion by a factor 4 for each of $\frac{1}{2}$, 1, and 2 times solar metallicity at three values of $\bar{Q}(H)$ and three of $T_{\text{ion}}$. The absolute abundances of the metals were calculated by first altering O/H whilst maintaining solar ratios to achieve the desired metallicity (e.g., $\frac{1}{4} Z_{\odot}$) and then performing the depletion/enhancement of the chosen elements. Since
the nucleogenic status of N is uncertain, our second depletion/enhancement grid investigates the effect on the output spectra of altering the N/O ratio. This grid is otherwise identical to the C, Mg, Si grid. Finally, because some of our diagnostics employ forbidden sulfur lines, we consider the effect of changing the S/O ratio for nine models with solar abundances. The three depletion/enhancement grids comprise a total of 189 models.

We propose to show in the following section how to utilize these model grids to determine $\bar{Q}(H)$, $T_{\text{ion}}$, and element-averaged metallicity for a large variety of H II regions which may be observed. However, since such analysis depends in the main on only a few of the total number of lines that could be observed, it would seem desirable to list for some standard model all of the important computed line intensities. These are shown in Table 1 for the model selected, which has parameters $\bar{Q}(H) = 10^8$ cm s$^{-1}$, $T_{\text{ion}} = 40,000$ K, and $Z = Z_\odot$ (reference solar abundances are from Allen 1973 to assist comparison with earlier work). The parameters were chosen to place this model approximately in the middle of the computed range of models for solar metallicity. In accordance with standard practice, all values are quoted relative to $I(H\beta) = 100$. The intensities of the other Balmer lines can be deduced from Brocklehurst's (1971) calculations using our computed recombination temperature of 6780 K. The radial structure of the standard model is illustrated in Figure 1 and deserves some comment. The top two plots in Figure 1 give the radial dependence of electron temperature and free electron number density, and ionization parameter in the nebula, whilst the radial ionization structure of the principal coolants is depicted in the other plots. Over most of the radius, we see that $T_e$ increases slowly away from the ionizing photon source, whilst $Q(H, r)$ decreases. The slow increase in the temperature is due to the "hardening" of the residual stellar ionizing radiation field as
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NOTE—Absolute intensity of $H\beta = 8.344 \times 10^{-16}$ ergs cm$^{-2}$ s$^{-1}$ sr$^{-1}$

$^a$Wavelength in $\mu$m

$^b$Integrated two-photon continuum
Figure 1. The ionization structure of the standard model for varying radius, $r$, expressed in terms of the actual Strömgren radius, $R$. Top left, the radial dependence of the electron temperature and number density of the free electron gas. Top right, the radial dependence of the ionization parameter $Q(H, r)$. The other plots show the radial ionization structure for the most abundant elements, H, He, C, N, O, and S.
soft photons near the ionization thresholds are absorbed. Thus, the mean energy delivered to the electron gas per photoionization increases. The temperature drops suddenly at approximately 96% of the Strömgren radius, resulting from exhaustion of the ionizing photons between the ionization edge of Ne⁺ (21.564 eV) and the He⁺ ionization edge (24.587 eV). Finally, the ionization of hydrogen declines as the number of ionizing photons runs out at the Strömgren radius, and the model terminates shortly thereafter when $N_{\text{H}^+}/N_{\text{H}}$ falls below 1%.

IV. DIAGNOSTIC DIAGRAMS

Since every input parameter to the H II region models has some effect on the predicted spectrum, it is difficult to produce a set of diagnostic diagrams which are instructive and yet not so complex as to be unusable. In the diagrams described below, we attempt to form line ratios which differentiate between the three principal influences on the output spectrum—namely, (a) element-averaged metallicity in the star and nebula, (b) ionization parameter in the nebula, and (c) ionization temperature of the exciting star—in such a way that these quantities may be determined for any observed H II region.

a) Excitation Diagrams of Baldwin, Phillips, and Terlevich

We first consider the loci of theoretical models on the three excitation diagrams of BPT which show significant correlations in the observational data. In Figure 2 we plot the positions of the models from our “solar” grid on the excitation diagram (5007/4861) versus (3727/5007) Comparing with the observational data (Fig. 3), we note that the theoretical models
Figure 2. The relationship between the relative fluxes \((5007/4861)\) vs. \((3727/5007)\) for the grid of models with solar abundances. Isotherms for ionization temperatures of 37,000 K and 56,000 K are labeled with the numbers 37 and 56 respectively; intermediate values 38,500, 40,000, 45,000, and 50,000 K are unlabeled for clarity. Lines of constant mean ionization parameter \(\bar{Q}(\text{H}) = 1 \times 10^7 \text{ cm s}^{-1}\) and \(\bar{Q}(\text{H}) = 1 \times 10^9 \text{ cm s}^{-1}\) are indicated by 7 and 9 respectively, with intermediate values \(\bar{Q}(\text{H}) = 3 \times 10^7, 1 \times 10^8,\) and \(3 \times 10^8 \text{ cm s}^{-1}\) also shown.
Figure 3. The positions of H II regions in our observational data base on the diagram (5007/4861) vs. (3727/5007). The solid line indicates the position of the upper envelope of the theoretical models shown in Fig. 4.
closely reproduce the locus of \( \text{HII} \) regions found on the diagram, although there are some observational points which clearly fall outside the envelope of models with solar abundances. When we consider the effect of abundance variations on this diagram (Fig. 4), several features become apparent. From the positions of the \( \text{HII} \) region models, we can infer the existence of an upper envelope for the positions that \( \text{HII} \) regions can occupy on this type of diagram, the latter being defined by models of approximately one-half solar abundance or less. For other sets of abundances the models fall systematically below this envelope, with the ratio \( I \left( [\text{OIII}] \lambda 5007 \right) / I (\text{H} \beta) \) decreasing with increasing \( Z \) above \( \sim \frac{1}{2} Z_\odot \), confirming the usefulness of this diagram in separating objects photoionized by OB stars from other types of excitation mechanism. Figure 3 observationally confirms the existence of such an upper envelope, since no object is found above it.

Next we consider the excitation diagrams which involve ratios with the \( [\text{NII}] \lambda 6584 \) line. We plot our solar abundance models in Figures 5 and 6 for the diagrams \( (6584/6563) \) vs. \( (3727/5007) \) and \( (5007/4861) \) vs. \( (6584/6563) \) respectively. In both cases the models reproduce the observed distribution of \( \text{HII} \) regions (Figs. 7 and 8), although there is an apparent discrepancy in the strength of the \( [\text{NII}] \) line between the models and the data. Translating the models to lower nitrogen line strength by about 0.2 dex results in better agreement for both diagrams. The qualitative structure of the diagrams may be understood as follows. As we progress from high to low \( \overline{Q}(\text{H}) \) and \( T_{\text{ion}} \), the number of photons capable of ionizing \( \text{O}^+ \) decreases, and so correspondingly does the size of the \( \text{O}^{++} \) zone and hence the total \( [\text{OIII}] \) emission. At the same time, the zone containing the singly ionized species is steadily becoming larger until it eventually fills effectively all the ionized zone, at which point the ratio of the intensities of the singly ionized species
Figure 4. Theoretical trajectories of variable metallicity models on the (5007/4861) vs. (3727/5007) diagram. Lines of constant $\bar{Q}(H) = 10^7$, $10^8$, and $10^9$ cm s$^{-1}$ and $T_{\text{ion}} = 37,000$, 40,000, and 50,000 K are illustrated for solar abundance ratio models. Tick marks indicate metallicities of $Z = 1/4$, $1/2$, $3/4$, and $3/2 Z_\odot$ while filled circles indicate a metallicity of $2 Z_\odot$. 
Figure 5. As Fig. 2, but for the line ratios (6584/6563) vs. (3727/5007).
Figure 6. As Fig. 2, but for the line ratios (5007/4861) vs. (6584/6563).
Figure 7. As Fig. 3, but for the diagram (6584/6563) vs. (3727/5007).
Figure 8. As Fig. 3, but for the diagram (5007/4861) vs. (6584/6563).
to Hβ becomes constant. Because of the difference in ionization potentials, this happens first for [O II], and later for [N II]. Decreasing the mean photon energy still further will eventually result in a reduction in the sizes of the singly ionized zones as the hydrogen transition zone becomes more important. This is reflected in the relative strengths of the corresponding emission lines. A similar effect is also seen in the diagram relating (5007/4861) vs. (3727/5007). For each value of the metal abundance we would expect that the locus of models for “low enough” $\bar{Q}(H)$, $T_{\text{ion}}$ would form a straight line with slope $-1$. This regime is reached when $I \left( [\text{O II}] \lambda 3727 \right)$ is constant. For solar abundances, we may estimate from Figure 6 that $I \left( [\text{N II}] \lambda 6584 \right)$ levels out for log (5007/4861) $\approx -0.5$, and since [O II] $\lambda 3727$ enters this regime prior to [N II] $\lambda 6584$, we may conclude that the inverse correlation between the line ratios in Figure 2 must extend upward to at least log (5007/4861) $\approx -0.5$. Inspection of the diagram shows that this is indeed the case.

It is interesting to note the observed point at log (3727/5007) $\approx -1.45$ on Figures 3 and 7, lying a considerable distance from both the observed correlations and the theoretical envelopes. Employing the notation of McCall (1982), this point is identified as the H II region NGC 598 ($-0606-1708$). There is considerable evidence to suggest that this H II region is density bounded (i.e., the central OB association is capable of ionizing a greater volume of gas than is actually present in the nebula), whereas the other objects are all ionization bounded (McCall, Rybski, and Shields 1985).

Whilst the usefulness of these diagrams in differentiating between excitation mechanisms cannot be denied, their utility as diagnostics for H II regions is very limited because of the compression of the diagrams at small $\bar{Q}(H)$ and $T_{\text{ion}}$, and the inability to distinguish between changes in these
quantities and metal abundance over much of the diagrams. In addition, the diagrams involving ratios with nitrogen lines are particularly bad, since the position of the models depends critically on the assumed N/O ratio, which is in turn determined by the as yet uncertain nucleogenic state of N, as well as depending on the absolute metal abundance.

b) *Diagrams Involving [O i]λ6300*

Unlike BPT, who were seeking excitation diagrams which would enable them to discriminate between nebulae ionized by different processes and therefore required diagrams on which H II regions photoionized by OB associations were clustered in a small region of the diagram, we are seeking diagnostics which discriminate different physical conditions in H II regions and so prefer diagrams in which such objects occur with a considerable spread in line ratios.

The [O i]λ6300 line and its ratios with other oxygen ions can be expected to be particularly useful in this regard, since it is emitted in the transition zone of the H II region, which contains an appreciable fraction of neutral hydrogen. It will therefore be strong in H II regions with low ionization parameter and/or stellar temperature. In Figures 9 and 10 we present two such diagrams employing the line ratios (6300/5007) vs. (3727/5007) and (6300/6563) vs. (3727/5007) respectively. These diagrams, at solar abundance, are useful in diagnosing Q(H) and T\text{ion}, with tangent vectors for these two quantities being approximately orthogonal. Furthermore, the diagnostics cover a sufficiently large range of line intensity ratios that knowledge of the ratios to an accuracy of ~ 0.3 dex is sufficient to localize the properties of the object under consideration.
Figure 9. As Fig. 2, but for the line ratios (6300/5007) vs. (3727/5007).
Figure 10. As Fig. 2, but for the line ratios (6300/6563) vs. (3727/5007).
The relative sparseness of the observational data might seem to suggest that the [O i] λ6300 line is too weak to be accurately measured in the spectra of many extragalactic H II regions, but this is probably not in fact true. The reasons why the line strength has in the past been generally poorly determined are twofold: (1) instrumental broadening at low spectral resolution, which effectively degrades the signal-to-noise ratio in the line, and (2) inadequate subtraction of the night sky λ6300 emission. At intermediate resolution, (1) is no longer a problem, whilst (2) is eliminated for galaxies with redshifts of only a few hundred km s⁻¹. The advent of new-generation high-speed spectrographs now allows observations to be conducted at the necessary resolution for objects where previously only low spectral resolution studies could be contemplated.

The effect of changing abundances on these diagnostic diagrams is shown in Figures 11 and 12. For \( Z \gtrsim Z_\odot \) and for large \( \overline{Q}(H) \) the grids show considerable distortion compared with those of solar metallicity and small \( \overline{Q}(H) \), although they have similar qualitative structure. Figures 9 and 11 illustrate that the line ratio \( I \left( [O \, i] \lambda 6300 \right) / I \left( [O \, iii] \lambda 5007 \right) \) is strongly dependent on both \( \overline{Q}(H) \), with decreasing ionization parameter resulting in increased emission from the low-ionization species relative to the high-ionization species, and metal abundance, where higher \( Z \) results in an increase in the line ratio. The explanation of the latter dependence is straightforward, since higher metal abundance results in increased cooling, a lower mean \( T_e \), but a steeper temperature gradient through the nebula resulting in a reduction in the size of the \( O^{++} \) zone, and a larger transition zone in the H II region where the ionization states of oxygen and hydrogen are locked together by charge exchange, enhancing the [O i] emission.
Figure 11. As Fig. 4, but for the diagram (6300/5007) vs. (3727/5007).
Figure 12. As Fig. 4, but for the diagram (6300/6563) vs. (3727/5007).
In Figures 13 and 14 we plot those few H II regions for which [O i] ȝ6300 has been measured. It is apparent that these objects show a considerable range in \( \overline{Q}(\text{H}) \), but all cluster around \( T_{\text{ion}} = 41,500 \text{ K} \) with relatively small scatter. The variation in \( \overline{Q}(\text{H}) \) is easy to explain, since this can result from either differences in initial mass function, age, or richness of the OB association exciting the H II region or density, clumpiness, or spatial distribution of the ionized material, or both. The constancy of ionization temperature is at first sight a more remarkable result. However, if we consider theoretical tracks on the H-R diagram for evolving OB stars (e.g., Maeder 1981), the explanation for this effect becomes apparent. The stars principally responsible for the ionizing photons will, as pointed out in § III, be those with \( T_{\text{eff}} \) close to \( T_{\text{max}} \) (the temperature of the hottest stars in the cluster) and, since the total number of photons emitted is proportional to the luminosity, with luminosity close to \( L_{\text{max}} \). Such stars will be located at approximately the position of the main-sequence turnoff. Theoretical isochrones for clusters of typical H II region ages, 4–8 million years, have main-sequence turnoffs which occur at very nearly constant \( T_{\text{eff}} \), and this is illustrated particularly well in Figure 2 of Isserstedt (1984), which indicates a total variation in effective temperature of the order of 3000 K for isochrones between 4 and 8 million years. This is of the same order as the scatter in Figure 13. The difference between 41,500 K and the mean temperature of the main-sequence turnoff derived from stellar evolutionary tracks is a measure of the difference between \( T_{\text{ion}} \), which our modeling code uses, and \( T_{\text{eff}} \) for the ionizing stars in H II regions.

Application of the above result to the first excitation diagram of BPT leads to a further interesting conclusion. Compare the observed locus of H II regions on the diagram (5007/4861) vs. (3727/5007) (Fig. 3) with the
Figure 13. As Fig. 3, but for the diagram (6300/5007) vs. (3727/5007).
Figure 14. As Fig. 3, but for the diagram (6300/6563) vs. (3727/5007).
theoretical diagnostic (Fig. 4). If we assert that the H II regions all have approximately the same ionization temperature, then in order to make the observational and theoretical diagrams consistent, it is necessary to invoke the existence of a correlation between $\bar{Q}(H)$ and $Z$. The value of $\langle T_{\text{ion}} \rangle$ deduced from Figure 13 implies that the highest-$\bar{Q}(H)$ objects have $Z \approx \frac{1}{4} Z_\odot$, whilst the H II regions with lowest ionization parameter suggest $Z \approx 2 Z_\odot$ for them; from Figures 3 and 4, we find $Z = Z_\odot$ for an apparent $\bar{Q}(H) \approx 3 \times 10^7$. Observationally, this result is not particularly surprising, since it is well known that those objects with large ionization parameter and low abundances are the isolated extragalactic H II regions and giant loop H II regions such as those found in the LMC or M33. The chemically enriched H II regions, on the other hand, tend to occur in early-type spirals on the inner edges of spiral arms where star formation is enhanced by the occurrence of density waves. Our result implies that these H II regions have, in general, larger mean gas densities than their lower-$Z$ counterparts, and hence the intrinsic ionization parameters for the high-metallicity objects will tend to be larger than the apparent $\bar{Q}(H)$ derived from our diagnostics. There is a real absence of H II regions with both high $Z$ and high apparent $\bar{Q}(H)$ in our sample. One possible explanation of this result follows. Since the number of ionizing photons depends primarily on the most luminous stars and therefore, at constant $T_{\text{eff}}$, on the most massive stars, it is plausible the above effect is a result of differences in the upper cutoff of the initial mass function for the metal-rich and metal-poor populations. At low metal abundances, the upper IMF will be enhanced because of the increased Jeans mass, resulting in objects with larger apparent $\bar{Q}(H)$. Conversely, the reduced Jeans mass for the metal-rich nebulae may result in a lower IMF cutoff and hence objects with smaller apparent values of $\bar{Q}(H)$. 
c) Diagrams Involving Composite Line Ratios

Finally, we consider diagnostic diagrams which employ composite line ratios. We have selected two diagrams in which tangent vectors for the quantities $Q(H)$ and $T_{\text{ion}}$ are approximately orthogonal, and which extend over a large range of line ratios. In Figure 15 we plot our detailed solar grid for the diagnostic $(3727 \cdot 3727/4861 \cdot 5007)$ vs. $(6300 \cdot 6300/3727 \cdot 6563)$, whilst the ratio $(6731 \cdot 6731/6563 \cdot 9069)$ vs. $(6300 \cdot 6300/3727 \cdot 6563)$ is plotted in Figure 16. As before, our comments relating to the use of the [O i] $\lambda 6300$ line apply to these line ratios also. The use of the sulfur lines also requires some justification. Only the single [S ii] $\lambda 6731$ line is employed in preference to the doublet $\lambda \lambda 6716,6731$ because this enables us to carry over our results to higher densities than would be the case if the contribution from [S ii] $\lambda 6716$ was included, since the latter line has a much lower critical density for collisional de-excitation than the former. In this way, our results may be directly applied to even the most dense H ii regions observed, provided only that the scaling law for $Q(H)$ with density introduced in § III is applied to our models. The near infrared [S iii] $\lambda 9069$ line has usually not been observed in H ii region spectra in the past, but the advent of red-sensitive CCD detectors combined with careful sky-subtraction techniques should mean that this line is no more difficult to measure accurately than many other lines in the visible spectrum. Abundance tracks for these two diagnostics are illustrated in Figures 17 and 18, and demonstrate the utility of these diagrams. Abundance changes have much less effect on these diagnostics than on previously described diagrams, particularly in the region of large $Q(H)$, where changing metallicity from $Z_{\odot}$ to $2 Z_{\odot}$ typically corresponds to a change in the composite line ratios of $\lesssim 0.5$ dex. The diagnostics described here neatly
Figure 15. As Fig. 2, but for the composite line ratios \((3727 \cdot 3727/4861 \cdot 5007)\) vs. \((6300 \cdot 6300/3727 \cdot 6563)\).
log (3727.3727/4861.5007)

log (6300.6300/3727.6563)
Figure 16. As Fig. 2, but for the composite line ratios \((6731 \cdot 6731/6563 \cdot 9069)\) vs. \((6300 \cdot 6300/3727 \cdot 6563)\).
Figure 17. As Fig. 4, but for the composite line ratios \((3727 \cdot 3727/4861 \cdot 5007)\) vs. \((6300 \cdot 6300/3727 \cdot 6563)\).
log (3727.3727/4861.5007)

\[
\log \left( \frac{6300.6300}{3727.6563} \right)
\]
Figure 18. As Fig. 4, but for the composite line ratios \((6731 \cdot 6731/6563 \cdot 9069)\) vs. \((6300 \cdot 6300/3727 \cdot 6563)\).
log \left( \frac{6731.6731}{6563.9069} \right)

\begin{align*}
\log (6300.6300/6563.9063) \\
\log (6300.6300/3727.6563)
\end{align*}
complement the diagrams outlined in the preceding subsection in which abundance changes have little effect for small values of $\overline{Q}(H)$ but significant effect for larger ionization parameters. With respect to abundance changes, the diagnostic employing the sulfur lines has greater immunity, but since the $[\text{S} \, \text{III}] \lambda 9069$ line has often not been measured in the past, the applicability of this diagram to previously published data is somewhat limited. The observational data set for the diagnostic involving only ratios of oxygen (and Balmer) lines is plotted in Figure 19.

Next we consider the effect on these diagnostics of altering the relative abundance ratios of the heavy elements. The results of depleting C, Mg, and Si, which may be locked up in refractory grains, by factors of 2 and 4 are shown in Figures 20, 21, and 22 for reference metallicities of $1 \over 2$, 1, and 2 times solar respectively for the first of our composite line ratio diagnostics, and in Figures 23, 24, and 25 for the diagnostic which involves ratios with the sulfur lines. Visual inspection of the figures indicates that the effect of depleting the refractory elements on the observed line ratios simulates a lower apparent $\overline{Q}(H)$ and a slightly higher $T_{\text{ion}}$. For reference metal abundances $\sim 1 \over 2 Z_\odot$ or less, the effect is essentially negligible for the degrees of depletion we are considering but become progressively more significant as the reference metallicity is increased. Such behavior is expected, since the cooling due to a given ion is proportional to the absolute abundance of that ion. Depleting the refractory elements leads to a decrease in the gas cooling by "unseen" coolants in the ultraviolet and infrared (specifically Mg II $\lambda 2798$, [C II] $158 \mu m$, and [Si II] $34.8 \mu m$) and results in a strengthening of the visible lines. In addition to the refractory elements, we should consider the effects of changing the N/O abundance ratio, since this depends on the nucleogenic
Figure 19. As Fig. 3, but for the composite line ratios \((3727 \cdot 3727/4861 \cdot 5007)\) vs. \((6300 \cdot 6300/3727 \cdot 6563)\).
\[ \log \left( \frac{3727.3727}{4861.5007} \right) \]

vs

\[ \log \left( \frac{6300.6300}{3727.6563} \right) \]
Figure 20. Theoretical trajectories for variable depletion of C, Mg, and Si for the diagram $(3727 \cdot 3727/4861 \cdot 5007)$ vs. $(6300 \cdot 6300/3727 \cdot 6563)$ for a reference metallicity of $\frac{1}{2} Z_\odot$. Lines of constant $\bar{Q}(H) = 10^7$, $10^8$, and $10^9$ cm s$^{-1}$ and $T_{\text{ion}} = 37,000$, 40,000, and 50,000 K are illustrated for the reference metallicity (no depletion) models. Tick marks indicate models with a C/O ratio of $\frac{1}{2}$, while filled circles indicate a C/O ratio of $\frac{1}{4}$. 
Figure 21. As Fig. 20, but for a reference metallicity of $1 \, Z_\odot$. 
Figure 22. As Fig. 20, but for a reference metallicity of $2 \, Z_\odot$. 
Figure 23. As Fig. 20, but for the composite line ratios \((6731 \cdot 6731/6563 \cdot 9069)\) vs. \((6300 \cdot 6300/3727 \cdot 6563)\).
Figure 24. As Fig. 21, but for the composite line ratios \((6731 \cdot 6731/6563 \cdot 9069)\) vs. \((6300 \cdot 6300/3727 \cdot 6563)\).
Figure 25. As Fig. 22, but for the composite line ratios \((6731 \cdot 6731/6563 \cdot 9069)\) vs. \((6300 \cdot 6300/3727 \cdot 6563)\).
state of nitrogen. The results of depleting N abundance are illustrated in Figures 26–31. Decreasing the relative nitrogen abundance reduces the cooling of the gas due primarily to the visible [N II] lines, although the infrared [N II] lines at 121.6 μm and 203.6 μm, and the [N III] 57.3 μm line are significant contributors. Fortunately, as may be seen from the figures, at the levels of depletion considered here, and for \( Z \lesssim 2 Z_\odot \), the effect of depleting nitrogen may be ignored. Finally, since our diagnostics involve ratios with the sulfur lines, we consider the results of changing the S/O ratio. Only depletion and enhancement of sulfur relative to oxygen each by a factor of 2 are calculated for solar reference abundance, since there is little evidence to suggest that the S/O ratio is variable in H II regions (Kaler 1981). In Figures 32 and 33 we plot variable S tracks for the two composite line ratio diagnostics, and inspection of these diagrams suggests that variations of up to a factor of 2 (up or down) in the S/O ratio can probably be ignored. Once again, altering the S/O ratio has the effect of altering the relative competition of the different coolants in the nebula, and in the case of sulfur, the lines involved are the visible [S II] and near-infrared [S III] lines, together with the infrared [S III] lines at 18.7 μm and 33.6 μm.

This completes the set of diagnostic diagrams. To estimate \( \overline{Q}(H) \), \( T_{\text{ion}} \), and \( Z \) in an observed H II region, the following procedure is suggested. First, assuming initially \( T_{\text{ion}} \approx 41,500 \) K and \( Z \approx Z_\odot \), estimate \( \overline{Q}(H) \) from either Figures 11 and 12 or Figures 17 and 18. If \( \overline{Q}(H) \) is large, the latter figures should be used to minimize errors because of the uncertain metallicity, otherwise the former figures can be used. From the observed empirical correlation, Figure 3, an initial estimate of \( Z \) can be found, and if this is too far from solar, the above steps should be repeated. Next, using this estimate of the metallicity, \( T_{\text{ion}} \) and \( \overline{Q}(H) \) may be estimated from any of Figures 11, 12, 17,
Figure 26. As Fig. 20, but for variable depletion of N.
Figure 27. As Fig. 21, but for variable depletion of N.
Figure 28. As Fig. 22, but for variable depletion of N.
Figure 29. As Fig. 23, but for variable depletion of N.
Figure 30. As Fig. 24, but for variable depletion of N.
Figure 31. As Fig. 25, but for variable depletion of N.
Figure 32. Theoretical trajectories for variable depletion/enhancement of S for the diagram \((3727 \cdot 3727/4861 \cdot 5007)\) vs. \((6300 \cdot 6300/3727 \cdot 6563)\) for a reference metallicity of \(1Z_\odot\). Lines of constant \(\mathcal{Q}(\text{H}) = 10^7, 10^8, \text{and } 10^9\) \(\text{cm s}^{-1}\) and \(T_{\text{ion}} = 37,000, 40,000, \text{and } 50,000\) K are illustrated for the reference metallicity (no depletion) models. Tick marks indicate models with an S/O ratio of \(\frac{1}{2}\), while filled circles indicate a S/O ratio of 2.
Figure 33. As Fig. 32, but for the composite line ratios \((6731 \cdot 6731/6563 \cdot 9069)\) vs. \((6300 \cdot 6300/3727 \cdot 6563)\).
or 18, choosing whichever figure shows the smallest dependence on $Z$ in the 
$[T_{\text{ion}}, \bar{Q}(H)]$ region of interest. Once $T_{\text{ion}}$ and $\bar{Q}(H)$ are determined, $Z$ can be estimated from whichever diagram shows the greatest dependence on $Z$ in the region of interest. If $Z \gtrsim Z_\odot$, it may be necessary to consider the possibility that the refractory elements are depleted at this point, and the amount of depletion can be estimated from Figures 20–25. It is now possible to make an improved estimate of $T_{\text{ion}}$ and $\bar{Q}(H)$ and so iterate the above process until convergence is achieved. In practice, only one or two iterations are sufficient to achieve self-consistency of the conditions derived from different diagnostics to within the observational errors.

V. CONCLUSIONS

We have computed a new homogeneous set of photoionization models with conditions appropriate to observed H II regions. The primary objective of these computations was to construct a comprehensive set of diagnostic diagrams from which the ionization parameter in an observed H II region, and the ionization temperature of its exciting star or stars, could be derived from ratios of the intensities of prominent emission lines. It is also possible to determine the element-averaged metallicity in the nebula using the diagrams presented here, although the main aim of this paper was to demonstrate how $\bar{Q}(H)$ and $T_{\text{ion}}$ could be derived essentially independently of $Z$, and hence many of the diagnostics were chosen for their small $Z$-dependence. We shall address the problem of how relative abundances can be determined in a later paper.

The utility of these diagnostics is clearly demonstrated by comparison of the loci of current observational data on the diagrams (Figs. 3, 7, 8, 13,
14, and 19) with the corresponding theoretical diagnostic diagrams derived from the models (Figs. 4, 5, 6, 11, 12, and 17 respectively), since that region of parameter space delineated by our grid of models envelops virtually all observed H II regions. We also note that interpretation of the observational data in the light of our diagnostic diagrams does not require implausible values for any of the derived parameters.

As may be apparent from the figures, no single line ratio that we have examined is particularly good for estimating any specific parameter over the full range of conditions considered here, but rather pairs of line ratios (as used in the diagnostics) should be employed to derive the conditions in the nebula. If the procedure suggested in § IV is followed, then $\overline{Q}(H)$ and $T_{\text{ion}}$ in a particular H II region may be estimated with reasonable precision, and $Z$ with rather less precision. The mean ionization temperature of the exciting star(s) may be determined from Figures 11, 17, and 18 relatively independently of both ionization parameter and metallicity, particularly for $\overline{Q}(H) \lesssim 10^8 \text{ cm s}^{-1}$. Employing the iterative procedure described in the previous section, $T_{\text{ion}}$ may be estimated with a precision of a few hundred kelvin for $37,000 \lesssim T_{\text{ion}} \lesssim 40,000$ K, increasing to approximately 1000 K for $T_{\text{ion}} \sim 50,000$ K. Similarly, the mean ionization parameter in the nebula is best estimated from Figures 12, 17, and 18, except for the very lowest values of $\overline{Q}(H)$, where Figure 11 should be used. In these figures, the dependence on metallicity of this parameter is more pronounced than the dependence of $T_{\text{ion}}$ on $Z$; nevertheless it should be possible to estimate $\overline{Q}(H)$ to a precision of order 0.2 dex for $\overline{Q}(H) \gtrsim 10^8 \text{ cm s}^{-1}$, and $\sim 0.3$ dex for $\overline{Q}(H) \sim 10^7 \text{ cm s}^{-1}$. As noted above, the element-averaged metallicity in an H II region is a more difficult parameter to determine precisely using these
diagnostics and can be reasonably estimated only using the iterative technique prescribed earlier, which should yield a value for $Z$ with a precision of at least 0.3 dex. It is not in general possible to determine relative elemental abundances using the diagnostics presented here, since, as described in § IVc, altering the N/O or S/O ratios has relatively little influence on the topology of the diagrams. Nevertheless, depletion of the refractory elements for overall metallicities $Z \gtrsim Z_\odot$ may be estimated to a precision of about 0.3 dex from Figures 22 and 25. It is important that the reader be aware that, even discounting model-dependent factors, there will be many circumstances in nature such as highly complex density and geometrical structure, ionizing stars not concentrated centrally in the nebula, non–ionization-boundedness, and so on, where one or more basic assumptions of these models may not be satisfied. Clearly, blind application of these results is not in order. However, if one is certain that such complications can be neglected in a particular case, application of these diagnostics in the manner prescribed above should lead to valuable estimates of $\overline{Q}(H)$, $T_{\text{ion}}$, and $Z$ within the nebula.

Comparison of the theoretical models with current observational data suggests that the ionization temperature of the principal stars in the ionizing OB associations is approximately constant, $\langle T_{\text{ion}} \rangle = 41,500$ K, independent of metal abundance and ionization parameter. We also find a correlation between metallicity and ionization parameter in the sense that high $\overline{Q}(H)$ is correlated with low $Z$.

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THEORETICAL MODELS FOR H\textsc{ii} REGIONS.

II. THE EXTRAGALACTIC H\textsc{ii} REGION

ABUNDANCE SEQUENCE

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ABSTRACT

With the aid of the extensive, homogeneous grid of theoretical photoionization models described in the first paper of this series, we have generated a multiline fit to the observed emission-line spectral sequence of extragalactic H II regions. It is possible to produce an excellent fit between the (rather narrow) emission-line ratio sequences that are observed and the theoretical sequences, provided that the average ionization parameter is strongly coupled with metallicity, and provided that nitrogen is a product of secondary nucleosynthesis.

Using this theoretical sequence of H II region models, we have recalibrated the semiempirical abundance diagnostic ratios used by Alloin et al. (1979), Pagel et al. (1979), and McCall, Rybski, and Shields (1985) and have generated new abundance diagnostic ratios. We find that the correlation between ionization parameter and abundance has the effect of changing the previous abundance calibration toward lower abundances, particularly for the most metal-rich H II regions. Finally, we give a new technique to derive abundances from H II region spectra.

Subject headings: galaxies: evolution — nebulae: abundances — nebulae: H II regions
I. INTRODUCTION

The spectrophotometry of giant H II regions in external galaxies has been the principal datum used to derive the abundances and abundance gradients of elements lighter than calcium. Since these elements, in particular oxygen and neon, are produced in the massive Population I stars, the interpretation of the observational material is of fundamental importance to our understanding of the evolution of galaxies.

In the past, much effort has been devoted to attempts to derive explicit elemental abundances from very high signal-to-noise spectra of individual H II regions. Formerly, the semiempirical ionization correction factor technique pioneered by Peimbert and Costero (1969) has been employed with considerable success to derive abundances in many galaxies (e.g., Peimbert and Torres-Peimbert 1974, 1976; Dufour 1975, 1977; Smith 1975; Pagel et al. 1978; Lequeux et al. 1979). More recently, as theoretical photoionization models have improved, these have been applied toward direct derivation of the abundances of individual HII regions (e.g., Shields and Searle 1978; Dufour et al. 1980; Dufour, Shields, and Talbot 1982). However, both of these methods depend critically on the detection of the temperature-sensitive line [O III] λ4363, which is very weak in, or entirely absent from, the spectra of metal-rich H II regions.

An alternative avenue of approach to the abundance problem is suggested by the fact that the spectra of extragalactic H II regions appear to represent a one-parameter sequence. This was first suggested by Searle (1971) who felt that the excitation, being probably controlled by the oxygen abundance, would represent an appropriate classification index. Sarazin (1976)
developed this idea and attempted to fit the whole sequence with theoretical models. He concluded that, in addition to the abundance variation, there must also be an excitation variation or a softening of the radiation field at higher metallicity. As more data have been accumulated, this sequence of H II region spectra has looked better (see, for example, the compilation by Baldwin, Phillips, and Terlevich 1981, or the very large sample of McCall, Rybski, and Shields 1985). The major question therefore revolves around what is the most appropriate emission-line ratio to use for abundance sequencing. Pagel et al. (1979) have suggested that the ratio \([\text{[O} II] \lambda 3727 + \text{[O} III] \lambda \lambda 4959, 5007]/\text{H} \beta\) is better than \([\text{O} III] \lambda \lambda 4959, 5007/\text{H} \beta\) because it is less sensitive to the geometry of the gas distribution with respect to the ionizing radiation. This appears to be amply borne out by further observation (Pagel, Edmunds, and Smith 1980; Edmunds and Pagel 1984; McCall, Rybski, and Shields 1985).

To derive an absolute abundance from such a sequence is more difficult. Pagel and his co-workers rely heavily on model fits to a metal-rich H II region in M101, S5, to fix the abundance scale at the upper end. In the third paper in this series (Evans 1986; hereafter Paper III) we will show that this "fiducial" point may be seriously misplaced. Alloin et al. (1979) argue that a safer approach may be to determine the electron temperature in the O++ zone via a semiempirical route involving the \([\text{[O} III] \lambda \lambda 4959, 5007/[\text{N} II] \lambda \lambda 6548, 6584\) ratio and then to derive the oxygen abundance from the abundance–electron temperature correlation. However, the success of this method depends critically on the assumed nucleosynthetic origin of nitrogen, which has been variously argued to be either a primary or secondary element (see § IV below).
In the first paper of this series (Evans and Dopita 1985; hereafter Paper I), we described computation of an extensive grid of models directed toward the production of a set of diagnostic diagrams which would enable the ionization parameter of H II regions and the ionization temperature of their exciting stars to be estimated in a manner that is largely independent of nebular and stellar chemical abundances. This is an essential first step toward the correct theoretical calibration of the abundance scale of extragalactic H II regions. In Paper I we discovered that the ionization temperature of the stars showed remarkably little variation with abundance, within the limitations of the available data, but that the ionization parameter shows a strong inverse correlation with metallicity. In this paper we will use this result as the starting point of an attempt to fit simultaneously all the important line ratios observed in extragalactic H II regions. As a result, we are able to both calibrate the abundance sequence in an absolute manner and to suggest new abundance sequencing ratios which may be useful from an observational viewpoint.

II. THE OBSERVATIONAL DATA BASE

In this paper we follow Paper I in selecting for the data base the compilation of Baldwin, Phillips, and Terlevich (1981; hereafter BPT) and the very extensive homogeneous data set of McCall (1982) which is substantially that published by McCall, Rybski, and Shields (1985). The BPT set is composed of most of the published high-quality data available to them. This sample has severe selection effects. For example, it is strongly biased toward the highest surface brightness H II regions in the Magellanic Clouds, blue compact galaxies, and giant H II regions (such as NGC 604 in M33)
which tend to occur in the outer parts of their parent galaxies. This in turn means that the sample is strongly biased toward lower abundance objects. The McCall (1982) sample is much more representative of the HII region population. Galaxies were selected on the basis of high equivalent width of Hα and at various radial positions within the galaxies. However, the galaxies chosen tend to be of high absolute magnitude, and this fact, together with the fact that the sample is rich in HII regions in the inner parts of galaxies, means that many more high-abundance objects were observed. Thus the two samples are somewhat complementary for the purpose of ensuring a good coverage over a wide range of abundances.

III. THE THEORETICAL MODELS

A full description of the theoretical photoionization models used here is given in Paper I. Suffice it to say here that the basic grid of models consists of steady state spherically symmetric dust-free nebulae of uniform density of hydrogen atoms plus ions (10 cm$^{-3}$) and constant helium abundance. The density is chosen to be sufficiently low as to preclude the possibility of collisional de-excitation of optical forbidden lines. The central ionizing OB association was approximated by a stellar atmosphere photon source with a single ionization temperature and the metallicity of the stellar atmosphere was kept the same as the surrounding nebula. The log $g = 4.0$ models of Hummer and Mihalas (1970) were used with the interpolation scheme developed by Shields and Searle (1978).

With these assumptions, the three parameters that have a major effect on the emission-line spectrum are chemical abundance, ionization parameter, and ionization temperature of the exciting stars. Our basic net of models,
described in Paper I, was cast wide enough to encompass all the likely values of these parameters and all the variety of the observed spectra.

Three subsidiary grids were also developed to gain an understanding of the effects of changing element abundance ratios on the emission-line spectrum. Specifically, these were (i) a grid allowing changes in the (C + Mg + Si)/O ratio to investigate the effects of depletion onto refractory grains, (ii) a grid allowing changes in the N/O ratio to investigate the nucleogenic status of nitrogen, and (iii) a grid allowing changes in the S/O ratio, which may reflect the initial mass function (IMF) for the more massive stars. Together, these grids offer an excellent insight into the spectral characteristics of H II regions and render it feasible to attempt a multiparameter fit to the observed spectral sequence in external galaxies.

IV. FITTING PROCEDURE

a) Initial Assumptions

In Paper I, we developed a set of diagnostic diagrams to enable the ionization parameter of the H II region and the ionization temperature of the central star to be determined largely independently of the chemical abundance in the nebula. These diagrams involved line ratios formed principally from the [O i] λ6300, [O ii] λ3727, [O iii] λ5007, [S ii] λ6731, and [S iii] λ9069 lines, as well as the Balmer lines of hydrogen. Unfortunately, the data base is very sparse in measurements of the [O i] λ6300 line and the [S iii] λ9069 line, and so a satisfactory diagnosis is possible over relatively few H II regions. However, this was sufficient to show that the ionization parameter varies over a very wide range of nearly two orders of magnitude. However,
the ionization temperature does not show great variability, the data points clustering about $T_{\text{ion}} = 41,500$ K with a total scatter of order 3000 K. There is no evidence to support the idea that the ionization temperature and the ionization parameter are coupled in the H II regions for which a complete analysis was possible.

Using the first excitation diagram of BPT, in which the $[\text{O III}]/[\text{O III}]$ forbidden-line ratio, log (3727/5007), is plotted against log (5007/4861), the distribution of the observational points can be reconciled with the theoretical curves only if the ionization parameter is itself correlated with metallicity. The sense of this is that high chemical abundance is correlated with low ionization parameter.

On the basis of Paper I, we take as the point of departure for the fitting process a fixed ionization temperature of 41,500 K, and an assumed correlation between ionization parameter, $Q(\text{H})$ (defined in Paper I), and chemical abundance, $12 + \log (\text{O/H})$. The next problem is to discover the form of this correlation.

b) The $Q(\text{H})-Z$ Correlation

In Paper I, we found that by far the best $Q(\text{H})$ indicator is the composite line ratio involving the forbidden lines of sulfur, $(6731 \cdot 6731/6563 \cdot 9069)$. This ratio changes by 1.5 magnitudes for every magnitude change in $Q(\text{H})$ and is substantially independent of ionization temperature or Z. Unfortunately, the data base on the $[\text{S III}] \lambda 9069$ line is essentially nonexistent. Fortunately, it is the $[\text{S II}] \lambda 6731$ line that is the most sensitive to $Q(\text{H})$, so that the simple ratio $(6731/6563)$ is still adequate as a $Q(\text{H})$ discriminant,
provided that $Q(H)$ is not too low or that the abundance of sulfur relative to oxygen is not greatly variable.

In Figure 1, we plot the $[S\,\text{II}]\lambda 6731/\text{H}$ ratio against the Pagel et al. (1979) abundance discriminant $([O\,\text{II}]\lambda 3727 + [O\,\text{III}]\lambda \lambda 4959, 5007)/H\beta$. The theoretical grid is for an ionization temperature of 41, 500 K and varying $Q(H)$ and $Z$. The $Q(H)-Z$ correlation is evident in this diagram. However, at the relatively low values of $Q(H)$ which characterize the bulk of H II regions, the Pagel et al. (1979) abundance discriminant begins to compact and become ambiguous. We therefore require to find an abundance indicator that does not suffer from this problem.

We find that the Alloin et al. (1979) discriminant ratio $[O\,\text{III}]\lambda \lambda 4959, 5007/[N\,\text{II}]\lambda \lambda 6548, 6584$ is not very helpful, at least at this stage, because it is very dependent on the assumed nucleogenic status of nitrogen, and furthermore the $[O\,\text{III}]$ line strength is dependent on $Q(H)$.

The conditions required to obtain a useful abundance indicator are that it must involve only the bright optical lines between 3727 Å and 6731 Å, it should retain sensitivity at high abundance where the $[O\,\text{III}]$ lines become weak or absent, and it should not use the $[N\,\text{II}]$ lines. Thus, the only possible lines that can be used are the $[O\,\text{II}]\lambda 3727$, $[S\,\text{II}]\lambda \lambda 6716, 6731$, and Balmer lines. By trial and error we discovered that the composite ratio $(3727\cdot 3727/4861\cdot 6731)$ is very suitable, since it shows good $Z$ sensitivity throughout the range encompassed by the observed H II regions, shows very little sensitivity to $Q(H)$, and is only slightly more sensitive to variations in
Figure 1. The simple $Q(H)$ discriminant, ($6731/6563$) plotted against the Pagel et al. (1979) abundance sensitive ratio $([\text{O II}] \lambda 3727 + [\text{O III}] \lambda \lambda 4959, 5007)/H\beta$. The theoretical grid of models is for an ionization temperature of $41,500 \text{K}$, and elemental abundances as defined in Table 1. Lines of constant mean ionization parameter $\log Q(H) = 6.5 \text{cm s}^{-1}$ and $\log Q(H) = 8.0 \text{cm s}^{-1}$ are labeled with 6.5 and 8.0, respectively, with intermediate values $\log Q(H) = 7.0$ and $7.5 \text{cm s}^{-1}$ also shown. Lines of constant metallicity $Z = 1/4, 1/2, 3/4, 3/2, \text{and } 2 Z_\odot$ are illustrated. The positions of $\text{H II}$ regions in our observational data base are indicated by filled circles.
the ionization temperature than the Pagel et al. (1979) abundance indicator. In Figure 2, we plot the [S II] λ6731/Hα ratio against this abundance discriminant. The $Q(H)-Z$ correlation is now clear and unambiguous.

It might be argued that sulfur abundance variations could produce the correlation of Figure 2. However, if this were so, we would require a massive variation on the S/O ratio; sulfur would have to be at least a secondary nucleosynthetic element. Such a conclusion would be completely at variance with what we know about the nucleogenic origin of sulfur (Weaver, Zimmerman, and Woosley 1978; Clegg, Lambert, and Tomkin 1981; Nomoto, Thielemann, and Yokoi 1984) and with a detailed analysis of observational results on supernova remnants (Dopita et al. 1984), of H II regions (Dennel and Stasińska 1983), and planetary nebulae in our own Galaxy (Kaler 1981). These studies show no detectable variations in S/O abundance ratios. If we assume that the S/O abundance ratio is fixed, then Figure 2 can be used to derive the $Q(H)-Z$ relationship. However, we need the absolute value of the S/O abundance ratio to be able to do this, since the $Q(H)$ value derived in Figure 2 is very sensitive to the assumed S/O abundance ratio. Fortunately, the first of the BPT diagrams, which depends only on line ratios of oxygen ions, is also useful as a $Q(H)-Z$ discriminant, provided that the assumption of constant ionization temperature is valid. We plot this in Figure 3. The separation is not as good as in Figure 2, but the trend and mean value can be derived. The discrepancy between the loci of the observational points in Figures 2 and 3 is largely due to the fact that the data sample in Figure 2 is incomplete at high values of $Q(H)$ (low $Z$) because the [S II] λ6731 line is either too weak to be measured or has very large errors for the low abundance objects in the BPT data base. Nevertheless, there is some degree of inconsistency between the figures. A possible cause for this may be due to
Figure 2. As Fig. 1, but employing the abundance discriminant suggested in the text, \((3727 \cdot 3727/4861 \cdot 6731)\).
$\log \left( \frac{6731}{6563} \right)$

$\log \left( \frac{3727.3727}{4861.6731} \right)$
Figure 3. As Fig. 1, but for the first of the BPT diagrams, (5007/4861) vs. (3727/5007).
uncertainty in the rate of the $H^0 + O^{++} \rightleftharpoons H^+ + O^+$ charge exchange reaction, which will weaken $I([O\text{ III}]\lambda5007)$ at lower values of $Q(H)$ because of the presence of partially ionized gas. The inconsistencies between the figures cannot be significant, however, since the abundance sequence derived below accurately tracks the locus of observed $H\text{ II}$ regions, and the chemical abundances derived from independent diagnostic line ratios are internally consistent to within the errors.

We have used Figure 2 to extract the form of the $Q(H)-Z$ relation, and Figure 3 to extract the $S/O$ abundance ratio which renders Figures 2 and 3 most nearly self-consistent. We have fitted the data to the simple functional form

$$12 + \log(O/H) = A - B \times \log Q(H), \quad Q(H)_{\text{min}} < Q(H) < Q(H)_{\text{max}},$$

where $A = 13.15$, $B = 0.5903$, $\log Q(H)_{\text{min}} = 6.7$, and $\log Q(H)_{\text{max}} = 8.4$, respectively. Within the substantial scatter at a given $Z$, this represents a very good fit to the observations. The accuracy with which the oxygen abundance can be derived from the abundance sequence, together with an example of its application to $H\text{ II}$ regions in the spiral galaxy M101, is discussed in Paper III.

The question of why there should be a $Q(H)-Z$ correlation is important enough to warrant a digression at this point. The possible explanations are (i) there is a correlation between the IMF and $Z$, (ii) the correlation is the result of dust absorption, or (iii) there are environmental effects which change the “geometry” at high $Z$.

In Paper I we have already discussed the first of these alternatives, and will not develop it further here.
The second alternative is related to a suggestion by Sarazin (1976) that the excitation gradients seen in H II regions are the result of nongray dust absorption. Certainly, if the dust has an absorption curve that is an increasing function of frequency, this will very effectively "soften" the radiation field and give rise to low-excitation H II regions in dusty environments. The dusty models of Sarazin (1976, 1977), Dufour et al. (1980), and Stasińska (1980) have many characteristics of dust-free models with a lower ionization temperature, but this is because of the unrealistic assumption that the dust absorption cross section varies as $\nu$ or $\nu^2$. It seems most likely that actual dust has an absorption peaked at $\sim 16-17$ eV, falling off at higher frequencies (Martin and Ferland 1980). This behavior makes the net stellar radiation which is absorbed by the gas appear to be harder than that emitted by the star; that is, it makes the star look hotter than it really is. Increasing the amount of "real" dust (based on current predictions of its UV cross sections) makes $\overline{Q}(H)$ apparently increase by making the star appear to be hotter, which is the opposite of the observed $\overline{Q}(H)$--$Z$ correlation. We emphasize again that we found no strong evidence to support the idea of a varying ionization temperature. Thus if dust absorption is important in driving a $\overline{Q}(H)$--$Z$ correlation, it must be through it possessing a gray rather than frequency-dependent opacity. Petrosian, Silk, and Field (1972) have developed analytic approximations to the ionization balance of dusty Strömgren spheres. If, within an H II region, a fraction $f$ of the stellar ionizing photons is absorbed by the gas, then the mean ionization parameter is approximately given by

$$\overline{Q}(H) = f L_C / 4\pi (y_0 R/2)^2 N,$$

where $L_C$ is the luminosity of the star in ionizing photons per second, $R$ is the dust-free Strömgren radius, and $y_0$ is the fractional radius of the ionized
zone, compared with the Strömgren radius, in the presence of dust. Equation (8) of Petrosian, Silk, and Field (1972) gives an expression for $f$ and $y_0$. Although $Q(H)$ does indeed decrease with increasing dust content, the rate of variation is slow, and unreasonably large values of dust absorption would be required to produce the observed correlation of $Q(H)$ and $Z$. We therefore conclude that dust absorption effects are not primarily responsible.

The third possibility, that environmental effects cause a changing $Q(H)$, is probably the most likely explanation. In general, H II regions are selected for observation because they have a high surface brightness. The surface brightness and the $Q(H)$ values are correlated. The Strömgren condition is

$$L_C = \frac{4\pi}{3} R^3 N^2 \epsilon \alpha_B,$$

(2)

where $\epsilon$ is the volume filling factor and $\alpha_B$ is the effective recombination coefficient for hydrogen. The mean surface flux at H$\beta$ is given by

$$S_{H\beta} = \frac{4}{3} R N_H^2 \epsilon \alpha_{\text{eff}} h \nu_{H\beta},$$

(3)

where $\alpha_{\text{eff}}$ is the effective recombination coefficient for H$\beta$. Combining equations (1)–(3) we have, for a dust-free H II region,

$$S_{H\beta} = Q(H) \left( \frac{N_H^2}{N} \right) (\alpha_{\text{eff}}/\alpha_B) h \nu_{H\beta}$$

(4)

$$\approx Q(H) \left[ N/ (1 + Z(\text{He}))^2 \right] (\alpha_{\text{eff}}/\alpha_B) h \nu_{H\beta},$$

(5)

since $N \approx N_H [1 + Z(\text{He})]$, where $Z(\text{He})$ is the relative abundance of helium by number with respect to hydrogen, and we have assumed helium to be singly ionized. Equations (4) and (5) show that high-density, high-$Q(H)$ H II regions will be preferentially observed. Since such H II regions are not observed in the high-$Z$ regime, we must conclude that there is a real absence
of high-$\bar{Q}(H)$, high-$Z$ objects in galaxies. The most obvious physical reason for this might be that the mean density of H II regions increases in the inner regions of galaxies where high values of $Z$ are located. This is not unreasonable, since the surface density of gas tends to increase in these regions (Paper III). An alternative explanation might be that the specific rate of star formation of massive stars is lower in high-$Z$ regions, and thus the mean value of $L_*$ is lower. These two alternatives could be discriminated between by a program of absolute photometry in the Balmer lines. The referee suggested an alternative explanation, namely, that $\epsilon$ decreases with $Z$. Presumably, $\epsilon$ is not unity because most of the volume of the H II region is occupied by shocked stellar wind, which is in turn accelerated by radiation pressure on heavy element ions in the stellar atmosphere, yielding a correlation between volume filling factor and metallicity.

c) **Nucleogenic Status of Nitrogen**

A question that has been discussed for many years is whether nitrogen is enriched as a primary element (in which case N/O is constant) or whether it is a secondary element (which implies N/O varying as O/H; Talbot and Arnett 1974). The evidence from supernova remnants implies a secondary origin (Dopita et al. 1984), and the secondary nature of nitrogen has already been suggested for H II regions (Dufour, Shields, and Talbot 1982; Mathis, Chu, and Peterson 1985). On the other hand, H II region data have suggested that a primary enrichment component is present, but that this varies in its importance from galaxy to galaxy (Smith 1975; Edmunds and Pagel 1978; Pagel et al. 1978; Alloin et al. 1979; Pagel and Edmunds 1981).
Since we have now established a statistical relationship between $T_{\text{ion}}$, $\bar{Q}(H)$, and $Z$, we are now in a position to examine this question. The diagnostic diagrams of BPT which involve $[\text{N II}]$ ratios are not particularly useful in this regard, since a clean separation of the various parameters is not possible. However, the ratio $[\text{O II}] \lambda 3727/[\text{N II}] \lambda 6584$ is much more useful, since this is sensitive to the N/O ratio, but depends less on the other parameters. In Figure 4, we plot this ratio against our abundance discriminant $(3727 \cdot 3727/4861 \cdot 6731)$. The observed points show very little scatter in the high abundance limit, which suggests that at this limit, at least, the various galaxies share a common mode of nitrogen enrichment. The two theoretical sequences shown are for nitrogen assumed primary, with a solar N/O ratio at solar abundance, and for nitrogen assumed secondary, likewise with a solar N/O ratio at solar abundance. Clearly, the latter curve is a much better fit to the observed points, which strongly argues for nitrogen as a secondary element, at least at high $Z$. The large amount of scatter at the low-$Z$ end is real and indicates that there is a different source of nitrogen enrichment in this abundance regime.

The ratio $[\text{O III}] \lambda 4959, 5007/[\text{N II}] \lambda \lambda 6548, 6584$, which was used by Alloin et al. (1979) as a nebular temperature indicator, and therefore indirectly as an abundance indicator, shows considerable scatter when plotted against our abundance indicator (Fig. 5, in which the two theoretical curves are similar to those of Fig. 4). Also, note that the total range covered by the observed $\text{H II}$ regions in the Alloin et al. (1979) ratio is much greater than in the $[\text{O II}] \lambda 3727/[\text{N II}] \lambda 6584$ ratio, but that the differences between the theoretical sequences for primary and secondary nitrogen enrichment are considerably smaller in Figure 5 than in Figure 4. The physical reason for both the scatter of the points and this range is that the Alloin et al. (1979)
Figure 4. Theoretical sequences employing the $\bar{Q}(\text{H})$–$Z$ relationship derived in the text and "solar" abundance ratios given in Table 1, showing the difference between primary and secondary nitrogen enrichment for the line ratio $(3727/6584)$ vs. $(3727 \cdot 3727/4861 \cdot 6731)$. Both sequences are normalized to the same N/O ratio at solar oxygen abundance. Tick marks indicate metallicities of $Z = 1/4$, $1/2$, $3/4$, and $3/2 \, Z_\odot$, while open circles indicate a metallicity of $2 \, Z_\odot$. The positions of H II regions in our observational data base are indicated by filled circles.
log (3727/6584)

log (3727.3727/4861.6731)
Figure 5. As Fig. 4, but for the Alloin et al. (1979) abundance sensitive line ratio $[\text{O} \, \text{iii}] \lambda\lambda4959, \, 5007/[\text{N} \, \text{ii}] \lambda\lambda6548, \, 6584$ vs. $(3727 \cdot 3727/4861 \cdot 6731)$. 
ratio is very sensitive to the value of $\overline{Q}(H)$. The range therefore reflects the $\overline{Q}(H)-Z$ correlation and the scatter the intrinsic scatter in the value of $\overline{Q}(H)$ at any given abundance. Without a proper relationship between $\overline{Q}(H)$ and $Z$, the nucleogenic status of nitrogen becomes uncertain.

The measurement of the nitrogen yield relative to the oxygen yield in individual galaxies can be used as a method of investigating the stellar initial mass function. According to the theory of Renzini and Voli (1981), nitrogen is synthesized in stars of 4–8 solar masses during various dredge-up phases. On the other hand, the oxygen yield is controlled by the rate of production of massive stars, so that, given an adequate theoretical basis, a secondary nitrogen yield can be used to put an observational constraint on the relative time-integrated star formation rates of intermediate mass stars and stars in the 15–50 solar mass range. However, only the first and second dredge-up phases produce secondary nitrogen. Renzini and Voli (1981) point out that when the third dredge-up phase occurs in conjunction with hot-bottom burning, primary nitrogen can be produced. This will occur for stars with a mass greater than some critical value, ~ 6.8 solar masses. Thus, scatter in the N/O–O relation can be caused by a variation in this primary yield and will be a measure of the relative enrichment resulting from the more massive and less massive intermediate mass stars. An alternative source of primary nitrogen is by direct production in supermassive stars (Woosley and Weaver 1982).

The scatter at the low-abundance end of Figure 4 is similar to, although less extreme than, that found by Pagel and Edmunds (1981). It appears that the more massive disk galaxies conform to a purely secondary slope down to low abundance, but that low-mass irregulars and blue compact
galaxies have N/O ratios which tend to be systematically lower at a given O abundance. From the above discussion, this could be either the result of a shallower IMF in the latter group, or a result of a variable efficiency of dredge-up in the hot-bottom burning phase, or a result of a past burst of supermassive star formation in the more massive galaxies.

V. COMPARISON WITH OBSERVATIONS

Following the procedure outlined in the previous section we have generated a theoretical sequence of H II regions that should reproduce the observed relative intensities of the [O II] λ3727, [O III] λλ4959, 5007, [S II] λλ6716,6731, [N II] λλ6548,6584, and Balmer lines. This sequence is characterized by a constant ionization temperature, $T_{\text{ion}} = 41,500 \text{ K}$, and the adopted set of elemental abundances given in Table 1 for “solar” composition. All abundance ratios are kept in their solar ratios at other metallicities, except for nitrogen which is treated as a secondary element with respect to oxygen. The adopted $Q(H)$ versus oxygen abundance is

$$\log Q(H) = 22.28 - 1.694 \times [12 + \log (O/H)], \quad 8.20 \lesssim 12 + \log (O/H) \lesssim 9.20.$$ 

We will now show that this sequence does in fact reproduce the observations in the diagnostic plots that are commonly used for excitation and abundance diagnostics.

a) Excitation Diagrams of Baldwin, Phillips, and Terlevich

The first of these, the plot of (5007/4861) versus (3727/5007), was used to derive the S/O abundance ratio (Fig. 3, above) and therefore should a priori yield a good fit to the observational data. To confirm this, we compare
TABLE 1

**ADOPTED “SOLAR” ABUNDANCES**

<table>
<thead>
<tr>
<th>Element</th>
<th>Number&lt;sup&gt;a&lt;/sup&gt;</th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>12.00</td>
</tr>
<tr>
<td>He</td>
<td>10.93</td>
</tr>
<tr>
<td>C</td>
<td>8.52</td>
</tr>
<tr>
<td>N</td>
<td>7.68</td>
</tr>
<tr>
<td>O</td>
<td>8.82</td>
</tr>
<tr>
<td>Ne</td>
<td>7.92</td>
</tr>
<tr>
<td>Mg</td>
<td>7.42</td>
</tr>
<tr>
<td>Si</td>
<td>7.52</td>
</tr>
<tr>
<td>S</td>
<td>7.30</td>
</tr>
<tr>
<td>Cl</td>
<td>5.6</td>
</tr>
<tr>
<td>Ar</td>
<td>6.8</td>
</tr>
</tbody>
</table>

<sup>a</sup>Log abundance by number relative to H = 12.00.
the final sequence of models to the observations in Figure 6. The excitation diagrams which use the [N II] lines are useful as a check that we have correctly solved the nitrogen abundance problem. The sequence of models is compared with the observations on the (6584/6563) versus (3727/5007) and the (5007/4861) versus (6584/6563) line ratio diagrams in Figures 7 and 8.

b) Pagel et al. (1979) and Alloin et al. (1979) Abundance Indicators

We have already pointed out that the Pagel et al. (1979) abundance indicator is also sensitive to $Q(H)$. However, the effect of the $Q(H)$–Z correlation we have derived is to enhance the utility of the $([\text{O II}] \lambda 3727 + [\text{O III}] \lambda \lambda 4959, 5007)/H\beta$ ratio as an abundance indicator. The physical reason for this is because, at constant $Q(H)$, the electron temperature of the nebula increases as the oxygen abundance decreases. Since the flux in the forbidden lines increases rapidly with electron temperature and the effective recombination rate for hydrogen decreases with electron temperature, the Pagel et al. (1979) ratio increases with decreasing abundance. However, this trend cannot continue indefinitely, and the ratio maximizes at some particular metal abundance. The forbidden-line emission maximizes when the collisional excitation rate peaks and decreases at lower abundances (higher $T_e$) where free-free and H, He recombination cooling dominate the forbidden lines. The effect of superposing a $Q(H)$–Z correlation is to push this maximum toward lower metallicity, so increasing the abundance range over which the Pagel et al. (1979) ratio is monotonic in its behavior. In Figure 9, we plot the Pagel et al. (1979) ratio against our own abundance sensitive ratio, $(3727 \cdot 3727/4861 \cdot 6731)$. Clearly, the theoretical sequence is an excellent fit to the observed sequence.
Figure 6. The final theoretical sequence plotted on the first BPT figure, (5007/4861) vs. (3727/5007).
Figure 7. As Fig. 6, but for the second BPT figure, (6584/6563) vs. (3727/5007).
Figure 8. As Fig. 6, but for the third BPT figure, (5007/4861) vs. (6584/6563).
Figure 9. The Pagel et al. (1979) abundance sensitive line ratio, ([O II] $\lambda 3727 +$ [O III] $\lambda \lambda 4959, 5007)/H\beta$, plotted against the abundance discriminant suggested in the text, ($3727 \cdot 3727/4861 \cdot 6731$), for the final theoretical sequence.
A consequence of the $\overline{Q}(H) - Z$ correlation is to change the absolute calibration of the abundance scale for H II regions, particularly at high $Z$. This occurs because the lower $\overline{Q}(H)$ at the high metallicity extreme allows the electron temperature to fall, and so quench the optical forbidden lines. For an oxygen abundance $12 + \log (O/H)$ much greater than 9.2, the H II region spectrum will simply consist of recombination lines in the visible. The effect of our recalibration of the abundance scale in H II regions is shown in Figure 10.

The Alloin et al. (1979) $[O \, iii] \lambda\lambda 4959,5007/[N \, ii] \lambda\lambda 6548,6584$ ratio is not very useful as an abundance indicator, because it is so sensitive to the intrinsic scatter in $\overline{Q}(H)$ and because, as we discussed above, there appears to be real scatter in the N/O–O abundance relation at low abundances. This probably accounts for the large scatter in the observational points of Figure 11, in which we plot the Alloin et al. (1979) ratio against our abundance indicator. Nevertheless, the fit at high $Z$ is good, which gives us confidence in the accuracy of our calibration in this regime.

As a temperature indicator, on the other hand, the Alloin et al. (1979) ratio is much more useful, particularly at the high abundance end. Indeed, as we indicated in the introduction, this ratio was originally intended to be used for this purpose. In Figure 12 we plot the predicted $[O \, iii] \lambda\lambda 4959,5007/[N \, ii] \lambda\lambda 6548,6584$ ratio against the mean electron temperature in the O $^{++}$ zone, $\langle T_{[O \, iii]} \rangle$, for our model sequence and for the Alloin et al. (1979) empirical calibration of the observational material. The fact that these are in close agreement shows that our calibration sequence predicts the correct electron temperatures, and since the temperature is critically dependent on both $\overline{Q}(H)$ and $Z$, this agreement gives us more confidence in the $\overline{Q}(H) - Z$
Figure 10. Calibration of oxygen abundance vs. the Pagel et al. (1979) abundance indicator ([O ii] λ3727 + [O iii] λλ4959, 5007)/Hβ derived from the theoretical sequence. Also shown are the previous calibrations of Edmunds and Pagel (EP; 1984) and McCall, Rybski, and Shields (MRS; 1985).
Figure 11. The Alloin et al. (ACJV; 1979) abundance sensitive line ratio $\text{[O III]} \lambda \lambda 4959, 5007/\text{[N II]} \lambda \lambda 6548, 6584$, plotted against the abundance discriminant $(3727 \cdot 3727/4861 \cdot 6731)$ for the final theoretical sequence.
log (4,959,500/654,865,844)

log (3727.3727/4861.6731)
Figure 12. Calibration of [O III] λ4959, 5007/[N II] λλ6548, 6584 vs. electron temperature in the O++ zone, (T_{O III}), derived from the theoretical sequence. Also shown is the calibration derived by Alloin et al. (1979).
\[
\log(4.959,5007/6548,6584) \\
\langle T_{\text{[OIII]}} \rangle \times 10^{-3}
\]
calibration in the high abundance limit. We regard this as important, since our recalibration of the abundance scale for H II regions differs most severely from that which is commonly adopted at the high-Z end.

VI. A METHOD FOR DERIVING CHEMICAL ABUNDANCES OF H II REGIONS

Since our sequence of models successfully describes the variety of H II region spectra that are observed, we are now in a position to invert the question and ask whether, from an observational measurement of only the brightest optical lines, a set of chemical abundances can be derived for a given H II region.

a) The Heavy Elements

The brightest optical emission lines are those of [O II] \( \lambda 3727 \), [O III] \( \lambda \lambda 4959, 5007 \), [N II] \( \lambda \lambda 6548, 6584 \), and [S II] \( \lambda \lambda 6716, 6731 \). Thus we should aim to derive O, N, and S abundances. In Figures 13a–13d, we use our theoretical sequence to plot, as a function of oxygen abundance, the ratios \( ([O \text{ II}] \lambda 3727 + [O \text{ III}] \lambda \lambda 4959, 5007) / /H\beta \) (as in Pagel et al. 1979), \( [S \text{ II}] \lambda 6731 / /H\alpha \), \( [O \text{ II}] \lambda 3727 / [N \text{ II}] \lambda 6584 \), and finally our abundance indicator ratio. In each plot, the solid line depicts the theoretical sequence derived above, while the dashed lines labeled "\( N \times 2 \)," "\( N \div 2 \)," "\( S \times 2 \)," and "\( S \div 2 \)" indicate the sequence with nitrogen or sulfur abundances multiplied or divided by two at each point. To derive theoretical abundances from these diagrams we recommend the following procedure.
Figure 13. (a) Theoretical sequence calibration of the abundance sensitive line ratio ([O II] λ3727+[O III] λλ4959, 5007)/Hβ vs. 12+log (O/H), (b) theoretical sequence calibration of the line ratio (6731/6563) vs. 12 + log (O/H), (c) theoretical sequence calibration of the line ratio (3727/6584) vs. 12 + log (O/H), and (d) theoretical sequence calibration of the line ratio (3727 · 3727/4861 · 6731) vs. 12 + log (O/H). In each figure, the adopted theoretical sequence is indicated by a solid line, while dashed lines illustrate the sequence with nitrogen or sulfur abundances increased or decreased by a factor of 2 at each point.
\[ \log \left( \frac{3727}{6584} \right) \]
1. Use each of these ratios to derive “independent” estimates of $12 + \log (O/H)$ from the theoretical sequence and take the mean.

2. Next, use this mean to estimate theoretical $[\text{N II}] \, \lambda 6584$ and $[\text{S II}] \, \lambda 6731$ line intensities from the sequence.

3. Use these theoretical values with the observed oxygen line intensities to refine the estimate of the oxygen abundance from Figures 13a, 13c, and 13d and iterate between steps 2 and 3 until the difference between iterations is less than 0.01 dex.

4. With this oxygen abundance, compare the predicted and observed $[\text{N II}] \, \lambda 6584$ and $[\text{S II}] \, \lambda 6731$ line strengths in Figures 13c and 13d to obtain the corrected nitrogen and sulfur abundances, using the scaling between the line intensity and the abundance given in the figures. Since the strength of the sulfur line is very dependent on $Q(H)$, it should be recognized that the sulfur abundance derived by this method is rather uncertain.

5. If the derived nitrogen or sulfur abundance is far from that employed in the adopted sequence, it may be necessary to iterate steps 1–4 interpolating on the figures to the correct nitrogen and sulfur abundances.

It is important to realize that the accuracy with which chemical abundances may be derived using this procedure will often be limited by the accuracy with which reddening corrections for the observational data can be determined. This is particularly true for ratios involving $[\text{O II}] \, \lambda 3727$ for
which the reddening correction is not trivial. The use of reddening corrections derived from Hβ/radio measurements is not valid because of the possible presence of regions of complete obscuration in the optical. Possibly the most accurate method for deriving the [O ii] λ3727 intensity is by comparison with higher order Balmer emission lines, although this is not possible if there is appreciable underlying continuum contributing a component of Balmer absorption.

b) Helium

The helium abundance varies over a very restricted range compared to that encountered for the heavy elements. This is the justification for using a constant helium abundance in our theoretical models. If we wish to derive an accurate helium abundance, it is therefore of paramount importance to have accurate ionization correction factors (Peimbert and Torres-Peimbert 1974, 1976). These depend critically on $\Theta(H)$, and since $\Theta(H)$ and $Z$ are correlated, then this implies that the ionization correction factors depend on the heavy element abundance as well. In Figure 14, we plot, for our $\Theta(H)-Z$ correlation the theoretical variation of the line intensities relative to Hβ of the triplet λ4471 and λ5876 lines and the singlet λ6678 line. Since there is real scatter in $\Theta(H)$ at a given $Z$, we also show the effect of varying $\Theta(H)$.

Another important factor which may affect the accuracy of any abundance estimate is the line transfer in the nebula. It is generally assumed that, for helium as well as hydrogen, the nebula is optically thick in the Lyman series lines (case B). This assumption is almost certainly valid for the
Figure 14. Calibration of the line ratios He I λ4471/Hβ, He I λ5876/Hβ, and He I λ6678/Hβ vs. 12 + log (O/H). Final theoretical sequence is indicated by the heavy line, while the other lines illustrate the line ratios for log $\langle Q(H) \rangle = 6.5, 7.0, 7.5, and 8.0$ cm$^{-1}$. 
helium triplet series, but may not be true for certain nebular geometries in the singlet lines (Brocklehurst 1971, 1972; Robbins and Robinson 1971).

The recombination coefficients are electron temperature dependent, so that in principle it is important to know this. However, in practice, this is not a problem, since the temperature dependence of the ratio of hydrogen and helium recombination lines in the optical is typically very weak (Brocklehurst 1971).

A more insidious problem is the effect of helium blanketing in the exciting star, since this directly affects the number of ionizing photons capable of ionizing helium, and therefore the extent of the zone of the nebula which contains ionized helium. However, since our sequence correctly describes the excitation of the H II regions at different metallicities, we believe that, if this effect is present, we have correctly compensated for it in our adopted $\overline{Q}(H) - Z$ relationship.

On the basis of these considerations, we recommend the following procedure for the derivation of the helium abundance.

1. Having determined the heavy element abundance by the above procedure, read off the $\overline{Q}(H)$ value which applies to the observed H II region using the $\overline{Q}(H) - Z$ diagnostic diagrams, Figures 1, 2, or 3.

2. From Figure 14, read off the predicted line strengths of the helium lines.

3. Compute the helium abundance from each of the line ratios, assuming that the line strength scales directly as the abundance. If the value obtained for the singlet line does not agree with that obtained for the
triplet lines, this is an indication that the assumption of case B may not be valid, in which case only the triplet lines should be used to derive the helium abundance and the result should be treated with caution.

Abundance estimates for individual H II regions derived by the method proposed here are probably not very reliable, but when many H II regions are observed the method should be valid in a statistical sense. In any event, as we shall show in Paper III of this series, this method makes a useful point of departure for more detailed modeling.

VII. CONCLUSIONS

Employing the homogeneous grid of photoionization models described in Paper I, we have generated a theoretical fit to the observed spectral sequence of extragalactic H II regions. Comparison of the region of parameter space spanned by the theoretical models of Paper I with the observed distribution of H II regions demonstrates that the latter form a narrow emission-line ratio spectral sequence. In this paper, we have derived the correlation between ionization parameter and metallicity suggested in Paper I, and have computed the sequence of theoretical photoionization models necessary to calibrate the observed H II region spectral sequence in terms of elemental abundances.

We have established the correlation between \( \overline{Q}(H) \) and oxygen abundance over the range of metallicities observed (\( \sim \frac{1}{4} - 2 Z_\odot \)), and have modeled the correlation with a simple functional form which fits the observed emission line data. An explanation for the derived \( \overline{Q}(H) - Z \) correlation has been proposed in § IVb.
Comparison of the models with the observational data implies that nitrogen must be enriched as a secondary element, except at very low abundances where there is sufficient scatter in the data to suggest that there may be a primary component of nitrogen at low $Z$. The implications of the latter were briefly discussed in § IVc.

We have demonstrated that the theoretical sequence proposed in this paper reproduces the observed sequences of H II regions on a number of diagrams commonly used for excitation and abundance diagnostics, and this gives us faith in the validity of the theoretical sequence. We have employed our sequence to recalibrate the semiempirical abundance sensitive line ratios of Pagel et al. (1979), Edmunds and Pagel (1984), and McCall, Rybski, and Shields (1985). The major consequence of this recalibration is to change the absolute calibration of the abundance scale at high $Z$. For example, at a metallicity of $\sim 2 Z_\odot$, our calibration of the oxygen abundance is $\sim 0.25$ dex lower than the calibrations of Edmunds and Pagel (1984) and McCall, Rybski, and Shields (1985). Our calibration of electron temperature in the O$^{++}$ zone agrees with that found empirically by Alloin et al. (1979) over much of the range of conditions observed, but our models illustrate that the Alloin et al. (1979) ratio is not particularly useful as an abundance discriminant because of its inherent sensitivity to the intrinsic scatter in observed $\overline{Q}(H)$ and because of the scatter in the N/O–O abundance relation at low $Z$.

Finally, we have prescribed a method for deriving oxygen, nitrogen, and sulfur abundances from bright emission-line ratios in H II regions by utilizing both previously employed abundance sensitive line ratios, and a new abundance discriminant proposed in this paper, $(3727 \cdot 3727/4861 \cdot 6731)$. We
have also presented sufficient theoretical data to enable helium abundances to be derived from measurements of the intensities of He I emission lines.

In the third paper in this series, we will apply the calibration and techniques described here to derive abundances in H II regions, and the abundance gradient, in the bright northern spiral galaxy M101.

We wish to thank the Anglo-Australian Observatory for use of their computing facilities in calculating many of the models described here. We also wish to thank the referee, John Mathis, for many valuable suggestions for improving the quality of this paper. One of us (I.N.E.) acknowledges the receipt of an Australian Commonwealth Postgraduate Research Award.
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III. THE ABUNDANCE GRADIENT IN M101

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ABSTRACT

The theoretical H II region abundance sequence calibration described in the second paper in this series has been employed to determine oxygen and other heavy element abundances in a selection of well-observed H II regions in M101. Comparison of abundances derived from the abundance sequence with abundances derived from “exact” photoionization modeling demonstrate that the accuracy with which H II region abundances may be derived from the sequence is \( \sim 0.15 \) dex. The data have been employed to measure radial abundance gradients and heavy element yields for oxygen, nitrogen, and sulfur in M101.

The abundance gradient and heavy element yield data suggest that the production of elements by massive stars (oxygen, neon) is enhanced in the inner regions of the disk of M101, while the production of heavy elements (S, Ar, Ca, Fe) by low and intermediate mass stars is enhanced in the outer disk. A model for galaxy disk formation is suggested which is at least qualitatively capable of explaining these observations.

Subject headings: galaxies: evolution — galaxies: individual — nebulae: abundances — nebulae: H II regions
I. INTRODUCTION

In recent years considerable effort has been applied to the task of developing an abundance calibrated sequence for giant extragalactic H II regions which employs only ratios of prominent emission lines to derive elemental abundances over the full range of abundances observed. Formerly, the semiempirical ionization correction factor technique of Peimbert and Costero (1969) was used to derive abundances in many H II regions (e.g., Peimbert and Torres-Peimbert 1974, 1976; Dufour 1975, 1977; Smith 1975; Pagel et al. 1978; Lequeux et al. 1979), but this method relies upon detection of the temperature-sensitive line [O III] λ4363 which is either very faint or not visible in the spectra of metal-rich H II regions. Sarazin (1976) attempted to fit the entire sequence of H II regions with theoretical models and concluded that there must be an excitation variation in addition to the abundance variation in order to fit the data at high metallicity. Pagel et al. (1979) proposed an empirical calibration of oxygen abundance using the line ratio ([O II] λ3727 + [O III] λλ4959, 5007)/Hβ and extended this work (Pagel, Edmunds, and Smith 1980; Edmunds and Pagel 1984) following theoretical calculations of Dufour et al. (1980). This calibration has also been studied by McCall (1982; see also McCall, Rybski, and Shields 1985), who employed a large homogeneous data set and photoionization modeling in order to calibrate the sequence. Recently, Evans and Dopita (1985, hereafter Paper I) computed an extensive homogeneous grid of photoionization models suitable for diagnosing the physical conditions in H II regions and employed these models to recalibrate, on a theoretical basis, the H II region abundance sequence (Dopita and Evans 1986, hereafter Paper II).
In this paper, the abundance calibration defined in Paper II is employed to derive oxygen abundances for number of H II regions in the bright northern spiral M101, a nearby, almost face-on Sc galaxy with prominent and well-studied H II regions. Theoretical photoionization models are computed for a subset of the H II regions studied in order to assess the accuracy with which oxygen abundances can be derived using the abundance sequence calibration as suggested in Paper II. These data are combined to derive the oxygen abundance gradient in M101 and also to examine the radial abundance dependence of other elements. Finally, the implications of these results for galaxy evolution and chemical enrichment models are discussed.

II. THE OBSERVATIONAL DATA BASE

a) H II Region Spectrophotometry

The spectrophotometric data employed in this paper are taken from the work of Smith (1975), Shields and Searle (1978, hereafter SS), McCall (1982), and Rayo, Peimbert, and Torres-Peimbert (1982, hereafter RPT). Reddening-corrected line intensity data are utilized for every H II region with measured [O II] λ3727, [O III] λλ4959,5007, [N II] λλ6548,6584, and [S II] λλ6716,6731. Where more than one author provides data for a given H II region, the most recent data are used. For each H II region, the source for the measured line strengths is given in Table 1, together with additional information relevant to the observations. The radial distance of each H II region from the nucleus of the galaxy projected onto the plane of the galactic disk is indicated in Table 1 in the column headed $\rho R_0$, where the adopted isophotal radius is taken to be $R_0 = 14'06'' = 16.62$ kpc and the adopted distance to M101 is
### TABLE 1

**Spectrophotometric Data Sources**

<table>
<thead>
<tr>
<th>Object</th>
<th>( \rho R_0 ) kpc</th>
<th>Instrument(^a)</th>
<th>Reference(^b)</th>
</tr>
</thead>
<tbody>
<tr>
<td>S1</td>
<td>1.66</td>
<td>IDS</td>
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<td>Smith No. 3</td>
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<tr>
<td>H40</td>
<td>3.49</td>
<td>IIDS</td>
<td>2</td>
</tr>
<tr>
<td>S5</td>
<td>3.82</td>
<td>MCS</td>
<td>3</td>
</tr>
<tr>
<td>H47</td>
<td>4.32</td>
<td>IIDS</td>
<td>2</td>
</tr>
<tr>
<td>H69-24</td>
<td>5.30</td>
<td>IDS</td>
<td>4</td>
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<tr>
<td>NGC 5461</td>
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<td>2</td>
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<tr>
<td>H69-63</td>
<td>5.72</td>
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<td>H69-142</td>
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<td>NGC 5455</td>
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<td>MCS</td>
<td>3</td>
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<td>4</td>
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<td>NGC 5471</td>
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<td>IIDS</td>
<td>2</td>
</tr>
</tbody>
</table>

\(^a\)IDS: Image Dissector Scanner; IIDS: Intensified Image Dissector Scanner; MCS: Multichannel Spectrometer

\(^b\)(1) Smith *et al.* 1975; (2) RPT; (3) SS; (4) McCall 1982.
4.06 Mpc (McCall 1982). The inclination of the galaxy to the line of sight is taken to be 18° while the position angle of the line of nodes is 39° (Bosma, Goss, and Allen 1981).

The spectrophotometry assembled here is somewhat inhomogeneous with regard to both instrumental photometric accuracy and also the signal-to-noise ratio of individual observations. It is unlikely, however, that instrumental errors will dominate over variations in measured line intensities which can result simply from observing the emission from different locations within the H II regions, either because different size apertures are employed or slightly different positions are measured by different observers. For example, both RPT and Sedwick and Aller (1981) have measured line intensities for the bright H II regions NGC 5461 and NGC 5471, but comparison of the two data sets indicate discrepancies in the reddening-corrected line intensities from the "same" object of up to ~ 0.15 dex, while the logarithmic reddening corrections, C(H/β), deduced from the two sets of data vary by ~ 0.3 dex for the same object. In this connection it is interesting to note that [O II] λ3727 shows substantial variations between the two sets of data. When comparing observed line strengths with predictions from theoretical photoionization models, it is important to realize that the line intensities computed in the models are integrated emission over the whole nebula, while observed intensities usually result from measurements of the brightest central region of the nebula only. As a result there may well be an observational bias which decreases the apparent intensities of lines emitted by lower ionization species (which are found in the hydrogen transition zone and the boundaries of the nebula) relative to the intensities of the lines emitted by the high ionization species found near the center of the nebula. This bias must be considered
when employing ratios with emission lines likely to be so affected, such as [O I] $\lambda$6300, for example.

\[ \text{b) Surface Density Data} \]

In order to interpret the abundance gradients derived in § IIIc in terms of chemical enrichment models and elemental yields, it is necessary to know the present day radial distribution of the gas to total mass surface densities in the disk.

The gas surface density is derived from the observed neutral and molecular hydrogen distributions according to the expression

\[
\sigma_{\text{gas}} = 1.30 [\sigma_{\text{H}_1} + \sigma_{\text{H}_2}],
\]

where $\sigma_x$ is the surface density of the quantity $x$ in units of $M_\odot \text{pc}^{-2}$. The factor 1.30 takes into account the contribution of the helium mass to the gas density assuming $N(\text{He})/N(\text{H}) = 0.075$, which was derived from the mean helium abundance from the theoretical photoionization models computed in § IIIb. The $\text{H}_1$ surface density distribution is taken from McCall (1982) who derived it from the $\text{H}_1$ column density measurements of Bosma, Goss, and Allen (1981). The molecular hydrogen surface density is derived from millimeter CO observations of Solomon et al. (1983) after correction to the adopted distance of the galaxy. The correction factor employed to convert $^{12}\text{CO}$ surface integrated intensity to molecular hydrogen surface density is quoted by Solomon et al. (1983) also. The total gas surface density determined by equation (1) is well represented by an exponential with a scale length of 7.3 kpc over a range of radius from 1.5 kpc to 12 kpc, except in the
region 3–4 kpc where a slight deficiency of gas relative to the fitted exponential is observed.

The total mass surface density radial distribution for M101 was taken from McCall (1982) who employed a Monnet and Simien (1977) thick exponential disk model to fit the rotation curve measurements of Rogstad and Shostak (1972) and Bosma, Goss, and Allen (1981). He derived a total mass surface density which varies as

\[ \log \sigma_T = \log \sigma_e - 0.7290 (R/R_e - 1), \]

where \( \log \sigma_e = 2.596 \, M_\odot \, \text{pc}^{-2} \) and \( R_e = 3.88 \, \text{kpc} \), from which a total disk mass of \( 7.1 \times 10^{10} \, M_\odot \) may be derived. Comparison of the theoretical rotation curve derived from the exponential disk model with the observations indicates that the mass distribution should be reliable in the region \( 2 \, \text{kpc} \lesssim R \lesssim 8 \, \text{kpc} \). At larger radii, the model fit deteriorates rapidly, and indeed at radii larger than 7' (~ 8.25 kpc at the distance of M101) Bosma, Goss, and Allen (1981) claim that the velocity field is too irregular to allow an accurate rotation curve to be derived. At radii less than \( \sim 2 \, \text{kpc} \), the spheroidal component starts to contribute significantly to the total mass surface density, and so the disk contribution is correspondingly uncertain.

III. ABUNDANCES IN H II REGIONS AND
THE ABUNDANCE GRADIENT IN M101

a) Abundances from the Theoretical Sequence of Paper II

For the majority of H II regions indicated in Table 1, the oxygen abundances have been estimated using reddening-corrected emission-line ratios
from the theoretical abundance sequence described in Paper II, employing the techniques suggested there. In some cases, however, the recommended procedure did not converge, usually because one or more of the abundance estimators yielded an initial value of $12 + \log (O/H)$ at substantial variance with the others. In such cases the oxygen abundance was derived solely from the line ratio $([\text{O} \, \text{ii}] \lambda 3727 + [\text{O} \, \text{iii}] \lambda \lambda 4959, 5007)/H\beta$ which, to first order, depends only on the oxygen abundance and is independent of the O/N and O/S ratios. For the low abundance H II region NGC 5471, no abundance estimate was derived from the abundance sequence, since the line ratios indicate $12 + \log (O/H) \approx 8.2$ for this object, and the abundance estimators have essentially no discrimination at such low abundances. Instead, the abundance of NGC 5471 was derived solely from individual theoretical photoionization models (see § IIIb). The results of the oxygen abundance determinations from the abundance sequence of Paper II are shown in Table 2.

The formal error in the oxygen abundance derived from consistency of the three estimators when the technique suggested in Paper II is applied is typically small, of order 0.05 dex. This is particularly true for high metallicity ($Z \gtrsim Z_\odot$) H II regions since the abundance estimators become progressively less sensitive to errors in the line ratios as $Z$ increases. For most objects, it is probable that the total error in the oxygen abundance will be dominated by errors resulting from differences between the actual physical conditions (e.g., ionization parameter, stellar temperature) in the nebula and the corresponding conditions adopted for the abundance sequence derived in Paper II. If the physical conditions change relative to the adopted sequence in a systematic way with radius, as has been suggested for stellar temperature (SS), for example, then the abundance gradients derived from the sequence may be in error. Although there is an apparent change in stellar temperature
<table>
<thead>
<tr>
<th>Object</th>
<th>$12 + \log (O/H)$</th>
</tr>
</thead>
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<tr>
<td>S1</td>
<td>9.08 ± 0.02</td>
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<tr>
<td>H108+111</td>
<td>9.06 ± 0.01</td>
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<tr>
<td>Smith No. 3</td>
<td>8.92 ± 0.04</td>
</tr>
<tr>
<td>H40</td>
<td>8.85 ± 0.01</td>
</tr>
<tr>
<td>S5</td>
<td>8.96 ± 0.01</td>
</tr>
<tr>
<td>H47</td>
<td>8.96 ± 0.02</td>
</tr>
<tr>
<td>H69–24</td>
<td>8.88 ± 0.12</td>
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<tr>
<td>NGC 5461</td>
<td>8.58^a</td>
</tr>
<tr>
<td>H69–63</td>
<td>8.75 ± 0.02</td>
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<td>H69–142</td>
<td>8.73 ± 0.01</td>
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<td>NGC 5462</td>
<td>8.67^a</td>
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<td>8.39 ± 0.13</td>
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<tr>
<td>S12</td>
<td>8.31^a</td>
</tr>
</tbody>
</table>

^a Derived from ([O II] $\lambda$3727 + [O III] $\lambda\lambda$4959, 5007)/H$\beta$ only
with radius in the individual H II region models presented in the next sub-
section, comparison of the slopes of the abundance gradients derived from
the abundance sequence alone with the those derived only from the "exact"
photoionization models suggests that either the stellar temperature does not
vary in a systematic fashion with radius, or that the effect of changing stellar
temperature on the derived abundance gradients is not important, or both.

b) Abundances from Theoretical Photoionization Models

We have computed individual photoionization models for four H II re-
gions in M101 using the multipurpose modeling code MAPPINGS, described
in Paper I (§ III) and references cited therein. The objects modeled are
NGC 5471, NGC 5461, and H40 (RPT) which have flux estimates for many
faint optical emission lines which can be employed to constrain the model pa-
rameters, and the nebula S5 (SS). The latter object has been included since
previous semiempirical calibrations of the extragalactic H II region abundance
sequence (Pagel et al. 1979; McCall 1982) have relied upon theoretical models
of this object to define the high-Z behavior of the abundance sequence.

Except as noted below, the H II region models are identical in struc-
ture to those described in Paper I (§ III), which should be referred to for a
more detailed description of the calculations. Each H II region was modeled
as a steady-state spherically symmetric nebula consisting of infinitesimal fil-
aments of gas with volume filling factor \( \epsilon \), surrounding a centrally located
source of ionizing photons which is modeled as a single star with ionization
temperature \( T_{\text{ion}} \). The stellar atmosphere flux is derived from the \( \log g = 4.0 \)
models of Hummer and Mihalas (1970) interpolated to the desired \( T_{\text{ion}} \) and
the same metal abundance set as employed for the nebula using the technique of SS.

The parameters which define a particular model are the number of Lyman continuum photons, $L_C$; the number density of hydrogen atoms plus ions, $N_H$; the ionization temperature of the central source, $T_{\text{ion}}$; the ionization parameter (defined in Paper I), $\overline{Q}(\text{H})$; and the chemical abundance set employed. The Lyman continuum flux was adjusted to give a value,

$$L_C = \int_{\nu_m}^{\infty} \left( \frac{L_\nu}{h \nu} \right) d\nu,$$

equal to that inferred from the observed Hβ luminosity. The density of the models was fixed on the basis of observations of density-sensitive emission-line ratios (principally $\text{[S II]} \lambda 6716/\lambda 6731$). The relative abundances of the elements He, N, O, and S (all models), and Ne and Ar (except for the S5 model), together with $\overline{Q}(\text{H})$ and $T_{\text{ion}}$ were adjusted to fit the observed emission line strengths. The abundances of the other elements (and, in the case of S5, Ne and Ar) were fixed in their solar ratio (Allen 1973) to the oxygen abundance. Chemical abundances derived in this manner are likely to be more accurate than abundances deduced from either observed or model electron temperatures using the ionization correction factor technique, for the following reasons. First, determinations based on observed electron temperatures may have substantial errors, particularly for high-metallicity objects, since the temperature-sensitive line ratios rely upon measurements of weak auroral transitions. On the other hand, model electron temperatures may be very sensitive to the (usually unknown) geometrical structure of the nebula and other inadequacies in the models, resulting in potentially large errors in derived abundances. Second, the ionization correction factors themselves are
difficult to determine, and are best computed from theoretical nebular models anyway (Mathis 1982, 1985). Altering $T_{\text{ion}}$ changes the "hardness" of the ionizing spectrum, with a larger value of $T_{\text{ion}}$ resulting in a spectrum with relatively more high energy photons which will produce a larger transition zone at the edge of the nebula and hence stronger emission from lines, such as $[\text{O} \, \text{I}] \lambda 6300$, produced in that zone. Since both $L_C$ and the total number density of atoms plus ions, $N$, are fixed, then from Paper I ($\S$ IIIc), for a spherically symmetric nebula without an empty zone,

$$Q(\text{H}) = \frac{L_C}{4\pi \bar{r}^2 N}$$

$$= \left[ \frac{16}{97} L_C N \epsilon^2 a_B^2 \right]^{1/3}$$

$$\propto \epsilon^{2/3},$$

since $L_C = \left(4\pi/3\right) R^3 N^2 \epsilon a_B$ and $\bar{r} = \frac{1}{2} R$ where $R$ is the Strömgren radius of the nebula, and $a_B$ is the case B recombination coefficient for hydrogen calculated at $T = 10^4$ K. Thus $Q(\text{H})$ is altered by changing $\epsilon$, and so the geometry of the nebula determines the ionization parameter. A larger $Q(\text{H})$ implies a larger volume filling factor (up to the point where $\epsilon = 1$, which places an implicit limit on how great a value $Q(\text{H})$ can attain) and hence a more compact and more uniform nebula with higher opacity and greater emission from the high ionization species located close to the central star.

The initial model for NGC 5471 used the oxygen abundance estimated by RPT, and the Lyman continuum flux was fixed at $L_C = 2.1 \times 10^{51}$ s$^{-1}$ on the basis of the observed H$\beta$ flux. Trial and error led to a model with $12 + \log (\text{O/H}) = 8.20$, $T_{\text{ion}} = 50,000$ K, $Q(\text{H}) = 4.00 \times 10^8$ cm s$^{-1}$, and a density of $300$ cm$^{-3}$. The parameters of the final model are presented in Table 3, while the observed and predicted line intensities are presented in Table 4. Inspection of the table demonstrates the quality of the fit, which accurately
<table>
<thead>
<tr>
<th>Parameter</th>
<th>NGC 5471</th>
<th>NGC 5461</th>
<th>H40</th>
</tr>
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<tr>
<td>$T_{\text{ion}}$ K</td>
<td>50,000</td>
<td>43,000</td>
<td>41,000</td>
</tr>
<tr>
<td>$L_C$ s$^{-1}$</td>
<td>$2.1 \times 10^{51}$</td>
<td>$2.8 \times 10^{51}$</td>
<td>$7.1 \times 10^{50}$</td>
</tr>
<tr>
<td>$Q(H)$ cm s$^{-1}$</td>
<td>$4.00 \times 10^{8}$</td>
<td>$1.80 \times 10^{8}$</td>
<td>$6.66 \times 10^{7}$</td>
</tr>
<tr>
<td>$N_H$ cm$^{-3}$</td>
<td>300</td>
<td>250</td>
<td>90</td>
</tr>
<tr>
<td>$\epsilon$</td>
<td>0.050</td>
<td>0.014</td>
<td>0.011</td>
</tr>
<tr>
<td>$R_{\text{pc}}$</td>
<td>25.9</td>
<td>48.6</td>
<td>57.4</td>
</tr>
<tr>
<td>He/H</td>
<td>0.074</td>
<td>0.077</td>
<td>0.061</td>
</tr>
<tr>
<td>12 + log (O/H)</td>
<td>8.20</td>
<td>8.76</td>
<td>8.99</td>
</tr>
<tr>
<td>12 + log (N/H)</td>
<td>6.71</td>
<td>7.46</td>
<td>7.79</td>
</tr>
<tr>
<td>O/S</td>
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<td>42.5</td>
<td>69.4</td>
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<td>O/Ne</td>
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<tr>
<td>O/Ar</td>
<td>123</td>
<td>366</td>
<td>443</td>
</tr>
<tr>
<td>Ion</td>
<td>NGC 5471</td>
<td>NGC 5461</td>
<td>H40</td>
</tr>
<tr>
<td>-----</td>
<td>----------</td>
<td>----------</td>
<td>-----</td>
</tr>
<tr>
<td>[O II] λ3727</td>
<td>+0.16</td>
<td>+0.19</td>
<td>+0.39</td>
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<tr>
<td>[Ne III] λ3869</td>
<td>-0.20</td>
<td>-0.22</td>
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<tr>
<td>[Ne III], H7 λ3968</td>
<td>-0.46</td>
<td>-0.46</td>
<td>-0.64</td>
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<td>[S II] λλ4068, 76</td>
<td>-1.89</td>
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<tr>
<td>Hδ λ4102</td>
<td>-0.59</td>
<td>-0.59</td>
<td>-0.59</td>
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<td>Hγ λ4340</td>
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<td>-0.31</td>
</tr>
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<td>[O III] λλ4363</td>
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<td>He i λ4471</td>
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</tr>
<tr>
<td>Hβ λ4861</td>
<td>+0.00</td>
<td>+0.00</td>
<td>+0.00</td>
</tr>
<tr>
<td>[O III] λ4959</td>
<td>+0.33</td>
<td>+0.41</td>
<td>+0.00</td>
</tr>
<tr>
<td>[O III] λ5007</td>
<td>+0.83</td>
<td>+0.87</td>
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<tr>
<td>[N I] λ5200</td>
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<td>-1.02</td>
<td>-0.96</td>
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<tr>
<td>[O I] λ6300</td>
<td>-1.66</td>
<td>-1.58</td>
<td>-1.92</td>
</tr>
<tr>
<td>[S II] λλ6310</td>
<td>-1.90</td>
<td>-1.34</td>
<td>-1.99</td>
</tr>
<tr>
<td>[N II] λ6548</td>
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<td>-1.61</td>
<td>-0.98</td>
</tr>
<tr>
<td>He λ6563</td>
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<td>+0.45</td>
<td>+0.45</td>
</tr>
<tr>
<td>[N II] λ6584</td>
<td>-1.13</td>
<td>-1.14</td>
<td>-0.51</td>
</tr>
<tr>
<td>He i λ6678</td>
<td>-1.58</td>
<td>-1.56</td>
<td>-1.52</td>
</tr>
<tr>
<td>[S II] λ6716</td>
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<td>-1.11</td>
<td>-0.97</td>
</tr>
<tr>
<td>[S II] λ6731</td>
<td>-1.18</td>
<td>-1.19</td>
<td>-1.05</td>
</tr>
<tr>
<td>He i λ7065</td>
<td>-1.67</td>
<td>-1.87</td>
<td>-1.69</td>
</tr>
<tr>
<td>[Ar III] λ7136</td>
<td>-1.25</td>
<td>-1.26</td>
<td>-1.12</td>
</tr>
<tr>
<td>[O II] λλ7320, 30</td>
<td>-1.50</td>
<td>-1.32</td>
<td>-1.52</td>
</tr>
</tbody>
</table>

**NOTE**—log \( I_{\text{obs}} \) is the observed logarithmic line intensity relative to Hβ; log \( I_{\text{mod}} \) is the predicted logarithmic line intensity relative to Hβ.
reproduces both the absolute H$\beta$ luminosity and also the relative intensities of the majority of the optical forbidden lines. In general, the temperatures of the various ionized zones are well reproduced by the model, although the temperature of the O$^+$ zone is slightly overestimated. This is shown by comparison of the predicted and observed [O ii] $\lambda\lambda$7320, 7330/[O ii] $\lambda$3727 ratios. The [S iii] $\lambda$6310 line is predicted to be much stronger than actually observed, and this is also true of the [S iii] $\lambda$λ9069, 9532 lines compared to the measurements of SS (log $\{I ([S \, iii] \lambda\lambda 9069, 9532) / I (H\beta)\} = +0.26$ predicted versus $-0.20$ observed). Geometrical differences between the model and the nebula, or temperature fluctuations in the nebula, may be responsible for the discrepancy between the observed and predicted line intensities. Increasing the ionization fraction of S$^{++}$ would result in a better match to the [S iii]/[S ii] line ratios and between the sulfur lines and H$\beta$ at a lower sulfur abundance, and in this connection it is interesting to note that RPT derive a sulfur abundance 0.45 dex lower than that derived here. The [N i] $\lambda$5200 doublet is predicted too weak by a factor of $\sim 2$, but this line is emitted in the hydrogen transition zone and its intensity is strongly affected by both the density and geometrical structure of the edge of the nebula. Finally, the He i $\lambda$7065 line is stronger than predicted, and this is due to enhanced emission of this line because of resonance fluorescence by self-absorption of $\lambda$3889 photons due to the large optical depth.

The parameters for the photoionization models, and the observed and predicted line intensities of NGC 5461 and H40 are also displayed in Tables 3 and 4. Many of the comments made in regard to the model of NGC 5471 apply to these models as well. For NGC 5461, the data in Table 4 suggest that the temperature of the O$^{++}$ zone is predicted to be too small since the auroral [O iii] $\lambda$4363 line is 0.23 dex weaker than observed. This translates to
an overestimate of the oxygen abundance by no more than 0.15 dex. However, it is relevant to note that for both of these models, which have ionizing source temperatures much lower than the NGC 5471 model, the strength of the [Ne III] λ3869 line is predicted (substantially in the case of H40) weaker than observed. This is due to absorption edges in the stellar atmospheres employed. More realistic models for the ionizing OB associations which include stars covering a range of temperatures but yielding the same average $\langle T_{\text{ion}} \rangle$ would probably ameliorate the problem since the hotter stars in the cluster contribute sufficient Ne$^+$ ionizing photons to maintain the [Ne III] line intensities. In an attempt to best fit the majority of the observed lines, the Ne abundance was increased above its solar ratio for these models. This has two effects. First, it implies that the Ne abundances are somewhat uncertain. Second, it enhances the cooling of the Ne$^{++}$ zone due to the λ3869 and 15.6 μm emission lines and hence also artificially decreases the temperature of the O$^{++}$ zone (which is very nearly coextensive with the Ne$^{++}$ zone) in the models. As a result, the theoretical temperature of the O$^{++}$ zone as derived from the ratio of the auroral to nebular [O III] lines is too low.

The model of S5 was constructed in a similar manner to the previous models, employing parameters derived from the abundance sequence as a starting point. Trial and error once again led to the final model presented in Table 5. Comparison with the observations (SS; McCall, Rybski, and Shields 1985) demonstrates that the fit is at least as good as the model computed by SS which is also reproduced in Table 5. If the oxygen abundance is derived solely on the basis of ([O II] λ3727 + [O III] λλ4959, 5007)/Hβ from the abundance sequence, the result is very close to $12 + \log (O/H) = 9.00$ (1.5 $Z_\odot$), and so in Table 5 the 1.5 $Z_\odot$ model employed in the theoretical abundance sequence (Paper II) is also presented. Inspection of the model
### TABLE 5
PHOTOIONIZATION MODELS FOR S5

#### A. LINE INTENSITIES

<table>
<thead>
<tr>
<th>Ion</th>
<th>( \log I_{\text{obs}} )</th>
<th>( \log I_{\text{mod}} )</th>
<th>( \log I_{\text{SS}} )</th>
<th>( \log I_{1.5 Z_{\odot}} )</th>
<th>( \log I_{\text{SS} \text{par}} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \text{O} \ II \ \lambda 3727 )</td>
<td>+0.26 ± 0.05</td>
<td>+0.23</td>
<td>+0.26</td>
<td>+0.21</td>
<td>−0.25</td>
</tr>
<tr>
<td>( \text{O} \ III \ \lambda 4363 )</td>
<td>&lt; −2.0</td>
<td>−3.69</td>
<td>−3.77</td>
<td>−3.77</td>
<td>−5.19</td>
</tr>
<tr>
<td>( \text{O} \ III \ \lambda 5007 )</td>
<td>−0.62 ± 0.06</td>
<td>−0.62</td>
<td>−0.57</td>
<td>−0.62</td>
<td>−1.39</td>
</tr>
<tr>
<td>( \text{N} \ II \ \lambda 5755 )</td>
<td>&lt; −2.4</td>
<td>−2.45</td>
<td>−2.47</td>
<td>−2.51</td>
<td>−2.91</td>
</tr>
<tr>
<td>He \ I \ \lambda 5876 )</td>
<td>−1.05 ± 0.05</td>
<td>−1.03</td>
<td>−1.05</td>
<td>−0.90</td>
<td>−1.03</td>
</tr>
<tr>
<td>( \text{O} \ I \ \lambda 6300 )</td>
<td>−1.83 ± 0.07</td>
<td>−1.62</td>
<td>−1.27</td>
<td>−1.24</td>
<td>−1.67</td>
</tr>
<tr>
<td>( \text{S} \ III \ \lambda 6310 )</td>
<td>&lt; −2.4</td>
<td>−2.17</td>
<td>−2.22</td>
<td>−2.16</td>
<td>−2.72</td>
</tr>
<tr>
<td>( \text{N} \ II \ \lambda 6584 )</td>
<td>−0.05 ± 0.06</td>
<td>−0.04</td>
<td>+0.10</td>
<td>+0.00</td>
<td>−0.09</td>
</tr>
<tr>
<td>( \text{S} \ II \ \lambda 6731 )</td>
<td>−0.58 ± 0.05</td>
<td>−0.56</td>
<td>−0.55</td>
<td>−0.52</td>
<td>−0.64</td>
</tr>
<tr>
<td>( \text{S} \ III \ \lambda 9069 )</td>
<td>−0.47 ± 0.10</td>
<td>−0.34</td>
<td>−0.50</td>
<td>−0.26</td>
<td>−0.47</td>
</tr>
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</table>

#### B. MODEL PARAMETERS

<table>
<thead>
<tr>
<th>Parameter</th>
<th>mod</th>
<th>SS, SS\text{par}</th>
<th>1.5 ( Z_{\odot} )</th>
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</thead>
<tbody>
<tr>
<td>( T_{\text{ion}} \ K )</td>
<td>38,000</td>
<td>38,000</td>
<td>41,500</td>
</tr>
<tr>
<td>( L_C \ \text{s}^{-1} )</td>
<td>( 9.6 \times 10^{50} )</td>
<td>( 9.0 \times 10^{50} )</td>
<td>( 2.7 \times 10^{46} )</td>
</tr>
<tr>
<td>( Q(H) \ \text{cm s}^{-1} )</td>
<td>( 5.26 \times 10^7 )</td>
<td>( 5.14 \times 10^7 )</td>
<td>( 1.11 \times 10^7 )</td>
</tr>
<tr>
<td>( N_H \ \text{cm}^{-3} )</td>
<td>35</td>
<td>24</td>
<td>10</td>
</tr>
<tr>
<td>( \epsilon )</td>
<td>0.010</td>
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<tr>
<td>( R_{\text{pc}} )</td>
<td>130</td>
<td>150</td>
<td>2.26</td>
</tr>
<tr>
<td>He/H</td>
<td>0.085</td>
<td>0.082</td>
<td>0.085</td>
</tr>
<tr>
<td>12 + log (O/H)</td>
<td>8.88</td>
<td>9.11</td>
<td>9.00</td>
</tr>
<tr>
<td>12 + log (N/H)</td>
<td>7.95</td>
<td>8.32</td>
<td>8.04</td>
</tr>
<tr>
<td>O/S</td>
<td>33.0</td>
<td>32.3</td>
<td>33.0</td>
</tr>
</tbody>
</table>

**NOTES**—\( \log I_{\text{obs}} \) is the observed logarithmic line intensity relative to H\( \beta \); \( \log I_{\text{model}} \) is the predicted logarithmic line intensity relative to H\( \beta \) for model, where model is either “mod” for the “best estimate” model presented here, “SS” for the model computed by SS, “1.5 \( Z_{\odot} \)” for the 1.5 \( Z_{\odot} \) model from the abundance sequence, or “SS\text{par}” for the model with the parameters determined by SS computed using MAPPINGS.

\( a \)This model had an empty zone \( (N_H = 0) \) with radius \( \frac{1}{2} R \).
indicates that it too is a reasonably good fit to the observations, although the \( [S\,\text{iii}] \lambda\lambda 9069, 9532 \) lines are predicted slightly too strong and \([O\,\text{i}] \lambda 6300\) somewhat too strong. An attempt was made to compute a model of S5 employing the parameters used by SS in order to demonstrate the effect upon the predicted spectrum of updated atomic data and the inclusion of other potentially important atomic processes, such as charge exchange reactions and low temperature dielectronic recombination, whose rates have been recently determined. In this case the model spectrum differed *substantially* from the observations (see Table 5), particularly with regard to the intensities of the \([O\,\text{iii}] \lambda\lambda 4959, 5007\) lines. The results indicate that S5 cannot have an oxygen abundance as high as that previously suggested by SS and demonstrate the importance of employing state-of-the-art atomic data and including *all* relevant atomic processes when computing theoretical nebular models. This is particularly true for regions containing substantial fractions of partially ionized gas, where charge exchange reactions with neutral hydrogen can significantly alter the ionization state of the plasma. Comparison with an earlier model of S5 computed with the MAPPINGS code (Binette 1982) employing the same model parameters, but earlier atomic data and the charge exchange reactions \( O^+ + H^0 \rightleftharpoons O^0 + H^+ \) and \( N^+ + H^0 \rightleftharpoons N^0 + H^+ \) only, illustrates that \( \log \left\{ I \left([O\,\text{iii}] \lambda 5007 \right) / I (H\beta) \right\} \) has decreased from \(-0.34\) to \(-1.39\) and \( \log \left\{ I \left([O\,\text{ii}] \lambda 3727 \right) / I (H\beta) \right\} \) from \(+0.22\) to \(-0.25\). Similarly, recent computations by Shields (1985) employing the same model parameters and code as SS, but with new atomic data, indicate that charge exchange reduced the ionization fraction of \( O^{++} \) from 0.076 in the original model of SS to 0.036, while increased collision strengths for \( S^+ \) and \( S^{++} \) (Mendoza 1983) reduced the mean electron temperature of the \( O^{++} \) zone from 5600 K to 4600 K, leading to \( \log \left\{ I \left([O\,\text{iii}] \lambda 5007 \right) / I (H\beta) \right\} = -1.33 \) versus \(-0.57\) computed by SS.
The calibration by Pagel et al. (1979) of the semiempirical abundance sequence at high metallicity was based almost exclusively on the photoionization model of S5 given in SS. McCall (1982) also computed a model for S5 using Shields' computer code and atomic data that was current in 1982. He derived a similar oxygen abundance to that quoted in SS and employed this as the primary calibrator for his calibration of the H II region abundance sequence. Since both of these authors employed the line ratio \([\text{[O II]} \lambda 3727 + \text{[O III]} \lambda \lambda 4959, 5007]/\text{H}\beta\) which relies on the strengths of the \([\text{O III]} \lambda \lambda 4959, 5007\) to deduce the oxygen abundance, the recalibration of the oxygen abundance of S5 presented here suggests that both of these previous calibrations of the abundance sequence may be systematically in error at high metallicities. Applying the oxygen abundance–line strength calibration for S5 derived here would result in a lower abundance derived from the same value of \([\text{[O II]} \lambda 3727 + \text{[O III]} \lambda \lambda 4959, 5007]/\text{H}\beta\) for high metallicities. Such a calibration would then approach the calibration derived on the basis of theoretical photoionization modeling of Paper II.

Comparison of the oxygen abundances derived by exact modeling with abundances derived from the abundance sequence allows an estimate of the accuracy with which \(12 + \log (O/H)\) may be derived from the abundance sequence. For the three objects in this sample for which this is possible, the RMS differences between the oxygen abundances derived from the sequence and those derived from the models is 0.14 dex. This is considerably larger than the typical “formal” errors defined in § IIIa on the basis of homogeneity of the three abundance-sensitive diagnostic line ratios, and is representative of differences between the physical conditions present in the “exact” nebular models and the conditions adopted for the abundance sequence. It is possible that systematic errors may arise if there is a systematic change of conditions.
away from those adopted for the sequence with metallicity. There is no evidence for this in the data, but the number of points over which a complete diagnosis has been achieved is small.

Uncertainty in the calculated oxygen abundances resulting from differences between the actual nebular geometry and the geometry assumed in the “exact” models is more difficult to quantify. For each of the H II regions modeled individually, several models with a variety of nebular geometries were computed in order to arrive at the “best estimate” model which most accurately reproduces all of the observed line intensities. In the case of S5, it is not possible to reproduce the observed line ratios with any models with an oxygen abundance more than \( \sim 0.15 \) dex larger or 0.1 dex smaller than the adopted value. Even more stringent limits are possible for the other objects modeled individually because of the higher quality of the data and the greater number of lines from different ionic species for which intensity measurements are available. It is unlikely that the true oxygen abundance in H40 or NGC 5461 differs from the adopted value by more than \( \pm 0.1 \) dex, while for NGC 5471 the adopted abundance is accurate to \( \pm 0.05 \) dex.

The accuracy with which the oxygen abundance may apparently be determined compares favorably with other methods such as the semiempirical ionization correction factor technique (Peimbert and Costero 1969), and this is particularly true for higher metallicity objects where the calibration is most useful and most necessary.

c) The Abundance Gradient

The results shown in Tables 3, 4, and 5 demonstrate that O/H increases by almost 1 dex from the outermost to the innermost H II regions
observed in M101. In Figure 1 the oxygen abundances derived in § IIIa and § IIIb are plotted versus $\rho$ for each of the H II regions in Table 1. The data are well fitted by an exponential relationship, $O/H \propto \exp(-\rho/a)$, but not to a power law, $O/H \propto \rho^{-a}$, or by a linear relation, $O/H \propto a - \rho$. The solid line in Figure 1 represents the weighted best exponential fit to the data points. Each data point was weighted on the basis of its estimated total error, which was considered to consist of the sum of a "random" component and a "systematic" component, according to the following prescription. The "random" component was calculated as follows: (i) for those points with abundances derived from the abundance sequence employing all three abundance estimators, the formal error in the oxygen abundance was employed; (ii) those points with oxygen abundances derived solely from $([\text{O} \, \text{II}] \lambda 3727 + [\text{O} \, \text{III}] \lambda \lambda 4959, 5007)/H\beta$ are given an error of $\pm 0.09$ dex which is twice the mean error for the points in (i) above; and (iii) abundances derived from theoretical photoionization models were ascribed zero random error. The probable "systematic" errors resulting from possible differences between the adopted model conditions and the true nebular conditions were estimated to be $\pm 0.15$ dex for $12 + \log (O/H) = 9.1$ decreasing linearly to $\pm 0.05$ dex at $12 + \log (O/H) = 8.2$. The quoted systematic errors are not standard errors, but rather their meaning is that it is extremely unlikely that the difference between the actual nebular abundances and the calculated abundances will exceed the stated errors. This leads to an oxygen abundance gradient $\Delta \log (O/H) / \Delta \rho = -1.24 \pm 0.10$ dex, which corresponds to $-0.0744 \pm 0.0060$ dex kpc$^{-1}$ at the adopted distance of M101. The derived oxygen abundance gradient is slightly steeper than, but consistent with, that
Figure 1. The derived radial oxygen abundance gradient in M101. The filled circles indicate points derived from the abundance sequence employing all three abundance estimators, the open squares represent points derived from the sequence employing the line ratio ([O II] λ3727 + [O III] λλ4959, 5007)/Hβ only, while the open circles represent points modeled “exactly.” The error bars are computed on the basis of internal consistency of the three abundance indicators. The solid line indicates the best fit to the data.
derived by RPT, $\Delta \log (O/\Pi) / \Delta \rho = -1.02 \pm 0.35$ dex (corrected for the different value of $R_0$ adopted), and is about the same as that measured in the solar vicinity (Talent and Dufour 1979; Peimbert 1979).

In Figure 2, the N/O ratio is derived as a function of oxygen abundance. Also shown are the positions of the solar value (Allen 1973) and the Orion nebula (RPT). The N/O ratios in M101 are about a factor of 2 smaller than those in Orion and also the solar vicinity. The N/O gradient is discussed further in § IV. The open circles in Figure 2 represent those objects that were modeled individually, while the filled circles indicate determinations from the abundance sequence using the technique suggested in Paper II. The H II regions for which the oxygen abundance data were derived solely from the $([O \ II] \lambda 3727 + [O \ III] \lambda \lambda 4959, 5007)/H\beta$ relationship were not employed to derive N/O ratios. The uncertainty in the derived N/O ratio is much less than for the O/H ratio and arises mainly from uncertainties in the measured line intensities. The solid line in Figure 2 is a linear regression fitted to the data weighted by the observational errors and yields an N/O gradient of $\Delta \log (N/O) / \Delta \log (O/H) = +0.63 \pm 0.14$ dex, corresponding to an N/H gradient of $-0.118 \pm 0.026$ dex kpc$^{-1}$.

The S/O gradient has also been derived from the data as suggested in Paper II, yielding $\Delta \log (S/O) / \Delta \log (O/H) = -0.51 \pm 0.16$ dex, which may be recast as an S/H gradient of $-0.035 \pm 0.011$ dex kpc$^{-1}$ (Fig. 3). The quoted errors include both a contribution from the observational uncertainties in the line intensities and also a contribution to the uncertainty in S/O which arises from the strong dependence of the $[S \ II] \lambda 6731$ line intensity on $Q(H)$. For those H II regions individually modeled, the value of $Q(H)$ is constrained primarily by the observed value of $I ([O \ II] \lambda 3727) / I ([O \ III] \lambda 5007)$
Figure 2. The N/O ratio as a function of oxygen abundance. The open circles represent points modeled "exactly," while the filled circles indicate nitrogen abundances derived using the technique suggested in Paper II. Also shown are the solar value and the Orion nebula.
Figure 3. As Fig. 2, but for the S/O ratio.
$12 + \log (O/H)$ vs. $\log (S/O)$

- Points represent different data sets.
- The line is a fitted trend line.
- "SUN" indicates a specific data point or group.
and can be estimated to an accuracy of approximately ±0.15 dex, which corresponds to an error in S/O of no more than 0.1 dex. It is interesting to note that the sign of the S/O gradient is the opposite of the O/H gradient, which implies that there is some mechanism which enhances the sulfur abundance relative to the oxygen abundance in the outer regions of the disk of M101. A possible explanation for this will be discussed in § IV below. The derived value for the S/O gradient depends strongly on the sulfur abundance adopted for NGC 5471. However, the model presented in Table 4 predicts the [S III] λ6310 line intensity to be smaller than observed, and this is also true of the predicted intensities of the [S III] λλ9069,9532 lines compared with the measurements of SS, suggesting that if the sulfur abundance had been derived from measurements of the [S III], rather than [S II], line intensities, then a significantly lower sulfur abundance would be derived for this object. It is clearly preferable, however, to be consistent when deriving the sulfur abundances by employing the same datum for each of the H II regions. Since [S III] line intensity measurements are not available for the majority of the H II regions, this necessitated employing the [S II] line observations only. However, even if NGC 5471 is excluded from the derivation of the S/O gradient in M101, the resulting S/O gradient deduced from all the other H II regions is compatible with the gradient deduced when NGC 5471 is included (with the adopted sulfur abundance) to within the statistical errors.

The Ne/O and Ar/O gradients have also been derived from the photoionization models of NGC 5471, NGC 5461, and H40. Unfortunately, these were the only objects in the sample with measured neon and argon line strengths. Furthermore, for the reasons outlined earlier, the fitted intensities of the [Ne III] lines in the models were not particularly good so
that the neon abundances probably have large errors. The argon abundances were the result of fitting only a single emission line, [Ar III] \( \lambda 7136 \), and may be somewhat uncertain also. Nevertheless, both the Ne/O and Ar/O gradients can be explained qualitatively, as shall be shown in § IV, and so the results are presented for completeness. The derived best fits for the Ne and Ar gradients are \( \Delta \log (\text{Ne/O}) / \Delta \log (\text{O/H}) = +0.27 \pm 0.19 \) dex and \( \Delta \log (\text{Ar/O}) / \Delta \log (\text{O/H}) = -0.73 \pm 0.13 \) dex, or an Ne/H gradient of \(-0.092 \pm 0.065 \) dex kpc\(^{-1}\) and an Ar/H gradient of \(-0.0195 \pm 0.0035 \) dex kpc\(^{-1}\) respectively.

IV. IMPLICATIONS FOR CHEMICAL ENRICHMENT IN GALAXIES

There is evidence in the literature to suggest that disk formation in galaxies occurs over a considerable period of time (e.g., Larson 1976; Jones and Wyse 1983), with the inner regions of the disk forming earlier in the history of the galaxy than the outer disk. For example, large abundance gradients increasing toward the center of a galaxy imply that the inner disk has undergone more cycles of chemical enrichment (and is therefore older) than the metal poor outer disk. In a recent paper, Dopita (1985) has proposed a law of star formation which is apparently applicable to all disk galaxies. He demonstrates that the specific star-formation rate (the SFR per unit total mass), \( \dot{M}_*/M_T \), is linearly related to the ratio of gas to total mass surface densities, \( \sigma_g/\sigma_T \), and that \( \dot{M}_*/M_T \) decreases exponentially with age, but the gas content declines to a finite limit. From the observed outward-increasing gradient in \( \sigma_g/\sigma_T \) in M101 it is possible to infer that if initially all of the material is in gaseous form, or at least is homogeneous, then the inner disk must have formed earlier in time than the outer disk, and that \( \dot{M}_*/M_T \) would
have been considerably higher there and then. Dopita (1985) suggests that
disk formation occurs first in the center of a galaxy and proceeds to greater
radii as the gaseous protodisk collapses to a disk morphology, and suggests
that beyond the Holmberg radius, disk formation may still be under way.

Such a model for disk formation is capable of explaining, at least
qualitatively, the differences between the abundance gradients of the vari-
ous elements presented in the preceding section. The rapid burst of star
formation early in the the history of the inner regions of the disk would
have produced substantial heating of the interstellar medium (ISM) from
events such as supernovae and hot stellar winds, and this would have re-
sulted in a larger Jeans mass. As a consequence of the enhanced Jeans mass,
the high-mass region of the initial mass function (IMF) may have been en-
hanced (McCall, Rybski, and Shields 1985), resulting in the formation of
a proportionately greater number of high-mass stars. Such stars are pre-
cisely those responsible for the nucleosynthesis of oxygen ($M_\ast \gtrsim 12\,M_\odot$)
and also neon ($12\,M_\odot \lesssim M_\ast \lesssim 25\,M_\odot$). Hence one would expect that oxy-
gen and neon abundances should be enhanced wherever the upper IMF is
enhanced. It has been suggested that intermediate mass stars (4–8\,M_\odot)\nmay be a source of primary nitrogen (Edmunds and Pagel 1978; Renzini
and Voli 1981). During dredge-up in stars of this mass range, fresh $^{12}\text{C}$ is
mixed into the hydrogen-rich zone after each pulse, and can be partly con-
verted into $^{13}\text{C}$ and $^{14}\text{N}$ via the CN cycle (Alloin et al. 1979). Very massive
stars ($\sim 100\,M_\odot$) may also contribute to primary nitrogen production di-
rectly through the $3\alpha$ process in their very hot ($\sim 10^8\text{K}$) cores (Woosley
and Weaver 1982), and abundances of ring H II regions such as NGC 2359
and NGC 6888 (Peimbert, Torres-Peimbert, and Rayo 1978; Talent and Du-
four 1979; Kwitter 1981) observationally support this idea. Consequently, the
nitrogen abundance gradient should fall somewhere between purely primary enrichment and purely secondary enrichment, depending upon the degree of primary N production which is very uncertain. This is exactly what is observed (Fig. 2). At large radii in the galaxy disk, the lower specific star-formation rate results in a less enhancement of the upper IMF and hence fewer high-mass stars are produced. Instead, a proportionately greater number of low- and intermediate-mass stars ($\lesssim 8 M_\odot$) are formed and hence heavy element (S, Ar, Ca, Fe) production from enrichment due to intermediate-mass stars and carbon deflagration supernovae is enhanced. One would expect, as a consequence of this, that heavy element abundance gradients would be *flatter* than the oxygen abundance gradient, and this is also observed.

Effects such as these can be quantified, in a limited sense, by calculation of the yields of individual elements. For an element $i$, the *yield*, $p_i$, is defined by

$$p_i = M_i/M_*,$$

where $M_i$ is the mass of that element that a generation of stars ejects into the ISM and $M_*$ is the mass of that generation that remains locked up in long-lived stars and compact remnants. Consider a simple model of galactic evolution in which it is assumed that the disk is stratified into isolated, well-mixed, concentric cylindrical zones within each of which the instantaneous recycling approximation applies and that gas is converted into stars according to a constant IMF in each zone. In such a model the heavy element yield for the element $i$ is given by

$$p_i = Z_i/\ln (1/\mu),$$

(2)

where $Z_i$ is the mass-fraction of the element $i$ in the zone and $\mu = \sigma_g/\sigma_T$ is the ratio of remaining gas to total mass of the zone. Assuming that this
model is applicable to M101, heavy element yields have been derived using equation (2) for the elements oxygen, nitrogen, and sulfur at three radii within the disk (Table 6). The mass-fraction of each element was derived from its abundance gradient determined in the previous section. The gas and total mass surface density data cited in § II were employed to calculate $\mu$. The computed yields are of dubious accuracy but should show the trends even if the absolute values are poorly calculated. The reason for this is the assumption that the abundances of the elements, the gas surface density, and the total mass surface density vary purely exponentially with radius, albeit with different scale lengths and normalizations. Furthermore, modifications to the simple model of galaxy evolution, such as metal-enhanced star formation (Talbot and Arnett 1975), dynamical collapse (Tinsley and Larson 1978; Chiosi 1980), or radial infall of gas (Mayor and Vigroux 1981) may substantially alter the yield computed above. Nevertheless, the values in Table 6 clearly establish an inwardly increasing yield for the elements nitrogen and oxygen, but an outwardly increasing sulfur yield. The nitrogen yield increases inward, although it is produced mainly in stars of intermediate mass, because of the large secondary enrichment contribution to the total nitrogen production. Per unit mass of processed material, a larger fraction of the mass is enriched into sulfur (and by analogy to other heavy elements also) in the outer regions of the disk relative to the inner disk, while at smaller radii in the disk the situation is reversed. These results are in qualitative agreement with the abundance gradients deduced above for these elements and imply that there must be proportionately more high-mass stars in the inner disk and proportionately more low- and intermediate-mass stars at larger radii in the disk. The implication of differences between the slopes of the individual element yields with radius within the galaxy is that the total heavy element
<table>
<thead>
<tr>
<th>$R$ kpc</th>
<th>$\frac{1}{\mu}$</th>
<th>$12 + \log (\text{O/H})$</th>
<th>$p_N$</th>
<th>$p_O$</th>
<th>$p_S$</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>33.8</td>
<td>9.06</td>
<td>$2.2 \times 10^{-4}$</td>
<td>$3.9 \times 10^{-3}$</td>
<td>$1.0 \times 10^{-4}$</td>
</tr>
<tr>
<td>5</td>
<td>14.0</td>
<td>8.84</td>
<td>$1.5 \times 10^{-4}$</td>
<td>$3.2 \times 10^{-3}$</td>
<td>$1.2 \times 10^{-4}$</td>
</tr>
<tr>
<td>8</td>
<td>5.7</td>
<td>8.62</td>
<td>$1.2 \times 10^{-4}$</td>
<td>$2.9 \times 10^{-3}$</td>
<td>$1.6 \times 10^{-4}$</td>
</tr>
</tbody>
</table>
yield, $p = \sum_i p_i$, summed over all the elements heavier than helium, is not a particularly useful quantity in characterizing chemical enrichment because the different enrichment sources and characteristic enrichment time scales render such a sum rather meaningless.

V. CONCLUSIONS

In this paper, the theoretical abundance sequence calibration of Paper II has been applied to spectrophotometric data gathered by several authors for a number of H II regions observed in the bright spiral galaxy M101 in order to estimate elemental abundances. Oxygen abundances were found to range from $12 + \log (O/H) = 8.20$ for the outermost observed region (NGC 5471) to $12 + \log (O/H) = 9.08$ for the innermost region (S1). Comparison of oxygen abundances derived from the abundance sequence with those derived from "exact" photoionization modeling suggests that the accuracy with which the oxygen abundance of an H II region may be estimated from the abundance sequence by employing the method suggested in Paper II is typically $\sim 0.15$ dex.

The high-abundance H II region S5 has been individually modeled using the computer code MAPPINGS (Paper I), resulting in a new oxygen abundance determination of $12 + \log (O/H) = 8.88$, considerably lower than the previous determinations of SS and McCall (1982). It was shown that the oxygen abundance of S5 cannot be as high as has been previously suggested by SS. The implications of these results upon previous semiempirical calibrations of the extragalactic H II region abundance sequence (Pagel et al. 1979; McCall 1982; McCall, Rybski, and Shields 1985) which have employed previous models of S5 to calibrate the high metallicity end of the sequence are discussed.
These data have been combined in order to measure the abundance gradient in M101. Unlike previous determinations of the oxygen gradient (SS; RPT) which have employed very few (typically three) data points, the significantly larger sample used here means that the slope of the gradient can be determined with greater precision and hence that the shape of the gradient can be measured with confidence. The oxygen gradient is found to be very closely exponential with a slope of $\Delta \log (O/H) / \Delta \rho = -1.24 \pm 0.10$ dex. The data have also allowed determinations of the abundance gradients of the elements N, S, Ne, and Ar. The slope of the N/H abundance gradient is steeper than the O/H gradient, but not so steep as N/O $\propto$ O/H. The neon gradient is also apparently steeper than the oxygen gradient, whereas the sulfur and argon gradients are evidently shallower than the oxygen gradient.

The implications of the derived chemical abundance gradients upon chemical evolution and galaxy formation models are discussed. A model of disk formation in which the inner regions of the protodisk collapse to a disk morphology earlier in the history of the galaxy than the outer regions has been proposed which, together with recent results concerning star formation in disk galaxies (Dopita 1985), seems to qualitatively explain the different radial gradients in elemental abundances, and also the individual element abundance yields.

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H II REGION ABUNDANCES IN SEYFERT GALAXIES

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The theoretical H\textsc{ii} region abundance sequence calibration of Dopita and Evans (1986) has been applied to optical spectrophotometry of 23 H\textsc{ii} regions located in the inner disk regions of two Seyfert 1 and two Seyfert 2 galaxies, including the prototype Seyfert 2, NGC 1068, in order to determine oxygen, nitrogen, and sulfur abundances. The mean oxygen abundance derived for each galaxy ranges between solar abundance and twice solar abundance. There is no evidence for abnormal N/O or S/O abundance ratios in any of the H\textsc{ii} regions we observed.

The observations suggest that the abundances derived for the H\textsc{ii} regions may be adopted as nuclear abundances and employed to constrain theoretical models of the Seyfert nucleus. The observations then place limits on the influence which the active nucleus can have on chemical enrichment of the local interstellar medium.

*Subject headings*: galaxies: individual — galaxies: seyfert — nebulae: abundances — nebulae: H\textsc{ii} regions
I. INTRODUCTION

In recent years, considerable effort, both observational and theoretical, has been directed toward the study of active galactic nuclei in an attempt to understand the mechanism by which the nucleus is powered, and the effect of the nuclear activity on the surrounding galaxy. Many authors have computed theoretical photoionization and shock models for objects covering a range of nuclear activity from LINERS to the broad- and narrow-line regions of Seyfert galaxies and quasars (see, for example, Kwan and Krolik 1981; Ferland and Netzer 1983; Halpern and Steiner 1983; Kwan 1984). In these models it has been frequently assumed a priori that the gas has a solar chemical composition, or approximately so, often with little or no observational basis for such an assumption. Since the most abundant elements (C, N, O, Ne) determine the line cooling in the gas, and in dense, hot regions where collisional ionization and Auger processes are significant may dominate the overall ionization balance, it is essential to employ accurate elemental abundances in order to correctly model the nuclear regions.

Because of uncertainties in physical processes and reddening corrections, it is not, in general, possible to estimate elemental abundances directly from observations of the nuclear spectrum except by way of self-consistency requirements for theoretical models. Hence, an alternate method for estimating the nuclear chemical composition must be sought. We propose that the most appropriate way of estimating nuclear elemental abundances is to adopt the abundances found in the galactic disk close to the nucleus, either from studies of near-nuclear H II regions (since such objects are more likely to have similar abundances to the nucleus due to their proximity than
H II regions further out in the disk), or, where such regions do not exist, from extrapolation of the radial abundance gradient to the nucleus.

Comparison of abundances found in near-nuclear H II regions in Seyfert galaxies with those found in normal galaxies may also enable us to quantify any effects which the Seyfert nucleus may have upon chemical enrichment processes which occur in the interstellar medium (ISM). The most likely such effects are enhancement of the supernova rate and related nucleosynthetic processes triggered by compression of the ISM by winds, shock and ionization fronts from the nucleus, and increased production of early-type stars in H II regions formed as a result of the high-level of turbulent activity near the nucleus. Bursts of star-formation triggered by the nucleus may alter the relative enrichment of different elements in the ISM through modification of the stellar mass function.

In this paper we derive chemical abundances for 23 near-nuclear H II regions in two Seyfert 1 and two Seyfert 2 galaxies, including the prototypical Seyfert 2, NGC 1068. In section II we present our observational data set, from which we derive oxygen, nitrogen, and sulfur abundances in section III. In section IV, we discuss our reasons for believing that the H II region abundances we deduce may be adopted to constrain theoretical models of the Seyfert nuclei, and consider whether or not the high photon flux near the active nucleus may affect our abundance determinations by altering the ionization balance of near-nuclear H II regions. In section V we present our final conclusions.
II. OBSERVATIONS

The optical spectra were obtained under photometric conditions at the 3.9 m Anglo-Australian Telescope on the nights of 1983 May 11–12 and 12–13 (NGC 3783, NGC 4507, and NGC 6814), and on 1983 November 9–10 (NGC 1068). The Royal Greenwich Observatory spectrograph was used with the Image Photon Counting System (IPCS; Boksenberg 1972) as detector. A grating of 250 lines mm\(^{-1}\) blazed in the blue was used in first order with a slit width of 300 \(\mu\)m (2\('\)01 on the sky), giving a spectral resolution of 8\(\AA\) and a spectral coverage of 3200–7400\(\AA\). The external memory was formatted to give 64 spectra (96 spectra for the NGC 1068 observations), each 2040 pixels long, separated by 1\('\)15 on the sky.

These spectra were reduced by the following procedure. First, pixel to pixel variations in the response of the detector were removed by division of the data by a normalized flat field obtained by summing two long exposures of an unfiltered tungsten lamp in third order red. Second, each spectrum was rebinned to a linear wavelength scale by making a two-dimensional third order polynomial fit to the calibration arcs. Third, the mean of those spectra judged to be free of nebular or stellar contributions was subtracted from each spectrum to correct for night-sky emission. Fourth, the spectra were converted to absolute flux by correcting for extinction via observations of Oke (1974) white dwarf standard stars. Finally, the spectra of individual H II regions were obtained by co-adding all the spectra (or spatial increments) in which the object was detected.

The corrections for reddening applied to the observed fluxes were computed by assuming that the intrinsic Balmer decrement results from pure
case B recombination (Brocklehurst 1971) for an adopted nebular temperature of 8000 K, and employing the reddening curve of Seaton (1979). The spectra were first corrected for galactic extinction using the value of $A_B$ tabulated by de Vaucouleurs, de Vaucouleurs, and Corwin (1976) for the line of sight to the parent galaxy. Next, the data were shifted to rest velocity and the observed ratio of $I(\text{H}\alpha)/I(\text{H}\beta)$ was used to determine the extragalactic extinction. The latter correction employed a "normal" galactic reddening law, since most of the extinction to extragalactic H II regions results from dust surrounding the nebula, rather than dust mixed with the ionized gas (Brand, Coulson, and Zealey 1981; McCall, Rybski, and Shields 1985).

In some of the spectra the Balmer decrement steepens toward the series limit, indicating that a component of Balmer absorption is present. In the worst cases, the emission component of H$\gamma$ is annihilated. The Balmer absorption arises from both the underlying galaxy-disk continuum and the continuum due to the ionizing OB association in the H II region. To attempt to minimize the effect of the absorption on the emission-line intensity measurements, data from nearby spatial increments judged to be free of nebular contributions were summed together to form an average spectrum of the underlying continuum, and this spectrum was then scaled according to the shapes and intensities of prominent absorption features, and subtracted from the H II region data. The separation of the H II region emission spectrum from the underlying continuum is particularly difficult since in many cases the extent of the nebular emission implies that data from adjacent spatial increments cannot be used to estimate the continuum spectrum. Large point-to-point variations in the stellar age and the presence of A and B stars in the vicinity of the H II region, or a very strong but localized OB association continuum, means that the continuum subtracted is not identical to the
continuum underlying the H\textsc{ii} region spectrum. The most likely result is to overestimate the observed $I(\text{H}\alpha)/I(\text{H}\beta)$ emission-line ratio, and hence the reddening. This is evident in some of the spectra in Table 1 where $I(\text{H}\gamma)$ is depressed relative to the theoretical value after the interstellar reddening has been removed on the basis of the observed $I(\text{H}\alpha)/I(\text{H}\beta)$ ratios. In such cases, caution needs to be applied when interpreting the data, but without additional high signal-to-noise spectrophotometry with both higher spectral and spatial resolutions, it is difficult to improve in these specific cases. However, in general, the technique is reasonably effective in removing the underlying absorption, but introduces increased uncertainties in the measured emission-line intensities, particularly for the higher order Balmer lines.

A further problem encountered when applying this procedure to NGC 1068 is the presence of weak optical emission over much of the inner disk region of the galaxy. The underlying emission was artificially removed before subtracting the averaged galaxy continuum spectrum from the H\textsc{ii} region spectra, but this procedure has unavoidably introduced additional uncertainties in the measured intensities of the nebular emission lines, particularly for objects with low surface brightness. Nevertheless, the methods used should result in more reliable emission-line intensity measurements since, to first order, the effects of the underlying absorption have been reduced.

In Figure 1 we present a representative sky subtracted and dereddened, but not continuum subtracted, spectrum from an H\textsc{ii} region in each of the four galaxies studied here. We employ the notation of McCall, Rybski, and Shields (1985) to identify and locate the H\textsc{ii} regions observed. Observed
Figure 1. Representative spectra from H II regions in each of the four galaxies studied here. (a) NGC 1068 (−027−033), (b) NGC 3783 (−010−012), (c) NGC 4507 (+001−019), and (d) NGC 6814 (+027−002).
Flux (erg cm\(^{-2}\cdot s\cdot \AA^{-1}\cdot 10^{14})

Wavelength

Flux (erg cm\(^{-2}\cdot s\cdot \AA^{-1}\cdot 10^{14})

(b)

\times 10
Flux (erg cm\(^{-2}\) s\(^{-1}\) Å\(^{-1}\) x 10\(^{14}\))

Wavelength

Flux (erg cm\(^{-2}\) s\(^{-1}\) Å\(^{-1}\) x 10\(^{14}\))

Wavelength

(c)

x5
Flux (erg cm$^{-2}$ s$^{-1}$ Å$^{-1}$ $\times 10^{14}$)

(d)

$\times 2.5$

Wavelength

4000  5000  6000  7000
TABLE 1

OBSERVED ($I_\lambda$) AND REDDENING CORRECTED ($F_\lambda$) FLUXES

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<thead>
<tr>
<th>Ion</th>
<th>$I_\lambda$</th>
<th>$F_\lambda$</th>
<th>$I_\lambda$</th>
<th>$F_\lambda$</th>
<th>$I_\lambda$</th>
<th>$F_\lambda$</th>
<th>$I_\lambda$</th>
<th>$F_\lambda$</th>
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<td>[Ne v] $\lambda$3426</td>
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<tr>
<td>[O II] $\lambda$3727</td>
<td>138</td>
<td>349</td>
<td>133</td>
<td>352</td>
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<td>13.4</td>
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<td>H$\beta$ $\lambda$4861</td>
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<td>100</td>
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<td>[O iii] $\lambda$4959</td>
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<td>H$\alpha$ $\lambda$6563</td>
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$\log F(H\beta)$: $-12.51$, $-12.33$, $-12.88$, $-12.26$

$C(H\beta)$: 1.35, 1.41, 0.56, 1.26
### Table 1 (continued)

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TABLE 1 (CONTINUED)

OBSERVED ($I_\lambda$) AND REDDENING CORRECTED ($F_\lambda$) FLUXES

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$\log F(H\beta)$: $-13.34$ $-12.28$ $-13.13$ $-12.48$

$C(H\beta)$: 0.98 0.75 1.07 1.58
TABLE 1 (CONTINUED)

OBSERVED ($I_\lambda$) AND REDDENING CORRECTED ($F_\lambda$) FLUXES

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TABLE 1 (CONTINUED)

OBSERVED (Iₜ) AND REDDENING CORRECTED (Fₓ) FLUXES

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**Observed (Iₜ) and Reddening Corrected (Fₓ) Fluxes**

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<td>[Ne v] λ3426</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>[O ii] λ3727</td>
<td>&lt;12</td>
<td>&lt;37</td>
<td>23: 70:</td>
</tr>
<tr>
<td>[Ne iii] λ3868</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>He i, H7 λ3889</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>[Ne iii], He λ3969</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Hδ λ4102</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Hγ λ4340</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>He ii λ4686</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>Hβ λ4861</td>
<td>100</td>
<td>100</td>
<td>100</td>
</tr>
<tr>
<td>[O iii] λ4959</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>[O iii] λ5007</td>
<td>&lt;18</td>
<td>&lt;16</td>
<td>&lt;14</td>
</tr>
<tr>
<td>[N i] λ5200</td>
<td>...</td>
<td>...</td>
<td>26 18</td>
</tr>
<tr>
<td>He i λ5876</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>[O i] λ6300</td>
<td>...</td>
<td>...</td>
<td>...</td>
</tr>
<tr>
<td>[N ii] λ6548</td>
<td>75:: 21::</td>
<td>194</td>
<td>57 147 39</td>
</tr>
<tr>
<td>Hα λ6563</td>
<td>1055</td>
<td>291</td>
<td>995 291 1111 291</td>
</tr>
<tr>
<td>[N ii] λ6584</td>
<td>154</td>
<td>42</td>
<td>323</td>
</tr>
<tr>
<td>[S ii] λ6716</td>
<td>76:: 19::</td>
<td>130</td>
<td>35 105 25</td>
</tr>
<tr>
<td>[S ii] λ6731</td>
<td>59:: 15::</td>
<td>89</td>
<td>24 44: 11:</td>
</tr>
<tr>
<td>log $F$(Hβ)</td>
<td>-13.72</td>
<td>-13.62</td>
<td>-13.23</td>
</tr>
<tr>
<td>$C$(Hβ)</td>
<td>1.68</td>
<td>1.61</td>
<td>1.75</td>
</tr>
</tbody>
</table>
(sky and galaxy continuum subtracted) and reddening-corrected emission-line intensities relative to $I(H\beta) = 100$ are given in Table 1 for all the reduced $H\text{II}$ region spectra. For each spectrum, we also list in Table 1 the absolute measured $H\beta$ flux (corrected for extinction) and the logarithmic reddening constant at $H\beta$, $C(H\beta)$, computed above.

III. $H\text{II}$ REGION ABUNDANCES

For each of the $H\text{II}$ regions listed in Table 1, we have estimated total oxygen, nitrogen, and sulfur abundances from the reddening-corrected emission-line ratios using the theoretical calibration of the extragalactic $H\text{II}$ region abundance sequence by Dopita and Evans (1986), and employing the techniques suggested in that paper. The results of the abundance determinations from the sequence are shown in Table 2. Error estimates were computed in the following manner, as suggested by Evans (1986) which should be referred to for more detail. The uncertainty in the computed oxygen abundance was treated as a sum of two components: a "random" component, deduced from the consistency of the three different abundance estimators recommended by Dopita and Evans (1986); and a "systematic" component resulting from possible differences between the actual nebular conditions and the nebular conditions adopted in the models used to calibrate the abundance sequence. The latter were estimated not to exceed $\pm 0.15$ dex for $12 + \log (O/H) = 9.1$ decreasing linearly to $\pm 0.05$ dex for $12 + \log (O/H) = 8.2$ (Evans 1986). It should be emphasized that the systematic errors dominate for high oxygen abundances, and that they are not standard errors, but rather their meaning is that it is extremely unlikely that the difference between the actual nebular abundances and the calculated abundances will exceed the
### Table 2

**Abundances Derived From The Abundance Sequence**

<table>
<thead>
<tr>
<th>Object</th>
<th>$12 + \log (O/H)$</th>
<th>$\log (N/O)$</th>
<th>$\log (S/O)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>NGC 1068 (-018+009)</td>
<td>8.76 ± 0.12</td>
<td>-0.75 ± 0.04</td>
<td>-1.33 ± 0.06</td>
</tr>
<tr>
<td>NGC 1068 (-022-009)</td>
<td>8.74 ± 0.11</td>
<td>-0.76 ± 0.04</td>
<td>-1.46 ± 0.06</td>
</tr>
<tr>
<td>NGC 1068 (-027-033)</td>
<td>9.07 ± 0.15</td>
<td>-0.79 ± 0.02</td>
<td>-1.54 ± 0.04</td>
</tr>
<tr>
<td>NGC 1068 (-029-038)</td>
<td>8.98 ± 0.14</td>
<td>-0.80 ± 0.02</td>
<td>-1.61 ± 0.04</td>
</tr>
<tr>
<td>NGC 1068 (-031-049)</td>
<td>8.89 ± 0.14</td>
<td>-0.92 ± 0.06</td>
<td>-1.61 ± 0.14</td>
</tr>
<tr>
<td>NGC 1068 (+023-016)</td>
<td>8.97 ± 0.14</td>
<td>-0.91 ± 0.02</td>
<td>-1.53 ± 0.04</td>
</tr>
<tr>
<td>NGC 1068 (+027+048)</td>
<td>8.91 ± 0.14</td>
<td>-0.78 ± 0.10</td>
<td>-1.48 ± 0.18</td>
</tr>
<tr>
<td>NGC 1068 (+024+032)</td>
<td>8.69 ± 0.11</td>
<td>-0.82 ± 0.10</td>
<td>-1.50 ± 0.14</td>
</tr>
<tr>
<td>NGC 1068 (+022+021)</td>
<td>8.95 ± 0.16</td>
<td>-0.86 ± 0.04</td>
<td>-1.58 ± 0.08</td>
</tr>
<tr>
<td>NGC 1068 (+020+012)</td>
<td>9.08 ± 0.15</td>
<td>-0.75 ± 0.02</td>
<td>-1.52 ± 0.04</td>
</tr>
<tr>
<td>NGC 1068 (+019+004)</td>
<td>8.83 ± 0.16</td>
<td>-0.62 ± 0.04</td>
<td>-1.41 ± 0.06</td>
</tr>
<tr>
<td>NGC 1068 (+017-003)</td>
<td>8.64 ± 0.13&lt;sup&gt;a&lt;/sup&gt;</td>
<td>-0.67 ± 0.12</td>
<td>-1.35 ± 0.32</td>
</tr>
<tr>
<td>NGC 3783 (+010-012)</td>
<td>8.94 ± 0.13</td>
<td>-0.83 ± 0.06</td>
<td>-1.60 ± 0.14</td>
</tr>
<tr>
<td>NGC 3783 (+004-014)</td>
<td>8.74 ± 0.14</td>
<td>-0.87 ± 0.06</td>
<td>-1.61 ± 0.12</td>
</tr>
<tr>
<td>NGC 3783 (+016-028)</td>
<td>8.88 ± 0.13</td>
<td>-1.16 ± 0.16</td>
<td>-1.47 ± 0.24</td>
</tr>
<tr>
<td>NGC 4507 (+001-019)</td>
<td>8.71 ± 0.12</td>
<td>-0.89 ± 0.02</td>
<td>-1.45 ± 0.12</td>
</tr>
<tr>
<td>NGC 4507 (-007-019)</td>
<td>8.85 ± 0.12</td>
<td>-0.97 ± 0.02</td>
<td>-1.50 ± 0.04</td>
</tr>
<tr>
<td>NGC 4507 (-013-018)</td>
<td>8.82 ± 0.13</td>
<td>-0.91 ± 0.04</td>
<td>-1.53 ± 0.12</td>
</tr>
<tr>
<td>NGC 4507 (-021-017)</td>
<td>8.82 ± 0.12</td>
<td>-0.92 ± 0.04</td>
<td>-1.59 ± 0.14</td>
</tr>
<tr>
<td>NGC 6814 (+016-016)</td>
<td>9.15 ± 0.16</td>
<td>-0.98 ± 0.36</td>
<td>-1.55 ± 0.50</td>
</tr>
<tr>
<td>NGC 6814 (+021-010)</td>
<td>9.09 ± 0.15</td>
<td>-0.83 ± 0.18</td>
<td>-1.51 ± 0.26</td>
</tr>
<tr>
<td>NGC 6814 (+027-002)</td>
<td>9.12 ± 0.15</td>
<td>-0.78 ± 0.18</td>
<td>-1.62 ± 0.30</td>
</tr>
</tbody>
</table>

<sup>a</sup>Derived from ([O II] $\lambda$3727 + [O III] $\lambda$4959, 5007) /H$\beta$ only.
stated errors. The uncertainty in the N/O ratio, which is less temperature sensitive than the ratios of either element alone with respect to hydrogen, is generally less than the uncertainty in the O/H ratio and arises mainly from uncertainties in the measured line intensities. Likewise, the uncertainty in the S/O ratio arises primarily from uncertainties in the measured line intensities, although in this case there is also a contribution which arises from the strong dependence of the intensity of the [S II] \( \lambda 6731 \) emission line on the ionization parameter \( \langle Q(H) \rangle \), defined by Evans and Dopita 1985.

We derive the mean oxygen, nitrogen, and sulfur abundances for the inner disk region of each galaxy from the H II region observations separately below.

\textbf{a) NGC 1068}

We have estimated elemental abundances in thirteen H II regions observed in the prototype Seyfert 2 galaxy NGC 1068 covering the range of radii from 20\arcsec–60\arcsec from the nucleus. This sample is sufficient to enable us to establish whether or not a strong radial abundance gradient is present in the inner disk region of this galaxy. The true radial distance of each H II region to the nucleus of the galaxy projected onto the plane of the galactic disk was computed from the apparent radial distance assuming that the position angle of the major axis of the galaxy is 52\degree (Nishimura, Kaneko, and Toyama 1984) and that the inclination of the galactic disk to the line of sight is given by \( \sec i = 1.18 \) (de Vaucouleurs, de Vaucouleurs, and Corwin 1976). The adopted isophotal radius of NGC 1068 is taken to be \( R_0 = 3'32'' = 11.68 \text{kpc} \),
and the adopted distance \((H_0 = 100 \, h^{-1} \text{km s}^{-1} \text{Mpc}^{-1})\) is 11.34 \(h\) kpc (de Vaucouleurs, de Vaucouleurs, and Corwin 1976).

In Figure 2 we plot the oxygen abundance derived for each \(\text{H} \, \text{II}\) region versus its fractional isophotal radius, \(\rho\). A first inspection of the figure suggests that there is no clear evidence for a radial gradient in oxygen abundance for the sample of \(\text{H} \, \text{II}\) regions which we observed, and that considerable scatter in oxygen abundance from region to region is evident. However, it is well established that weak \([\text{O} \, \text{III}] \lambda \lambda 4959, 5007\) emission extends over much of the inner disk region of NGC 1068 (Burbidge, Burbidge, and Prendergast 1958; Bertola 1968; Walker 1968; Balick and Heckman 1979) extending out as far as 50" from the nucleus along the major axis of the galaxy (Nishimura, Kaneko, and Toyama 1984). In addition, we detect extended emission from other lines also. The cause of this weak extended emission is not well established, but may be due to absorption of low-energy X-ray photons emitted from the Seyfert nucleus by warm \((\sim 10^4 \text{K})\) interstellar clouds (Evans and Dopita 1986). The excess line-emission arising from the underlying component, together with the increased uncertainties resulting from the subtraction of the averaged disk absorption spectrum, significantly increase the total uncertainties in the measured emission-line ratios (and hence abundance estimates) for \(\text{H} \, \text{II}\) regions with low surface brightness. The excess line-emission emanating from the underlying component results in an underestimate of the oxygen abundance for those objects with relatively strong background emission. On the basis of the signal-to-noise ratios of the observed spectra, we estimate that this effect is unimportant for objects with a mean apparent \(\text{H} \beta\) surface brightness greater than \(\sim 5 \times 10^{-16} \text{erg cm}^{-2} \text{s}^{-1} \text{arcsec}^{-2}\), and becomes increasingly important with decreasing surface brightness. In Figure 2, \(\text{H} \, \text{II}\) regions which have \(S_{\text{H} \beta} > 5 \times 10^{-16} \text{erg cm}^{-2} \text{s}^{-1} \text{arcsec}^{-2}\)
Figure 2. The oxygen abundances derived for the H II regions in NGC 1068 plotted against fractional isophotal radius, $\rho$. The filled circles represent those regions with $S_{H\beta} > 5 \times 10^{-16}$ erg cm$^{-2}$ s$^{-1}$ arcsec$^{-2}$, while the open circles indicate those regions with lower mean surface brightnesses likely to be affected by the underlying disk emission. The diamonds locate H II regions whose spectra are likely to be affected by the high-excitation emission to the NE of the nucleus.
are indicated by filled circles, while those with lower \( S_{\text{H}\beta} \) are marked with open circles. A further complication is the presence of an extended region of high-excitation emission to the NE of the nucleus. This region shows strong lines of \([\text{Ne} \text{v}]\ \lambda\lambda3346,3426\) and also \(\text{He}\ \Pi\ \lambda4686\) superposed on normal \(\text{H}\ \Pi\) region spectra, and has been interpreted as emission from ordinary \(\text{H}\ \Pi\) regions superposed on emission from a region photoionized by a power-law X-ray spectrum emanating from the Seyfert nucleus (Evans and Dopita 1986). The theoretical photoionization models presented in that paper suggest that the high-excitation region can contribute a considerable fraction of the total \([\text{O} \text{iii}]\ \lambda\lambda4959,5007\) emission observed. Diamonds are used in Figure 2 to indicate \(\text{H}\ \Pi\) regions likely to be significantly affected by this emission. If we consider only those \(\text{H}\ \Pi\) regions unlikely to be affected by either of the above complicating factors (the filled circles in Fig. 2), we find no evidence for a radial gradient in oxygen abundance over the range of \(\rho\) observed, and estimate the mean oxygen abundance to be \(12 + \log (\text{O}/\text{H}) = 9.02 \pm 0.07\), with only a small amount of scatter.

For the same \(\text{H}\ \Pi\) regions used to derive the mean oxygen abundance, we deduce mean nitrogen to oxygen and sulfur to oxygen ratios of \(\log (\text{N}/\text{O}) = -0.81 \pm 0.07\) and \(\log (\text{S}/\text{O}) = -1.55 \pm 0.04\) respectively. These values are comparable to the solar values (Allen 1973), \(\log (\text{N}/\text{O}) = -0.86\) and \(\log (\text{S}/\text{O}) = -1.62\), indicating that neither element is overabundant relative to oxygen, but that oxygen is mildly overabundant (by 0.2 dex) relative to the solar value in the inner \(\text{H}\ \Pi\) regions of NGC 1068.

b) \textit{NGC 3783}

Three \(\text{H}\ \Pi\) regions were observed in the Seyfert 1 galaxy NGC 3783.
Two of the H\II regions were situated \( \sim 15'' \) from the nucleus in the inner ring of this theta-type barred spiral near the southern end of the bar, while the third H\II region was located at approximately twice the radius of the other two in a spiral arm SW of the nucleus. Compared to the H\II regions in NGC 1068, the H\II regions in NGC 3783 have much lower mean surface brightnesses. Consequently, our spectra of these objects have somewhat lower signal-to-noise ratios. Combined with the apparently lower degree of excitation found in these H\II regions (e.g., Fig. 1) this implies that only upper limits could be established for the intensity of [O\III] \( \lambda 5007 \) in each case. However, [O\II] \( \lambda 3727 \) was readily detected, as were the other lines necessary to derive an abundance estimate. The abundances computed using the upper limits for the [O\III] \( \lambda 5007 \) line intensities did not deviate either consistently or significantly from those made with estimators not employing the [O\III] \( \lambda 5007 \) line. Hence we have confidence that our abundance estimates for these objects are not biased by the lack of a positive detection of this line.

The mean oxygen abundance derived from the three H\II regions is given by \( 12 + \log (O/H) = 8.86 \pm 0.08 \). There are insufficient data for this galaxy to establish whether or not a radial abundance gradient exists, but the morphology of the galaxy argues strongly against the presence of a steep abundance gradient since the bar-forming potential in the stellar disk of the galaxy is expected to produce considerable radial mixing of the ISM (Schwarz 1981; see also § IV below). The mean nitrogen to oxygen abundance ratio for the three H\II regions is \( \log (N/O) = -1.00 \pm 0.15 \), while the mean sulfur to oxygen ratio is \( \log (S/O) = -1.54 \pm 0.10 \). Within the errors the oxygen, nitrogen, and sulfur abundances in the H\II regions we observed are neither underabundant nor overabundant compared to the solar values.
c) NGC 4507

For the Seyfert 2 galaxy NGC 4507, four H II regions were observed with galactocentric radii between 19" and 26". As for NGC 3783 and NGC 6814 (§ IIId below), the limited range of galactocentric radii makes it impossible for us to derive an abundance gradient from these data. Only mean abundances can be determined. Inspection of the representative spectrum shown in Figure 1 indicates that the H II regions we observed in this galaxy have the lowest mean oxygen abundance of our sample, and, as expected since the ionization parameter and oxygen abundance are inversely correlated (Dopita and Evans 1986), high excitation. The abundances derived from the sequence confirm the qualitative results suggested by the figure, and we derive a mean oxygen abundance from the observations of $12 + \log (O/H) = 8.80 \pm 0.06$, with N/O and S/O ratios given by $\log (N/O) = -0.92 \pm 0.02$ and $\log (S/O) = -1.53 \pm 0.02$ respectively. Even though these H II regions represent the lowest mean abundances in our sample, we note that they are not significantly lower than the solar values.

d) NGC 6814

Three H II regions were observed in the Seyfert 1 galaxy NGC 6814, covering a range of galactocentric radii between 23" and 27". It is immediately apparent from the weakness of the forbidden lines (e.g., Fig. 1) that the three H II regions have a considerably higher than solar oxygen abundance and a very low ionization parameter. Indeed, in the case of NGC 6814 (+027—002), there is a clear detection of the low excitation [N I] $\lambda\lambda5198, 5201$ doublet which is emitted in the hydrogen transition zone where a significant fraction of neutral hydrogen exists. For each spectrum, only upper limits for
the intensities of the [O iii] λ5007 line could be established, and in one case only an upper limit could be set for the intensity of [O ii] λ3727 while for the other objects the detection was marginal (2σ–3σ). Even so, the good agreement found between the oxygen abundance determinations computed using the three different estimators recommended by Dopita and Evans (1986), for each of the H II regions, gives us confidence in the values derived. We find a mean oxygen abundance given by \(12 + \log (O/H) = 9.12 \pm 0.09\), which is a factor of two larger than the solar value, and is 0.24 dex higher than the oxygen abundance measured in the high-abundance H II region S5 in M101 (Evans 1986). On the other hand, the relative abundances of nitrogen and sulfur to oxygen are more typically solar, with values of \(\log (N/O) = -0.86 \pm 0.06\) and \(\log (S/O) = -1.56 \pm 0.03\) respectively.

IV. DISCUSSION

The results presented in the previous section suggest that the abundances of the elements oxygen, nitrogen, and sulfur present in the inner regions of the Seyfert galaxies which we studied are typically solar, or perhaps somewhat overabundant with respect to solar. None of the H II regions in the four galaxies studied show any evidence for oxygen abundances significantly lower than solar, and this is also true for other Seyfert galaxies for which abundance measurements in H II regions have been conducted (e.g., Pagel et al. 1979; Hawley and Phillips 1980).

The lack of any evidence to suggest that N/O or S/O abundance ratios are abnormal in any of the H II regions in our sample indicates that preferential enrichment or depletion of these elements relative to oxygen cannot be important in determining the local chemical composition of the ISM in
the inner disk regions of the galaxies we observed. This suggests, for example, that enhancements of the supernova or star-formation rates and related nucleosynthetic processes triggered by nuclear shocks and winds compressing the local ISM are either too insignificant to effect the overall chemical enrichment of inner disk, or that such processes do not greatly modify the local stellar mass function over the timescale of the nuclear activity. With the advent of *Space Telescope*, it should be possible to discriminate between these possibilities by a program of spatially-resolved spectrophotometry of the nuclear regions.

Whether or not a direct correlation exists between elemental abundances and Seyfert activity is both uncertain and difficult to establish. There is evidence to suggest that Seyfert galaxies occur with only a narrow range of morphological types. Sérsic (1973) pointed out that many Seyferts tend to be barred spirals, while de Vaucouleurs (1974) noted that Seyfert galaxies tend to have Hubble types earlier than Sbc, and Adams (1977) indicated that many Seyferts have ring structures. Simkin, Su, and Schwarz (1980) have constructed theoretical disk models which reproduce the range of morphological types observed, and suggest that they may form an evolutionary sequence. In particular, correlations are observed between morphological type parameterized by age along the theoretical evolutionary sequence and quantities, such as the FWZI of the Balmer lines or the X-ray luminosity, characterizing the degree of activity for Seyfert 1 nuclei (Su and Simkin 1980). At the same time, it is well known that irregular galaxies and late-type spirals tend to contain H II regions with low metal abundances, and that metallicity tends to increase as one progresses from late-type galaxies to early-type galaxies, and with increasing luminosity. Hence it is certainly possible that the limited range of metal abundances seen in Seyfert galaxies is due only to the
correlation of metal abundance with galaxy morphology and the restricted range of morphological types occupied by Seyfert galaxies, but is causally unrelated in any way to the Seyfert activity itself.

More significant for models of Seyfert galaxies and their nuclei is the apparent lack of strong radial abundance gradients. Our data for NGC 1068 suggest that no obvious gradient in metal abundance is present in this galaxy, at least in the inner region of the disk over which our observations range. Likewise, there is no evidence for large abundance gradients in the Seyfert galaxies NGC 1365 (Pagel et al. 1979) and NGC 1566 (Hawley and Phillips 1980) which have well studied H II regions. Furthermore, neither of the active galaxies M51 and M83 show evidence for large abundance gradients. The former galaxy exhibits “Seyfert like” nuclear activity (Rose and Searle 1982; Rose and Cecil 1983), and there are indications of active sites situated outside the nucleus, possibly originating from a bi-directional nuclear jet (Ford et al. 1985). The latter galaxy has been classified as having a starburst nucleus (Bohlin et al. 1983). On the other hand, we find that abundance gradients tend to be quite pronounced in late-type spirals, such as M33 (Dopita, D’Odorico, and Benvenuti 1980) and M101 (Evans 1986), which do not exhibit strong nuclear activity.

The lack of steep abundance gradients in Seyfert galaxies is almost certainly related to their limited range of morphologies, following the suggestion of Searle (1971) and Smith (1975) that a correlation exists between abundance gradients and morphological type. One reason for such a correlation has been suggested by Schwarz (1979, 1981) who demonstrated that in a gravitational potential produced by a stellar background with a sharply peaked central density distribution, a rotating gaseous disk would develop a sequence
of spiral and then ringlike patterns when perturbed by a rotating $2\theta$ potential with the appropriate pattern speed. Su and Simkin (1980) showed that the range of morphologies observed for Seyfert galaxies were well fitted by the theoretical disk model. As the model sequence evolved, the gas in the inner regions of the disk developed a strong flow into the nuclear regions on a timescale short compared with the age of the galaxy. Models with radial inflow of gas are also required to adequately explain observed abundance gradients in normal spiral galaxies (e.g., Tinsley and Larson 1978; Mayor and Vigroux 1981; Lacey and Fall 1985), and are expected to be present in most galaxy disks. When combined with the outflow of material from the active nucleus, predicted by a number of models (e.g., Kippenhahn, Mestel, and Perry 1975; Blandford and Konigl 1979; Krolik and Vrtilek 1984) and observed in some cases (e.g., Cecil and Rose 1984; Heckman, Miley, and Green 1984; Wamsteker and Barr 1985), this implies that substantial radial mixing of the ISM must take place in the inner regions of the disk, minimizing the formation of abundance gradients and possibly also enhancing star-formation through turbulent motions and compression. A major consequence of the radial mixing predicted by such models is that the chemical composition of the gas which makes up the narrow-line region, and possibly also the broad-line region, will be similar to the chemical composition to the H ii regions found in the inner disk. Hence, measurements of elemental abundances in near-nuclear H ii regions may be used to constrain theoretical models of the active nuclear regions.

Let us now consider whether the high ionizing luminosity of the active nucleus may affect the gas in near-nuclear H ii regions. At small radii from the nucleus, it seems highly probable that the intense photon flux from the nuclear ionizing spectrum would either dominate or at least significantly alter
the ionization balance in an H II region, unless the latter is somehow shielded from the central source. Large changes in the ionization balance of H II regions arising from the nuclear ionizing photon flux would almost certainly render invalid abundance determinations from those objects. Besides directly altering the ionization balance within the H II regions, the nuclear spectrum may ionize the lower density interstellar medium and clouds surrounding them. An example of this is NGC 1068, where both high-excitation emission is seen superposed with H II region spectra to the NE of the nucleus (Evans and Dopita 1986), and low-level underlying emission is observed over much of the inner 2–3 kpc of the disk. The radius within the disk to which such effects may be important depends upon the shape of the ionizing spectrum and the ionizing luminosity of the central source, and the column density and absorption cross section of the intervening material. Assuming isotropic emission from the nuclear photon source, and a uniformly dense interstellar medium, we can estimate the radius in the disk at which the nuclear photon source should have negligible effect on the ionization balance in the H II regions as follows. The ionization parameter due to the central source, at any radius r from the nucleus, is given by

\[ Q(H, r) = \frac{L_C}{4\pi r^2 N}, \]

where \( L_C \) is the ionizing photon luminosity and \( N \) is the number density of atoms plus ions for the intervening material. The lowest value of the ionization parameter in low-excitation (metal rich) H II regions is \( \sim 5 \times 10^6 \text{ cm}^{-1} \) (Dopita and Evans 1986), so if we assume that a value of \( Q(H, r) = 2 \times 10^6 \text{ cm}^{-1} \) represents a level where the ionization due to the nuclear source is insignificant relative to the local ionization due to the OB association illuminating the H II region, and taking \( N = 0.3 \text{ cm}^{-3} \) as
being representative of the intervening interstellar medium in the disk, we find

\[ r_{\text{max}} \approx 2.7L_{42}^{1/2} \text{kpc}, \]

where \( r_{\text{max}} \) is the radius in kpc where the ionization parameter declines to \( 2 \times 10^6 \text{cm s}^{-1} \), \( L_{42} \) is the 0.5–4.5 keV X-ray luminosity in units of \( 10^{42} \text{erg s}^{-1} \), and we have assumed for simplicity that the nuclear ionizing spectrum can be represented as a power-law, \( F_\nu \propto \nu^\alpha \), with spectral index \( \alpha = -1 \). For example, for NGC 1068 where the 0.5–4.5 keV X-ray luminosity is \( \sim 7.2 \times 10^{41} \text{erg s}^{-1} \) (Lawrence and Elvis 1982), we find \( r_{\text{max}} \approx 2.3 \text{kpc} \), which is in good agreement with the extent of the underlying disk emission in that galaxy. The presence of density inhomogeneities, such as interstellar or molecular clouds, or regions of low-density coronal gas in pressure equilibrium with the interstellar medium expected to exist in the strong X-ray fields of active galactic nuclei (Lepp et al. 1985), will alter \( r_{\text{max}} \), but the above expression gives an approximate estimate for the extent of the nuclear influence. When attempting to derive abundances from H II regions with radii \( r \lesssim r_{\text{max}} \) one should be appropriately cautious, although the increased number density within the H II region will considerably reduce the effective ionization parameter of the nuclear spectrum relative to the input value at the edge of the H II region. For H II regions with \( r \approx r_{\text{max}} \) the most likely effects of the nuclear spectrum will be increased emission from low ionization species which exist in the hydrogen transition zone at the edge of the nebula, and contamination of the pure H II region spectrum by emission from the lower density warm ISM surrounding the region.
V. CONCLUSIONS

We have applied the theoretical abundance sequence calibration of Dopita and Evans (1986) to low resolution spectrophotometry of 23 H II regions in two Seyfert 1 and two Seyfert 2 galaxies in order to estimate elemental abundances. The mean oxygen abundance derived from the H II region observations in each galaxy ranges from approximately solar abundance to twice solar abundance. In all cases we find that the ratios of nitrogen abundance and sulfur abundance to oxygen abundance are about the same as the solar values, indicating that these elements are not preferentially enriched or depleted relative to oxygen. This implies that processes excited by the nuclear activity which would result in preferential chemical enrichment cannot be a significant factor in determining the local chemical composition of the ISM.

The absence of a steep abundance gradient in the inner regions of NGC 1068, combined with similar results for other Seyfert and active galaxies, implies that substantial radial mixing of the ISM must occur in the inner disks of these galaxies. Consequently, we conclude that elemental abundances found in near-nuclear H II regions could be adopted as nuclear abundances as a constraint on theoretical models for the narrow- and broad-line regions of the Seyfert nucleus. It is somewhat fortuitous that the abundances we measure are approximately solar, or slightly higher, since the majority of theoretical models which have to date been reasonably successful in explaining the emission-line intensities and continua emitted by Seyfert and other active nuclei have often, a priori, assumed a solar abundance set.

For H II regions lying within a few kpc from the nucleus, the influence of the nuclear ionizing spectrum on the ionization balance should be taken into
account when interpreting the spectra of the H\textsc{ii} regions to derive elemental abundances. The most likely effect of the nuclear luminosity is to increase the forbidden-line emission, resulting in artificially low abundance estimates for very near-nuclear H\textsc{ii} regions. This effect is in fact evident in the data for the H\textsc{ii} regions in NGC 1068 with very small fractional radii.

The overabundance of the elements, and the relatively small range of abundances displayed by our sample of galaxies is an interesting result that needs confirmation in a larger sample of Seyfert and other active galaxies. In addition, further theoretical studies of the chemical and dynamical evolution of the nuclear regions are required to establish whether or not there is a causal relationship between strong radial flows and mixing of the local ISM near the nucleus and the nuclear activity. For example, one can envisage that the gas close to the nucleus could behave as a relaxation oscillator. Strong radial flows to the nucleus could give rise to starburst activity through compression of the ISM, and the formation of a nuclear accretion disk. The increasing activity and turbulence may result in the formation of a Seyfert nucleus and an outflowing nuclear wind. The latter may eventually dissipate the circumnuclear gas and cut off the nuclear activity, after which a new radial flow could result, thus repeating the process.

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HIGH-EXCITATION EXTRA-NUCLEAR GAS
IN THE SEYFERT GALAXY NGC 1068

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ABSTRACT

Optical spectrophotometry of candidate near-nuclear H II regions in the disk of the Seyfert galaxy NGC 1068 indicates the presence of high-excitation extra-nuclear emission. The optical spectra appear to be very similar to ordinary H II region spectra with the addition of strong lines of [Ne v] λλ3346, 3426 and He II λ4686. We interpret this as the superposition of an H II region spectrum with the high-excitation emission, and present theoretical nebular models which suggest that the high-excitation gas is most likely photoionized by a power-law spectrum, probably from the nearby Seyfert nucleus.

Subject headings: galaxies: individual — galaxies: seyfert — nebulae: general — nebulae: H II regions
I. INTRODUCTION

The bright prototype Seyfert 2 galaxy NGC 1068 has been the subject of a number of recent investigations. For example, Alloin et al. (1983) have demonstrated the existence of complex large-scale mass motions near the nucleus, and the impact of such activity on the surrounding galaxy disk has recently been discussed by Atherton, Reay, and Taylor (1985). Nishimura, Kaneko, and Toyama (1984) have illustrated that low-level emission is present over the inner 2–3 kpc of the galaxy, while Telesco et al. (1984) have established the presence of a luminous infrared disk covering the inner 3 kpc at a wavelength of 10 μm. In the near-IR, Hall et al. (1981) have detected shocked molecular hydrogen near the nucleus, and Scoville, Young, and Lucy (1983) have discussed the role of such gas in the process of star formation. Pedlar et al. (1983) and Wilson and Ulvestadt (1983) have studied the radio jets emanating from the nucleus, and their effect on the surrounding interstellar medium.

In this Letter, we report new observations of candidate near-nuclear H II regions, carried out as part of a study of H II region abundances in Seyfert galaxies (Evans and Dopita 1986), which demonstrate the existence of high-excitation extra-nuclear emission in NGC 1068. We present theoretical nebular models for the data which suggest that the observed emission is a superposition of an ordinary H II region spectrum and emission from a region photoionized by the power-law spectrum emanating from the nearby Seyfert nucleus.
II. OBSERVATIONS AND REDUCTIONS

The optical spectra were obtained under photometric conditions at the 3.9 m Anglo-Australian Telescope on the night of 1983 November 8–9. The Royal Greenwich Observatory spectrograph was used with the Image Photon Counting System (IPCS; Boksenberg 1972) as detector. The instrumental configuration was chosen to give 96 spectra, each separated by 1''15 on the sky, with a spectral resolution of 8 Å and a spectral coverage of 3200–7400 Å. A slit width of 300 μm (2''01 on the sky) was employed for these observations. The spectra were reduced to absolute flux in the normal manner (see, for example, Dopita, Binette, and Schwartz 1982), and the spectra of individual knots were obtained by co-adding all the spectra (or spatial increments) in which the knot was detected.

The reddening corrections applied to the observed fluxes were initially determined from the data based on the assumption that the intrinsic Balmer decrement is due purely to recombination for an adopted nebular temperature of 8000 K. The theoretical models computed in § III suggest that a steeper Balmer decrement is more appropriate, and so the reddening corrections were later recalculated on the basis of these models. In some of the spectra underlying Balmer absorption due to the galaxy is evident, but optical emission is present over the entire region observed, and hence the underlying galaxy continuum could not be accurately subtracted from the total spectra. Consequently, measurements of the emission line intensities of higher order Balmer lines are somewhat uncertain, and so only the observed $I(\text{H}\alpha)/I(\text{H}\beta)$ ratio was employed to estimate the amount of interstellar reddening.
III. RESULTS AND DISCUSSION

Our observations indicate the presence of a large region of highly ionized nebulosity that extends over a linear dimension of 1.9h kpc at the distance of NGC 1068 ($H_0 = 100h^{-1} \text{km s}^{-1} \text{Mpc}^{-1}$), equivalent to 35'' on the sky, along a P. A. of 10° centered on $\alpha = 02^h 40^m 08^s$, $\delta = -00^\circ 13' 19''$ (1950.0). A typical spectrum is shown in Figure 1. The presence of the high-excitation lines [Ne v] $\lambda\lambda 3346, 3426$ is immediately evident, and He ii $\lambda 4686$ is visible also. In Figure 2 we plot our observations on the excitation diagram ([Ne v] $\lambda 3426$/[Ne iii] $\lambda 3869$) versus ([O iii] $\lambda 5007$/[O ii] $\lambda 3727$), together with the data set of Baldwin, Phillips, and Terlevich (1981) for a number of other types of emission-line nebulosity. The crosses indicate the region of parameter space populated by planetary nebulae, while diamonds are used to indicate objects photoionized by power-law spectra. Normal H ii regions and shock-heated objects emit negligible amounts of [Ne v] $\lambda 3426$. The open circles indicate the location of the knots we have observed, prior to correction for interstellar reddening, while the filled circles indicate the results of applying the reddening correction described above. Inspection of the figure demonstrates the anomalously high [Ne v] $\lambda 3426$ line intensities from these knots, even before any reddening correction is applied. The apparent ratios of [Ne v] $\lambda 3426$ to [Ne iii] $\lambda 3869$ are higher in these knots than any of the other objects in the Baldwin, Phillips, and Terlevich data set, and are typically 0.8 dex larger than in the nucleus of NGC 1068. On the other hand, the [Ne iii] $\lambda 3869$ line strengths are typical of ordinary H ii regions, implying that the neon abundance is not abnormally high. Similarly, the [O iii] $\lambda\lambda 4959, 5007$ line intensities are typical of ordinary H ii regions and do not reflect the degree of ionization suggested by the [Ne v] $\lambda 3426$ line strengths.
Figure 1. A typical IPCS spectrum of one of the knots. Note particularly the high-excitation $\text{[Ne v]} \lambda\lambda 3346, 3426$ and $\text{He } II \lambda 4686$ lines.
Figure 2. The excitation diagram ([Ne v] $\lambda$3426/[Ne iii] $\lambda$3869) versus ([O iii] $\lambda$5007/[O ii] $\lambda$3727). The positions of the observed knots prior to dereddening is indicated by open circles, while filled circles mark the positions after correction for interstellar reddening. Crosses mark the location of planetary nebulae in the Baldwin, Phillips, and Terlevich sample, and diamonds indicate the positions of objects from the same sample which are photoionized by a power-law spectrum.
When placed on the other excitation diagrams of Baldwin, Phillips, and Terlevich, the knots occupy similar positions to ordinary H\textsc{ii} regions, except that $I ([\text{N}\text{\sc{ii}}] \lambda 6584) / I (\text{H}\alpha)$ is typically 0.3 dex larger in the knots than the median values for H\textsc{ii} regions. Such a difference is within the scatter for real H\textsc{ii} regions, and could be readily accounted for by a small increase in nitrogen abundance (Dopita and Evans 1986). From our optical spectra, the knots are atypical of H\textsc{ii} regions only in the sense that they show strong [Ne v] $\lambda 3346, 3426$ and He ii $\lambda 4686$ emission.

It has been well established that [O iii] $\lambda \lambda 4959, 5007$ emission extends outwards from the nucleus of NGC 1068 for a considerable distance in the direction of P. A. 30° (Burbidge, Burbidge, and Prendergast 1959; Bertola 1968; Walker 1968). Balick and Heckman (1979) measured strong [O iii] $\lambda 5007$ emission 15″ NE of the nucleus, while Nishimura, Kaneko, and Toyama (1984) detected [O iii] $\lambda 5007$ emission up to 50″ out from the nucleus along the major axis of the galaxy (P. A. 52°).

The presence of extended emission over a very large region to the NE of the nucleus of NGC 1068 raises the possibility that our spectra consist of a superposition of emission from normal H\textsc{ii} regions together with emission from a separate region responsible for the high-excitation lines. The resolution of our data is too low to allow us to determine if there are differences in radial velocities or line profiles between the high- and low-excitation lines. However, in this context it is interesting to note that knots showing [Ne v] $\lambda 3426$ emission appear to follow a spur of “high” (FWHM > 85 km s$^{-1}$) H\alpha linewidth with a P. A. of approximately 20°, and located about 10″ N and 20″ E of the nucleus (Atherton, Reay, and Taylor 1984), although the linear extent of the [Ne v] $\lambda 3426$ emission is larger than the extent of the spur.
Atherton, Reay, and Taylor (1984) interpret regions of high linewidth as being due to a very high level of turbulent gas motions in the disk due to the activity of the Seyfert nucleus, but the presence of localized high-excitation emission suggests that there may be a contribution from localized activity also.

The intensity of the $[\text{Ne} \, v] \lambda 3426$ line in these spectra precludes the possibility that an ordinary stellar source is responsible for photoionizing the high-excitation gas. From a range of models computed using our general purpose modeling code MAPPINGS (Binette 1982; Binette, Dopita, and Tuohy 1985; Evans and Dopita 1985), it would appear that a power-law spectrum is most likely to be capable of producing the degree of ionization necessary to give rise to the strength of the $[\text{Ne} \, v] \lambda 3426$ emission observed, provided that we assume that the observed spectra consist of a superposition of ordinary $\text{H} \, \text{ii}$ region spectra and emission from the high-excitation gas. It does not seem to be possible to reproduce both the high- and low-excitation line intensities observed with a plasma photoionized by a single input ionizing spectrum.

To test this hypothesis, we computed a series of theoretical models consisting of the sum of an ordinary $\text{H} \, \text{ii}$ region and a region photoionized by a power-law spectrum. The summed model spectra were then compared with the mean spectrum of the observed knots. The models were homogeneous in the sense that identical elemental abundances were employed for the high- and low-excitation regions, but otherwise the two regions were treated distinctly. The actual elemental abundances employed were determined from the models for the low-excitation region, since the majority of the optical forbidden lines are emitted by that region, and their intensities
depend strongly on the adopted abundances. By contrast, the emission from
the high-excitation region depends only weakly on the adopted abundances.

The high-excitation region was modeled as a single-zone plane-parallel
slab of gas illuminated on one face by a power-law with index $\alpha = -1$ (defined
by $F_\nu \propto \nu^\alpha$), although the models are relatively insensitive to the assumed
spectral index for $-1.5 \lesssim \alpha \lesssim -0.5$. Initially, we employed a power-law spec-
trum which extended from a turn-on energy of 7.64 eV to a high-energy cut-
off of 5 keV. However, with such an ionizing spectrum, we found that it was
not possible to reproduce the observed low ratio of $I(\text{He}^\text{II} \lambda 4686)/I(\text{H}\beta)$
while simultaneously maintaining sufficiently strong $[\text{Ne}^\text{v}] \lambda 3426$ emission.
Based on the assumption that the Seyfert nucleus is the source of the ion-
izing photons, we increased the turn-on energy of the power-law to 40 Ryd
in order to simulate the absorption of low-energy photons by the interven-
ing interstellar medium (ISM) and dense molecular clouds observed near
the nucleus (Hall et al. 1981). Increasing the turn-on energy has the ef-
fact of decreasing the number of photons capable of ionizing He$^+$ (ionization
energy $E_{\text{f}}(\text{He}^+) = 54.52$ eV) relative to the number of photons capable of
ionizing Ne$^{+3}$ (ionization energy $E_{\text{f}}(\text{Ne}^{+3}) = 97.11$ eV). This reduces the
intensity of the He$^{\text{II}} \lambda 4686$ recombination line compared to the $[\text{Ne}^\text{v}] \lambda 3426$
forbidden line. One potential source of $[\text{Ne}^\text{v}] \lambda 3426$ emission is Auger cas-
cade following K-shell photoionization of Ne$^{+2}$ with a threshold of $\sim 900$ eV.
The value adopted for the turn-on energy was chosen on the basis of stud-
ies of photoelectric absorption of soft X-rays by the ISM (Hayakawa 1973)
and the presence of the strong oxygen K-edge discontinuity in the absorption
cross section at $\sim 0.53$ keV. Provided that the turn-on energy is substantially
greater than $E_{\text{f}}(\text{He}^+)$ the value chosen is not critical, and varying it over the
range $\sim 20$–60 Ryd has only a small effect on the computed spectrum. The
ratio of $I ([\text{Ne} \text{ v}] \lambda 3426) / I (\text{He} \text{ II} \lambda 4686)$ from the model is then solely determined by the mean ionization parameter in the gas, $\bar{Q}(\text{H})$ (defined by Evans and Dopita 1985). The observed ratio of $I ([\text{Ne} \text{ v}] \lambda 3426) / I (\text{He} \text{ II} \lambda 4686)$ is achieved when $\bar{Q}(\text{H}) \approx 7 \times 10^8 \text{cm s}^{-1}$, and this results in a plasma with a mean electron temperature close to 40,000 K. Such a plasma emits strongly in the $[\text{Ne} \text{ v}] \lambda \lambda 3346, 3426$, $[\text{O} \text{ iii}] \lambda \lambda 4959, 5007$, and $\text{He} \text{ II} \lambda 4686$ lines, and the Balmer lines of hydrogen, but little else, in the visible spectrum. Most of the line cooling in the plasma occurs in the very strong $\text{O vi} \lambda 1034$ and $\text{He} \text{ II} \lambda 304$ UV resonance lines. The density of the high-excitation gas must be considerably lower than the density of the gas comprising the $\text{H II}$ region, otherwise the photon flux from the power-law source would dominate the ionization in the $\text{H II}$ region as well, unless the latter were somehow shielded from the central source. If we assume that the power-law spectrum contributes no more than $\sim 5\%$ of the ionization within the $\text{H II}$ region, then the ratio of ionization parameters in the high- and low-excitation (see below) gas places an upper limit on the density of the high-excitation gas of $\sim 0.03 \text{cm}^{-3}$ assuming $N = 30 \text{cm}^{-3}$ in the $\text{H II}$ region. Furthermore, the mean density of the intervening column between the nuclear source and the high-excitation gas cannot exceed $\sim 0.003 \text{cm}^{-3}$ otherwise the observed X-ray luminosity (Lawrence and Elvis 1982) would be incapable of providing sufficient photon flux to ionize the high-excitation region (assuming isotropic emission). Such a low mean density can be achieved by assuming that the ISM is in multi-phase pressure equilibrium (Lepp et al. 1985, and references cited therein), with the bulk of the gas in the low-density coronal phase. These conditions are expected to hold in the hard X-ray field present near a Seyfert nucleus. However, the mean density of the intervening column may be somewhat
higher, $\sim 0.01-0.03 \text{cm}^{-3}$, following recent studies which indicate the presence of a hidden Seyfert 1 nucleus in NGC 1068 which is directing X-ray emission anisotropically in the approximate direction of the high-excitation region (Antonucci and Miller 1985; Krolik and Begelman 1986).

Once the relative intensities of the lines emitted by the high-excitation gas have been established, the absolute intensity of the emission can be determined by comparison of the predicted intensity of $[\text{Ne v}] \lambda 3426$ with the observed spectrum. The predicted high-excitation contribution can then be subtracted from the observed spectrum in order to estimate the contribution of the low-excitation (or H II region) spectrum to the total emission. The H II region models computed to determine this contribution to the model spectrum were identical in structure to those described by Evans (1986), which should be referred to for a detailed description of the calculations. Suffice it to say here that the H II region was treated as a steady-state spherically symmetric nebula consisting of infinitesimal filaments of gas with uniform density of hydrogen atoms plus ions, $N_H = 30 \text{cm}^{-3}$, with volume filling factor $\epsilon = 0.1$. The centrally located source of ionizing photons is modeled as a single star with ionization temperature $T_{\text{ion}}$. The stellar atmosphere flux is derived from the log $g = 4.0$ models of Hummer and Mihalas (1970) using the interpolation scheme developed by Shields and Searle (1978).

Locating the "observed" H II region spectrum on the diagnostic diagrams of Evans and Dopita (1985) suggested that a low $\overline{Q}(H)$ ($\sim 3 \times 10^7 \text{cm s}^{-1}$) and a high $T_{\text{ion}}$ ($\sim 56,000 \text{K}$), together with a metallicity of $\sim \frac{3}{4} Z_\odot$, is required to correctly model the emission. Trial and error led to a final model with $12 + \log (O/H) = 8.70$, $T_{\text{ion}} = 60,000 \text{K}$, and $\overline{Q}(H) = 1.33 \times 10^7 \text{cm s}^{-1}$. The He, N, and S abundances were allowed to vary in
their ratio to O in order to fit the observations, while the other elements (and in particular Ne) were fixed in their “solar” ratio (Allen 1973) to oxygen. The ionization temperature of the stellar atmosphere required is much higher than the mean found by Evans and Dopita (1985) and employed for their calibration of the H II region abundance sequence (Dopita and Evans 1986). However, one of the knots observed showed a prominent (~ twice $I(H\beta)$) broad emission feature centered near 4660Å, and we identify this as a blend of C III and C IV permitted lines indicative of the presence of WC stars. Such stars would have the effect of biasing the $T_{\text{ion}}$ required to model the mean observed spectrum towards a greater temperature than normal.

In Table 1 we present the intensities of the mean observed spectrum of the knots, together with the theoretical contributions of the high- and low-excitation regions according to our models, and the sum of the contributions of the models. The principal model parameters are also presented in the table. Inspection of the table illustrates the excellent agreement between the theoretical models and the mean observed spectrum. Indeed, the only line for which a significant discrepancy exists is [Ne III] $\lambda$3869, which is predicted to be a factor of two weaker than observed. As described by Evans (1986), this is due to absorption edges in the stellar atmosphere models employed, and arises because of our simplistic assumption that the OB associations responsible for producing the ionizing photons which give rise to the H II region contribution to the spectra can be modeled as a single stellar atmosphere with $T_{\text{ion}}$ equal to the cluster mean ionization temperature.

On the basis of the agreement between the observed and predicted spectra, we propose that the data can be best explained by a superposition of emission from a normal H II region and emission from a high-excitation
## TABLE 1

**PHOTOIONIZATION MODELS**

### A. LINE INTENSITIES

<table>
<thead>
<tr>
<th>Ion</th>
<th>( \log I_{\text{obs}} )</th>
<th>( \log I_{\text{high exc}} )</th>
<th>( \log I_{\text{low exc}} )</th>
<th>( \log I_{\text{total}} )</th>
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<tr>
<td>([\text{Ne v}] \lambda 3426)</td>
<td>(+0.09 \pm 0.07)</td>
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<td>(-11.25)</td>
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<td>([\text{O ii}] \lambda 3727)</td>
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<td>(+0.29)</td>
<td>(+0.31)</td>
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<tr>
<td>([\text{Ne iii}] \lambda 3869)</td>
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<td>(-2.14)</td>
<td>(-1.15)</td>
<td>(-1.11)</td>
</tr>
<tr>
<td>(\text{H}\delta \lambda 4102)</td>
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<td>(-0.98)</td>
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</tr>
<tr>
<td>(\text{H}\gamma \lambda 4340)</td>
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<td>(-0.73)</td>
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<tr>
<td>([\text{O iii}] \lambda 4363)</td>
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<td>(-1.16)</td>
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<td>(\text{He ii} \lambda 4686)</td>
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<tr>
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### B. MODEL PARAMETERS

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<thead>
<tr>
<th>Parameter</th>
<th>high exc</th>
<th>low exc</th>
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<tr>
<td>(T_{\text{ion}} \text{K})</td>
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<tr>
<td>(\alpha)</td>
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<td>(\ldots)</td>
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<tr>
<td>(\overline{Q}(\text{H}) \text{cms}^{-1})</td>
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<td>(1.33 \times 10^7)</td>
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<tr>
<td>(N_H \text{ cm}^{-3})</td>
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<td>(0.1)</td>
</tr>
<tr>
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<td>(\ldots)</td>
</tr>
<tr>
<td>(\text{He}/\text{H})</td>
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<td>(0.082)</td>
</tr>
<tr>
<td>(12 + \log (\text{O}/\text{H}))</td>
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<td>(8.70)</td>
</tr>
<tr>
<td>(12 + \log (\text{N}/\text{H}))</td>
<td>(8.19)</td>
<td>(8.19)</td>
</tr>
<tr>
<td>(\text{O} / \text{S})</td>
<td>(34.4)</td>
<td>(34.4)</td>
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</tbody>
</table>

**NOTES**—\(\log I_{\text{obs}}\) is the observed logarithmic line intensity relative to \(\text{H}\beta\); \(\log I_{\text{high exc}}\) and \(\log I_{\text{low exc}}\) are the predicted contributions of the models for the high- and low-excitation regions respectively; \(\log I_{\text{total}}\) is the sum predicted line intensities from the models.
region. The high-excitation emission is due to photoionization of gas in an interstellar cloud by the power-law spectrum emanating (presumably) from the nearby Seyfert nucleus. X-ray photons with energies lower than ~ 40Ryd are absorbed by warm (~ 10,000 K) interstellar clouds in the intervening ISM, and this may be at least partly responsible for the [O iii] λλ4959, 5007 emission observed underlying the central 2–3 kpc of the disk. As pointed out by Atherton, Reay, and Taylor (1985), the active nucleus must also pressurize the interstellar cloud, either through interaction of the radio jets (Blandford and Konigl 1979), sub-relativistic winds (Krolik and Vrtilek 1984), or radiation pressure (Kippenhahn, Mestel, and Perry 1975), and this must be responsible for the large turbulent line widths which they detect. Such turbulence will enhance the likelihood of star formation in the interstellar clouds, giving rise to the creation of H II regions and further star formation. Whether or not the high-excitation emission is related to interaction of the nearby radio jets with the interstellar clouds cannot be ascertained from our data. High resolution narrow band imaging of the central region of NGC 1068 in [Ne v] λ3426 would be useful to delineate the extent of the high-excitation emission and enable us to map the regions photoionized by the (nuclear) power-law spectrum.

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DISCUSSION AND CONCLUSIONS

This investigation has presented a new calibration of the H II region abundance sequence derived from theoretical photoionization modeling employing the most recent atomic data available, and has utilized the calibration to initiate studies of elemental abundances in near-nuclear H II regions in a sample of Seyfert galaxies. The detailed results of this study are articulated in the papers which comprise this dissertation and will not be repeated at length here. However, the major contributions of this investigation are summarized here, together with indications of areas which warrant further research which follow naturally from this study.

A large homogeneous set of photoionization models with conditions applicable to H II regions has been computed using the general purpose modeling code MAPPINGS. From the grid of models a set of diagnostic diagrams has been developed which enables one to estimate the mean ionization parameter and element-averaged metallicity in the nebula, and the mean ionization temperature of the exciting stars. Comparison of the theoretical models with current observational data suggests that the ionization temperature of the principal stars in the ionizing OB associations cluster about $T_{\text{ion}} = 41,500$ K with a total scatter of order 3000 K. The distribution of the observed H II regions can be reconciled with the theoretical models only if the ionization parameter is correlated with metallicity, in the sense that high $Q$(H) is correlated with low $Z$. These results indicate that the observed distribution of H II regions form a one-dimensional emission-line spectral sequence which can be parameterized by metal abundance.

By correctly establishing the correlation between ionization parameter and abundance, the sequence of theoretical photoionization models necessary
to calibrate the observed spectral sequence in terms of elemental abundances has been computed. Comparison of the observational data with the theoretical sequence implies that nitrogen must be enriched as a secondary element of nucleosynthesis, except at very low abundances. The theoretical sequence reproduces the observed sequences of H II regions on a number of diagrams commonly used for abundance and excitation diagnostics, and has been employed to recalibrate the semiempirical abundance sensitive line ratios recommended by Pagel et al. (1979) and others. The major consequence of this recalibration is to reduce the absolute calibration of the abundance scale at high metallicity. A method has been prescribed for deriving oxygen, nitrogen, and sulfur abundances from ratios of prominent emission lines, and helium abundances from the intensities of He I emission lines.

Comparison of oxygen abundances derived from the abundance sequence with those derived from "exact" photoionization modeling for a number of H II regions in the spiral galaxy M101 indicates that oxygen abundances may be estimated from the sequence with an accuracy of ~ 0.15 dex. The photoionization models also demonstrate that the H II region S5, which was employed by Pagel et al. (1979) and McCall (1982) to calibrate the high-metallicity end of the abundance sequence, has a considerably lower oxygen abundance than previously thought. The differences between the previous abundance determinations and the one presented here result from different adopted values for atomic rate coefficients which have been updated in the intervening period. Employing the newly derived oxygen abundance for S5 indicates that the previous empirical calibrations of the abundance sequence would resemble the theoretical sequence computed here. The elemental abundances derived from the exact photoionization model data have
been combined with abundances estimated from the sequence for several additional H II regions in M101 in order to measure the slope and shape of the radial oxygen abundance gradient in that galaxy, and indicate that the latter is very closely exponential. The implications of the derived O, N, S, Ne, and Ar abundance gradients on galaxy formation and chemical evolution models were discussed, and a simple model for disk formation which is capable of qualitatively explaining the observed differences between the slopes of the radial abundance gradients for the different elements was proposed.

Following the calibration and verification of the abundance sequence, it was applied to spectrophotometry of a number of H II regions in a sample of Seyfert galaxies to estimate elemental abundances. The mean oxygen abundances derived for near-nuclear H II regions in the four galaxies in the sample were found to fall in the range ~ 1–2 times solar abundance. None of the objects in the sample showed any evidence for preferential enhancement or depletion of nitrogen or sulfur abundances relative to the oxygen abundance. The absence of a steep abundance gradient in the inner regions of NGC 1068, combined with similar results for other Seyfert and active galaxies, implies that substantial radial flows and mixing of the local interstellar medium must occur in the inner disks of these galaxies, as several authors have suggested on theoretical grounds (Simkin, Su, and Schwarz 1980; Schwarz 1981; Lacey and Fall 1985). Consequently, it is apparent that elemental abundances found in near-nuclear H II regions may be adopted as nuclear abundances as a constraint on theoretical models of the nucleus, although for H II regions lying within a few kpc from the nucleus, it may be necessary to consider the influence of the nuclear ionizing spectrum on the local ionization balance within the H II regions when deriving elemental abundances from the emission-line spectra.
Spectrophotometry of an emission-line region in the prototype Seyfert 2 galaxy NGC 1068 which exhibits very intense [Ne v] λλ3346, 3426 and He II λ4686 emission in addition to normal H II region spectral features, was presented. Comparison of the spectrophotometry with theoretical photoionization models suggests that this can be interpreted as a superposition of a spectrum from an ordinary H II region and emission from a high-excitation region photoionized by a power-law spectrum emanating from the Seyfert nucleus. These spectra provide an example of the potential pitfalls of which one must be aware when estimating elemental abundances in H II regions within a few kpc from an active galactic nucleus, and demonstrate the interaction of the nuclear ionizing spectrum with the gas in the disk of the galaxy at a radius of \( \sim 1.5 \) kpc from the nucleus.

Some questions are raised by this study which clearly warrant further investigation. For example, what will be the effect on the photoionization models (and hence the diagnostic diagrams and the abundance sequence calibration) of changes in atomic data resulting from new and more accurate experimental and theoretical studies? The primary causes of differences between the abundance sequence calibration presented here and the previous calibrations of Pagel et al. (1979) and McCall (1982) are changes in the rate of the charge exchange reaction \( \text{O}^{++} + \text{H}^0 \rightarrow \text{O}^+ + \text{H}^+ \) and increased collision strengths for \( S^+ \) and \( S^{++} \) following recent quantum mechanical calculations. On the other hand, the theoretical abundance sequence reproduces the observed sequences of H II regions on a number of diagnostic diagrams involving ratios of different ionic and atomic species. This gives one faith in the validity of the theoretical sequence calibration and suggests that any changes which may arise as a result of updates to atomic data will not significantly alter the conclusions presented here.
Additional high quality spectrophotometric data are needed to determine if the assumptions of constant $T_{\text{ion}}$ and the linearity of the $Q(H) - Z$ relationship are strictly valid. To the degree of accuracy which can be achieved with the existing data set, these relationships appear to be valid, but there are few H II regions for which a complete diagnosis is possible. There is some evidence from individual photoionization modeling of H II regions to suggest that there may be a correlation between $T_{\text{ion}}$ and $Z$, but the loci of observed H II regions on those diagnostic diagrams best suited to determining the ionization temperatures of the exciting stars indicate that the contrary is true. More accurate models and better complete spectrophotometry covering the entire visible spectrum is needed for a large sample of objects to definitively resolve this question. In either case, the effect on the abundance sequence calibration is apparently small. The assumption of a linear relationship between $Q(H)$ and $Z$ was made by selecting the simplest functional form which yielded a good fit to the data. Clearly, however, $Q(H)$ cannot increase indefinitely with decreasing metal abundance. Hence the functional form must change at low metallicity, and quite possibly at high abundances also. Once again, an improved data set and better models are needed to settle this question. It may be possible to establish the correct functional form of the $Q(H) - Z$ relationship on theoretical grounds from star-formation theory if, for example, there is a correlation between the stellar IMF and $Z$, or from galaxy-formation theory if $Q(H)$ depends on environmental effects in the galaxy disk which change the "geometry."

The nucleogenic status of nitrogen also bears further investigation. There is strong evidence in the data to suggest that secondary enrichment of nitrogen predominates for high metallicities. However, there is considerable scatter at low abundances, suggesting that there is a different source of
nitrogen enrichment in this abundance regime. The sources of the primary enrichment, and the abundance at which this component ceases to contribute significantly to the overall nitrogen enrichment are uncertain. The influence of the local IMF and the environment in which the H II region is located, are unknown and must be established through further studies.

The feasibility of measuring more precise radial abundance gradients for different elements over a larger range of abundances than previously possible, such as presented here for M101, enables more precise comparisons between the data and galaxy disk formation, evolution, and chemical enrichment models, and should help to establish those scenarios which are plausible. The disk-formation model presented earlier is a very simple example, and much more quantitative and rigorous work needs to be done in this area. Such studies also have a bearing on star-formation models (and vice-versa) and when combined with results from nucleosynthesis theory yield constraints on the shape of the stellar IMF.

Further studies of a larger sample of H II regions in Seyfert and other active galaxies are essential to generalize the conclusions obtained from the small sample described earlier. In particular, they are necessary to confirm that the elemental abundances measured in near-nuclear H II regions can be adopted as nuclear abundances. Statistical studies of abundance versus degree of nuclear activity are required in order to evaluate suggestions that these objects form an evolutionary sequence, and to investigate the influence of the nuclear activity on the ionization balance of the gas in the surrounding disk. Further theoretical studies of the chemical and dynamical evolution of the nuclear regions are required to establish whether a causal relationship exists between strong radial flows and mixing of the local interstellar medium.
near the nucleus and nuclear activity. Once constraints on elemental abundances in the narrow- and broad-line nuclear regions have been established from these studies, one can sensibly proceed to the next step in constructing self-consistent models to determine the ionizing spectrum emitted by the central active nuclear source.
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