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ATLAS5* AT THE UNIVERSITY OF LONDON (SAM1)

II. USER'S GUIDE.

by

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*A program for the calculation of model stellar atmospheres.

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ABSTRACT

The computer program ATLAS5 calculates model atmospheres in radiative and convective equilibrium. The approximations used limit the program to plane-parallel, horizontally homogeneous, steady-state, non-moving atmospheres with energy and abundances constant with depth.

The original version of the program was written in FORTRAN IV by R. L. Kurucz of the Smithsonian Astrophysical Observatory (Kurucz 1970). The original version of the program was implemented on the CDC 6600 of the University of London Computer Centre by Dr. J. D. Argyros. A considerably modified version, written by S. L. Wright and J. D. Argyros, has been implemented on the CDC 6600 of the University of London Computer Centre and the IBM 360 of the University College London Computer Centre. In order to distinguish between the different versions of the program, we have decided to call the modified version SAM1.

This report describes all of the facilities available with SAM1 including a complete description of the output produced by the program. Information is given to help the user select appropriate model parameters, and to suggest ways of recovering from the various error conditions that may arise when running the program. The appendices give a brief description of how the program works, a complete list of all the options available, and details of how to run the program on the computers mentioned above.

PREFACE

A complete description of all the changes that have been made to the original version of ATLAS5, and details of the implementation of the program at the University of London have been given by Wright and Argyros (1975). Although many details of the program have been changed, the general structure of the program is the same as that described by Kurucz (1970). The user who is interested in the details of the program should refer to the two references mentioned above.

IMPORTANT NOTE

The length of a single precision word is 60 bits for CDC machines and 32 bits for IBM machines. Therefore to make both versions of the program essentially equivalent the IBM version has been written in double precision. This however introduces some problems because of the different format of floating point numbers in the two versions. The input subroutines have been written in such a way that the output produced by both versions can be read in by either version of the program (with the exception of the data concerning molecules). It is strongly recommended, however, that the user should use D-format numbers with the IBM version and E-format numbers with the CDC version.

Throughout this report examples are given with D-format numbers. The user who wishes to use the CDC version should convert all these to E-format numbers.

0. INTRODUCTION

The art of model atmosphere construction has reached the stage that it is now relatively easy to calculate a so-called 'classical' model atmosphere ; i.e. a plane-parallel atmosphere in hydrostatic and radiative equilibrium (with allowance for convection using a mixing-length theory), and in L.T.E. . It is also easy to calculate a non-L.T.E. atmosphere provided that one makes the assumption that the bound-bound radiative rates are in detailed balance, which is a very good approximation if one is only interested in the line wings and continuum.

Thus it is now feasible to write a model atmosphere program in such a way that an astronomer who requires a model can obtain one very easily without having to bother himself with the details of the programming. The model atmosphere program, ATLAS5, written by R. L. Kurucz of the Smithsonian Astrophysical Observatory is such a program. Of course no computer program is infallible, thus a reasonably comprehensive manual is required to help the user to overcome any problem that may arise. This report is intended to be a completely self-contained guide to the use of a version of ATLAS5 which we have called SAM1.

All the information and data that the program requires are read from data cards. These 'control cards' are very easy to code and can control all the available options of SAM1. Chapter 1 of this report gives details of the basic control cards that are required. Chapter 2 describes the output with reference to a sample model calculation which the user should run. Chapter 3 describes all the other options available. Chapter 4 gives some general ideas as to how the parameters for the model atmosphere should be selected. The error messages that the program generates are described in chapter 5 along with some suggestions as to what to do when these errors occur. Some utility programs are used in conjunction with SAM1, and these are described in chapter 6. Appendix I is a brief description of how SAM1 works. All users (including those with experience in constructing model stellar atmospheres) are recommended to read Appendix I after running

the sample model. A complete list of all the options together with their default values and other useful information, is given in Appendix II. Appendix III gives the Job Control Cards for running SAM1 and its associated programs on the CDC 6600 of the University of London Computer Centre and the IBM 360 of the University College London Computer Centre.

The user should treat the program as a 'grey box' which, when provided with reasonably sensible physical information, produces a 'classical' model atmosphere. No program as complex and as flexible as SAM1 can ever be treated as a 'black box'. The user has to be aware of the physical principles and assumptions on which the program has been based. If the program is supplied with information which is physically unrealistic or which violates the assumptions on which the program is based, then the user can expect the program to produce a completely non-physical model or, more likely, fail to produce a model at all.

Although this report was produced with SAM1 specifically in mind, it can be used in conjuction with other versions of ATLAS5. All the facilities which are different from, or not available in, the original version of ATLAS5 are marked with an asterisk.

1. BASIC CONTROL CARDS

1.0 Introduction

In order for SAM1 to compute a stellar atmosphere model, the following information must be specified:

a) The physical parameters of the required model (T_{eff}, surface gravity etc.)

b) The physical processes to be included in the calculation.

c) Whether certain information is to be read in, or calculated by the program.

d) The type and form of output required.

Apart from a few parameters which must be specified, SAM1 assumes default values for parameters which are not explicitly given. The default values of parameters (where applicable) are given in detail in Appendix II.

1.1 Format of the control cards

The information that SAM1 requires is punched onto data cards in a free-field format, i.e. the data are not constrained to lie between certain columns of a data card, or on a particular data card. Thus these 'control cards' are easy for the user to punch up, reducing possibilities for error and making more efficient use of the user's and computer's time. Because of this free-field input, all numeric data must be preceded by an identifying 'code word'. In addition there are some code words which do not require any numeric data.

The free-field input subroutines can recognise two types of data:

i) A string of alphabetic characters, of which only the first six are used by the program.

ii) A number in a valid I,F,E, or D format, of which only the first 15 significant digits are used by the program.

In all cases the end of the character string or number is indicated by a blank or a comma. Code words can also be ended by an equal sign.

Throughout this report the characters that the program recognises will be underlined, and numbers will be represented by: n1, n2, ... etc.

The rules for punching up a set of data cards are as follows :

i. All the data associated with a particular code word must appear on the same data card as the code word, unless otherwise stated.

ii. More than one set of code words and associated data may appear on the same data card.

iii. The data card(s) on which a code word and its associated data are punched can appear anywhere in the deck of data cards, unless otherwise stated.

iv. No blank cards may appear in the deck of data cards.

An example of how the program handles a typical data card should make the technique easy to understand. Suppose the program encountered the following data card :

TEFF 10000. GRAVITY 4 LTE

card column 1 card column 80

The program searches through the card until a character string terminated by a comma, blank or equal sign is encountered (all numeric data are ignored during this search). If this string is not a valid code word, an error message is printed and the run is terminated. The code word TEFF requires one number, therefore the card is searched (ignoring all alphabetic information) until a character string beginning with a digit, decimal point or sign and ending with a blank or a comma is found. This character string is interpreted as a number. If the string is not in a valid Fortran IV format then the result is unpredictable. Having completed reading in the data associated with this code word, the program searches for the next code word (GRAVIT) and its associated data (again one number). If the end of a data card is reached while the program is looking for the next code word, a new card is read in and the search is continued. The program continues reading in data until it encounters a code word which tells it to perform some other operation.

The following example is completely equivalent to the above example :

TEFF=1.D+04 LTE GRAVITY (IN LOGS) 4.00

1.2 Information required by SAM1

The following information must be given to SAM1 in each run :

a) An effective temperature for the model, T_{eff}.

TEFF n1

n1 is the effective temperature in ^{o}K.

b) A surface gravity for the model, g.

GRAVITY n1

n1 is the surface gravity in cm sec^{-2}. However if n1 is less than 10 it is treated as $\log_{10} g$. Thus GRAVITY 10000. is equivalent to GRAVIT 4.00.

c) A set of depth points at which the variables are to be calculated. There are several ways of specifying the depth points (see chapter 3). Normally to construct an initial model the following method is used :

CALCULATE n1 n2 n3

n1 is the number of depth points (maximum 40). n2 is the $\log_{10}$ Rosseland depth at the first depth point. n3 is the $\log_{10}$ Rosseland spacing between depth points.

e.g. CALCULATE MODEL AT 40 DEPTHS FROM -3.5 SPACING .125

The CALCULATE control card can only be used after T_{eff} and g have been defined.

d) A set of frequency points at which the radiation field is to be calculated.

Each frequency point in SAM1 is given a unique identifying frequency number. The frequency points are numbered from 1 in order of increasing frequency. As well as requiring frequency points, SAM1 needs a set of integration weights corresponding to these frequencies to enable integrations over frequency to be calculated. A utility program, FRESET, is provided (see section 6.1) which calculates an appropriate set of weights. The user inputs a name for the frequency set and a set of frequency points into FRESET, which produces a punched card output that can be read by SAM1. This punched card output is headed by a control card :

READ FREQUENCIES n1 n2 n3 name

n1 is the total number of frequency points, n2 and n3 are the

frequency numbers of the limiting frequencies that are used in the integration over frequency. FRESET sets n2 = 1 and n3 = n1. The user does not need to bother about n2 and n3 at this stage. Details of how to use these options are given in section 3.2 a. Name is simply a name (of up to six characters) used to identify the frequency set. This control card is followed by n1 triplets of frequency number, frequency and integration weight on as many cards as are required.

The number of iterations to be performed.

ITERATIONS n1 n2

n1 is the sequence number of the last iteration of this calculation. n2 is the sequence number of the first iteration of this calculation.

e.g. ITERATIONS 15 STARTING AT 11

This card tells SAM1 to perform 5 iterations in all. The iterations will be numbered 11, 12, ... 15. Thus a model which is calculated in more than one computer run can be given a logical sequence of iteration numbers. The maximum iteration number allowed is 30.

In addition to the above information which must be specified in each run, two other code words are required in order to run SAM1 :

BEGIN

When this code word is encountered, SAM1 stops reading in data and starts the model atmosphere calculation. After the specified number of iterations have been completed, SAM1 resumes reading in data starting at the card after the BEGIN code word. Thus the user can perform another model atmosphere calculation in the same SAM1 run. N.B. All the data from the previous calculation is still available and can be used to start the new calculation.

END

This code word signifies the end of the SAM1 run. SAM1 stops after reading this code word.

Given the above information SAM1 can compute a model atmosphere by assuming default values for all the other parameters.

1.3 Other basic (but optional) control cards.

a) A title for the model can be specified using (e.g.)

TITLE PURE HYDROGEN ATMOSPHERE WITH ELECTRON SCATTERING

The code word must start in column 1 of a data card. Columns 7 to 80 of this card are then printed as a title to the summary table.

b) The type of calculation to be performed can be identified with :

LTE or NLTE

The code word LTE tells SAM1 to calculate an atmosphere in Local Thermodynamic Equilibrium (L.T.E.). The code word NLTE tells SAM1 to calculate an atmosphere such that the populations of the level of H^- and the first six levels of atomic hydrogen are calculated self-consistently with the rest of the atmosphere. (assuming the lines are in detailed balance). The default for this option is LTE therefore the code word LTE need not be punched on the data set if an L.T.E. atmosphere is required.

c) The opacity sources to be included in the calculation are specified by :

OPACITY IFOP n1 n2 n3 ..... n20

n1, n2, ... n20 are twenty switches, a 1 indicating that the opacity is ON, and a 0 indicating that the opacity is switched OFF. The opacity sources available in SAM1, with their default settings, are given in table 1, below. Note that this option overrides all of the default settings so that a completely new set of switch positions must be specified.

e.g. OPACITY IFOP 1 1 1 1 0 0 0 0 0 0 0 1 0 1 0 0 0 0 0 0

In this example only the opacities H1, H2PLUS, HMINUS, HRAY, ELECTRON, and HLINES have been included.

TABLE 1

DEFAULT SETTINGS OF OPACITY SOURCES

i)	H1	ON	xi)	HOT	OFF
ii)	H2PLUS	ON	xii)	ELECTRON	ON
iii)	HMINUS	ON	xiii)	H2RAY	OFF
iv)	HRAY	ON	xiv)	HLINES	OFF
v)	HE1	ON	xv)	LINES	OFF
vi)	HE2	ON	xvi)	LINESCAT	OFF
vii)	HEMINUS	OFF	xvii)	XLINES	OFF
viii)	HERAY	OFF	xviii)	XLSCAT	OFF
ix)	COOL	ON	xix)	XCONT	OFF
x)	LUKE	OFF	xx)	XSCAT	OFF

Alternatively one can use the forms:

OPACITY ON cw1 cw2 ...

OPACITY OFF cw1, cw2, ...

In this case the opacities corresponding to the code words cw1, cw2 etc. are either switched ON or OFF according to the code word following OPACITY. Default options are taken for those opacities not listed.

e.g. OPACITY ON HLINES

OPACITY OFF HE1, HE2 COOL

In this example, the opacity HLINES which is normally OFF is included, while the opacities HE1, HE2, COOL have been omitted. The opacities H1, H2PLUS, HMINUS and HRAY are included because of the default settings. Thus the two examples given in this section are equivalent. Details of the opacities are given in Appendix II.

Output options.

PRINT n1 n2 ...

PUNCH n1 n2 ...

Each integer n1, n2 etc. tells SAM1 what information the user wants to be printed and/or punched out after each iteration of the model. One integer is required for each iteration to

be performed. Details of all the available options are given in chapters 2 and 3.

As an example, consider the set of cards :

ITERATIONS 16 STARTING AT 11

PRINT 1 1 1 1 1 2 PUNCH 0 0 0 0 0 2

This tells SAM1 to perform iterations 11 to 16. The output from iterations 11 to 15 will be in the format corresponding to PRINT=1 and PUNCH=0. The output for iteration 16 will be in the format corresponding to PRINT=2, and PUNCH=2.

The default options are : PRINT=1 for all iterations except the last, when it is PRINT=2. The default for PUNCH is PUNCH=0 for all iterations.

2. A SAMPLE MODEL CALCULATION

2.1 Introduction

In this chapter the standard output of SAM1 is described with reference to a sample model calculation which the user should run.

2.2 Running the sample model

Using the data given in Table 2,p.41 and the Job Control Cards from Appendix III, the user should run the program FRESET to obtain the quadrature weights to be used in the frequency integrals. Combining the card output from FRESET with the following control cards, SAM1 should be run using the Job Control Cards from Appendix III.

```
                TEFF   10000      GRAVITY  4
                TITLE  SAMPLE MODEL
                CALCULATE MODEL   40  -4.5   0.16666666666666666666
                ITERATIONS  5  STARTING AT  1
                PRINT  2 1 0 1 2    PUNCH  0 0 0 0 1
                READ FREQUENCIES   75  ...
                                .
output from     FRESET          .
                                .
                                .
                  75  ...
                BEGIN
                END
```

2.3 Output from the sample model

Printout

The page numbers used in this section refer to the output produced by SAM1.

1. The first two pages give information about the options selected, and the starting model to be used.

Page 1 - options selected

Item	Parameters
1	Effective temperature, $\log_{10}$ surface gravity, LTE/NLTE model.
2	Title of the model.
3	Abundance scaling factor and abundances of H and He (see section 3.3 a).
4	The abundance of other elements (in logs relative to the total number) before the scaling factor is applied.
5	Twenty opacity switches.
6	Switches for the physical processes to be included.
	IFCORR - perform a temperature correction.
	IFPRES - calculate the pressure.
	IFSURF - calculate the flux or intensity.
	IFSCAT - include scattering.
	IFCONV - include convection.
	MIXLTH - mixing length/scale height for convection.
	IFMOL - include molecules in the equilibrium equations.
	IFTURB - include turbulence in the pressure calculation.
	TRBFDG, TRBPOW, TRBSND, TRBCON - constants used in the turbulence calculation.
7	Iterations to be performed.
8	IFPRNT - print switches for each iteration. IFPNCH - punch switches for each iteration.
9	Frequency points and quadrature weights.
10	Default opacity table message (unless the user has read in another opacity table).

Refer to chapter 3 for details of those options that have not yet been described.

[illegible] - the starting model

[illegible]	Heading	Explanation
[illegible]		depth point label.
[illegible]	RHOX	mass depth variable see Appendix 1.
[illegible]	T	temperature in ^{o}K.
[illegible]	P	pressure in dynes cm^{-2}.
[illegible]	XNE	electron number density in cm^{-3}.
[illegible]	ABROSS	the Rosseland opacity in g^{-1} cm^{2}.
[illegible]	PRAD	radiation pressure in dynes cm^{-2}.
[illegible]	VTURB	turbulent velocity in kms sec^{-1}.
[illegible]	BHYD	departure coefficients for H.
[illegible]	BMIN	departure coefficient for H^{-}.

[illegible] Pages [illegible] - 7 are the output for the first iteration given by the [illegible] option.

[illegible] - radiation field quantities at the surface of the atmosphere.

[illegible]	Heading	Explanation
[illegible]		frequency identification number.
[illegible]	WAVE	wavelength in nanometers.
[illegible]	HLAMBDA	Eddington flux, $H_{\lambda} = \mathcal{F}_{\lambda}/4\pi$ ergs cm^{-2} sec^{-1} nm^{-1}.
[illegible]	LOG H	$\log_{10} H_{\lambda}$
[illegible]	MAG	$-2.5\log_{10} H_{\lambda}$
[illegible]	FREQUENCY	frequency in Hz
[illegible]	HNU	Eddington flux, $H_{\nu} = \mathcal{F}_{\nu}/4\pi$ ergs cm^{-2} sec^{-1} Hz^{-1}.
[illegible]	LOG H	$\log_{10} H_{\nu}$
[illegible]	MAG	$-2.5\log_{10} H_{\nu}$
[illegible]	TAUONE	$\log_{10}$ RHOX where the monochromatic optical depth is 1.
[illegible]	TAUNU	$\log_{10}$ optical depth at the last depth point.
[illegible]		frequency identification number.

Page 4 - the temperature correction table.

Column	Heading	Explanation
1		depth identification number.
2	RHOX	the mass depth variable, gm cm^{-2}
3	T	the old temperature in ^{o}K.
4	DTLAMB	temp. correction for the upper layers, ^{o}K
5	DTSURF	temp. correction for the middle layers, ^{o}K
6	DTFLUX	temp. correction for the lower layers, ^{o}K
7	T1	total temperature correction, ^{o}K
8	CONV/TOTAL	fraction of convective flux (only if IFCONV=2)
9	ERROR	percentage flux error = $(\mathcal{H} - H)/\mathcal{H} * 100.$ where $\mathcal{H} = \sigma \frac{T_{eff}^4}{4\pi}$, $H = \int_0^\infty H_\nu d\nu + H_{conv.}$
10	DERIV	percentage error in the flux derivative $= 100. * (\frac{dH}{d\tau_{Ross}}) / \ldots$

[illegible] - convection parameters.

Column	Heading	Explanation
[illegible]		depth identification number
[illegible]	RHOX	mass depth variable, gm cm^{-2}
[illegible]	PTOTAL	total pressure, dynes cm^{-2}
[illegible]	PTURB	turbulent pressure, dynes cm^{-2}
[illegible]	GRDADB	adiabatic gradient
[illegible]	DLTDLP	$\frac{d(\ln T)}{d(\ln P)}$
[illegible]	VELSND	velocity of sound, cm sec^{-1}
[illegible]	DLRDLT	$\frac{d(\ln \rho)}{d(\ln T)}$ ρ = density in gm cm^{-3}
[illegible]	HEATCP	specific heat at constant pressure
[illegible]	HSCALE	pressure scale height, cm
[illegible]	VCONV	convective velocity, cm sec^{-1}
[illegible]	FLXCNV	convective flux, ergs cm^{-2} sec^{-1}

[illegible]

Column	Heading	Explanation
[illegible]		depth identification number
[illegible]	XNATOM	atomic number density, cm^{-3}
[illegible]	ACCRAD	$\frac{4\pi}{c} \int_0^\infty k_\nu H_\nu \, d\nu$
[illegible]	PRAD	radiation pressure = $\int$ ACCRAD dM, dynes cm^{-2}
[illegible]	XNFPH1	number density/partition function for H
[illegible]	XNFPH2	" " H^+
[illegible]	XNFPHE1	" " He
[illegible]	XNFPHE2	" " He^+
[illegible]	XNFPHE3	" " He^{++}

Page 7 - a summary table. T_{eff}, g, the title of the model and the iteration number are given as a heading to the table.

Column	Heading	Explanation
1		depth identification number
2	RHOX	mass depth variable, gm cm^{-2}
3	TEMP	revised temperature, ^{o}K
4	PRESSURE	gas pressure, dynes cm^{-2}
5	ELECTRON NUMBER	electron number density, cm^{-3}
6	DENSITY	gas density, gm cm^{-3}
7	ROSSELAND MEAN	Rosseland mean opacity, gm^{-1} cm^{2}
8	HEIGHT (KM)	height above $\tau_{Ross} = 1$, km
9	ROSSELAND DEPTH	Rosseland mean optical depth
10	FRACTION CONV FLUX	fraction of the total flux which is convective
11	VTURB	turbulent velocity, kms sec^{-1}
12 + 13	PER CENT FLUX ERROR DERIV	percentage error in the flux and flux derivative.

The temperature and RHOX in this table have been corrected according to the last temperature correction, and therefore will not be consistent with the rest of the table until the model has converged.

Underneath the table is the total integrated flux $\mathcal{H} = \frac{\sigma T_{eff}^{4}}{4\pi}$, and a message telling the user which file the restart data has been written to, see Appendix III.

- Pages 8 and 9 are the output for the second iteration given by the PRINT 1 option.

- Page 10 has only the RESTART DATA message, as the PRINT 0 option suppresses all the output.

- Pages 11 and 12 are the output from iteration 4 given by the PRINT 1 option.

- Page 13 gives a table of electron contributions which is only printed out for the last iteration of a model. Columns 2 to 11 give the fraction of the total electron density contributed by each element (indicated by the column heading). Columns 12 to 21 give the number of electrons contributed by one atom of each element.

- Pages 14 to 18 give the output (PRINT 2) for the last iteration.

Punchout:

No punched card output is produced for the first four iterations because of the PUNCH 0 option. The punchout for the last iteration (PUNCH 1) contains sufficient information for SAM1 to read it in and continue with the model calculation. Compare your punchout with the control cards described in chapters 1 and 3.

3. OTHER AVAILABLE OPTIONS

3.0 Introduction

The control cards described in chapter 1 enable the user to construct 'standard' model atmospheres, and they are all that are required by the casual user. However the great advantage with this program is that the user can exercise considerable control over the processes that are included in the model calculation. The program also provides facilities for the user to define a starting model, and to scale models onto different depth grids. These and other options, including the extended output facility, are described in this chapter.

3.1 Control of physical processes

*a) SAM1 usually performs a temperature correction after each iteration i.e.

CORRECTION 1

which sets IFCORR=1 (this is the default and therefore does not need to be specified explicitly in the data deck). However the temperature correction can be switched off by specifying :

CORRECTION 0

which sets IFCORR=0.

b) The pressure and number densities of various species are normally calculated i.e.

PRESSURE ON

which sets IFPRES=1 (this is the default and therefore does not need to be specified). However if this is not required, specify :

PRESSURE OFF

which sets IFPRES=0.

c) Turbulent pressure is not normally included in the pressure

calculation i.e.

TURBULENCE OFF

which sets IFTURB=0, TRBFDG=0, TRBPOW=0, TRBSND=0, TRBCON=0 (this is the default). If turbulence is to be included, specify :

TURBULENCE ON n1 n2 n3 n4

which sets IFTURB=1, TRBFDG=n1, TRBPOW=n2, TRBSND=n3, TRBCON=n4. The turbulent velocity is given by :

VTURB = TRBFDG*RHO**TRBPOW + TRBSND*VELSND/1.D5 + TRBCON, kms sec^{-1}

The turbulent pressure is then :

PTURB = RHO* (VTURB*1.D5) ** 2/2. dynes cm^{-2}

where RHO is the density in gm cm^{-3}.

N.B. For this option to work IFCONV must be greater than 0, see section 3.1 d.

To include the calculation of convective variables use :

CONVECTION n1 n2

which sets MIXLTH=n1 and IFCONV=n2. MIXLTH is the ratio of mixing length to pressure scale height. If IFCONV=0, convective variables are not calculated. If IFCONV=1, convective variables are calculated unless IFPRES=0 or MIXLTH=0.0. If IFCONV=2, then convective variables are calculated and the temperature correction is performed so as to keep the total flux (radiative + convective) constant with depth. The default setting is :

CONVECTION 1.0 1

SAM1 has a facility for including molecules in the equilibrium equations which is brought into play with the code words :

MOLECULES ON

which sets IFMOL=1 (default IFMOL=0). This option requires a special set of data which must commence on the first card after the READ code word. There are two cases :

- If IFPRES=1 then SAM1 requires one data card for each species, including atoms, to be included in the equilibrium equations. Each data card must contain a code identifying the molecule or atom and the six coefficients that go into the polynominal form

of the Saha equation (see Appendix I). The data cards must be in the format (F18.2, F7.3, 5D11.4) for IBM machines, or in the format (F18.2, F 7.3, 5E11.4) for CDC machines. These data cards must follow the BEGIN card, the end of the data is indicated by a zero molecular code or a blank card. The maximum number of species allowed is 100, in which there must not be more than 25 different elements. For atoms, the six coefficients can be set to zero, in which case SAM1 uses the internal table of atomic partition functions.

The code for identifying atoms and molecules is as follows : The atomic number for each component is treated as a base 100 digit, and the digits are ordered increasing from left to right to form a number e.g. 11. refers to sodium, 608. is carbon monoxide etc. An electron component is written 00 e.g. H^- is 100. . A positive charge is written after the decimal point e.g. 2.02 is He^{++}.

ii) If IFPRES=0 then SAM1 expects to find the data deck which has been punched out by the PUNCH 5 option in a previous run of the model. This data must follow the BEGIN card.

f) SAM1 usually solves the radiative transfer problem exactly (see Appendix I) i.e.

SCATTERING ON

which sets IFSCAT=1 (this is the default). However, SAM1 can solve the radiative transfer problem approximately by ignoring the scattering component i.e. by setting $\alpha_\nu = 0.0$. This option is specified by :

SCATTERING OFF

which sets IFSCAT=0. This option saves computer time and should be specified if the user only requires an approximate solution to the transfer problem, or if the scattering component is negligible.

3.2 Input and calculation options

a) The control card which introduces the frequencies and integration weights is :

READ FREQUENCIES n1 n2 n3 name

n1 is the number of frequency points, n2 and n3 are the frequency numbers of the limiting frequencies that are used in the integration over frequency. Name is a name (of up to six characters) used to identify the frequency set. Following this card are n1 triplets of frequency number, frequency, and integration weight, in any order and on as many cards as are necessary. Each card may contain any number of complete triplets.

The user can adjust n2 and n3 such that only the sequential set of frequencies from frequency number n2 to frequency number n3 are used in calculating the integrals over frequency. Thus if, for example, there is a region of very high opacity (such as the region beyond the Lyman jump, < 91.2nm, in cool stars) at the beginning and/or end of the set of frequencies; then this region can be excluded from the calculation. The model will not be affected by the exclusion of such regions, and the execution time of the program will be smaller.

b) A starting temperature distribution can be specified using the control card :

READ STARTING n1 n2

Starting on the next card, n2 pairs of depth variable and the corresponding temperature are read in from as many cards as are necessary. n1=1 means that the depth variable is the Rosseland mean optical depth, n1=2 means that the depth variable is RHOX.

c) The user can define an ititial set of departure coefficients using :

READ DEPARTURE n1

SAM1 reads in n1 cards each containing : RHOX, six departure coefficients for atomic hydrogen, and the departure coefficient for H^-.

d) A complete model can be read in using the control card :

READ DECK n1

Following this card are n1 pairs of cards. On the first card of each pair there must appear : RHOX, temperature, total pressure, electron number density, Rosseland opacity, radiation pressure, and turbulent velocity. The second card of each pair must contain : the last temperature correction, the flux error, the flux derivative error, the six departure coefficients for H, and the departure coefficient of H^-. If this deck is to be used as a starting model the calculation only depends on RHOX, temperature, radiation pressure, turbulent pressure and the departure coefficients. Therefore if the other quantities are not known they can be set to zero.

e) The user can map a model onto a new set of depth points using :

CHANGE n1 n2, n3, n4, ...

SAM1 reads n1 new RHOX's (n2, n3, ...) on as many cards as are necessary. This card is used, only after a model has been defined, to change the depth point spacing, or to extrapolate to greater or smaller depths. SAM1 interpolates all the necessary quantities onto the new RHOX scale and sets the number of depth points to n1.

f) The user can scale a model to a new effective temperature, gravity and set of depth points using the control card :

SCALE n1 n2 n3 n4 n5

n1, n2, n3 have the same significance as on a CALCULATE card, n4 is the new effective temperature and n5 is the new gravity. This card must come after the old model has been defined. Thus suppose a converged model had been read in for a 10000 ^{o}K, log g = 4 atmosphere. Then to obtain a starting model for a 10000^{o}K, log g = 3 atmosphere one could use the following control card :

SCALE MODEL 40 -4.5 .1666666666666666 TEFF = 10000 GRAVITY 3.0

3.3 Miscellaneous options

a) There are two ways in which the user can change the elemental abundances used in the model calculation (default abundances are given in Appendix II).

i) The abundance of each individual element can be changed using the card :

ABUNDANCE CHANGE n1 n2 , n3 n4 , n5 n6 , ...

n1, n3 .. are atomic numbers, n2, n4 .. are the corresponding abundances (relative to the total number). A negative number is treated as a logarithm.

ii) All the abundances except H and He are multiplied by a scaling factor before the calculation is begun. This scaling factor is specified using the following control card :

ABUNDANCE SCALE n1

where n1 is the scaling factor (default value 1.0). Thus one could, for example, simulate a metal defficient star by using an appropriate scaling factor (e.g. 0.1).

b) Once a converged model has been obtained, the user can print and/or punch out the surface intensity of the model at specified angles by running the model in the usual way with the additional control card :

SURFACE INTENSITY n1 n2, n3, n4, ...

SAM1 reads n1 μ's, n2, n3 ..., from as many cards as are necessary ($\mu = \cos\theta$, where θ is the angle from the normal of the ray). The maximum value of n1 is 20.

e.g. SURFACE INTENSITY 10 1.0 .9 .8 .7 .6 .5 .4 .3
.2 .1

see section 3.4 for details of the printout/punchout.
N.B. With this option in effect, SAM1 does not calculate a temperature correction, and only the table of surface intensities is printed, see section 3.4, a,i).

c) Instead of using frequencies the user can define a set of equally spaced wavelengths to be used in the model calculation. The control

card is :

WAVELENGTH n1 n2 n3

where n1 is the starting wavelength, n2 is the wavelength spacing, n3 is the final wavelength. All wavelengths must be given in nanometers.

* d) If the internal opacity table (see Appendix I) is not appropriate for the user's calculation, a new opacity table can be generated by the utility program OPTAB (see section 6.2). The normal punchout from OPTAB is a deck of cards headed by the control card :

KAPPA n1

where n1 is the number of pressure and temperature points at which the table has been calculated. This deck can go anywhere before the BEGIN card.

* e) The output from the punch options can be written on media other than punched cards (magnetic tape, disk etc.) by using appropriate Job Control Cards (see Appendix III). The user can read this information back into SAM1 using the control card :

MODEL n1

where n1 is the unit number corresponding to the data set on which the information is written. Only data which corresponds to valid control cards is recognised, all other information is ignored. When the control card BEGIN is encountered on unit n1, control is returned to the normal input stream (unit 5). Thus the user can read in a model and then change some of the options before beginning the calculation. For an example see section 4.1.

3.4. Output options

So far the PRINT options 0, 1, 2 and the PUNCH options 0, 1 have been described with reference to a 'standard' model calculation. Some of the options described earlier in this chapter will produce output of their own under these PRINT/PUNCH options. This output is described below.

a) Output from special options.

i) If the SURFACE INTENSITY option has been specified, then instead of the table of surface fluxes being printed out (cf. page 3 of the sample output) the following information is printed out for each wavelength :

wavelength, frequency, TAUONE, TAUNU (see page 15) followed by μ and its corresponding intensity (in ergs cm^{-2} sec^{-1} $sterad^{-1}$) for all the μ's specified on the control card. No other information is printed when this option is in effect.

ii) If the NLTE option has been specified then three extra tables are printed if the PRINT option > 0 :

1) A table of statistical equilibrium rates and the departure coefficient for H^-.

Column	Heading	Explanation
1		depth identification number
2	RHOX	mass depth variable
3	QELECT	electron collision rate
4	QASSOC	associative detachment rate
5	QCHARGE	charge cancellation rate
6	QRDKHM	radiative de-excitation rate
7	QRDHMK	radiative excitation rate
8	BMIN	departure coefficient for H^-

2) A table giving all the radiative and collisonal rates for H, K represents the continuum, (only printed if IFPRNT > 1).

3) A table of the departure coefficients for H.

iii) If IFMOL=1 then three extra self-explanatory tables are produced. The first occurs after the first two tables of the printout and is simply a printout of the data read in. The others appear in the printout for the last iteration. The second table gives some useful variables, and the third gives the number densities of all the species considered at each depth.

b) Other basic output options.

i) There are two other basic PRINT options :
PRINT 3 gives all the output as for PRINT 2 plus the following table at each frequency :

Column	Heading	Explanation
1		depth identification number
2	RHOX	mass depth variable
3	TAUNU	the optical depth, τ_ν
4	ABTOT	the total opacity, κ_ν
5	ALPHA	the scattering fraction of the source function, α_ν (see Appendix I).
6	BNU	the Planck function
7	SNU	the source function
8	JNU	the mean intensity
9	JMINS	JNU - SNU = $\frac{dH_\nu}{d\tau_\nu}$
10	HNU	the Eddington flux $H_\nu = \mathcal{F}_\nu/4\pi$

PRINT 4 option gives all the tables as for the PRINT 2 option plus a table at each frequency giving the $\log_{10}$ opacity per gram of stellar material for each opacity source at each depth point.

These two PRINT options are not recommended very highly as they produce a large amount of output which is not readily digestible. If the type of information output by these options is required, then the user will probably find that the options described in section 3.5 are more suitable.

ii) The other basic PUNCH options are :

*1) PUNCH 2 which gives all the output from the PUNCH 1 option plus the surface flux at each frequency. The format is :

FLUX n1 n2

n1 is the wavelength in nanometers, n2 is $\log_{10}$ HNU in ergs cm^{-2} sec^{-1} Hz^{-1}. If however the SURFACE INTENSITY option has been specified then the surface intensity is punched in the format :

INTENSITY n1 n2 n3 , n4 n5 , etc.

where n1 is the wavelength and the pairs (n2, n3) etc. are the μ and corresponding $\log_{10}$ surface intensity.

2) PUNCH 5 which gives the output from the PUNCH 2 option plus a table of number densities/partition functions for all the molecules included. This option can only be used if IFMOL=1.

3.5 Extended output options

The extended output option provides the following facilities :

i) The model can be mapped onto a mean or monochromatic optical depth grid specified by the user. The only limitation is that the frequency of the monochromatic depth must be one of the frequencies used in the integration over frequency.

ii) The output from the PRINT 3 option, mapped onto the users depth grid, can be output at specified frequencies.

iii) A table of opacity for each opacity source included in the calculation can be mapped onto the users depth grid and output for specified frequencies.

a) Control cards

The control cards required by the extended output facility must appear between the two special code words :

CALL DUMMYR

and RETURN

Information following these code words must appear on a new card. Between these two code words the following information may appear :

SAMPLE n1 n2 n3 n4 n5 ....

Each frequency used in the integration process is provided with a unique identifying integer starting from unity. This control card gives the number of frequencies (n1) to be used by the program in its modified sections. The list of frequency identifiers (n2, n3, n4 ...) on as many cards as are required, corresponds to those frequencies which will appear in the output lists. If the extended versions of either PRINT 3 or 4 is selected, then this control card and a list of frequency identifiers (even if only one) must appear.

DEPTH n1 n2 n3 n4 n5 n6

This control card specifies the number of optical depths (n1) at which the model atmosphere is required, and the number of depths used for the extended PRINT 3 and 4 options. The frequency identifier (n2) specifies the frequency of the following list (n3, n4, n5 ...), on as many cards as are required, of n1 monochromatic optical depths. If the frequency identifier is 0, then the optical depths are on a Rosseland mean optical depth scale.

e.g. In the sample model the frequency 5.99585D14 (500nm) is frequency number 25, therefore to map a model onto a τ_{500nm} depth grid we could use the following control cards :

```
MODEL  READ FROM UNIT 12
CALL
DEPTH  5  25
  1.D-2  1.D-1  1.  0.5D1  10.
RETURN
ITERATIONS  6  6  PRINT  12
BEGIN
END
```

b) Use of the extended output options

The extended output options are brought into play by specifying the following PRINT and PUNCH options :

i) PRINT 12. This option gives all the output as for the PRINT 2 option plus a table giving the model atmosphere mapped onto the optical depth grid specified by the user with the DEPTH control card.

ii) PRINT 13. This option produces all the output associated with the PRINT 12 option plus a table at each frequency (specified on the SAMPLE control card) giving the radiation field parameters mapped onto the depth grid as given on the DEPTH control card.

iii) PRINT 14. This option produces all the output associated with the PRINT 12 option plus a table giving the $\log_{10}$ opacity at each frequency and depth (specified on the DEPTH and SAMPLE control cards)

for each opacity source used in the calculation.

c) PUNCH 3. This option produces all the output as for the PUNCH 2 option plus a punchout of the information given by the PRINT 13 option.

d) PUNCH 4. This option produces all the output as for the PUNCH 2 option plus a punchout of the information given by the PRINT 14 option.

N.B.

Because of the way in which the input subroutines have been written the punch card output from either machine is directly readable by the other machine, with no alterations to the deck of cards.

4. NOTES ON THE SELECTION OF PARAMETERS

4.0 Introduction

This chapter describes the general technique of calculating a model stellar atmosphere, and provides some hints as to the selection of model parameters.

4.1 Running a model atmosphere

The general procedure for running a model stellar atmosphere is as follows :

a) Bearing in mind the opacity sources to be included in the model and its effective temperature, the user selects a set of frequency points. These frequency points are punched onto data cards and the program FRESET is run as described in section 6.1.

b) The internal opacity table which is used to calculate the initial structure of the model atmosphere is tabulated for $3000 < T < 30000\ ^{o}K$ and $10^{-2} < P < 10^{6}$ dynes/cm^{2}. Thus if the effective temperature and gravity of the model are such that the temperatures and pressures in the model lie well outside these ranges then a poor starting model will be produced. This will mean that the model will take a long time to converge if it converges at all. Very generally speaking the temperature structure will be acceptable for effective temperature in the range $3500 < T_{eff} < 15000$. If the temperature and pressures look to be within acceptable limits and the abundances and/or opacity sources are not radically different from the default values (see Appendix II) then the internal opacity table will probably give a reasonably good starting model. If however it is decided that the internal table will not be good enough then the user will have to calculate a new opacity table using the utility program OPTAB (see section 6.2).

c) The user selects all the other parameters for the model and codes the appropriate control cards. The method of coding the control cards is given in chapters 1 and 3. Usually a fairly small number of iterations (about 6 to 10) are specified for the first run if the

user has no idea of how many iterations will be required to produce a converged model. The control cards are included with the output from FRESET (and OPTAB if required) and run with the Job Control Cards for the appropriate computer.

From looking at the trend in the flux and flux derivative errors (given in the summary table at the end of each iteration) from iteration to iteration the user should be able to estimate how many more iterations are required in order to obtain a model atmosphere converged to the required accuracy. It is important to use both errors to determine whether the model is converging, as the flux error can become very small even when the flux derivative error is still quite large and the model has not yet converged.

Having determined how many more iterations are required the user can restart the model calculation with the following set of control cards :

```
MODEL  READ FROM UNIT  n1
ITERATIONS  n2  STARTING AT  n3
PRINT .....      PUNCH .......
BEGIN
END
```

where n1 is the logical unit number of the restart data file (see the RESTART DATA message at the end of the last iteration), n2 is the iteration number of the last iteration to be performed, and n3 is the iteration number of the first iteration to be performed in this run. If the data has been punched onto cards, the model can be restarted using the following control cards :

```
MODEL  READ FROM UNIT  5
TEFF ...
.
.
.
:
.
BEGIN   ITERATION 10 COMPLETED
ITERATIONS  ........
.
.
.
.
BEGIN
END
```

DECK OF CARDS PRODUCED BY ANY PUNCH OPTION

4.2 Selection of model parameters

a) TEFF and GRAVITY

In principle these can take any value the user wishes, however it must be born in mind that a different opacity table may be required (see the discussion in section 4.1 b).

b) The set of depth points

The selection of a set of depth points is largely a matter of experience. A logarithmic distribution of points is best (hence the format of the CALCULATE card). It has been found that the set of points used to construct the sample model (see section 2.1) is quite good for a large number of models. Certainly for stability, the number of depth points must be fairly large, i.e. 30 - 40 (the maximum number of depth points allowed in this implementation is 40). Especial care should be taken with cool ($T_{eff} < 4000^{o}K$) or very hot ($T_{eff} > 30000^{o}K$) models as they very easily 'blow up' if the depth points are ill-chosen (see chapter 5). Obtaining a usable depth point grid in these cases is largely a matter of trial and error.

c) The set of frequency points

Again the selection of a set of frequency points is largely a matter of experience. Sufficient frequency points must be supplied to adequately represent the distribution of the emergent flux, including discontinuities etc.. In practice a minimum of 50 frequency points should be used (the maximum number of points allowed in this implementation is 500).

The range of frequency points must be such that it includes that part of the spectrum where the model emits the vast majority of its flux. Otherwise a completely un-physical model will result when the constraint of radiative equilibrium is imposed. As well as frequency points, the user must supply appropriate integration weights for these points so that integrals over frequency can be calculated. A utility program is provided to calculate these weights (see section 6.1).

The utility program enables the user to very easily include frequency points very close together but on either side of an opacity discontinuity e.g. the Balmer jump. A list of all the

discontinuities included in SAM1 for each opacity source is given in Appendix II. The user does not have to explicitly include frequency points to cover all the opacity discontinuities for each opacity source included in the calculation. However the true flux distribution of the model can be seen more easily if all the major discontinuities are included.

d) The number of iterations

No criteria can be given to determine the number of iterations required to obtain a converged model atmosphere. The user must look at the trend in the flux and flux derivative errors from iteration to iteration and decide how many iterations will be required to obtain the degree of convergence required for any particular application. SAM1 produces sufficient information in easily accesible form after each iteration, to enable the user to restart the calculation without having to recompute the model from the beginning again.

Models which include convective flux in the temperature correction i.e. IFCONV=2, converge much more slowly than pure radiative models. They also tend to have fairly large errors in the last few depth points which are very difficult to get rid of. However these last few points generally do not affect the emergent flux distribution, therefore one can tolerate fairly large errors here.

5. ERROR MESSAGES

5.0 Introduction

There are basically two types of error message. The first type is concerned with the format of the control cards input to the program. If the program cannot understand any control card an appropriate error message is produced. The second type is concerned with errors that occur during the calculation of the model atmosphere. If, for any reason, during the calculation the numbers produced by the program become physically unrealistic or violate the assumptions on which the program is based, then an error message will be produced and the calculation stopped. This chapter describes the error messages which can be produced and gives some suggestions as to what the user should do when an error occurs.

5.1 Error messages and what to do about them

a) Input error messages

These messages are produced when the program cannot understand the input data. In each case the message is followed by the text which was being processed when the error was detected. This line does not necessarily contain the error, which may have occurred on a previous data card.

i) I DO NOT UNDERSTAND .....

This error occurs when the program encounters some undecodable text while searching for a code word. It probably means that a code word has been mis-spelt, or the arguments to the previous code word are wrong.

*ii) DUMMYR DOES NOT UNDERSTAND .....

If the program cannot decode the control cards occuring between the CALL and the RETURN code words then this error is produced. Only the control cards for the extended output option can appear between these two code words.

iii) IWORDF HAS READ OFF THE END .....

This means that the program was searching for a code word when it encountered the end of a card. The user should check the format of the card.

iv) FREEFF HAS READ OFF THE END .....

In this case the program was searching for a number when the end of card was encountered. The format of the card should be checked.

These errors can be avoided by careful checking of the control cards, making sure that the code words are spelt correctly and that parameters which must appear on the same control card do so.

b) Execution error messages

One or more of the following messages may be produced if the user has failed to supply one of the fundamental model parameters, see section 1.2.

WHAT TEFF
WHAT GRAVITY
HOW MANY FREQUENCIES
HOW MANY DEPTHS
HOW MANY ITERATIONS

The following error messages are produced when an error occurs in the calculation of a model. The most common situations are that an iteration loop fails to converge, or that a parameter becomes unphysical (such as a negative pressure).

i) MOLECULES OFF

This message is produced if the user has attempted to calculate the number density of a molecule when the MOLECULES option is switched off (IFMOL=Ø).

*ii) NO DATA FOR MOLECULE .....

This message is produced if the user has attempted to calculate the number density of a molecule when the required information for that molecule has not been read in.

iii) TOO MANY MOLECULES

This means that the user has supplied data for more than 100 molecules.

*iv) PRESSURE FAILS TO CONVERGE AT DEPTH ....

The iterative scheme used to calculate the pressure has not converged for the depth indicated. This probably means that the temperature

at this depth is well outside the range of temperatures for which the opacity table has been tabulated. There are two solutions to this problem :

1) Change the depth points so that the model does not go so deep in the atmosphere. This may not be a satisfactory solution for many reasons, but provided the revised model is stable and has an optical thickness of at least 10, then the model should be satisfactory.

2) Perhaps the better solution is to recalculate the opacity table so that the temperatures in the model fall within the range of tabulation.

* v) XNE DOES NOT CONVERGE FOR DEPTH ....
or CONVEC : XNE DOES NOT CONVERGE AT DEPTH ....

This message indicates that the iterative scheme used to calculate the electron number density (XNE) has not converged at the depth specified. This error normally occurs when the depth points extend too deep in the atmosphere. Thus the solution is to change the depth grid so that the depth points occur higher up in the atmosphere.

* vi) THE MODEL HAS BLOWN UP AT DEPTH ....

This error occurs when a depth point has an optical depth which is smaller than the optical depth of a point which is physically higher in the atmosphere. The solution is to move the depth grid higher in the atmosphere and/or change the distribution of the depth points. This error can also occur if the starting model is a bad one, which probably means that the opacity table is not good enough for the model. So the problem may be cured by recalculating the opacity table.

The user will probably have noticed that a lot of these errors are caused by the parameters of the model lying outside the ranges for which they have been tabulated in the program. Thus the user should always take care to check that the parameters of the model are within permisible bounds.

The user should also carefully look at the final converged model atmosphere to make sure that it makes sense physically. Two things

which must be checked are :

1) That the frequency points cover that region of the spectrum where the majority of the stellar flux is emitted, and

2) That the model has an optical depth of at least 10 at all the frequencies.

Provided that these two conditions are satisfied, then the model atmosphere produced by the program is probably a good representation of the physics that was put into the program.

6. UTILITY PROGRAMS

6.0 Introduction

In this chapter the two utility programs which are used in conjunction with SAM1 are described :

FRESET: which calculates integration weights for the integrals over frequency.

OPTAB : which calculates an opacity table used in constructing the starting model.

6.1 FRESET

The input to FRESET consists of a name for the frequency set and a list of all the frequencies for which the integration weights are to be calculated. The name of the frequency set (up to six characters long) must appear at the beginning of the first card. The list of frequencies (in any order) are read in free-field format (i.e. they can appear anywhere on a card as long as the numbers are separated by a blank or a comma). Any number which is less than 10^6 is treated as a wavelength in nanometers. Any alphabetic characters may occur in among the data to clarify the information. The end of the data is denoted by a 0.

The output from FRESET is a listing of the frequencies and corresponding integration weights, and a punched card deck which can be read by SAM1.

FRESET has a useful facility to enable the user to easily cope with opacity discontinuities (e.g. the Balmer jump). If a minus sign is put in front of a frequency then FRESET takes the absolute value of the frequency and splits it into two frequencies, one either side of the discontinuity. As many points as required can be inserted between any two discontinuities. However these points should be evenly distributed in frequency. FRESET can be quite sensitive to the distribution of the frequency points. If it does not like the distribution, some of the integration weights will be negative. When this happens the distribution should be changed and/or extra points included until all weights are positive. There are sometimes problems

about negative weights near the ends of the frequency set, this can be overcome by making the end points discontinuities.

TABLE 2

EXAMPLE DATA SET FOR FRESET

```
COOL
H EDGES  -3.28805D15 -8.220125D14 -3.6533889D14 -2.05503125D14
-1.31522D14 -9.1334722D13 6.713061D13 5.1375781D13 4.059321D13
-3.28805D13
C  -2.7254D15 -2.4196D15 -2.0761D15  AL  -1.443D15  MG -1.848851D15
-1.1925797D15 -7.9804046D14  SI  -1.9723165D15 -1.7879689D15
-1.515292D15  OTHER POINTS  1.95D14 2.3D14 2.6D14 3.0D14 3.3D14
4.D14 4.5D14 5.D14 5.5D14 5.99585D14 6.5D14 7.D14 7.5D14 8.5D14 9.D14
9.3D14 1.D15 1.05D15 1.1D15 1.15D15 1.25D15 1.3D15 1.35D15 1.4D15
1.55D15 1.6D15 1.65D15 1.75D15 1.82D15 1.9D15 2.02D15 2.2D15 2.3D15
2.5D15 2.6D15 2.8D15 3.D15    0.
```

*6.2 OPTAB

The utility program OPTAB is controlled in the same way as SAM1. The user presents the required information to OPTAB in the form of control cards and then tells it to start the calculation with the BEGIN code word. The code words recognised by OPTAB are the following :

TITLE	see	page	10
OPACITY	"	"	10
ABUNDANCE	"	"	25
MOLECULES	"	"	21
READ FREQUENCIES	"		8
WAVELENGTH	"	"	25
BEGIN	"	"	9
END	"	"	9

OPTAB also has a special control card to tell it the temperature and pressure values of the tabulation :

CALCULATE DECK n1 n2 n3
n4 n5 n6 .....

where n1 is the number of temperature and pressure points in the tabulation. n2 is the starting number and n3 is the finishing number of the part of the table to be calculated in this run. This card must be followed by cards containing n1 values of $\log_{10}$ temperature followed by n1 values of $\log_{10}$ pressure.

OPTAB must be told the values of temperature and pressure for which the table is to be calculated, and a set of frequency points and integration weights. The defaults for the other parameters are the same as those for SAM1. The frequency points used should be selected using the same criteria as are the points for a model atmosphere calculation, bearing in mind the temperature range of the opacity table.

Thus the default opacity table can be produced with the following deck of control cards :

```
TITLE       STANDARD OPACITY DECK
CALCULATE DECK  30  1  30
 3.5 3.525 3.55 3.575 3.6 3.625 3.65 3.675 3.7 3.725 3.75 3.775
 3.8 3.825 3.85 3.875 3.9 3.925 3.95 3.975 4.0 4.05 4.1 4.15
 4.2 4.25 4.3 4.35 4.4 4.45
 -2. -1.4 -1. -0.5 0. 0.5 1.0 1.25 1.5 1.75 2.0 2.25 2.5 2.75 3.
 3.2 3.4 3.6 3.8 4.0 4.2 4.4 4.6 4.8 5.0 5.2 5.4 5.6 5.8 6.0
READ FREQUENCIES  75 1  75   COOL
        .
        .
        .
BEGIN
END
```

N.B.

OPTAB uses a lot of computer time, so a new opacity table should only by calculated when really necessary.

APPENDIX I

How SAM1 works

Introduction

The calculation of a model stellar atmosphere is a straightforward process, once several assumptions and approximations have been made to simplify the problem both physically and computationally. We simplify the problem by assuming :

1) The atmosphere is in a steady state.

2) The energy source of the star lies far below the atmosphere and the flux of energy is constant with depth in the atmosphere (also that no energy comes into the atmosphere from above). The total flux from the star is usually specified by an effective temperature T_{eff}, such that :

$$\text{Flux} = \sigma T_{eff}^{4} \qquad \sigma = 5.66956 \times 10^{-5} \text{ ergs cm}^{-2}\text{sec}^{-1}{}^{o}\text{K}^{-4}$$

3) The atmosphere is homogeneous except in the normal direction.

4) The atmosphere is thin relative to the radius of the star, so we can consider plane-parallel layers instead of concentric shells.

5) The atmosphere is in hydrostatic equilibrium.

Given these assumptions, we go through an iteration procedure to determine the parameters that describe the model atmosphere : we guess the temperature at a set of depth points in the atmosphere, and calculate the pressure, number densities, and opacity at each depth. From these quantities we determine the radiation field and convective flux at each depth. The total flux at each depth does not, in general, equal the prescribed constant flux, so we change the temperature distribution according to a 'temperature correction' scheme. We repeat the whole process with successive temperature distributions for a given number of iterations.

The co-ordinate system

Because of the simplifications that have been introduced into the atmospheres problems, we can completely describe the models produced by SAM1 using only two co-ordinates, depth and frequency. The physical

structure of a model (temperature, pressure etc.) is defined by the values of the variables at a set of discrete depth points. The radiation field at each depth is described by the values of the variables (mean intensity, flux, etc.) at a set of discrete frequency points.

The main depth variable used in the program is a mass variable, called RHOX (given the symbol M) which is defined by :

$$M_i = - \int_0^{x_i} \rho \, dx \qquad (1)$$

ρ = density x = geometrical depth in the atmosphere (+ve towards the observer)

RHOX, and all optical depth variables, are measured positive into the atmosphere (away from the observer) hence the negative sign in (1). All optical depth variables can be calculated using RHOX e.g.

$$\tau_\nu = \int_{M_1}^{M_n} \kappa_\nu \, dM \qquad (2)$$

Because of its useful scaling properties a Rosseland mean optical depth is also used. It is defined by :

$$\tau_{Ross} = \int_{M_1}^{M_n} \kappa_{Ross} \, dM \qquad (3)$$

where κ_{Ross} is the Rosseland mean opacity defined by :

$$\frac{1}{\kappa_{Ross}} = \frac{\int_0^\infty \left[\frac{1}{\kappa_\nu + \sigma_\nu}\right] \frac{dB_\nu}{dT} \, d\nu}{\int_0^\infty \frac{dB_\nu}{dT} \, d\nu} \qquad (4)$$

κ_ν = mass absorption coefficient, σ_ν = mass scattering coefficient,
B_ν = the Plank function, T = temperature.

For the second co-ordinate, frequency, we select as many frequency points as are necessary to represent the distribution of the emergent flux. In the model calculation, integrals over frequency of various radiation field variables, f_ν are required. These are calculated using previously determined integration weights, w_i , i.e.

$$\int_0^\infty f_\nu d\nu = \sum_i w_i f_{\nu_i} \qquad (5)$$

A utility program is supplied (see section 6.1) to determine these weights.

1) Construction of the initial model

There are several different options which the user can choose to define a starting model (see section 3.2). If one of these options is used SAM1 fills in any missing information and proceeds to step 2. If, however, the user does not have a starting model then the CALCULATE option (see section 1.2) can be used to generate a starting model. With this option the user specifies a set of logarithmically spaced values of τ_{Ross}. A temperature distribution is then calculated using :

$$T(\tau) = T_{eff} \{0.75\ (0.71 + \tau - 0.1331 \exp(-3.4453\tau))\}^{\frac{1}{4}} \qquad (6)$$

The next step is to integrate the equation of hydrostatic equilibrium (equation 7) to obtain the pressure structure of the model.

$$\frac{dP_{tot}}{d\tau_{Ross}} = \frac{g}{\kappa_{Ross}} \qquad (7)$$

$$P_{tot} = P_{gas} + P_{rad} + P_{turb} \qquad (8)$$

$$P_{rad} = \frac{4\pi}{C} \int_0^\infty K_\nu d\nu = \frac{4\pi}{C} \int_0^M \int_0^\infty k_\nu H_\nu d\nu dM \qquad (9)$$

$$P_{turb} = \frac{1}{3} \rho\, v^2_{turb} \text{ where } V_{turb} = A + Bv_{sound} + C\rho^D \qquad (10)$$

In equation (8), P_{tot} is the total pressure, P_{rad} is the radiation pressure given by equation (9) where K_ν is the second moment of the intensity, and H_ν is the first moment, often called the Eddington Flux. P_{turb} is an empirical estimate of the turbulent pressure caused by the random motion of small gas elements, given by equation (10). The constants A,B,C,D in equation (10) can be specified by the user. However P_{turb} is not normally included in the pressure calculation. Initially we do not know the radiation field, the density or the sound velocity, therefore we set $P_{turb} = 0$, and make an estimate of the radiation pressure using

$$P_{rad} = \frac{4\sigma}{3c} \left(T^4 - T_0^4 \right) \qquad (11)$$

Equation (7) is integrated as follows. A guess is made for κ_{Ross} at a τ_{Ross} near the surface, and the simple difference equation corresponding to (7) is solved for P_{tot}. P_{gas} is then calculated from (8).

Using this P_{gas} and the temperature at this depth, a new κ_{Ross} is found by interpolating in a table of κ_{Ross} as a function of pressure and temperature. With this new κ_{Ross} the difference equation can be solved again to give a new P_{gas}. Iteration between κ_{Ross} and P_{gas} continues until they are consistent to some specified error. Having determined the upper boundary condition, equation (7) is solved to find the pressure at all depths using Hammings predictor-corrector method.

The internal table of κ_{Ross} was calculated using 'normal' abundances and the default opacity sources (see Appendix II), for temperatures in the range 3100 to 28000 ^{0}K and pressures in the range 10^{-2} to 10^{6} dynes cm^{-2}. If the temperatures and/or pressures in the user's model are outside these ranges, or if the abundances and/or opacity sources included in the model are significantly different from the default values, the initial pressure structure will not be very good. This will lead to slow convergence, or the model may just 'blow up'. Thus the facility has been provided to enable the user to calculate a new table of κ_{Ross} using the utility program OPTAB (see section 6.2). The output from OPTAB can be read in by SAM1 and used instead of the internal table.

Having obtained the pressure, RHOX can be calculated from equation (12).

$$P_{tot} = gM \qquad (12)$$

2) Calculation of number densities

Although we explicitly need only those number densities that are required for the calculation of the opacity, number densities of other species must be considered because of their indirect effects. Thus we have to calculate number densities of all species that contribute a significant number of electrons, also in calculating molecular number densities we need to know what other molecules are competing for the available atoms. In order to calculate equilibrium number densities, we set up as many equations as there are constraints. The first set of constraints are on the abundances - the total number density of atoms of each element must be a given fraction of the total number of atoms. The other constraints are the conservation of charge, and the perfect gas law. Each term in the equilibrium equations can be written as a

function of neutral atom and electron number densities by means of a Saha equation :

$$n^{k+}_{12..m} = \frac{n_1 n_2 \cdots n_m}{(n_e)^k} \quad E(T) \qquad (13)$$

where the species $n^{k+}_{12..m}$ has m atoms and k + ve charges.

In SAM1 the Saha functions, E(T), for atoms are provided as an internal table. However for molecules the Saha functions are approximated by :

$$E(T) = \exp(A/kT_{ev} - B + CT - DT^2 + ET^3 - FT^4 - 1.5(m-k-1)\ln T) \qquad (14)$$

T_{ev} is the temperature in electron volts.
The coefficients A,B,C,D,E,F must be supplied by the user (see section 3.1, e).

The resulting set of equilibrium equations contain only the number densities of neutral atoms and the electron number density. Because the equilibrium equations are non-linear, they are solved using a Newton-Raphson technique. However if there are no molecules there are no cross-terms linking the equations, and a simple iterative scheme can be used. Once the neutral atom number densities and the electron number density are known, the number densities of other species can be obtained from equations such as (13). The only elements which are considered to contribute a significant number of electrons are : H,He,C,Na,Mg,Al,Si,K,Ca,Fe.

3) Calculation of the radiation field.

Using the opacity sources requested by the user, the total absorption and scattering coefficients can be calculated. The source function S_ν can then be calculated by solving the integral equation (15).

$$S_\nu = (1 - \alpha_\nu)\overline{S}_\nu + \alpha_\nu J_\nu \qquad (15)$$

where $\alpha_\nu = \frac{\sigma_\nu}{\kappa_\nu + \sigma_\nu}$, $\overline{S}_\nu = \frac{\Sigma \kappa_\nu(l \rightarrow u) S_\nu(l-u)}{\kappa_\nu}$, $\kappa_\nu = \Sigma \kappa_\nu(l \rightarrow u)$

κ_ν (l-u) is the mass absorption coefficient for the transition l-u and S_ν (l-u) is the corresponding source function. α_ν is the scattering part of the source function, κ_ν is the total mass absorption coefficient, σ_ν is the total mass scattering coefficient. J_ν is the

mean intensity. Equation (15) is solved by the integral equation technique given by Kurucz (1969). Having obtained the source function, the mean intensity, J_ν , and the flux, H_ν , are obtained using methods described by Kurucz (1969). Given these radiation field quantities all the other quantities such as the total Rosseland opacity, radiation pressure etc. can be calculated.

4) Enforcing the constraint of radiative equilibrium.

The radiation field that has just been calculated does not satisfy the constraint of radiative and convective equilibrium i.e.

$$\int_0^\infty H_\nu d\nu + H_{conv} \neq \frac{\sigma T_{eff}^4}{4\pi} \qquad (16)$$

where H_{conv} is the convective flux which can be calculated with a simple Bohm-Vitense mixing length theory if requested by the user, otherwise it is set to zero. In order to bring the model closer to a state of radiative and convective equilibrium the temperature at each depth must be corrected. SAM1 uses an approximation to the Bohm-Vitense temperature correction method (see Bohm-Vitense (1964)) to correct the surface layers of the model. A modified Avrett-Krook method is used to correct the rest of the model (see Avrett and Krook (1963)).

These methods change the depth points as well as the temperatures, thus the depth points at which the final model is tabulated are not normally the same as the points used in the starting model.

5) Finishing off the iteration

If the user has requested a non-L.T.E. model, then the statistical equilibrium equations are set up and solved to give the departure coefficients for the first six levels of atomic hydrogen and the departure coefficient for H^-. These departure coefficients are then included in the calculation of electron number densities, opacities etc. in the next iteration. Finally the geometric height in the atmosphere, turbulent pressure etc. are calculated.

SAM1 then starts the next iteration by calculating the new P_{tot} using equation (12) with the new set of rhox's obtained in step 4.

A new P_{gas} can be obtained from equation (8) using the new P_{tot} together with the new P_{rad} calculated in step 3, and the new P_{turb} calculated in this step. The calculation then proceeds from step 2.

This process continues for the number of iterations requested by the user.

Appendix II

Summary of available options

The options available with SAM1 are listed below in alphabetical order. Those characters which are recognised by the program as representing that option are underlined. At the end of each entry there is a list of the places in the main text which refer to that particular option. The defining reference is underlined. An 'I' after a reference indicates an indirect reference, i.e. while the option is not specifically mentioned, the contents of that section are relevant to the option. The number that appears in brackets refers to the page number in this report. Options which are different from, or not available in, ATLAS5 are marked with an asterisk.

ABUNDANCE CHANGE n1 n2

changes the abundance (per number) of element n1 to the value n2 (-ve means a $\log_{10}$). Default abundances are given in table 3 p. 58.

3.3,a,i(25); 6.2(41)

ABUNDANCE SCALE n1

causes all the abundances (except H and He) to be multiplied by n1.

3.3,a,ii(25); 6.2(41)

ATLAS

This control card, which has not been classified in the main text, allows the user to read in a model punched by ATLAS5. The card should be placed before a deck of ATLAS5 control cards. This option is cancelled by the execution of a BEGIN card.

*
BEGIN

normally causes the calculation to start, however if data is being read in under the MODEL n1 option, then BEGIN causes the program to resume reading from the main input stream (unit 5).

1.2,f(9); 2.1(13); 3.1,e(21,22); 3.3 (26); 3.5,a(30); 4.1,e(33); 6.2(41,42)

CALCULATE n1 n2 n3

sets up a grid of n1 depth points from $\log_{10}$ τ_{Ross} = n2 with $\log_{10}$ spacing = n3

1.2,c(8); 2.1(13); 3.2,f(24); 4.2,b(34)I; Appendix I(45)

*
CALCULATE DECK n1 n2 n3

introduces n1 values of $\log_{10}$ temperature and $\log_{10}$ pressure to be used to calculate part of an opacity table (from pressure number n2 to n3).

6.2(41,42)

*
CALL

must preceed the extended output option control cards.

3.5,a(29,30); 5.1,a,ii(36)

CHANGE n1 n2, n3, ...

maps an already defined model onto n1 new rhox values n2, n3, ...

3.2,e(24); 4.2,b(34)I

*
CONVECTION n1 n2

sets MIXLTH=n1 ans IFCONV=n2. Defaults MIXLTH=1.0, IFCONV=1

3.1,d(21); 4.2,d(35)I

* CORRECTION n1

sets IFCORR=n1. If n1=0 no temperature correction is performed. The default is IFCORR=1, which performs a normal temperature correction.

3.1,a(20)

DECK

see under CALCULATE DECK AND READ DECK.

DEPARTURE

see under READ DEPARTURE.

* DEPTH n1 n2 n3, n4, ...

specifies n1 optical depths (n3, n4, ...) at frequency identifier n2, which are used in the extended output options.

3.5(30)

END

marks the end of the input data and stops the program.

1.2,g(9); 2.1(13); 3.5,a(30); 4.1,e(33); 6.2(41,42)

FREQUENCIES

see under READ FREQUENCIES.

GRAVITY n1

sets the surface gravity to n1 (if n1 less than 10, it is treated as a $\log_{10}$)

1.1(7); 1.2,b(8); 2.1(13); 4.1,b(32); 4.2,a(34)

IFOP

see under OPACITY IFOP

* ITERATIONS n1 n2

indicates that n1-n2+1 iterations are to be performed, numbered from n2.

1.2,e(9); 1.3,d(12); 2.1(13); 3.5,a(30); 4.1,e(33); 4.2,d(35)I

INTENSITY

see under SURFACE INTENSITY

* KAPPA n1

causes an opacity table to be read in.

3.3,d(26); 4.1,b(32)I; 6.2(41,42)I

LTE

specifies that the calculation should be performed assuming L.T.E.
see also under NLTE.

1.1(7); 1.3,b(10)

* MODEL n1

tells the program to read data from unit n1. See also under BEGIN.

3.3,e(26); 4.1,e(33)

MOLECULES ON

sets IFMOL=1, to allow molecules to be included in the equilibrium equations.
Default IFMOL=0. Some molecular constants are given in table 4 p. 58, 59.

3.1,e(21); 3.4,a,iii(27); 3.4,b,ii(29); 5.1,b(37); 6.2(41)

NLTE

specifies that a non-L.T.E. calculation is to be performed.

1.3,b(10); 3.4,a,ii(27)

OFF

ON

are opposite switch settings for use with other options. See MOLECULES, OPACITY, PRESSURE, TURBULENCE, SCATTERING.

OPACITY IFOP n1, n2, ..., n20

causes the twenty opacity switches to be reset.

1.3,c(10); 6.2(41)

OPACITY ON cw1, cw2, ...

OPACITY OFF cw1, cw2, ...

cause the opacities specified by cw1, cw2, ... to be switched ON or OFF.

1.3,c(11); 6.2(41)

The opacity sources included in SAM1 are described in Table 5. p.60.

PRESSURE OFF

suppresses the calculation of pressure and number densities. IFPRES is set to 0. Default IFPRES=1.

3.1,b(20)

PRINT n1

indicates the print option required. Default n1=1 for all iterations except the last, when n1=2.

n1 = 0 suppresses the output.

1 print emergent flux and summary table.

2 print temperature correction, surface flux, model etc.

3 print 2 plus TAUNU, SNU, etc. at each frequency.

4 print 2 plus all opacities at all frequencies.

*12 print 2 plus the model mapped onto the specified grid.

*13 print 12 plus TAUNU etc. at selected depths and frequencies.

*14 print 12 plus opacities at selected depths and frequencies.

1.3,d(11); 2.1(13); 2.2(15-19); 3.4(26-29); 3.5(29,30); 4.1,e(33)

PUNCH n1

indicates the punch option required. Default n1=0 for all iterations.

n1 = 0 suppresses all punch output.

1 punch the model.

2 punch 1 plus the surface flux at each wavelength.

*3 punch 2 plus punch of PRINT 13 information.

*4 punch 2 plus punch of PRINT 14 information.

5 punch 2 plus molecular number densities/partition functions.

1.3,d(10,11); 2.1(13); 2.2(19); 3.1,b,ii(22); 3.4(26-28); 4.1,e(33)

*READ DECK n1

introduces a complete model structure at n1 depths.

3.2,d(20)

READ DEPARTURE n1

introduces n1 sets of departure coefficients.

3.2,c(23)

READ FREQUENCIES n1 n2 n3 name

introduces the frequency points and integration weights. n1 is the number of frequencies, the integration runs from n2 to n3, name is an identifier.

1.2,d(8); 2.1(13); 3.2,a(23); 4.1,a(32)I; 4.2,c(34)I; 6.1(40)I; 6.2(41,42)

*READ STARTING n1 n2

introduces n2 pairs of depth variable and temperature. n1=1 means that the depth variable is the Rosseland mean optical depth, n1=2 means the depth variable is RHOX.

3.2,b(23)

*RETURN

indicates the end of the extended output control cards.

3.5,a(29); 5.2,a,ii(36)

*SAMPLE n1 n2, n3, ...

indicates the frequency identifiers of the frequencies to be used in the extended output options.

3.5,a(29)

SCALE n1 n2 n3 n4 n5

enables the user to scale an already defined model to a new T_{eff}, g and depth grid. n1, n2, n3 have the same meaning as on a CALCULATE card, n4 is the new T_{eff}, and n5 is the new gravity.

3.2,f(24); 4.2,b(34)I

SCATTERING OFF

sets IFSCAT=0, indicating the transfer solution is to ignore scattering.

3.1,f(22)

STARTING

see under READ STARTING

SURFACE INTENSITY n1 n2, n3, ...

sets IFSURF=1. The surface intensity will be printed out for n1 μ's, n2, ...

3.3,b(25); 3.4,a.i(27); 3.4,b,ii(28)

TEFF n1

sets the effective temperature to n1.

1.1(7); 1.2,a(8); 2.1(13); 4.1,b(32)I; 4.2,a(34)

TITLE title

inputs a title for the model.

1.3,a(10); 2.1(13); 6.2(41,42)

TURBULENCE ON n1 n2 n3 n4

sets IFTURB=1 and TRBFDG=n1, TRBPOW=n2, TRBSND=n3, TRBCON=n4. Default OFF.

3.1,c(21)

WAVELENGTH n1 n2 n3

defines a grid of equally spaced wavelengths starting at n1, ending at n2 with spacing n3.

3.3,c(26); 6.2(41)

TABLE 3

TABLE OF ELEMENTAL ABUNDANCES

H	0.900	HE	0.100												
LI	-11.60	BE	-9.60	B	-9.20	C	-3.50	N	-4.12	O	-3.28	F	-6.60	NE	-3.50
NA	-6.18	MG	-4.57	AL	-5.65	SI	-4.50	P	-6.62	S	-4.84	CL	-6.60	AR	-5.30
K	-7.00	CA	-5.72	SC	-9.01	TI	-7.55	V	-8.13	CR	-6.58	MN	-7.17	FE	-4.50
CO	-8.40	NI	-6.97	CU	-7.30	ZN	-7.63	GA	-9.11	GE	-8.73	AS	-9.70	SE	-8.80
BR	-9.40	KR	-8.80	RB	-9.42	SR	-9.23	Y	-9.60	ZR	-9.60	NB	-10.30	MO	-10.00
TC	-20.00	RU	-10.40	RH	-11.20	PD	-10.70	AG	-11.30	CD	-9.98	IN	-10.34	SN	-10.34
SB	-10.40	TE	-10.00	I	-10.60	XE	-10.00	CS	-10.90	BA	-10.15	LA	-10.60	CE	-10.40
PR	-11.20	ND	-10.50	PM	-20.00	SM	-11.00	EU	-11.30	GD	-10.90	TB	-11.60	DY	-10.80
HO	-11.50	ER	-11.10	TM	-11.90	YB	-10.90	LU	-11.70	HF	-11.40	TA	-11.70	W	-10.90
RE	-11.40	OS	-10.70	IR	-10.80	PT	-10.40	AU	-11.30	HG	-11.10	TL	-11.50	PB	-10.15
BI	-11.30	PO	-20.00	AT	-20.00	RN	-20.00	FR	-20.00	RA	-20.00	AC	-20.00	TH	-11.70
PA	-20.00	U	-12.00	NP	-20.00	PU	-20.00	AM	-20.00	CM	-20.00	BK	-20.00	CF	-20.00
ES	-20.00														

TABLE 4

CONSTANTS FOR MOLECULAR PARTITION FUNCTIONS

CODE	A	B	C	D	E	F
101.00	4.477	0.4663D 02	0.1803D-02	0.5024D-06	0.8142D-10	0.5050D-14
103.00	2.429	0.4494D 02	0.2245D-02	0.5518D-06	0.8062D-10	0.4762D-14
104.00	2.211	0.4382D 02	0.1989D-02	0.4923D-06	0.7372D-10	0.4435D-14
105.00	3.001	0.4640D 02	0.1883D-02	0.4642D-06	0.6965D-10	0.4153D-14
106.00	3.470	0.4551D 02	0.1711D-02	0.3632D-06	0.5016D-10	0.2872D-14
107.00	3.699	0.4524D 02	0.1843D-02	0.4900D-06	0.7735D-10	0.4764D-14
108.00	4.395	0.4575D 02	0.1700D-02	0.4490D-06	0.7086D-10	0.4365D-14
109.00	5.844	0.4662D 02	0.1538D-02	0.4041D-06	0.6441D-10	0.3982D-14
111.00	2.050	0.4471D 02	0.2416D-02	0.6104D-06	0.9049D-10	0.5371D-14
112.00	1.999	0.4344D 02	0.2215D-02	0.5488D-06	0.8116D-10	0.4803D-14
113.00	2.901	0.4569D 02	0.1840D-02	0.4124D-06	0.5761D-10	0.3277D-14
114.00	3.190	0.4477D 02	0.1686D-02	0.3737D-06	0.5086D-10	0.2828D-14
115.00	3.300	0.4468D 02	0.1896D-02	0.4674D-06	0.6806D-10	0.4026D-14
116.00	3.530	0.4527D 02	0.1860D-02	0.4733D-06	0.7169D-10	0.4304D-14
117.00	4.431	0.4589D 02	0.1564D-02	0.3960D-06	0.6211D-10	0.3828D-14
303.00	1.095	0.4453D 02	0.2634D-02	0.6537D-06	0.9453D-10	0.5565D-14
308.00	3.599	0.4614D 02	0.2226D-02	0.5390D-06	0.7689D-10	0.4473D-14
309.00	5.904	0.4671D 02	0.2307D-02	0.5706D-06	0.8263D-10	0.4837D-14
317.00	4.959	0.4614D 02	0.2609D-02	0.6995D-06	0.1062D-09	0.6377D-14
408.00	4.596	0.4678D 02	0.1949D-02	0.4703D-06	0.7233D-10	0.4420D-14
409.00	6.305	0.4561D 02	0.2020D-02	0.4806D-06	0.6888D-10	0.4020D-14
417.00	4.899	0.4519D 02	0.2377D-02	0.6226D-06	0.9390D-10	0.5619D-14
505.00	2.775	0.4765D 02	0.2395D-02	0.6099D-06	0.9975D-10	0.5234D-14
507.00	4.002	0.4630D 02	0.2133D-02	0.5297D-06	0.7766D-10	0.4562D-14
508.00	8.142	0.4802D 02	0.1729D-02	0.3908D-06	0.5465D-10	0.3108D-14
509.00	8.499	0.4823D 02	0.1891D-02	0.4359D-06	0.6126D-10	0.3490D-14
516.00	5.117	0.4742D 02	0.1895D-02	0.4332D-06	0.5959D-10	0.3273D-14
517.00	5.117	0.4770D 02	0.2336D-02	0.6058D-06	0.9061D-10	0.5345D-14
606.00	6.156	0.4964D 02	0.3481D-02	0.1049D-05	0.1685D-09	0.1037D-13
607.00	8.109	0.4785D 02	0.1866D-02	0.4618D-06	0.7159D-10	0.4375D-14
608.00	11.108	0.4917D 02	0.1580D-02	0.3435D-06	0.4687D-10	0.2656D-14
609.00	4.966	0.4737D 02	0.2017D-02	0.4776D-06	0.6740D-10	0.3847D-14
615.00	6.895	0.4751D 02	0.2117D-02	0.4953D-06	0.7281D-10	0.4401D-14
616.00	7.892	0.4855D 02	0.1738D-02	0.3695D-06	0.4761D-10	0.2559D-14
617.00	3.340	0.4701D 02	0.2459D-02	0.6535D-06	0.9826D-10	0.5817D-14
707.00	9.763	0.4870D 02	0.1922D-02	0.4914D-06	0.7469D-10	0.4540D-14
708.00	6.508	0.4737D 02	0.1984D-02	0.4928D-06	0.7293D-10	0.4335D-14
709.00	2.819	0.4677D 02	0.2241D-02	0.5510D-06	0.7990D-10	0.4646D-14
714.00	4.510	0.4715D 02	0.1872D-02	0.4125D-06	0.5395D-10	0.2905D-14
715.00	7.111	0.4768D 02	0.2246D-02	0.5575D-06	0.7911D-10	0.4575D-14
716.00	4.987	0.4699D 02	0.2258D-02	0.5734D-06	0.8395D-10	0.4920D-14
808.00	5.116	0.4863D 02	0.1632D-02	0.3392D-06	0.4603D-10	0.2584D-14
811.00	3.079	0.4642D 02	0.2622D-02	0.6850D-06	0.1020D-09	0.6054D-14
812.00	3.903	0.4657D 02	0.2300D-02	0.4385D-06	0.5323D-10	0.2847D-14
813.00	4.987	0.4756D 02	0.2010D-02	0.4565D-06	0.6239D-10	0.3467D-14
814.00	8.310	0.4848D 02	0.1551D-02	0.2907D-06	0.3281D-10	0.1549D-14
815.00	6.071	0.4731D 02	0.2417D-02	0.6210D-06	0.8997D-10	0.5250D-14
816.00	5.358	0.4749D 02	0.1699D-02	0.3506D-06	0.4450D-10	0.2365D-14
817.00	2.745	0.4683D 02	0.2108D-02	0.5134D-06	0.7441D-10	0.4317D-14
909.00	1.592	0.4863D 02	0.2016D-02	0.4605D-06	0.6429D-10	0.3630D-14
911.00	4.953	0.4672D 02	0.2757D-02	0.7406D-06	0.1121D-09	0.6707D-14
912.00	3.200	0.4547D 02	0.2509D-02	0.6524D-06	0.9717D-10	0.5756D-14
913.00	6.790	0.4779D 02	0.2136D-02	0.5067D-06	0.7140D-10	0.4053D-14
914.00	5.420	0.4690D 02	0.2106D-02	0.4986D-06	0.6860D-10	0.3797D-14
916.00	3.338	0.4671D 02	0.1921D-02	0.4300D-06	0.5806D-10	0.3208D-14
917.00	2.616	0.4768D 02	0.2141D-02	0.5324D-06	0.7815D-10	0.4563D-14
1111.00	0.730	0.4515D 02	0.3692D-02	0.1075D-05	0.1702D-09	0.1046D-13
1117.00	4.222	0.4615D 02	0.3004D-02	0.8513D-06	0.1330D-09	0.8096D-14
1216.00	2.901	0.4608D 02	0.2614D-02	0.6884D-06	0.1025D-09	0.6076D-14
1217.00	2.701	0.4500D 02	0.2845D-02	0.7969D-06	0.1237D-09	0.7494D-14
1313.00	1.604	0.4756D 02	0.2910D-02	0.7781D-06	0.1175D-09	0.6950D-14
1317.00	5.074	0.4728D 02	0.2544D-02	0.6757D-06	0.1010D-09	0.6005D-14
1414.00	3.252	0.4718D 02	0.2026D-02	0.4519D-06	0.5742D-10	0.2958D-14
1416.00	6.418	0.4799D 02	0.1793D-02	0.3753D-06	0.4597D-10	0.2324D-14
1417.00	4.002	0.4654D 02	0.2553D-02	0.6846D-06	0.1021D-09	0.5973D-14
1515.00	5.033	0.4822D 02	0.2690D-02	0.7036D-06	0.1008D-09	0.5849D-14
1516.00	5.637	0.4692D 02	0.2764D-02	0.7435D-06	0.1095D-09	0.6420D-14
1616.00	4.380	0.4769D 02	0.1903D-02	0.4236D-06	0.5595D-10	0.3044D-14
1617.00	2.749	0.4757D 02	0.3563D-02	0.1090D-05	0.1757D-09	0.1081D-13
1717.00	2.476	0.4802D 02	0.2918D-02	0.6537D-06	0.1006D-09	0.6043D-14

TABLE 4 cont.

CONSTANTS FOR MOLECULAR PARTITION FUNCTIONS

CODE	A	B	C	D	E	F
10106.00	8.850	0.9346D 02	0.2237D-02	0.2947D-06	0.2771D-10	0.1219D-14
10108.00	9.511	0.9316D 02	0.2653D-02	0.5695D-06	0.8393D-10	0.5042D-14
10116.00	7.514	0.9205D 02	0.2751D-02	0.5122D-06	0.6619D-10	0.3654D-14
10308.00	8.894	0.9268D 02	0.3519D-02	0.7018D-06	0.1086D-09	0.6249D-14
10607.00	13.135	0.9609D 02	0.3411D-02	0.6738D-06	0.8767D-10	0.4837D-14
10608.00	12.311	0.9419D 02	0.3025D-02	0.5969D-06	0.7722D-10	0.4235D-14
10811.00	8.286	0.9270D 02	0.4370D-02	0.1098D-05	0.1624D-09	0.9622D-14
10812.00	6.823	0.9145D 02	0.3973D-02	0.9476D-06	0.1369D-09	0.8010D-14
30308.00	7.366	0.9434D 02	0.4556D-02	0.1062D-05	0.1467D-09	0.8357D-14
40909.00	13.202	0.9754D 02	0.3476D-02	0.7463D-06	0.9069D-10	0.4690D-14
40917.00	11.168	0.9669D 02	0.4598D-02	0.1029D-05	0.1401D-09	0.7833D-14
41717.00	9.449	0.9719D 02	0.5379D-02	0.1339D-05	0.1944D-09	0.1130D-13
50808.00	14.587	0.9907D 02	0.4523D-02	0.9755D-06	0.1201D-09	0.6937D-14
50809.00	15.397	0.9930D 02	0.4010D-02	0.8217D-06	0.1055D-09	0.5652D-14
50817.00	13.416	0.9902D 02	0.4617D-02	0.1060D-05	0.1470D-09	0.8299D-14
50909.00	13.251	0.9661D 02	0.4309D-02	0.9904D-06	0.1364D-09	0.7673D-14
50917.00	11.196	0.9550D 02	0.4955D-02	0.1244D-05	0.1810D-09	0.1048D-13
51717.00	9.141	0.9572D 02	0.5539D-02	0.1481D-05	0.2230D-09	0.1319D-13
60606.00	13.957	0.1008D 03	0.3991D-02	0.8103D-06	0.1017D-09	0.5362D-14
60717.00	12.126	0.9884D 02	0.4869D-02	0.1167D-05	0.1663D-09	0.9567D-14
60808.00	16.561	0.1010D 03	0.3366D-02	0.5777D-06	0.6387D-10	0.3053D-14
60816.00	14.210	0.1000D 03	0.3976D-02	0.7806D-06	0.9593D-10	0.4969D-14
60909.00	10.268	0.9779D 02	0.3764D-02	0.7731D-06	0.9926D-10	0.5306D-14
61616.00	11.881	0.1004D 03	0.4542D-02	0.9836D-06	0.1284D-09	0.6921D-14
70708.00	11.440	0.9917D 02	0.3992D-02	0.8112D-06	0.1052D-09	0.5731D-14
70808.00	9.621	0.9762D 02	0.3689D-02	0.7514D-06	0.9673D-10	0.5229D-14
70909.00	6.056	0.9632D 02	0.4439D-02	0.1028D-05	0.1421D-09	0.7987D-14
80814.00	13.447	0.1000D 03	0.3748D-02	0.6548D-06	0.6866D-10	0.3001D-14
80816.00	11.023	0.9841D 02	0.3785D-02	0.7703D-06	0.9748D-10	0.5159D-14
80817.00	5.244	0.9736D 02	0.4372D-02	0.9979D-06	0.1379D-09	0.7749D-14
80913.00	12.703	0.9914D 02	0.5349D-02	0.1283D-05	0.1804D-09	0.1021D-13
80916.00	7.482	0.9651D 02	0.4090D-02	0.8932D-06	0.1180D-09	0.6419D-14
81313.00	10.615	0.9748D 02	0.4554D-02	0.1056D-05	0.1453D-09	0.8125D-14
81317.00	11.108	0.9875D 02	0.5934D-02	0.1525D-05	0.2236D-09	0.1300D-13
81617.00	7.696	0.9601D 02	0.4673D-02	0.1134D-05	0.1611D-09	0.9206D-14
81717.00	4.226	0.9711D 02	0.4903D-02	0.1234D-05	0.1802D-09	0.1048D-13
90912.00	10.812	0.9818D 02	0.5333D-02	0.1276D-05	0.1793D-09	0.1019D-13
90914.00	11.835	0.9749D 02	0.4374D-02	0.9918D-06	0.1330D-09	0.7263D-14
90916.00	6.674	0.9742D 02	0.4430D-02	0.1021D-05	0.1399D-09	0.7804D-14
121717.00	8.360	0.9759D 02	0.6573D-02	0.1791D-05	0.2718D-09	0.1618D-13
141414.00	7.588	0.9976D 02	0.5519D-02	0.1328D-05	0.1810D-09	0.9918D-14
141717.00	8.902	0.9647D 02	0.5582D-02	0.1487D-05	0.2215D-09	0.1298D-13
161717.00	5.545	0.9661D 02	0.5601D-02	0.1502D-05	0.2257D-09	0.1333D-13
1010105.00	11.697	0.1404D 03	0.3631D-02	0.5393D-06	0.5877D-10	0.2927D-14
1010106.00	12.600	0.1403D 03	0.4124D-02	0.7248D-06	0.8941D-10	0.4810D-14
1010107.00	12.004	0.1397D 03	0.3565D-02	0.5705D-06	0.6898D-10	0.3756D-14
1010115.00	9.809	0.1392D 03	0.4286D-02	0.6773D-06	0.7112D-10	0.3340D-14
1010606.00	16.864	0.1449D 03	0.5101D-02	0.9249D-06	0.1131D-09	0.5929D-14
1050808.00	19.005	0.1456D 03	0.4759D-02	0.8475D-06	0.1002D-09	0.5106D-14
4040808.00	16.308	0.1459D 03	0.6961D-02	0.1538D-05	0.2064D-09	0.1146D-13
5050808.00	21.561	0.1511D 03	0.7348D-02	0.1655D-05	0.2258D-09	0.1259D-13
6060707.00	21.323	0.1507D 03	0.7597D-02	0.1776D-05	0.2484D-09	0.1414D-13
6080909.00	18.010	0.1493D 03	0.5654D-02	0.1065D-05	0.1262D-09	0.6336D-14
6080917.00	16.353	0.1483D 03	0.6495D-02	0.1393D-05	0.1833D-09	0.9961D-14
6081717.00	14.698	0.1488D 03	0.7379D-02	0.1742D-05	0.2443D-09	0.1386D-13
6090909.00	14.907	0.1492D 03	0.5737D-02	0.1084D-05	0.1282D-09	0.6406D-14
7070909.00	10.459	0.1482D 03	0.7099D-02	0.1605D-05	0.2190D-09	0.1222D-13
7090909.00	8.498	0.1489D 03	0.6958D-02	0.1527D-05	0.2028D-09	0.1107D-13
8080816.00	14.568	0.1514D 03	0.6010D-02	0.1178D-05	0.1433D-09	0.7339D-14
8081313.00	15.827	0.1505D 03	0.6743D-02	0.1431D-05	0.1851D-09	0.9906D-14
8090916.00	11.166	0.1488D 03	0.7031D-02	0.1556D-05	0.2073D-09	0.1131D-13
8161717.00	10.044	0.1479D 03	0.8671D-02	0.2220D-05	0.3251D-09	0.1889D-13
9090915.00	15.220	0.1492D 03	0.7811D-02	0.1840D-05	0.2542D-09	0.1425D-13
9091111.00	12.416	0.1462D 03	0.1103D-01	0.3079D-05	0.4704D-09	0.2810D-13
9091616.00	9.634	0.1489D 03	0.8108D-02	0.1960D-05	0.2755D-09	0.1557D-13
11111717.00	10.590	0.1454D 03	0.1163D-01	0.3352D-05	0.5215D-09	0.3146D-13
15151515.00	12.320	0.1510D 03	0.9896D-02	0.2590D-05	0.3745D-09	0.2170D-13
15171717.00	10.038	0.1483D 03	0.1001D-01	0.2734D-05	0.4131D-09	0.2448D-13
16161717.00	8.382	0.1480D 03	0.9684D-02	0.2605D-05	0.3904D-09	0.2299D-13
101010106.00	17.019	0.1886D 03	0.3786D-02	0.2398D-06	0.4969D-11	0.1368D-14
101010114.00	13.329	0.1881D 03	0.5422D-02	0.6785D-06	0.4887D-10	0.1207D-14
101040808.00	19.626	0.1930D 03	0.5103D-02	0.5837D-06	0.3864D-10	0.8844D-15
505080808.00	28.019	0.2006D 03	0.9320D-02	0.2041D-05	0.2732D-09	0.1504D-13
609090909.00	19.911	0.2028D 03	0.8550D-02	0.1624D-05	0.1968D-09	0.1000D-13
617171717.00	13.406	0.2024D 03	0.1229D-01	0.3173D-05	0.4672D-09	0.2723D-13
707080808.00	19.793	0.2522D 03	0.1214D-01	0.2646D-05	0.3521D-09	0.1932D-13
808090916.00	18.367	0.2021D 03	0.8955D-02	0.1843D-05	0.2330D-09	0.1225D-13
909090914.00	24.676	0.2024D 03	0.1022D-01	0.2316D-05	0.3130D-09	0.1720D-13
909090916.00	13.344	0.2011D 03	0.1026D-01	0.2322D-05	0.3135D-09	0.1724D-13
1417171717.00	16.323	0.2017D 03	0.1327D-01	0.3548D-05	0.5309D-09	0.3120D-13
10101010606.00	23.067	0.2382D 03	0.6007D-02	0.6428D-06	0.3609D-10	0.3636D-15
10103030808.00	20.465	0.2409D 03	0.1108D-01	0.2395D-05	0.3206D-09	0.1782D-13
10108081111.00	18.921	0.2414D 03	0.1333D-01	0.3251D-05	0.4689D-09	0.2721D-13

TABLE 5

Opacity Sources in SAM1

The opacity sources available in our standard version of SAM1 are the same as those given by Kurucz (1970). Improved opacity subroutines are available and will be described in a later publication. The opacity edges for these sources are given in Table 6, p.62.

i) H1
Bound-free and free-free opacity of atomic hydrogen. Eight bound levels are explicitly included.

ii) H2PLUS
Bound-free and free-free opacity of H_2^+.

iii) HMINUS
Bound-free and free-free opacity of H^-.

iv) HRAY
Rayleigh scattering from atomic hydrogen.

v) HE1
Bound-free and free-free opacity of atomic helium. Eleven bound levels are explicitly included.

vi) HE2
Bound-free and free-free opacity of He^+. Nine bound levels are explicitly included.

vii) HEMINUS
Free-free opacity of He^-.

viii) HERAY
Rayleigh scattering from atomic helium.

ix) COOL

This includes the free-free and bound-free opacity from the lowest levels of Mg and Si, and the bound-free opacity from the lowest levels of C, Al. As is suggested by the name, these opacity sources are significant for fairly cool atmospheres, i.e. $T_{eff} \leq 10000\ ^{o}K$.

x) LUKE

This includes the free-free and bound-free opacity from the lowest levels of Si^{+} and Ca^{+}, and the bound-free of N, O, Mg^{+}. These opacities are significant for 'warm atmospheres', i.e. $10^{4} \leq T_{eff} \leq 3 \times 10^{4}\ ^{o}K$.

xi) HOT

This includes bound-free opacities for the lowest levels of C^{+} to C^{3+}, N^{+} to N^{4+}, O^{+} to O^{5+}, Ne to Ne^{5+}. These all fall in the Lyman continuum of hydrogen and consequently are only important at temperatures high enough for the Lyman continuum to be somewhat transparent.

xii) ELECTRON

The opacity due to isotropic electron scattering.

xiii) H2RAY

Rayleigh scattering from the hydrogen molecule.

xiv) HLINES

This opacity source is an approximation to the stark-broadened hydrogen line opacity, it only simulates the effect of the lines on the continuum and should not be used to calculate detailed line profiles. It approximates the lines from all levels up to n=4, and also includes a pseudo-continuum term to allow for the effect of overlapping lines as you approach the series limit.

xv) to xx) The remaining opacity subroutines are in fact dummy subroutines which are provided to allow the user to define his own opacity subroutines and use them in SAM1 without having to change major parts of the program. For details of how to do this the user should refer to Kurucz (1970) and Wright and Argyros (1975).

TABLE 6

TABLE OF ABSORPTION EDGES

The following table represents a list of the absorption edges which it is possible to use in SAM1. The tabulation has been done for monotonically decreasing wavelength. The following notation has been used:

Following each entry there appears one of the three letters l, i, h or a blank. If it is a blank, the entry is either for hydrogen or helium; for any other entry:

l=low temperature absorption edge;
i=intermediate temperature edge;
h=high temperature absorption edge.

In the column labelled Level, the entry represents the level from which the corresponding photoionization occurs. Normally this produces the next ionization stage in its ground state. If a photoionization process produces the next ionization stage in one of its excited states then the term corresponding to that state is printed in parentheses, e.g.:

Ne II $2p^5\ ^2p$ ($2p^4\ ^1s$) etc.

Atomic Species	Level	Absorption Edge Frequency	Wavelength (nanometres)	
H I	6s	9.1334694E 13	3282.35	
H I	5s	1.3152200E 14	2279.41	
H I	4s	2.0550303E 14	1458.32	
He I	$3p\ ^1P$	3.6279965E 14	826.33	
H I	3s	3.6533851E 14	820.59	
He I	$3d\ ^3D + 3d\ ^1D$	3.6589954E 14	819.33	
He I	$3p\ ^3P$	3.8209962E 14	784.59	
He I	$3s\ ^1S$	4.0309959E 14	743.72	
Mg I	$3d\ ^3D$	4.1113494E 14	729.13	l
Mg I	$4p\ ^3P$	4.1440958E 14	723.42	l
He I	$3s\ ^3S$	4.5139955E 14	663.41	
Mg I	$3d\ ^1D$	4.5772084E 14	654.97	l
Si I	$3d\ ^3P$	4.6135099E 14	649.11	l
Si I	$4p\ ^1D$	4.7216401E 14	634.93	l
Si I	$3d\ ^3F$	4.7386443E 14	632.65	l
Si I	$4p\ ^3D$	5.3295900E 14	562.51	l
Si I	$3d\ ^1D$	5.5723899E 14	538.00	l
Mg I	$3p\ ^1P$	7.9804009E 14	375.55	l
He I	$2p\ ^1P$	8.1464980E 14	368.00	
H I	2s	8.2201245E 14	364.71	
Si II	$5p\ ^2P$	8.3824984E 14	357.64	i
He I	$2p\ ^3P$	8.7606971E 14	342.20	
Si II	$4d\ ^2D$	9.2378921E 14	324.52	i
He I	$2s\ ^1S$	9.6024973E 14	312.20	
He I	$2s\ ^3S$	1.1525993E 15	260.10	
Mg I	$3p\ ^3P$	1.1925795E 15	251.33	l
Al I	$3p\ ^2P$	1.4429998E 15	207.76	l
Si I	$3p^2\ ^1S$	1.5152918E 15	197.84	l
Si II	$4p\ ^2P$	1.5171537E 15	197.60	i
Si II	$3d\ ^2D$	1.5736320E 15	190.51	i
Si I	$3p^2\ ^1D$	1.7379678E 15	167.67	l
Mg I	$3s^2\ ^1S$	1.8488508E 15	162.13	l
Si I	$3p^2\ ^3P$	1.9723150E 15	152.00	l
C I	$2p^2\ ^1S$	2.0760986E 15	144.40	l
Ca II	$4p\ ^2P$	2.1107789E 15	142.03	i
C I	$2p^2\ ^1D$	2.4195985E 15	123.90	l
Ca II	$3d\ ^2D$	2.4601269E 15	121.86	i
Mg II	$3p\ ^2P$	2.5643059E 15	116.91	i
N I	$2p^3\ ^2P$	2.6533170E 15	112.99	i
C I	$2p^2\ ^3P$	2.7253983E 15	110.00	l

TABLE 6 cont.

Atomic Species	Level	Absorption Edge Frequency	Wavelength (nanometres)	
Ca II	4s ²S	2.8704539E 15	104.44	i
N I	2p³ ²D	2.9415340E 15	101.92	i
O I	2p⁴ ³P	3.2890495E 15	91.18	i
H 1	1s	3.2890495E 15	91.18	
N I	2p³ ⁴S	3.5179148E 15	85.22	i
Mg II	3s ²S	3.6354920E 15	82.45	i
Si II	3p ²P	3.9466718E 15	75.96	i
C II	2p ²P (2p ³P)	4.1499448E 15	72.24	a
C II	2p² ²S (2p ³P)	4.5743377E 15	65.54	h
C II	2p² ²D (2p ³P)	5.2207690E 15	57.42	h
Ne I	2p⁶ ¹S	5.2223066E 15	57.41	h
C II	2p ²P	5.8325749E 15	50.38	h
He I	1s² ¹S	5.9446943E 15	50.43	
C II	2p² ⁴P (2p ³P)	6.1770220E 15	48.53	a
N II	2p² ¹S	6.1810592E 15	48.50	h
N II	2p² ¹D	6.7118756E 15	44.73	h
N II	2p² ³P	7.1583790E 15	41.33	h
O II	2p³ ²P	7.2344879E 15	41.15	h
O II	2p³ ²D	7.6936003E 15	38.97	h
O II	2p³ ²P (2p² ¹D)	7.8859508E 15	38.02	h
O II	2p³ ²D (2p² ¹D)	8.2350765E 15	36.14	h
O II	2p³ ⁴S	8.4376830E 15	35.28	a
C III	2p ¹P	8.5099623E 15	35.23	a
O II	2p³ ²P (2p² ¹S)	8.5728535E 15	34.97	a
Ne II	2p⁵ ²P	9.9063676E 15	30.25	a
C III	2p ³P	1.0006926E 16	29.95	h
N III	2p² ²D (2p ³P)	1.0450775E 16	28.66	h
Ne II	2p⁵ ²P (2p⁴ ¹D)	1.0671508E 16	28.09	a
N III	2p ²P	1.1867335E 16	25.14	h
Ne II	2p⁵ ²P (2p⁴ ¹S)	1.1568125E 16	25.92	h
C III	2s² ¹S	1.1578390E 16	25.89	h
N III	2p² ⁴P (2p ³P)	1.1772192E 16	25.47	h
O III	2p² ¹S	1.1988136E 16	25.01	a
O III	2p² ¹D	1.2075028E 16	23.65	h
O III	2p² ³P	1.3276487E 16	22.53	h
O III	2p³ ⁵S (2p² ⁴P)	1.3514655E 16	22.02	h
C IV	2s ²S	1.3659315E 16	21.95	h
N IV	2p ¹P	1.4614807E 16	20.24	a
Ne III	2p⁴ ¹S (2p³ ²P)	1.4900315E 16	20.12	h
Ne III	2p⁴ ³P	1.5333888E 16	19.55	h
C IV	2s ²S	1.5594515E 16	19.22	h
Ne III	2p⁴ ¹D (2p³ ²D)	1.5796877E 16	18.98	a
Ne III	2p⁴ ¹D (2p³ ²P)	1.6432047E 16	18.24	h
Ne III	2p⁴ ³P (2p³ ²D)	1.6582077E 16	18.10	h
N IV	2p ³P	1.6714007E 16	17.94	a
Ne III	2p⁴ ³P (2p³ ²P)	1.7197247E 16	17.43	h
O IV	2p² ²D (2p ³P)	1.7378387E 16	17.25	h
O IV	2p ²P	1.8710785E 16	16.02	a
N IV	2s² ¹S	1.8732977E 16	16.00	h
O IV	2p² ⁴P (2p ³P)	1.9035965E 16	15.75	h
Ne IV	2p⁴ ⁴P (2p³ ⁵S)	2.0607378E 16	14.55	a
N V	2p ²P	2.1254917E 16	14.10	h
Ne IV	2p³ ²P	2.1526084E 16	13.86	h
Ne IV	2p³ ²D	2.2261266E 16	13.47	h
Ne IV	2p³ ²P (2p² ¹D)	2.2511624E 16	13.32	h
O V	2p ¹P	2.2730004E 16	13.16	h
Ne IV	2p³ ²D (2p² ¹D)	2.3176777E 16	12.94	a
Ne IV	2p³ ⁴S	2.3489455E 16	12.76	h
Ne IV	2p³ ²P (2p² ¹S)	2.3519103E 16	12.75	h
N V	2s ²S	2.3697248E 16	12.67	h
O V	2p ³P	2.5075436E 16	11.95	h
O V	2s² ¹S	2.7540645E 16	10.89	h
Ne V	2p² ¹S	2.8648480E 16	10.45	h
Ne V	2p² ¹D	2.9655976E 16	10.11	h
Ne V	2p² ³P	3.0541504E 16	9.82	h
Ne V	2p³ ⁵S (2p² ⁴P)	3.0851403E 16	9.72	h
O VI	2s ²S	3.3396863E 16	8.98	h
Ne VI	2p ²P	3.8167504E 16	7.85	h

Appendix III

Job Control Cards

This Appendix gives all the information required for running SAM1 and its associated programs at the University of London (correct as of May 1975). Users who are interested in the implementation of the program should refer to Wright and Argyros (1975). The first section of the Appendix gives details about the Input/Output files required by the programs, the second section gives the Job Control Cards that are needed to run the programs on the IBM 360/65 of the University College London Computer Centre, and the third gives the Job Control Cards required to run the programs on the CDC 6600 of the University of London Computer Centre.

In order to clearly distinguish between the letter O and the number zero, we have put a slash through every zero.

III.1 I/O file usage

Unit Number	Normal usage
5	punched card input to the programs
6	lineprinter output from the programs
7	punched card output from the programs
1Ø	scratch disk file needed by SAM1
11	" " " " " "
12	disk file for SAM1 restart data
13	" " " " " "

The procedure that SAM1 uses for storing the restart data is as follows: On the first iteration the restart data is written to unit 12, which is then rewound. The restart data for the next iteration is written to unit 13, which is then rewound. This process of writing the data alternately to units 12 and 13 continues until the Job terminates. This system ensures that under any eventuality, e.g. a System crash, or the Job time allocation is exceeded, the user can restart the calculation from the last, or last but one iteration.

III.2 IBM Job Control Cards

a) SAM1

```
 i)      //jbnumber JOB (17Ø,SAM1,t,l,c), 'heading'
 ii)     //ONE EXEC GO,PROG=UCAQØ35A,LIB=UCPGMLIB
 iii)    //G.FTØ7FØØ1  DD SYSOUT=B
 iv)     //G.FT1ØFØØ1 DD UNIT=DRUM,SPACE=(CYL,(5,1)),
 v)      //  DCB=(RECFM=VS,BLKSIZE=81Ø)
 vi)     //G.FT11FØØ1 DD UNIT=DRUM,SPACE=(CYL,(5,1)),
 vii)    //  DCB=(RECFM=VS,BLKSIZE=81Ø)
 viii)   //G.FT12FØØ1 DD UNIT=devtype,VOL=SER=vname,DSNAME=dname,
 ix)     //  DISP=OLD,DCB=(RECFM=FB,LRECL=8Ø,BLKSIZE=88Ø)
 x)      //G.FT13FØØ1 DD UNIT=dectype,VOL=SER=vname,DSNAME=dname,
 xi)     //  DISP=OLD,DCB=(RECFM=FB,LRECL=8Ø,BLKSIZE=88Ø)
 xii)    //G.SYSIN DD *
                              :
                        SAM1 control cards
                              :
 xiii)   /*
 xiv)    //
```

On card i), jbnumber should be replaced by the users Job number, t is the time requested in minutes and seconds in the format MM.SS or just MM, l is the number of lines requested in thousands, c is the number of punched cards requested, heading can be replaced by up to twenty characters. If the user does not want the output from unit 7 on punched cards, he can replace card iii) with an appropriate DD card. Cards iv) to vii) define the scratch data files for units 1Ø and 11. Cards viii) to xi) define the disk files for units 12 and 13 assuming they have already been created. Some resident system disk space is available for storage of users data with certain restrictions (see Kennington, 1975), it is very convenient to use this for storing the restart data files. To do this, replace devtype by 2314, replace vname by 4CØØ2, and replace dname by a valid user Job number. These files can be created with the following Job step:

```
//NULL EXEC NULL
//ALLOC DD UNIT=2314,VOL=SER=4CØØ2,DSNAME=dname1,
//  DISP=(NEW,KEEP),SPACE=(TRK,3)
//ALLOC DD UNIT=2314,VOL=SER=4CØØ2,DSNAME=dname2,
//  DISP=(NEW,KEEP),SPACE=(TRK,3)
```

These cards can go immediately after the JOB card i), or can be run as a separate Job.

The time taken for a model calculation depends on a large number of parameters (number of iterations, number of frequencies, opacity sources included etc.), therefore a feel for the parameters required on the JOB card can only be gained by experience. A suitable JOB card for running the sample model discussed in section 2.1 would be:

```
//jbnumber JOB (17Ø,SAM1,7,2,3ØØ),'SAM1 SAMPLE MODEL'
```

b) FRESET

```
 i)    //jbnumber JOB (12Ø, FSET,t,l,c), 'heading'
 ii)   //ONE EXEC GO,PROG=UCAQØ358,LIB=UCPGMLIB
 iii)  //G.FTØ7FØØ1 DD SYSOUT=B
 iv)   //G.SYSIN DD *
                          :
                  data for FRESET
                          :
 v)    /*
 vi)   //
```

Suitable parameters for running FRESET to obtain the information required for the sample model would be : t=ØØ.1Ø , l=1 , c=5Ø.

c) OPTAB

```
 i)    //jbnumber JOB (17Ø,OTAB,t,l,c), 'heading'
 ii)   //ONE EXEC GO,PROG=UCAQØ359,LIB=UCPGMLIB
 iii)  //G.FTØ7FØØ1 DD SYSOUT=B
 iv)   //G.SYSIN DD *
                          .
                  data for OPTAB
                          .
 v)    /*
 vi)   //
```

III.3 CDC Job Control Cards

a) SAM1

```
 i)      JOB(jbnumbr, Jj,M66ØØ,LC1,Tt,PCc)
 ii)     ATTACH(SAM1,SAM1,ID=UCAQØ34)
 iii)    ATTACH(TAPE14,pfname1)
 iv)     ATTACH(TAPE15,pfname2)
 v)      REQUEST(TAPE12,*PF)
 vi)     REQUEST(TAPE13,*PF)
 vii)    RFL(141ØØØ)
 viii)   SAM1.
 ix)     SYS(EXIT)
 x)      EXIT.
 xi)     CATALOG(TAPE12,pfname3)
 xii)    CATALOG(TAPE13,pfname4)
 xiii)   -EOR-
           :
         SAM1 control cards
           :
 xiv)    -EOR-
 xv)     -EOI-
```

On card i), jbnumbr should be replaced by the users Job number (note that 7 character Job numbers are used on the CDC machine, as opposed to 8 character job numbers on the IBM machine). The value of j depends on the system resources requested by the rest of the parameters on this card (see Williams and Manning, 1973). The parameters t,l,c are the time in seconds, the number of output lines, and the number of punched cards requested, respectively. Cards iii) and iv) are optional in the sense that they are only required if a run is to be continued using the restart data written by a previous run. Note that under the present permanent file system at ULCC it is not possible to make this data available on units 12 and 13. Therefore the data written to units 12,13 and CATALOGed with permanent file names pfname1 and pfname2 respectively in a previous run, are ATTACHed as shown; the restart data can then be read in using MODEL 14 or MODEL 15. Cards v) and vi) tell the system that the data written to logical units 12 and 13 (which have local file names TAPE12 and TAPE13 respectively) are to be saved as permanent

files. If the user does not wish to save the restart data then cards v), vi), and ix) to xii) inclusive can be omitted. Card vii) is required because of a bug in the CDC loader, and card viii) initiates execution of the program.

If at any time during the run a fatal error occurs, then execution will continue from card x). If the run is completed successfully then card ix) causes card x) to be skipped. Thus cards ix) and x) ensure that the system will execute cards xi) and xii) whether the run was successful or not. Cards xi) and xii) make the files TAPE12 and TAPE13 permanent, with permanent file names pfname3 and pfname4 respectively. The end of record indicator, card xiii) consists of a 7,8,9 punch in column one of a card, and must appear before the data set for the run. The end of information mark consisting of a 6,7,8,9 punch in column one of a card, ensures that the job is read in correctly. One of the better features of the operating system is that on any fatal error (including exceeding the time limit) an extra few seconds are given to the user, in which he can perform any operation starting at an EXIT. card. This is more than ample time to ensure that the restart data is made permanent as in this example.

The time taken for a model calculation depends on a large number of parameters, therefore a feel for the parameters required on the JOB card can only be gained by experience. A suitable JOB card for running the sample model calculation of section 2.1 is:

JOB(jbnumbr,J9,M66ØØ,LC2ØØØ,T1ØØ,PC3ØØ)

b) FRESET

```
 i)    JOB(jbnumbr,Jj,M66ØØ,LC1,Tt,PCc)
 ii)   ATTACH(FRESET,FRESET,ID=UCAQØ34)
 iii)  FRESET.
 iv)   -EOR-
         :
       data for FRESET
         :
 v)    -EOI-
```

The following Job card parameters should be sufficient for most cases: j=6, l=1ØØØ, t=5, PC2ØØ.

c) OPTAB

```
i)      JOB(jbnumbr,Jj,M66ØØ,LC1,Tt,PCc)
ii)     ATTACH(OPTAB,OPTAB,ID=UCAØØ34)
iii)    RFL(141ØØØ)
iv)     OPTAB.
v)      -EOR-
          :
        data for OPTAB
          :
vi)     -EOI-
```

Parameters for a typical run would be : j=9 , l=1ØØØ , t=12Ø , c=4ØØ

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