PL-TR-94-2196

INFRARED PLASMA EMISSIONS

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31 May 1994

Final Report
20 November 1989 - 31 May 1994

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Directorate of Geophysics
AIR FORCE MATERIEL COMMAND
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REPORT DOCUMENTATION PAGE

Form Approved OMB No. 0704-0188

1. AGENCY USE ONLY *(Leave blank)*	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	31 May 1994	Final (20 November 1989-31 May 1994)

4. TITLE AND SUBTITLE

Infrared Plasma Emissions

5. FUNDING NUMBERS

PE: 61102F
PR: 2310 TA G4 WU CC
Contract:
F19628-90-C-0025

6. AUTHOR(S)

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7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

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8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)

Phillips Laboratory
29 Randolph Road
Hanscom AFB, MA 01731-3010
Contract Manager: Dean Kimball/GPOS

10. SPONSORING/MONITORING AGENCY REPORT NUMBER

PL-TR-94-2196

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT

Approved for public release; distribution unlimited

12b. DISTRIBUTION CODE

13. ABSTRACT *(Maximum 200 words)*

In this final report, we present the infrared spectrum of a laser-produced oxygen plasma. We have focused on extending the spectral range of observation of OI Rydberg emissions to 13 μm. We report the first observations of OI Rydberg line emission in the 8-13 μm wavelength region. We also present observations of Bremsstrahlung emission that compare favorably with recent theoretical results of Lin.

We have developed a model called APOSTLE which predicts the line-broadened emission spectrum from an OI plasma. We describe the theoretical and functional basis for the model. The model results are discussed and compared with the data obtained in the plasma experiment.

14. SUBJECT TERMS				15. NUMBER OF PAGES
Plasma	Infrared	Emissions	Rydberg	128
Laser	Stark Broadening		Bremsstrahlung	16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
Unclassified	Unclassified	Unclassified	SAR

CLASSIFIED BY:

DECLASSIFY ON:

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Preface

This final scientific report summarizes work performed for the period November 1989 to March 1994 under PL contract no. F-19628-90-C-0025. The objective of this contract was to enhance our understanding of nuclear induced atmospheric plasma processes which give rise to optical and infrared radiation emission which can impact target discrimination capabilities of surveillance acquisition and tracking systems. This objective was achieved through (1) the benchmarking of Defense Nuclear Agency's EGG-22 plasma emission code against experimental observations and recent theoretical continuum emissivity coefficients and (2) the development of the APOSTLE spectral line broadening model.

In 1980, the Air Force Phillips Laboratory (then the Geophysics Laboratory) initiated an investigation into the spectral characteristics of atmospheric plasmas. The first results were reported in Applied Optics[1]. It became clear with the early results that theoretical treatments for spectral line broadening in a plasma was not well developed. Thus, we developed the APOSTLE (Atmospheric Plasma Optical Spectral-Temporal Line Emission) code to describe the spectral emission characteristics of the plasmas. This code was developed in parallel with the experimental program and thus is well benchmarked against data. While subtle differences between the code predictions and the data persist, the overall agreement is excellent.

1. INTRODUCTION

The study of recombining laser-produced plasmas plays an important role in understanding the chemical dynamics and temporal behavior in ion-electron recombination processes in the disturbed upper atmosphere. During these processes, atomic oxygen is expected to be the strongest emitter since N^+ will charge transfer with O due to its lower ionization energy. This charge transfer will then result in a persistence of a high O^+ density for which recombination and radiative decay become important.

There have been few infrared spectroscopy studies of laser-produced atmospheric plasmas. Initial experiments[1] demonstrated that laser-produced plasmas can be used to achieve very high levels of atomic excitation. Additionally, laser produced plasmas have been shown to be strong sources of bremsstrahlung radiation.[1,2]

Spectral investigation of these plasmas began as early as 1964[3] and most of the work since then has been in the visible region.[2] In previous infrared studies , Laurie and Baird[4] and Lurie *et al.*[5] reported observations of IR line emission in the spectral range 1.80-3.10 μm and 5.7-7.5 μm from high-lying OI states (Rydberg) in a laser-produced recombining oxygen plasma. The observed OI spectral lines, particularly near 7.45 μm, were unusually broad (0.04-0.17 μm) and originated from Rydberg states with the principal quantum number between 3 and 6. Brown *et al.*[6] measured OI transitions originating from n=6 and 7 by laser absorption spectroscopy occurring at wavelengths as long as 12.35 μm. Similarly, broad emission lines are observed by Winkelmann and Tilgner[7] for ArI at 4.6, 7.4, and 12.3 μm in an argon plasma jet. These studies suggest a large Stark broadening effect for the hydrogen states, which give rise to these inter-Rydberg IR transitions. Studies of the Rydberg line emissions of alkali and alkaline-earth atoms have shown that the Stark shifts increase in magnitude as the principal quantum number of the initial energy level of the Rydberg atom increases.[8] In other words, as the size of the electron shell increases, the bond between the optical electron and the core becomes weaker, resulting in greater influence of the external electric fields. For an oxygen plasma, OI transition probabilities have been calculated[9] for n=7-6 and 8-7 transitions near 12.35 and 19.1 μm, but there are no prior published measurements.

Collisional-Stark broadening of emission lines from a relaxing plasma has been examined by a combination of spectroscopic techniques and theoretical treatments. Line shape analysis provides determinations of charged particle density and radiative transfer characteristics in stellar atmospheres, laser fusion plasmas, and laboratory discharges.[10,11] There is excellent agreement between experiment and theory with respect to the Stark-broadened lines of atomic hydrogen and it

is common practice to seed laboratory plasmas with hydrogen to determine electron densities.[12,13] Konjevic and Roberts[14] and Konjevic *et al.*[15] have critically reviewed and tabulated the experimental data of Stark widths and shifts of spectral lines of non-hydrogenic atoms. These data are compared with the extensive theoretical calculations of Griem[10] for the lighter elements up to Ca (as well as Cs) and with results of Dimitrijevic and Konjevic[16] for some heavier elements. In general, the agreement with these semi-classical calculations[10,16] is within 20%. For some of the heavier elements, the discrepancies are larger.

Several experiments have tested the predictions of Stark broadening theories for some plasma-broadened neutral oxygen lines.[17,18,19,20,21,22,23,24] Plasma sources used in these investigations include well-stabilized arcs, a gerdin-type generator, shock tubes, and RF discharges. For these LTE (local thermodynamic equilibrium) plasmas, the electronic temperature of the radiator is determined typically from absolute line intensity measurements and ranges from 10,000 K to 14,000 K. The electron density is in the range of $(1\text{-}10)\times10^{16}$ cm^{-3} from H_β line width measurements. There is generally good agreement (within 30%) between the experimental and calculated line widths and shifts. The comparisons for oxygen (OI) and other neutral atoms are almost entirely for spectral lines emitted in the near-UV and visible. There is little information available on Stark broadening of infrared spectral lines. Though, line widths and shifts have been measured for several ArI, NI, and SI lines in the near-IR, λ=1-2μm.[21,22,23,24,25,26,27] Typically these line widths are poorly predicted by theory. Stark broadening parameters have been calculated[11] for other non-hydrogenic atoms, particularly for isolated spectral lines of He and Na and for longer wavelengths,[28] but there are no experimental data with which to compare. Laboratory measurements of atomic oxygen emission line profiles between 1 and 3 μm have been made by Assous[21] at an electron density of about 3×10^{16} cm^{-3} in an induction-heated oxygen plasma. The experimentally determined line widths and shifts are in poor to good agreement with different calculations depending on the theoretical method used. Baird and Alexiou[29,30] have performed Stark line broadening calculations for high angular momentum states of atomic oxygen, principally the n=6 to 5 transitions near 7.45 μm. These semi-classical calculations were used to investigate the sensitivity of the OI line widths to electron densities and temperatures.

The determinations of Stark electron-broadening parameters by existing semi-classical[31,48,32,33,34] or fully quantum mechanical[34,35,36] theoretical methods generally require heavy computational demands even for single line calculations. A large number of atomic inter-Rydberg transitions and nearby perturbing levels are required to calculate plasma broadened IR spectral line emission. To

interpret these data, an efficient, yet accurate, calculation method is needed. Due to the lack of Stark broadening parameters for OI IR transition with $\lambda > 2$ μm, a modified version of present theoretical methods is used to predict the IR spectrum of laser-produced oxygen plasma. First, the Anderson formalism[37] is used to produce an efficient model of electron collisional broadening. The impact approximation model is then coupled to a quasi-static model of Hooper[38] to account for ion collisional broadening. While previous efforts have concentrated in the visible and near-IR region of the spectrum, the present study predicts spectra over a wide spectral range. With increasing levels of approximation within the model one can obtain Stark broadened spectra over a large spectral range with decreasing computational demands.

In this final report we present the infrared spectrum of a laser-produced oxygen plasma. We have focused on extending the spectral range of observation of OI Rydberg emission to 13 μm. We report here the first observations of OI Rydberg line emission in the wavelength region 8-13 μm. Additionally, we present observations of Bremsstrahlung radiation that compare favorably in shape and magnitude with recent theoretical emissivity coefficients by Lin[39] for free-free transitions in the field of a neutral oxygen atom. The data are also compared to the continuum theories of John and Williams[40] and Geltman[41] as well as the empirical values of Taylor and Caledonia.[42]

We have developed a model to predict the plasma OI line emission spectrum. We describe here the theoretical basis and the functionality of the model. The line emission model is used in conjunction with Lin's[39] emissivity coefficients to characterize the plasma conditions. These results are compared to the data and discussed in the rest of this report. In Chapter 2, the issues addressed under this contract are described. In Chapter 3, the experimental apparatus used in this study is described and procedures for data reduction is outlined. The observations are presented in Chapter 4. In Chapters 5 and 6, we present the validation of EGG-22 through comparison with Lin's emissivity coefficients and we describe the APOSTLE line emission model. The results of line and continuum emission modelling are compared with the data in the Chapter 7. Finally, a user's manual for the model is included in Appendix A. In Appendix B, we list the source code and in Appendix C, we list APOSTLE predicted line positions and Einstein coefficients.

2. LINUS ISSUES

Previous work on the LINUS project motivated the need to extend the spectral range of observation to validate existing plasma radiance models. The extended range allowed us to investigate more completely the behavior of continuum emission from a laser produced oxygen plasma. This investigation was parallel to the development of new emissivity coefficients for electron-neutral collisions for atomic oxygen. The data reported herein is in good agreement with these new coefficients and provided benchmarking for the EGG-22 plasma radiance model.

The literature review also revealed a lack of information on the subject of collisional-Stark broadening of OI infrared lines. Thus we developed a computationally efficient model of collisional Stark broadening of line emissions from atomic oxygen within a laser-induced plasma. The model is based on a combination of earlier theories of Stark broadening and is in good agreement with previous experimental and theoretical works. The model was used to generate spectra for a wide range of parameters. The comparison of the many numerically computed spectra and the experimentally measured spectral emissions provided estimates of OI electronic temperature and electron density and temperature. Finally, application of the model to the LWIR region of the OI spectrum shows Stark broadening effects from collisional broadening in lower density plasmas ($N_e \sim 10^{13}$ cm^{-3}).

The goal of this investigation was to validate the EGG-22 plasma radiance model. The data presented in this final report was acquired using the LINUS experiment at Phillips laboratory. In particular, the issues addressed in this contract were

1. Parametric Issues: The parameters used to characterize the plasma conditions are O-atom density, electron density, electron temperature, and emitter electronic temperature. The electronic temperature is derived from the continuum subtracted spectrum. In conjunction with Saha equilibrium, the simultaneous fit of the continuum and line emission models give the best parameter estimates that describe the plasma conditions.

2. Thermalization issues: OI Ryderg states are collisionally coupled when there are a sufficient number of thermalizing collisions. State populations are measured in the observed line emission spectrum. Complete Local thermodynamic equilibrium (LTE) is not expected to occur in the plasma but Saha equilibrium is expected. Spectral calculations were performed

using the ARCHON chemical kinetics code to model state populations of a recombination model where deviations from equilibrium are expected.

3. Validation of EGG22: The EGG-22 plasma radiance model is compared with lin's theoretical emissivity coefficients for *e*-O collisional interactions. These new coefficients are also compared to data and to previous theories.

4. LWIR line emission observation: We have extended the spectral of OI line emission observation to 13 μm. First observations of composite lines occurring at 10.4 and 12.35 are reported here.

3. EXPERIMENTAL

A. LINUS Experimental Platform

The apparatus used for this study is similar to that used by Lurie and Baird[4] and is illustrated in Figure 1. The apparatus was used to acquire a continuous infrared spectrum from 3.5-13.0 μm. The beam from a Quanta-Ray Nd:YAG laser (model DCR 1A, λ=1.064 mm, 10 ns fwhm multilongitudinal pulse, 10 Hz repetition rate) was propagated in the plane of the optical table, deflected vertically using a corner cube prism, and focused with a 51 mm focal length biconvex lens into a cubical cell fitted with uncoated ZnSe windows.

The radiation from the laser-produced plasma was collected at 90° to the laser beam axis and imaged onto the entrance slit of a 0.5 m f/6.9 grating monochromator (SPEX Industries Model 1870) using two 100 mm focal length uncoated ZnSe plano-convex lenses. Two gratings and three filters were used to cover the broad spectral range. The combinations are given in Table 1. The long-pass filters were used to block higher-order emissions.

Table 1. Gratings and interference filters used to acquire a continuous infrared spectrum across the spectral range 3.5-13.0 μm.

Spectral Region (μm)	Long-pass Filter (μm)	Grating
3.5-6.3	3.3	150 grooves/mm
6.3-8.0	6.1	150 grooves/mm
6.3-13.0	6.1	75 grooves/mm
8.0-13.0	8.8	75 grooves/mm

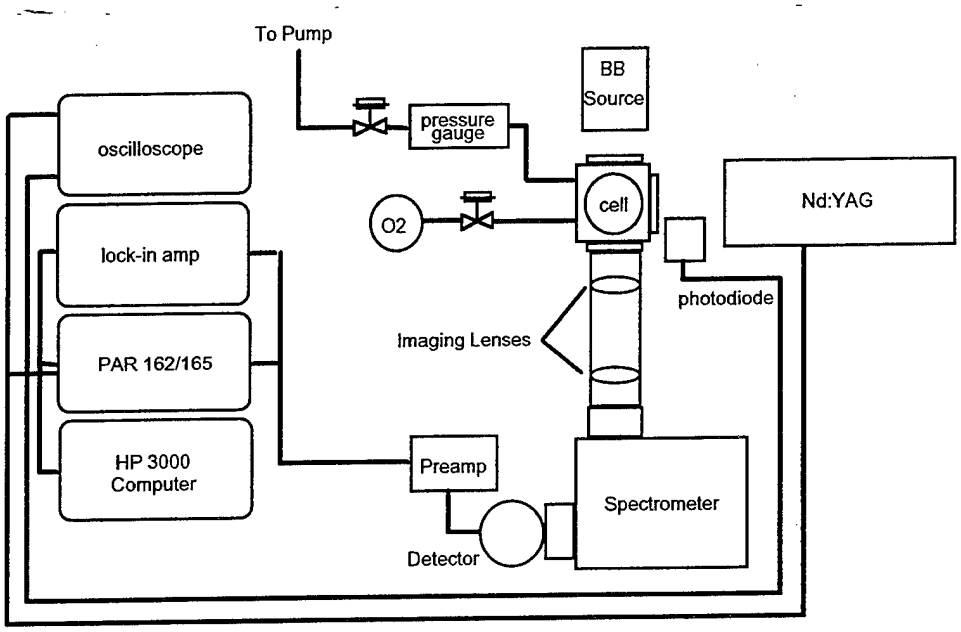

Figure 1. Experimental Apparatus used for acquisition of a continuous 3.5-13.0 μm emission spectrum from a laser produced oxygen plasma.

A liquid nitrogen cooled HgCdTe detector (Santa Barbara Research Center, 5 mm square element) operated in the photo conductive mode with a matched preamplifier (SBRC Model A110, 80 db voltage gain) was used to detect the infrared emissions. The detector is well suited for use in the spectral range 3-13 μm and has a detectivity of $\sim 10^{10}$ cm $Hz^{-1/2}$ W^{-1} near 6 μm yielding an estimated NESR of $\sim 10^{-6}$ W cm^{-2} sr^{-1} μm^{-1}. In the MWIR region (3.5-8.0 μm), the $4p^5$ P-$3d^5$ D transition near 6 μm has a signal-to-noise ratio of ~40. In the LWIR region (8.0-13.0 μm), the 10.4 μm line emission has a signal-to-noise ratio of ~15.

OI visible diagnostic information relating to energy deposition was monitored using a Hamamatsu photomultiplier tube fitted with a narrow band pass filter (20 nm) near 715.8 nm and a neutral density filter (O.D.=4.0). The line emission of interest in this window is the $3p'(^1D)$-$3s'(^1D^0)$ transition originating from a state with a Rydberg-like energy of 116631 cm^{-1} (Ionization potential = 109837 cm^{-1}). Stability of the 715.8 nm signal during all data acquisition ensured stable energy deposition.

In this study, the plasma was produced from 110 torr high purity O_2 (Matheson, 99.995%). A laser pulse energy of 780 mJ created an estimated intensity of $2x10^{13}$ W cm^{-2} in the focal plane. The resulting plasma emission region appeared cylindrically shaped and approximately 6 mm long and 2 mm in diameter. During all data acquisition, the entire optical path was enclosed in

plexiglass and purged with dry nitrogen to minimize CO_2 and H_2O absorption effects on the measured plasma emissions.

B. Data Acquisition and Reduction

Data acquisition was performed with a Princeton Applied Research model 162 boxcar averager operated in conjunction with a model 165 gated integrator using a 0.6 μs aperture duration. Fifty laser shots were averaged per wavelength increment. Measurements were taken with an aperture delay time of 20 μs. The output of the boxcar averager was sent to a HP Model 9000 series 310 computer which averaged 50 laser shots per wavelength increment.

The absolute spectral response of the system was determined with an Infrared Industries model 408 blackbody source operated at 1000°C where the signal processing of the blackbody emissions was done with a Stanford Research Systems lock-in amplifier. The wavelength accuracy of the system was calibrated using a HeNe laser in the sixth and higher orders.

Individual scans were recorded digitally on the HP computer and transfered to an IBM PC compatible computer at Mission Research Corporation. Information about the scan was recorded and used for the data reduction process. The spectral response of the system was then derived from a comparison of the observed blackbody emission spectra with the theoretical blackbody function. Figure 2 illustrates the optical path traversed by the emissions being studied.

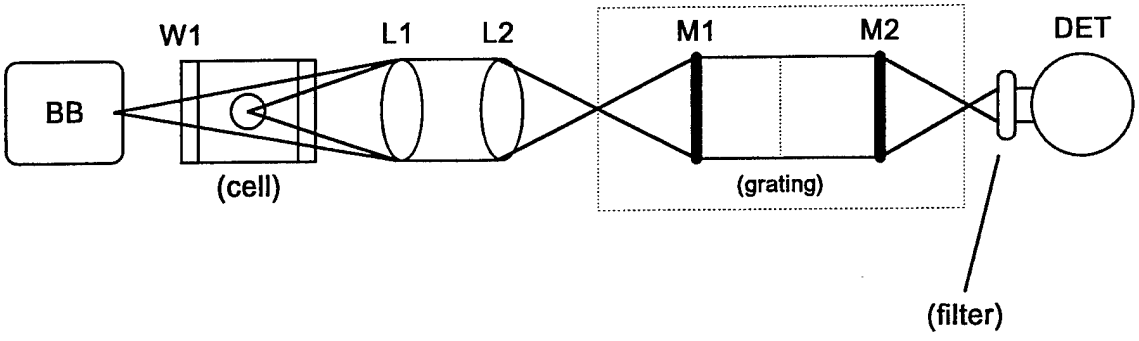

Figure 2. Optical path of emission in the experiment.

The measured voltage output of the detector (mV) for a given source spectral radiance, Φ (W cm^{-2} $sr^{-1}$$\mu m^{-1}$), is given by:[67]

$$S_p(\lambda) = R(\lambda) A_p \Omega_{L1} \frac{\Omega_{M1}\Omega_{DET}}{\Omega_{L2}\Omega_{M2}} T(\lambda) \int_{\lambda-\Delta\lambda}^{\lambda+\Delta\lambda} \Phi(\lambda) d\lambda \tag{1}$$

where,

R = Instrument Spectral Response,

$\Omega_{L1}, \Omega_{L2}, \Omega_{M1}, \Omega_{M2}, \Omega_{DET}$ = Solid angles subtended by mirrors 1 and 2, lenses 1 and 2, and the detector,

A_p = Apparent disk of the spark,

$T(\lambda)$ = Total transmittance excluding window 1.

Using the theoretical blackbody function, $N(\lambda,T)$, The spectral response is written as,

$$R(\lambda) = \frac{S_{BB}(\lambda)}{A_{BB}\Omega_{BB} \frac{\Omega_{M1}\Omega_{DET}}{\Omega_{L2}\Omega_{M2}} T^*(\lambda) N(\lambda,T) \Delta\lambda_{BB}(\lambda)} \tag{2}$$

where,

$T^*(\lambda) = T_{W1}(\lambda) T(\lambda)$ is the total transmittance including window 1,

$\int_{\lambda-\Delta\lambda}^{\lambda+\Delta\lambda} \Phi(\lambda) d\lambda \cong \Phi(\lambda) \Delta\lambda_p(\lambda)$ and $\Delta\lambda_p$ is the instrument resolution.

Substituting equation (28) into (27) yields the spectral radiance of the observed plasma emissions,

$$\Phi(\lambda) = \frac{A_B\Omega_B}{A_p\Omega_p} \frac{S_p(\lambda)}{S_B(\lambda)} \frac{\Delta\lambda_B(\lambda)}{\Delta\lambda_p(\lambda)} T_{W1}(\lambda) N(\lambda,T) = CalibrationFactor \frac{S_p(\lambda)}{\Delta\lambda_p(\lambda)} \tag{3}$$

4. OBSERVATIONS

Figure 3 shows the IR spectrum of the laser-produced oxygen plasma. The spectrum can be described by the spectral sum of continuum radiation and collisionally broadened line emission. The plasma consists of excited and ionized atoms and electrons which radiate and recombine to

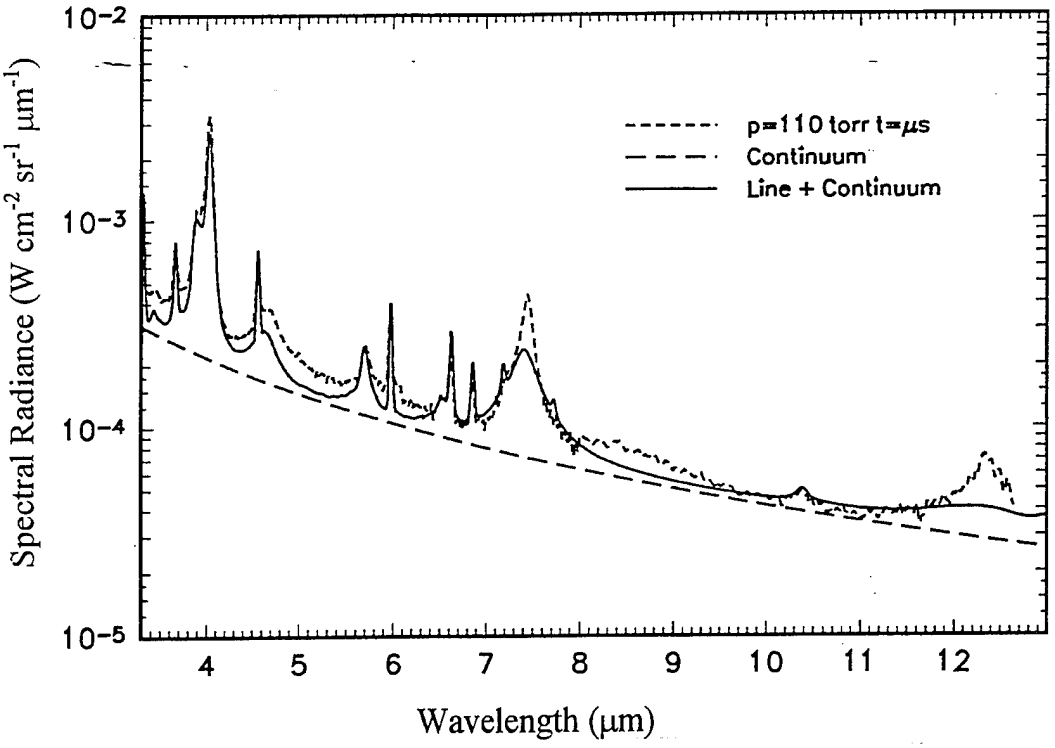

Figure 3. The short-dashed curve is the IR emission spectrum of the laser-produced oxygen plasma at an aperature time delay of 20 μs. The plasma was created from 110 torr O_2 and the measurement is of the center of the emission region. The medium-dashed curve is the continuum model and the solid curve is the sum of the continuum and line emission models.

form electronically excited neutral atomic oxygen. Initially (≤1 μs), infrared emission from the plasma is mostly recombination and continuum radiation which decreases rapidly as radiative and collisional relaxation processes progress. At 20 μs, the major species are O, O^+, and electrons with electron-to-neutral density ratio <1%.[43]

Significant continuum radiation persists throughout the plasma lifetime. Continuum radiation occurs through both electron recombination with ions (free-bound or recombination radiation), and electron collisions with ions and neutral atoms (free-free transitions or bremsstrahlung radiation). Since bremsstrahlung radiation from electron-neutral atom interactions is not a Coulombic process, the interaction is short-ranged. As such, bremsstrahlung radiation due to electron-atom interactions is expected to dominate only after ~10 μs; prior to this electron-ion interactions dominate. The observed continuum spectrum is modelled using a theory for free-free transitions in the field of a neutral which is superposed with the line emission component of the spectrum.

The infrared line emission spectrum is produced by inter-Rydberg state transitions. These states are populated by recombination and collisional processes. Initial studies of the thermal

equilibration time between electrons and atoms suggest that thermalization is achieved in approximately 6 μs.[43] Collisional coupling is then expected to occur for those Rydberg states within kT_e of the ionization potential. Consequently, Saha equilibrium is assumed to describe the Rydberg state population distribution. Emitter line profiles in a laser-produced plasma are broadened through the Stark effect by ions and collisions with electrons. Collisional-Stark broadening of spectral lines is significant even at low electron densities (10^{13} cm^{-3}). We developed a collisional-Stark broadening model to predict the line emission spectrum. The model is described in detail in Chapter 6 and only pertinent information is reviewed here. The line emission model predicts the spectrum using electron density, N_e, electron temperature, T_e, ion temperature, T_i, and emitter electronic temperature, T_{el}, as free parameters. For this study, we set $T_e = T_{el}$, where the empirically derived temperature was used in the spectral calculation.

We examine the characteristics of the plasma by simultaneously fitting continuum and line emission models to the observed spectrum. The parameters used to characterize the plasma conditions are O-atom density, electron density, electron temperature, and emitter electronic temperature. The electronic temperature is derived from the continuum subtracted spectrum. In conjunction with Saha equilibrium, the simultaneous fit of the continuum and line emission models give the best parameter estimates that describe the plasma conditions. These results are discussed below. The line emission model fitting is described in further detail in Chapter 7.

A. Line Emission

The continuum subtracted spectrum is shown in Figure 4. Table 2 is a listing of the line positions of the spectral features observed in the region 3.5 to 13 μm, their transition assignments, predicted Einstein coefficients and observed line widths. The observed transitions are illustrated in energy-level diagrams in Figure 5. It should be noted that the line widths are to be interpreted only qualitatively since there is a high degree of spectral blending.

The feature near 10.4 μm is given a composite line assignment dominated by $6d^5D$-$6p^5P$ and $5p^3P$-$4d^3D$. The broad feature near 12.35 μm occurs at the long wavelength edge of the detector responsivity and, therefore, the line shape of the feature is not entirely realized. This feature is predicted to be dominated by six transitions: 7 g,h,$i^{3,5}$ G,H,I -6f,g,$h^{3,5}$ F,G,H. This is the first reported observation of the 10.4 and 12.35 μm emission from a laser produced plasma.

We have examined the integrated intensities of 5 transitions in the spectrum that exhibit the least blending with other features for state population and electronic temperature determination.

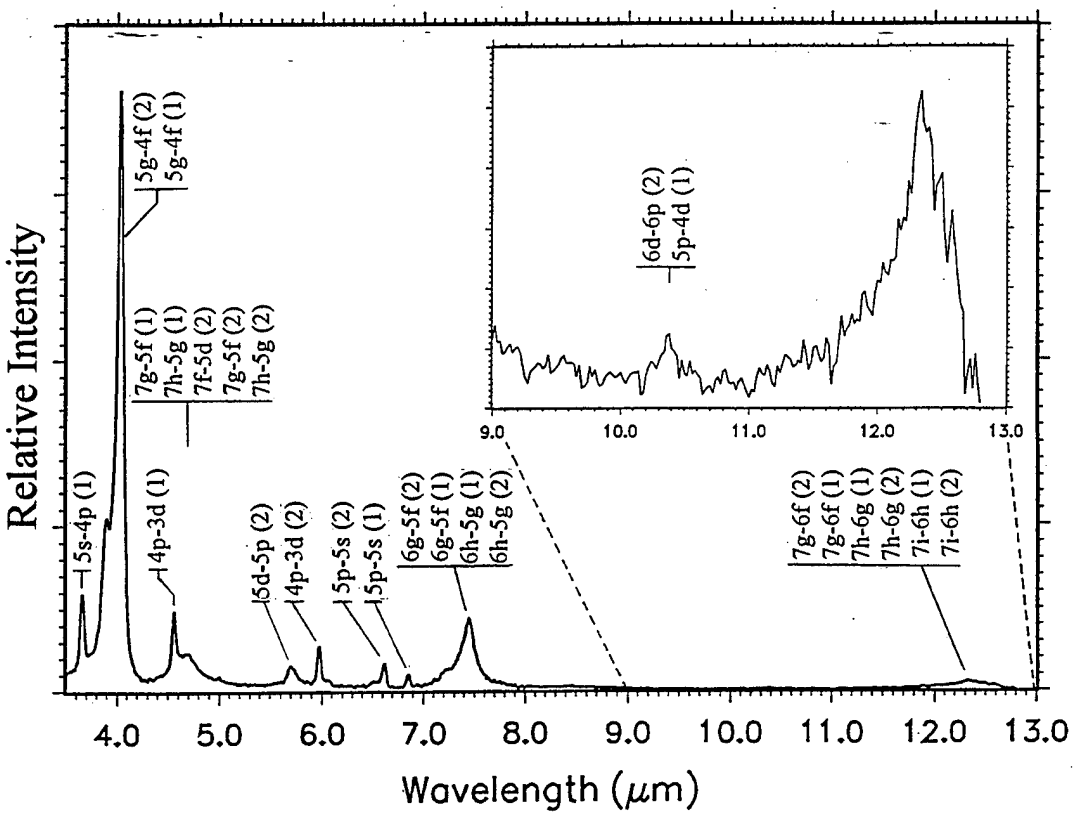

Figure 4. The OI line emission spectrum was obtained by subtracting the power law fit to Lin's emissivity coefficients shown in Figure 3.

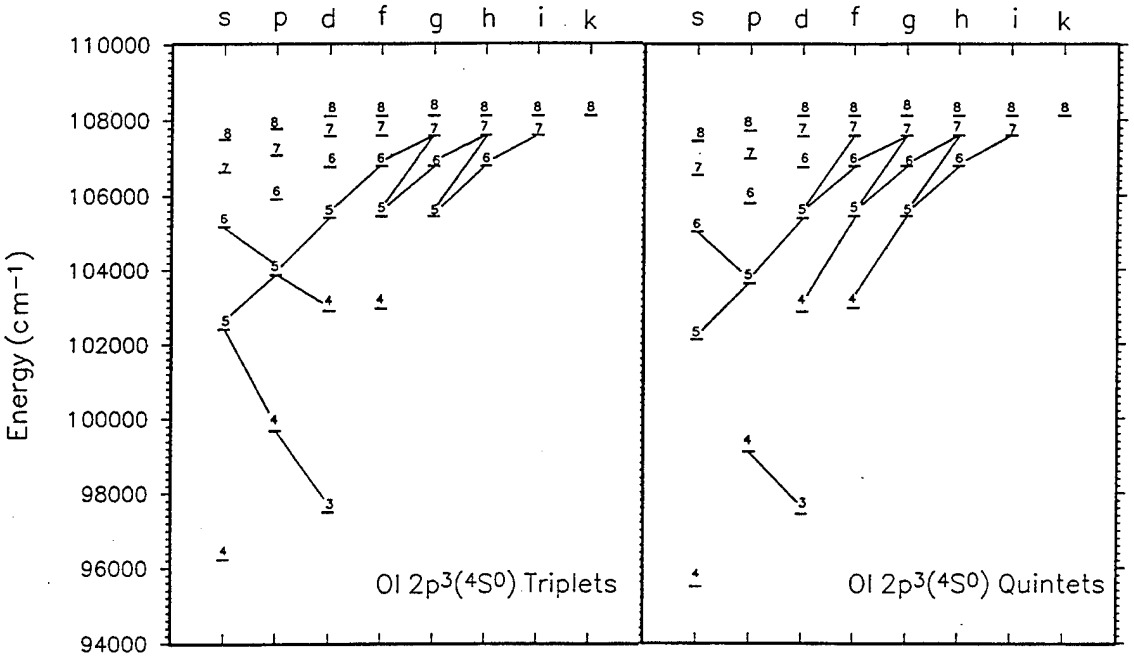

Figure 5. Energy level diagram illustrating the major transitions observed in the line emission spectrum from 3.5 to 13.0 μm.

TABLE 2. Observed line positions, assignments, calculated Einstein coefficients, and approximate line widths in LINUS IR plasma spectra at 20 μs.

Observed Feature (μm)	Wavelength[a] (μm)	Transition Assignment[a] (spin in parantheses)	gA[a] (s^{-1})	approximate FWHM[b] (μm)
3.67	3.6618	5s-4p (1)	$1.227x10^{7}$	0.04
3.89	3.8819	5f-4d (2)	$9.603x10^{7}$	0.04
3.94	3.9474	5f-4d (1)	$5.794x10^{7}$	0.02
4.04	4.0496	5g-4f (2)	$1.916x10^{8}$	0.04
	4.0499	5g-4f (1)	$1.149x10^{8}$	
4.56	4.5607	4p-3d (1)	$9.371x10^{6}$	0.04
	4.6510	7g-5f (1)	$1.481x10^{7}$	
	4.6511	7h-5g (1)	$1.680x10^{7}$	
4.62	4.5254	7f-5d (2)	$1.585x10^{7}$	0.2
	4.6507	7g-5f (2)	$2.469x10^{7}$	
	4.6511	7h-5g (2)	$2.799x10^{7}$	
5.69	5.6842	5d-5p (2)	$4.146x10^{7}$	0.1
5.98	5.9773	4p-3d (2)	$7.405x10^{6}$	0.04
6.51	6.4978	5d-5p (1)	$1.995x10^{7}$	0.06
6.61	6.6249	5p-5s (2)	$1.514x10^{7}$	0.05
6.86	6.8583	5p-5s (1)	$8.911x10^{6}$	0.04
7.19	7.1786	6s-5p (2)	$8.170x10^{6}$	---
	7.2664	6f-5d (1)	$1.615x10^{7}$	
	7.4281	6g-5f (2)	$5.032x10^{7}$	
7.44	7.4285	6g-5f (1)	$3.020x10^{7}$	
	7.4556	6h-5g (1)	$5.431x10^{7}$	0.15
	7.4556	6h-5g (2)	$9.052x10^{7}$	
10.38	10.3859	6d-6p (2)	$1.408x10^{7}$	0.2
	10.3995	5p-4d (1)	$3.435x10^{6}$	
	12.3629	7g-6f (2)	$1.694x10^{7}$	
	12.3644	7g-6f (1)	$1.017x10^{7}$	
12.35	12.3648	7h-6g (1)	$1.757x10^{7}$	0.5
	12.3648	7h-6g (2)	$2.929x10^{7}$	
	12.3625[c]	7i-6h (1)	$2.892x10^{7}$	
	12.3625[c]	7i-6h (2)	$4.821x10^{7}$	

[a] Taken from Chung *et al.*[12]

[b] Only approximate since there is a high degree of blending associated with these features.

These transitions include: $5s^3P$-$4p^3S$, $4p^3P$-$3d^3D$, $4p^5P$-$3d^5D$, $5p^5D$-$5s^5P$, and $5p^3P$-$5s^3S$, occurring near 3.67, 4.56, 5.98, 6.61, and 6.86 μm respectively. Assuming Saha equilibrium, the integrated intensity ($Wcm^{-2}sr^{-1}$) of the spectral distribution of a transition is given by:

$$I = \frac{d}{4\pi}\frac{N_0}{Z} g \exp\left(-\frac{hcF}{kT}\right) A \frac{hc}{\lambda} \tag{4}$$

where N_0 is the total atom density divided by the partition function, F the emitting state term value, T the electronic temperature, A the Einstein coefficient, and λ the transition wavelength. The degeneracy, g is given by $(2l+1)(2s+1)$. The path length, d, was calculated with a Lagrangian hydrodynamics model. The model predicted that the plasma emission region is approximately 6 mm long and 2 mm in diameter which is consistent with visual observation. Since the monochromator slit was perpendicular to the long axis of the emission region, a path length of 2 mm was used in the analysis of the data. Linearization of equation (4) yields the following relationship:

$$\ln\left[\frac{I}{gAhc/\lambda}\right] = -\frac{1}{T}\left(\frac{hcF}{k}\right) + \ln\left[\frac{dN_0}{4\pi Z}\right] \tag{5}$$

Figure 6 shows the results of the left hand side of equation (5) plotted against hcF/k for the five transitions. An electronic temperature of 8000 ± 1000 K is derived from the slope of the least squares fit to the data. The intercept determined from the least squares, which reveals information about the absolute number density, is not used in the analysis since a large error bar is associated with that number. The uncertainty in the derived temperature is the standard deviation associated with the fit. The error bars on the data points were derived from the following sources: (1) signal-to-noise estimations near each feature which resulted in individual intensity errors varying across the range 4-9%, and (2) 10% estimated area in the total intensity of the spectrum based on repetitions of the same experiment. In the error analysis, linear detector response with respect to signal was assumed. The derived electronic temperature was then used in the line emission modelling to obtain an estimate of the electron density.

The five transitions used for electronic temperature estimation were also used to estimate state populations. By determining the ratio of the relative integrated line intensities, the relative emitting state populations are measured. Table 3 lists the ratios of the transition probabilities, observed intensities multiplied with their respective transition energies, measured upper state populations and energies. A term diagram is shown for the five transitions in figure 7.

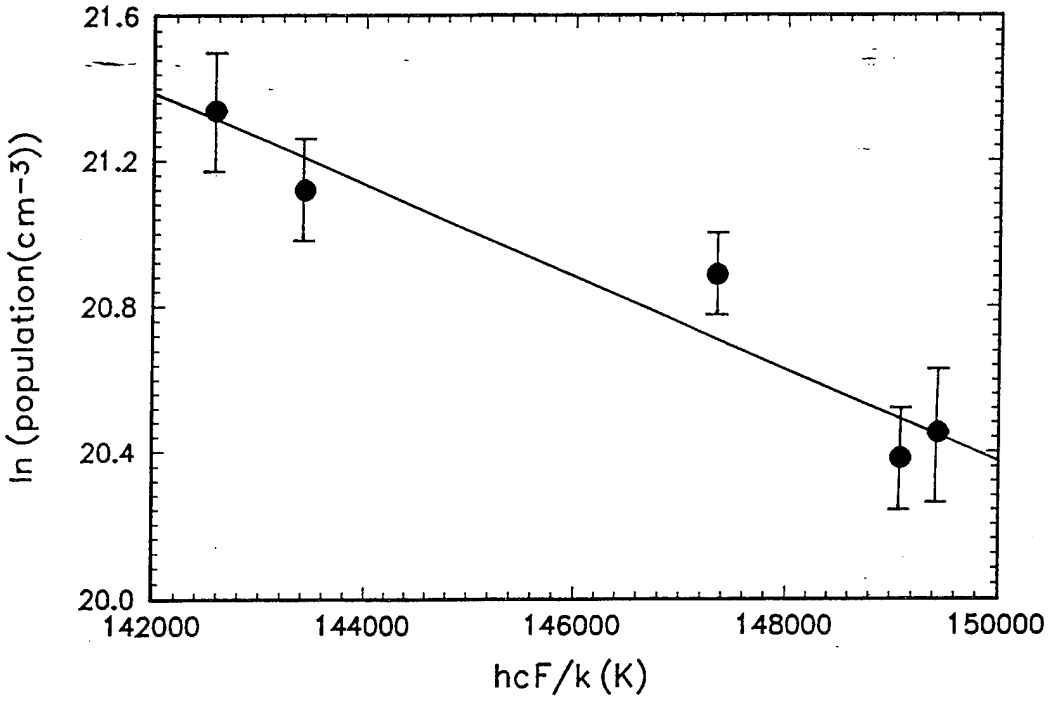

Figure 6. The electronic temperature is determined from a least squares fit the plot of the left-hand side of equation (5) against hcF/k. The least squares fit is shown as the solid line which is associated with an electronic temperature of 8000± 1000 K where the uncertainty reflects the standard deviation of the fit.

TABLE 3. Measured relative populations.

Upper State Ratio	Energies (cm^{-1})	N_i/N_j	g_iA_i/g_jA_j	I_iE_i/I_jE_i
4p(1)/5s(1)	99681, 102412	1.26 ± 0.06	0.763	0.964
4p(1)/4p(2)	99681, 99094	0.80 ± 0.05	1.265	1.018
4p(1)/5p(2)	99681, 103626	2.1 ± 0.2	0.619	1.290
4p(1)/5p(1)	99681, 103870	2.0 ± 0.2	1.051	2.050
5s(1)/4p(2)	102412, 99094	0.61 ± 0.04	1.657	1.056
5s(1)/5p(2)	102412, 103626	1.6 ± 0.1	0.811	1.338
5s(1)/5p(1)	102412, 103870	1.5 ± 0.2	1.377	2.126
4p(2)/5p(2)	99094, 103626	2.6 ± 0.2	0.489	1.267
4p(2)/5p(1)	99094, 103870	2.5 ± 0.3	0.831	2.013
5p(2)/5p(1)	103626, 103870	1.2 ± 0.1	1.669	1.589

Inspection of Table 3 shows the measured populations to decrease with increasing state energy. This suggests that these states are collisionally coupled. Electronic population of the Rydberg states are associated with more loosely bound electrons and are thus more susceptible to external effects induced by the plasma. Under Saha equilibrium conditions, thermalization through

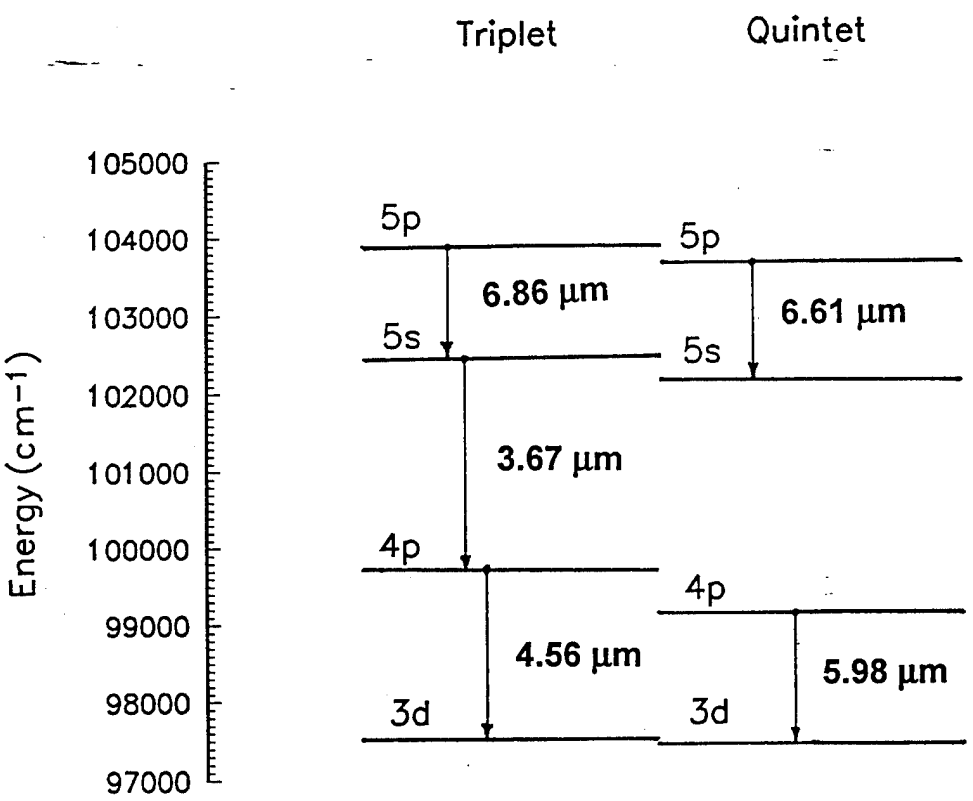

Figure 7. Term diagram for the five transitions used for the electronic temperature determination and state population measurement.

collisions with electrons determines the population distribution. The distribution reflects the electron temperature ($T_{el} = T_e$). Specifically, those Rydberg states within kT_e of the ionization potential may display coupled electron and electronic temperatures.

B. Continuum

The electron and atomic oxygen densities can be estimated from the continuum if the electron temperature is known, the plasma is collision dominated, and the form of the continuum is known. Figure 3 shows the power law fit to the theoretical emissivity coefficients of Lin.[39] The electron density was determined from the line emission modelling and the electronic temperature was measured from the spectroscopic analysis of integrated line intensities.

From the continuum fit, the product of the path length and electron and atomic oxygen densities can be determined by from:

$$\varepsilon(\lambda,T) = dN_e N_o J(\lambda,T) \tag{6}$$

where $J(\lambda,T)$ is the power law fit to Lin's emissivity coefficients.[39] The electron and atomic oxygen densities were uniquely determined using equation (6) and the Saha equilibrium condition. Saha equilibrium predicts the ratio of the square of the electron density to the oxygen density given the electron temperature:[44]

$$\frac{N_e^2}{N_o} = \left(\frac{2\pi mkT}{h^2}\right)^{3/2} \frac{2g_+}{g_o} e^{-(I-E_o)/kT} \tag{7}$$

where E_o is the multiplet averaged ground state energy, I is the ionization limit, T is electron temperature, m is the electron mass, and g_+ and g_o are the multiplet average ground state degeneracies for the ion and neutral. Using the spectroscopically determined temperature, the electron and atomic oxygen densities are estimated to be $8\text{x}10^{15}$ and $5\text{x}10^{18}$ cm^{-3} respectively. Using these values in eq. (6) results in an effective path length of 0.016 cm.

5. BREMSSTRAHLUNG RADIATION

Continuum emission in the laser-produced plasma is due to free-free (Bremsstrahlung) and free-bound processes. Continuum emission due to bremsstrahlung radiation by electron-ion collisions and recombination are well understood, and the reader is guided towards the previous LINUS final report for additional information. For bremsstrahlung radiation due to electron-neutral collisions (F-F(N)) we outline the threoretical developments that were concurrent with experimental program.

Bremsstrahlung radiation due to electron-neutral collisions in the EGG-22 plasma radiance model is based on the work by Zel'dovich and Raizer.[45] The expression for the F-F(N) emission coefficient may be expressed as,[45]

$$\varepsilon_{FF} = \frac{32\pi e^2\sigma}{3c^3}\left(\frac{2}{\pi m^3 kT}\right)^{1/2}\left[2(kT)^2 + 2h\nu kT + (h\nu)^2\right] N_a N_e \exp\left(-\frac{h\nu}{kT}\right) \tag{8}$$

The formulation of equation (8) is not regarded as exact since different temperature and energy dependencies can be derived based on different representations of the electron-neutral atom interaction. This formulation is the one presently used in the EGG-22 plasma radiance model. The cross section for interaction is not well established here but has a direct impact on the coefficient.

EGG-22 uses cross sections derived from the experimental results of Taylor and Caledonia[42] which are expressed in terms of radiative absorption coefficients. However, the measurements were only made at 2, 3.5, and 5 μm and at only one electron temperature. Thus, there is considerable uncertainty in extrapolating and interpolating these results to different wavelengths.

Lin's treatment[39] of the emissivity coefficient for free-free transitions in the field of a neutral oxygen atom is fully quantum mechanical and implements polarized orbitals. In Tables 4, 5, and 6, we list the values for Lin's emissivity coefficients[39] and the values predicted by EGG-22 for electron temperatures of 10000 K, 25000 K, and 50000 K in the wavelength range 1 to 30 μm. Figure 8 is a plot the emissivity coefficients for each of the three temperatures. There is reasonably good agreement between Lin's coefficients[39] and EGG22 at 10000 K. However, there is markedly different behavior as the electron temperature is increased. The distinguishing characteristic is that Lin's coefficients[39] increase with increasing electron temperature whereas the prediction by EGG-22 shows just the opposite. This result is surprising since intuitively, Bremsstrahlung emission due to electron-neutral collisions should decrease due to the decreasing residence time of the electron near the atom decreases as the electron's effective temperature increases. Discussions with Lin[39] have indicated that the "intuitive" decrease with increasing temperature may be fallacious and the apparent increase is due to energetic wave- function overlap in this region. It is probably academic however, since at 50000 K, electron-neutral Bremsstrahlung emission is a minor source of radiance (the gas is nearly 100% ionized).

In figure 9, Lin's theoretical coefficients are compared with those of John and Williams[40], Geltman[41], and the empirical coefficients of Taylor and Caledonia.[42] The theories agree within a factor of two with one another. There is considerable disagreement however, between the theoretical and the empirical values.

TABLE 4. Bremsstrahlung emissivity coefficients for free-free in the field of a neutral at an electron temperature T_e=10000 K.

λ	Chun Lin	EGG-22	Ratio
1	4.3(-36)	1.5(-35)	0.29
5	3.7(-37)	6.5(-37)	0.57
9	1.2(-37)	1.5(-37)	0.80
13	6.0(-38)	5.9(-38)	1.0
17	3.6(-38)	2.9(-38)	1.2
21	2.3(-38)	1.7(-38)	1.4
25	1.7(-38)	1.1(-38)	1.6
29	1.2(-38)	7.2(-39)	1.7

TABLE 5. Bremsstrahlung emissivity coefficients for free-free in the field of a neutral at an electron temperature T_e=25000 K.

λ	Chun Lin	EGG-22	Ratio
1	2.4(-35)	2.3(-35)	1.0
5	1.3(-36)	4.9(-37)	2.7
9	4.0(-37)	1.1(-37)	3.6
13	1.9(-37)	4.0(-38)	4.8
17	1.1(-37)	1.9(-38)	5.8
21	7.3(-38)	1.1(-38)	6.6
25	5.2(-38)	7.0(-39)	7.4
29	3.8(-38)	4.7(-39)	8.1

TABLE 6. Bremsstrahlung emissivity coefficients for free-free in the field of a neutral at an electron temperature T_e=50000 K.

λ	Chun Lin	EGG-22	Ratio
1	5.2(-35)	1.8(-35)	2.9
5	2.4(-36)	3.7(-37)	6.5
9	7.6(-37)	7.8(-38)	9.7
13	3.7(-37)	2.9(-38)	12
17	2.1(-37)	1.4(-38)	15
21	1.4(-37)	8.0(-39)	18
25	9.9(-38)	5.0(-39)	20
29	7.4(-38)	3.4(-39)	22

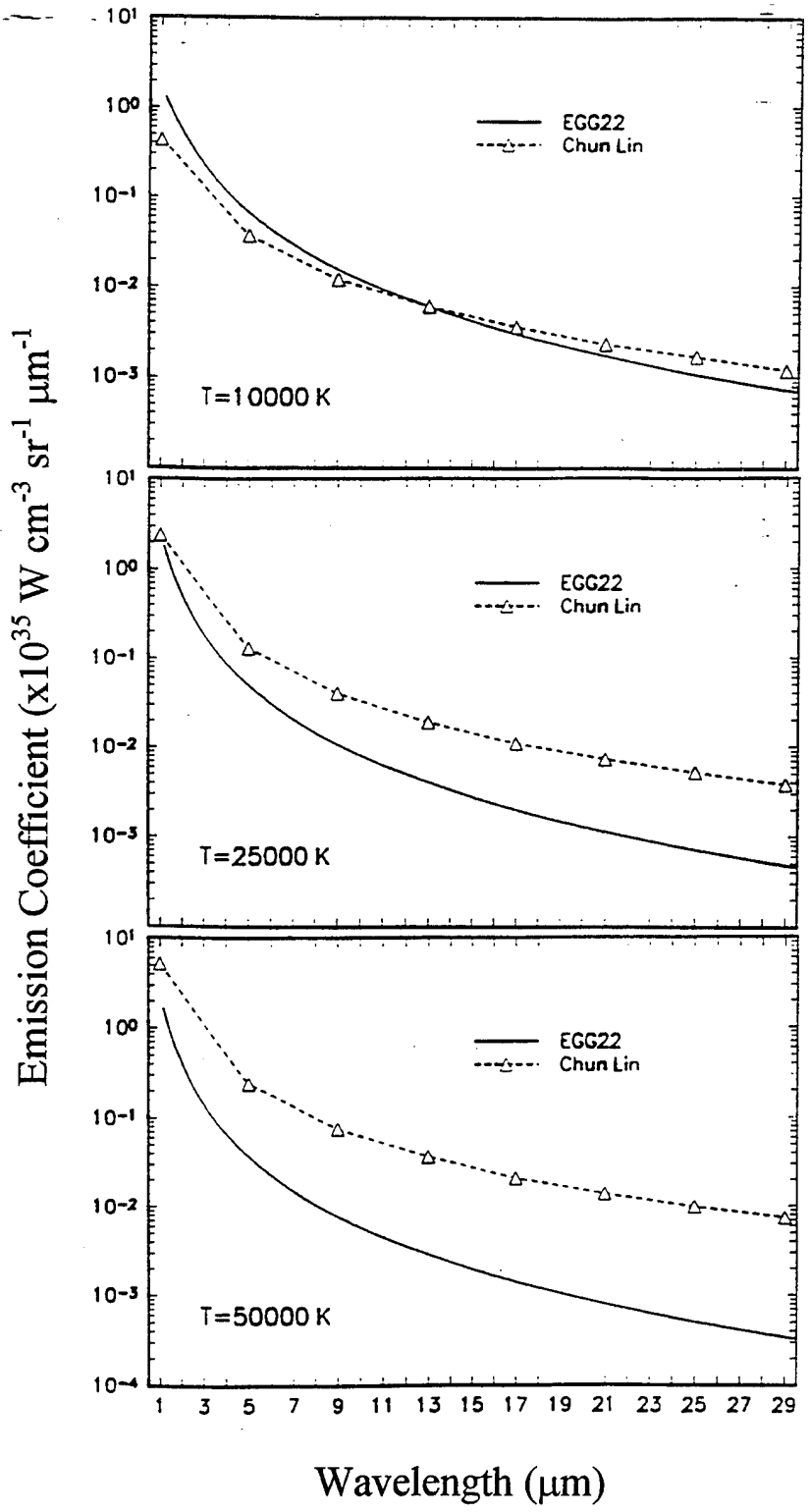

Figure 8. Comparison of EGG-22 and theoretical emissivity coefficients for free-free transitions in the field of a neutral oxygen atom.

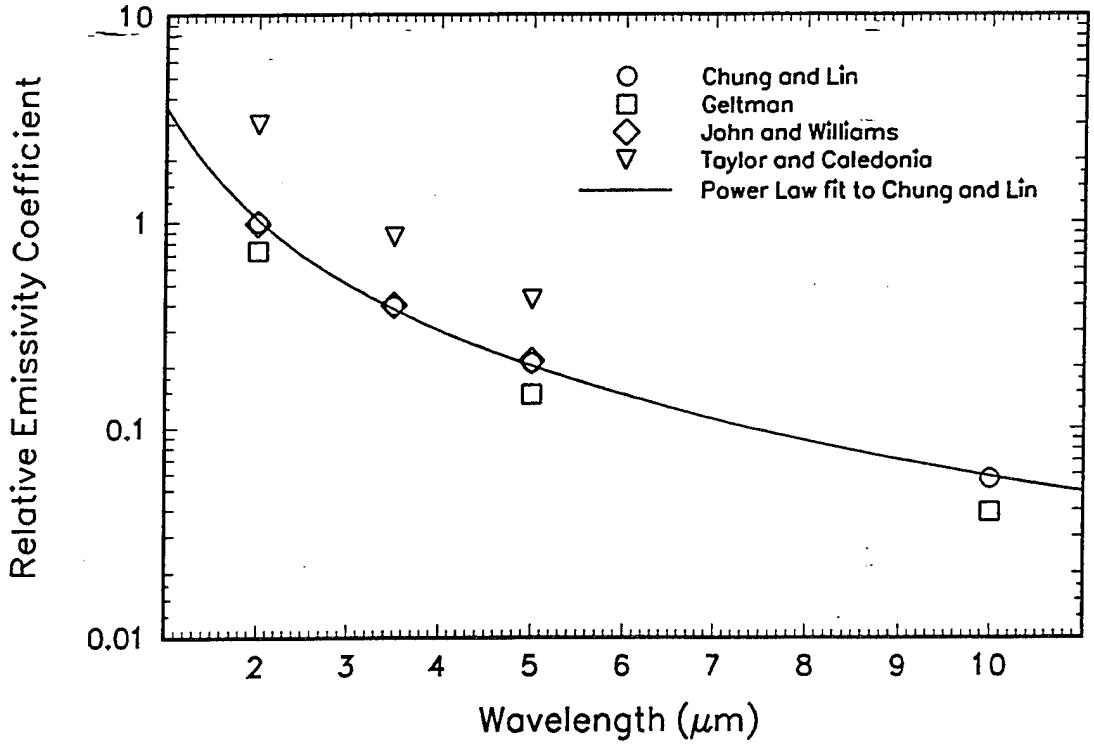

Figure 9. Comparison of theoretical and empirical emissivity coefficients for free-free transitions in the field of a neutral oxygen atom. All values are for an electron temperature of 10000 K. All values are relative Lin's emissivity coefficient at 2μm.

6. APOSTLE LINE BROADENING MODEL

A. Theory

A foundational work of pressure broadening of spectral lines was produced by Anderson[37] in 1949. Early treatments of pressure broadening assumed that collisions are adiabatic,[60,65,66] *i.e.*, no energy transfer takes place during a collision. The adiabatic assumption is usually applicable in the optical regime because energy transfer in an electron-atom collision is insufficient to induce such transitions. Anderson[37] included inelastic collisions and, thus, the applicability of his theory can be extended to the microwave and infrared regions. By assuming that the colliding neutral particles follow classical paths, the line width and shift can be described in terms of a semi-classical scattering operator. The scattering operator matrix is then evaluated using a second-order expansion approximation.[11,32,36,37,] These methods were further developed by Tsao and Curnutte[46] and Kolb and Griem[47].

Most collisional-Stark broadening calculations[31,32,34,35] are performed using extensions of the classical path impact theory developed by Anderson[37] for self-broadening of neutral emitters. The theory has been adapted and extended to a radiating plasma by Griem, Baranger, Sahal-Brechot,

and Cooper and their co-workers.[11,31,32, 33,48] The theory of collisional broadening[10,11] encompasses two limiting cases: (1) the impact approximation based on instantaneous collisions where the collision is short in comparison to the time between collisions, and (2) the quasi-static approximation based on slowly moving perturbers. For a plasma, the impact approximation describes electron impact on the radiating atom and the quasi-static approximation describes the ion-radiator collision effects. The quasi-static approximation is used to statistically represent ion-collisional influences as external electric fields (microfields). The ion-produced microfields vary so slowly that their time-dependence can be neglected. In this case, the calculation reduces to that of the static Stark effect, taking into account the statistical distribution of the electric fields at the radiator. In plasmas with atoms excited to sufficiently high n states, the small energy differences between perturbing levels become comparable to the line widths (overlapping lines) and the quasi-static line splitting is significant.[3] For lower-lying Rydberg levels whose components of different orbital angular momentum are well-separated in energy (isolated lines), the line broadening is caused mainly by collisions with electrons. There is an increase in the electron-impact width with increasing n and l of the upper state for lines belonging to a spectral series.[8] In many plasmas the electric fields produced by electrons colliding with the radiators vary so rapidly (i.e., collisions are short in duration) that the corresponding line widths and shifts depend only on net changes in the radiator states.

The determination of collisionally broadened[10,11] linewidths is divided into the effects of low-frequency perturbers (ions) using the quasi-static approximation and of the high frequency perturbers (electrons) using the impact approximation. To develop a "fast" computational model of line broadening over a large spectral range, we use the approximations of Anderson[37] for electron collisional effects and the model of Hooper[38] for ion collisional effects. The approximation criteria are examined in detail as some spectral features fall outside the limits of model validity. Such cases are flagged as inappropriate estimates.

1. Ion Collisional Broadening

The quasi-static approximation is valid if the splitting caused by the perturber field, $\Delta\omega$, is large compared to the inverse of the duration of the collision, $1/\tau_p$, or

$$\Delta\omega >> \frac{1}{\tau_p} \approx \frac{u_p}{b_p} \tag{9}$$

where u_p is the velocity of the perturber and b_p is its characteristic impact parameter. For long range Coulomb interactions, b_p is limited by plasma shielding effects and can be approximated by the Debye length, λ_D.

The use of the quasi-static approximation for the ions is equivalent to representing the ions by a normalized distribution function, $\mathcal{P}(E)$, of static electric fields, E. $\mathcal{P}(E)$ depends on the ion mass, density, and temperature. By adopting this physical picture for the ions, the standard quantum mechanical theory for Stark effect is applicable.

The Stark effect is described by the Stark Hamiltonian, which is the product of the electric dipole moment, $e\mathbf{r}$, and the electric field, E. The selection rules for electric dipole induced transitions are Δs=0, Δl=+1,-1, Δm_l=+1,0,-1. The presence of the Stark field has two effects. First, the energy levels of the m_l magnetic substates are shifted, *i.e.*, their degeneracy is lifted. For all atoms except hydrogen, the amount of energy shift is proportional to the square of m_l. Therefore, the line shifting is not symmetric about the unperturbed line. Second, lines forbidden by the electric dipole selection rules become allowed due to the mixing of states. The presence of an electric field results in spectra with split and broadened lines. The Stark shifted line positions, ω_{ij}, and corresponding perturbed wave functions are determined by diagonalization of the Stark Hamiltonian. The electric dipole transition moments are calculated using the resulting wave functions and energies. After calculating the energy levels and wave functions for a particular field, the Einstein coefficients are calculated according to:[49]

$$A_{ij} = \frac{64\pi^4 \tilde{\omega}_{ij}^3}{3h} \left| \langle i | e\mathbf{r} | j \rangle \right|^2 \tag{10}$$

where h is Planck's constant, the transition frequency is in wavenumbers.

The basis set for the Stark Hamiltonian matrix assumes L-S coupling and is defined by the spin, s, the principal number, n, the orbital angular momentum, l, and the magnetic quantum number, m_l. The diagonal matrix elements of the Hamiltonian are the unperturbed energy levels for oxygen atom, the majority of which have been documented by Moore[50]. States not listed in Moore are calculated using the polarization formulas in Edlen[51] and the polarizability constants in Isberg[52]. The formulas are based on the theory of Born and Heisenberg[53] and of Waller[54], who modifies the hydrogenic term formula for the interaction of the valence electron with the core electrons. The off-diagonal elements of the Stark Hamiltonian matrix are calculated by multiplying the dipole

moment matrix elements by the ion-induced field. The radial part of the dipole moment matrix element is obtained from the calculations of Chung *et al.*[9] and Lin.[55] These calculations employ a frozen core representation of the oxygen wave functions. For transitions higher than *h-g*, the radial matrix elements are calculated from the tables in Oertel and Shomo[56], which are extensions of the Coulomb approximation calculations of Bates and Damgaard.[57] The signs of these matrix elements may differ from those of Lin[55] depending on whether n'- n'' is even or odd because of a difference in the phase definition in the wave functions. Formulas for the angular component, consisting of direction cosine matrix elements, are based on the standard approach given by Condon and Shortley.[49]

The ion-induced field in the Stark Hamiltonian is given by Holtsmark[58] to be $2.6eN_p^{2/3}$. Since the temporal dependence of the ion field is difficult to characterize experimentally or theoretically, the accepted approach is to statistically simulate the effect of the quasi-static ions by a plasma microfield distribution. Using this approach, a microfield distribution has been calculated by Baranger and Mozer.[59] Hooper[38] further refined the theory by including correlation among all perturbers and allowing independent input for plasma density and ion and electron temperature. The microfield distribution used in the present model is based on Hooper's approach for the case of a low frequency electric microfield distribution at a neutral point.

2. Electron impact Broadening

Most theories on electron impact broadening are based on three assumptions: the classical path, impact, and binary assumptions. The classical path approximation assumes that the perturber path is straight for neutral radiators and hyperbolic for charged radiators. The impact approximation assumes that the duration of the collision is short compared to the time between collisions. The binary approximation assumes that a collision involves two species: the radiator and one perturber. These approximations allow one to express the interaction of the electron perturber and the neutral emitter as a definite function of time, $H_1(t)$. The classical path approximation is particularly useful in treating Stark broadening of spectral lines emitted in plasmas because the interparticle forces are long range Coulomb forces and the broadening is dominated by many weak collisions. The impact approximation can be invoked if the duration of a perturbing collision, τ_p, is much shorter than the time between perturbing collisions, τ_b, is small compared to the time between collisions. The duration of the collision can be approximated by dividing the largest impact parameter for

producing an emission disturbance, b_p, by the average perturber velocity, u_p. Therefore, the impact approximation can be used when

$$\tau_p \approx \frac{b_p}{u_p} << \tau_b \approx \frac{1}{N u_p \pi b_p^2} \tag{11}$$

This is essentially identical with the criterion for the binary collision approximation:

$$\frac{4}{3}\pi b_p^3 N_p << 1 \tag{12}$$

The impact approximation also implies the opposite of the criterion of the quasi-static approximation[2], that is

$$\Delta\omega << \frac{u_p}{b_p} \tag{13}$$

where $\Delta\omega$ defines the region around the line center that can be confidently modeled under impact approximation theory. The largest possible impact parameter for a perturbing collision is limited by the Debye length, λ_D. For electrons as perturbers with average velocity, $u = \left(8kT_e / \pi m_e\right)^{1/2}$, equation (13) can be reduced to $\Delta\omega < \omega_{pe}$ where ω_{pe} is the electron plasma frequency.

Anderson[37] states that the impact approximation is equivalent to assuming that all emission lines are either well resolved or not at all resolved when compared to the linewidth, i.e., degenerate levels. This simplification was removed by Kolb[47] who generalized Anderson's method to include overlapping lines. We return to Anderson's theory for reason of model efficiency. The comparison of the calculations with those using more complex theory and with experimental data will test the success of the approximations used.

Under the impact approximation, the spectral distribution of a single transition is Lorentzian[60]

$$L(\tilde{\omega} - \tilde{\omega}_{ij}) = \frac{\delta\tilde{\omega}_{ij} / \pi}{(\tilde{\omega} - \tilde{\omega}_{ij} - \Delta\tilde{\omega}_{ij})^2 + \delta\tilde{\omega}_{ij}^{\,2}} \tag{14}$$

where $\delta\tilde{\omega}_{ij}$ is the half width at half the maximum line intensity and $\Delta\tilde{\omega}_{ij}$ is the line shift due to electron impact. Once the electron collisional broadening width and shift are determined then equation (14) can be used to construct the total line emission spectrum through summation over all electric dipole allowed transitions.

The line broadening cross section, σ_b and line shift cross section, σ_s, for an electron-radiator collision are related to the linewidth and lineshift by

$$\delta\tilde{\omega}_{ij} = N_e u_e \sigma_b \tag{15}$$

$$\Delta\tilde{\omega}_{ij} = N_e u_e \sigma_s \tag{16}$$

The cross sections are calculated from Anderson's[37] equation (52)

$$\sigma = \sigma_b + i\sigma_s = \int_0^\infty 2\pi S(b)db \tag{17}$$

where b is the impact parameter and $S(b)$ may be interpreted as the probability of an electron collision disturbing the emission of radiation. $S(b)$ is written in terms of the time-development matrix, $T(t)$, which is approximated by[37]

$$T(t) = \frac{2\pi}{ih}\exp\left[-\int_{-\infty}^{t} H_1(t')dt'\right] \tag{18}$$

where t is time and H_1 is the interaction Hamiltonian. Additionally, the classical path, impact and binary approximations greatly simplify the Hamiltonian describing the interaction of the perturber and emitter. The interaction Hamiltonian for the electron-neutral interaction is:

$$H_1 = -\frac{e^2}{r_c} + \frac{e^2}{\sqrt{r_c^2 - 2r_c r_a + r_a^2}} \tag{19}$$

where the distances from the O^+ nucleus to the perturbing and emitting electron are, respectively, r_c and r_a The first term is the Coulomb attraction between the perturbing electron and the oxygen nucleus and the second term is the Coulomb repulsion between the perturbing electron and the emitting electron.

Expanding the second term in equation (19) in (r_a/r_c), and retaining the first order terms, one obtains the point-dipole charge interaction Hamiltonian

$$H_1 = e^2 \cos\gamma \frac{r_a}{r_c^2} \tag{20}$$

with γ as the angle between vectors r_c and r_a. To express the interaction Hamiltonian in spherical coordinates (r,θ,ϕ), we choose the electron-atom collision to occur in a plane with $\phi_c = 0$ and define the relationship of collision parameters to r_c and θ_c by invoking the classical path approximation through

$$\begin{aligned} \cos\theta_c &= \bar{u}t / r_c \\ \sin\theta_c &= b / r_c \\ r_c^2 &= b^2 + \bar{u}^2 t^2 \end{aligned} \tag{21}$$

where $\bar{u}$ is average electron velocity, t is time, b is the impact parameter. By substituting the relations in equation (21) into equation (20) through

$$\cos\gamma = \cos\theta_a \cos\theta_c + \sin\theta_a \sin\theta_c \cos(\phi_a - \phi_c) \tag{22}$$

the Hamiltonian becomes

$$H_1 = \frac{e^2 r_a}{r_c^3}(\lambda_{za}\bar{u}t + \lambda_{xa}b) \tag{23}$$

where $\lambda_{za} = \cos\theta_a$ and $\lambda_{xa} = \sin\theta_a \cos\phi_a$ are direction cosines of the emitting electron. To obtain a tractable expression for $T(t)$ of equation (18), it is expanded in terms of powers of a matrix, P,

$$P = \frac{2\pi}{h}\int_{-\infty}^{\infty} H_1(t)dt \tag{24}$$

The expression for $S(b)$ is then written in terms of powers of the matrix P which result from the expansion of $T(t)$:

$$S(b) = S_0 + S_1 + S_2 + \ldots \tag{25}$$

S_0 is zero for all situations.[33] As stated in Anderson[37], the first-order term, S_1 is imaginary and, thus, the first "shift" term of the expansion. For the present problem S_1 is also zero as it depends on the interaction matrix elements that are zero due to symmetry (Anderson's equation[37] (54*b*)). S_2 has two types of second-order terms and are named in Anderson[37] as $(S_2)_{middle}$ and $(S_2)_{outer}$ (Anderson's equations[37] (54*c*',*c*")). $(S_2)_{middle}$ is zero for the same reason as S_1. The only non-zero term in the second-order approximation is $(S_2)_{outer}$. $S(b)$ is subsequently expressed as

$$S(b) \approx S_2(b) = \frac{1}{2}\left[\sum_{m_i}\frac{\langle i,m_i|P^2|i,m_i\rangle}{2l_i+1} + \sum_{m_f}\frac{\langle f,m_f|P^2|f,m_f\rangle}{2l_f+1}\right] \tag{26}$$

where $|i\rangle = |n_i l_i\rangle$ and $|f\rangle = |n_f l_f\rangle$ are the initial and final states. This term gives the probability of a transition being caused by a collision averaged over the initial and final states. The line shift cross section is zero for the second-order approximation. The *P*-matrix element is given by

$$\langle a|P|b\rangle = \frac{2\pi}{h}\int_{-\infty}^{+\infty}\exp(i\omega_{ab}t)\langle a|H_1(t)|b\rangle dt \tag{27}$$

where ω_{ab} is the transition frequency. The states $\langle a| = \langle nlm|$ and $|b\rangle = |n'l'm'\rangle$ are the wave functions of the radiator with the primed states being the perturbing states. With H_1 given by equation (23), the *P*-matrix element becomes

$$\langle a|P|b\rangle = \frac{4\pi e^2}{h}\left[iM_{za}\int_0^{t_D} \frac{ut\sin(\omega_{ab}t)dt}{(b^2+u^2t^2)^{3/2}} + M_{xa}\int_0^{t_D} \frac{b\cos(\omega_{ab}t)dt}{(b^2+u^2t^2)^{3/2}}\right] \tag{28}$$

where $M_{za} = \langle a|r_a\lambda_{za}|b\rangle$, $M_{xa} = \langle a|r_a\lambda_{xa}|b\rangle$ and λ's are the direction cosines. The computation of the P matrix element requires solution to the time integrals. To account for correlation effects between electrons that shield the perturbing electron's electric field, a cutoff in the scattering integration over impact parameter is applied at the Debye length, λ_D. The introduction of a collision operator cutoff sets the upper integration limit, t_D, at

$$t_D = \frac{1}{v}(\lambda_D{}^2 - b^2)^{1/2} \tag{29}$$

Once the matrix element of P for a particular impact parameter is calculated, then $S(b)$ is obtained through equation (26). Because $S(b)$ diverges at small b values, a strong-collision cutoff (b_{min}) is applied to suppress the divergence in the integration.[8,62,64] A Lorentz-Weisskopf type term is used to approximate the contribution of strong collisions to the broadening cross section by assuming that the phase shifts and inelastic effects produced by the electron-atom collisions are so large that the scattering operator matrix elements either oscillate rapidly between +1 and -1 or approach 0. The maximum impact parameter, b_{max}, outside which $S(b)$ is taken as zero, is determined by Debye shielding as mentioned earlier. Although Griem[31] and Chappell *et al.*[62] argue that the maximum impact parameter should be 1.123 λ_D and 0.682 λ_D respectively, little difference was observed in the calculated spectra when these values were used. The maximum impact parameter use here is 1.0 λ_D. Only small errors are introduced into line width calculations by the above second-order expansion and impact parameter cutoff procedures.

3. Additional Approximations

The time integral (eq. (28)) is solved numerically using a weighted trapezoidal routine. Because the numerical solution to the integrals is time consuming, an approximate analytic solution is obtained by allowing t_D to go to infinity. The integral can then be expressed analytically in terms of modified Bessel functions of integer order.

The computational demands of spectral models have motivated the need for greater levels of approximation. Along with the above theoretical and numerical approximations, we have included the options to make the following additional approximations in calculating the spectral line widths: one may choose to use (1) unperturbed wave functions and energy levels, (2) ion-perturbed energy levels only, or (3) ion-perturbed wave functions and energy levels. These three approximation levels are termed the *unperturbed*, *semi-perturbed,* and *perturbed* cases, respectively. If the wave functions and energies are not perturbed significantly by the ions, then the calculations of electron broadened line widths can be simplified by using the unperturbed wave functions and energies. For the *unperturbed* case, the calculations are performed for transitions between two n, l states with no ion collisional effects incorporated into the solution. For the *semi-perturbed* and *perturbed* cases, the calculation of $S(b)$ is performed for transitions between two n, l, m states. The summation over m_i and division by $2l_i+1$ in equation (26) are omitted since the magnetic substates are treated explicitly. These approximations are only justified by comparison to data and published linewidth calculations.

The levels of approximation, perturbed, semi-perturbed and unperturbed were examined for computational efficiency and degrading effects. Computational efficiency depends on the number of microfield intervals, number of basis states, and the number of lines in a spectral range. However, the unperturbed calculations are about a factor of 10 faster than the semi-perturbed calculations. The fully perturbed calculations are from 10 to >1000 times slower than the semi-perturbed calculations. From performing many unperturbed and semi-perturbed calculations, it is found that the unperturbed lines are sometimes 30% narrower than lines from semi-perturbed calculations. A fully perturbed calculation and a semi-perturbed calculation over the spectral range 3.5μm to 8μm showed very little difference in the structure. The semi-perturbed calculations were used in the comparisons presented below.

B. APOSTLE Model

The APOSTLE model was designed for computational efficiency to provide calculated spectra over large spectral ranges. APOSTLE consists of three modules, executed sequentially: *mfd*, *stark,* and *linshape*. The objective of APOSTLE is to predict the characteristic nature of a collisionally broadened spectra arising from a laser induced plasma.

In essence, the approach of the APOSTLE model lies in the determination of the spectral Radiance ($Wcm^{-3}sr^{-1}(cm^{-1})^{-1}$) of a collisional-Stark broadened line:

$$I(\tilde{\omega}-\tilde{\omega}_{ij}) = N_i A_{ij} \varepsilon_{ij} L(\tilde{\omega}-\tilde{\omega}_{ij}) \tag{30}$$

where A_{ij} is the Einstein coefficient, ε_{ij} is the energy of the transition and $L(\tilde{\omega}-\tilde{\omega}_{ij})$ is given by equation (14). The upper state population, N_i is given by:

$$N_i = \frac{N_0 g_i}{Z} \exp\left(-\frac{hcF_i}{kT}\right) \tag{31}$$

Figure 10 shows the modular design of APOSTLE. The first module performs the task of computing the ion microfield probability distribution. This code is executed first for which its output used as the input for the second module, *stark*. *Stark* is the main module responsible for computing the line positions, Einstein coefficients, state populations, and spectral distribution half-widths. The output

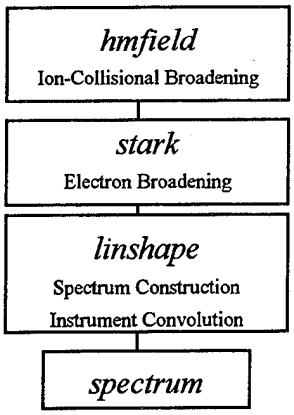

Figure 10. Modular design of the APOSTLE model.

of *stark* is then used in the third module, *linshape*, which constructs the spectrum according to equation (30), then convolves the spectrum with a user specified instrumental line shape.

The first code in the APOSTLE suite, *mfd*, is used to calculate the Stark effect on the oxygen Rydberg lines induced by the presence of ionic species. The computer code was written by C. F. Hooper[72] and it is used in the APOSTLE model in unmodified form. The only documentation available exists in the form of comments in the FORTRAN source code. The physical basis for the

code has been published by Hooper.[58] The output of *mfd* is a set of weighted electric field strengths with the corresponding probabilities of producing these field strengths. This output file, a graphical example of which is given in Figure 11, is used as an input file for the spectral-line-broadening code *stark*.

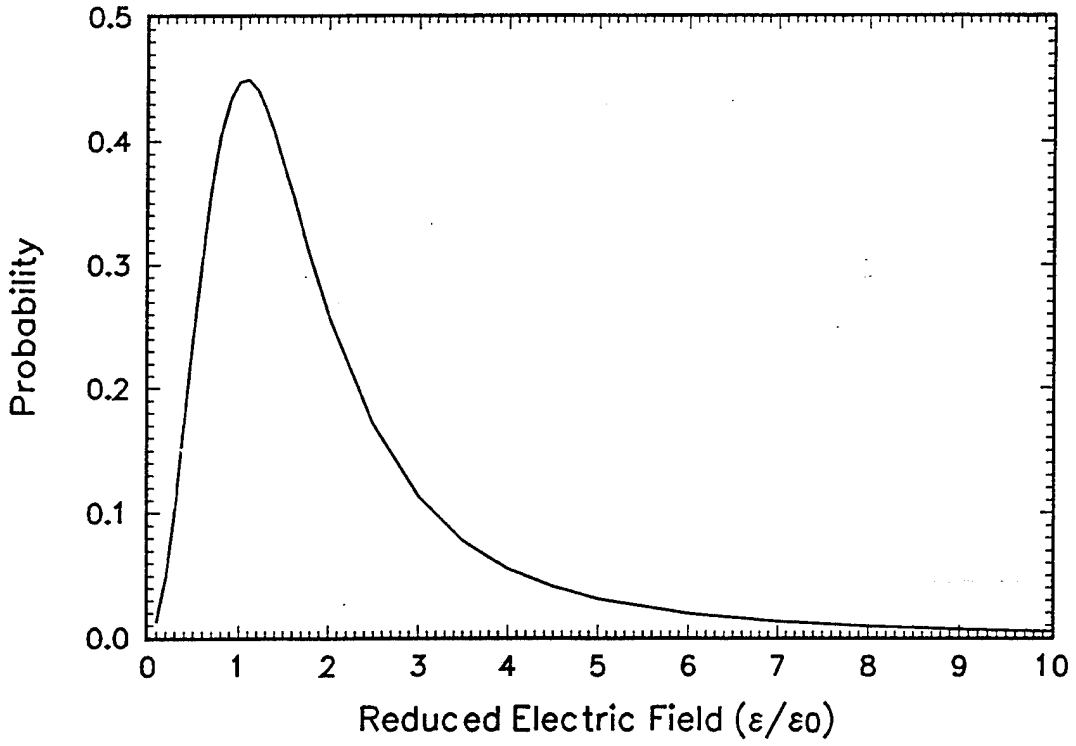

Figure 11. The APOSTLE calculated electric field probability distribution for ion-collisional broadening.

The effect of collisional-Stark broadening of the oxygen Rydberg spectral lines, by both ion and electron perturbers is calculated in *stark*. Figure 12 illustrates the block structure of the APOSTLE *stark* module. The *stark* module function is to calculate line positions, Einstein coefficients, state populations, and spectral line widths. The calculation is performed iteratively over the ion microfield distribution according to the basis set, microfield, spectral range, and parameters provided. State populations are calculated internally using to eq (24) according to the electronic temperature or will also accept populations calculated independently.

Figure 13 is a plot of gA with λ (product of the Einsten coefficient and upper state degeneracy) under unperturbed, zero-field conditions from 2-30 μm. These values are tabulated in Appendix C. The figure shows a general tendency of decreasing values of gA with λ with gA varying over more than four orders of magnitude. However, five prominent groups of transitions can be readily

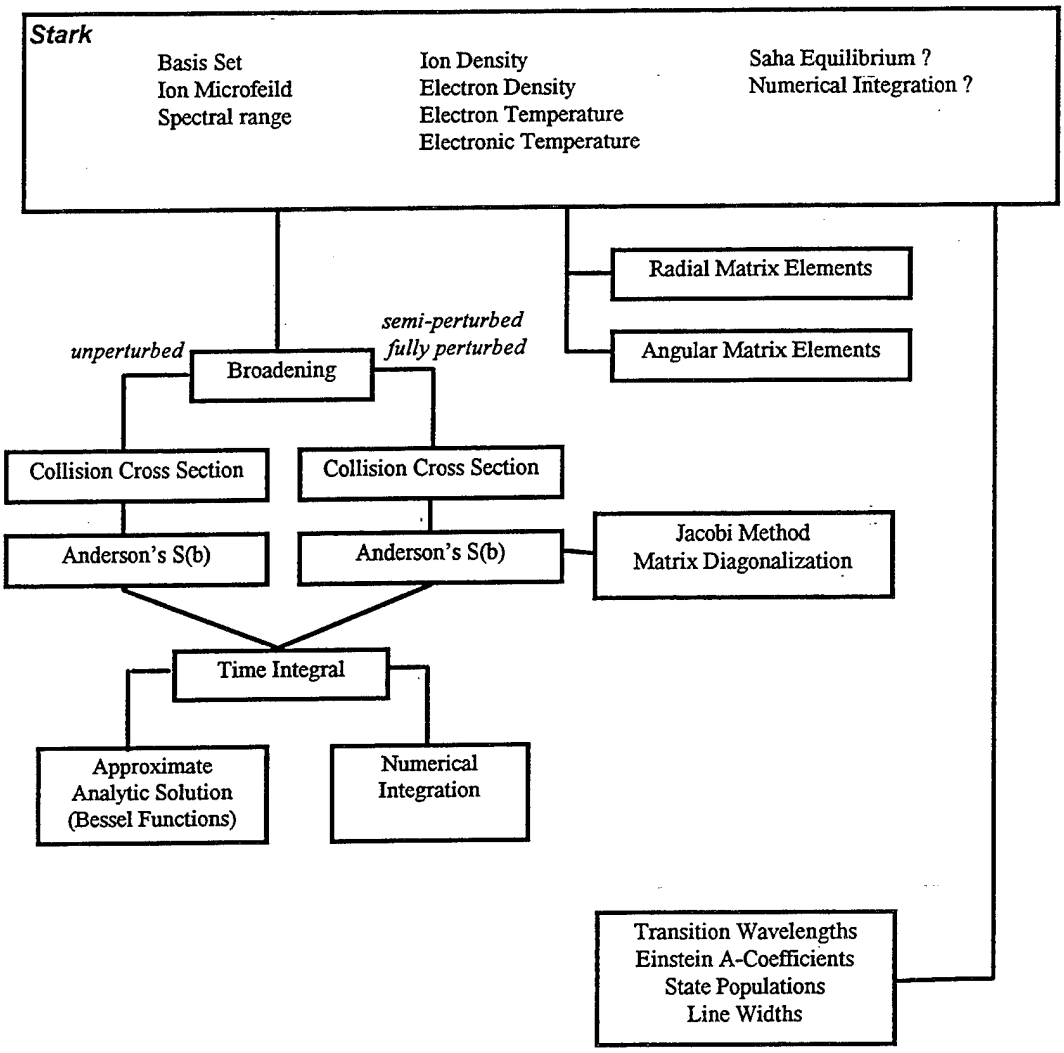

Figure 12. Block structure of the APOSTLE *stark* module.

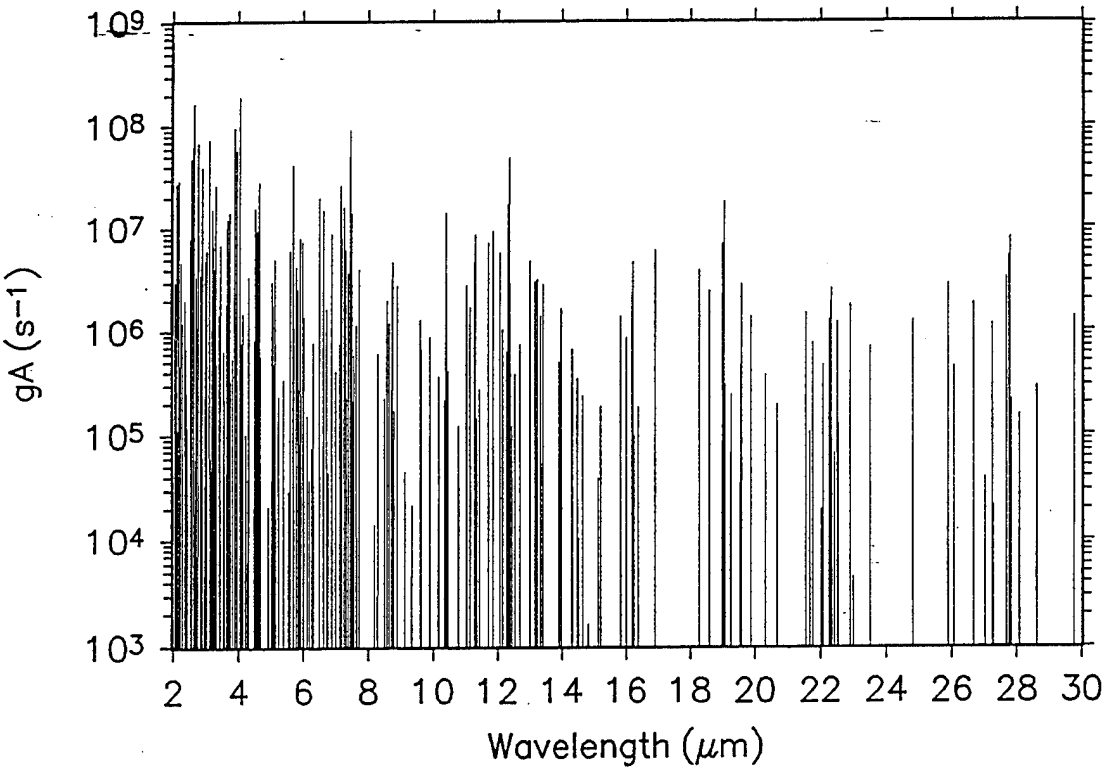

Figure 13. Plot of gA as function of λ as predicted by the APOSTLE model in the absence of collisional-Stark broadening.

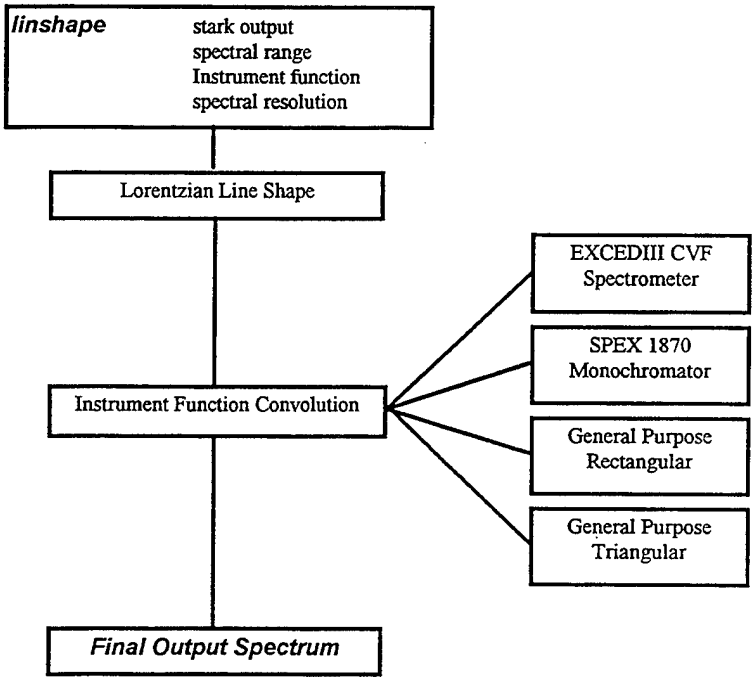

Figure 14. Block structure of the APOSTLE *linshape* module.

observed in the plot: 4.04 μm, 7.45 μm, 12.35μm, 19.0 μm, and 27.8 μm. The line position, Einstein coefficients, upper state populations, and electron-broadened half-widths define the output of *stark* which is used in the third APOSTLE module, *linshape*.

The third module in the APOSTLE model, *linshape*, performs the construction of the instrumentally convolved spectrum from the line-by-line broadening information from *stark*. This is accomplished in two steps: first, the Lorentzian spectral distribution is constructed for each transition from the line positions, Einstein coefficients, upper state populations, and spectral half-widths for each transition. Second, the spectrum is then convolved with an instrumental line shape (ILS) function which is user flexible and computed internally. Figure 14 illustrates the structure of *linshape*.

The total spectral radiance of the spectrum is obtained from the summation of eq (23) over all transitions. In wavelength space ($Wcm^{-3}sr^{-1}\mu m^{-1}$) this is equal to,

$$I(\lambda) = \frac{1}{\lambda^2}\sum_{i,j} I(\tilde{\omega} - \tilde{\omega}_{ij}) \tag{32}$$

From this, the unconvolved spectrum is convolved with the ILS function, $f(\lambda)$:

$$I^*(\lambda) = \int I(\lambda) f(\lambda - \lambda')d\lambda' \tag{33}$$

Presently, options available include a function for a SPEX Industries model 1870 grating monochromator, EXCEDEIII CVF4 (circularly variable filter) spectrometer, and two general purpose ILS functions (triangular and rectangular) requiring user input resolution. Figure 15 illustrates a typical situation of the convolution of an unconvolved Lorentz distribution with the SPEX ILS function. In this figure, the ILS is characterized by a fwhm of ~0.032 μm.

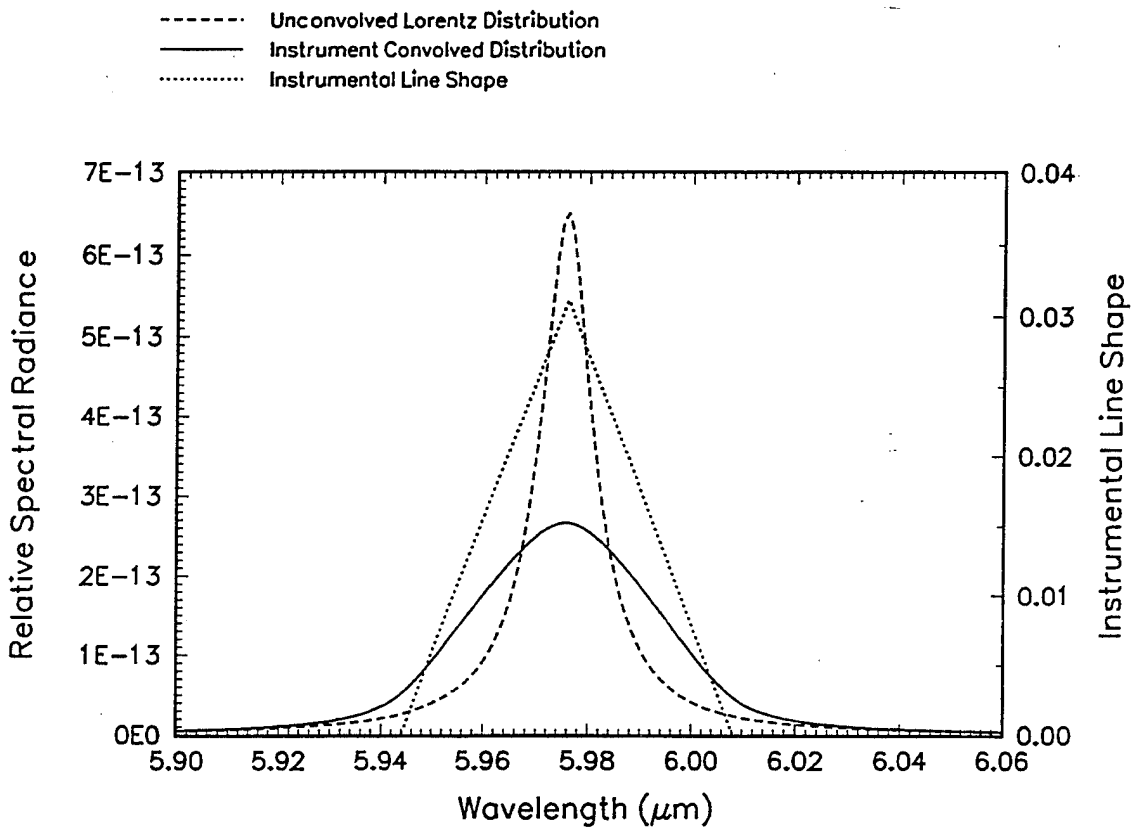

Figure 15. Example of the effect convolution of triangular instrumental line shape with a collisional-Stark broadened line.

7. APOSTLE MODEL VS. DATA

A. Collisionally Dominated Plasma

The line emission model provides a spectral prediction to the laser-produced oxygen plasma IR spectrum in Chapter 4. The results of the fitting procedure are shown in figure 3. For the fitting procedure the parameter space (T_e, T_{el}, N_e) of the line model was explored. The basis set consisted of 62 states (31 triplets and 31 quintets) with the highest principal quantum number, n=8. The plasma density was varied between $2x10^{15}$ cm^{-3} to $2x10^{16}$ cm^{-3}, and electron and electronic temperature parameters were varied between 5000K to 50,000K in 5000K intervals, and 5000K to 20,000K in 5000K intervals, respectively. The spectral calculations have been done with the semi-perturbed approximation of the model due to the computational demands of a fully perturbed calculation. A fully perturbed calculation was performed for a single set of parameters and compared to a semi-perturbed calculation at the same values. The results showed very little difference over the broad spectral range that was compared ($3\mu m < \lambda < 12\mu m$).

The model was fit to the data using the empirically derived electronic temperature and atomic oxygen density. Using these values, an absolute Boltzmann state population distribution was generated. Stark broadening is relatively insensitive to electron temperature[14] but there are slight variations in shapes of some features. The fitting procedure was the variation of the electron density to give the best model-data agreement in the line widths of the $4p^5P$-$3d^5D$ (5.976 μm) and the $5d^5D$-$5p^5P$ (5.6847 μm) transitions. This resulted in an estimated electron density of $8x10^{15}$ cm^{-3}.

In general, the agreement between model and data is good, although the model is excessively broadened for the 7.45 and 12.35 μm emission features. Integrated band intensities over three spectral bands were calculated to investigate the discrepancy of the model prediction at 7.45 and 12.35 μm. Table 7 lists the calculated integrated intensities for model and data.

TABLE 7. Model vs. Data comparison of band integrated intensities.

Wavelength Band (μm)	Data (Wcm^{-2} Sr^{-1})	APOSTLE(Wcm^{-2} Sr^{-1})
3.8-4.3	$4x10^{-4}$	$3x10^{-4}$
6.9-8.0	$1x10^{-4}$	$9x10^{-5}$
10.8-12.35	$2x10^{-5}$	$1x10^{-5}$

Comparing the values in the first and second bands, the model prediction and experiment are in good agreement, thus suggesting only a line shape mismatch at 7.45 μm. In third wavelength band, it is possible that the discrepancy observed may be due in part to the poor detector responsivity beyond 12.5μm. The disagreement of model and measurement for 7.45μm and 12.35μm features may be partly due to the fact that these features consist of strongly overlapping lines. The present model assumes that the lineshape for overlapping lines is the sum of the individual transition spectral distributions. Interference effects from overlapping lines may narrow the linewidth. To obtain a better agreement for multiplet lineshape, it is necessary to use the more complex expression for the lineshape of overlapping lines.[47]

Additionally, the plasma conditions may not be sufficiently described by Saha equilibrium. An examination of the constants of thermal equilibration suggests that equilibrium conditions between electron kinetic and other temperatures do not exist at early times within laser induced plasma emission region. The initial energy deposition of the laser beam into the focal region dissociates, fully ionizes and multiply ionizes the oxygen gas. Excess energy elevates the electron temperature. The ions quickly heat up and the plasma begins an expansion from the deposition region. Chemical kinetics calculations[43] indicate that recombination rapidly changes the gas from a fully ionized to partially ionized plasma within $3x10^{-7}$ s. At 10^{-6} s, the ions should be in approximate equilibrium with the now dominant neutral O atoms due to the fast ion-neutral thermal transfer time constant (10^{-10} s). The equilibration time between the light electrons and heavy particles is significantly longer (about $6x10^{-6}$ s). Thus, the species kinetic temperatures may not be equal at the measurement time. This result is observed in modeling of a laser induced plasma done by Milroy et al. (1979)[63].

Finally, it is worthwhile to examine the uncertainties in the calculations of the spectral emissions. The uncertainty in the plasma parameters is harder to quantify. Uncertainty in the electron density and temperature determinations is estimated to be from 30% to 50% based on changes in the spectra as the plasma parameters are varied. In addition, the model calculation is for spatially homogeneous conditions. The line-of-sight integration of the laser-induced plasma is most certainly not homogeneous. Given these uncertainties, the comparison of model with experiment is satisfactory.

B. ARCHON Chemical Kinetics Modelling

At this juncture, the possibility of non-thermal state populations can now be investigated. This investigation was carried out with the use of the ARCHON chemical kinetics model. The reaction set model, along with rate coefficients is listed in Table 8.

TABLE 8. ARCHON reaction set model.

Reaction	Process Type	a	b	c
$O^{5+} + e + e \rightarrow O^{4+} + e$	three-body	8.7×10^{-18}	-4.5	0
$O^{5+} + e \rightarrow O^{4+} + e$	dielectronic	1.7×10^{-10}	-1.5	5.6
$O^{5+} + e \rightarrow O^{4+} + e$	radiative	2.2×10^{-9}	-0.7	0
$O^{4+} + e + e \rightarrow O^{3+} + e$	three-body	4.5×10^{-18}	-4.5	0
$O^{4+} + e \rightarrow O^{3+} + e$	dielectronic	1.1×10^{-10}	-1.5	5.6
$O^{4+} + e \rightarrow O^{3+} + e$	radiative	8.9×10^{-10}	-0.7	0
$O^{3+} + e + e \rightarrow O^{2+} + e$	three-body	1.9×10^{-18}	-4.5	0
$O^{3+} + e \rightarrow O^{2+} + e$	dielectronic	6.2×10^{-11}	-1.5	5.6
$O^{3+} + e \rightarrow O^{2+} + e$	radiative	2.8×10^{-11}	-0.7	0
$O^{2+} + e + e \rightarrow O^{+} + e$	three-body	5.6×10^{-19}	-4.5	0
$O^{2+} + e \rightarrow O^{+} + e$	dielectronic	2.8×10^{-11}	-1.5	5.6
$O^{2+} + e \rightarrow O^{+} + e$	radiative	5.6×10^{-11}	-0.7	0
$O^{+} + e + e \rightarrow O + e$	three-body	7.4×10^{-20}	-4.5	0
$O + e \rightarrow O^{+} + e + e$	re-ionization	3.9×10^{-12}	1.5	162
$O^{+} + e \rightarrow O^{2+} + e + e$	re-ionization	1.2×10^{-13}	1.5	400
$O^{2+} + e \rightarrow O^{3+} + e + e$	re-ionization	1.8×10^{-14}	1.5	640
$O^{3+} + e \rightarrow O^{4+} + e + e$	re-ionization	4.7×10^{-15}	1.5	890
$O^{4+} + e \rightarrow O^{5+} + e + e$	re-ionization	1.3×10^{-15}	1.5	1300
$O+ + e \rightarrow O(n=11,l)$	recombination	$1\times10^{-12}/g_i$	-1.5	5.6
$O(n_i,l_i) \rightarrow O(n_f,l_f) + h\nu$	radiative cascade			

The details of the calculation are discussed in the *Infrared Emissions Final Report.*[43] However only the pertinent details will be discussed here. It is to be noted here that the present calculation is preliminary. The reaction set does not include oxygen atom impact excitation or quenching reactions. Collision cross sections for the former are at present unavailable. The model was chosen only to illustrate the effect of electron recombination with singly-ionized oxygen on the IR plasma spectrum, particularly the 7.45 μm emission feature. The initial conditions were chosen to match the initial cell conditions before the laser pulse, which were 110 torr O_2. The time dependence of the electron temperature was obtained from the earlier SALE calculations.[43]

Several calculations were made with different reaction set models, the results of which are not documented here. The desired result was to predict the 7.45 μm spectral distribution.

The calculation yielded the recombination driven state populations which were subsequently used for APOSTLE spectral calculations. Figure 16 shows the resulting triplet state population distribution (the quintet state distribution is similar) compared to a Boltzmann distribution at 10000 K. Figure 17 shows the resulting synthetic spectrum, compared to the previously best fit thermal model spectrum and the experimental spectrum at 20 μs. The normalization of the two model spectra were chosen to be coincident with the observed peak intensities of the 5.69, 5.98, 6.61, and 6.86 μm features for the thermal model and the peak intensity of the 7.45 μm feature for the non-thermal case. Although the spectral fit is poor for the 5.69, 5.98, 6.61, and 6.86 μm features in the non-thermal case, the spectral distribution of the 7.45 μm feature is reproduced with a much higher quality. It was also observed that the 4.04 μm feature appears to be relatively insensitive to either thermal or non-thermal populations. It appears that some features are modelled well using an collisionally-coupled populations and others using a non-thermal model.

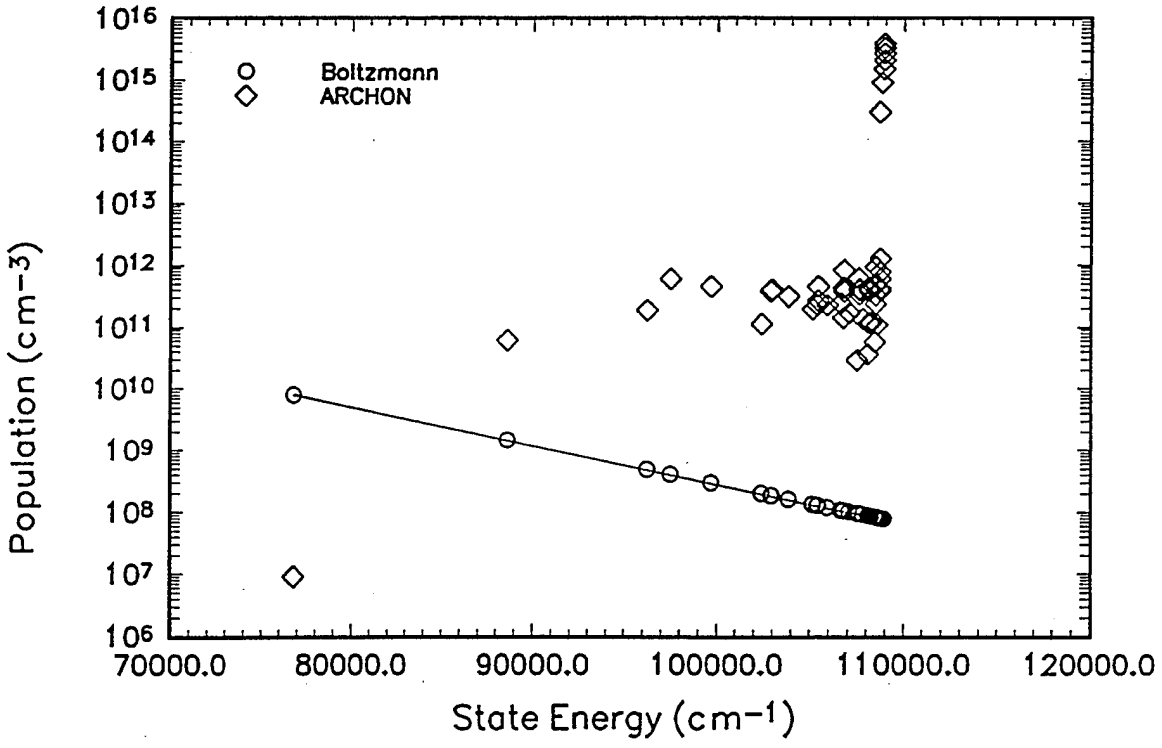

Figure 16. Comparison of the triplet Boltzmann state population distribution and the ARCHON calculation.

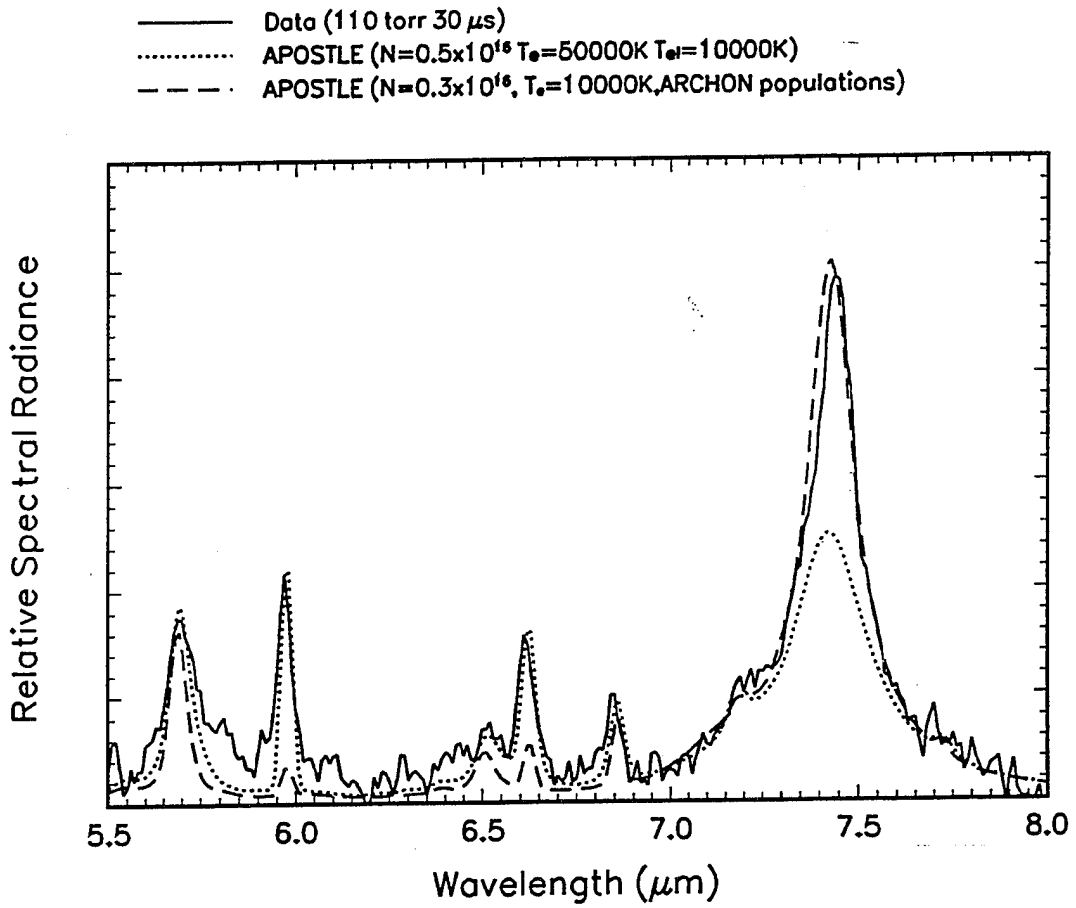

Figure 17. Comparison the APOSTLE predicted spectrum using collisionally-coupled state populations and the ARCHON calculated state populations.

8. SUMMARY AND CONCLUSIONS

We have obtained a time resolved infrared spectra from the center of a recombining laser produced oxygen plasma. Measurements were acquired in the spectral range from 3.5 to 13.0 μm at an aperture delay time of 20 μs. The transitions near 10.4, and 12.35 μm are first reported observations in emission. The 10.4 μm feature is a composite line dominated by the $6d^5D$-$6p^5P$ and $5p^3P$-$4d^3D$ transitions and the 12.35 μm feature is dominated by the $7g,h,i^{3,5}$ G,H,I-$6f,g,h^{3,5}$ F,G,H transitions.

In general, there is excellent agreement between line and continuum emission models and data. An electronic temperature of 8000 ± 1000 K was derived from the spectroscopic analysis of the data. Using this value, the electron density was estimated at $8x10^{15}$ cm^{-3} from the line emission

model. Lin's theoretical emissivity coefficients[39] were then used in conjunction with the assumption of Saha equilibrium to estimate the atomic oxygen density and the path length. The path length was derived to be 0.016 cm and the atomic oxygen density was estimated to be 5 $x10^{18}$ cm^{-3} suggesting that the ionization level was <1%.

Although a single temperature was assumed to describe the state population distribution, this conclusion should not be interpreted rigorously since the plasma emission region may be inhomogeneous and inconsistent with collisional equilibrium conditions. However, the deduced temperature and density values were found to be in good agreement with the physical description of the plasma conditions given the experimental uncertainties.

The key issues surrounding the parametric characterization of the LINUS plasma include the temporal development of electron, ion, and neutral densities and temperature. These parameters determine the characteristic of the emission processes that unfold in the plasma relaxation. At early times, the observed radiance from the plasma is known to be continuum dominated, consisting mostly of Free-Free transitions in the field of an ion, Free-Bound processes, and Free-Free transitions in the field of a neutral. These processes are strongly dependent on the parameters densities and temperatures.

The present contract was coincident with the development of a new theoretical description for bremsstrahlung radiation due to electron-neutral collisions. This new model was compared to previous theories and the EGG-22 plasma radiance model. The agreement between EGG-22 and the new coefficients was good for an electron temperature of 10000 K thus validating EGG-22. The difference between Lin's coefficients and EGG-22 at higher temperatures is probably academic however, since at higher temperatures, the gas is nearly 100% ionized, and bremsstrahlung radiation due to F-F(N) becomes a minor source of radiation.

The present model of the Stark line broadening problem is based on the standard theory of Stark effect using the quasi-static approximation and impact theory of Anderson.[37] Many calculations in the four-dimensional parameter space (N_e, T_e, T_i, T_{ei}) of the model were used to provide a best estimate of the plasma parameters within the measured spark region of a laser induced oxygen plasma. It is possible that the electron temperature departs from the OI electronic temperature during the early time of the spark ($t<10^{-5}s$). However, the line spectrum is fairly insensitive to electron temperature and no estimates of T_e were obtained directly from lineshapes. The electron density and electronic temperature observed in the laser induced oxygen plasma were consistent with Saha equilibrium suggesting the plasma was collisionally dominated. These conclusions

compare favorably with previous atomic oxygen linewidth calculations and experimental studies of laser produced plasmas. The above favorable comparisons give confidence in the model results except for lines at 7.45μm and 12.45μm where approximation criteria failed. Although the present approach has been only applied to OI as radiator, the model should be applicable to emitters in a plasma that satisfy L-S coupling.

Two important issues related to the LINUS IR emission spectrum are homogeneity of the emission region and the attainment of local thermodynamic equilibrium. Thermal and non-thermal state population modelling was performed which was then used for APOSTLE spectral calculations. Non-thermal state populations were modelled with ARCHON using a reaction set model consisting primarily of three-body, dielectronic, and radiative recombination, and radiative decay. The 7.45 μm line shape was predicted with a much higher quality than that predicted using thermal populations. It was concluded that the different spectral character of the 7.45 μm emission could be due to at least two causes: insufficient treatment of overlapping lines or non-thermal state populations.

Spatial imaging of the LINUS plasma emission region was unfortunately not accomplished in the present study. This is a key issue important to understanding the plasma development and subsequent relaxation. The experimental observation of spatial information could also be used to benchmark the SALE hydrodynamic calculations[43], as well as directly address the issues of homogeneity and collisional-radiative processes.

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APPENDIX A

APOSTLE USER'S MANUAL

I. INTRODUCTION

The APOSTLE computer code modules are written and FORTRAN 77 and are most efficiently executed on a computer with at least a i386 CPU with math coprocessor. The source code was developed as a three module program with Lahey and SVS brand compilers. In the past, the code has also executed succesfully and SUN 386i workstation and the Apollo DN1000 computer. There is minimal "user-friendliness" code in the model. If a program execution is failing, it is advised to first check the input files for inconsistencies. If all parameters in the input files appear consistent, then one or more of those parameters may be outside the range of validity of the model.

The FORTRAN structure of each module is written compactly; that is, all subroutines and functions are contained in the source code module file. This design was meant to make source code compilation easier. Compilation is performed for each module, thus there should be three executables after compilation.

The APOSTLE program package should reside in one subdirectory. This is achieved by simply copying the source code, all of the input files, and external data files to a "C:\APOSTLE" subdirectory. A typical subdirectory listing may appear like:

```
Volume in drive C is MS-DOS_5
 Volume Serial Number is 18E2-8248
 Directory of C:\APOSTLE

.            <DIR>      04-21-94   8:36a
..           <DIR>      04-21-94   8:36a
README            3559 01-11-94  11:36a
M31S1    DAT       814 04-15-91   2:20p
M31S2    DAT       814 04-15-91   2:20p
M53S1    DAT      1387 09-20-91  11:40a
M53S2    DAT      1387 09-20-91  11:43a
M54S1    DAT      1415 04-07-93   8:48a
STARK    FOR    105430 06-24-94  11:55a
LINSHAPE FOR     23126 05-23-94  11:57a
MFD      FOR     97707 01-09-94  11:34a
MFD      SET       362 01-07-94  11:22a
STARK1   SET      1194 06-24-94  11:46a
STARK2   SET      1194 06-24-94  11:47a
LINSHAPE SET       796 05-23-94  10:16a
```

All files with the `*.set` filename extensions are input files for the executables. These input files are edited manually before program execution. The information in the input files are commented and are meant to be self-explanatory. The format of the input files are structured as: parameters in column 1 and definitions/comments written in column 13. All data input is not formatted. The files `M31S1.DAT`, `M31S2.DAT`, `M53S1.DAT`, `M53S2.DAT` and

M54S1.DAT contain basis set information which is read in at the time of executables. The names of the *.set files should never be changed since each program module searches the subdirectory for these files. Additionally, all input parameters in the input files should be in upper case. With these input files, a typical APOSTLE synthetic spectral calculation can be acheived in 4 steps:

(1) edit input files

(2) execute mfd.exe (microfield distribution) module

(3) execute stark.exe (collisional stark broadening) module.

(4) execute linshape.exe (line shape construction and instrument convolution) module

In the first step, the edited input files define the values of the parameters used by the model. These input files reside in the subdirectory where the output files will be written. It is useful to store the program executables in a "C:\BIN" subdirectory and including this subdirectory in the path statement of the AUTOEXEC.BAT file of the computer. The input files are edited using standard editors such as the MS-DOS editor "EDIT" or the Borland editor BRIEF. Once the input files are edited, program execution is carried out by typing the program module name at the DOS prompt. Program execution may also carried out through the use of batch files.

In the second step, the mfd module is executed to create the microfield distribution. When the microfield distribution is created, the information is written to hard disk. In the third step, the stark module is executed. The calculation is looped over two iterations for spin 1 and spin 2. Thus there will be two output files from the stark module. The third and final step, is the construction of the spectrum from the line broadening information calculated by the stark module. Two files are written to hard disk: the instrument convolved spectrum and the unconvolved spectrum.

The following sections of this appendix describe the model I/O. Only partial output content is exemplified here due to the voluminous nature of the output files. The example input files may be used as a test case. The values of the input parameters for the test case have been chosen to reduce the program run time.

II. MODULE I/O

A. MFD

The first module executed is the ion microfield probability distribution module (mfd.exe). Figure A1 gives an example of the input file (mfd.set) for producing a microfield distribution

for an electron density of $8x10^{15}$ cm^{-3} and an electron temperature of 10000 K. The output in this example is a single file (N8_0T10.H15) consisting of a set of electric field strengths with the corresponding probabilities of producing these field strengths. There are a total of 51 sample points in the microfield distribution. The incremental spacing of this distribution is not constant.

input	*variable*	*description*
N8_0T10.H15	OUTFIL	OUTPUT FILENAME
0	IH	LOW FREQ.=0, HI FREQ.=1
0.8	EDENS	ELECTRON DENSITY XE16
10000.	TE	ELECTRON TEMP. IN K
1.1	ALPHA	INITIAL ESTIMATE (1.1)
0	R	RATIO OF TYPE 2 TO TYPE 1 PERTURBERS (0)
1.0	TRATIO	RATIO OF ELECTRON TO ION TEMPERATURE (1.0)
0	XI	NET RADIATOR CHARGE (0.0)
1	Z1	NET CHARGE OF TYPE 1 PERTURBER (1)
1	Z2	NET CHARGE OF TYPE 2 PERTURBER (1)
0.1	DALPHA1	VALUE FOR THE ALPHA-VALUE SEARCH (0.1)

Figure A1. The input file, mfd.set, is used to define the input parameters for the mfd module.

B. STARK

The stark module calculates the line broadening information for spectrum construction. This output is used for the lineshape module. During execution, the information is written to the screen. The stark module reads in the input files (STARK1.SET and STARK2.SET), an example of which is given in Figure A2, and all the external files (M31S1.DAT, M31S2.DAT, N8_0T10.H15, and possibly an externally calculated population file). In this example, a collisional-stark broadening calculation is performed for an electron density of $8x10^{15}$ cm^{-3} and electron temperature of 10000 K.

input	*variable*	*description*
M31S1.DAT	NAMEIN	BASIS STATE FILENAME
0.8	XIDENS	ION DENSITY (1E16CM-3)
0.8	EDENS	ELECTRON DENSITY (1E16
10000.	ETEMP	ELECTRON TEMPERATURE (K)
10000.	TEL	ELECTRONIC TEMPERATURE
4.0	WVMIN	MINIMUM WAVELENGTH
4.1	WVMAX	MAXIMUM WAVELENGTH
STARK1.DAT	NAMEOUT	OUTPUT FILENAME
N8_0T10.H15	NAMEFD	MICROFIELD FILENAME

```
51              NEPT        NUMBER OF ELECTRIC FIELD POINTS
5               NINC        SAMPLED INCREMENT
S               EBROAD      E-BROADENING: U,S,OR P?
C               ZEMAVG      IF U READ(R) OR CALCULATE(C)
NONE            NAMEWID     READ FROM FILE --->
Y               POPBOLTZ    POPULATION: BOLTZMANN? (Y/N)
N               NAMEPOP     IF N, READ FROM POP. FILE:
N               NAINT       NUMERICAL INTEGRATION?
10              NGAUSS      Quadrature intervals
```

Figure A2. The input file `STARK1.SET` used to define the input parameters for the stark module.

The input files (`stark1.set` and `stark2.set`) contains 18 lines each. The parameters in these files have the following definitions:

`NAMEIN` = name of the basis state filename

`XIDENS` = ion density in units of 10^{16} cm^{-3}

`EDENS` = electron density in units of 10^{16} cm^{-3}

`ETEMP` = electron temperature (K)

`TEL` = electronic temperature (K)

`WVMIN` = starting wavelength (μm)

`WVMAX` = ending wavelength of spectral range (μm)

`NAMEOUT` = name of the output file used in the linshape module

`NAMEFD` = name of the microfield distribution file

`NEPT` = number of points in the microfield distribution (51)

`NINC` = incremental sampling of the microfield distribution

`EBROAD` = electron broadening cases which have the following choices:

- `u` - unperturbed energies and unperturbed wavefunctions
- `s` - ion-pertubed energies and unperturbed wavefunctions
- `p` - ion-perturbed energies and perturbed wavefunctions

`ZEMAVG` = for the unperturbed case, either [`R`]ead values of electron widths from a file or [`C`]alculate the values

`NAMEWID` = if `ZEMAVG=[R]`, file name to be read containing electron widths

`POPBOLTZ` = if[`Y`]es, then a relative Boltzmann distribution is calculated internally according to the input electronic temperature

NAMEPOP = in POPBOLTZ=[N], the name of the file containing the state population distribution

NAINT = numerical integration [Y/N]

NGAUSS = if NAINT=[N], number of gaussian quadrature intervals

The first line is the basis state filename (m31s1.dat or m31s2.dat) and has the following format,

```
S
NBASIS
N1      L1    EN1L1    IGROUP1
N2      L2    EN2L2    IGROUP2
.       .     .        .
.       .     .        .
```

where the parameters in the basis state file have the following definitions:

S = spin angular momentum quantum number

NBASIS = number states in the file

N = principal quantum number

L = orbital angular momentum quantum number

ENL = term value of the unperturbed state (cm^{-1})

IGROUP = group number

The order of the basis states in the basis state file is from large L to small L. Basis states which have the same group number can perturb one another if the electric dipole selection rules are obeyed.

Independently calculated state population distributions may be read by the stark module.

```
N1      L1    POPL1
N2      L2    POPL2
.       .     .
.       .     .
```

The program reads the first value of the microfield distribution, calculates the line broadening information for all transitions that lie in the input spectral range, then iterates to the next microfield distribution sample point. For example, if `ninc=5`, then every fifth distribution sample point is used for the broadening calculation and there will be 11 iterations of the calculation.

Figure A3 shows partial output of the stark module. In the figure, the first three lines are the values for the electron density ($x10^{16}$ (cm^{-3})), the electron temperature (K), and electronic temperature (K). The next block of information is the line broadening information. The columns of numbers following the densities and temperatures are: 1) the wavelength of the transition (μm), 2) Einstein coefficient (s^{-1}), 3) population (cm^{-3}), 4) halfwidth of the lorentztian distribution (cm^{-1}), 5) weighted electric field strength probability, 6) product of the upper term value and hc/k (K), and 7) transition assignment. The line shape module only reads the first four columns of information. The last three contain extraneous information.

```
 8.0000E-01
  10000.0000
  10000.0000
  7.482   9.6503E+04   5.1219E+05   1.4340E+01   1.3550E-02   155566.    8j- 6h
  3.768   5.2238E+04   1.7196E+07   4.8400E+01   4.5491E-01   155518.    8h- 5f
  8.890   1.6921E+03   9.6574E+06   1.6519E+01   3.0673E-02   155008.    7h- 7s
  4.401   5.8237E+04   2.8403E+06   1.6016E+01   5.0093E-03   154949.    8i- 5d
     .         .            .            .            .          .          .
     .         .            .            .            .          .          .
     .         .            .            .            .          .          .
  3.538   1.3098E+03   6.2842E+05   2.1680E+00   8.3124E-04   156984.    8j- 6h
  4.775   2.5185E+04   2.1550E+05   1.5064E+01   2.8505E-04   156236.    8i- 7p
 10.733   2.8651E+04   1.3376E+05   4.6791E+00   1.3553E-04   153029.    7i- 6g
     -1. -1. -1. -1.
     12565     0.408849E+01
```

Figure A3. Example information from the stark1.dat output file of the stark module.

C. LINSHAPE

the linshape module constructs the spectrum from the line broadening information calculated by the stark module. The file in Figure A4 is an example of the input for the linshape module. There will be two such files; one for spin 1 information and one for spin 2 information. Typically, these are named `stark1.dat` and `stark2.dat`

input	*variable*	*description*
STARK1.DAT	NAMEIN1	CODE-B OUTPUT FOR SPIN 1
STARK2.DAT	NAMEIN2	CODE-B OUTPUT FOR SPIN 2
OUTPUT.SYN	ENAMEW	OUTPUT FILENAME (CONVOLVED SPECTRA
2.E+17	DENS	TOTAL ATOM DENSITY (CM-3)
1.0	PTHLEN	PATH LENGTH (CM) [0.6 CM FROM SALE RESULTS]
4.0	WVST	START WAVELENGTH (MICRONS)
4.1	WVEN	END WAVELENGTH (MICRONS)
0.001	R	INTERNAL RESOLUTION (MICRONS) (LINUS:0.001
0.02	REXT	EXTERNAL RESOLUTION (MICRONS)
S	SPEC	N=NONE,S=SPEX,C=CVF
3.	SLIT	SLIT WIDTH IN MM
0.03	DELAMDA	MICRONS
T	INSTFNT	T=TRIANGULAR,R=RECTANGULAR

Figure A4. The input file, linshape.set used to define the input parameters for the linshape module.

The parameters in the linshape module input file have the following definitions,

NAMEIN1 = name of the spin 1 output file from the stark module

NAMEIN2 = name of the spin 2 output file from the stark module

ENAMEW = name of the output file from the linshape module

DENS = total atomic oxygen density (cm^{-3})

PTHLEN = path length associated with the emission region

WVST = starting wavelength of the spectral region (μm)

WVEN = ending wavelength of the spectral region(μm)

R = internal grid spacing(μm)

REXT = external grid spacing(μm)

SPEC = instrumental resolution (FWHM)

SLIT = slit width in mm

DELAMDA = if spex =[n], fwhm of the instrument resolution

INSTFNT = shape of the resolution

There are two grid spacings associated with the output of the linshape module. The external grid spacing is design for hard space saving. If the external grid spacing is equal to the internal grid spacing, every spectral sample in the spectrum is included in the output file (output.syn). A note is

made here that too large of an internal grid-spacing will result in insufficient sampling of the spectral distribution which may lead to erroneous line shape construction and instrumental convolution. Additionally, the external grid spacing should never exceed the internal grid spacing.

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APPENDIX B

SOURCE CODE

CODE A: Ion microfield probability distribution

```
      PROGRAM mfd
      implicit real*8 (a-h,o-z)
      character*12 outfil
      common/freq/ih
      common/micro/a,r,Tratio,xi,z1,z2,e(101),pe(101),alpha
      common/li1i2/rl(200),fl1(200),fl2(200),nl
      parameter(pi=3.14159D+00)
      parameter(ekb=1.38066D-16)
      parameter(e0=4.8026D-10)
      parameter(e02=e0*e0)

9000 format(3x,'edens  =',f8.2/3x,'Te     =',f8.2/3x,'alph   =',f8.2
     &      /3x,'r      =',f8.2/3x,'Tratio =',f8.2/3x,'xi     =',f8.2
     &      /3x,'z1     =',f8.2/3x,'z2     =',f8.2/3x,'dalph1 =',f8.2/)

         read(*,'(a)') outfil
         read(*,*) ih
         read(*,*) edens
         read(*,*) Te
         read(*,*) alph
         read(*,*) r
         read(*,*) Tratio
         read(*,*) xi
         read(*,*) z1
         read(*,*) z2
         read(*,*) dalph1

         open (7,file=outfil,status='unknown')
         write(*,9000) edens,Te,alph,r,Tratio,xi,z1,z2,dalph1

         edens=edens*(1.0D+16)
         rm1=3.0d0/(4.0d0*pi*edens)
         rm=(rm1)**(1./3.)
         elambda=sqrt((ekb*Te*rm1)/(3.0d0*e02))
         a=rm/elambda

         write(*,*) '   Computing microfield distribution...'

         call alser(alph,dalph1)
         call geni1
         call geni2
         call trans
         call afit

      close(1)
      stop
      end
```

CODE B: Collisional Stark Broadening

```
C*****************************STARK.FOR************************************
C                                                                          *
C           COLLISIONAL STARK BROADENING MODEL FOR ATOMIC OXYGEN           *
C                                                                          *
C                    MISSION RESEARCH CORPORATION                          *
C                       1 TARA BLVD SUITE 302                              *
C                        NASHUA NH 03062-2801                              *
C                                                                          *
C  THIS IS THE MAIN PROGRAM IN THE STARK LINE BROADENING MODEL.            *
C  SUCCESFUL COMPILATION AND LINKAGE WITH ASSOCIATED SUBROUTINES           *
C  THE EXECUTABLE PROGRAM HANDLES FOUR TASKS:                              *
C       1. READS IN INPUT PARAMETERS IN THE FORM OF AN INIT-FILE,          *
C       2. CALCULATES ION-PERTURBED ENERGY LEVELS AND WAVEFUNCTIONS,       *
C          TRANSITION WAVELENGTHS, TRANSITION PROBABILITIES, AND           *
C          RELATIVE POPULATIONS,                                           *
C       3. CALULATES ELECTRON-BROADENED LINEWIDTHS, AND                    *
C       4. WRITES THE OUTPUT FILE.                                         *
C                                                                          *
C  LOGICAL UNIT ASSIGNMENTS:                                               *
C                                                                          *
C    ( 2)     (NAMEOUT)       OUTPUT FILE: LINE, A-COEF, POP, E-BROAD      *
C    (14)     (NAMEPOP)       NAME OF NON-BOLTZMANN POP. FILE IF USED      *
C    (11)     (NAMEIN)        NAME OF BASIS STATE FILE                     *
C    (21)     (NAMEFD)        NAME OF HOOPER MICROFIELD FILE               *
C    (22)     (NAMEWID)       NAME OF E-BROAD. FILE IF NOT CALC. THIS RUN  *
C    (31)     (OUTRANGE.DAT) NAME OF E-BROAD. FILE IF CALC. THIS RUN       *
C                                                                          *
C**************************************************************************

      PROGRAM STARK
      IMPLICIT REAL*8 (A-H,O-Z)
      PARAMETER(BK=1.3807D-16)
      PARAMETER(PI=3.141592654D+00)
      PARAMETER(A0=0.529177D-08)
      PARAMETER(E0=4.80324D-10)
      PARAMETER(EMASS=9.10953D-28)
      PARAMETER(ECOUL=1.6D-19)
      PARAMETER(C0=2.997925D+10)
      PARAMETER(H0=6.6261961D-27)
      PARAMETER(HBAR=1.05459D-34)
      PARAMETER(COEFF=0.5D0*(2.D0*9.D11*A0*ECOUL**2/HBAR)**2)
      PARAMETER(IDMN=55)
      PARAMETER(INML=500)
      PARAMETER(ITRN=12*INML)

      CHARACTER*1 PERTURB,EBROAD,NAINT
      CHARACTER*1 ZEMAVG,POPBOLTZ,ORB(0:8)
      CHARACTER*24 NAMEIN,NAMEOUT,NAMEFD,NAMEWID,NAMEPOP

      DATA ORB/'S','P','D','F','G','H','I','J','K'/

      DIMENSION E(IDMN),PQN(IDMN),XLB(IDMN),IGROUP(IDMN)
      DIMENSION RME(10,20,20)
      DIMENSION ZNEW(INML,INML),EM(INML),PQNW(INML),
     &          XLW(INML),XMW(INML),NEND(INML)
      DIMENSION XG(100),WG(100)
      DIMENSION A(IDMN,IDMN),WR(IDMN),Z(IDMN,IDMN)
      DIMENSION XM(INML),EZWIDTH(IDMN,IDMN),XINDEW(INML)
      DIMENSION AMP2(ITRN),WWRI(ITRN),WWRJ(ITRN),XLAMB(ITRN)
      DIMENSION XEF(102),PF(102),ELWIDTH(ITRN)
      DIMENSION POP(IDMN,0:IDMN)
      DIMENSION IPQNW(ITRN),JPQNW(ITRN),IXLW(ITRN),JXLW(ITRN)
```

```
      COMMON/CONSTANTS/EVELOC,DEBYELN,DEBROGLN
      COMMON/ANS/PERTURB,EBROAD,NAINT
      COMMON/EZPARAM/E,PQN,XLB,IGROUP,NBASIS
      COMMON/RADIAL/RME
      COMMON/PLASM/EDENS,ETEMP,SPIN
      COMMON/IPARAM/NSTATE,NINIT,NFIN
      COMMON/FPARAM/ZNEW,EM,PQNW,XLW,XMW,NEND
      COMMON/GAUSS/ XG,WG,NGAUSS

 1299 FORMAT(1X,'K = ',I10, 'IS TOO LARGE',I10)
 1301 FORMAT(1X,F7.3,1P,4(2X,E10.4),2X,0P,F7.0,2X,I2,A,'-',I2,A)
 2000 FORMAT(3X, '-1. -1. -1. -1.')
 3000 FORMAT(1X,I10,2X,E14.6)
 9005 FORMAT(5X,I2,3X,I2,3X,1P,E12.3,3X,E12.3,3X,E12.3)

      DO 9999 ISPIN=1,2  ! END OF LOOP NEAR MAIN PROGRAM END STATEMENT

      IF(ISPIN.EQ.1) THEN
         WRITE(*,*) ' STARK BROADENING - SPIN 1...'
         OPEN(7,FILE='STARK1.SET',STATUS='OLD')
      ELSE IF (ISPIN.EQ.2) THEN
         WRITE(*,*) ' STARK BROADENING - SPIN 2...'
         OPEN(7,FILE='STARK2.SET',STATUS='OLD')
      END IF

      READ(7,'(A)')NAMEIN
      READ(7,*)XIDENS
      READ(7,*)EDENS
      READ(7,*)ETEMP
      READ(7,*)TEL
      READ(7,*)WVMIN
      READ(7,*)WVMAX
      READ(7,'(A)')NAMEOUT
      READ(7,'(A)')NAMEFD
      READ(7,*)NEPT
      READ(7,*)NINC
      READ(7,'(A)')EBROAD
      READ(7,'(A)')ZEMAVG
      READ(7,'(A)')NAMEWID
      READ(7,'(A)')POPBOLTZ
      READ(7,'(A)')NAMEPOP
      READ(7,'(A)')NAINT
      READ(7,*)NGAUSS

      CALL GAULEG(XG,WG,NGAUSS)    ! SETUP GAUSSIAN INTEGRATION

         NSTART=1
         ISTOP=0
         OPEN (2,FILE=NAMEOUT,STATUS='NEW')
         WRITE(2,'(1PE12.4)')XIDENS
         WRITE(2,'(F12.4)')ETEMP
         WRITE(2,'(F12.4)')TEL
      EDENS=EDENS*1.D16     ! ELECTRON DENSITY IN UNITS OF 1E16/CM3
      NM=IDMN

      IF (POPBOLTZ.EQ.'N') THEN
         OPEN(14,FILE=NAMEPOP,STATUS='OLD')  ! USER SUPPLIED POPULATION
         DO 20 I=1,100
            READ(14,*)NPQN,NXL,POP(NPQN,NXL)
            IF (NPQN.EQ.3.AND.NXL.EQ.0) GO TO 21
20       CONTINUE
21       CONTINUE
      ENDIF

      EVCM=8065.479           ! CONSTANTS AND UNIT CONVERSION FACTORS
      E02 = E0*E0
      CONST3 = (H0*C0)
```

```
      CONST5 = CONST3/BK      !CONST5 = 1/(0.695 CM-1/K)

      DO 30 I = 1,102     ! INITIALIZATION OF MICROFIELD VARIABLES
         XEF(I) = 0.0
         PF(I) = 0.0
30    CONTINUE

      DO 40 I = 1,IDMN    ! INITIALIZATION OF A(I,J)
      DO 40 J = 1,IDMN
         A(I,J) = 0.0
         Z(I,J) = 0.0
40    CONTINUE
      DO 41 I=1,ITRN
         ELWIDTH(I)=0.
41    CONTINUE

      OPEN(11,FILE=NAMEIN, STATUS = 'OLD') ! INPUT BASIS STATES IN
      READ(11,*)SPIN                       ! ORDER OF DECREASING L
      READ(11,*)NBASIS
         DO 50 I=1,NBASIS
         READ(11,*)PQN(I),XLB(I),E(I),IGROUP(I)
50    CONTINUE
      CLOSE(11)

      IF (SPIN.EQ.1.) CALL RADMATX1    ! READ IN RADIAL
      IF (SPIN.EQ.2.) CALL RADMATX2    ! MATRIX ELEMENTS
      LMAX=INT(XLB(1))
      MMAX=LMAX+1

      DO 51 I=1,MMAX                ! CALCULATE POSITIVE ML VALUES
         XM(I)=FLOAT(I-1)
51    CONTINUE

C STATIC ELECTRIC FIELDS DUE TO ION DENSITY, XIDENS=ION DENSITY IN
C UNITS OF 1E16 CM-3

      IF (EDENS.EQ.0.) EBROAD='N'
      IF (XIDENS.EQ.0.) THEN
         PF(1)=1.0
         XEF(1)=1.
         XEF(2)=2.
         NEPT=1
         NINC=1
      ELSE
         EDN = XIDENS*(1.0D+16)
         RM1 = 0.75/(PI*EDN)
         RM = RM1**(1./3.)
         RM2 = RM**2
         ELAMBDA = BK*ETEMP
         ELAMBDA = ELAMBDA*RM1
         ELAMBDA = SQRT(ELAMBDA/(3.0*E02))
         AA = RM/ELAMBDA
         AA=AA
         EF0 = ((300.0)*E0)/RM2     ! FIELD STRENGTH IN VOLTS/CM
         OPEN (21, FILE = NAMEFD, STATUS = 'OLD')  ! INPUT HOOPER'S
         DO 60 KN=1,NEPT                           ! MICROFIELD
            READ(21,*)XEF(KN),PF(KN)               ! DISTRIBUTION
60       CONTINUE
         CLOSE(21)
      END IF
      KH = ISTOP

C EVALUATE BROADENING: EVALUATE ELECTRON VELOCITY, DEBYE LENGTH,
C DEBROGLIE WAVELENGTH.

      EVELOC=SQRT(8.*BK*ETEMP/(PI*EMASS))
      DEBYELN=SQRT(BK*ETEMP/(4.*PI*EDENS*E0**2))
```

```
      DEBROGLN=H0/(EMASS*EVELOC)/(2.*PI)

C EVALUATE ELECTRON WIDTH FOR UNPERTURBED CASE:

      IF (EBROAD.EQ.'U') THEN
        IF (ZEMAVG.EQ.'R') THEN
           OPEN (22, FILE = NAMEWID, STATUS = 'OLD')
           DO 100 IE=1,NBASIS
           DO 100 JE=IE+1,NBASIS
              EZWIDTH(IE,JE)=0.
              READ(22,*)IDUM,JDUM,DUM,EZWIDTH(IE,JE)
                IDUM=IDUM    ! SET DUMMY VARIABLES EQUAL TO SELF FOR
                JDUM=JDUM    ! A CLEAN COMPILE
                DUM=DUM      !
              EZWIDTH(JE,IE)=EZWIDTH(IE,JE)
100        CONTINUE
         ELSE IF (ZEMAVG.EQ.'C') THEN
           DO 110 IE=1,NBASIS
           DO 110 JE=IE+1,NBASIS
              IF (IE.NE.JE) THEN
                 EZWIDTH(IE,JE)=0.
                 NINIT=IE
                 NFIN=JE
                 CALL ELBAVG(EWIDTH,XSECT)
                 EZWIDTH(IE,JE)=EWIDTH
                 EZWIDTH(JE,IE)=EZWIDTH(IE,JE)
             END IF
110        CONTINUE
         ENDIF
      ENDIF

      DO 1000 KN = NSTART,NEPT,NINC ! LOOP THRU QUASISTAT FIELD: FIND
         NSTATE=0                   ! TRANSITIONS FOR EA FIELD VALUE

         DO 1100 ML=1,MMAX     ! BLOCK DIAGONALIZATION ACCORDING TO ML
            N=0
            DO 1105 I=1,NBASIS                              ! DETERMINE
               IF (XLB(I).LT.ABS(XM(ML))) GO TO 1106 ! SIZE OF
               N=N+1                                        ! MATRIX TO BE
1105        CONTINUE                                        ! DIAGONALIZED
1106        CONTINUE

C CALCULATE OFF-DIAGONAL MATRIX ELEMENTS (ANGULAR AND RADIAL)

            DO 1110 I=1,N
            DO 1110 J=I+1,N
               CALL ANGME(XLB(I),XM(ML),XLB(J),XM(ML),AME)
               IF (AME.EQ.0.) THEN
                  A(I,J)=0.
               ELSE
                  XLN1=XLB(I)
                  XLN2=XLB(J)
                  PN1=PQN(I)
                  PN2=PQN(J)
                  IF (XLN1.LT.XLN2) THEN
                     XLN1=XLN2
                     PTEMP=PN2
                     PN2=PN1
                     PN1=PTEMP
                  END IF
                  IXLN1=INT(XLN1)
                  IPN1=INT(PN1)
                  IPN2=INT(PN2)
                  RADIALME=RME(IXLN1,IPN1,IPN2)
                  IF (RADIALME.EQ.0.) THEN
                     WRITE(2,*)IXLN1,IPN1,IPN2,RADIALME
                  END IF
```

```
                  A(I,J)=-AME*RADIALME*A0*XEF(KN)*EF0*EVCM
               END IF
               A(J,I)=A(I,J)
1110        CONTINUE

            DO 1120 I=1,N    ! DIAGONAL ELEMENTS ARE THE ZERO FIELD
               A(I,I)=E(I)   ! ENERGY LEVELS
1120        CONTINUE

            CALL JACOBI(A,N,NM,WR,Z,NROT)    ! MATRIX DIAGONALIZATION

C RELABEL ML STATES

            DO 1130 I=1,N
               NSTATE=NSTATE+1
               XINDEW(NSTATE)=FLOAT(I)
               NEND(NSTATE)=N
               EM(NSTATE)=WR(I)
               XMW(NSTATE)=XM(ML)
               PQNW(NSTATE)=PQN(I)
               XLW(NSTATE)=XLB(I)
               IF (N.EQ.1) THEN
                   ZNEW(1,NSTATE)=Z(1,1)
               ELSE
                  DO 1131 K=1,N
                     ZNEW(K,NSTATE) = Z(K,I)
1131              CONTINUE
               ENDIF
1130        CONTINUE
1100     CONTINUE

C EVALUATED TRANSITION FREQUENCIES AND PROBABILITIES:

         K=0
         DO 1200 IM=1,NSTATE
         DO 1200 JM=IM+1,NSTATE
            WWWX = ABS(XMW(IM)-XMW(JM))
            WWX  = ABS(EM(IM)-EM(JM))
            XLAMBDA = 10000.0/MAX(100.0D0,WWX)
            IF (WWWX    .LE. 1.    .AND.
     &          WWX     .GE. 100.0 .AND.
     &          XLAMBDA .LE. WVMAX .AND.
     &          XLAMBDA .GE. WVMIN
     &         ) THEN

C EVALUATE DIPOLE MOMENT MATRIX ELEMENTS BETWEEN PERTURBED
C WAVEFUNCTIONS FOR A DELTA ML=0,+1,-1 TRANSITION

               TAMP=0.
               DO 1210 II=1,NEND(IM)
               DO 1210 JJ=1,NEND(JM)
                  CALL ANGME(XLB(II),XMW(IM),XLB(JJ),XMW(JM),AME)
                  IF (AME.NE.0.) THEN
                     XLN1=XLB(II)
                     XLN2=XLB(JJ)
                     PN1=PQN(II)
                     PN2=PQN(JJ)
                     IF (XLN1.LT.XLN2) THEN
                        XLN1=XLN2
                        PTEMP=PN2
                        PN2=PN1
                        PN1=PTEMP
                     END IF
                     IXLN1=INT(XLN1)
                     IPN1=INT(PN1)
                     IPN2=INT(PN2)
                     RADIALME=RME(IXLN1,IPN1,IPN2)
```

```
                  IF (RADIALME.EQ.0.) THEN
                     WRITE(2,*)SPIN,XLN1,PN1,PN2,RADIALME
                  END IF
                  TAMP=TAMP+ZNEW(II,IM)*ZNEW(JJ,JM)*AME*RADIALME
               END IF
1210           CONTINUE
               ZA=TAMP*E0*A0
               ZA2 = ZA**2
               ZA2 = ZA2*((WWX)**3)
               ZA2 = ZA2*(64*(PI**4)/(3*H0))

C ACCOUNT FOR ML=-ML DEGENERACY:

               IF ((XMW(IM).NE.0.) .OR. (XMW(JM).NE.0.)) ZA2=2.*ZA2
               IF (ZA2.LT.0.) WRITE(2,*)IM,JM,ZA2
               IF(ZA2 .GE. 1000.0) THEN
                  K = K + 1
                  XLAMB(K) = XLAMBDA
                  WWRI(K) = EM(IM)
                  WWRJ(K) = EM(JM)
                  AMP2(K) = ZA2
                  IPQNW(K)=PQNW(IM)
                  JPQNW(K)=PQNW(JM)
                  IXLW(K)=XLW(IM)
                  JXLW(K)=XLW(JM)
                  IF (EBROAD.EQ.'U') THEN
                     ICOUNT=INT(XINDEW(IM))
                     JCOUNT=INT(XINDEW(JM))
                     ELWIDTH(K)=EZWIDTH(ICOUNT,JCOUNT)
                  ELSE IF (EBROAD.EQ.'S') THEN
                     PERTURB='N'
                     NINIT=IM
                     NFIN=JM
                     CALL ELECBR(EWIDTH)
                     ELWIDTH(K)=EWIDTH
                  ELSE IF (EBROAD.EQ.'P') THEN
                     PERTURB='Y'
                     NINIT=IM
                     NFIN=JM
                     CALL ELECBR(EWIDTH)
                     ELWIDTH(K)=EWIDTH
                  ENDIF
               ENDIF
            END IF
1200     CONTINUE
         IF (K.GT.ITRN) THEN
            OPEN(31,FILE='OUTRANGE.DAT',STATUS='UNKNOWN')
            WRITE(31,1299) K,KN
            CLOSE(31)
         ENDIF
         KH = KH + K
         AMP2SUM=0.

C DETERMINE THE UPPER LEVEL POPULATION OF A TRANSITION:

         DO 1300 KI = 1,K
            IF (WWRI(KI) .GE. WWRJ(KI)) THEN
               WWE = WWRI(KI)
               DENP=POP(IPQNW(KI),IXLW(KI))
            ELSE
               WWE = WWRJ(KI)
               DENP=POP(JPQNW(KI),JXLW(KI))
            END IF
            ENERGY = WWE*CONST5
            DEN = (2.*SPIN+1)*EXP(-ENERGY/TEL)
            IF (POPBOLTZ.EQ.'N') DEN=DENP
            IF (KN.EQ.1) THEN
```

```
               DELX=(XEF(1+NINC)-XEF(1))
            ELSE IF ((NEPT-KN).LT.NINC)THEN
               DELX=XEF(KN)-XEF(KN-NINC)
            ELSE
               DELX=0.5*((XEF(KN)-XEF(KN-NINC))
     &              +(XEF(KN+NINC)-XEF(KN)))
            END IF
            DEN = DEN*PF(KN)*DELX           ! WEIGHT DENSITY BY
            IF (EDENS.EQ.0) ELWIDTH(KI)=-2. ! MF DISTRIB. P(E)DE

            IF (DEN.EQ.0.) GOTO 1290
          WRITE(2,1301) XLAMB(KI),AMP2(KI),DEN,ELWIDTH(KI),PF(KN),
     &      ENERGY,IPQNW(KI),ORB(IXLW(KI)),JPQNW(KI),ORB(JXLW(KI))
          WRITE(*,1301) XLAMB(KI),AMP2(KI),DEN,ELWIDTH(KI),PF(KN),
     &      ENERGY,IPQNW(KI),ORB(IXLW(KI)),JPQNW(KI),ORB(JXLW(KI))
1290        CONTINUE

            AMP2SUM=AMP2SUM+AMP2(KI)
1300      CONTINUE
          WRITE(*,*) ' END OF PASS: ',KN
1000    CONTINUE


        WRITE(2,2000)
        WRITE(2,3000) KH,AMP2SUM/(1.D8)
        CLOSE(2)

 9999   CONTINUE
        STOP
        END


        SUBROUTINE ELBAVG(EWIDTH,XSECT)
C*************************************************************************
C                                                                        *
C     THIS SUBROUTINE CALCULATES ELECTRON WIDTHS USING                   *
C     UNPERTURBED WAVEFUNCTIONS AND ENERGY LEVELS WITH                   *
C     WITH AN ANALYTICAL APPROXIMATION FOR THE INTEGRAL                  *
C                                                                        *
C*************************************************************************
        IMPLICIT REAL*8 (A-H,O-Z)
        PARAMETER(C0=2.997925D+10)
        PARAMETER(IDMN=55)          ! MUST BE > NBASIS
        PARAMETER(INML=500)         ! MUST BE > # OF M TRANSITIONS
        PARAMETER(ITRN=12*INML)     ! MUST > (L+1)*INML
        COMMON/CONSTANTS/EVELOC,DEBYELN,DEBROGLN
        COMMON/ANS/PERTURB,EBROAD,NAINT
        COMMON/EZPARAM/E,PQN,XLB,IGROUP,NBASIS
        COMMON/RADIAL/RME
        COMMON/PLASM/EDENS,ETEMP,SPIN
        COMMON/INTEGL/WAB,B,XMEXSUM2,XMEZSUM2
        COMMON/IPARAM/NSTATE,NINIT,NFIN
        CHARACTER*1 PERTURB,EBROAD,NAINT
        DIMENSION E(IDMN),PQN(IDMN),XLB(IDMN),IGROUP(IDMN)
        DIMENSION RME(10,20,20)
        DIMENSION XMEXSUM2(2,IDMN),XMEZSUM2(2,IDMN)
        DIMENSION XMW(IDMN),XMP(IDMN)
        EXTERNAL F3

C L=1 IS THE INITIAL STATE OF THE TRANSITION
C L=2 IS THE FINAL STATE OF THE TRANSTION

        DO 1000 L=1,2
          IF (L.EQ.1) NTRANS=NINIT
          IF (L.EQ.2) NTRANS=NFIN
           DO 1100  MP=1,NBASIS
              XMEXSUM2(L,MP)=0.
```

```
            XMEZSUM2(L,MP)=0.
            IF (MP.NE.NTRANS  .AND.
     &           IGROUP(MP).EQ.IGROUP(NTRANS) .AND.
     &           ABS( XLB(NTRANS)-XLB(MP) ).LE.1. .AND.
     &           ABS( XLB(NTRANS)-XLB(MP) ).NE.0.) THEN
               XLN1=XLB(NTRANS)
               XLN2=XLB(MP)
               PN1=PQN(NTRANS)
               PN2=PQN(MP)
               IF (XLN1.LT.XLN2) THEN
                  XLN1=XLN2
                  PTEMP=PN2
                  PN2=PN1
                  PN1=PTEMP
               ENDIF
               IXLN1=INT(XLN1)
               IPN1=INT(PN1)
               IPN2=INT(PN2)
               MLEND=INT(XLB(NTRANS)+1.)
               MPLEND=INT(XLB(MP)+1.)
               IF (MLEND.GE.IDMN .OR. MPLEND.GE.IDMN) THEN
                 WRITE(*,*)'MLEND',MLEND,'MPLEND',MPLEND,IDMN
               ENDIF
               DO 1110 ML=1,MLEND
                  XMW(ML)=XLB(NTRANS)-FLOAT(ML)+1.
                  DO 1111 MPL=1,MPLEND
                     XMP(MPL)=XLB(MP)-FLOAT(MPL)+1.
                     XXXX = ABS(XMW(ML)-XMP(MPL))
                     IF (XXXX.LE.1.) THEN
                        IF (XXXX.EQ.1.) THEN
                           CALL ANGXME(XLB(NTRANS),XMW(ML),XLB(MP),
     &                                 XMP(MPL),AME)
                           CZ=2.
                           XMEM=AME*RME(IXLN1,IPN1,IPN2)
                           XMEXSUM2(L,MP)=XMEXSUM2(L,MP)+CZ*XMEM**2
                        ELSE IF (XXXX.EQ.0.) THEN
                           CALL ANGZME(XLB(NTRANS),XMW(ML),XLB(MP),
     &                                 XMP(MPL),AME)
                           CZ=2.
                           IF ((XMP(MPL).EQ.0.).AND.(XMW(ML).EQ.0.))
     &                        CZ=1.
                           XMEM=AME*RME(IXLN1,IPN1,IPN2)
                           XMEZSUM2(L,MP)=XMEZSUM2(L,MP)+CZ*XMEM**2
                        ENDIF
                     ENDIF
1111              CONTINUE
1110           CONTINUE
            ENDIF
1100     CONTINUE
1000  CONTINUE

C INTEGRATE FROM SMALL B TO LARGE B

      AA=0.0D0
      BB=DEBYELN
      CALL QGAUS(F3,AA,BB,XSECT)

C CALCULATION OF CROSS SECTION AND ELECTRON BROADENED LINE HALF-WIDTH
C IN WAVENUMBER

C      XSECTD=DEBROGLN**2
      EWIDTH=EDENS*EVELOC*XSECT/C0  ! WHERE'S THE 2*PI ?
      IF (EWIDTH.LT.1.E-4) EWIDTH=0.
      RETURN
      END
```

```
      SUBROUTINE S2U(TD,S2C)
C*************************************************************************
C THE FOLLOWING SUBROUTINE CALCULATES THE QUANTITY S2(B)                  *
C*************************************************************************
      IMPLICIT REAL*8 (A-H,O-Z)
      PARAMETER(BK=1.3807D-16)
      PARAMETER(PI=3.141592654D+00)
      PARAMETER(A0=0.529177D-08)
      PARAMETER(ECOUL=1.6D-19)
      PARAMETER(C0=2.997925D+10)
      PARAMETER(HBAR=1.05459D-34)
      PARAMETER(COEFF=0.5D0*(2.D0*9.D11*A0*ECOUL**2/HBAR)**2)
      PARAMETER(IDMN=55)       ! MUST BE > NBASIS
      PARAMETER(INML=500)      ! MUST BE > # OF TRANSITIONS
      PARAMETER(ITRN=12*INML) ! MUST BE > (L+1)*INML

      COMMON/CONSTANTS/EVELOC,DEBYELN,DEBROGLN
      COMMON/ANS/PERTURB,EBROAD,NAINT
      COMMON/EZPARAM/E,PQN,XLB,IGROUP,NBASIS
      COMMON/INTEGL/WAB,B,XMEXSUM2,XMEZSUM2
      COMMON/IPARAM/NSTATE,NINIT,NFIN
      CHARACTER*1 PERTURB,EBROAD,NAINT
      DIMENSION E(IDMN),PQN(IDMN),XLB(IDMN),IGROUP(IDMN)
      DIMENSION XMEXSUM2(2,IDMN),XMEZSUM2(2,IDMN)
      DIMENSION S2SUM(2)
      EXTERNAL BESSK0,BESSK1,BESSI0,BESSI1,F1,F2

C L=1 IS THE INITIAL STATE OF THE TRANSITION
C L=2 IS THE FINAL STATE OF THE TRANSITION

      XCO=2.*PI*C0
      ZERO=0.D0
      DO 100 L = 1,2
         IF (L.EQ.1) NTRANS=NINIT
         IF (L.EQ.2) NTRANS=NFIN
         S2SUM(L)=0.
         DO 110  MP=1,NBASIS
            IF (XMEXSUM2(L,MP).NE.0. .OR.
     &          XMEZSUM2(L,MP).NE.0.) THEN
               WAB=ABS(E(MP)-E(NTRANS))*XCO
               IF (NAINT.EQ.'Y') THEN
                 CALL QROMB(F1,ZERO,TD,X1T)
                 CALL QROMB(F2,ZERO,TD,X2T)
               ELSE
                 AVAR=B*WAB/EVELOC
                 BK0=BESSK0(AVAR)
                 IF (BK0.LT.1.E-30) BK0=0.
                 X1T=AVAR*BK0/(B*EVELOC)
                 BK1=BESSK1(AVAR)
                 IF (BK1.LT.1.E-30) BK1=0.
                 X2T=BK1*WAB/EVELOC**2
               ENDIF
               S2T=XMEZSUM2(L,MP)*X1T**2+XMEXSUM2(L,MP)*X2T**2
               S2SUM(L)=S2SUM(L)+S2T
            ENDIF
110      CONTINUE
         S2SUM(L)=S2SUM(L)/(2.*XLB(NTRANS)+1.)
100   CONTINUE
      S2C=COEFF*(S2SUM(1)+S2SUM(2))
      RETURN
      END


      FUNCTION F1(TIME)
C*************************************************************************
C TIME INTEGRANDS                                                         *
C*************************************************************************
```

```
      IMPLICIT REAL*8 (A-H,O-Z)

C MUST BE  GREATER THAN NBASIS (55)
      PARAMETER(IDMN=55)
      COMMON/CONSTANTS/EVELOC,DEBYELN,DEBROGLN
      COMMON/INTEGL/WAB,B,XMEXSUM2,XMEZSUM2
      DIMENSION XMEXSUM2(2,IDMN),XMEZSUM2(2,IDMN)
      F1TOP=EVELOC*TIME*SIN(WAB*TIME)
      F1BOT=SQRT((B**2+(EVELOC*TIME)**2)**3)
      F1=F1TOP/F1BOT
      RETURN
      END


      FUNCTION F2(TIME)
      IMPLICIT REAL*8 (A-H,O-Z)

      PARAMETER(IDMN=55)    ! MUST BE > NBASIS
      COMMON/CONSTANTS/EVELOC,DEBYELN,DEBROGLN
      COMMON/INTEGL/WAB,B,XMEXSUM2,XMEZSUM2
      DIMENSION XMEXSUM2(2,IDMN),XMEZSUM2(2,IDMN)

      F2TOP=B*COS(WAB*TIME)
      F2BOT=SQRT((B**2+(EVELOC*TIME)**2)**3)
      F2=F2TOP/F2BOT
      RETURN
      END


      FUNCTION F3(CS)
      IMPLICIT REAL*8 (A-H,O-Z)
      PARAMETER(IDMN=55)    ! MUST BE > NBASIS
      COMMON/CONSTANTS/EVELOC,DEBYELN,DEBROGLN
      COMMON/INTEGL/WAB,B,XMEXSUM2,XMEZSUM2
      DIMENSION XMEXSUM2(2,IDMN),XMEZSUM2(2,IDMN)

      B=CS
C     IF (B.LT.DEBROGLN) THEN
        IF (B.LE.0.0D0) THEN
          F3 = 0.D0
          RETURN
      ELSE
        HYPO=MAX(0.D0,DEBYELN**2-B**2)
        TD=SQRT(HYPO)/EVELOC
        CALL S2U(TD,S2C)
        S2C = MIN(S2C,1.D0)
        F3=S2C*B
        RETURN
      ENDIF
      END


      SUBROUTINE ELECBR(EWIDTH)
C*************************************************************************
C  THIS SUBROUTINE CALCULATES ELECTRON WIDTHS FOR THE SEMI-PERTURBED      *
C  AND FULY-PERTURBED CASES WITH AN ANALYTICAL APPROXIMATION FOR THE      *
C  INTEGRAL                                                               *
C*************************************************************************
      IMPLICIT REAL*8 (A-H,O-Z)
      PARAMETER(PI=3.141592654D+00)
      PARAMETER(C0=2.997925D+10)
      PARAMETER(IDMN=55)   ! MUST BE > NBASIS
      PARAMETER(INML=500) ! MUST BE > INML
      PARAMETER(ITRN=12*INML)   ! MUST BE > (L+1)*INML
      COMMON/CONSTANTS/EVELOC,DEBYELN,DEBROGLN
      COMMON/ANS/PERTURB,EBROAD,NAINT
      COMMON/FPARAM/ZNEW,EM,PQNW,XLW,XMW,NEND
```

```
      COMMON/INTEGL/WAB,B,XMEXSUM2,XMEZSUM2
      COMMON/IPARAM/NSTATE,NINIT,NFIN
      COMMON/PLASM/EDENS,ETEMP,SPIN
      CHARACTER*1 PERTURB,EBROAD,NAINT
      DIMENSION ZNEW(INML,INML),EM(INML),PQNW(INML),XLW(INML),
     &          XMW(INML),NEND(INML)
      DIMENSION XMEXSUM2(2,IDMN),XMEZSUM2(2,IDMN)
      EXTERNAL F4

C UNITS

C      AA=DEBROGLN
C      BB=DEBYELN
C      CALL QGAUS(F4,AA,BB,XSECT)
C      XSECT=XSECT+PI*DEBROGLN*DEBROGLN
      AA=0.0D0
      BB=DEBYELN
      CALL QGAUS(F4,AA,BB,XSECT)

C CALCULATION OF CROSS SECTION AND ELECTRON HALF-WIDTH IN WAVENUMBER

C      XSECTD=PI*DEBROGLN**2
      EWIDTH=EDENS*EVELOC*XSECT/C0
      IF (EWIDTH.LT.1.E-4) EWIDTH=0.
      RETURN
      END


      SUBROUTINE S2SPBESS(TD,S2)
C*****************************************************************************
C  THE FOLLOWING SOUBROUTINE CALCULATES THE QUANTITY S2(B)                    *
C*****************************************************************************
      IMPLICIT REAL*8 (A-H,O-Z)
      PARAMETER(PI=3.141592654D+00)
      PARAMETER(A0=0.529177D-08)
      PARAMETER(ECOUL=1.6D-19)
      PARAMETER(C0=2.997925D+10)
      PARAMETER(HBAR=1.05459D-34)
      PARAMETER(COEFF=0.5D0*(2.D0*9.D11*A0*ECOUL**2/HBAR)**2)
      PARAMETER(IDMN=55)       ! MUST BE > NBASIS
      PARAMETER(INML=500)      ! MUST BE > # OF TRANSITIONS
      PARAMETER(ITRN=12*INML) ! MUST BE > (L+1)*INML
      COMMON/CONSTANTS/EVELOC,DEBYELN,DEBROGLN
      COMMON/ANS/PERTURB,EBROAD,NAINT
      COMMON/EZPARAM/E,PQN,XLB,IGROUP,NBASIS
      COMMON/FPARAM/ZNEW,EM,PQNW,XLW,XMW,NEND
      COMMON/RADIAL/RME
      COMMON/INTEGL/WAB,B,XMEXSUM2,XMEZSUM2
      COMMON/IPARAM/NSTATE,NINIT,NFIN
      COMMON/PLASM/EDENS,ETEMP,SPIN
      CHARACTER*1 PERTURB,EBROAD,NAINT
      DIMENSION E(IDMN),PQN(IDMN),XLB(IDMN),IGROUP(IDMN)
      DIMENSION ZNEW(INML,INML),EM(INML),PQNW(INML),XLW(INML),
     &                    XMW(INML),NEND(INML)
      DIMENSION RME(10,20,20)
      DIMENSION XMEXSUM2(2,IDMN),XMEZSUM2(2,IDMN)
      DIMENSION S2SUM(2)
      EXTERNAL BESSK0,BESSK1,BESSI0,BESSI1,F1,F2

C L=1 IS THE INITIAL STATE OF THE TRANSITION
C L=2 IS THE FINAL STATE OF THE TRANSITION

      XC0=2.*PI*C0
      ZERO=0.0D0
      DO 1000 L=1,2
         IF (L.EQ.1) NTRANS=NINIT
         IF (L.EQ.2) NTRANS=NFIN
```

```
          S2SUM(L)=0.
          DO 1100  M=1,NSTATE
             IF (M.NE.NTRANS) THEN

C ION-PERTURBED STATES AND ENERGIES

                IF (PERTURB.EQ.'Y') THEN
                   WAB=ABS(EM(NTRANS)-EM(M))*XCO
                   IF (NAINT.EQ.'Y') THEN
                     CALL QROMB(F1,ZERO,TD,X1T)
                     CALL QROMB(F2,ZERO,TD,X2T)
                   ELSE
                     AVAR=B*WAB/EVELOC
                     BK0=BESSK0(AVAR)
                     IF (BK0.LT.1.E-30) BK0=0.
                     X1T=AVAR*BK0/(B*EVELOC)
                     BK1=BESSK1(AVAR)
                     IF (BK1.LT.1.E-30) BK1=0.
                     X2T=BK1*WAB/EVELOC**2
                   ENDIF
                   DO 1110 II=1,NEND(NTRANS)
                      IF (ABS(ZNEW(II,NTRANS)).GT.0.01) THEN
                         DO 1111 JJ=1,NEND(M)
                            IF (ABS(ZNEW(JJ,M)).GT.0.01) THEN
                               CALL ANGZME(XLB(II),XMW(NTRANS),
     &                                     XLB(JJ),XMW(M),AZME)
                               CALL ANGXME(XLB(II),XMW(NTRANS),
     &                                     XLB(JJ),XMW(M),AXME)
                               IF ((AZME.NE.0.).OR.(AXME.NE.0.)) THEN
                                  XLN1=XLB(II)
                                  XLN2=XLB(JJ)
                                  PN1=PQN(II)
                                  PN2=PQN(JJ)
                                  IF (XLN1.LT.XLN2) THEN
                                     XLN1=XLN2
                                     PTEMP=PN2
                                     PN2=PN1
                                     PN1=PTEMP
                                  ENDIF
                                  IXLN1=INT(XLN1)
                                  IPN1=INT(PN1)
                                  IPN2=INT(PN2)
                                  RADIALME=RME(IXLN1,IPN1,IPN2)
                                  IF (RADIALME.NE.0.) THEN
                                     XMEZM=AZME*RADIALME*ZNEW(II,NTRANS)
     &                                    *ZNEW(JJ,M)
                                     XMEXM=AXME*RADIALME*ZNEW(II,NTRANS)
     &                                    *ZNEW(JJ,M)
                                     CZ=1.
                                     IF ((XMW(M).NE.0.) .OR.
     &                                   (XMW(NTRANS).NE.0.)) CZ=2.
                                     S2T= CZ*(XMEZM**2)*X1T**2
     &                                  + 2.*(XMEXM**2)*X2T**2
                                     S2SUM(L)=S2SUM(L)+S2T
                                  ENDIF
                               ENDIF
                            ENDIF
1111                     CONTINUE
                      ENDIF
1110                CONTINUE
                ELSE

C SEMI-PERTURBED CASE: UNPERTURBED WAVEFUNCTIONS AND PERTURBED ENERGIES

                   CALL ANGME(XLW(NTRANS),XMW(NTRANS),
     &                        XLW(M     ),XMW(M     ),AME)
                   IF (AME.NE.0.) THEN
```

```
                    CALL ANGZME(XLW(NTRANS),XMW(NTRANS),
     &                         XLW(M),XMW(M),AZME)
                    CALL ANGXME(XLW(NTRANS),XMW(NTRANS),
     &                         XLW(M),XMW(M),AXME)
                    XLN1=XLW(NTRANS)
                    XLN2=XLW(M)
                    PN1=PQNW(NTRANS)
                    PN2=PQNW(M)
                    IF (XLN1.LT.XLN2) THEN
                       XLN1=XLN2
                       PTEMP=PN2
                       PN2=PN1
                       PN1=PTEMP
                    ENDIF
                    IXLN1=INT(XLN1)
                    IPN1=INT(PN1)
                    IPN2=INT(PN2)
                    XMEZM = AZME*RME(IXLN1,IPN1,IPN2)
                    XMEXM = AXME*RME(IXLN1,IPN1,IPN2)
                    WAB=ABS(EM(M)-EM(NTRANS))*XCO
                    IF (NAINT.EQ.'Y') THEN
                      CALL QROMB(F1,ZERO,TD,X1T)
                      CALL QROMB(F2,ZERO,TD,X2T)
                    ELSE
                      AVAR=B*WAB/EVELOC
                      BK0=BESSK0(AVAR)
                      IF (BK0.LT.1.E-30) BK0=0.
                      X1T=AVAR*BK0/(B*EVELOC)
                      BK1=BESSK1(AVAR)
                      IF (BK1.LT.1.E-30) BK1=0.
                      X2T=BK1*WAB/EVELOC**2
                    ENDIF
                    CZ=1.
                    IF ((XMW(M).NE.0.).OR.(XMW(NTRANS).NE.0.))CZ=2.
                    S2T=CZ*(XMEZM**2)*X1T**2 + 2.*(XMEXM**2)*X2T**2
                    S2SUM(L)=S2SUM(L)+S2T
                  ENDIF
                ENDIF
              ENDIF
1100        CONTINUE
1000    CONTINUE
        S2=COEFF*(S2SUM(1)+S2SUM(2))
        RETURN
        END


        FUNCTION F4(CS)
        IMPLICIT REAL*8 (A-H,O-Z)
        PARAMETER(IDMN=55)   ! MUST BE > NBASIS
        COMMON/CONSTANTS/EVELOC,DEBYELN,DEBROGLN
        COMMON/INTEGL/WAB,B,XMEXSUM2,XMEZSUM2
        DIMENSION XMEXSUM2(2,IDMN),XMEZSUM2(2,IDMN)

        B=CS
C        IF (B.LE.0) THEN
        IF (B.LE.DEBROGLN) THEN
          F4 = 0.
          RETURN
        ELSE
          HYPO=MAX(0.D0,DEBYELN**2-B**2)
          TD=SQRT(HYPO)/EVELOC
          CALL S2SPBESS(TD,S2C)
          S2C = MIN(S2C,1.D0)
          F4=S2C*B
          RETURN
        ENDIF
        END
```

```
      SUBROUTINE ANGME(XL1,XM1,XL2,XM2,AME)
C*****************************************************************************
C  ANGULAR MATRIX ELEMENT FORMULAS FROM CHUN LIN                              *
C*****************************************************************************
      IMPLICIT REAL*8 (A-H,O-Z)
      DELL=XL2-XL1
      DELM=XM2-XM1
      AME=0.
      IF (DELL.EQ.1) THEN
        IF (DELM.EQ.1) THEN
          AME = -SQRT((XL1+XM1+1.)*(XL1+XM1+2.)
     &          /(2.0*(2.*XL1+1.)*(2.*XL1+3.)))
        ELSE IF (DELM.EQ.-1.) THEN
          AME =  SQRT((XL1-XM1+1.)*(XL1-XM1+2.)
     &          /(2.0*(2.*XL1+1.)*(2.*XL1+3.)))
        ELSE IF (DELM.EQ.0.) THEN
          AME =  SQRT((XL1-XM1+1.)*(XL1+XM1+1.)
     &          /((2.*XL1+1.)*(2.*XL1+3.)))
        ENDIF
      ELSE IF (DELL.EQ.-1.) THEN
        IF (DELM.EQ.1.) THEN
          AME =  SQRT((XL1-XM1)*(XL1-XM1-1.)
     &          /(2.0*(2.*XL1-1.)*(2.*XL1+1.)))
        ELSE IF (DELM.EQ.-1.) THEN
          AME = -SQRT((XL1+XM1)*(XL1+XM1-1.)
     &          /(2.0*(2.*XL1-1.)*(2.*XL1+1.)))
        ELSE IF (DELM.EQ.0.) THEN
          AME =  SQRT((XL1+XM1)*(XL1-XM1)
     &          /((2.*XL1-1.)*(2.*XL1+1.)))
        ENDIF
      ENDIF
      RETURN
      END


      SUBROUTINE ANGZME(XL1,XM1,XL2,XM2,AME)
C*****************************************************************************
C  Z-DIRECTION COSINES ANGULAR MATRIX ELEMENT FORMULAS FROM CHUN LIN           *
C*****************************************************************************
      IMPLICIT REAL*8 (A-H,O-Z)

      DELL=XL2-XL1
      DELM=XM2-XM1
      AME=0.
      IF (DELL.EQ.1.) THEN
        IF (DELM.EQ.0.) THEN
          AME =  SQRT((XL1-XM1+1.)*(XL1+XM1+1.)
     &          /((2.*XL1+1.)*(2.*XL1+3.)))
        ENDIF
      ELSE IF (DELL.EQ.-1.) THEN
        IF (DELM.EQ.0.) THEN
          AME =  SQRT((XL1+XM1)*(XL1-XM1)
     &          /((2.*XL1-1.)*(2.*XL1+1.)))
        ENDIF
      ENDIF
      RETURN
      END


      SUBROUTINE ANGXME(XL1,XM1,XL2,XM2,AME)
C*****************************************************************************
C  X-DIRECTION COSINES ANGULAR MATRIX ELEMENT FORMULAS FROM CHUN LIN           *
C*****************************************************************************
      IMPLICIT REAL*8 (A-H,O-Z)
```

```
      DELL=XL2-XL1
      DELM=XM2-XM1
      AME=0.
      IF (DELL.EQ.1.) THEN
        IF (DELM.EQ.1.) THEN
          AME = -0.5*SQRT((XL1+XM1+1.)*(XL1+XM1+2.)
     &          /((2.*XL1+1.)*(2.*XL1+3.)))
        ELSE IF (DELM.EQ.-1.) THEN
          AME =  0.5*SQRT((XL1-XM1+1.)*(XL1-XM1+2.)
     &          /((2.*XL1+1.)*(2.*XL1+3.)))
        ENDIF
      ELSE IF (DELL.EQ.-1.) THEN
        IF (DELM.EQ.1.) THEN
          AME =  0.5*SQRT((XL1-XM1)*(XL1-XM1-1.)
     &               /((2.*XL1-1.)*(2.*XL1+1.)))
        ELSE IF (DELM.EQ.-1.) THEN
          AME = -0.5*SQRT((XL1+XM1)*(XL1+XM1-1.)
     &               /((2.*XL1-1.)*(2.*XL1+1.)))
        ENDIF
      ENDIF
      RETURN
      END


C*********************************************************************
C  FUNCTION INTEGRATOR FROM NUMERICAL RECIPES [PRESS ET AL.].        *
C                                                                    *
C  RETURNS AS SS THE INTEGRAL OF THE FUNCTION FUNC FROM A TO B.      *
C  INTEGRATION IS PERFORMED BY ROMBERG'S METHOD OF ORDER 2K, WHERE,  *
C  E.G., K=2 IS SIMPSON'S RULE.                                      *
C*********************************************************************

      SUBROUTINE QROMB(FUNC,A,B,SS)
C*********************************************************************
C  HERE EPS IS THE FRACTIONAL ACCURACY DESIRED, AS DETERMINED BY THE  *
C  EXTRAPOLATION ERROR ESTIMATE; JMAX LIMITS THE TOTAL NUMBER OF STEPS;*
C  K IS THE NUMBER OF POINTS USED IN THE EXTRAPOLATION. THE S AND H   *
C  PARAMETERS STORE THE SUCCESSIVE TRAPEZOIDAL APPROXIMATIONS         *
C  AND THEIR RELATIVE STEP-SIZES.                                     *
C*********************************************************************
      IMPLICIT REAL*8(A-H,O-Z)
      PARAMETER (EPS=1.E-3, JMAX=150, JMAXP=JMAX+1, K=2, KM=K-1)

   DIMENSION S(JMAXP), H(JMAXP)
       EXTERNAL FUNC
   H(1)=1.
   DO 11 J=1,JMAX
      CALL TRAPZD(FUNC,A,B,S(J),J)
      IF (J.GE.K) THEN
         CALL POLINT(H(J-KM),S(J-KM),K,0.,SS,DSS)
      IF (ABS(DSS).LT.EPS*ABS(SS)) RETURN
      ENDIF
      S(J+1)=S(J)

C  THE FOLLOWING IS A KEY STEP.  THE FACTOR IS 0.25 EVEN THOUGH THE
C  STEP-SIZE IS DECREASED BY ONLY 0.5.  THIS MAKES THE EXTRAPOLATION
C  A POLYNOMIAL IN H**2 AS ALLOWED BY EQUATION (4.2.1), NOT JUST A
C  POLYNOMIAL IN H.

      H(J+1)=0.25*H(J)
11    CONTINUE
      WRITE(*,*)J,DSS,EPS*SS
      WRITE(*,*)'TOO MANY STEPS.'
      RETURN
      END
```

```
      SUBROUTINE TRAPZD(FUNC,A,B,S,N)
C*****************************************************************************
C  THIS ROUTINE COMPUTES THE N'TH STAGE OF REFINEMENT OF AN EXTENDED          *
C  TRAPEZOIDAL RULE.  FUNC IS INPUT AS THE NAME OF THE FUNCTION TO BE         *
C  INTEGRATED BETWEEN LIMITS A AND B, ALSO INPUT.  WHEN CALLED WITH N=1,      *
C  THE ROUTINE RETURNS AS S THE CRUDEST ESTIMATE OF THE INTEGRAL OF F(X).     *
C  SUBSEQUENT CALLS WITH N=2,3,... (IN THAT SEQUENTIAL ORDER) WILL IMPROVE*
C  THE ACCURACY OF S BY ADDING 2**(N-2) ADDITIONAL INTERIOR POINTS.           *
C  S SHOULD NOT BE MODIFIED BETWEEN SEQUENTIAL CALLS.                         *
C*****************************************************************************
      IMPLICIT REAL*8(A-H,O-Z)

       EXTERNAL FUNC
       IF (N.EQ.1) THEN
     S=0.5*(B-A)*(FUNC(A)+FUNC(B))

C IT IS THE NUMBER OF POINTS TO BE ADDED ON THE NEXT CALL.

     IT=1
       ELSE
     TNM=FLOAT(IT)

C DEL IS THE SPACING OF THE POINTS TO BE ADDED

     DEL=(B-A)/TNM
          X=A+0.5*DEL
          SUM=0.
     DO 11 J=1,IT
        SUM=SUM+FUNC(X)
             X=X+DEL
11         CONTINUE

C THE FOLLOWING REPLACES S BY ITS REFINED VALUE.

           S=0.5*(S+(B-A)*SUM/TNM)
         IT=2*IT
   ENDIF
   RETURN
   END


   SUBROUTINE POLINT(XA,YA,N,X,Y,DY)
C*****************************************************************************
C  GIVEN ARRAYS XA AND YA, EACH OF LENGTH N, AND GIVEN A VALUE X,             *
C  THIS ROUTINE RETURNS A VALUE Y, AND AN ERROR ESTIMATE DY.                  *
C  IF P(X) IS THE POLYNOMIAL OF DEGREE N-1 SUCH THAT P(XAI)=YAI,              *
C  I=1,...,N, THEN THE RETURNED VALUE Y=P(X).                                 *
C*****************************************************************************
        IMPLICIT REAL*8(A-H,O-Z)
   PARAMETER (NMAX=50)
   DIMENSION XA(N),YA(N),C(NMAX),D(NMAX)

   NS=1
   DIF=ABS(X-XA(1))
   DO 11 I=1,N
      DIFT=ABS(X-XA(I))
      IF (DIFT.LT.DIF) THEN
         NS=I
         DIF=DIFT
      ENDIF
      C(I)=YA(I)
      D(I)=YA(I)
11    CONTINUE
      Y=YA(NS)
   NS=NS-1
   DO 13 M=1,N-1
      DO 12 I=1,N-M
```

```
        HO=XA(I)-X
   HP=XA(I+M)-X
   W=C(I+1)-D(I)
   DEN=HO-HP
   IF (DEN.EQ.0.) PAUSE
   DEN=W/DEN
   D(I)=HP*DEN
   C(I)=HO*DEN
12       CONTINUE
         IF (2*NS.LT.N-M) THEN
         DY=C(NS+1)
      ELSE
         DY=D(NS)
   NS=NS-1
      ENDIF
      Y=Y+DY
13    CONTINUE
      RETURN
   END


      FUNCTION BESSK0(X)
C*************************************************************************
C  RETURNS THE MODIFIED BESSEL FUNCTION K0(X) FOR POSITIVE REAL X        *
C  EVALUATION OF THE MODIFIED BESSEL FUNCTION TAKEN FROM NUMERICAL       *
C  RECIPES [PRESS ET AL.].                                               *
C*************************************************************************

      IMPLICIT REAL*8 (A-H,O-Z)
      DATA P1,P2,P3,P4,P5,P6,P7
     &   /-0.57721566D+00,+0.42278420D+00,+0.23069756D+00,
     &    +0.34885900D-01,+0.26269800D-02,+0.10750000D-03,
     &    +0.74000000D-05/
      DATA Q1,Q2,Q3,Q4,Q5,Q6,Q7
     &   /+1.25331414D+00,-0.78323580D-01,+0.21895680D-01,
     &    -0.10624460D-01,+0.58787200D-02,-0.25154000D-02,
     &    +0.53208000D-03/
      IF (X.LE.2.0) THEN
         Y=X*X/4.0
         BESSK0=(-LOG(X/2.0)*BESSI0(X))+(P1+Y*(P2+Y*(P3+
     &             Y*(P4+Y*(P5+Y*(P6+Y*P7))))))
      ELSE
         Y=(2.0/X)
         BESSK0=(EXP(-X)/SQRT(X))*(Q1+Y*(Q2+Y*(Q3+
     &          Y*(Q4+Y*(Q5+Y*(Q6+Y*Q7))))))
      ENDIF
      RETURN
      END


      FUNCTION BESSK1(X)
C*************************************************************************
C  RETURNS THE MODIFIED BESSEL FUNCTION K1(X) FOR POSITIVE REAL X        *
C*************************************************************************
      IMPLICIT REAL*8 (A-H,O-Z)
      DATA P1,P2,P3,P4,P5,P6,P7
     &   /+1.00000000D+00,+0.15443144D+00,-0.67278579D+00,
     &    -0.18156897D+00,-0.19194020D-01,-0.11040400D-02,
     &    -0.46860000D-04/
      DATA Q1,Q2,Q3,Q4,Q5,Q6,Q7
     &   /+1.25331414D+00,+0.23498619D+00,-0.36556200D-01,
     &    +0.15042680D-01,-0.78035300D-02,+0.32561400D-02,
     &    -0.68245000D-03/
      IF (X.LE.2.0) THEN
         Y=X*X/4.0
         BESSK1=(LOG(X/2.0)*BESSI1(X))+(1.0/X)*(P1+Y*(P2+
     &           Y*(P3+Y*(P4+Y*(P5+Y*(P6+Y*P7))))))
```

```
      ELSE
         Y=(2.0/X)
         BESSK1=(EXP(-X)/SQRT(X))*(Q1+Y*(Q2+Y*(Q3+
     &           Y*(Q4+Y*(Q5+Y*(Q6+Y*Q7))))))
      ENDIF
      RETURN
      END


      FUNCTION BESSI0(X)
C*************************************************************************
C  RETURNS THE MODIFIED BESSEL FUNCTION I0(X) FOR ANY REAL X             *
C*************************************************************************

      IMPLICIT REAL*8 (A-H,O-Z)
      DATA P1,P2,P3,P4,P5,P6,P7
     &   /+1.00000000D+00,+3.5156229D+00,+3.0899424D+00,
     &    +1.20674920D+00,+0.2659732D+00,+0.3607680D-01,
     &    +0.45813000D-02/
      DATA Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8,Q9
     &   /+0.39894228D+00,+0.1328592D-01,+0.2253190D-02,
     &    -0.15756500D-02,+0.9162810D-02,-0.2057706D-01,
     &    +0.26355370D-01,-0.1647633D-01,+0.3923770D-02/
      IF (ABS(X).LT.3.75) THEN
         Y=(X/3.75)**2
         BESSI0=P1+Y*(P2+Y*(P3+Y*(P4+Y*(P5+Y*(P6+Y*P7)))))
      ELSE
         AX=ABS(X)
         Y=(3.75/AX)
         BESSI0=(EXP(AX)/SQRT(AX))*(Q1+Y*(Q2+Y*(Q3+Y*(Q4+
     &           Y*(Q5+Y*(Q6+Y*(Q7+Y*(Q8+Y*Q9))))))))
      ENDIF
      RETURN
      END


      FUNCTION BESSI1(X)
C*************************************************************************
C  RETURNS THE MODIFIED BESSEL FUNCTION I1(X) FOR ANY REAL X             *
C*************************************************************************

      IMPLICIT REAL*8 (A-H,O-Z)
      DATA P1,P2,P3,P4,P5,P6,P7
     &   /+0.50000000D+00,+0.87890594D+00,+0.51498869D+00,
     &    +0.15084934D+00,+0.26587330D-01,+0.30153200D-02,
     &    +0.32411000D-03/
      DATA Q1,Q2,Q3,Q4,Q5,Q6,Q7,Q8,Q9
     &   /+0.39894228D+00,-0.39880240D-01,-0.36201800D-02,
     &    +0.16380100D-02,-0.10315550D-01,+0.22829670D-01,
     &    -0.28953120D-01,+0.17876540D-01,-0.42005900D-02/
      IF (ABS(X).LT.3.75) THEN
         Y=(X/3.75)**2
         BESSI1=X*(P1+Y*(P2+Y*(P3+Y*(P4+Y*(P5+Y*(P6+Y*P7))))))
      ELSE
         AX=ABS(X)
         Y=(3.75/AX)
         BESSI1=(EXP(AX)/SQRT(AX))*(Q1+Y*(Q2+Y*(Q3+Y*(Q4+
     &           Y*(Q5+Y*(Q6+Y*(Q7+Y*(Q8+Y*Q9))))))))
      ENDIF
      RETURN
      END


      SUBROUTINE JACOBI(A,N,NP,D,V,NROT)
C*************************************************************************
C  MATRIX DIAGONALIZATION FROM NUMERICAL RECIPES [PRESS ET AL.]          *
C  USING THE JACOBI METHOD                                               *
```

```
C*************************************************************************
      IMPLICIT REAL*8 (A-H,O-Z)
      PARAMETER(NMAX=100)
      DIMENSION A(NP,NP),D(NP),V(NP,NP),B(NMAX),Z(NMAX)
      DO 12 IP=1,N
         DO 11 IQ=1,N
            V(IP,IQ)=0.
11       CONTINUE
         V(IP,IP)=1.
12    CONTINUE
      DO 13 IP=1,N
         B(IP)=A(IP,IP)
         D(IP)=B(IP)
         Z(IP)=0.
13    CONTINUE
      NROT=0
      DO 24 I=1,50
         SM=0.
         DO 15 IP=1,N-1
            DO 14 IQ=IP+1,N
               SM=SM+ABS(A(IP,IQ))
14          CONTINUE
15       CONTINUE
         IF (SM.EQ.0.) RETURN
         IF (I.LT.4) THEN
            TRESH=0.2*SM/N**2
         ELSE
            TRESH=0.
         ENDIF
         DO 22 IP=1,N-1
            DO 21 IQ=IP+1,N
               G=100.*ABS(A(IP,IQ))
               IF ((I.GT.4).AND.(ABS(D(IP))+G.EQ.ABS(D(IP)))
     &             .AND.(ABS(D(IQ))+G.EQ.ABS(D(IQ)))) THEN
                  A(IP,IQ)=0.
               ELSE IF (ABS(A(IP,IQ)).GT.TRESH) THEN
                  H=D(IQ)-D(IP)
                  IF (ABS(H)+G.EQ.ABS(H)) THEN
                     T=A(IP,IQ)/H
                  ELSE
                     THETA=0.5*H/A(IP,IQ)
                     T=1./(ABS(THETA)+SQRT(1.+THETA**2))
                     IF (THETA.LT.0.)T=-T
                  ENDIF
                  C=1./SQRT(1.+T**2)
                  S=T*C
                  TAU=S/(1.+C)
                  H=T*A(IP,IQ)
                  Z(IP)=Z(IP)-H
                  Z(IQ)=Z(IQ)+H
                  D(IP)=D(IP)-H
                  D(IQ)=D(IQ)+H
                  A(IP,IQ)=0.
                  DO 16 J=1,IP-1
                     G=A(J,IP)
                     H=A(J,IQ)
                     A(J,IP)=G-S*(H+G*TAU)
                     A(J,IQ)=H+S*(G-H*TAU)
16                CONTINUE
                  DO 17 J=IP+1,IQ-1
                     G=A(IP,J)
                     H=A(J,IQ)
                     A(IP,J)=G-S*(H+G*TAU)
                     A(J,IQ)=H+S*(G-H*TAU)
17                CONTINUE
                  DO 18 J=IQ+1,N
                     G=A(IP,J)
```

```
                  H=A(IQ,J)
                  A(IP,J)=G-S*(H+G*TAU)
                  A(IQ,J)=H+S*(G-H*TAU)
18               CONTINUE
                 DO 19 J=1,N
                  G=V(J,IP)
                  H=V(J,IQ)
                  V(J,IP)=G-S*(H+G*TAU)
                  V(J,IQ)=H+S*(G-H*TAU)
19               CONTINUE
                 NROT=NROT+1
               ENDIF
21           CONTINUE
22         CONTINUE
           DO 23 IP=1,N
             B(IP)=B(IP)+Z(IP)
             D(IP)=B(IP)
             Z(IP)=0.
23         CONTINUE
24       CONTINUE
         RETURN
         END


         SUBROUTINE QGAUS(FUNC,A,B,SS)
C*****************************************************************************
C  QGAUS(FUNC,A,B,SS) RETURNS AS SS THE INTEGRAL OF THE FUNCTION, FUNC,      *
C  BETWEEN A AND  B, BY TEN POINT GUASSIAN LEGENDRE INTEGRATION: THE         *
C  FUNCTION IS EVALUATED EXACTLY TEN TIMES AT INTERIOR POINTS IN THE         *
C  RANGE OF INTEGRATION.                                                     *
C                                                                            *
C  WITH THE LOWER AND UPPER LIMITS OF INTEGRATION AND GIVEN N, GAULEG        *
C  RETURNS ARRAYS X AND W OF LENGTH N, CONTAINING THE ABSCISSAS AND          *
C  WEIGHTS OF THE GAUSS-LEGENDRE N-POINT QUADRATURE FORMULA                  *
C*****************************************************************************
         IMPLICIT REAL*8 (A-H,O-Z)
         COMMON/GAUSS/ X,W,N
         PARAMETER (NN=100)
C        DIMENSION YY(NN),XX(NN)
         DIMENSION X(NN),W(NN)
         EXTERNAL FUNC

         XR=B-A
         SS=0
         DO 100 J=1,N
           DX=XR*X(J)
           SS=SS+W(J)*FUNC((A+DX))
C           XX(J)=X(J)
C           YY(J)=FUNC((A+DX))
  100    CONTINUE
         SS=SS*XR
C         DO 12 J=1,N
C         WRITE(*,*)XX(J),YY(J)
C12      CONTINUE
         RETURN
         END


         SUBROUTINE GAULEG(X,W,N)
         IMPLICIT REAL*8 (A-H,O-Z)
         COMMON/ANS/PERTURB,EBROAD,NAINT
         CHARACTER*1 PERTURB,EBROAD,NAINT
         DIMENSION X(N),W(N)

         XINT=1.
         IF (NAINT.EQ.'N') THEN
           N=MIN(10,N)
```

```
        W(N)=XINT/2.
        X(N)=1.-W(N)/2.
        DO 110 I=1,N-2
          W(N-I)=W(N-I+1)/2.
          X(N-I)=X(N-I+1)-W(N-I+1)/2.-W(N-I)/2.
  110   CONTINUE
        W(1)=W(2)
        X(1)=X(2)-W(2)/2.-W(1)/2.
      ELSE
        DX=XINT/FLOAT(N)
        W(1)=DX
        X(1)=DX/2.
        DO 120 I=2,N
          W(I)=W(1)
          X(I)=X(I-1)+W(I)/2.+W(I-1)/2.
  120   CONTINUE
      ENDIF
      RETURN
      END

C*************************************************************************
C  THE FOLLOWING TWO SUBROUTINES CONTAIN THE RADIAL MATRIX.               *
C  ELEMENTS FOR OXYGEN CALCULATED BY CHUN LIN FOR SPIN 1 (TRIPLET)        *
C  AND SPIN 2 (QUINTET)                                                   *
C*************************************************************************

      SUBROUTINE RADMATX1
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/RADIAL/RME1
      DIMENSION RME1(10,20,20)

C THE DATA FORMAT IS RME1(L1,PN1,PN2); L1-L2=+1

C P-S TRANSITION:

      RME1(1, 3, 3) = -5.69980E+00
      RME1(1, 4, 3) = -1.32130E-01
      RME1(1, 5, 3) =  5.70950E-03
      RME1(1, 6, 3) =  2.18900E-02
      RME1(1, 7, 3) =  2.24800E-02
      RME1(1, 8, 3) =  2.03440E-02
      RME1(1, 9, 3) =  1.79130E-02
      RME1(1,10, 3) =  1.57220E-02
      RME1(1,11, 3) =  1.38520E-02
      RME1(1,12, 3) =  1.22820E-02
      RME1(1,13, 3) =  1.09640E-02
      RME1(1,14, 3) =  9.85310E-03
      RME1(1,15, 3) =  8.90960E-03
      RME1(1, 3, 4) =  4.33920E+00
      RME1(1, 4, 4) = -1.25200E+01
      RME1(1, 5, 4) = -6.49010E-01
      RME1(1, 6, 4) = -1.62430E-01
      RME1(1, 7, 4) = -6.06670E-02
      RME1(1, 8, 4) = -2.67710E-02
      RME1(1, 9, 4) = -1.26120E-02
      RME1(1,10, 4) = -5.85800E-03
      RME1(1,11, 4) = -2.35970E-03
      RME1(1,12, 4) = -4.47990E-04
      RME1(1,13, 4) =  6.28850E-04
      RME1(1,14, 4) =  1.24150E-03
      RME1(1,15, 4) =  1.58520E-03
      RME1(1, 3, 5) =  1.10210E+00
      RME1(1, 4, 5) =  9.95550E+00
      RME1(1, 5, 5) = -2.17500E+01
      RME1(1, 6, 5) = -1.39390E+00
      RME1(1, 7, 5) = -4.24680E-01
      RME1(1, 8, 5) = -1.97530E-01
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RME1(1, 9, 5) = -1.12670E-01
RME1(1,10, 5) = -7.25610E-02
RME1(1,11, 5) = -5.06750E-02
RME1(1,12, 5) = -3.74970E-02
RME1(1,13, 5) = -2.89740E-02
RME1(1,14, 5) = -2.31520E-02
RME1(1,15, 5) = -1.89980E-02
RME1(1, 3, 6) =  5.86310E-01
RME1(1, 4, 6) =  2.29000E+00
RME1(1, 5, 6) =  1.74950E+01
RME1(1, 6, 6) = -3.34100E+01
RME1(1, 7, 6) = -2.35630E+00
RME1(1, 8, 6) = -7.71360E-01
RME1(1, 9, 6) = -3.81740E-01
RME1(1,10, 6) = -2.29910E-01
RME1(1,11, 6) = -1.55340E-01
RME1(1,12, 6) = -1.13150E-01
RME1(1,13, 6) = -8.68770E-02
RME1(1,14, 6) = -6.93560E-02
RME1(1,15, 6) = -5.70160E-02
RME1(1, 3, 7) =  3.87520E-01
RME1(1, 4, 7) =  1.18020E+00
RME1(1, 5, 7) =  3.80550E+00
RME1(1, 6, 7) =  2.69780E+01
RME1(1, 7, 7) = -4.75060E+01
RME1(1, 8, 7) = -3.53100E+00
RME1(1, 9, 7) = -1.19830E+00
RME1(1,10, 7) = -6.09970E-01
RME1(1,11, 7) = -3.75860E-01
RME1(1,12, 7) = -2.58760E-01
RME1(1,13, 7) = -1.91440E-01
RME1(1,14, 7) = -1.48930E-01
RME1(1,15, 7) = -1.20200E-01
RME1(1, 3, 8) =  2.84040E-01
RME1(1, 4, 8) =  7.69880E-01
RME1(1, 5, 8) =  1.91670E+00
RME1(1, 6, 8) =  5.65600E+00
RME1(1, 7, 8) =  3.84140E+01
RME1(1, 8, 8) = -6.40400E+01
RME1(1, 9, 8) = -4.91670E+00
RME1(1,10, 8) = -1.70370E+00
RME1(1,11, 8) = -8.80780E-01
RME1(1,12, 8) = -5.49260E-01
RME1(1,13, 8) = -3.81740E-01
RME1(1,14, 8) = -2.84600E-01
RME1(1,15, 8) = -2.22810E-01
RME1(1, 3, 9) =  2.21200E-01
RME1(1, 4, 9) =  5.61350E-01
RME1(1, 5, 9) =  1.23580E+00
RME1(1, 6, 9) =  2.79890E+00
RME1(1, 7, 9) =  7.84300E+00
RME1(1, 8, 9) =  5.18060E+01
RME1(1, 9, 9) = -8.30120E+01
RME1(1,10, 9) = -6.51240E+00
RME1(1,11, 9) = -2.28680E+00
RME1(1,12, 9) = -1.19330E+00
RME1(1,13, 9) = -7.46390E-01
RME1(1,14, 9) = -5.23640E-01
RME1(1,15, 9) = -3.92070E-01
RME1(1, 3,10) =  1.79280E-01
RME1(1, 4,10) =  4.36520E-01
RME1(1, 5,10) =  8.95540E-01
RME1(1, 6,10) =  1.78620E+00
RME1(1, 7,10) =  3.82690E+00
RME1(1, 8,10) =  1.03670E+01
RME1(1, 9,10) =  6.71580E+01
RME1(1,10,10) = -1.04420E+02
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RME1(1,11,10) = -8.31800E+00
RME1(1,12,10) = -2.94700E+00
RME1(1,13,10) = -1.54720E+00
RME1(1,14,10) = -9.75820E-01
RME1(1,15,10) = -6.84070E-01
RME1(1, 3,11) =  1.49490E-01
RME1(1, 4,11) =  3.53970E-01
RME1(1, 5,11) =  6.94220E-01
RME1(1, 6,11) =  1.28650E+00
RME1(1, 7,11) =  2.42090E+00
RME1(1, 8,11) =  5.00070E+00
RME1(1, 9,11) =  1.32280E+01
RME1(1,10,11) =  8.44680E+01
RME1(1,11,11) = -1.28270E+02
RME1(1,12,11) = -1.03330E+01
RME1(1,13,11) = -3.68400E+00
RME1(1,14,11) = -1.94200E+00
RME1(1,15,11) = -1.22820E+00
RME1(1, 3,12) =  1.27340E-01
RME1(1, 4,12) =  2.95600E-01
RME1(1, 5,12) =  5.62180E-01
RME1(1, 6,12) =  9.93600E-01
RME1(1, 7,12) =  1.73350E+00
RME1(1, 8,12) =  3.13950E+00
RME1(1, 9,12) =  6.32030E+00
RME1(1,10,12) =  1.64270E+01
RME1(1,11,12) =  1.03740E+02
RME1(1,12,12) = -1.54560E+02
RME1(1,13,12) = -1.25570E+01
RME1(1,14,12) = -4.49770E+00
RME1(1,15,12) = -2.37760E+00
RME1(1, 3,13) =  1.10300E-01
RME1(1, 4,13) =  2.52310E-01
RME1(1, 5,13) =  4.69360E-01
RME1(1, 6,13) =  8.02860E-01
RME1(1, 7,13) =  1.33370E+00
RME1(1, 8,13) =  2.23630E+00
RME1(1, 9,13) =  3.94190E+00
RME1(1,10,13) =  7.78570E+00
RME1(1,11,13) =  1.99630E+01
RME1(1,12,13) =  1.24970E+02
RME1(1,13,13) = -1.83280E+02
RME1(1,14,13) = -1.49910E+01
RME1(1,15,13) = -5.38780E+00
RME1(1, 3,14) =  9.68160E-02
RME1(1, 4,14) =  2.19020E-01
RME1(1, 5,14) =  4.00780E-01
RME1(1, 6,14) =  6.69510E-01
RME1(1, 7,14) =  1.07500E+00
RME1(1, 8,14) =  1.71420E+00
RME1(1, 9,14) =  2.79450E+00
RME1(1,10,14) =  4.82790E+00
RME1(1,11,14) =  9.39680E+00
RME1(1,12,14) =  2.38360E+01
RME1(1,13,14) =  1.48160E+02
RME1(1,14,14) = -2.14460E+02
RME1(1,15,14) = -1.76330E+01
RME1(1, 3,15) =  8.59250E-02
RME1(1, 4,15) =  1.92710E-01
RME1(1, 5,15) =  3.48190E-01
RME1(1, 6,15) =  5.71410E-01
RME1(1, 7,15) =  8.94980E-01
RME1(1, 8,15) =  1.37800E+00
RME1(1, 9,15) =  2.13460E+00
RME1(1,10,15) =  3.40800E+00
RME1(1,11,15) =  5.79760E+00
RME1(1,12,15) =  1.11540E+01
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      RME1(1,13,15) =  2.80470E+01
      RME1(1,14,15) =  1.73320E+02
      RME1(1,15,15) = -2.48060E+02

C D-P TRANSITION:
      RME1(2, 3, 3) = -7.15410E+00
      RME1(2, 4, 3) = -1.39930E+00
      RME1(2, 5, 3) = -6.29180E-01
      RME1(2, 6, 3) = -3.76330E-01
      RME1(2, 7, 3) = -2.58990E-01
      RME1(2, 8, 3) = -1.93390E-01
      RME1(2, 9, 3) = -1.52230E-01
      RME1(2,10, 3) = -1.24280E-01
      RME1(2,11, 3) = -1.04220E-01
      RME1(2,12, 3) = -8.91940E-02
      RME1(2,13, 3) = -7.75690E-02
      RME1(2,14, 3) = -6.83390E-02
      RME1(2,15, 3) = -6.08530E-02
      RME1(2, 3, 4) =  8.55100E+00
      RME1(2, 4, 4) = -1.33950E+01
      RME1(2, 5, 4) = -2.95390E+00
      RME1(2, 6, 4) = -1.40360E+00
      RME1(2, 7, 4) = -8.65420E-01
      RME1(2, 8, 4) = -6.07120E-01
      RME1(2, 9, 4) = -4.59440E-01
      RME1(2,10, 4) = -3.65270E-01
      RME1(2,11, 4) = -3.00580E-01
      RME1(2,12, 4) = -2.53700E-01
      RME1(2,13, 4) = -2.18310E-01
      RME1(2,14, 4) = -1.90750E-01
      RME1(2,15, 4) = -1.68750E-01
      RME1(2, 3, 5) =  6.36840E-01
      RME1(2, 4, 5) =  1.78280E+01
      RME1(2, 5, 5) = -2.12180E+01
      RME1(2, 6, 5) = -4.84580E+00
      RME1(2, 7, 5) = -2.34510E+00
      RME1(2, 8, 5) = -1.46100E+00
      RME1(2, 9, 5) = -1.03180E+00
      RME1(2,10, 5) = -7.84600E-01
      RME1(2,11, 5) = -6.26200E-01
      RME1(2,12, 5) = -5.16990E-01
      RME1(2,13, 5) = -4.37600E-01
      RME1(2,14, 5) = -3.77540E-01
      RME1(2,15, 5) = -3.30670E-01
      RME1(2, 3, 6) =  2.93510E-01
      RME1(2, 4, 6) =  1.21350E+00
      RME1(2, 5, 6) =  2.96800E+01
      RME1(2, 6, 6) = -3.06380E+01
      RME1(2, 7, 6) = -7.08620E+00
      RME1(2, 8, 6) = -3.45110E+00
      RME1(2, 9, 6) = -2.15720E+00
      RME1(2,10, 6) = -1.52660E+00
      RME1(2,11, 6) = -1.16280E+00
      RME1(2,12, 6) = -9.29310E-01
      RME1(2,13, 6) = -7.68240E-01
      RME1(2,14, 6) = -6.51090E-01
      RME1(2,15, 6) = -5.62430E-01
      RME1(2, 3, 7) =  1.85080E-01
      RME1(2, 4, 7) =  5.38970E-01
      RME1(2, 5, 7) =  1.85100E+00
      RME1(2, 6, 7) =  4.41860E+01
      RME1(2, 7, 7) = -4.16630E+01
      RME1(2, 8, 7) = -9.67780E+00
      RME1(2, 9, 7) = -4.72020E+00
      RME1(2,10, 7) = -2.95140E+00
      RME1(2,11, 7) = -2.08870E+00
      RME1(2,12, 7) = -1.59090E+00
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RME1(2,13, 7) = -1.27170E+00
RME1(2,14, 7) = -1.05150E+00
RME1(2,15, 7) = -8.91480E-01
RME1(2, 3, 8) =  1.32810E-01
RME1(2, 4, 8) =  3.35450E-01
RME1(2, 5, 8) =  7.93510E-01
RME1(2, 6, 8) =  2.54910E+00
RME1(2, 7, 8) =  6.13660E+01
RME1(2, 8, 8) = -5.42960E+01
RME1(2, 9, 8) = -1.26230E+01
RME1(2,10, 8) = -6.15250E+00
RME1(2,11, 8) = -3.84280E+00
RME1(2,12, 8) = -2.71690E+00
RME1(2,13, 8) = -2.06780E+00
RME1(2,14, 8) = -1.65190E+00
RME1(2,15, 8) = -1.36540E+00
RME1(2, 3, 9) =  1.02290E-01
RME1(2, 4, 9) =  2.39580E-01
RME1(2, 5, 9) =  4.86770E-01
RME1(2, 6, 9) =  1.05730E+00
RME1(2, 7, 9) =  3.30630E+00
RME1(2, 8, 9) =  8.12280E+01
RME1(2, 9, 9) = -6.85380E+01
RME1(2,10, 9) = -1.59220E+01
RME1(2,11, 9) = -7.74810E+00
RME1(2,12, 9) = -4.83120E+00
RME1(2,13, 9) = -3.41070E+00
RME1(2,14, 9) = -2.59260E+00
RME1(2,15, 9) = -2.06920E+00
RME1(2, 3,10) =  8.23880E-02
RME1(2, 4,10) =  1.84310E-01
RME1(2, 5,10) =  3.45340E-01
RME1(2, 6,10) =  6.39150E-01
RME1(2, 7,10) =  1.32980E+00
RME1(2, 8,10) =  4.12150E+00
RME1(2, 9,10) =  1.03770E+02
RME1(2,10,10) = -8.43920E+01
RME1(2,11,10) = -1.95770E+01
RME1(2,12,10) = -9.50710E+00
RME1(2,13,10) = -5.91650E+00
RME1(2,14,10) = -4.16970E+00
RME1(2,15,10) = -3.16520E+00
RME1(2, 3,11) =  6.84510E-02
RME1(2, 4,11) =  1.48550E-01
RME1(2, 5,11) =  2.64870E-01
RME1(2, 6,11) =  4.50120E-01
RME1(2, 7,11) =  7.92440E-01
RME1(2, 8,11) =  1.61050E+00
RME1(2, 9,11) =  4.99410E+00
RME1(2,10,11) =  1.29000E+02
RME1(2,11,11) = -1.01860E+02
RME1(2,12,11) = -2.35870E+01
RME1(2,13,11) = -1.14300E+01
RME1(2,14,11) = -7.09850E+00
RME1(2,15,11) = -4.99390E+00
RME1(2, 3,12) =  5.81860E-02
RME1(2, 4,12) =  1.23600E-01
RME1(2, 5,12) =  2.13230E-01
RME1(2, 6,12) =  3.43860E-01
RME1(2, 7,12) =  5.53800E-01
RME1(2, 8,12) =  9.46510E-01
RME1(2, 9,12) =  1.89970E+00
RME1(2,10,12) =  5.92330E+00
RME1(2,11,12) =  1.56920E+02
RME1(2,12,12) = -1.20930E+02
RME1(2,13,12) = -2.79520E+01
RME1(2,14,12) = -1.35160E+01
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      RME1(2,15,12) = -8.37730E+00
      RME1(2, 3,13) =  5.03360E-02
      RME1(2, 4,13) =  1.05270E-01
      RME1(2, 5,13) =  1.77400E-01
      RME1(2, 6,13) =  2.76250E-01
      RME1(2, 7,13) =  4.21220E-01
      RME1(2, 8,13) =  6.36380E-01
      RME1(2, 9,13) =  1.10130E+00
      RME1(2,10,13) =  2.19680E+00
      RME1(2,11,13) =  6.90900E+00
      RME1(2,12,13) =  1.87530E+02
      RME1(2,13,13) = -1.41620E+02
      RME1(2,14,13) = -3.26740E+01
      RME1(2,15,13) = -1.57660E+01
      RME1(2, 3,14) =  4.41560E-02
      RME1(2, 4,14) =  9.12600E-02
      RME1(2, 5,14) =  1.51170E-01
      RME1(2, 6,14) =  2.29610E-01
      RME1(2, 7,14) =  3.37560E-01
      RME1(2, 8,14) =  4.96980E-01
      RME1(2, 9,14) =  7.57900E-01
      RME1(2,10,14) =  1.25680E+00
      RME1(2,11,14) =  2.50180E+00
      RME1(2,12,14) =  7.95070E+00
      RME1(2,13,14) =  2.20810E+02
      RME1(2,14,14) = -1.63920E+02
      RME1(2,15,14) = -3.77520E+01
      RME1(2, 3,15) =  3.91790E-02
      RME1(2, 4,15) =  8.02320E-02
      RME1(2, 5,15) =  1.31170E-01
      RME1(2, 6,15) =  1.95600E-01
      RME1(2, 7,15) =  2.80130E-01
      RME1(2, 8,15) =  3.97070E-01
      RME1(2, 9,15) =  5.71090E-01
      RME1(2,10,15) =  8.58310E-01
      RME1(2,11,15) =  1.41300E+00
      RME1(2,12,15) =  2.81460E+00
      RME1(2,13,15) =  9.04840E+00
      RME1(2,14,15) =  2.56790E+02
      RME1(2,15,15) = -1.87830E+02

C F-D TRANSITION:
      RME1(3, 4, 3) =  1.01970E+01
      RME1(3, 5, 3) =  3.32020E+00
      RME1(3, 6, 3) =  1.80170E+00
      RME1(3, 7, 3) =  1.19090E+00
      RME1(3, 8, 3) =  8.71790E-01
      RME1(3, 9, 3) =  6.78720E-01
      RME1(3,10, 3) =  5.50490E-01
      RME1(3,11, 3) =  4.59680E-01
      RME1(3,12, 3) =  3.92290E-01
      RME1(3,13, 3) =  3.40480E-01
      RME1(3,14, 3) =  2.99530E-01
      RME1(3,15, 3) =  2.66430E-01
      RME1(3, 4, 4) = -1.58900E+01
      RME1(3, 5, 4) =  1.39800E+01
      RME1(3, 6, 4) =  5.16890E+00
      RME1(3, 7, 4) =  2.92980E+00
      RME1(3, 8, 4) =  1.97770E+00
      RME1(3, 9, 4) =  1.46600E+00
      RME1(3,10, 4) =  1.15120E+00
      RME1(3,11, 4) =  9.39850E-01
      RME1(3,12, 4) =  7.88960E-01
      RME1(3,13, 4) =  6.76310E-01
      RME1(3,14, 4) =  5.89260E-01
      RME1(3,15, 4) =  5.20160E-01
      RME1(3, 4, 5) =  1.69840E+00
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RME1(3, 5, 5) = -3.00270E+01
RME1(3, 6, 5) =  1.84360E+01
RME1(3, 7, 5) =  7.06310E+00
RME1(3, 8, 5) =  4.06580E+00
RME1(3, 9, 5) =  2.76790E+00
RME1(3,10, 5) =  2.06300E+00
RME1(3,11, 5) =  1.62660E+00
RME1(3,12, 5) =  1.33230E+00
RME1(3,13, 5) =  1.12160E+00
RME1(3,14, 5) =  9.63850E-01
RME1(3,15, 5) =  8.41730E-01
RME1(3, 4, 6) =  5.77150E-01
RME1(3, 5, 6) =  3.73100E+00
RME1(3, 6, 6) = -4.68020E+01
RME1(3, 7, 6) =  2.35480E+01
RME1(3, 8, 6) =  9.11450E+00
RME1(3, 9, 6) =  5.27190E+00
RME1(3,10, 6) =  3.59870E+00
RME1(3,11, 6) =  2.68730E+00
RME1(3,12, 6) =  2.12220E+00
RME1(3,13, 6) =  1.74070E+00
RME1(3,14, 6) =  1.46740E+00
RME1(3,15, 6) =  1.26270E+00
RME1(3, 4, 7) =  3.13170E-01
RME1(3, 5, 7) =  1.28370E+00
RME1(3, 6, 7) =  6.40080E+00
RME1(3, 7, 7) = -6.64540E+01
RME1(3, 8, 7) =  2.93100E+01
RME1(3, 9, 7) =  1.13570E+01
RME1(3,10, 7) =  6.56990E+00
RME1(3,11, 7) =  4.48460E+00
RME1(3,12, 7) =  3.34900E+00
RME1(3,13, 7) =  2.64520E+00
RME1(3,14, 7) =  2.17040E+00
RME1(3,15, 7) =  1.83040E+00
RME1(3, 4, 8) =  2.05950E-01
RME1(3, 5, 8) =  6.97910E-01
RME1(3, 6, 8) =  2.21520E+00
RME1(3, 7, 8) =  9.72160E+00
RME1(3, 8, 8) = -8.90490E+01
RME1(3, 9, 8) =  3.57170E+01
RME1(3,10, 8) =  1.38040E+01
RME1(3,11, 8) =  7.96990E+00
RME1(3,12, 8) =  5.43260E+00
RME1(3,13, 8) =  4.05300E+00
RME1(3,14, 8) =  3.19920E+00
RME1(3,15, 8) =  2.62400E+00
RME1(3, 4, 9) =  1.50080E-01
RME1(3, 5, 9) =  4.58710E-01
RME1(3, 6, 9) =  1.20440E+00
RME1(3, 7, 9) =  3.37440E+00
RME1(3, 8, 9) =  1.36980E+01
RME1(3, 9, 9) = -1.14620E+02
RME1(3,10, 9) =  4.27690E+01
RME1(3,11, 9) =  1.64610E+01
RME1(3,12, 9) =  9.47720E+00
RME1(3,13, 9) =  6.44660E+00
RME1(3,14, 9) =  4.80220E+00
RME1(3,15, 9) =  3.78650E+00
RME1(3, 4,10) =  1.16470E-01
RME1(3, 5,10) =  3.33970E-01
RME1(3, 6,10) =  7.90460E-01
RME1(3, 7,10) =  1.83300E+00
RME1(3, 8,10) =  4.76130E+00
RME1(3, 9,10) =  1.83310E+01
RME1(3,10,10) = -1.43160E+02
RME1(3,11,10) =  5.04630E+01
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      RME1(3,12,10) =  1.93340E+01
      RME1(3,13,10) =  1.10950E+01
      RME1(3,14,10) =  7.52880E+00
      RME1(3,15,10) =  5.59830E+00
      RME1(3, 4,11) =  9.42750E-02
      RME1(3, 5,11) =  2.58990E-01
      RME1(3, 6,11) =  5.74630E-01
      RME1(3, 7,11) =  1.20100E+00
      RME1(3, 8,11) =  2.58350E+00
      RME1(3, 9,11) =  6.37600E+00
      RME1(3,10,11) =  2.36240E+01
      RME1(3,11,11) = -1.74700E+02
      RME1(3,12,11) =  5.87990E+01
      RME1(3,13,11) =  2.24230E+01
      RME1(3,14,11) =  1.28250E+01
      RME1(3,15,11) =  8.68090E+00
      RME1(3, 4,12) =  7.86350E-02
      RME1(3, 5,12) =  2.09570E-01
      RME1(3, 6,12) =  4.45070E-01
      RME1(3, 7,12) =  8.71570E-01
      RME1(3, 8,12) =  1.68970E+00
      RME1(3, 9,12) =  3.45520E+00
      RME1(3,10,12) =  8.21830E+00
      RME1(3,11,12) =  2.95750E+01
      RME1(3,12,12) = -2.09230E+02
      RME1(3,13,12) =  6.77760E+01
      RME1(3,14,12) =  2.57300E+01
      RME1(3,15,12) =  1.46680E+01
      RME1(3, 4,13) =  6.70770E-02
      RME1(3, 5,13) =  1.74800E-01
      RME1(3, 6,13) =  3.59820E-01
      RME1(3, 7,13) =  6.74080E-01
      RME1(3, 8,13) =  1.22400E+00
      RME1(3, 9,13) =  2.25590E+00
      RME1(3,10,13) =  4.44780E+00
      RME1(3,11,13) =  1.02880E+01
      RME1(3,12,13) =  3.61870E+01
      RME1(3,13,13) = -2.46750E+02
      RME1(3,14,13) =  7.73940E+01
      RME1(3,15,13) =  2.92550E+01
      RME1(3, 4,14) =  5.82180E-02
      RME1(3, 5,14) =  1.49140E-01
      RME1(3, 6,14) =  2.99950E-01
      RME1(3, 7,14) =  5.44320E-01
      RME1(3, 8,14) =  9.45240E-01
      RME1(3, 9,14) =  1.63140E+00
      RME1(3,10,14) =  2.89920E+00
      RME1(3,11,14) =  5.56100E+00
      RME1(3,12,14) =  1.25850E+01
      RME1(3,13,14) =  4.34580E+01
      RME1(3,14,14) = -2.87270E+02
      RME1(3,15,14) =  8.76520E+01
      RME1(3, 4,15) =  5.12330E-02
      RME1(3, 5,15) =  1.29500E-01
      RME1(3, 6,15) =  2.55840E-01
      RME1(3, 7,15) =  4.53370E-01
      RME1(3, 8,15) =  7.62330E-01
      RME1(3, 9,15) =  1.25790E+00
      RME1(3,10,15) =  2.09330E+00
      RME1(3,11,15) =  3.61920E+00
      RME1(3,12,15) =  6.79460E+00
      RME1(3,13,15) =  1.51090E+01
      RME1(3,14,15) =  5.13900E+01
      RME1(3,15,15) = -3.30790E+02

C G-F TRANSITION:
      RME1(4, 5, 4) =  1.77200E+01
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RME1(4, 6, 4) =  5.25090E+00
RME1(4, 7, 4) =  2.69850E+00
RME1(4, 8, 4) =  1.72450E+00
RME1(4, 9, 4) =  1.23510E+00
RME1(4,10, 4) =  9.47600E-01
RME1(4,11, 4) =  7.60920E-01
RME1(4,12, 4) =  6.30990E-01
RME1(4,13, 4) =  5.35870E-01
RME1(4,14, 4) =  4.63520E-01
RME1(4,15, 4) =  4.06800E-01
RME1(4, 5, 5) = -2.25000E+01
RME1(4, 6, 5) =  2.25640E+01
RME1(4, 7, 5) =  7.82850E+00
RME1(4, 8, 5) =  4.26610E+00
RME1(4, 9, 5) =  2.80620E+00
RME1(4,10, 5) =  2.04360E+00
RME1(4,11, 5) =  1.58500E+00
RME1(4,12, 5) =  1.28250E+00
RME1(4,13, 5) =  1.06970E+00
RME1(4,14, 5) =  9.12640E-01
RME1(4,15, 5) =  7.92420E-01
RME1(4, 5, 6) =  2.01870E+00
RME1(4, 6, 6) = -4.02490E+01
RME1(4, 7, 6) =  2.81160E+01
RME1(4, 8, 6) =  1.02940E+01
RME1(4, 9, 6) =  5.75420E+00
RME1(4,10, 6) =  3.83880E+00
RME1(4,11, 6) =  2.82030E+00
RME1(4,12, 6) =  2.20050E+00
RME1(4,13, 6) =  1.78850E+00
RME1(4,14, 6) =  1.49690E+00
RME1(4,15, 6) =  1.28080E+00
RME1(4, 5, 7) =  6.36100E-01
RME1(4, 6, 7) =  4.25990E+00
RME1(4, 7, 7) = -6.03180E+01
RME1(4, 8, 7) =  3.43500E+01
RME1(4, 9, 7) =  1.28550E+01
RME1(4,10, 7) =  7.27030E+00
RME1(4,11, 7) =  4.88400E+00
RME1(4,12, 7) =  3.60450E+00
RME1(4,13, 7) =  2.82140E+00
RME1(4,14, 7) =  2.29880E+00
RME1(4,15, 7) =  1.92780E+00
RME1(4, 5, 8) =  3.28470E-01
RME1(4, 6, 8) =  1.38160E+00
RME1(4, 7, 8) =  7.11540E+00
RME1(4, 8, 8) = -8.31380E+01
RME1(4, 9, 8) =  4.12540E+01
RME1(4,10, 8) =  1.55790E+01
RME1(4,11, 8) =  8.85540E+00
RME1(4,12, 8) =  5.96740E+00
RME1(4,13, 8) =  4.41330E+00
RME1(4,14, 8) =  3.45990E+00
RME1(4,15, 8) =  2.82250E+00
RME1(4, 5, 9) =  2.08880E-01
RME1(4, 6, 9) =  7.21280E-01
RME1(4, 7, 9) =  2.34700E+00
RME1(4, 8, 9) =  1.06040E+01
RME1(4, 9, 9) = -1.08840E+02
RME1(4,10, 9) =  4.88210E+01
RME1(4,11, 9) =  1.84910E+01
RME1(4,12, 9) =  1.05290E+01
RME1(4,13, 9) =  7.10230E+00
RME1(4,14, 9) =  5.25620E+00
RME1(4,15, 9) =  4.12280E+00
RME1(4, 5,10) =  1.48690E-01
RME1(4, 6,10) =  4.60710E-01
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      RME1(4, 7,10) =  1.23320E+00
      RME1(4, 8,10) =  3.53600E+00
      RME1(4, 9,10) =  1.47330E+01
      RME1(4,10,10) = -1.37480E+02
      RME1(4,11,10) =  5.70480E+01
      RME1(4,12,10) =  2.16050E+01
      RME1(4,13,10) =  1.23010E+01
      RME1(4,14,10) =  8.29600E+00
      RME1(4,15,10) =  6.13850E+00
      RME1(4, 5,11) =  1.13460E-01
      RME1(4, 6,11) =  3.28540E-01
      RME1(4, 7,11) =  7.89550E-01
      RME1(4, 8,11) =  1.86530E+00
      RME1(4, 9,11) =  4.94920E+00
      RME1(4,10,11) =  1.95060E+01
      RME1(4,11,11) = -1.69070E+02
      RME1(4,12,11) =  6.59310E+01
      RME1(4,13,11) =  2.49300E+01
      RME1(4,14,11) =  1.41770E+01
      RME1(4,15,11) =  9.55330E+00
      RME1(4, 5,12) =  9.07080E-02
      RME1(4, 6,12) =  2.50890E-01
      RME1(4, 7,12) =  5.63460E-01
      RME1(4, 8,12) =  1.19580E+00
      RME1(4, 9,12) =  2.61750E+00
      RME1(4,10,12) =  6.58690E+00
      RME1(4,11,12) =  2.49240E+01
      RME1(4,12,12) = -2.03650E+02
      RME1(4,13,12) =  7.54690E+01
      RME1(4,14,12) =  2.84690E+01
      RME1(4,15,12) =  1.61630E+01
      RME1(4, 5,13) =  7.49670E-02
      RME1(4, 6,13) =  2.00660E-01
      RME1(4, 7,13) =  4.30330E-01
      RME1(4, 8,13) =  8.53470E-01
      RME1(4, 9,13) =  1.67900E+00
      RME1(4,10,13) =  3.48950E+00
      RME1(4,11,13) =  8.44910E+00
      RME1(4,12,13) =  3.09880E+01
      RME1(4,13,13) = -2.41200E+02
      RME1(4,14,13) =  8.56610E+01
      RME1(4,15,13) =  3.22250E+01
      RME1(4, 5,14) =  6.35040E-02
      RME1(4, 6,14) =  1.65880E-01
      RME1(4, 7,14) =  3.44130E-01
      RME1(4, 8,14) =  6.51630E-01
      RME1(4, 9,14) =  1.19820E+00
      RME1(4,10,14) =  2.23890E+00
      RME1(4,11,14) =  4.48110E+00
      RME1(4,12,14) =  1.05360E+01
      RME1(4,13,14) =  3.77000E+01
      RME1(4,14,14) = -2.81740E+02
      RME1(4,15,14) =  9.65060E+01
      RME1(4, 5,15) =  5.48260E-02
      RME1(4, 6,15) =  1.40550E-01
      RME1(4, 7,15) =  2.84430E-01
      RME1(4, 8,15) =  5.20870E-01
      RME1(4, 9,15) =  9.14350E-01
      RME1(4,10,15) =  1.59710E+00
      RME1(4,11,15) =  2.87510E+00
      RME1(4,12,15) =  5.59200E+00
      RME1(4,13,15) =  1.28470E+01
      RME1(4,14,15) =  4.50600E+01
      RME1(4,15,15) = -3.25280E+02

C H-G TRANSITION:
      RME1(5, 6, 5) =  2.72140E+01
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RME1(5, 7, 5) =  7.45730E+00
RME1(5, 8, 5) =  3.64220E+00
RME1(5, 9, 5) =  2.24990E+00
RME1(5,10, 5) =  1.57310E+00
RME1(5,11, 5) =  1.18630E+00
RME1(5,12, 5) =  9.40500E-01
RME1(5,13, 5) =  7.72520E-01
RME1(5,14, 5) =  6.51350E-01
RME1(5,15, 5) =  5.60300E-01
RME1(5, 6, 6) = -2.98490E+01
RME1(5, 7, 6) =  3.30640E+01
RME1(5, 8, 6) =  1.08660E+01
RME1(5, 9, 6) =  5.70590E+00
RME1(5,10, 6) =  3.65590E+00
RME1(5,11, 6) =  2.61200E+00
RME1(5,12, 6) =  1.99720E+00
RME1(5,13, 6) =  1.59880E+00
RME1(5,14, 6) =  1.32250E+00
RME1(5,15, 6) =  1.12110E+00
RME1(5, 6, 7) =  2.37410E+00
RME1(5, 7, 7) = -5.14380E+01
RME1(5, 8, 7) =  3.96420E+01
RME1(5, 9, 7) =  1.39590E+01
RME1(5,10, 7) =  7.58760E+00
RME1(5,11, 7) =  4.95900E+00
RME1(5,12, 7) =  3.58760E+00
RME1(5,13, 7) =  2.76640E+00
RME1(5,14, 7) =  2.22800E+00
RME1(5,15, 7) =  1.85140E+00
RME1(5, 6, 8) =  6.99500E-01
RME1(5, 7, 8) =  4.86810E+00
RME1(5, 8, 8) = -7.49390E+01
RME1(5, 9, 8) =  4.69160E+01
RME1(5,10, 8) =  1.70590E+01
RME1(5,11, 8) =  9.44250E+00
RME1(5,12, 8) =  6.24060E+00
RME1(5,13, 8) =  4.54820E+00
RME1(5,14, 8) =  3.52540E+00
RME1(5,15, 8) =  2.85010E+00
RME1(5, 6, 9) =  3.44840E-01
RME1(5, 7, 9) =  1.49470E+00
RME1(5, 8, 9) =  7.96580E+00
RME1(5, 9, 9) = -1.01020E+02
RME1(5,10, 9) =  5.48700E+01
RME1(5,11, 9) =  2.02750E+01
RME1(5,12, 9) =  1.13330E+01
RME1(5,13, 9) =  7.53780E+00
RME1(5,14, 9) =  5.51750E+00
RME1(5,15, 9) =  4.29100E+00
RME1(5, 6,10) =  2.12130E-01
RME1(5, 7,10) =  7.50780E-01
RME1(5, 8,10) =  2.50910E+00
RME1(5, 9,10) =  1.16910E+01
RME1(5,10,10) = -1.29900E+02
RME1(5,11,10) =  6.34950E+01
RME1(5,12,10) =  2.36530E+01
RME1(5,13,10) =  1.32910E+01
RME1(5,14,10) =  8.87100E+00
RME1(5,15,10) =  6.50930E+00
RME1(5, 6,11) =  1.47360E-01
RME1(5, 7,11) =  4.66180E-01
RME1(5, 8,11) =  1.27560E+00
RME1(5, 9,11) =  3.74640E+00
RME1(5,10,11) =  1.60520E+01
RME1(5,11,11) = -1.61660E+02
RME1(5,12,11) =  7.27850E+01
RME1(5,13,11) =  2.72170E+01
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      RME1(5,14,11) =  1.53330E+01
      RME1(5,15,11) =  1.02520E+01
      RME1(5, 6,12) =  1.10410E-01
      RME1(5, 7,12) =  3.25440E-01
      RME1(5, 8,12) =  7.96860E-01
      RME1(5, 9,12) =  1.92030E+00
      RME1(5,10,12) =  5.20740E+00
      RME1(5,11,12) =  2.10520E+01
      RME1(5,12,12) = -1.96350E+02
      RME1(5,13,12) =  8.27370E+01
      RME1(5,14,12) =  3.09790E+01
      RME1(5,15,12) =  1.74700E+01
      RME1(5, 6,13) =  8.70370E-02
      RME1(5, 7,13) =  2.44490E-01
      RME1(5, 8,13) =  5.58050E-01
      RME1(5, 9,13) =  1.20460E+00
      RME1(5,10,13) =  2.68490E+00
      RME1(5,11,13) =  6.89240E+00
      RME1(5,12,13) =  2.66960E+01
      RME1(5,13,13) = -2.34000E+02
      RME1(5,14,13) =  9.33470E+01
      RME1(5,15,13) =  3.49480E+01
      RME1(5, 6,14) =  7.11510E-02
      RME1(5, 7,14) =  1.93060E-01
      RME1(5, 8,14) =  4.19960E-01
      RME1(5, 9,14) =  8.45380E-01
      RME1(5,10,14) =  1.68920E+00
      RME1(5,11,14) =  3.56930E+00
      RME1(5,12,14) =  8.80160E+00
      RME1(5,13,14) =  3.29840E+01
      RME1(5,14,14) = -2.74610E+02
      RME1(5,15,14) =  1.04610E+02
      RME1(5, 6,15) =  5.97550E-02
      RME1(5, 7,15) =  1.57980E-01
      RME1(5, 8,15) =  3.31920E-01
      RME1(5, 9,15) =  6.36860E-01
      RME1(5,10,15) =  1.18710E+00
      RME1(5,11,15) =  2.25030E+00
      RME1(5,12,15) =  4.57310E+00
      RME1(5,13,15) =  1.09350E+01
      RME1(5,14,15) =  3.99170E+01
      RME1(5,15,15) = -3.18190E+02

C I-H TRANSITION:
      RME1(6, 7, 6) =  3.87110E+01
      RME1(6, 8, 6) =  9.90570E+00
      RME1(6, 9, 6) =  4.61860E+00
      RME1(6,10, 6) =  2.76000E+00
      RME1(6,11, 6) =  2.60000E+00
      RME1(6, 7, 7) = -3.78590E+01
      RME1(6, 8, 7) =  4.55660E+01
      RME1(6, 9, 7) =  1.42540E+01
      RME1(6,10, 7) =  7.22410E+00
      RME1(6,11, 7) =  4.50280E+00
      RME1(6, 7, 8) =  2.72970E+00
      RME1(6, 8, 8) = -6.34980E+01
      RME1(6, 9, 8) =  5.31590E+01
      RME1(6,10, 8) =  1.80360E+01
      RME1(6,11, 8) =  9.53800E+00
      RME1(6,12, 8) = -6.09830E+00
      RME1(6, 7, 9) =  7.57200E-01
      RME1(6, 8, 9) =  5.47990E+00
      RME1(6, 9, 9) = -9.05600E+01
      RME1(6,10, 9) =  6.14650E+01
      RME1(6,11, 9) =  2.17300E+01
      RME1(6,12, 9) =  1.17660E+01
      RME1(6, 7,10) =  3.55900E-01
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      RME1(6, 8,10) =  1.60020E+00
      RME1(6, 9,10) =  8.82050E+01
      RME1(6,10,10) = -1.20000E+02
      RME1(6,11,10) =  7.04630E+01
      RME1(6,12,10) =  2.54780E+01
      RME1(6, 7,11) =  2.12000E-01
      RME1(6, 8,11) =  7.74700E-01
      RME1(6, 9,11) =  2.66250E+00
      RME1(6,10,11) =  1.27800E+01
      RME1(6,11,11) = -1.52120E+02
      RME1(6,12,11) =  8.01380E+01
      RME1(6, 8,12) =  4.69900E-01
      RME1(6, 9,12) =  1.31310E+00
      RME1(6,10,12) =  3.94800E+00
      RME1(6,11,12) =  1.73870E+01
      RME1(6,12,12) = -1.87060E+02

C K-I TRANSITION:
      RME1(7, 8, 7) =  5.20000E+01
      RME1(7,11, 7) =  5.03000E+00
      RME1(7, 8, 8) = -4.64760E+01
      RME1(7,11, 8) =  1.03000E+01
      RME1(7, 8,11) =  6.00000E-01
      RME1(7,11,11) = -1.40010E+02
      RETURN
      END


      SUBROUTINE RADMATX2
      IMPLICIT REAL*8 (A-H,O-Z)
      COMMON/RADIAL/RME2
      DIMENSION RME2(10,20,20)

C THE DATA FORMAT IS RME2(L1,PN1,PN2); L1-L2=+1

C P-S TRANSITION:
      RME2(1, 3, 3) = -5.24460E+00
      RME2(1, 4, 3) = -1.79310E-01
      RME2(1, 5, 3) = -1.60130E-02
      RME2(1, 6, 3) =  8.80620E-03
      RME2(1, 7, 3) =  1.34420E-02
      RME2(1, 8, 3) =  1.35570E-02
      RME2(1, 9, 3) =  1.25430E-02
      RME2(1,10, 3) =  1.13150E-02
      RME2(1,11, 3) =  1.01430E-02
      RME2(1,12, 3) =  9.09840E-03
      RME2(1,13, 3) =  8.18920E-03
      RME2(1,14, 3) =  7.40360E-03
      RME2(1,15, 3) =  6.72510E-03
      RME2(1, 3, 4) =  4.25890E+00
      RME2(1, 4, 4) = -1.18480E+01
      RME2(1, 5, 4) = -7.11340E-01
      RME2(1, 6, 4) = -1.97560E-01
      RME2(1, 7, 4) = -8.34570E-02
      RME2(1, 8, 4) = -4.31970E-02
      RME2(1, 9, 4) = -2.52570E-02
      RME2(1,10, 4) = -1.60330E-02
      RME2(1,11, 4) = -1.08030E-02
      RME2(1,12, 4) = -7.61800E-03
      RME2(1,13, 4) = -5.56940E-03
      RME2(1,14, 4) = -4.19310E-03
      RME2(1,15, 4) = -3.23510E-03
      RME2(1, 3, 5) =  1.04630E+00
      RME2(1, 4, 5) =  9.78740E+00
      RME2(1, 5, 5) = -2.08420E+01
      RME2(1, 6, 5) = -1.48290E+00
      RME2(1, 7, 5) = -4.77560E-01
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RME2(1, 8, 5) = -2.32710E-01
RME2(1, 9, 5) = -1.38370E-01
RME2(1,10, 5) = -9.25230E-02
RME2(1,11, 5) = -6.68360E-02
RME2(1,12, 5) = -5.09760E-02
RME2(1,13, 5) = -4.04690E-02
RME2(1,14, 5) = -3.31250E-02
RME2(1,15, 5) = -2.77710E-02
RME2(1, 3, 6) =  5.53900E-01
RME2(1, 4, 6) =  2.19490E+00
RME2(1, 5, 6) =  1.72720E+01
RME2(1, 6, 6) = -3.22470E+01
RME2(1, 7, 6) = -2.48100E+00
RME2(1, 8, 6) = -8.46130E-01
RME2(1, 9, 6) = -4.31750E-01
RME2(1,10, 6) = -2.66600E-01
RME2(1,11, 6) = -1.83910E-01
RME2(1,12, 6) = -1.36340E-01
RME2(1,13, 6) = -1.06260E-01
RME2(1,14, 6) = -8.59080E-02
RME2(1,15, 6) = -7.14120E-02
RME2(1, 3, 7) =  3.65410E-01
RME2(1, 4, 7) =  1.12670E+00
RME2(1, 5, 7) =  3.67390E+00
RME2(1, 6, 7) =  2.67310E+01
RME2(1, 7, 7) = -4.60680E+01
RME2(1, 8, 7) = -3.70020E+00
RME2(1, 9, 7) = -1.29890E+00
RME2(1,10, 7) = -6.77160E-01
RME2(1,11, 7) = -4.25110E-01
RME2(1,12, 7) = -2.97110E-01
RME2(1,13, 7) = -2.22570E-01
RME2(1,14, 7) = -1.74960E-01
RME2(1,15, 7) = -1.42460E-01
RME2(1, 3, 8) =  2.67540E-01
RME2(1, 4, 8) =  7.34010E-01
RME2(1, 5, 8) =  1.84370E+00
RME2(1, 6, 8) =  5.48660E+00
RME2(1, 7, 8) =  3.81720E+01
RME2(1, 8, 8) = -6.23060E+01
RME2(1, 9, 8) = -5.13950E+00
RME2(1,10, 8) = -1.83450E+00
RME2(1,11, 8) = -9.67720E-01
RME2(1,12, 8) = -6.12820E-01
RME2(1,13, 8) = -4.31170E-01
RME2(1,14, 8) = -3.24690E-01
RME2(1,15, 8) = -2.56310E-01
RME2(1, 3, 9) =  2.08180E-01
RME2(1, 4, 9) =  5.34820E-01
RME2(1, 5, 9) =  1.18730E+00
RME2(1, 6, 9) =  2.70510E+00
RME2(1, 7, 9) =  7.63340E+00
RME2(1, 8, 9) =  5.15950E+01
RME2(1, 9, 9) = -8.09630E+01
RME2(1,10, 9) = -6.79790E+00
RME2(1,11, 9) = -2.45200E+00
RME2(1,12, 9) = -1.30260E+00
RME2(1,13, 9) = -8.28960E-01
RME2(1,14, 9) = -5.85380E-01
RME2(1,15, 9) = -4.42060E-01
RME2(1, 3,10) =  1.68610E-01
RME2(1, 4,10) =  4.15690E-01
RME2(1, 5,10) =  8.59870E-01
RME2(1, 6,10) =  1.72420E+00
RME2(1, 7,10) =  3.71050E+00
RME2(1, 8,10) =  1.01140E+01
RME2(1, 9,10) =  6.70020E+01
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RME2(1,10,10) = -1.02040E+02
RME2(1,11,10) = -8.67500E+00
RME2(1,12,10) = -3.15090E+00
RME2(1,13,10) = -1.68120E+00
RME2(1,14,10) = -1.07310E+00
RME2(1,15,10) = -7.59340E-01
RME2(1, 3,11) =  1.40520E-01
RME2(1, 4,11) =  3.36950E-01
RME2(1, 5,11) =  6.66340E-01
RME2(1, 6,11) =  1.24110E+00
RME2(1, 7,11) =  2.34420E+00
RME2(1, 8,11) =  4.85990E+00
RME2(1, 9,11) =  1.29300E+01
RME2(1,10,11) =  8.43930E+01
RME2(1,11,11) = -1.25530E+02
RME2(1,12,11) = -1.07700E+01
RME2(1,13,11) = -3.93070E+00
RME2(1,14,11) = -2.10320E+00
RME2(1,15,11) = -1.34480E+00
RME2(1, 3,12) =  1.19640E-01
RME2(1, 4,12) =  2.81290E-01
RME2(1, 5,12) =  5.39460E-01
RME2(1, 6,12) =  9.58220E-01
RME2(1, 7,12) =  1.67760E+00
RME2(1, 8,12) =  3.04680E+00
RME2(1, 9,12) =  6.15290E+00
RME2(1,10,12) =  1.60790E+01
RME2(1,11,12) =  1.03770E+02
RME2(1,12,12) = -1.51450E+02
RME2(1,13,12) = -1.30840E+01
RME2(1,14,12) = -4.79150E+00
RME2(1,15,12) = -2.56850E+00
RME2(1, 3,13) =  1.03580E-01
RME2(1, 4,13) =  2.40030E-01
RME2(1, 5,13) =  4.50290E-01
RME2(1, 6,13) =  7.74100E-01
RME2(1, 7,13) =  1.29030E+00
RME2(1, 8,13) =  2.16880E+00
RME2(1, 9,13) =  3.83170E+00
RME2(1,10,13) =  7.58960E+00
RME2(1,11,13) =  1.95630E+01
RME2(1,12,13) =  1.25130E+02
RME2(1,13,13) = -1.79780E+02
RME2(1,14,13) = -1.56160E+01
RME2(1,15,13) = -5.73290E+00
RME2(1, 3,14) =  9.08890E-02
RME2(1, 4,14) =  2.08310E-01
RME2(1, 5,14) =  3.84420E-01
RME2(1, 6,14) =  6.45420E-01
RME2(1, 7,14) =  1.03970E+00
RME2(1, 8,14) =  1.66190E+00
RME2(1, 9,14) =  2.71450E+00
RME2(1,10,14) =  4.69900E+00
RME2(1,11,14) =  9.16990E+00
RME2(1,12,14) =  2.33810E+01
RME2(1,13,14) =  1.48480E+02
RME2(1,14,14) = -2.10530E+02
RME2(1,15,14) = -1.83650E+01
RME2(1, 3,15) =  8.06370E-02
RME2(1, 4,15) =  1.83240E-01
RME2(1, 5,15) =  3.33920E-01
RME2(1, 6,15) =  5.50760E-01
RME2(1, 7,15) =  8.65480E-01
RME2(1, 8,15) =  1.33570E+00
RME2(1, 9,15) =  2.07270E+00
RME2(1,10,15) =  3.31450E+00
RME2(1,11,15) =  5.64840E+00
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      RME2(1,12,15) =  1.08940E+01
      RME2(1,13,15) =  2.75330E+01
      RME2(1,14,15) =  1.73810E+02
      RME2(1,15,15) = -2.43700E+02

C D-P TRANSITION:
      RME2(2, 3, 3) = -6.67490E+00
      RME2(2, 4, 3) = -1.50350E+00
      RME2(2, 5, 3) = -7.13760E-01
      RME2(2, 6, 3) = -4.39720E-01
      RME2(2, 7, 3) = -3.08170E-01
      RME2(2, 8, 3) = -2.32920E-01
      RME2(2, 9, 3) = -1.84880E-01
      RME2(2,10, 3) = -1.51870E-01
      RME2(2,11, 3) = -1.27930E-01
      RME2(2,12, 3) = -1.09870E-01
      RME2(2,13, 3) = -9.58090E-02
      RME2(2,14, 3) = -8.45900E-02
      RME2(2,15, 3) = -7.54550E-02
      RME2(2, 3, 4) =  8.83250E+00
      RME2(2, 4, 4) = -1.23150E+01
      RME2(2, 5, 4) = -3.09460E+00
      RME2(2, 6, 4) = -1.54110E+00
      RME2(2, 7, 4) = -9.74390E-01
      RME2(2, 8, 4) = -6.94260E-01
      RME2(2, 9, 4) = -5.30890E-01
      RME2(2,10, 4) = -4.25190E-01
      RME2(2,11, 4) = -3.51780E-01
      RME2(2,12, 4) = -2.98110E-01
      RME2(2,13, 4) = -2.57340E-01
      RME2(2,14, 4) = -2.25420E-01
      RME2(2,15, 4) = -1.99810E-01
      RME2(2, 3, 5) =  3.74890E-01
      RME2(2, 4, 5) =  1.84220E+01
      RME2(2, 5, 5) = -1.93880E+01
      RME2(2, 6, 5) = -5.00390E+00
      RME2(2, 7, 5) = -2.52640E+00
      RME2(2, 8, 5) = -1.60990E+00
      RME2(2, 9, 5) = -1.15300E+00
      RME2(2,10, 5) = -8.85250E-01
      RME2(2,11, 5) = -7.11370E-01
      RME2(2,12, 5) = -5.90290E-01
      RME2(2,13, 5) = -5.01590E-01
      RME2(2,14, 5) = -4.34060E-01
      RME2(2,15, 5) = -3.81090E-01
      RME2(2, 3, 6) =  1.70570E-01
      RME2(2, 4, 6) =  6.71120E-01
      RME2(2, 5, 6) =  3.06760E+01
      RME2(2, 6, 6) = -2.79070E+01
      RME2(2, 7, 6) = -7.25040E+00
      RME2(2, 8, 6) = -3.67240E+00
      RME2(2, 9, 6) = -2.34390E+00
      RME2(2,10, 6) = -1.68070E+00
      RME2(2,11, 6) = -1.29160E+00
      RME2(2,12, 6) = -1.03900E+00
      RME2(2,13, 6) = -8.63070E-01
      RME2(2,14, 6) = -7.34210E-01
      RME2(2,15, 6) = -6.36110E-01
      RME2(2, 3, 7) =  1.08290E-01
      RME2(2, 4, 7) =  2.88660E-01
      RME2(2, 5, 7) =  9.46780E-01
      RME2(2, 6, 7) =  4.56730E+01
      RME2(2, 7, 7) = -3.78740E+01
      RME2(2, 8, 7) = -9.84080E+00
      RME2(2, 9, 7) = -4.98080E+00
      RME2(2,10, 7) = -3.17610E+00
      RME2(2,11, 7) = -2.27570E+00
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RME2(2,12, 7) = -1.74820E+00
RME2(2,13, 7) = -1.40600E+00
RME2(2,14, 7) = -1.16810E+00
RME2(2,15, 7) = -9.93930E-01
RME2(2, 3, 8) =  7.81850E-02
RME2(2, 4, 8) =  1.80720E-01
RME2(2, 5, 8) =  3.82470E-01
RME2(2, 6, 8) =  1.19770E+00
RME2(2, 7, 8) =  6.34350E+01
RME2(2, 8, 8) = -4.92930E+01
RME2(2, 9, 8) = -1.27780E+01
RME2(2,10, 8) = -6.45260E+00
RME2(2,11, 8) = -4.10640E+00
RME2(2,12, 8) = -2.93770E+00
RME2(2,13, 8) = -2.25410E+00
RME2(2,14, 8) = -1.81160E+00
RME2(2,15, 8) = -1.50420E+00
RME2(2, 3, 9) =  6.04820E-02
RME2(2, 4, 9) =  1.30120E-01
RME2(2, 5, 9) =  2.35240E-01
RME2(2, 6, 9) =  4.50580E-01
RME2(2, 7, 9) =  1.42150E+00
RME2(2, 8, 9) =  8.39680E+01
RME2(2, 9, 9) = -6.21630E+01
RME2(2,10, 9) = -1.60640E+01
RME2(2,11, 9) = -8.08850E+00
RME2(2,12, 9) = -5.13510E+00
RME2(2,13, 9) = -3.66650E+00
RME2(2,14, 9) = -2.80910E+00
RME2(2,15, 9) = -2.25510E+00
RME2(2, 3,10) =  4.88670E-02
RME2(2, 4,10) =  1.00770E-01
RME2(2, 5,10) =  1.68540E-01
RME2(2, 6,10) =  2.71170E-01
RME2(2, 7,10) =  4.92210E-01
RME2(2, 8,10) =  1.61650E+00
RME2(2, 9,10) =  1.07280E+02
RME2(2,10,10) = -7.64840E+01
RME2(2,11,10) = -1.96990E+01
RME2(2,12,10) = -9.88900E+00
RME2(2,13,10) = -6.26210E+00
RME2(2,14,10) = -4.46200E+00
RME2(2,15,10) = -3.41300E+00
RME2(2, 3,11) =  4.06920E-02
RME2(2, 4,11) =  8.16280E-02
RME2(2, 5,11) =  1.30450E-01
RME2(2, 6,11) =  1.92990E-01
RME2(2, 7,11) =  2.88240E-01
RME2(2, 8,11) =  5.06950E-01
RME2(2, 9,11) =  1.78180E+00
RME2(2,10,11) =  1.33360E+02
RME2(2,11,11) = -9.22580E+01
RME2(2,12,11) = -2.36840E+01
RME2(2,13,11) = -1.18540E+01
RME2(2,14,11) = -7.48770E+00
RME2(2,15,11) = -5.32410E+00
RME2(2, 3,12) =  3.46460E-02
RME2(2, 4,12) =  6.81820E-02
RME2(2, 5,12) =  1.05800E-01
RME2(2, 6,12) =  1.49170E-01
RME2(2, 7,12) =  2.03410E-01
RME2(2, 8,12) =  2.86380E-01
RME2(2, 9,12) =  4.94570E-01
RME2(2,10,12) =  1.91690E+00
RME2(2,11,12) =  1.62220E+02
RME2(2,12,12) = -1.09480E+02
RME2(2,13,12) = -2.80190E+01
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      RME2(2,14,12) = -1.39850E+01
      RME2(2,15,12) = -8.81190E+00
      RME2(2, 3,13) =  3.00080E-02
      RME2(2, 4,13) =  5.82390E-02
      RME2(2, 5,13) =  8.85420E-02
      RME2(2, 6,13) =  1.21070E-01
      RME2(2, 7,13) =  1.56940E-01
      RME2(2, 8,13) =  1.99850E-01
      RME2(2, 9,13) =  2.65580E-01
      RME2(2,10,13) =  4.54940E-01
      RME2(2,11,13) =  2.02130E+00
      RME2(2,12,13) =  1.93860E+02
      RME2(2,13,13) = -1.28160E+02
      RME2(2,14,13) = -3.27050E+01
      RME2(2,15,13) = -1.62800E+01
      RME2(2, 3,14) =  2.63480E-02
      RME2(2, 4,14) =  5.06040E-02
      RME2(2, 5,14) =  7.58010E-02
      RME2(2, 6,14) =  1.01480E-01
      RME2(2, 7,14) =  1.27460E-01
      RME2(2, 8,14) =  1.53850E-01
      RME2(2, 9,14) =  1.82390E-01
      RME2(2,10,14) =  2.25870E-01
      RME2(2,11,14) =  3.87980E-01
      RME2(2,12,14) =  2.09480E+00
      RME2(2,13,14) =  2.28270E+02
      RME2(2,14,14) = -1.48290E+02
      RME2(2,15,14) = -3.77420E+01
      RME2(2, 3,15) =  2.33940E-02
      RME2(2, 4,15) =  4.45690E-02
      RME2(2, 5,15) =  6.60190E-02
      RME2(2, 6,15) =  8.70490E-02
      RME2(2, 7,15) =  1.07030E-01
      RME2(2, 8,15) =  1.25090E-01
      RME2(2, 9,15) =  1.40020E-01
      RME2(2,10,15) =  1.51100E-01
      RME2(2,11,15) =  1.67250E-01
      RME2(2,12,15) =  2.93620E-01
      RME2(2,13,15) =  2.13700E+00
      RME2(2,14,15) =  2.65460E+02
      RME2(2,15,15) = -1.69870E+02

C F-D TRANSITION:
      RME2(3, 4, 3) =  1.00470E+01
      RME2(3, 5, 3) =  3.32660E+00
      RME2(3, 6, 3) =  1.81760E+00
      RME2(3, 7, 3) =  1.20590E+00
      RME2(3, 8, 3) =  8.84760E-01
      RME2(3, 9, 3) =  6.89960E-01
      RME2(3,10, 3) =  5.60120E-01
      RME2(3,11, 3) =  4.68080E-01
      RME2(3,12, 3) =  3.99700E-01
      RME2(3,13, 3) =  3.47070E-01
      RME2(3,14, 3) =  3.05430E-01
      RME2(3,15, 3) =  2.71760E-01
      RME2(3, 4, 4) = -1.59620E+01
      RME2(3, 5, 4) =  1.35960E+01
      RME2(3, 6, 4) =  5.12770E+00
      RME2(3, 7, 4) =  2.92940E+00
      RME2(3, 8, 4) =  1.98590E+00
      RME2(3, 9, 4) =  1.47600E+00
      RME2(3,10, 4) =  1.16110E+00
      RME2(3,11, 4) =  9.49110E-01
      RME2(3,12, 4) =  7.97480E-01
      RME2(3,13, 4) =  6.84100E-01
      RME2(3,14, 4) =  5.96350E-01
      RME2(3,15, 4) =  5.26690E-01
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RME2(3, 4, 5) =  1.86750E+00
RME2(3, 5, 5) = -3.01440E+01
RME2(3, 6, 5) =  1.77680E+01
RME2(3, 7, 5) =  6.95340E+00
RME2(3, 8, 5) =  4.06320E+00
RME2(3, 9, 5) =  2.76020E+00
RME2(3,10, 5) =  2.06310E+00
RME2(3,11, 5) =  1.62990E+00
RME2(3,12, 5) =  1.33690E+00
RME2(3,13, 5) =  1.12660E+00
RME2(3,14, 5) =  9.68940E-01
RME2(3,15, 5) =  8.46710E-01
RME2(3, 4, 6) =  6.31830E-01
RME2(3, 5, 6) =  4.09330E+00
RME2(3, 6, 6) = -4.69590E+01
RME2(3, 7, 6) =  2.25510E+01
RME2(3, 8, 6) =  8.92190E+00
RME2(3, 9, 6) =  5.20480E+00
RME2(3,10, 6) =  3.56960E+00
RME2(3,11, 6) =  2.67360E+00
RME2(3,12, 6) =  2.11560E+00
RME2(3,13, 6) =  1.73790E+00
RME2(3,14, 6) =  1.46670E+00
RME2(3,15, 6) =  1.26320E+00
RME2(3, 4, 7) =  3.43270E-01
RME2(3, 5, 7) =  1.39640E+00
RME2(3, 6, 7) =  7.00710E+00
RME2(3, 7, 7) = -6.66460E+01
RME2(3, 8, 7) =  2.79380E+01
RME2(3, 9, 7) =  1.10680E+01
RME2(3,10, 7) =  6.45870E+00
RME2(3,11, 7) =  4.42980E+00
RME2(3,12, 7) =  3.31820E+00
RME2(3,13, 7) =  2.62630E+00
RME2(3,14, 7) =  2.15820E+00
RME2(3,15, 7) =  1.82220E+00
RME2(3, 4, 8) =  2.26100E-01
RME2(3, 5, 8) =  7.58660E-01
RME2(3, 6, 8) =  2.39860E+00
RME2(3, 7, 8) =  1.06220E+01
RME2(3, 8, 8) = -8.92730E+01
RME2(3, 9, 8) =  3.39250E+01
RME2(3,10, 8) =  1.34070E+01
RME2(3,11, 8) =  7.80860E+00
RME2(3,12, 8) =  5.34830E+00
RME2(3,13, 8) =  4.00240E+00
RME2(3,14, 8) =  3.16600E+00
RME2(3,15, 8) =  2.60090E+00
RME2(3, 4, 9) =  1.64990E-01
RME2(3, 5, 9) =  4.98900E-01
RME2(3, 6, 9) =  1.30170E+00
RME2(3, 7, 9) =  3.64100E+00
RME2(3, 8, 9) =  1.49420E+01
RME2(3, 9, 9) = -1.14870E+02
RME2(3,10, 9) =  4.05100E+01
RME2(3,11, 9) =  1.59450E+01
RME2(3,12, 9) =  9.26000E+00
RME2(3,13, 9) =  6.32920E+00
RME2(3,14, 9) =  4.72930E+00
RME2(3,15, 9) =  3.73700E+00
RME2(3, 4,10) =  1.28170E-01
RME2(3, 5,10) =  3.63470E-01
RME2(3, 6,10) =  8.54190E-01
RME2(3, 7,10) =  1.97270E+00
RME2(3, 8,10) =  5.12350E+00
RME2(3, 9,10) =  1.99690E+01
RME2(3,10,10) = -1.43440E+02
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      RME2(3,11,10) =  4.76890E+01
      RME2(3,12,10) =  1.86850E+01
      RME2(3,13,10) =  1.08160E+01
      RME2(3,14,10) =  7.37490E+00
      RME2(3,15,10) =  5.50090E+00
      RME2(3, 4,11) =  1.03830E-01
      RME2(3, 5,11) =  2.82060E-01
      RME2(3, 6,11) =  6.21120E-01
      RME2(3, 7,11) =  1.29170E+00
      RME2(3, 8,11) =  2.77120E+00
      RME2(3, 9,11) =  6.84600E+00
      RME2(3,10,11) =  2.57040E+01
      RME2(3,11,11) = -1.75010E+02
      RME2(3,12,11) =  5.54640E+01
      RME2(3,13,11) =  2.16290E+01
      RME2(3,14,11) =  1.24780E+01
      RME2(3,15,11) =  8.48710E+00
      RME2(3, 4,12) =  8.66610E-02
      RME2(3, 5,12) =  2.28350E-01
      RME2(3, 6,12) =  4.81260E-01
      RME2(3, 7,12) =  9.37350E-01
      RME2(3, 8,12) =  1.81070E+00
      RME2(3, 9,12) =  3.69650E+00
      RME2(3,10,12) =  8.80810E+00
      RME2(3,11,12) =  3.21470E+01
      RME2(3,12,12) = -2.09560E+02
      RME2(3,13,12) =  6.38340E+01
      RME2(3,14,12) =  2.47800E+01
      RME2(3,15,12) =  1.42490E+01
      RME2(3, 4,13) =  7.39600E-02
      RME2(3, 5,13) =  1.90550E-01
      RME2(3, 6,13) =  3.89200E-01
      RME2(3, 7,13) =  7.25070E-01
      RME2(3, 8,13) =  1.31140E+00
      RME2(3, 9,13) =  2.41050E+00
      RME2(3,10,13) =  4.74830E+00
      RME2(3,11,13) =  1.10100E+01
      RME2(3,12,13) =  3.92980E+01
      RME2(3,13,13) = -2.47100E+02
      RME2(3,14,13) =  7.27980E+01
      RME2(3,15,13) =  2.81370E+01
      RME2(3, 4,14) =  6.42180E-02
      RME2(3, 5,14) =  1.62640E-01
      RME2(3, 6,14) =  3.24540E-01
      RME2(3, 7,14) =  5.85630E-01
      RME2(3, 8,14) =  1.01270E+00
      RME2(3, 9,14) =  1.74250E+00
      RME2(3,10,14) =  3.09060E+00
      RME2(3,11,14) =  5.92610E+00
      RME2(3,12,14) =  1.34500E+01
      RME2(3,13,14) =  4.71580E+01
      RME2(3,14,14) = -2.87640E+02
      RME2(3,15,14) =  8.23550E+01
      RME2(3, 4,15) =  5.65310E-02
      RME2(3, 5,15) =  1.41270E-01
      RME2(3, 6,15) =  2.76900E-01
      RME2(3, 7,15) =  4.87880E-01
      RME2(3, 8,15) =  8.16790E-01
      RME2(3, 9,15) =  1.34340E+00
      RME2(3,10,15) =  2.23010E+00
      RME2(3,11,15) =  3.85060E+00
      RME2(3,12,15) =  7.22970E+00
      RME2(3,13,15) =  1.61200E+01
      RME2(3,14,15) =  5.57270E+01
      RME2(3,15,15) = -3.31180E+02

C G-F TRANSITION:
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RME2(4, 5, 4) =  1.77190E+01
RME2(4, 6, 4) =  5.25110E+00
RME2(4, 7, 4) =  2.69870E+00
RME2(4, 8, 4) =  1.72470E+00
RME2(4, 9, 4) =  1.23530E+00
RME2(4,10, 4) =  9.47740E-01
RME2(4,11, 4) =  7.61030E-01
RME2(4,12, 4) =  6.31090E-01
RME2(4,13, 4) =  5.35970E-01
RME2(4,14, 4) =  4.63600E-01
RME2(4,15, 4) =  4.06880E-01
RME2(4, 5, 5) = -2.25010E+01
RME2(4, 6, 5) =  2.25600E+01
RME2(4, 7, 5) =  7.82840E+00
RME2(4, 8, 5) =  4.26630E+00
RME2(4, 9, 5) =  2.80640E+00
RME2(4,10, 5) =  2.04380E+00
RME2(4,11, 5) =  1.58520E+00
RME2(4,12, 5) =  1.28270E+00
RME2(4,13, 5) =  1.06980E+00
RME2(4,14, 5) =  9.12770E-01
RME2(4,15, 5) =  7.92540E-01
RME2(4, 5, 6) =  2.02010E+00
RME2(4, 6, 6) = -4.02500E+01
RME2(4, 7, 6) =  2.81090E+01
RME2(4, 8, 6) =  1.02930E+01
RME2(4, 9, 6) =  5.75420E+00
RME2(4,10, 6) =  3.83890E+00
RME2(4,11, 6) =  2.82050E+00
RME2(4,12, 6) =  2.20070E+00
RME2(4,13, 6) =  1.78870E+00
RME2(4,14, 6) =  1.49710E+00
RME2(4,15, 6) =  1.28090E+00
RME2(4, 5, 7) =  6.36560E-01
RME2(4, 6, 7) =  4.26300E+00
RME2(4, 7, 7) = -6.03200E+01
RME2(4, 8, 7) =  3.43410E+01
RME2(4, 9, 7) =  1.28540E+01
RME2(4,10, 7) =  7.27010E+00
RME2(4,11, 7) =  4.88400E+00
RME2(4,12, 7) =  3.60460E+00
RME2(4,13, 7) =  2.82160E+00
RME2(4,14, 7) =  2.29890E+00
RME2(4,15, 7) =  1.92800E+00
RME2(4, 5, 8) =  3.28730E-01
RME2(4, 6, 8) =  1.38260E+00
RME2(4, 7, 8) =  7.12070E+00
RME2(4, 8, 8) = -8.31410E+01
RME2(4, 9, 8) =  4.12410E+01
RME2(4,10, 8) =  1.55760E+01
RME2(4,11, 8) =  8.85480E+00
RME2(4,12, 8) =  5.96720E+00
RME2(4,13, 8) =  4.41330E+00
RME2(4,14, 8) =  3.46000E+00
RME2(4,15, 8) =  2.82250E+00
RME2(4, 5, 9) =  2.09060E-01
RME2(4, 6, 9) =  7.21800E-01
RME2(4, 7, 9) =  2.34870E+00
RME2(4, 8, 9) =  1.06120E+01
RME2(4, 9, 9) = -1.08840E+02
RME2(4,10, 9) =  4.88040E+01
RME2(4,11, 9) =  1.84880E+01
RME2(4,12, 9) =  1.05280E+01
RME2(4,13, 9) =  7.10180E+00
RME2(4,14, 9) =  5.25600E+00
RME2(4,15, 9) =  4.12280E+00
RME2(4, 5,10) =  1.48810E-01
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RME2(4, 6,10) =  4.61060E-01
RME2(4, 7,10) =  1.23400E+00
RME2(4, 8,10) =  3.53830E+00
RME2(4, 9,10) =  1.47440E+01
RME2(4,10,10) = -1.37480E+02
RME2(4,11,10) =  5.70270E+01
RME2(4,12,10) =  2.16010E+01
RME2(4,13,10) =  1.22990E+01
RME2(4,14,10) =  8.29530E+00
RME2(4,15,10) =  6.13820E+00
RME2(4, 5,11) =  1.13560E-01
RME2(4, 6,11) =  3.28790E-01
RME2(4, 7,11) =  7.90120E-01
RME2(4, 8,11) =  1.86650E+00
RME2(4, 9,11) =  4.95240E+00
RME2(4,10,11) =  1.95200E+01
RME2(4,11,11) = -1.69080E+02
RME2(4,12,11) =  6.59050E+01
RME2(4,13,11) =  2.49250E+01
RME2(4,14,11) =  1.41750E+01
RME2(4,15,11) =  9.55230E+00
RME2(4, 5,12) =  9.07910E-02
RME2(4, 6,12) =  2.51090E-01
RME2(4, 7,12) =  5.63870E-01
RME2(4, 8,12) =  1.19660E+00
RME2(4, 9,12) =  2.61910E+00
RME2(4,10,12) =  6.59100E+00
RME2(4,11,12) =  2.49420E+01
RME2(4,12,12) = -2.03650E+02
RME2(4,13,12) =  7.54380E+01
RME2(4,14,12) =  2.84620E+01
RME2(4,15,12) =  1.61600E+01
RME2(4, 5,13) =  7.50360E-02
RME2(4, 6,13) =  2.00830E-01
RME2(4, 7,13) =  4.30650E-01
RME2(4, 8,13) =  8.54060E-01
RME2(4, 9,13) =  1.68010E+00
RME2(4,10,13) =  3.49160E+00
RME2(4,11,13) =  8.45430E+00
RME2(4,12,13) =  3.10100E+01
RME2(4,13,13) = -2.41210E+02
RME2(4,14,13) =  8.56250E+01
RME2(4,15,13) =  3.22170E+01
RME2(4, 5,14) =  6.35640E-02
RME2(4, 6,14) =  1.66020E-01
RME2(4, 7,14) =  3.44390E-01
RME2(4, 8,14) =  6.52090E-01
RME2(4, 9,14) =  1.19890E+00
RME2(4,10,14) =  2.24030E+00
RME2(4,11,14) =  4.48380E+00
RME2(4,12,14) =  1.05420E+01
RME2(4,13,14) =  3.77270E+01
RME2(4,14,14) = -2.81750E+02
RME2(4,15,14) =  9.64640E+01
RME2(4, 5,15) =  5.48790E-02
RME2(4, 6,15) =  1.40760E-01
RME2(4, 7,15) =  2.84640E-01
RME2(4, 8,15) =  5.21240E-01
RME2(4, 9,15) =  9.14950E-01
RME2(4,10,15) =  1.59810E+00
RME2(4,11,15) =  2.87690E+00
RME2(4,12,15) =  5.59530E+00
RME2(4,13,15) =  1.28550E+01
RME2(4,14,15) =  4.50920E+01
RME2(4,15,15) = -3.25280E+02

C H-G TRANSITION:
```

```
RME2(5, 6, 5) =  2.72140E+01
RME2(5, 7, 5) =  7.45730E+00
RME2(5, 8, 5) =  3.64320E+00
RME2(5, 9, 5) =  2.24990E+00
RME2(5,10, 5) =  1.57310E+00
RME2(5,11, 5) =  1.18630E+00
RME2(5,12, 5) =  9.40500E-01
RME2(5,13, 5) =  7.72520E-01
RME2(5,14, 5) =  6.51350E-01
RME2(5,15, 5) =  5.60300E-01
RME2(5, 6, 6) = -2.98490E+01
RME2(5, 7, 6) =  3.30640E+01
RME2(5, 8, 6) =  1.08660E+01
RME2(5, 9, 6) =  5.70590E+00
RME2(5,10, 6) =  3.65590E+00
RME2(5,11, 6) =  2.61200E+00
RME2(5,12, 6) =  1.99720E+00
RME2(5,13, 6) =  1.59880E+00
RME2(5,14, 6) =  1.32250E+00
RME2(5,15, 6) =  1.12110E+00
RME2(5, 6, 7) =  2.37410E+00
RME2(5, 7, 7) = -5.14390E+01
RME2(5, 8, 7) =  3.96420E+01
RME2(5, 9, 7) =  1.39590E+01
RME2(5,10, 7) =  7.58760E+00
RME2(5,11, 7) =  4.95900E+00
RME2(5,12, 7) =  3.58760E+00
RME2(5,13, 7) =  2.76640E+00
RME2(5,14, 7) =  2.22800E+00
RME2(5,15, 7) =  1.85140E+00
RME2(5, 6, 8) =  6.99500E-01
RME2(5, 7, 8) =  4.86810E+00
RME2(5, 8, 8) = -7.49390E+01
RME2(5, 9, 8) =  4.69160E+01
RME2(5,10, 8) =  1.70590E+01
RME2(5,11, 8) =  9.44250E+00
RME2(5,12, 8) =  6.24060E+00
RME2(5,13, 8) =  4.54820E+00
RME2(5,14, 8) =  3.52540E+00
RME2(5,15, 8) =  2.85010E+00
RME2(5, 6, 9) =  3.44840E-01
RME2(5, 7, 9) =  1.49470E+00
RME2(5, 8, 9) =  7.96580E+00
RME2(5, 9, 9) = -1.01020E+02
RME2(5,10, 9) =  5.48700E+01
RME2(5,11, 9) =  2.02750E+01
RME2(5,12, 9) =  1.13330E+01
RME2(5,13, 9) =  7.53780E+00
RME2(5,14, 9) =  5.51750E+00
RME2(5,15, 9) =  4.29010E+00
RME2(5, 6,10) =  2.12140E-01
RME2(5, 7,10) =  7.50780E-01
RME2(5, 8,10) =  2.50910E+00
RME2(5, 9,10) =  1.16910E+01
RME2(5,10,10) = -1.29900E+02
RME2(5,11,10) =  6.34950E+01
RME2(5,12,10) =  2.36530E+01
RME2(5,13,10) =  1.32910E+01
RME2(5,14,10) =  8.87100E+00
RME2(5,15,10) =  6.50930E+00
RME2(5, 6,11) =  1.47360E-01
RME2(5, 7,11) =  4.66180E-01
RME2(5, 8,11) =  1.27560E+00
RME2(5, 9,11) =  3.74640E+00
RME2(5,10,11) =  1.60520E+01
RME2(5,11,11) = -1.61660E+02
RME2(5,12,11) =  7.27850E+01
```

```
      RME2(5,13,11) =  2.72170E+01
      RME2(5,14,11) =  1.53330E+01
      RME2(5,15,11) =  1.02520E+01
      RME2(5, 6,12) =  1.10410E-01
      RME2(5, 7,12) =  3.25440E-01
      RME2(5, 8,12) =  7.96860E-01
      RME2(5, 9,12) =  1.92030E+00
      RME2(5,10,12) =  5.20740E+00
      RME2(5,11,12) =  2.10520E+01
      RME2(5,12,12) = -1.96350E+02
      RME2(5,13,12) =  8.27360E+01
      RME2(5,14,12) =  3.09790E+01
      RME2(5,15,12) =  1.74700E+01
      RME2(5, 6,13) =  8.70370E-02
      RME2(5, 7,13) =  2.44490E-01
      RME2(5, 8,13) =  5.58060E-01
      RME2(5, 9,13) =  1.20460E+00
      RME2(5,10,13) =  2.68500E+00
      RME2(5,11,13) =  6.89250E+00
      RME2(5,12,13) =  2.66960E+01
      RME2(5,13,13) = -2.34000E+02
      RME2(5,14,13) =  9.33460E+01
      RME2(5,15,13) =  3.49480E+01
      RME2(5, 6,14) =  7.11510E-02
      RME2(5, 7,14) =  1.93060E-01
      RME2(5, 8,14) =  4.19970E-01
      RME2(5, 9,14) =  8.45390E-01
      RME2(5,10,14) =  1.68920E+00
      RME2(5,11,14) =  3.56930E+00
      RME2(5,12,14) =  8.80170E+00
      RME2(5,13,14) =  3.29840E+01
      RME2(5,14,14) = -2.74610E+02
      RME2(5,15,14) =  1.04610E+02
      RME2(5, 6,15) =  5.95760E-02
      RME2(5, 7,15) =  1.57980E-01
      RME2(5, 8,15) =  3.31920E-01
      RME2(5, 9,15) =  6.36870E-01
      RME2(5,10,15) =  1.18710E+00
      RME2(5,11,15) =  2.25030E+00
      RME2(5,12,15) =  4.57310E+00
      RME2(5,13,15) =  1.09350E+01
      RME2(5,14,15) =  3.99170E+01
      RME2(5,15,15) = -3.18190E+02

C I-H TRANSITION:
      RME2(6, 7, 6) =  3.87110E+01
      RME2(6, 8, 6) =  9.90570E+00
      RME2(6, 9, 6) =  4.61860E+00
      RME2(6,10, 6) =  2.76000E+00
      RME2(6,11, 6) =  2.60000E+00
      RME2(6, 7, 7) = -3.78590E+01
      RME2(6, 8, 7) =  4.55660E+01
      RME2(6, 9, 7) =  1.42540E+01
      RME2(6,10, 7) =  7.22410E+00
      RME2(6,11, 7) =  4.50280E+00
      RME2(6, 7, 8) =  2.72970E+00
      RME2(6, 8, 8) = -6.34980E+01
      RME2(6, 9, 8) =  5.31590E+01
      RME2(6,10, 8) =  1.80360E+01
      RME2(6,11, 8) =  9.53800E+00
      RME2(6,12, 8) = -6.09830E+00
      RME2(6, 7, 9) =  7.57200E-01
      RME2(6, 8, 9) =  5.47990E+00
      RME2(6, 9, 9) = -9.05600E+01
      RME2(6,10, 9) =  6.14650E+01
      RME2(6,11, 9) =  2.17300E+01
      RME2(6,12, 9) =  1.17660E+01
```

```
      RME2(6, 7,10) =  3.55900E-01
      RME2(6, 8,10) =  1.60020E+00
      RME2(6, 9,10) =  8.82050E+01
      RME2(6,10,10) = -1.20000E+02
      RME2(6,11,10) =  7.04630E+01
      RME2(6,12,10) =  2.54780E+01
      RME2(6, 7,11) =  2.12000E-01
      RME2(6, 8,11) =  7.74700E-01
      RME2(6, 9,11) =  2.66250E+00
      RME2(6,10,11) =  1.27800E+01
      RME2(6,11,11) = -1.52120E+02
      RME2(6,12,11) =  8.01380E+01
      RME2(6, 8,12) =  4.69900E-01
      RME2(6, 9,12) =  1.31310E+00
      RME2(6,10,12) =  3.94800E+00
      RME2(6,11,12) =  1.73870E+01
      RME2(6,12,12) = -1.87060E+02

C K-I TRANSITION:
      RME2(7, 8, 7) =  5.20000E+01
      RME2(7,11, 7) =  5.03000E+00
      RME2(7, 8, 8) = -4.64760E+01
      RME2(7,11, 8) =  1.03000E+01
      RME2(7, 8,11) =  6.00000E-01
      RME2(7,11,11) = -1.40010E+02

      RETURN
      END
```

CODE C: Line Shape Construction and Instrument Convolution

```
C*************************LINSHAPE.FOR*********************************
C                                                                      *
C                      LINE SHAPE CONSTRUCTION                         *
C             AND INSTRUMENT FUNCTION CONVOLUTION PROGRAM              *
C                                                                      *
C                      LAST UPDATE: 20 MAY 1994                        *
C                                                                      *
C                     MISSION RESEARCH CORPORATION                     *
C                        1 TARA BLVD SUITE 302                         *
C                         NASHUA NH 03062-2801                         *
C                                                                      *
C                                                                      *
C  SPEC:       SWITCH FOR INSTRUMENT FUNCTION (SPEX SPECTROMETER, CVF  *
C               INTERFEROMETER, OR GENERIC).                           *
C  INSTFNT:    TRIANGULAR OR RECTANGULAR INSTRUMENT FUNCTION.          *
C  DELAMDA:    FWHM SUPPLIED ON INPUT FOR TRIANGULAR/RECTANGULAR INST. FN.*
C  ENAMEW:     OUTPUT FILE FOR CONVOLVED SPECTRA.                      *
C  NAMEIN1:    SPIN 1 OUTPUT FILE FROM CODE-B.                         *
C  NAMEIN2:    SPIN 2 OUTPUT FILE FROM CODE-B.                         *
C                                                                      *
C  I,J,N,M:    LOOP INDICES.                                           *
C  NP:         ARRAY SIZE LIMIT.                                       *
C  NUMLINE:    NUMBER OF TRANSITIONS (LINES) LOADED INTO PROGRAM.      *
C  NINC        NUMBER OF SAMPLES IN THE SPECTRUM.                      *
C  DIV:        LOOP INDICE (STEP) DETERMINE FROM EXTERNAL RESOLUTION.  *
C                                                                      *
C  PI:         3.1415927                                               *
C  HP,C0:      PLANCK'S CONSTANT AND SPEED OF LIGHT.                   *
C  FPI:        FOUR PI STERADIANS.                                     *
C  LINE:       LINE POSITION (MICRON).                                 *
C  A:          EINSTEIN A-COEFFICIENT (S-1).                           *
C  POP:        RELATIVE POPULATION OF THE UPPER STATE OF THE TRANSITION.*
C  DENS:       TOTAL ATOM DENSITY SUPPLIED ON INPUT (CM-3).            *
C  DDN:        ELECTRON DENSITY SUPPLIED BY CODE-B INPUT FILE.         *
C  TE:         ELECTRON TEMPERATURE SUPPLIED BY CODE-B INPUT FILE.     *
C  TEL:        ELECTRONIC TEMPERATURE SUPPLIED BY CODE-B INPUT FILE.   *
C  EWDTH:      HALF-WIDTH AT HALF MAX OF STARK WIDTH (CM-1).           *
C  A/C0        ROUGH APPROXIMATION OF NATURAL LINE WIDTH (CM-1)        *
C  LORLINE:    CALCULATED LORENTZ ARRAY AT EACH LINE (CM-1).           *
C  TOTRAD:     SUMMATION OF ALL LORENTZ ARRAYS FOR TOTAL CONTRIBUTION. *
C  WAVLEN:     WAVELENGTH ARRAY (MICRON).                              *
C  F:          WAVENUMBER SPACE VARIABLE (CM-1).                       *
C  F0:         LINE POSITION IN WAVENUMBER SPACE (CM-1).               *
C  XCONVL:     WAVELENGTH ARRAY PASSED BACK FROM CONVOLUTION SUBROUTINE.*
C  YCONVL:     CONVOLVED SPECTRUM ARRAY PASSED BACK FROM CONVOLUTION   *
C               SUBROUTINE.                                            *
C  R:          INTERNAL RESOLUTION FOR LORENTZ ARRAYS (MICRON).        *
C  REXT:       EXTERNAL RESOLUTION FOR CONVOLVED OUTPUT (MICRON).      *
C  ENRGY:      ENERGY OF TRANSITION (ERG).                             *
C  INTENS:     POPULATION, A-COEFFICIENT, AND TRANSITION ENERGY.       *
C  NUMER:      VARIABLE USED FOR OPTIMIZATION.                         *
C  HWHM2:      VARIABLE USED FOR OPTIMIZATION.                         *
C                                                                      *
C  SUBROUTINES:     LORENTZ, CONVOLV.                                 *
C  REAL FUNCTIONS:  SPEX, CVF.                                        *
C                                                                      *
C**********************************************************************

      PROGRAM LINSHAP7
      IMPLICIT NONE

      INTEGER I,J,N,M,NUMLINE,NP,NINC,DIV
      CHARACTER*1 SPEC,INSTFNT
```

```
      CHARACTER*12 ENAMEW,NAMEIN1,NAMEIN2
      REAL PI,HP,C0,HC,FPI
      REAL DELAMDA,WVST,WVEN,R,REXT,WAVLEN,F,F0,XCONVL,LINE
      REAL YCONVL,LORLINE,TOTRAD,INTENS
      REAL DDN,TE,TEL,A,POP,EWDTH,ENRGY,HWHM,SLIT,PTHLEN
      REAL PARTFUNC,Z,DENS
      PARAMETER (NP=50000)              ! ARRAY SIZE LIMIT
      PARAMETER (PI=3.14159D0)          ! PI
      PARAMETER (HP=6.6261961D-27)      ! PLANCK'S CONST ERG*S
      PARAMETER (C0=2.997925D+10)        ! SPEED OF LIGHT CMS-1
      PARAMETER (HC=HP*C0)              ! ERGCM
      PARAMETER (FPI=4.D0*PI)             ! 4PI SR
      DIMENSION YCONVL(NP),XCONVL(-300:NP)
      DIMENSION LORLINE(NP), TOTRAD(-300:NP)
      DIMENSION WAVLEN(-300:NP),F(-300:NP)
      DIMENSION LINE(50000),A(50000),POP(50000),EWDTH(50000)
      COMMON/SPEX/ SLIT

9001  FORMAT(1X,F8.4,2X,1P,E12.3)
9000  FORMAT(1X,F9.6,5X,1PE10.4)

      OPEN (10,FILE='LINSHAPE.SET',STATUS = 'OLD')

        READ(10,'(A12)') NAMEIN1        ! SPIN 1 CODE-B OUTPUT FILE
        READ(10,'(A12)') NAMEIN2        ! SPIN 2 CODE-B OUTPUT FILE
        READ(10,'(A12)') ENAMEW         ! CONVOLVED SPECTRA (OUTPUT)
        READ(10,*) DENS                 ! TOTAL ATOM DENSITY (CM-3)
        READ(10,*) PTHLEN               ! PATH LENGTH (CM)
        READ(10,*) WVST                 ! STARTING WAVELENGTH (MICRONS)
        READ(10,*) WVEN                 ! ENDING WAVELENGTH (MICRONS)
        READ(10,*) R                    ! INTERNAL RESOLUTION (MICRONS)
        READ(10,*) REXT                 ! EXTERNAL RESOLUTION (MICRONS)
        READ(10,'(A1)') SPEC            ! SWITCH FOR INSTRUMENT FUNCTION
        READ(10,*) SLIT                 ! SLIT WIDTH IN MILIMETERS
        READ(10,*) DELAMDA              ! FWHM IN MICRONS
        READ(10,'(A1)') INSTFNT         ! TRIANGULAR OR RECTANGULAR INSTR. FN.

      OPEN (11,FILE = NAMEIN1,STATUS = 'OLD')
      OPEN (12,FILE = NAMEIN2,STATUS = 'OLD')
      OPEN (13,FILE = ENAMEW,STATUS = 'UNKNOWN')
      OPEN (14,FILE = 'UNCONVL.DAT',STATUS = 'UNKNOWN')

      NINC=NINT((WVEN-WVST)/R)
      DIV=INT(REXT/R)
      IF(NINC.GT.NP)THEN
         WRITE(*,*)'   NINC > ',NP,' SPECTRAL RANGE IS TOO BIG'
         GO TO 9999
      ENDIF

C ARRAY INITIALIZATION:

      DO 1000 I=1,NINC
        WAVLEN(I)=WVST+FLOAT(I)*R    ! WAVELENGTH ARRAY (MICRONS)
        TOTRAD(I)=0.E0               ! RADIANCE ARRAY (WCM-3SR-1MICRON-1)
 1000   CONTINUE
      DO 1001 I=NINC,1,-1
        F(I)=1.D+4/WAVLEN(I)          ! WAVENUMBER ARRAY (CM-1)
 1001   CONTINUE

      WRITE(*,*) ' READING SPIN 1 LINE FILES...' ! SPIN 1

      READ(11,*)DDN     ! ELECTRON DENSITY.
      READ(11,*)TE      ! ELECTRON TEMPERATURE.
      READ(11,*)TEL     ! ELECTRONIC TEMPERATURE.
      DDN=DDN           ! THIS INFO IS LABELLING INFO FOR STARK OUTPUT.
      TE=TE             ! VARIABLES ARE RESTORED FOR A CLEAN COMPILE
```

```
      I=1
1090  READ(11,*,END=1100) LINE(I),A(I),POP(I),EWDTH(I)
      I=I+1
      GOTO 1090
1100  N=I-1
      Z=PARTFUNC(TEL)

      DO 1300 I=1,N
      IF (LINE(I).EQ.-1.) GOTO 1301
         EWDTH(I)=MAX(0.D0,EWDTH(I)) ! SEE EWIDTH=-2. FLAG IN CODE-B MAIN
         HWHM=EWDTH(I)+A(I)/C0       ! HWHM NATURAL LINE WIDTH LOWER LIMIT
         F0=1.D4/LINE(I)             ! CONVERSION FROM MICRONS TO WAVENUMBER
         LINE(I)=LINE(I)*1D-04       ! CONVERSION FROM MICRONS TO CM
         ENRGY=HC/LINE(I)            ! ENERGY OF TRANSITION (ERG)
         INTENS=1.D-7*ENRGY*A(I)*POP(I)*PTHLEN*DENS/(Z*FPI)
                                     ! WCM-2JSR-1 (1E-7W/ERGS-1)

         CALL LORENTZ(F(1),F0,INTENS,HWHM,LORLINE,NINC)

         DO 1200 J=1,NINC        ! SUM ALL LORENTZ DISTRIBUTIONS
            LORLINE(J)=LORLINE(J)*1.D4/(WAVLEN(J))**2
            TOTRAD(J)=TOTRAD(J)+LORLINE(J)
1200     CONTINUE

1300  CONTINUE
1301  CONTINUE

      WRITE(*,*) ' READING SPIN 2 LINE FILES...' ! SPIN 2

      READ(12,*)DDN     ! ELECTRON DENSITY.
      READ(12,*)TE      ! ELECTRON TEMPERATURE.
      READ(12,*)TEL     ! ELECTRONIC TEMPERATURE.
      DDN=DDN           ! THIS INFO IS LABELLING INFO OF STARK OUTPUT
      TE=TE             ! VARIABLES ARE RESTORED FOR A CLEAN COMPILE

      I=1
1390  READ(12,*,END=1400) LINE(I),A(I),POP(I),EWDTH(I)
      I=I+1
      GOTO 1390
1400  M=I-1
      Z=PARTFUNC(TEL)

      DO 1600 I=1,M
      IF (LINE(I).EQ.-1.) GO TO 1601
        EWDTH(I)=MAX(0.D0,EWDTH(I)) ! SEE EWIDTH=-2. FLAG IN CODE-B MAIN
        HWHM=EWDTH(I)+A(I)/C0       ! HWHM NATURAL LINE WIDTH LOWER LIMIT
        F0=1.D4/LINE(I)             ! CONVERSION FROM MICRONS TO WAVENUMBER
        LINE(I)=LINE(I)*1D-4        ! CONVERSION FROM MICRONS TO CM
        ENRGY=HC/LINE(I)            ! ENERGY OF TRANSITION (ERG)
        INTENS=1.D-7*ENRGY*A(I)*POP(I)*PTHLEN*DENS/(Z*FPI)
                                    ! WCM-2JSR-1 (1E-7W/ERGS-1)

        CALL LORENTZ(F(1),F0,INTENS,HWHM,LORLINE,NINC)

        DO 1500 J=1,NINC
           LORLINE(J)=LORLINE(J)*1.D4/(WAVLEN(J))**2
           TOTRAD(J)=TOTRAD(J)+LORLINE(J)
1500     CONTINUE

1600  CONTINUE
1601  CONTINUE

      NUMLINE=N+M
      WRITE(*,*) '   NUMBER OF SPIN 1 LINES= ',N
      WRITE(*,*) '   NUMBER OF SPIN 2 LINES= ',M
      WRITE(*,*) '   SUM OVER STATES (PARTITION FUNCTION)= '
      WRITE(*,*) '   TOTAL NUMBER OF LINES=  ',NUMLINE
```

```
      WRITE(*,*) ' CONVOLVING...'
      CALL CONVOLVE(WAVLEN,TOTRAD,XCONVL,YCONVL,NINC,
     &              DELAMDA,SPEC,INSTFNT)

      DO 1900 I=1,NINC,DIV
         WRITE(13,9000) XCONVL(I), YCONVL(I)
         WRITE(14,9000) WAVLEN(I),TOTRAD(I)
1900  CONTINUE

9999  CONTINUE

      CLOSE(11)
      CLOSE(12)
      CLOSE(13)
      CLOSE(14)

      STOP
      END


      SUBROUTINE LORENTZ(F,F0,INTENS,HWHM,LORLINE,NINC)
C*****************************************************************************
C                                                                              *
C THIS SUBROUTINE PASSES BACK A LORENTZIAN DISTRIBUTION FOR A                  *
C SINGLE LINE.                                                                 *
C                                                                              *
C  NINC        NUMBER OF SAMPLES IN THE SPECTRUM.                              *
C  F:          WAVENUMBER SPACE VARIABLE (CM-1).                               *
C  F0:         LINE POSITION IN WAVENUMBER SPACE (CM-1).                       *
C  INTENS:     POPULATION, A-COEFFICIENT, AND TRANSITION ENERGY.               *
C  NUMER:      VARIABLE USED FOR OPTIMIZATION.                                 *
C  HWHM2:      VARIABLE USED FOR OPTIMIZATION.                                 *
C  LORLINE:    CALCULATED LORENTZ ARRAY AT EACH LINE (CM-1).                   *
C                                                                              *
C*****************************************************************************

      IMPLICIT NONE
      INTEGER I,NINC
      REAL PI,HWHM,HWHM2,F,F0,LORLINE,NUMER,INTENS
      DIMENSION LORLINE(*),F(*)
      PARAMETER (PI=3.14159D0)

      NUMER=INTENS*HWHM/PI          ! LOOP OPTIMIZATION VARIABLE
      HWHM2=HWHM**2                 ! HWHM SQUARED. UNITS: CM-1

      DO 1000 I=1,NINC
      LORLINE(I)=NUMER/((F(I)-F0)**2+HWHM2)    ! LORENTZ DISTRIBUTION.
 1000 CONTINUE

      RETURN
      END


      REAL FUNCTION SPEX(WAVLEN)
C*****************************************************************************
C  THIS FUNCTION RETURNS THE VALUE OF FWHM FOR THE SPEX INSTRUMENT            *
C*****************************************************************************
      REAL SLIT,FWHM,WAVLEN
      COMMON/SPEX/ SLIT

      IF (WAVLEN.LT.8.0) THEN
         FWHM=SLIT*(-.000585*WAVLEN+.0142)
      ELSE IF (WAVLEN.LT.16.) THEN
         FWHM=SLIT*(-.000585*WAVLEN+.0284)
      ELSE
         FWHM=SLIT*(-.000585D0*WAVLEN+.0426D0)
```

```
      END IF
         SPEX=FWHM

      RETURN
      END


      REAL FUNCTION CVF(WAVLEN)
C*************************************************************************
C  THIS FUNCTION RETURNS FWHM FOR THE EXCEDE III CVF4 INSTRUMENT         *
C*************************************************************************

      IF (WAVLEN.LT.4.2E0) THEN
         FWHM=(-.00304709E0*WAVLEN+.0357227E0)*WAVLEN
      ELSE IF (WAVLEN.LT.7.35E0) THEN
         FWHM=(-.00231325E0*WAVLEN+.0406235E0)*WAVLEN
      ELSE IF (WAVLEN.LT.12.85E0) THEN
         FWHM=(-.00079086E0*WAVLEN+.037995E0)*WAVLEN
      ELSE
         FWHM=(-.000236616E0*WAVLEN+.03491286E0)*WAVLEN
      ENDIF
      CVF=FWHM

      RETURN
      END


      SUBROUTINE CONVOLVE(WAVLEN,TOTRAD,XCONVL,YCONVL,NINC,
     $  DELAMDA,SPEC,INSTFNT)
C*************************************************************************
C THIS SUBROUTINE CONVOLVES THE SUPERPOSED LORENTZIAN DISTRIBUTIONS WITH *
C EITHER A TRIANGULAR OR RECTANGULAR INSTRUMENT FUNCTION.               *
C*************************************************************************
        PARAMETER(INTVL=15000)
        CHARACTER*1 SPEC,INSTFNT
        DIMENSION YCONVL(INTVL),XCONVL(-300:INTVL),B(-300:INTVL)
        DIMENSION X(-300:INTVL),Y(-300:INTVL)
        DIMENSION WAVLEN(-300:INTVL),TOTRAD(-300:INTVL)
        COMMON/SPEX/ SLIT

        DO 100 I=1,NINC
           X(I)=WAVLEN(I)
           Y(I)=TOTRAD(I)
           XCONVL(I)=X(I)
 100    CONTINUE

C  IF SPEC = S THEN CALCULATE FWHM FOR SPEX INSTRUMENT
C  IF SPEC = C THEN CALCULATE FWHM FOR CVF INSTRUMENT

        IF (SPEC.EQ.'S') THEN
           FWHM1=SPEX(X(1))
        ELSE IF (SPEC.EQ.'C') THEN
           FWHM1=CVF(X(1))
        ELSE
           FWHM1=DELAMDA
        END IF

        DELX1=X(2)-X(1)
        NPT1=INT(FWHM1/DELX1)
        DO 120 M1=0,-NPT1,-1
           X(M1)=X(1)+FLOAT(M1-1)*DELX1
           XCONVL(M1)=X(M1)
           Y(M1)=0.E0
 120    CONTINUE

        IF (SPEC.EQ.'S') THEN
           FWHMN=SPEX(X(NINC))
```

```
         ELSE IF (SPEC.EQ.'C') THEN
            FWHMN=CVF(X(NINC))
         ELSE
            FWHMN=DELAMDA
         END IF

         DELXN=X(NINC)-X(NINC-1)
         NPTN=INT(FWHMN/DELXN)
         DO 130 MN=NINC+1,NINC+NPTN
            X(MN)=X(NINC)+(MN-NINC)*DELXN
            XCONVL(MN)=X(MN)
            Y(MN)=0.D0
 130     CONTINUE

C  CONVOLUTION WITH THE INSTRUMENT FUNCTION:

         DO 1000 I=1,NINC
            IENDR=0
            IENDL=0
            BJSUM=0.D0

            IF (SPEC.EQ.'S') THEN
               FWHM=SPEX(X(I))
            ELSE IF (SPEC.EQ.'C') THEN
               FWHM=CVF(X(I))
            ELSE
               FWHM=DELAMDA
            END IF

C CALCULATION FOR THE RIGHT SIDE OF THE INSTRUMENT FUNCTION:

            DO 150 J=I,NINC+200
               B(J)=0.D0
               DELX=ABS(X(I)-XCONVL(J))

C  TRIANGULAR INSTRUMENT FUNCTION:
               IF (INSTFNT.EQ.'T') THEN
                  IF (DELX.GT.FWHM) GO TO 155
                  B(J)=1.D0-(DELX/FWHM)
               ENDIF

C RECTANGULAR INSTRUMENT FUNCTION:
               IF (INSTFNT.EQ.'R') THEN
                  IF (DELX.GT.FWHM) GO TO 155
                  B(J)=1.D0
               ENDIF

C SPEX INSTRUMENT FUNCTION:
               IF (INSTFNT.EQ.'S') THEN
                  IF (DELX.GT.FWHM) GO TO 155
                  B(J)=1.D0-(DELX/FWHM)
               ENDIF

               IENDR=IENDR+1
               BJSUM=BJSUM+B(J)
 150       CONTINUE

C CALCULATION FOR THE LEFT SIDE OF THE INSTRUMENT FUNCTION

 155       DO 160 J=I-1,-NINC-200,-1
              B(J)=0.D0
              DELX=ABS(X(I)-XCONVL(J))

C  TRIANGULAR INSTRUMENT FUNCTION:
            IF (INSTFNT.EQ.'T') THEN
               IF (DELX.GT.FWHM) GO TO 190
               B(J)=1.D0-(DELX/FWHM)
```

```
            ENDIF

C RECTANGULAR INSTRUMENT FUNCTION:
            IF (INSTFNT.EQ.'R') THEN
               IF (DELX.GT.FWHM) GO TO 190
               B(J)=1.D0
            ENDIF

C SPEX INSTRUMENT FUNCTION:
            IF (INSTFNT.EQ.'S') THEN
               IF (DELX.GT.FWHM) GO TO 190
               B(J)=1.D0-(DELX/FWHM)
            ENDIF

            IENDL=IENDL+1
            BJSUM=BJSUM+B(J)
 160     CONTINUE

C NORMALIZATION OF WEIGHTING FACTORS

 190     DO 200 K=I-IENDL,I+IENDR-1
            B(K)=B(K)/BJSUM
 200     CONTINUE

C CONVOLUTION:

         YCONVL(I)=0.D0
         DO 300 L=I-IENDL,I+IENDR-1
            YCONVL(I)=YCONVL(I)+Y(L)*B(L)
300      CONTINUE
1000  CONTINUE

      RETURN
      END


      FUNCTION PARTFUNC(TEL)
      INTEGER S,N,L
      INTEGER NMAX,NMIN,LMAX,LMIN
      REAL F,PARTFUNC
      REAL KB,H,C,HC,KT,TEL,G
      DIMENSION F(30,30,0:3)
      COMMON/TERMS/F

      PARAMETER (KB=1.38066E-16)       ! BOLTZMANN CONST ERG/K.
      PARAMETER (H=6.62608E-27)       ! PLANCK'S CONST ERGS.
      PARAMETER (C=2.99792E+10)      ! SPEED OF LIGHT CM/S.
      PARAMETER (HC=H*C)

      CALL BASIS                 ! FILL ENERGY MATRIX WITH VALUES.

      KT=KB*TEL                  ! ELECTRONIC TEMPERATURE * BOLTZ CONST.
      PARTFUNC=0.0              ! PARTITION FUNCTION VARIABLE INITIALIZATION.

      DO 1000 S=0,2

         IF(S.EQ.0) THEN
            NMAX=2               ! THE LOOP INDICES ARE 'HARD WIRED' BECAUSE
            NMIN=2               ! OF THE DIFFERENCE IN SIZE OF THE BASIS SETS
            LMAX=1               ! WITH RESPECT TO SINGLETS, TRIPLETS AND
            LMIN=1               ! QUINTETS.
         END IF
         IF(S.EQ.1) THEN
            NMAX=11              ! LOOP INDICES FOR THE SPIN 1 BASIS STATES.
            NMIN=2
            LMAX=7
            LMIN=0
```

```
         END IF
         IF(S.EQ.2) THEN
            NMAX=11            ! LOOP INDICES FOR THE SPIN 2-BASIS STATES.
            NMIN=3
            LMAX=7
            LMIN=0
         END IF

      G=(2.D0*(FLOAT(S))+1.D0)*(2.D0*(FLOAT(S))+1.D0) ! DEGENERACY.
         DO 1200 L=LMAX,LMIN,-1                       ! FORMAT FOR CODE-B
            DO 1100 N=NMAX,NMIN,-1                    ! INPUT.
               IF(N.LE.L) GOTO 1200                   ! 'L=N-1'
               IF(N.EQ.2.AND.L.EQ.0) GOTO 1200        ! NO 2S STATE.
               IF(N.GE.9.AND.L.EQ.LMAX) GOTO 1100      ! NO 2S STATE.
               PARTFUNC=PARTFUNC+G*EXP(-HC*F(N,L,S)/KT)
1100     CONTINUE
1200     CONTINUE
1000  CONTINUE

      RETURN
      END


      SUBROUTINE BASIS
C*************************************************************************
C                                                                        *
C  THIS SUBROUTINE FILLS THE ARRAY, F(N,L,S), WITH THE ENERGY LEVELS OF  *
C  ATOMIC OXYGEN INCLUDING TRIPLETS, QUINTETS, AND THE THREE LOWEST      *
C  SINGLETS, I.E., 2P4(1D), 2P4(1S), AND 3S(1D). THE ARRAY INDICES ARE   *
C  PRINCIPAL QUANTUM NUMBER, THE VECTOR SUM OF THE ORBITAL MAGNETIC      *
C  QUANTUM NUMBER, AND SPIN.                                             *
C                                                                        *
C*************************************************************************
      REAL F
      DIMENSION F(30,30,0:3)
      COMMON/TERMS/F

      F(2,2,0) =   33792.5830     ! 2P4 (1D)
      F(2,1,1) =      77.9750     ! 2P4 (3P)
      F(2,2,0) =   15867.8620     ! 2P4 (1S)

      F(3,0,1) =   76794.9780
      F(3,0,2) =   73768.2000
      F(3,1,1) =   88630.9770
      F(3,1,2) =   86629.0890
      F(3,2,0) =  102662.0260     ! 3S (1D)
      F(3,2,1) =   97488.4760
      F(3,2,2) =   97420.7480

      F(4,0,1) =   96225.0490
      F(4,0,2) =   95476.7280
      F(4,1,1) =   99681.0510
      F(4,1,2) =   99094.0650
      F(4,2,2) =  102865.5620
      F(4,2,1) =  102908.4200
      F(4,3,2) =  102968.2490
      F(4,3,1) =  102968.3430

      F(5,0,1) =  102411.9950
      F(5,0,2) =  102116.6980
      F(5,1,1) =  103870.0200
      F(5,1,2) =  103626.2730
      F(5,2,1) =  105409.0080
      F(5,2,2) =  105385.3850
      F(5,3,1) =  105441.7240
      F(5,3,2) =  105441.6450
      F(5,4,1) =  105446.2900
```

F(5,4,2) = 105446.2900

F(6,0,1) = 105165.2320
F(6,0,2) = 105019.3070
F(6,1,1) = 105912.0310
F(6,1,2) = 105788.6840
F(6,2,1) = 106765.8030
F(6,2,2) = 106751.4620
F(6,3,1) = 106785.2010
F(6,3,2) = 106785.1600
F(6,4,1) = 106787.8910
F(6,4,2) = 106787.8910
F(6,5,1) = 106788.5800
F(6,5,2) = 106788.5800

F(7,0,1) = 106627.9340
F(7,0,2) = 106545.3540
F(7,1,1) = 107072.0000
F(7,1,2) = 106982.0000
F(7,2,1) = 107582.7770
F(7,2,2) = 107573.4870
F(7,3,1) = 107595.1470
F(7,3,2) = 107595.1400
F(7,4,1) = 107596.9600
F(7,4,2) = 107596.9600
F(7,5,1) = 107597.3600
F(7,5,2) = 107597.3600
F(7,6,1) = 107597.4800
F(7,6,2) = 107597.4800

F(8,0,1) = 107497.2240
F(8,0,2) = 107446.0360
F(8,1,1) = 107778.0000
F(8,1,2) = 107720.0000
F(8,2,1) = 108114.0000
F(8,2,2) = 108106.0790
F(8,3,1) = 108120.7900
F(8,3,2) = 108120.7900
F(8,4,1) = 108122.0200
F(8,4,2) = 108122.0200
F(8,5,1) = 108122.2900
F(8,5,2) = 108122.2900
F(8,6,1) = 108122.3800
F(8,6,2) = 108122.3800
F(8,7,1) = 108122.4100
F(8,7,2) = 108122.4100

F(9,0,1) = 108056.0000
F(9,0,2) = 108021.4000
F(9,1,1) = 108244.0000
F(9,1,2) = 108205.0000
F(9,2,1) = 108476.7000
F(9,2,2) = 108470.2000
F(9,3,1) = 108481.1100
F(9,3,2) = 108481.1100
F(9,4,1) = 108481.9800
F(9,4,2) = 108481.9800
F(9,5,1) = 108482.1800
F(9,5,2) = 108482.1800
F(9,6,1) = 108482.2400
F(9,6,2) = 108482.2400

F(10,0,1) = 108436.3000
F(10,0,2) = 108412.0000
F(10,1,1) = 108568.0000
F(10,1,2) = 108541.0000
F(10,2,1) = 108736.1000

```
F(10,2,2) = 108731.5000
F(10,3,1) = 108738.8200
F(10,3,2) = 108738.8200
F(10,4,1) = 108739.4600
F(10,4,2) = 108739.4600
F(10,5,1) = 108739.6100
F(10,5,2) = 108739.6100
F(10,6,1) = 108739.6500
F(10,6,2) = 108739.6500

F(11,0,1) = 108705.5000
F(11,0,2) = 108688.4000
F(11,1,1) = 108803.0000
F(11,1,2) = 108782.0000
F(11,2,1) = 108927.2000
F(11,2,2) = 108924.7300
F(11,3,1) = 108929.4800
F(11,3,2) = 108929.4800
F(11,4,1) = 108929.9600
F(11,4,2) = 108929.9600
F(11,5,1) = 108930.0700
F(11,5,2) = 108930.0700
F(11,6,1) = 108930.1100
F(11,6,2) = 108930.1100

RETURN
END
```

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APPENDIX C

APOSTLE OUTPUT
LINE POSITIONS, EINSTEIN COEFFICIENTS

OI Triplet Transitions (λ, Einstein Coefficient, and transition assignment)

2.0536	1.579E+05	8p- 4d
2.0550	8.621E+05	10d- 5p
2.0680	3.311E+05	11s- 5p
2.1337	1.611E+07	7f- 4d
2.1459	1.109E+05	7p- 5s
2.1605	1.755E+07	7g- 4f
2.1671	1.757E+05	7d- 4f
2.1708	1.265E+06	9d- 5p
2.1900	4.640E+05	10s- 5p
2.3563	1.983E+06	8d- 5p
2.3889	6.807E+05	9s- 5p
2.4018	2.548E+05	7p- 4d
2.5795	2.838E+07	6f- 4d
2.6181	3.735E+07	6g- 4f
2.6333	3.325E+05	6d- 4f
2.6934	3.421E+06	7d- 5p
2.7489	7.059E+03	11p- 6s
2.7569	1.065E+06	8s- 5p
2.8405	2.105E+06	11f- 5d
2.8571	5.062E+05	6p- 5s
2.8668	2.592E+06	11g- 5f
2.8691	5.178E+04	11d- 5f
2.8704	1.808E+06	11h- 5g
2.8709	1.322E+04	11f- 5g
2.8935	3.932E+07	4p- 4s
2.9388	1.266E+04	10p- 6s
2.9464	3.333E+04	11p- 5d
3.0032	2.865E+06	10f- 5d
3.0324	3.641E+06	10g- 5f
3.0355	7.270E+04	10d- 5f
3.0364	2.686E+06	10h- 5g
3.0372	1.918E+04	10f- 5g
3.0985	7.330E+07	4d- 4p
3.1656	4.569E+04	10p- 5d
3.2481	2.584E+04	9p- 6s
3.2551	4.049E+06	9f- 5d
3.2892	5.379E+06	9g- 5f
3.2939	4.304E+06	9h- 5g
3.2949	1.072E+05	9d- 5f
3.2951	2.964E+04	9f- 5g
3.3166	4.504E+05	11d- 6p
3.3293	4.850E+05	6p- 4d
3.4533	6.930E+06	6d- 5p
3.5274	6.562E+04	9p- 5d
3.5410	6.379E+05	10d- 6p
3.5798	2.192E+05	11s- 6p
3.6259	1.846E+06	7s- 5p
3.6617	1.227E+07	5s- 4p
3.6876	6.010E+06	8f- 5d
3.7309	8.518E+06	8g- 5f
3.7369	7.724E+06	8h- 5g
3.7390	5.017E+04	8f- 5g
3.7421	1.694E+05	8d- 5f
3.8274	6.449E+04	8p- 6s
3.8991	9.541E+05	9d- 6p
3.9474	5.793E+07	5f- 4d
3.9615	3.118E+05	10s- 6p
4.0356	1.161E+08	5g- 4f
4.0972	7.645E+05	5d- 4f
4.2212	1.017E+05	8p- 5d
4.5414	1.545E+06	8d- 6p
4.5609	9.367E+06	4p- 3d
4.5743	9.502E+06	7f- 5d
4.5976	8.834E+03	11p- 7s
4.6218	1.334E+06	11f- 6d
4.6399	1.491E+07	7g- 5f
4.6489	1.682E+07	7h- 5g
4.6536	9.759E+04	7f- 5g
4.6625	1.907E+06	11g- 6f
4.6643	4.691E+05	9s- 6p
4.6681	2.038E+06	11h- 6g
4.6685	5.916E+04	11d- 6f
4.6694	2.577E+04	11f- 6g
4.6696	2.421E+06	11i- 6h
4.6699	6.479E+03	11g- 6h
4.6706	2.949E+05	7d- 5f
4.9087	2.082E+04	11p- 6d
5.0684	1.813E+06	10f- 6d
5.1170	2.673E+06	10g- 6f
5.1237	3.019E+06	10h- 6g
5.1254	2.063E+06	10i- 6h
5.1258	3.831E+04	10f- 6g
5.1258	8.458E+04	10d- 6f
5.1259	1.015E+04	10g- 6h
5.1545	1.651E+04	10p- 7s
5.2445	2.339E+05	7p- 6s
5.3902	3.386E+05	11d- 7p
5.5488	2.906E+04	10p- 6d
5.8299	2.557E+06	9f- 6d
5.8935	3.932E+06	9g- 6f
5.9022	4.811E+06	9h- 6g
5.9044	3.779E+06	9i- 6h
5.9053	1.755E+04	9g- 6h
5.9059	6.139E+04	9f- 6g
5.9119	1.280E+05	9d- 6f
5.9854	2.846E+06	7d- 6p
6.0092	4.879E+05	10d- 7p
6.0133	1.915E+05	7p- 5d
6.1218	1.552E+05	11s- 7p
6.1879	3.683E+04	9p- 7s
6.3084	7.743E+05	8s- 6p
6.4978	1.994E+07	5d- 5p
6.7650	4.388E+04	9p- 6d
6.8586	8.910E+06	5p- 5s
7.1190	7.505E+05	9d- 7p
7.2664	1.615E+07	6f- 5d
7.3298	2.260E+05	10s- 7p
7.3801	3.768E+06	8f- 6d
7.4255	8.955E+05	11f- 7d
7.4285	3.019E+07	6g- 5f
7.4500	5.442E+07	6h- 5g
7.4688	2.378E+05	6f- 5g
7.4804	6.153E+06	8g- 6f
7.4917	1.379E+06	11g- 7f

7.4940	8.524E+06	8h- 6g
7.4974	8.489E+06	8i- 6h
7.4994	3.525E+04	8g- 6h
7.5013	1.770E+06	11h- 7g
7.5024	1.099E+05	8f- 6g
7.5033	1.750E+06	11i- 7h
7.5041	1.563E+04	11g- 7h
7.5042	3.878E+03	11h- 7i
7.5046	3.585E+04	11f- 7g
7.5072	6.215E+04	11d- 7f
7.5256	2.099E+05	8d- 6f
7.5524	5.891E+05	6d- 5f
7.6583	1.050E+04	11p- 8s
7.7207	4.041E+06	6s- 5p
8.1952	1.387E+04	11p- 7d
8.6502	1.216E+06	10f- 7d
8.6951	1.152E+05	8p- 7s
8.7017	2.724E+05	11d- 8p
8.7389	1.925E+06	10g- 7f
8.7516	2.610E+06	10h- 7g
8.7543	2.836E+06	10i- 7h
8.7556	6.881E+03	10h- 7i
8.7558	2.551E+04	10g- 7h
8.7576	5.503E+04	10f- 7g
8.7646	9.097E+04	10d- 7f
9.3390	2.165E+04	10p- 8s
9.5969	1.288E+06	8d- 7p
9.8795	8.190E+04	8p- 6d
10.1500	2.055E+04	10p- 7d
10.1626	3.561E+05	9s- 7p
10.3993	3.435E+06	5p- 4d
10.4373	4.046E+05	10d- 8p
10.7817	1.212E+05	11s- 8p
11.1317	1.705E+06	9f- 7d
11.2761	2.802E+06	9g- 7f
11.2966	4.107E+06	9h- 7g
11.3010	5.133E+06	9i- 7h
11.3033	1.448E+04	9h- 7i
11.3043	4.699E+04	9g- 7h
11.3103	9.254E+04	9f- 7g
11.3436	1.422E+05	9d- 7f
11.7127	7.100E+06	6d- 6p
12.0577	5.766E+06	7f- 6d
12.2627	6.280E+05	11f- 8d
12.3189	1.028E+07	7g- 6f
12.3538	1.762E+07	7h- 6g
12.3583	1.010E+06	11g- 8f
12.3625	2.892E+07	7i- 6h
12.3704	9.047E+04	7g- 6h
12.3755	1.429E+06	11h- 8g
12.3790	1.749E+06	11i- 8h
12.3810	1.153E+04	11h- 8i
12.3813	2.605E+04	11g- 8h
12.3845	4.452E+04	11f- 8g
12.3876	2.320E+05	7f- 6g
12.4006	6.381E+04	11d- 8f
12.5380	3.789E+05	7d- 6f
13.3869	1.325E+04	11p- 9s
13.3905	2.825E+06	6p- 6s
13.3909	6.118E+04	9p- 8s
13.9684	1.623E+06	7s- 6p
14.3123	6.605E+05	9d- 8p
14.5138	1.031E+04	11p- 8d
14.6370	2.327E+05	11d- 9p
15.1235	3.841E+04	9p- 7d
15.1906	1.863E+05	10s- 8p
16.0046	8.474E+05	10f- 8d
16.1637	1.397E+06	10g- 8f
16.1920	2.083E+06	10h- 8g
16.1980	2.791E+06	10i- 8h
16.2014	2.195E+04	10h- 8i
16.2030	4.497E+04	10g- 8h
16.2127	7.132E+04	10f- 8g
16.2520	9.628E+04	10d- 8f
18.5869	2.439E+06	8f- 7d
18.9799	4.195E+06	8g- 7f
19.0357	6.922E+06	8h- 7g
19.0469	1.096E+07	8i- 7h
19.0545	3.927E+04	8h- 7i
19.0600	1.040E+05	8g- 7h
19.0902	1.769E+05	8f- 7g
19.2733	2.407E+05	8d- 7f
19.5313	3.459E+04	10p- 9s
19.5780	2.811E+06	7d- 7p
19.8798	1.363E+06	6p- 5d

OI Quintet Transitions (λ, Einstein Coefficient, and transition assignment)

2.0554	2.660E+05	7p- 5s
2.0600	7.568E+04	8p- 4d
2.0644	3.061E+06	9d- 5p
2.0896	8.208E+05	10s- 5p
2.1143	2.758E+07	7f- 4d
2.1604	2.926E+07	7g- 4f
2.1714	3.497E+05	7d- 4f
2.2322	4.720E+06	8d- 5p
2.2753	1.212E+06	9s- 5p
2.4293	1.177E+05	7p- 4d
2.5334	7.951E+06	7d- 5p
2.5513	4.811E+07	6f- 4d
2.6180	1.919E+06	8s- 5p
2.6181	6.225E+07	6g- 4f
2.6433	6.568E+05	6d- 4f
2.6515	1.648E+08	4d- 4p
2.6577	1.825E+04	11p- 6s
2.7233	1.103E+06	6p- 5s
2.7645	6.729E+07	4p- 4s
2.8216	3.593E+06	11f- 5d
2.8395	3.144E+04	10p- 6s
2.8667	4.321E+06	11g- 5f
2.8704	3.013E+06	11h- 5g
2.8709	2.208E+04	11f- 5g
2.8710	1.021E+05	11d- 5f
2.9441	1.351E+04	11p- 5d
2.9820	4.877E+06	10f- 5d
3.0323	6.069E+06	10g- 5f
3.0364	4.476E+06	10h- 5g
3.0372	3.202E+04	10f- 5g
3.0396	1.429E+05	10d- 5f
3.1390	6.104E+04	9p- 6s
3.1690	1.808E+04	10p- 5d
3.1887	1.042E+06	11d- 6p
3.1998	1.548E+07	6d- 5p
3.2303	6.868E+06	9f- 5d
3.2891	8.967E+06	9g- 5f
3.2939	7.173E+06	9h- 5g
3.2951	4.949E+04	9f- 5g
3.3019	2.101E+05	9d- 5f
3.3084	2.679E+07	5s- 4p
3.3981	1.458E+06	10d- 6p
3.4210	2.279E+05	6p- 4d
3.4257	3.400E+06	7s- 5p
3.4486	3.804E+05	11s- 6p
3.5466	2.513E+04	9p- 5d
3.6558	1.027E+07	8f- 5d
3.7027	1.428E+05	8p- 6s
3.7292	2.146E+06	9d- 6p
3.7308	1.420E+07	8g- 5f
3.7369	1.288E+07	8h- 5g
3.7390	8.375E+04	8f- 5g
3.7531	3.308E+05	8d- 5f
3.8120	5.436E+05	10s- 6p
3.8819	9.602E+07	5f- 4d
4.0354	1.935E+08	5g- 4f
4.1371	1.496E+06	5d- 4f
4.2834	3.770E+04	8p- 5d
4.3152	3.400E+06	8d- 6p
4.4710	2.048E+04	11p- 7s
4.4789	8.249E+05	9s- 6p
4.5254	1.585E+07	7f- 5d
4.5913	2.244E+06	11f- 6d
4.6397	2.486E+07	7g- 5f
4.6489	2.803E+07	7h- 5g
4.6536	1.629E+05	7f- 5g
4.6624	3.180E+06	11g- 6f
4.6681	3.396E+06	11h- 6g
4.6694	4.302E+04	11f- 6g
4.6696	4.034E+06	11i- 6h
4.6699	1.080E+04	11g- 6h
4.6738	1.148E+05	11d- 6f
4.6908	5.740E+05	7d- 5f
4.9248	6.316E+03	11p- 6d
5.0109	3.691E+04	10p- 7s
5.0318	3.039E+06	10f- 6d
5.0950	4.713E+05	7p- 6s
5.1169	4.456E+06	10g- 6f
5.1237	5.032E+06	10h- 6g
5.1254	3.438E+06	10i- 6h
5.1258	6.395E+04	10f- 6g
5.1259	1.692E+04	10g- 6h
5.1379	1.635E+05	10d- 6f
5.1474	7.692E+05	11d- 7p
5.5880	8.536E+03	10p- 6d
5.6029	6.054E+06	7d- 6p
5.6847	4.145E+07	5d- 5p
5.7159	1.094E+06	10d- 7p
5.7815	4.259E+06	9f- 6d
5.8603	2.765E+05	11s- 7p
5.8934	6.553E+06	9g- 6f
5.9022	8.019E+06	9h- 6g
5.9044	6.298E+06	9i- 6h
5.9053	2.924E+04	9g- 6h
5.9059	1.025E+05	9f- 6g
5.9346	2.463E+05	9d- 6f
5.9761	7.404E+06	4p- 3d
6.0254	7.811E+04	9p- 7s
6.0337	1.388E+06	8s- 6p
6.2633	7.390E+04	7p- 5d
6.6244	1.513E+07	5p- 5s
6.7195	1.656E+06	9d- 7p
6.8798	1.263E+04	9p- 6d
6.9930	4.077E+05	10s- 7p
7.1440	2.631E+07	6f- 5d
7.1786	8.168E+06	6s- 5p
7.3029	6.210E+06	8f- 6d
7.3747	1.487E+06	11f- 7d
7.4281	5.031E+07	6g- 5f
7.4500	9.070E+07	6h- 5g
7.4690	3.968E+05	6f- 5g
7.4802	1.025E+07	8g- 6f
7.4852	2.262E+04	11p- 8s
7.4916	2.298E+06	11g- 7f

7.4940	1.421E+07	8h- 6g
7.4974	1.415E+07	8i- 6h
7.4994	5.875E+04	8g- 6h
7.5013	2.950E+06	11h- 7g
7.5024	1.834E+05	8f- 6g
7.5033	2.917E+06	11i- 7h
7.5041	2.604E+04	11g- 7h
7.5042	6.463E+03	11h- 7i
7.5046	5.984E+04	11f- 7g
7.5211	1.192E+05	11d- 7f
7.5705	4.029E+05	8d- 6f
7.6346	1.144E+06	6d- 5f
8.2746	2.970E+03	11p- 7d
8.3006	5.972E+05	11d- 8p
8.5132	2.247E+05	8p- 7s
8.5812	2.006E+06	10f- 7d
8.7388	3.209E+06	10g- 7f
8.7516	4.349E+06	10h- 7g
8.7543	4.727E+06	10i- 7h
8.7556	1.147E+04	10h- 7i
8.7558	4.252E+04	10g- 7h
8.7576	9.184E+04	10f- 7g
8.8000	1.735E+05	10d- 7f
8.8962	2.786E+06	8d- 7p
9.1327	4.475E+04	10p- 8s
9.6209	6.627E+05	9s- 7p
9.8863	8.728E+05	10d- 8p
10.3248	2.640E+04	8p- 6d
10.3263	2.172E+05	11s- 8p
10.3358	4.444E+03	10p- 7d
10.3866	1.408E+07	6d- 6p
11.0178	2.783E+06	9f- 7d
11.2760	4.669E+06	9g- 7f
11.2966	6.845E+06	9h- 7g
11.3010	8.555E+06	9i- 7h
11.3033	2.413E+04	9h- 7i
11.3043	7.832E+04	9g- 7h
11.3103	1.545E+05	9f- 7g
11.4278	2.699E+05	9d- 7f
11.8529	9.279E+06	7f- 6d
12.1448	1.034E+06	11f- 8d
12.3183	1.712E+07	7g- 6f
12.3538	2.936E+07	7h- 6g
12.3583	1.683E+06	11g- 8f
12.3625	4.820E+07	7i- 6h
12.3704	1.508E+05	7g- 6h
12.3755	2.382E+06	11h- 8g
12.3790	2.914E+06	11i- 8h
12.3810	1.922E+04	11h- 8i
12.3813	4.341E+04	11g- 8h
12.3845	7.430E+04	11f- 8g
12.3878	3.873E+05	7f- 6g
12.4387	1.212E+05	11d- 8f
12.6851	7.309E+05	7d- 6f
12.9975	4.796E+06	6p- 6s
13.1456	3.026E+06	5p- 4d
13.1475	2.679E+04	11p- 9s
13.1759	1.170E+05	9p- 8s
13.2158	3.135E+06	7s- 6p
13.3298	1.396E+06	9d- 8p
13.8941	4.941E+05	11d- 9p
14.4509	3.433E+05	10s- 8p
14.7946	1.608E+03	11p- 8d
15.8042	1.384E+06	10f- 8d
15.8350	1.031E+04	9p- 7d
16.1637	2.327E+06	10g- 8f
16.1920	3.471E+06	10h- 8g
16.1980	4.651E+06	10i- 8h
16.2014	3.659E+04	10h- 8i
16.2030	7.494E+04	10g- 8h
16.2127	1.190E+05	10f- 8g
16.3744	1.817E+05	10d- 8f
16.9065	6.013E+06	7d- 7p
18.2714	3.888E+06	8f- 7d
18.9796	6.988E+06	8g- 7f
18.9933	7.629E+05	10d- 9p
19.0357	1.154E+07	8h- 7g
19.0469	1.826E+07	8i- 7h
19.0545	6.545E+04	8h- 7i
19.0600	1.733E+05	8g- 7h
19.0902	2.953E+05	8f- 7g
19.2456	6.566E+04	10p- 9s
19.5718	4.573E+05	8d- 7f