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SPACE STATION CONTAMINATION STUDY: ASSESSMENT OF CONTAMINANT SPECTRAL BRIGHTNESS

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1. Introduction

Recent models of the gas concentrations induced around orbiting vehicles have predicted concentration enhancements up to 50 times ambient near ram surfaces at ·200 km. The number densities have yielded relatively large scale lengths, which means that the column abundances are significantly larger that anticipated ($·10^{14}$ cm^{-2} at 200 km). The molecules and atoms which make up the total abundance can either absorb, scatter, or emit radiation at the operating or sensing wavelengths of spectrometric, radiometric, and photometric instruments. Conservative preliminary estimates of the collisional excitation that could arise as a result of interactions between the instreaming ambient atmosphere and the gases generated in the environment of a low-Earth orbit (LEO) vehicle indicated that these would be significantly higher than the natural zodical background level + 10%, the criterion used in Space Station Contamination Requirements Document JSC-30426.

Previous requirements of atomic and molecular column densities specified in JSC-30426 appear to have been based largely on calculations of absorption effects. In retrospect, it is easily shown that emissive contamination is far more significant than absorptive contamination for the same column content.

Whereas the total column densities of 5 x 10^{13} cm^{-2} specified in JSC-30426 provide adequate controls on absorption, the same is not true for emissions. The results of this study will demonstrate that emissive contamination is significantly more severe than anticipated.

2. Background

The determination of the change to the natural brightness created by contaminants around a spacecraft is not a simple task. A host of excitation mechanisms exists and vary primarily with the flux and composition of incident ambients, which, in turn, depend on various geophysical parameters such as epoch of the solar cycle, season, time of day, altitude, and geographic location; that is, its position along the orbit. Superimposed on the well-defined behavior patterns are more sporadic fluctuations due to solar disturbances and magnetic activity, as well as effects of orographic origin such as gravity waves.

The gases in the contamination environment are generated by

five main mechanisms:

(1) Concentration enhancement of ambient gases which peaks in the ram direction

(2) Outgassing

(3) Leakage

(4) Venting

(5) Thruster firings

The effects of all five sources on contamination gases are calculated in the Science and Engineering Associates' (SEA) configuration contamination model. Table 1 lists a summary of the composition data obtained from SEA for this study.

In addition, the assessment of spectral brightness resulting from the ambient-contaminant interaction requires a knowledge of the details of cross sections and excitation mechanisms. The approach we adopted was to utilize the spectral brightness measurements made on Spacelab 1 and on the S3-4 spacecraft to identify source mechanisms, key cross sections and, hence, the abundance of contaminant species. These inferred abundances were then used to update the composition comprising the total column concentrations predicted by the SEA configuration contamination model for the Space Station and to scale the irradiances to four altitudes: 300, 350, 400, and 463 km. The contamination irradiances are compared with zodiacal natural background levels.

3. Modeling

The capability to model the spectral signatures due to the Space Station contaminant atomic and molecular species has been set in place. The model potentially provides the means for relatively accurate scaling of spectral features with altitude. However, in the current report, detailed scaling of specific features was not undertaken, because of the large demand on computer resources needed for such an effort. Instead, the full spectrum was computed at a single height (250 km for the vacuum ultraviolet, the near ultraviolet, and the visible; and 463 km for the infrared red) and scaled according to three factors given by $[N_2]^3$, $[N_2]^2[O]$, and $[N_2][O]^2$, which roughly cover the range of likely scaling factors. The curves labeled $[N_2][O]^2$ which are presented in Section 8 probably represent peak values for the computed brightnesses. The brightnesses derived are consistent with the column abundances calculated by the SEA model.

It was found that absorption effects were not significant for the species analyzed and thus results for absorption are not presented, and the JSC-30426 data provide adequate controls on

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Table 1. Composition Data

km	Total Density Ambient	Total RAM Density	Total NCD Without Freestream	Total Flux
200	1.03E + 10	3.83E + 11	3.01E + 14	6.33E + 15
250	3.33E + 9	1.15E + 11	1.07E + 14	5.31E + 14
300	1.38E + 9	4.57E + 10	3.38E + 13	8.34E + 13
350	6.50E + 8	2.18E + 10	1.67E + 13	2.04E + 13
400	3.35E + 8	1.16E + 10	9.58E + 12	6.60E + 12
450	1.83E + 8	6.62E + 9	4.83E + 12	2.05E + 12
500	1.04E + 8	4.23E + 9	3.07E + 12	8.79E + 11

km	H_2O	Organic NCD
200	5.98E + 11	5.98E + 11
200	5.86E + 11	6.67E + 11
300	5.40E + 11	3.07E + 11
350	5.60E + 11	4.40E + 11
400	5.80E + 11	7.73E + 11
450	5.40E + 11	3.00E + 11
500	5.40E + 11	3.00E + 11

km	Ambient O	NCD O	Ambient N_2	NCD N_2
200	2.59E + 9	6.09E + 13	7.26E + 9	2.21E + 14
250	1.08E + 9	2.38E + 13	2.12E + 9	6.22E + 13
300	5.68E + 8	1.14E + 13	7.71E + 8	2.03E + 13
350	3.26E + 8	6.77E + 12	3.09E + 8	8.50E + 12
400	1.98E + 8	4.25E + 12	1.31E + 8	3.78E + 12
450	1.23E + 8	2.44E + 12	5.73E + 7	1.48E + 12
500	7.75E + 7	1.53E + 12	2.57E + 7	6.64E + 11

<u>Units</u> – Number Density: cm^{-3}
Number Column Density (NCD): cm^{-2}

absorption. Note, however, that these exceed the constraints estimated for emission.

Since it was found that the SEA results at 463 km did not show a significant dependence on the ram direction, only representative results are presented at this stage. The dependence on ram increases significantly with decreasing altitude. The calculations we present here are representative of worst case conditions, namely, the ram direction, maximum solar activity, and maximum likely magnetic disturbance. Future work could provide reasonably good estimates for a variety of conditions. The spectral results shown in Section 8 show the altitude at which the spectral irradiances equal the zodiacal background.

4. Database

Because of the limited available data prior to Shuttle missions of detailed spectral measurements of the natural emissions at Shuttle altitudes, it proved very difficult initially to identify what components of the spectral intensities observed on S3-4 and Spacelab 1 could be attributed to contaminant sources. The Spacelab 1 array of spectrometers - the Imaging Spectrometric Observatory (ISO) - covered the spectral range from the EUV (`50 nm) to the far visible/near infrared, namely `800 nm. The first real progress in identifying a far-field vehicle signature was made by NRL personnel (Conway, et al., 1987) who demonstrated that nadir observations of the Lyman-Birge-Hopfield (LBH) bands of N_2 varied with altitude approximately as the cube of the concentration of N_2 - a non-natural signature. The same LBH spectral signature was observed on Spacelab 1 at 250 km at night in the nadir direction by the ISO (Torr, et al., 1985). The knowledge that this signature could be attributed to "vehicle glow" provided the information needed to identify a mechanism that could account for the LBH glow (Torr, et al., 1988). This undertaking led to predictions of similar effects for other molecular species provided by the SEA model. A series of successful identifications of spectral signatures of several molecules essentially led to a chain of predictions and confirmations of necessary accompanying emission features extending from the vacuum ultraviolet (VUV) to the near infrared (NIR), and predictions for the infrared (IR). With a working hypothesis in hand, which yielded results consistent with available measurements, irradiances could be calculated for Space Station using the mechanisms identified for Shuttle.

5. Vacuum Ultraviolet (VUV) Emissions

5.1 S3-4 LBH Glow

The fact that the LBH emissions were observed 90° to the ram direction suggests a gas-phase reaction, since the surfaces would

not be directly impacted. The Spacelab 1 spectral ratios preclude electron impact excitation. In the gas-phase, the incident ambients do not have sufficient energy to excite the LBH emission from normal, ground-state N_2 molecules. This indicates that the contaminant gases must have a significant population of long-lived electronically excited species. In the case of N_2, an obvious (if not the only) candidate is N_2 in the electronic A state.

The ISO data were examined for emissions from this state (the Vegard Kaplan - VK bands) and it was found that the column abundances inferred for $N_2(A)$ comprised up to ·0.01% of the total N_2 column concentration predicted by the SEA model. The collision cross section needed to excite $N_2(A)$ to the $N_2(a)$ state through collisions with ambient O and N_2 (which gives rise to the LBH emission) was estimated to be ·3.8 x 10^{-16} cm^2 to fit the S3-4 and Spacelab 1 data.

Consideration as to what surface chemistry could produce $N_2(A)$ led to the conclusion that similar excited states should at least be produced for O_2, NO, and CO, namely O_2 (a and b), NO(a), and CO(a and a'). The presence of other diatomic and polyatomic species is not precluded. The details of the surface chemistry are complex, and the products of surface reactions depend on the surfaces involved. Logically, there is no reason why collisional excitation of $N_2(A)$ would only excite the LBH bands, since there are several nearby upper states that should be excited. The same rationale also applies to the other molecules in question.

The ISO vacuum ultraviolet data exhibit a large continuum feature between ·140 and 180 nm. It was found that this continuum could be explained by synthesis of a number of VUV bands of N_2, NO, and CO, namely:

N_2: LBH, VK, and Ogawa-Tanaka-Wilkinson-Mulliken bands

NO: δ and ε bands

CO: Fourth Positive and Hopfield-Birge bands

The vibrational distributions of the molecules could be determined by spectral synthetic fitting of the data, and it became evident that the desorbed long-lived electronically excited precursors such as $N_2(A)$ were being produced in highly vibrationally excited levels, which, in turn, determined the vibrational distribution of the subsequent gas-phase collisionally excited bands. Figure 1 shows the composite synthesized spectrum for N_2, NO, and CO in the VUV at 250 km at 1.9 A wavelength resolution.

5.2 Scaling with Altitude

As mentioned in Section 3, detailed scaling of discrete spectral features was not done for the present work.
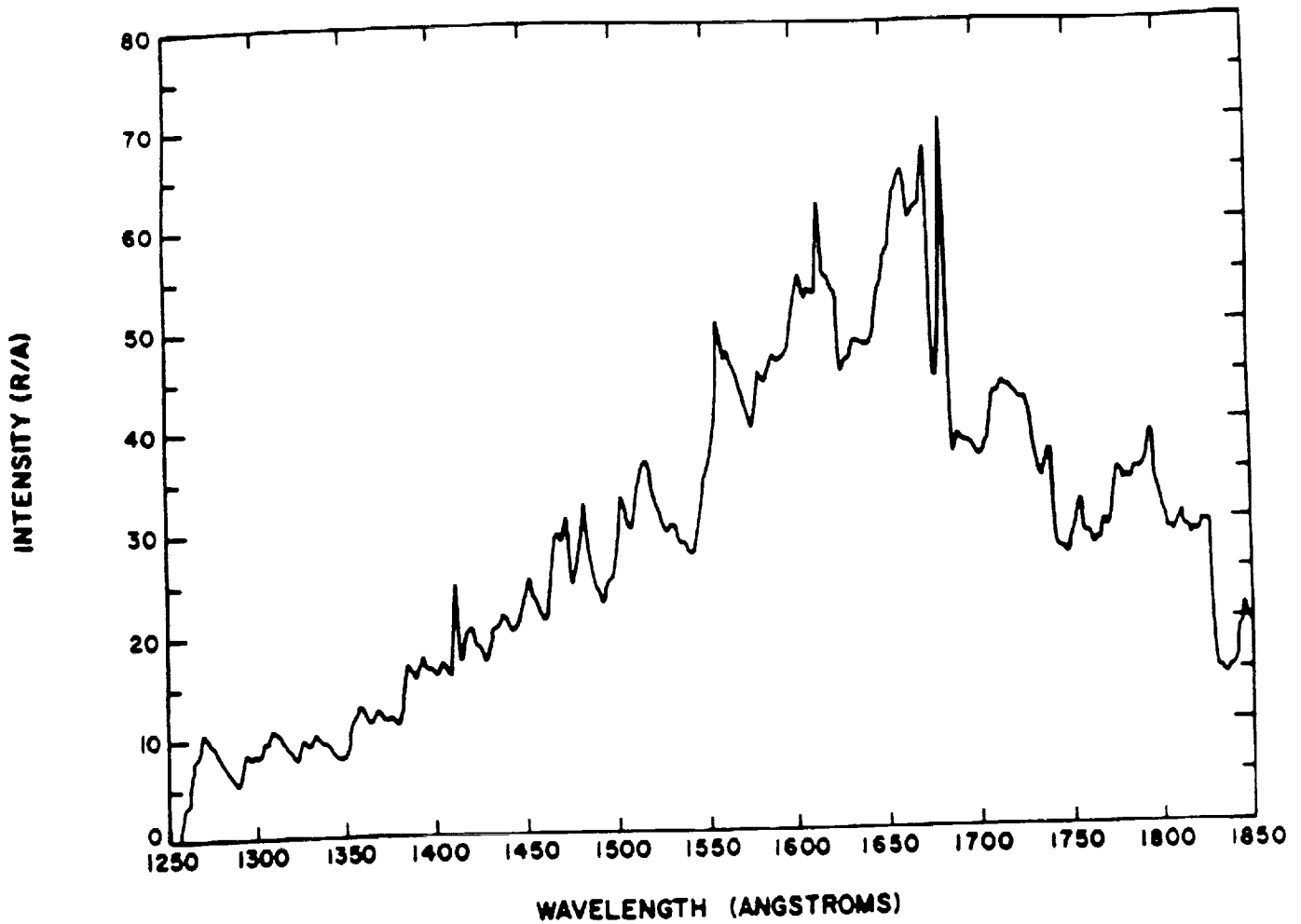
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Fig. 1. Synthesized vacuum ultraviolet spectrum for the conditions of Spacelab 1: Viewing direction - nadir (no ram data available); Altitude - 250 km; Date - Nov./Dec. 1983 - nighttime; Spectral resolution - 1.9A; Bands synthesized: N_2 - LBH, VK, Ogawa-Tanaka-Wilkinson-Mulliken; NO - δ and ϵ; CO - Fourth Positive, Hopfield-Birge. Note: 1 R/A = 10^6 photons cm^{-2} s^{-1} A^{-1}. The assumed steradiancy for the gas phase reactions is 4π.

Representative scaling has been done for the three factors $[N_2]^3$, $[N_2]^2[O]$, and $[N_2][O]^2$ for the overall spectrum to indicate possible or likely peak intensity levels. When the column abundance is dominated by Space Station sources, the scaling will be linear with respect to the ambient density.

6. Ultraviolet (UV) and Near Ultraviolet (NUV) Emissions

Given the information learned from the VUV on the column abundances of the various contaminant constituents, the bands expected for these molecules in the UV and NUV (~200-400 nm) were identified by synthetic spectral fitting of the ISO data, and then scaled to Space Station altitudes.

The ISO data exhibit very strong first negative bands of ionized molecular nitrogen with principal features at 391.4, 427.8, and 358.4 nm.

Although the study to date has not identified all the features observed in the ISO UV and NUV spectrum, several of the major systems were identified. These include:

CO^+: First Negative, Comet Tail

CO: Fourth Positive

N_2: Vegard Kaplan, Second Positive

O_2: Herzberg I, II, Chamberlain

NO appeared to be dominated by atmospheric emissions although a significant glow component could not be ruled out. In addition, a number of atomic lines could be matched by permitted O, N, O^+, and N^+ transitions. The forbidden transitions of O and N, namely, $O(^3P - {}^1D)$, $O(^3P - {}^1S)$, and $N(^4S - {}^2D)$, were also observed at levels which appear to significantly exceed their expected natural levels. In synthesizing the "far-field glow" spectrum, the assumption was therefore made that all the permitted and forbidden and atomic transitions are induced emissions. There is no difficulty in identifying potential source mechanisms. Preliminary estimates indicated that observed intensity levels could be accounted for, both through direct collisional excitation and chemiluminescence. While these sources would scale differently with altitude and composition, the difference is not large enough to significantly degrade the uncertainty of the present calculations. In the future, there is enormous scope for improving and quantifying the calculations. Representative synthetic UV and NUV spectra at 250 km for Spacelab 1 are shown in Figure 2.

7. Visible and Near-IR

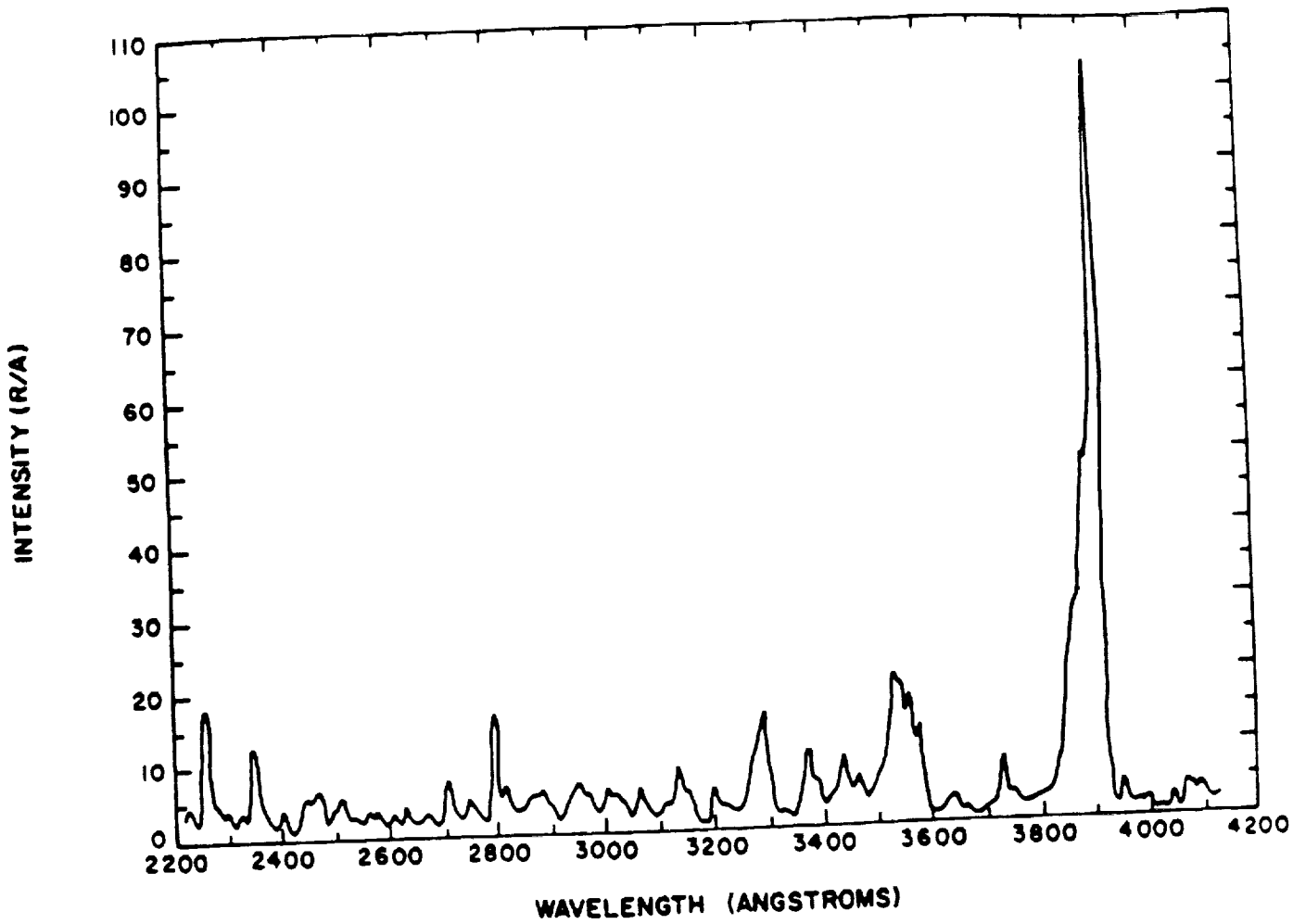In the case of the visible range, the assumption was made

Fig. 2. Synthesized near ultraviolet spectrum for Spacelab 1 conditions: Viewing direction - ram, dayside; Altitude - 250 km; Date - Nov./Dec. 1983; Spectral resolution - 2.5 Å; Bands synthesized: N_2 - First Negative, Vegard Kaplan, Second Positive; O_2 - Herzberg I, II, Chamberlain; NO - γ; CO - Fourth Positive (no Cameron bands observed); CO^+ - Comet Tail; Atomic Lines - O, N, O^+, N^+.

that the main source of emission would arise from the molecules identified through the VUV and UV. However time has precluded inclusion of several important CO and OH emissions.

Since the intensity of several "terrestrial species" significantly exceeded their expected natural levels, it was assumed that all the observed emissions could be attributed to contaminant sources. Likely candidate bands were synthesized, with the intensities being constrained only by the overall observed intensity envelope, since the actual observed spectra appear to be more complex, with possibly unidentified features contributing significantly. The following band systems were synthesized by fitting the ISO data

N_2: First Positive

O_2: Atmospheric

N_2^+: Meinel

The OH Meinel and CO Triplets, Herman, Angstrom, and Herzberg bands have not yet been synthesized, and their inclusion constitutes an important task for the future. Significant OH^+ has also not yet been ruled out. Expected atomic signatures for O, N, O^+ and N^+ were included.

Representative visible and NIR synthetic spectra for 250 km for Spacelab 1 are shown in Figure 3.

8. Altitude Variation

Figure 4 shows the altitude scaling adopted for the calculation of irradiances at the altitudes: 300, 350, 400, and 450 km.

Figures 5 to 7 show the VUV, NUV, and VIS results scaled to an altitude of 350 km for the NUV, 400 km for the VIS, and 450 km for the VUV (approximately the proposed nominal Station altitude). As mentioned earlier, significant directional differences in column abundances did not emerge for the Space Station from the SEA calculations for 463 km, where local sources of contamination greatly exceeded ram buildup.

We re-emphasize that the calculations reported here are highly preliminary and only reflect a best attempt (based on limited knowledge) to estimate worst case conditions. Many assumptions have been made; the scaling procedures used are crude. However, during the course of this work, the method has been established and given appropriate resources, the calculations could be significantly improved.

No attempt was made to model the spectral region between 800 and 1000 nm because insufficient experimental or theoretical information is currently available to generate useful results.
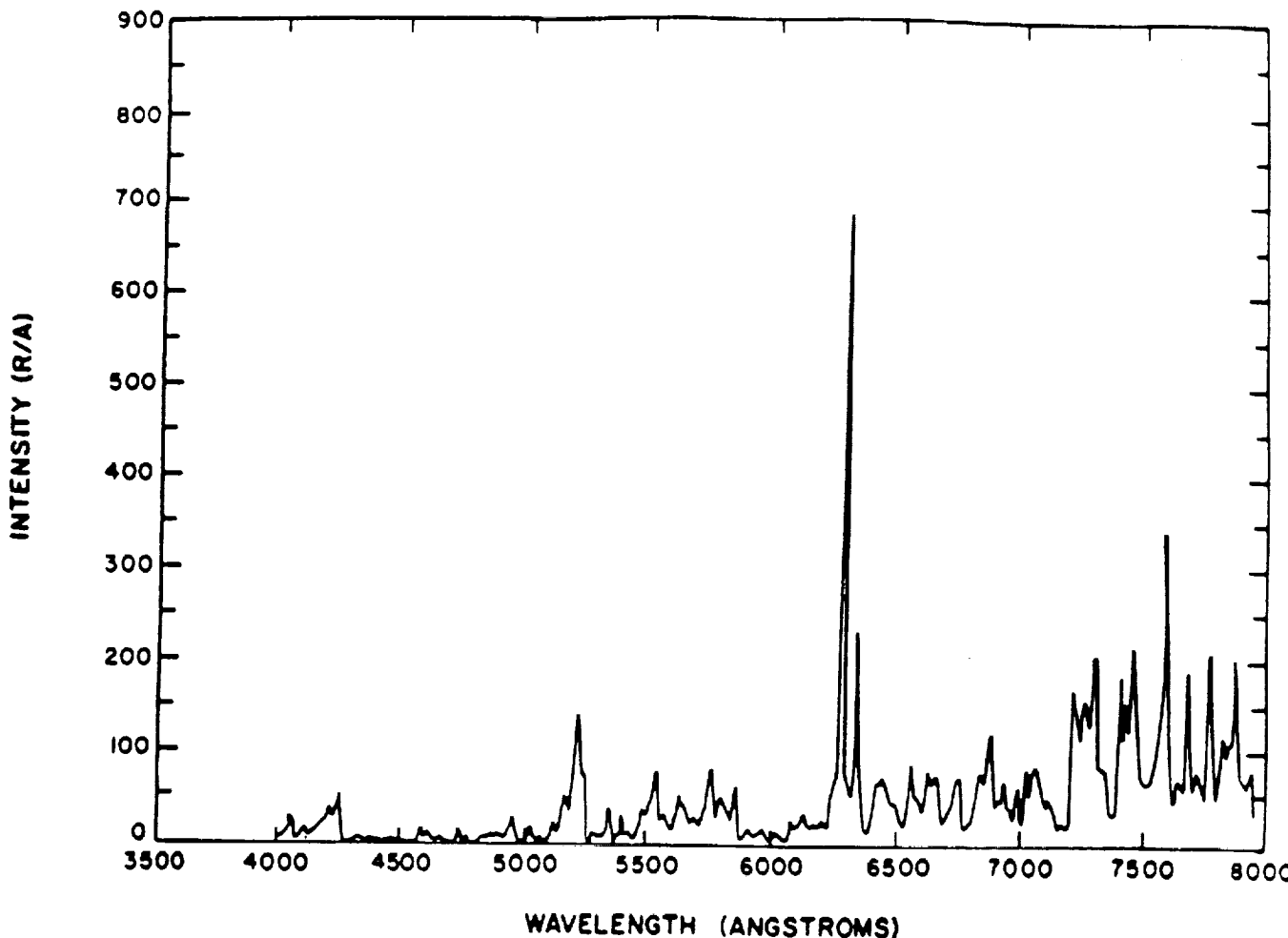
Fig. 3.   Synthesized visible spectrum and near infrared for
Spacelab 1 conditions: Viewing conditions - ram dayside; Altitude
- 250 km; Date - Nov./Dec. 1983; Spectral Resolution - 5.1 A;
Bands synthesized: N_2 - First Positive; O_2 - Atmospheric; N_2^+-
Meinel; Bands not yet synthesized: OH - Meinel; CO - Triplets,
Herman, Angstrom, Herzberg; Atomic Lines - O, N, O^+, N^+.
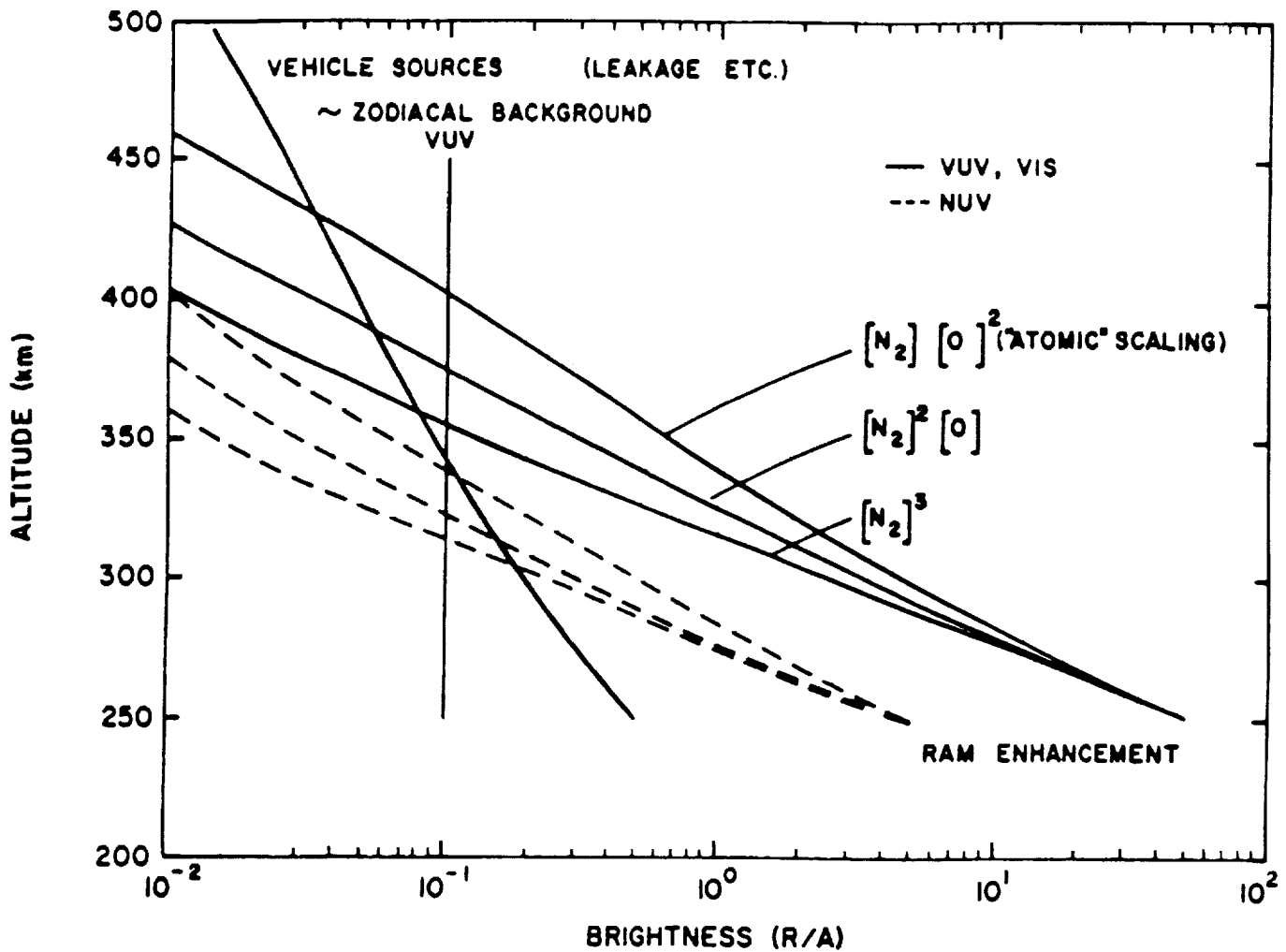
Fig. 4. Variation of the scaling factors with altitude used to extend the spectra synthesized at 250 km to high altitudes. The meanings of the scaling factors $[N_2]^3$, $[N_2]^2[O]$, and $[N_2][O]^2$ are discussed in Sections 5.2 and 8.
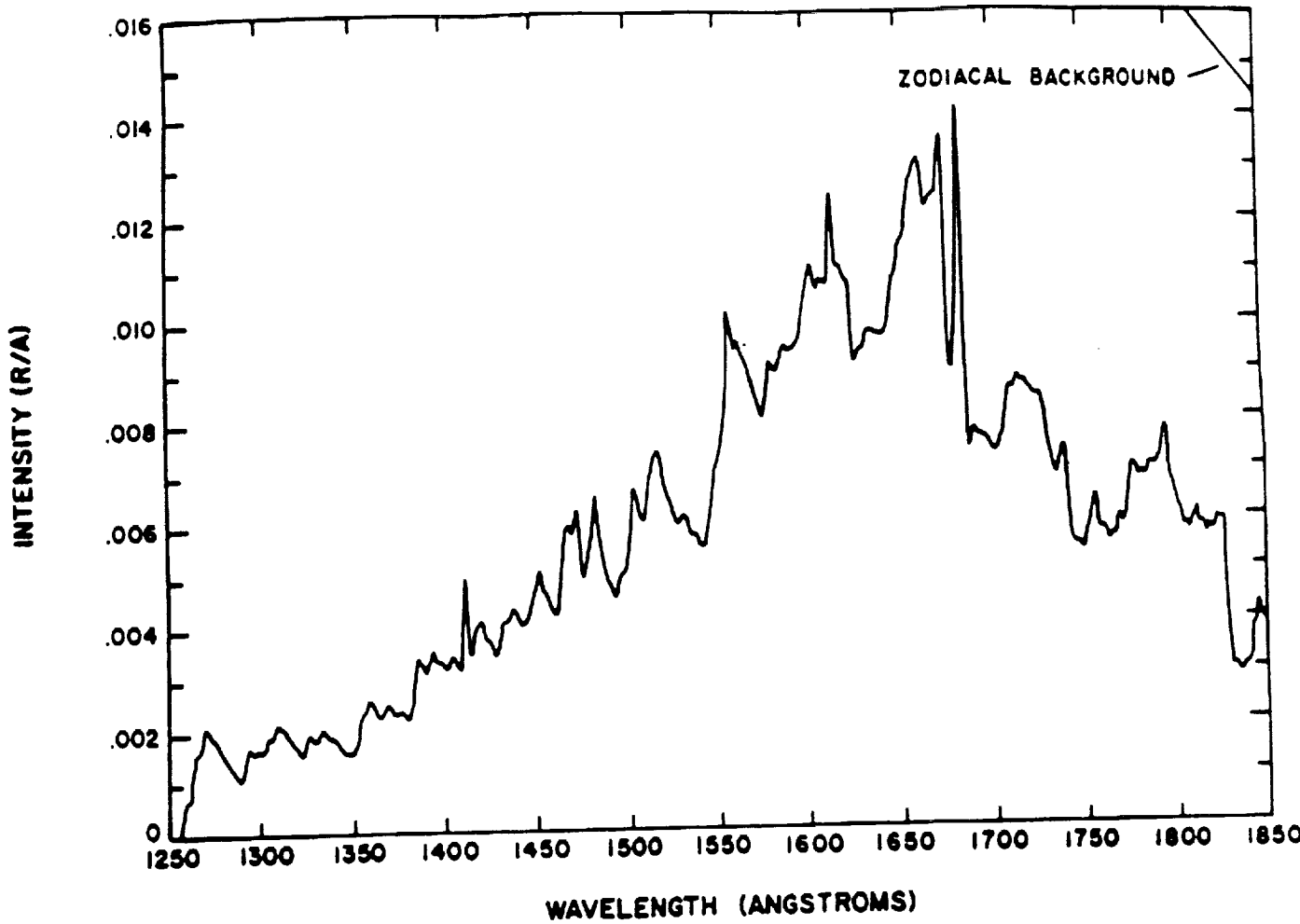
Fig. 5. Synthesized VUV spectrum at 450 km using $[N_2][O]^2$ scaling (that is, worst case). An estimated zodiacal background level is also shown.
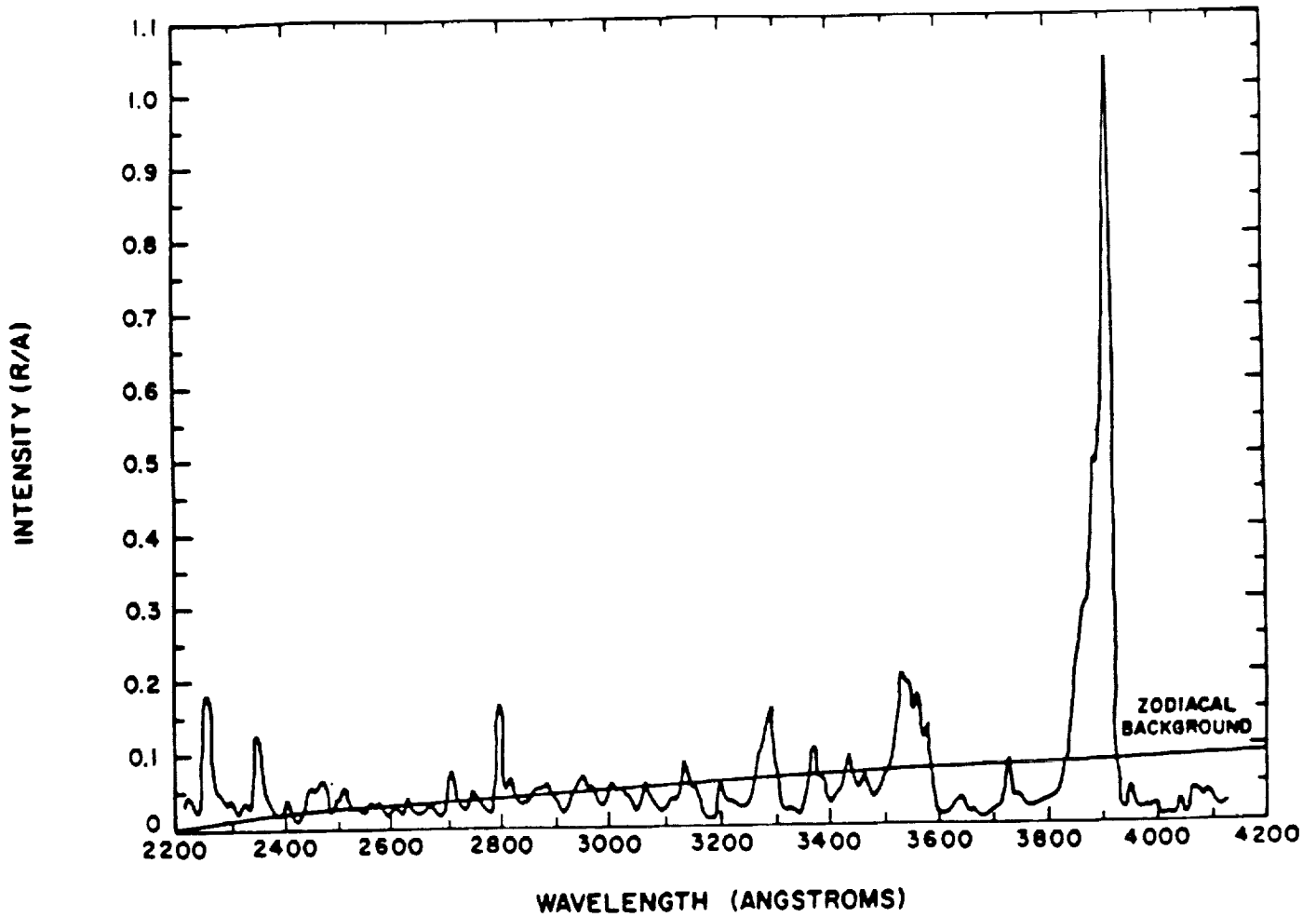
Fig. 6. Synthesized UV, NUV spectrum at 350 km using $[N_2][O]^2$ scaling (that is, worst case). The mean intensity is approximately equal to the zodiacal background at this level.
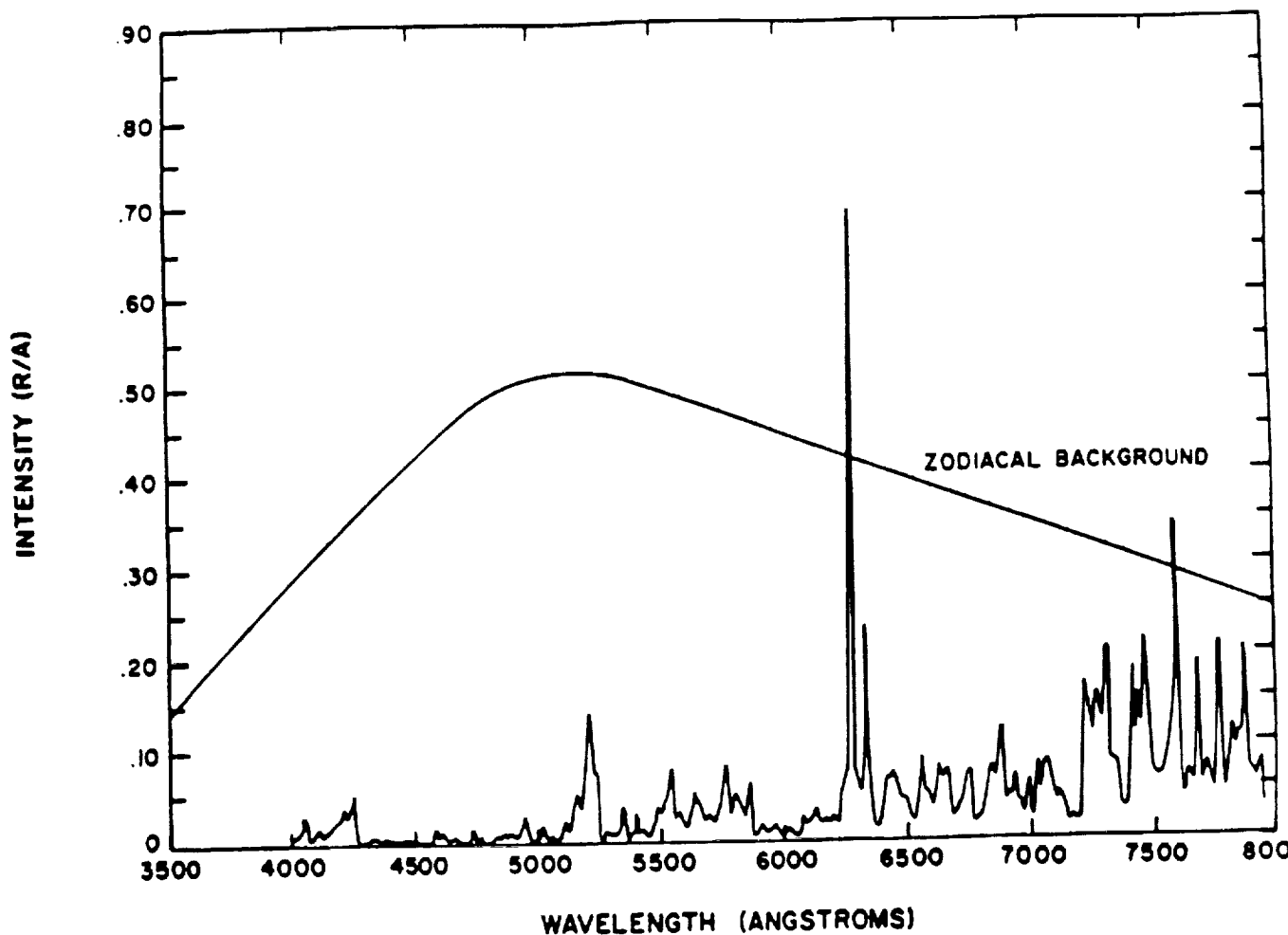
Fig. 7. Synthesized visible and near IR spectrum at 400 km using $[N_2][O]^2$ scaling (that is, worst case). At this altitude, with the exception of the $O(^3P-O^1D)$ feature, the contamination brightnesses lie well below the zodiacal background.

9. Natural Emissions

Figure 8 shows a representative calculation of natural irradiances due to thermospheric sources at 250 km tangential viewing for Spacelab 1 conditions for comparison with the contamination brightnesses reported in the preceding sections. The wavelength resolution is 5.1 A.

10. Conclusions and Recommendations

The results presented in this study show that spectral emissions which arise as a result of vehicle-ambient atmospheric interactions are significant and can become competitive with the natural zodiacal background up to altitudes as high as 400 km for the VUV and VIS for the worst case conditions used in this study. As mentioned in the text, the empirical database on the induced environment of space vehicles is very sparce, and these results are based on a number of assumptions and cannot be regarded as definitive at the present time. Since the technique for doing calculations of this kind was developed in its preliminary form for the purpose of this study, we are now in a position to provide greatly improved estimates of the contamination irradiances. The following tasks are considered most important in order to achieve a higher confidence level for the preliminary conclusions drawn here:

(1) The sensitivity of the SEA model to angular dependences in the collision cross section should be included since this could result in lower emissions in the non-ram direction and the calculations should be self-consistently done for various geophysical conditions. In the calculations presented here, data were utilized where available, namely, a mixture of night, day, ram, wake, etc.

(2) The calculations should be repeated for several viewing directions.

(3) We used very crude altitude scaling based on an 8 m disk and not on the Space Station geometry. The SEA calculations followed by this emission model should be repeated using the appropriate Station model. This is most essential.

(4) Several significant bands were not synthesized for the NUV visible and NIR. These should be included.

(5) The self-consistency of emissions across the full spectral range covered (EUV to IR) cannot be guaranteed at this time. Once a self-consistent calculation is done, the column number densities of each upper state could be tabulated. The sparseness of the database was a limitation in that snapshots of data had to be used where these were not taken under the same
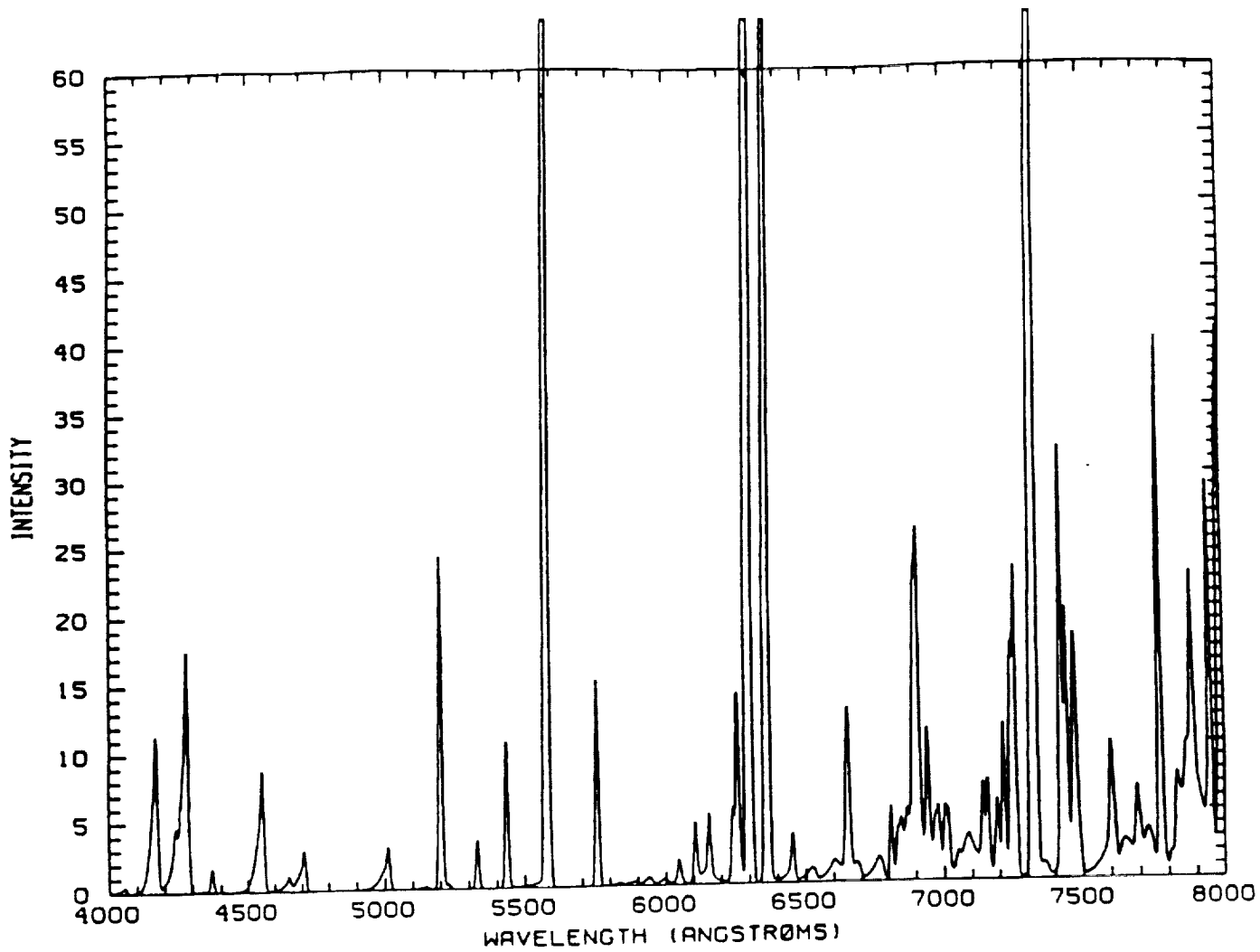
Fig. 8. Synthetic spectrum of the natural irradiances expected
for Spacelab 1 daytime conditions (Nov./Dec. 1983) at 250 km for
tangent viewing conditions. The sources were generated by a
comprehensive model of the photochemistry and dynamics of the
thermosphere. The units on the abscissa are (R/A).

conditions, e.g., sunlit, dark, wake, ram.

(6) Measurements of relevant neutral-neutral collision cross sections are needed for the 5 to 10 eV range.

(7) In situ optimized measurements of far-field glow are needed.

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