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THE SATURN SPECTRUM IN THE EUV - ELECTRON EXCITED HYDROGEN

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Abstract. Recent laboratory observations of electron excited H_2 in the EUV have brought about the realization that higher Rydberg series band systems make a significant contribution to the emission spectrum. Theoretical cross section estimates for the excitation of the D, D', B', B'' states agree with these results. Model calculations for particle excitation of the Saturn atmosphere, including the higher states, now show excellent agreement with Voyager auroral and dayside equatorial spectra. The model data also confirm the relative spectral response calibration of the Voyager instruments, providing a basis for accurate analysis of the excitation processes on both Jupiter and Saturn.

Introduction

Jupiter and Saturn dayside and auroral spectra in the EUV show particle excited emission in H_2 bands [see Broadfoot et al., 1981a, b; Clark, et al., 1982; Yung et al., 1982]. The early attempts at modeling EUV spectra obtained by the Voyager experiment in particular were not very satisfactory because the synthesized spectra could not account for substantial emission features shortward of 1250 A. Subsequent events have shown that excitation cross sections of the H_2 ($B\ ^1\Sigma_u^+ - X\ ^1\Sigma_g^+$) Lyman (L) and ($C\ ^1\Pi_u - X\ ^1\Sigma_g^+$) Werner (W) bands were not well established, and part of the difficulty is attributable to this fact. In addition to uncertain direct excitation cross sections, substantial cascade contributions by the E, F $^1\Sigma_g^+ - B\ ^1\Sigma_u^+$ transitions [Ajello et al., 1982a] had not been taken into account. A more recent discovery [Ajello et al., 1982b] in the laboratory has shown that higher Rydberg series members that start with the B and C states also make a strong contribution to the spectrum shortward of 1200 A. We point out in this brief report that the addition of the ground state transitions from the $B'\ ^1\Sigma_u^+$, $B''\ ^1\Sigma_u^+$, $D\ ^1\Pi_u$, and $D'\ ^1\Pi_u$ states have elevated the modeling process from one of confusion to a confidence that simple electron excitation of H_2 in the EUV is now understood. The model calculations also represent an independent confirmation of the measured relative spectral sensitivity of the Voyager EUV instruments in the 800 A - 1700 A region. Our purpose in this report is to briefly describe the excitation model and show the accuracy to which the simpler Voyager spectra of Saturn can now be fitted. We regard the results as an important benchmark for accurate analysis of the more complex spectra of Saturn and Jupiter.

Excitation Model

The model calculations of electron excited H_2 described below require estimates of collision strengths for the seven band systems contributing to the model. Among this group only the B, C and E, F states have measured cross sections. Published measurements to date are discussed in the recent work by Ajello et al. [1982a]. As discussed below, we calculate the collision strengths of the remaining four band systems using gaunt factors determined from the measured B and C states, and theoretical oscillator strengths. The laboratory measurements of the higher Rydberg series systems discussed below are uncalibrated and can be used only to show that the model calculations predict the observed spectral structure. Calibrated laboratory measurements for the H_2 systems in general have not been available below ~1100 A (see note added in proof).

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Energy Averaged Cross Sections

We assume in these calculations that the primary electrons have energies of 100 eV or higher. The cross sections averaged over electron energy distribution are estimated by making the further assumption that most of the emission is produced by secondary electrons, a condition that would be applicable if the primary electrons lose most or all of their energy to the atmosphere. The electron differential flux distribution applied to the calculation has the form E^{-n}, where E is electron energy and n = 1.4 [cf. Strobel and Shemansky, 1982]. The relative intensities of the bands are not very sensitive to the electron distribution unless large numbers of electrons fall in the energy range of the excitation thresholds. That is, rather drastic changes in electron energy distribution are required to produce a significant effect on the energy averaged excitation cross sections.

The shape functions of the collision strengths for the H_2 B and C states are taken from experimental data [Stone and Zipf, 1972; Ajello et al., 1982b]. The collision strengths tend to have a simple classical shape, requiring only two parameters in an analytic approximation. The gaunt factors for the Lyman and Werner bands at energies of 100 eV or larger differ by 10% or less, and on this basis the excitation process appears to be well behaved even for the first members of the Rydberg series. The cascade contribution of the E, F, $^1\Sigma_g^+$ state to the production of B state population is taken from the recent laboratory work by Ajello et al. [1982a]. Although the higher Rydberg series states have been detected in the laboratory [Ajello et al., 1982b] calibration of the measurements is not yet available. We therefore estimate the cross sections from calculated oscillator strengths [Miller and Krauss, 1967], for the B', B'', D and D' states, using the gaunt factors established for the B and C states. Oscillator strengths for the B and C states have been calculated in detail by Allison and Dalgarno [1970] and measured in absorption by Lewis [1974]. Relevant molecular data are listed in Table 1. The cross sections of the H_2 Lyman and Werner systems correspond to the present

TABLE 1. Molecular Data for H_2 Bands

Transition	1 E,eV	2 Q,10^{-17} cm^2	4 Q,10^{-17} cm^2	5 f	6 e,10^{-8} s^{-1}
C-X	12.70	2.09	3.08	0.330	2.86
D-X	14.12	0.51	.78	0.084	0.67
D'-X	14.73	0.16	.25	0.028	0.21
B-X	12.09	(3.34)[3]	3.53	0.279	(4.64)[3]
B'-X	13.84	0.41	0.63	0.054	0.54
B''-X	14.62	0.12	0.19	0.017	0.15
Total ionization	15.422	5.33	9.20		6.70

(1) Weighted mean threshold energy.

(2) Energy averaged cross-section for a differential electron flux distribution having the form $F_e \alpha E^{-1.4}$ el cm^{-2} s^{-1} ev^{-1}.

(3) Includes the E, F-B cascade component.

(4) Electron excitation cross-section at 100 eV.

(5) Absorption oscillator strength.

(6) Production rate per ground state molecule, for input primary electrons of 10 kev at a flux of 1 erg cm^{-2} s^{-1}.

analysis of the measurements by Ajello et al. [1982a]. The cross section for the Lyman system given in Table 1 differs with that given by Ajello et al. [1982a] but within measurement uncertainty. The uncertainty in the H_2 Lyman/Werner cross section ratio based strictly on the scatter in published theoretical and experimental numbers, is about 25% [see Ajello et al., 1982a]. Absolute cross section estimates in the literature show a somewhat greater divergence [Ajello et al., 1982a]. The present values for direct excitation of the B and C states are within 12% of the recent theoretical calculations of Hazi [1981], Fliflet and McKoy [1980], Chung and Lin [1978], and Lee and McKoy [see Ajello et al., 1982a].

The higher vibrational levels of the H_2 B and C states have branches into the dissociative continuum of the X state [Stephens and Dalgarno, 1972]. The continuum B-X transitions in particular are significant and are included in the model calculations.

The model calculations for fitting the observed data also required taking into account the e+H process. Detailed collisional equilibrium calculations [cf. Shemansky and Smith, 1981] were used to model the H Lyman series to the Rydberg limit, $n \to \infty$. Shape functions and cross sections for the 2s and 2p states calculated by Baluja et al. [1978] were used to establish atomic cross section data for the system. Further details will be given in a later publication.

Excitation Branching

The model calculations of the e+H_2 process assume that the H_2 ground state population is entirely in the v = 0 level, with the rotational population in thermal equilibrium. The calculations therefore represent the simplest possible ground state configuration. The relative excitation rates of the excited state vibrational levels were determined by using collision strengths calculated with a uniform shape factor (in threshold energy units) for each state and a constant gaunt factor at a given threshold energy unit, independent of excited vibrational level. The transition probabilities used in calculating the excitation rates for the B and C states are given by Allison and Dalgarno [1970] and Stephens and Dalgarno [1972]. The distribution of intensities among the bands of the H_2 Lyman and Werner systems were determined by using the Allison and Dalgarno [1970] tables. Vibrational and rotational energy data for the B-X, and C-X systems were obtained from Dabrowski and Herzberg [1974], Wilkinson [1968], Namioka [1964], and Herzberg and Howe [1959]. The remaining ground state connected band systems, B'-X, B''-X, D-X, D'-X included in the model were synthesized by using constant electronic transition moments to establish absolute transition probability tables. Molecular data for these systems were obtained from Monfils [1968], Spindler [1969a, b], Namioka [1964], Monfils [1965], Huber and Herzberg [1979], and Rothenberg and Davidson [1967]. Franck-Condon factors have not been published for the B''-X and D'-X systems. The transition probability data for these transitions were established through the fact that equilibrium internuclear distances for the B'' and D' states, were very nearly equal to those of the B' and D states, respectively, and would thus have very similar Franck-Condon factors for the ground state transitions. The contribution of the E, F $^1\Sigma_g^+$ state to the Lyman system was obtained by using the Franck-Condon factor calculations of Lin [1974] and other data obtained by Ajello et al. [1982a].

Rotational excitation transitions on electron impact were assumed to follow the optical line strength factors. Equations for the excitation-emission structure can be obtained from the authors on request.

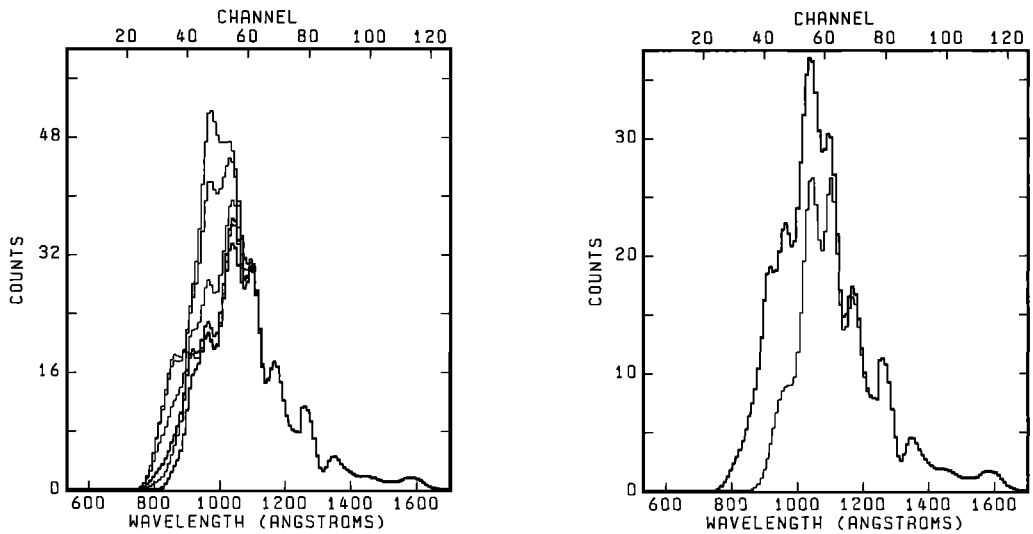

Fig. 1. Model spectra of electron excited H_2 in the signal format of the Voyager EUV spectrometer; resolution ~30 A. The neutral gas temperature in the model is 400 K. (a) Results for different abundances of foreground H_2 gas, 0.0; 1 x 10^{14}; 1 x 10^{15}; 1 x 10^{16}; 1 x 10^{17}; 1 x 10^{20} cm^{-2}. The last case (1 x 10^{20} cm^{-2}) also includes 1 x 10^{17} cm^{-2} of foreground atomic hydrogen. (b) Comparison of the model spectrum with and without the higher Rydberg series bands (see text). The heavy plotted line is the model calculation including 1 x 10^{16} cm^{-2} of foreground H_2. The light plotted line is the model under the same conditions but including only the H_2 Lyman and Werner band systems.

Optical Depth Effects

Emission in H_2 and H ground state connected transitions from the atmosphere of Jupiter and Saturn will always show optical depth effects, because the significant emissions have large transition probabilities. Observations above the atmosphere from an exobase source on either planet show strong extinction effects in these transitions. Transmission losses between source and observation point are therefore included in the model calculations. The calculations are based on single scattering losses only. The H_2 transitions and H Lyman-series transitions above Ly-α [cf. Cook et al., 1981] are ultimately lost through fluorescence. Line shape structure and the H_2 band absorption process is discussed by Festou et al. [1981].

Synthetic Spectra

Synthetic spectra of the band systems discussed above are shown in Figure 1a for various abundances of foreground H_2 gas, as they would appear in the output format of the Voyager EUV instruments [cf. Broadfoot et al., 1981]. The spectral calibration factors applied to the synthesis are those dermined by Holberg et al. [1982] at wavelengths longward of 1300 A. The response function applied to the shorter wavelength data is the original instrument calibration. Note that depths of foreground H_2 greater than $[H_2]\ell$ = 10^{16} cm^{-2} produce little change in the shape of the band structure because most of the v'' = 0 connected transitions have been removed by the scattering process. Figure 1b shows the decomposed synthetic spectrum for $[H_2]\ell$ = 10^{16} cm^{-2} indicating the calculated contributions of the B', B'', D, and D' states to the total emission. The effect on the shorter wavelength region of the spectrum is substantial and apparently is essential to the modeling process. The synthetic spectra shown here were all calculated at a temperature of 400 K. However, at the Voyager instrument resolution (~30 A) the spectral shape of the model is very insensitive temperature, because only the rotational level populations show a sensitivity over the expected range of temperatures. Nevertheless, the model does take rotational structure into account in order to calculate transmission properties.

The strong increase in instrument sensitivity toward shorter wavelengths allows measurement of electron excited atomic hydrogen emission to the Rydberg limit at 912 A. Optically thick foreground gas tends to remove the stronger members of the series starting with H Lyβ, to fluorescence in the Balmer series, and only the higher members near 920 A are transmitted. Figure 3 shows the electron excited atomic hydrogen component in a model calculation with an abundance of $[H]\ell$ = 5 x 10^{14} cm^{-2} in foreground atomic hydrogen.

Experimental Observations

Figure 2 shows a laboratory spectrum of electron excited H_2 obtained in a crossed beam experiment [Ajello et al., 1982b]; the apparatus has been described in a previous paper [Ajello and Srivastava, 1981]. This figure also shows the synthesized structure of the H_2 Werner system, but note that intensity scales cannot be compared. Although the spectrum of Figure 2 is not calibrated it is obvious that the higher H_2 Rydberg series transitions make a substantial contribution to the emission (see note added in proof). Werner band transitions begin to contribute measurably only at wavelengths longward of ~900 A, whereas relatively strong features are present at wavelengths down to 800 A.

This characteristic is also present in the Voyager spectra of auroral and dayside equatorial emission from Saturn, shown in Figures 3 and 4. Figure 3 shows a Voyager 1 auroral spectrum from the darkside north polar region. A model calculation of H_2 excitation with a foreground gas abundance of $[H_2]\ell$ = 10^{16} cm^{-2} combined with direct atomic hydrogen excitation with a foreground gas abundance of $[H]\ell$ = 5 x 10^{14} cm^{-2}, is shown over plotted on the observed spectrum in

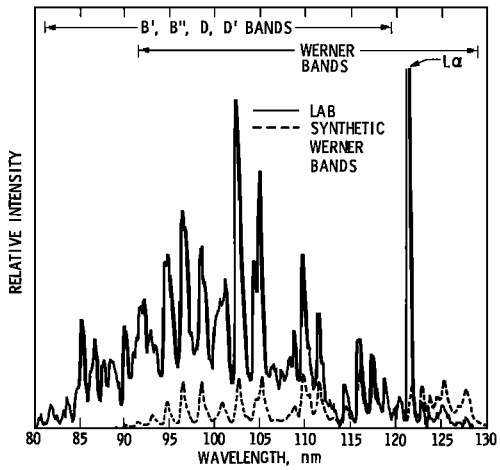

Fig. 2. A laboratory spectrum of electron excited H_2, after Ajello et al. [1982b]. The gas is excited in a crossed beam experiment, using a spectrometer resolution of ~5 A. The spectral response is not calibrated, but has a similar response function to that of the Voyager instruments. The dashed curve is a synthesized model comparison spectrum of the Werner bands, indicating the presence in the experimental data of other strong contributions in the short wavelength region. Note that the intensity scales of the laboratory and synthetic spectra are not comparable.

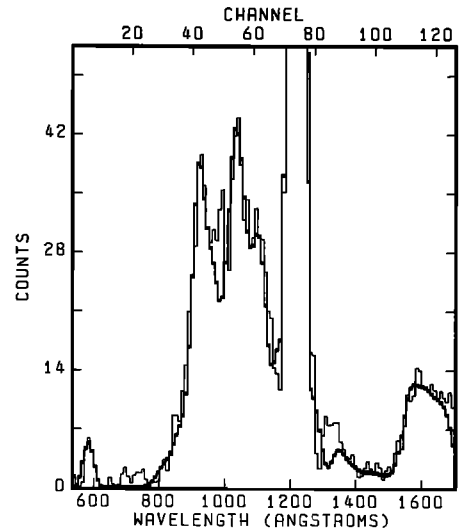

Fig. 4. A Voyager 1 Saturn equatorial dayside (65°-40° lat) spectrum, compared to a model of electron excited He, H and H_2. The plotted data is in the same format as Figure 3. The observations were obtained at a spacecraft event time of 316/0200 UT, with an integration interval of 10241 s. The model calculations were made with the same foreground gas parameters as those applied in Figure 3. The reduced absolute data is given in Table 2.

the figure. The model fit to the observed spectrum is clearly accurate with the exception of channels 49 and 50 just below 1000 A, and the 1100- to 1160-A region where ~15% differences occur. It is not certain whether the differences at channels 49 and 50 represent real signal or a noise event. The 1100- to 1160-A region of the spectra is known to be variable in observations of both Jupiter and Saturn (compare Figure 4) and is judged to be H_2 emission caused by complexity in the excitation mechanism. The model spectrum is fitted to the observed data by normalizing to the average signal between 1450 A and 1600 A. The 1450- to 1600-A region of the spectrum is entirely due to the B-X transition. The relative intensities of the short and long wavelength regions thus reflect the relative cross sections of the H_2 Lyman (B-X) system and the sum of the C-X, D-X, D'-X, B'-X, B''-X systems. The relative intensities and spectral shapes of these

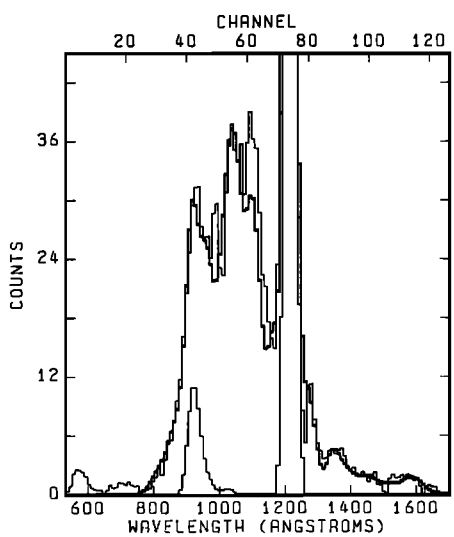

Fig. 3. A Voyager 1 spectrum of Saturn aurora on the darkside north polar region, compared to a model of electron excited H and H_2. The light plotted line is the observed reduced data obtained at a spacecraft event time of 319/0547 UT, with an integration interval of 4308 s. The heavy plotted line is the model calculated with foreground H_2 and H abundances of 1 x 10^{16} cm^{-2} and 5 x 10^{14} cm^{-2}, respectively. The lower light plotted line showing a peak near 920 A is the model spectrum of the electron excited H contribution to the total spectrum, transmitted through the foreground gas.

TABLE 2. Analysis of the Voyager 1 Saturn Equatorial Spectrum

Source	Intensity, R
H_2 (L + W)	916
HI (1216 A), e + H	1280
HI (1216 A), e + H_2	90
HI (1216 A), solar scatter	3500
HI 1216 A), total	4900
HI (1025 A), solar scatter	10
1660 A, solar scatter	(31) R/A
HeI (584 A)	2.4

Species	Foreground gas abundance, cm^{-2}
H_2	10^{16}
HI	5 x 10^{14}

Exobase Temperature: 400 K

regions in the model calculation depend on the measured relative cross sections of the B-X and C-X transitions, and the calculated cross sections for the remaining systems. The accuracy of the overall fit of the model and observed data then tends to reflect the independent relative calibrations of the laboratory and Voyager instruments. Although there is a free parameter of optical depth in the calculation, the freedom is limited by spectral shape and the fact that the spectrum changes very little (Figure 1) for abundances beyond $[H_2]\,\ell = 10^{15}$ cm^{-2}. The value $[H_2]\,\ell = 10^{15}$ cm^{-2} represents levels in the atmosphere at or above the exobase. Figure 4 shows a spectrum of the Saturn dayside equatorial region also indicating particle excitation of H and H_2. The model superposed on the observation shows a much better fit in the 1100- to 1160-A region in comparison with the case in Figure 3, suggesting differences in excitation conditions. The estimated abundances of foreground gas in this case are the same as the auroral spectrum of Figure 3. The strong emission longward of 1500 A in Figure 4 is dominated by reflection of solar radiation, which has been modeled by using calculations by G.R. Gladstone and Y.L. Yung (private communication, 1981). The excess emission near 1330 A (Figure 4) has not been identified. The dayside spectrum includes solar resonance scattered H Lyα (1216 A) and H Lyβ (1025 A) radiation apart from the electron excited components. The estimated intensities of the emission in the dayside spectrum and other data are given in Table 2. A neutral exospheric temperature of 400 K places the source location at an altitude of ~2200 km above the 1 bar level, at a number density $[H_2] = 7\times10^8$ cm^{-3}, just below the exobase. Further discussion of the implications of the analysis is reserved for a later publication.

Discussion

Higher members of the H_2 Rydberg series systems that start with the B and C states make a substantial contribution to the EUV emission spectrum. Earlier attempts to model the EUV spectrum of H_2 by using only the Werner and Lyman band systems showed distinct differences with Voyager observations [Broadfoot et al., 1981]. The strong difference spectrum raised questions concerning the complexity of the excitation mechanism, source species, and instrument calibration. The general confusion now appears to be removed by the inclusion of the higher series systems. The presence of these systems in H_2 absorption spectra and electron energy loss spectra [Lewis, 1974; Geiger and Schmoranzer, 1969] has been known for some time, but the realization of the strength of the contribution to the emission spectrum came only with the results of the recent research by Ajello and co-workers. The accuracy of the conformation of the model to the less complex weaker particle excitation in the Saturn exospheric region, should now allow an understanding of the more complex excitation processes that are obviously present in other spectra of Jupiter and Saturn.

Note added in proof: Calibrated laboratory spectra over the 700 A - 1700 A range have now been obtained (Ajello, Shemansky, Kwok and Yung, in preparation). Analysis of the data shows good agreement with the cross sections given in Table 1, with slight differences (<10%) in relative values. The absolute values given for 100 eV electrons in Table 1 are about 15% below the values obtained in the recent analysis. Quantitative measures of predissociation have also been obtained, but the effect on the model fit to the data presented here can be neglected for the purpose of the present analysis.

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