Visible to Near Infrared Emission Spectra of Electron-Excited \( \text{H}_2 \)

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ABSTRACT

The electron-impact induced fluorescence spectrum of \( \text{H}_2 \) at 100 eV from 700 nm to 950 nm at a spectral resolution of between 0.2 nm to 0.3 nm has been measured. The laboratory spectrum has been compared with our theoretical simulated spectrum obtained by calculating the lines emission cross sections from the upper states of \( g \) symmetry (EF, GK, HH, P, O ; I, R, J, S ) towards the states of \( u \) symmetry (B, C, B', D) of \( \text{H}_2 \). The nine above Born-Openheimer \( g \)-upper states have been coupled together as well as the four above Born-Openheimer \( u \)-lower states. The comparison seems adequate with few minor discrepancies.

1. Introduction

\( \text{H}_2 \) is the most abundant molecule and is an active component of stellar formation. Collisonal excitation by electrons is the source of both UV and Visible-Optical-IR (VOIR) \( \text{H}_2 \) florescence in circumstellar disks and certain classes of stars (Dalgarno et al. 1999). Intense \( \text{H}_2 \) transitions in the VOIR from various vibrational levels of the ground state have been observed in highly-collimated jets of matter from young stellar objects. These observed lines trace the colder molecular part of the post-shocked gas (Giannini et al. 2004).

With the successful missions of HST Space Telescope Imaging Spectrograph (STIS) and FUSE, UV astrophysical spectroscopy has undergone a quantum leap in resolving power \( (10^5) \) and precision \( (1\%) \) demanding higher accuracy of the measured cross sections and oscillator strengths for excitation, ionization and emission processes (Dalgarno et al. 1999).

In the last few years we have published analytical models based on laboratory measurements of the two most fundamental sets of electronic cross sections in UV astronomy, the \textit{Lyman} and \textit{Werner} band systems

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\begin{align*}
B^1\Sigma^+_u \rightarrow X^1\Sigma^+_g & \quad 1\sigma 2p\sigma \\
C^1\Pi^+_u \rightarrow X^1\Sigma^+_g & \quad 1\sigma 2p\sigma
\end{align*}
\]

These cross sections and models are now the basis for electron transport codes to predict UV emission spectra from secondary electron distributions in weakly ionized plasmas of astrophysical regimes (see (Liu et al. 2002), (Abgrall et al. 1999)). We have also demonstrated that the gerade series (EF \(^{1}\Sigma_g^+, GK \(^{1}\Sigma_g^-, HH \(^{1}\Sigma_g^-, I \(^{1}\Pi_g^+, J \(^{1}\Delta_g^+\) ... ) make a significant contribution (about 50% at 20 eV) to the UV spectrum of H₂ (Dziczek et al. 2000) via cascading to the n=2pσ B and 2pπ C states.

In this paper we present the optically thin VOIR spectrum of electron-excited H₂ corresponding to the cascading of the EF, GK, HH, ... g-states to the B, C, B’ and D u-states.

2. Experimental Apparatus

To measure VOIR spectra of atomic and molecular gas species, the Laboratory at JPL is equipped with an electron impact collision chamber in tandem with a SpectraPro-500i spectrograph. This is a 0.5 meter focal length monochromator with a triple grating turret covering the wavelength range of 195 nm to 1400 nm. The VOIR spectrum of H₂ is measured by crossing a magnetically collimated beam of electrons at 100 eV with a beam of H₂ gas formed by a capillary array. The emitted photons, corresponding to radiative decay of collisionally excited states of H₂, are detected at 90 degrees by the spectrograph equipped with a variable entrance slit and a CCD camera with 20 µm pixels.

3. Theoretical Simulated Spectrum and Comparison

We have calculated the lines emission cross sections from the upper state of g symmetry (EF, GK, HH, P, O ; I, R, J, S ) towards the states of u symmetry (B, C, B’, D). The excitation cross section of H₂ at 300 K was estimated by using the Franck-Condon approximation as in (Liu et al. 2003). We have calculated the transition emission probabilities of each rovibronic state belonging to g in a way similar as in (Abgrall et al. 2000) to obtain the rovibronic wavefunction of g symmetry states, we have coupled together the 9 above Born-Openheimer g-states, and to obtain those of u-rovibronic states, we have coupled together the 4 above Born-Openheimer u-states. The excitation rate of the different g-states was calculated as in (Liu et al. 2002). Figure 1 shows the comparison between the experimental data and the resulting synthetic spectrum.
Fig. 1.— The electron-excited H₂ spectrum at 100 eV from 700 nm to 900 nm is composed of two different sets of measurements obtained with different gratings at resolutions of 0.2 nm and 0.3 nm. It is compared to a synthetic spectrum convoluted (red curve) with a 0.3 nm Gaussian FWHM to represent the experimental function. The two open circles at around 752 nm and 890 nm correspond to the identified $EF - B(6-0)P(2)$ transition and to the mixture of $EF - B(3-0)P(2)$ and $EF - B(3-0)P(3)$ transitions, respectively. These transitions were used to normalized the two sets of experimental data to the synthetic spectrum.

4. Summary and Future Work

The laboratory capabilities at JPL are now extended towards the VOIR region, covering the wavelength range from 300 nm to 1200 nm. H₂ electron-impact induced fluorescence spectrum from 700 nm to 950 nm has been measured at resolutions of between 0.2 nm to 0.3 nm. Recent calculations are compared to the experimental measurements. The calculations include nine coupled gerade states and four coupled ungerade states. At the present stage only the $R$ and $P$ lines have been included in the simulation and we plan to compute the contributions of $Q$ branches from $\Sigma$-$\Pi$ and $\Pi$-$\Pi$ transitions. The comparison is satisfactory over the whole wavelength region. Minor discrepancies between experiment and theory are still present and are being investigated.
H$_2$ measurements at wavelengths as low as 300 nm are planned. These measurements will overlap with our previous reported measurements (220 nm to 530 nm) (James et al. 1998). We will extend our theoretical and experimental work for HD and D$_2$ in the VOIR.

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REFERENCES