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INTRODUCTION

The sensitivity of diatomic ro-vibronic band emission structure to isotopic composition provides a possibility of detecting the proportions of deuterium and tritium in the tokamak via the fusion relevant molecules BeD/BeT and CD/CT. Studies of the BeD $A\,^2\Pi$ - $X\,^2\Sigma$ transition at ~4990Å and the CD $A\,^2\Delta$ - $X\,^2\Pi$ transition at ~4320Å in the visible spectral region [4] from the JET tokamak have already shown the sensitivity of the band envelopes to the effective rotational and vibrational temperature.

Modelling parameters are not available for all BeH and CH isotopologues. Also distinguishing molecular features in JET tritium experiments are masked by unfavourable band head shifts, overlapping atomic lines and by the low levels of tritium introduced.

1. PREDICTION OF BAND STRUCTURE

Calculation of electronic spectra for diatomics containing beryllium or carbon and an isotope of hydrogen is based on the CALCAT program of [7]. It is suited to open shell diatomics where it proves easy to include all transitions without the need for tabulated Hönl-London factors. Initial assessment of spectral prediction, using the parameters of the $CD\,A\,^2\Delta$ - $X\,^2\Pi$ transition at ~4320Å of [6] following the formats of [1], with the experiment suggested a relatively poor fit. The equivalent parameterisation of the CH transition by contrast veries the data of [1]. Since the $CD\,X\,^2\Pi$ parameters are sound [8], we conclude that the laboratory CD emission spectrum should be re-evaluated.

Analysis of pre-tritium set-up shots indicated that the $B\,^2\Sigma$ - $X\,^2\Pi$ transition at ~3890Å was likely to show the most favourable tritide isotope shift. The $B\,^2\Sigma$ state is however shallow and very anharmonic. Laboratory data is not available for the CT $A\,^2\Delta$ - $X\,^2\Pi$ and $B\,^2\Sigma$ - $X\,^2\Pi$ transitions.

The above comments suggest caution in extrapolation of parameters from CD to CT based on equilibrium molecular constants and the Born-Oppenheimer separation. Cross-verifying isotopic scaling of molecular constants has been set up for the interconversion, but further corrections from separation violation may be required. The calculation relies on using a power series expansion in the vibrational quantum numbers to interpolate all the information from the tting of the experimental data for a particular isotopologue. The power series expansions take the form

$$
\begin{aligned}
G(v) &= \omega_e\,(v+1/2) - \omega_e x_e\,(v+1/2)^2 + \omega_e y_e(v+1/2)^3 + \omega_e z_e(v+1/2)^4 \\
P_v &= P_e + \alpha_P\,(v+1/2) - \beta_P\,(v+1/2)^2 + \ldots
\end{aligned}
\tag{1}
$$

for vibrational states and other parameters such as P_v respectively. Thus, for example, the centrifugal distortion D_v: D_e, α_D and β_D scale as $(\mu_1/\mu_2)^{-2}$, $(\mu_1/\mu_2)^{-5/2}$ and $(\mu_1/\mu_2)^{-3}$ respectively with μ_1 and μ_2 the reduced masses for the reference and required isotopologues. Figsures 1 and 2 show the simulations for $A\,^2\Delta$ - $X\,^2\Pi$ and $B\,^2\Sigma$ - $X\,^2\Pi$ transitions respectively.

Since the molecular spectral signals are relatively weak, the deuteride and tritide differences must be detected against a background of noise and unrelated atomic lines. Random noise has been added to the simulations (Fig.2(b)) which shows its masking effect.

Recent analyses and parameterisations are available for BeH, BeD and BeT [5]. The very small shift in the $A\ ^2\Pi$ - $X\ ^2\Sigma$ electron transition between the deuteride and tritide means that the band head position is not an effective distinguishing feature. The simulations (Fig. 3(a)) show the main variation in the overlapped sequence band envelope. Although the BeD band at ~4990Å occurs in a relatively line-free region, signal to noise ratios indicate that BeD/BeT proportions of ~1 are required for distinguishability.

2. OBSERVATIONS AND EXPERIMENTAL SPECTRAL ANALYSIS

Maximum tritium concentrations in the trace experiments were believed to be limited to <5%. For the measurements on BeD/BeT, since ambient beryllium levels in JET are low, heavy beryllium evaporation was carried out as a prelude to the experimental pulses. The discharge was initiated in pure tritium and the preferred spectral line-of-sight was directed close to the outer shoulder of the divertor from where the nascent plasma expands. However, outgassing greatly reduces the effective concentration. Two discharges were usable. Figure 3(b) shows the observed spectra in the initial and late phases of the pulse as the tritium concentration falls. Since wall absorbed tritium at this stage of the trace experiments was low, BeT formation was expected to be from plasma sources alone. As expected, an unambiguous BeT signature was not obtained. Monitoring of both CD/CT transitions was possible in a series of pulses. The CD/CT band simulations at 4320Å seemed to indicate that the line-like 2-2 band shift between deuteride and tritide might be diagnostic. Superposition of a number of atomic lines (including beryllium and chlorine) confuse an immediate conclusion. Some additional information is provided by the time history of the spectral emission. Thermal and density fluctuations in the observational lines-of-sight (due to typical plasma variations) generate, on the spectrometer sampling period, a varying signal which shows a differential variation between different emitters depending on their location and exciting conditions. The time history then provides a normalised 'time pattern', analogous to the 'position patterns' [2] used as an aid in solar spectral identication. Time patterns are shown in Fig.4 for a number of features in the vicinity of the CD/CT $A^2\Delta$ – $X^2\Pi$ band. The line features longward of 4305Å show a markedly different time pattern with much deeper variation than the molecular band components. The exception is the 'line' at 4316Å. which shows a pattern intermediate between the atomic and molecular patterns in both the pure deuterium and tritium gas puff cases. We conclude that this 'line' feature is a superposition of an atomic line and the CD 2-2 band.

The precise wavelength of the CT 2-2 band is uncertain and it is possible that it coincides with one of the atomic lines between 4308Å and 4313Å. The expectation is that CT and CD molecular band features will have identical time patterns. The present results therefore show no evidence of the CT 2-2 band either in isolation or superposition. From the theoretical simulations for CD and the observations, a threshold (~25% tritide) for the CT 2-2 band to be detectable in superposition with an atomic line can be inferred. If the CT 2-2 band is not in superposition, then the current experiments indicate a tritide concentration <10%.

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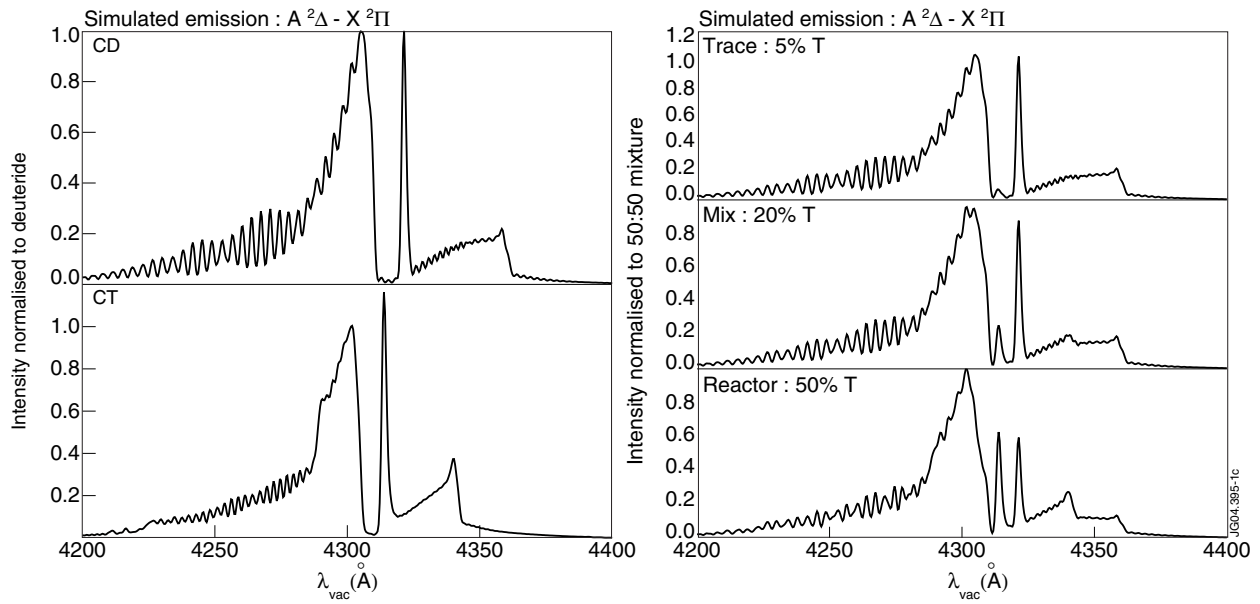
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Figure 1: (a) Simulated emission for CD and CT $A\,^2\Delta - X\,^2\Pi$ at $T_r = 0.3eV$ and $T_v = 0.3eV$. (b) Simulations of various CT/CD proportions.
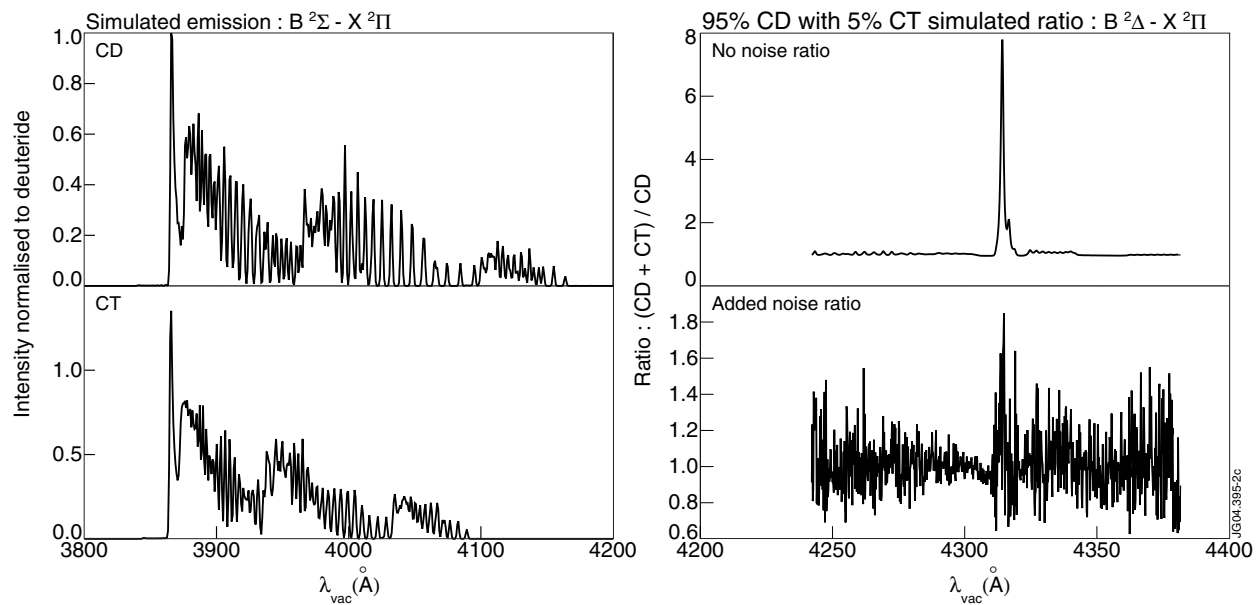

Figure 2: (a) Simulated emission for CD and CT $B\,^2\Sigma - X\,^2\Pi$ at $T_r = 0.3eV$ and $T_v = 0.3eV$. (b) The emission ratio for the $A\,^2\Delta - X\,^2\Pi$ band in the presence of simulated noise.

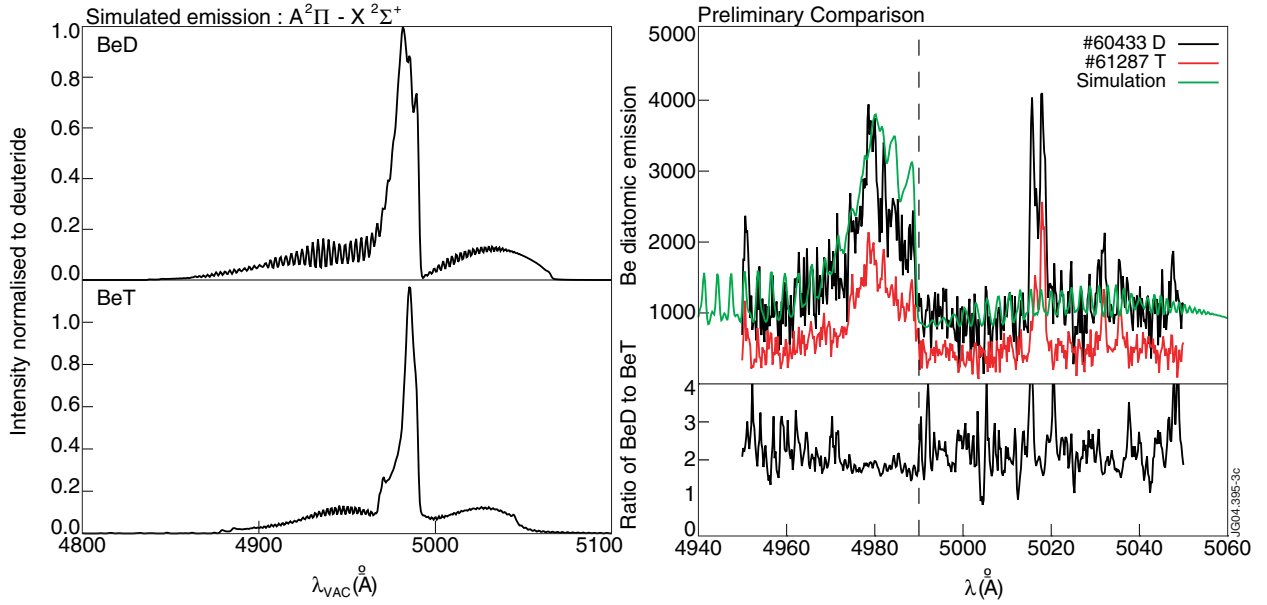Figure 3: (a) Simulated emission for BeD and BeT A $^2\Pi$ – X $^2\Pi$ at T_r = 0.3eV and T_v = 0.3eV. (b) Observed spectra before and after the tritium gas puff together with a superposed simulation.
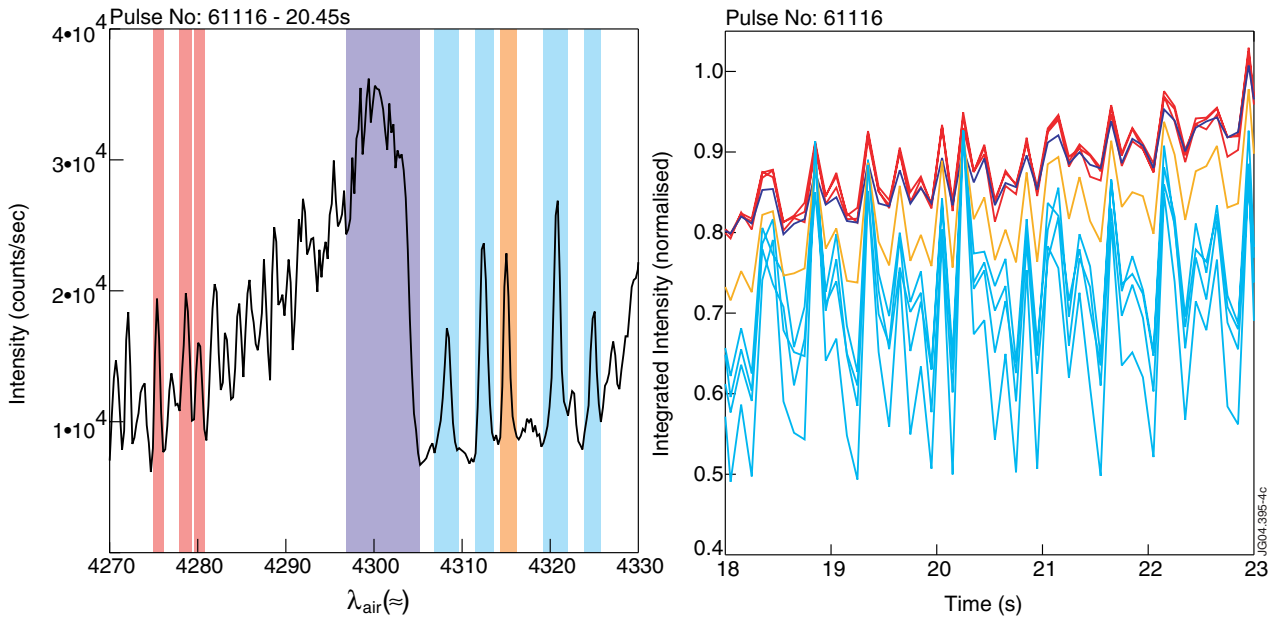

Figure 4: Time patterns of line features in the vicinity of the CD/CT A $^2\Delta$ – X $^2\Pi$. Pure molecular signatures are shown in red and pure atomic signatures in pale blue. Note that the band head region (dark blue) follows the molecular signature. The line in yellow shows a mixed signature interpreted as the 2-2 band blended with an atomic line.