# Astronomically inspired input data for SHIFTS

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Several hyperspectral data cubes have been prepared as input for SHIFTS, mostly for development and testing purposes. As part of his MSc thesis at the University of Lethbridge, John Lindner developed an input cube that models an optically thin molecular cloud (see chapter 7 of his thesis for the details of the model). The model represents a disk of dust with a radial temperature dependence and a ring-like region with CO molecules.

This model is available in various versions:

| Filename | Spectral elements | Comment |
|---|---|---|
| FullCloud2.sav | 1873 | The model with full spectral resolution |
| FullCloud3_lowRes.sav | 125 | The lower spectral resolution allows for shorter simulation runs |
| Fullcloud_10timespower.sav | 1873 | 10 times higher than the full model |
| FullCloud_special.sav | 188 | 10 times worse spectral resolution than the full model |
| | | |

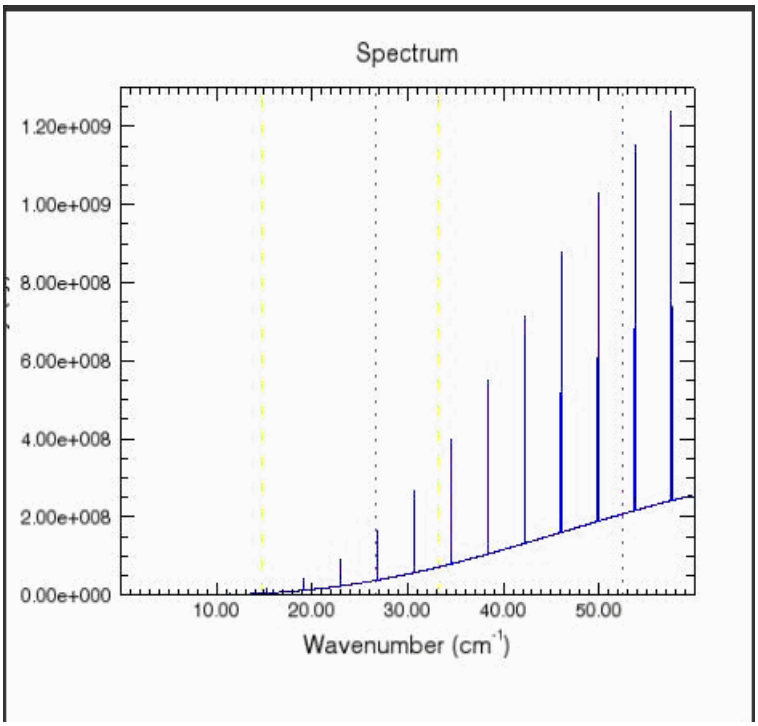


**Figure 1: Sample spectrum of the full model for the centre position of the hyperspectral cube**

# Chapter 7

# Simulated observation of molecular cloud

*" 'Yes indeed,' said the Unicorn. 'Now you have put a cogent question. What can we measure? Or perhaps I should say "What could we measure?" because (if I may speak for others) we are experts in the theory of measurement, not its practice.' "*

- John Lighton Synge, *Kandelman's Krim*, Jonathan Cape (1957).

This chapter describes the analysis of a simulated astronomical observation produced by the Simulator for the Herschel Imaging Fourier Transform Spectrometer (SHIFTS). Given the agreement between SHIFTS simulations and measured data obtained during from first proto-flight model (PFM1) tests (see Chapter 6), SHIFTS was employed to predict the performance of the Spectral and Photometric Imaging Receiver (SPIRE) spectrometer under nominal operational conditions. The results described herein demonstrate the advantages and challenges associated with use of this instrument. Section 7.1 describes the simple model used to simulate the far-infrared (FIR) emission of a disk of gas and dust. Given the simulated astronomical source (SAS), Section 7.2 analyzes and discusses the data products generated by SHIFTS.

## 7.1 Synthetic molecular cloud

One of the primary science goals of the SPIRE instrument is to characterize the early stages of star formation [4, 5]. As indicated in Section 1.1, star formation occurs in the dense regions of molecular clouds. A large fraction of the 200 – 670 μm emission (i.e., the band observed by the SPIRE spectrometer) from these clouds is due to the thermal radiation of dust grains (e.g., silicate and graphite) [9, 17, 157]. In addition to the radiating dust, there are numerous molecular emission lines present at these wavelengths [5]. This section describes the construction of a simple static model composed of continuum and line emission.

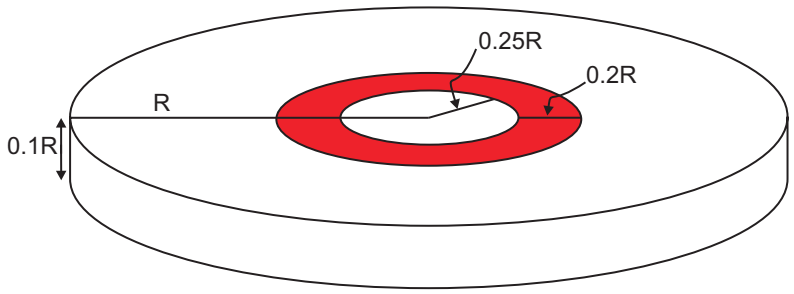


**Figure 7.1**: Inclined view of the simulated disk. In this figure, the radius $R$ is 1 parsec and the red ring represents the region where carbon monoxide molecules were present.

The model contained an obscured central luminosity source surrounded by a circular disk of dust. The basic assumptions in the model included the following: the entire disk was optically thin (i.e., no radiation emitted locally was absorbed locally); no stellar extinction occurred between the disk and the Herschel Space Observatory (HSO); the plane of the disk was not inclined with respect to the HSO; and the dust and gas components were at constant densities [15, 158].

Figure 7.1 shows the basic geometry of the model. As can be seen, the radius of the disk was 1 parsec (or pc; see Table A-1) with a thickness one-tenth its radius. At a distance of 1.6 kilo-parsecs from the Earth, the disk subtended an angle of 4.0 arcmin [15]. The distance and radius were specifically chosen so that the disk filled the field-of-view (FOV) of the SPIRE spectrometer; however, the values were representative of star-forming regions seen in the literature [32, 159, 160]. The disk was split into square blocks $0.06 \times 0.06$ pc across and 0.1 pc deep. This corresponded to a 7.8 arcsec angular spacing between each block and a solid angle of $1.4 \times 10^{-9}$ steradians. In addition to the dust component, a ring of carbon monoxide (CO) molecules was located between 0.25 and 0.45 pc (see Section 7.1.2). With each block, the conditions were assumed constant (i.e., each block was isopycnic, isothermal and isotropic).

To create the simulated astronomical source, we specified the initial conditions for the three associated arrays introduced in Section 4.2. The intial value, number of elements and step size of the right ascension and declination were determined from the geometry given above. For the wavenumber grid, the spacing of the SAS spectra, $\Delta\sigma_{\text{sim}}$, was fixed at 0.032 $\text{cm}^{-1}$ and the number of elements was set so that the Nyquist frequency was 60 $\text{cm}^{-1}$ (see Section 2.4). The spectrum of each block was then calculated using the specific intensities outlined in the following two sections.

### 7.1.1 Continuum component

To describe the continuum emission, each dust grain was modelled as a greybody [158, 161, 162]. For an optically thin distribution, the total dust emission is governed by

$$S_\sigma = \kappa_o m_d N_d \left(\frac{\sigma}{\sigma_o}\right)^\beta B_\nu(T_{\text{dust}}), \qquad [\text{W m}^{-2}\,\text{Hz}^{-1}\,\text{str}^{-1}] \quad (7.1)$$

where $N_d$ is the column density of dust (in $\mathrm{cm}^{-2}$), $m_d$ is the mass of a single dust grain (in g), $\sigma$ is the wavenumber (in $\mathrm{cm}^{-1}$), $\kappa_o$ is the dust opacity per unit mass column density (in $\mathrm{cm}^2\,\mathrm{g}^{-1}$) at a reference wavenumber $\sigma_o$ (in $\mathrm{cm}^{-1}$), $\beta$ is the emissivity index (unitless), and $B_\nu(T_{\mathrm{dust}})$ is the blackbody equation (see Equation 1.1) for a dust temperature $T_{\mathrm{dust}}$ (in K) [160, 163]. The product of the terms in the above equation, except for $B_\nu(T_{\mathrm{dust}})$, corresponds to the emissivity term, $\varepsilon_\nu$, in Equation 1.1.

To simulate the differential heating of the grains due to the central source, a radial temperature gradient was introduced between the blocks. The temperature of each block was defined as

$$T_{\mathrm{dust}} = T_o e^{-r/\gamma}, \qquad [\mathrm{K}] \tag{7.2}$$

where $T_o = 40\,\mathrm{K}$ was the temperature at the center of the cloud, $r$ was the radial distance from the center of the disk (in pc) and $\gamma = 1\ \mathrm{pc}^{-1}$ was a temperature gradient index [158]. Given $T_o$ and $\gamma$, the temperature at the edge of the disk was 11.5 K. This range is typical of temperatures seen in star-forming regions [33, 162, 164].

The other terms in Equation 7.1 would ordinarily have various frequency, radius and temperature dependences but were, for simplicity, fixed as constants. Assuming a dust density of $3.0\ \mathrm{g\,cm}^{-3}$ and a grain radius of 0.43 μm, the dust mass was $10^{-12}$ g [157, 158]. For the reference wavenumber and dust emissivity index, we assumed canonical values of 1000 $\mathrm{cm}^{-1}$ and 2.0, respectively [32, 158, 163]. Given the dust opacities listed in Johnstone *et al.* [32] and Motte *et al.* [160], we adopted a value of $\kappa_o = 0.04\ \mathrm{cm}^2\,\mathrm{g}^{-1}$. The column density of CO in molecular clouds such as the Orion Nebula and Cepheus A is on the order of $10^{16}\ \mathrm{cm}^{-2}$ [159, 165]. Given a gas-to-dust ratio of 150 and because our disk model was approximately one-tenth the thickness of the above molecular clouds, the dust column density was set to $6.7 \times 10^{12}\ \mathrm{cm}^{-2}$ [159, 165, 166].

Employing the above values, the effective dust emissivity in Equation 7.1 was 0.01 % at $\sigma = 20\ \mathrm{cm}^{-1}$ [72]. The resultant specific intensities in the simulated disk (approximately 10 to 500 $\mathrm{MJy\,str}^{-1}$) were in agreement with values seen in Motte, André & Neri [160].

### 7.1.2 Emission line component

In addition to the continuum emission described above, a ring of carbon monoxide molecules was included between 0.25 and 0.45 pc. Due to its ubiquity in star-forming regions, CO is frequently employed as a molecular tracer [167, 168]. To simplify the discussion, only a single isotope, $^{12}\mathrm{C}^{16}\mathrm{O}$, was included in our model.

Consider the radiative absorption and emission processes in a two energy level system as shown in Figure 7.2. The *Einstein A coefficient*, denoted by $A_{u\ell}$, is defined as the probability per unit time that a system in an upper quantum state $u$ will spontaneously drop to a lower quantum state $\ell$ and emit a photon with a frequency proportional to the energy difference between the two states.

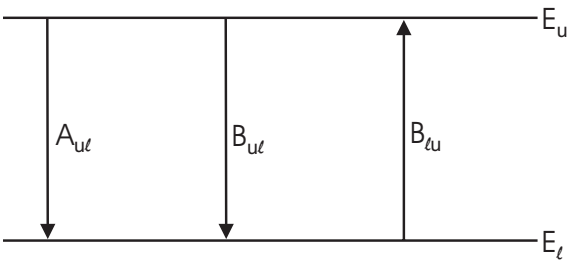


**Figure 7.2**: Emission and absorption in a two energy level system. The upper energy state, $E_u$, has a population of $N_u$ and a degeneracy of $g_u$, while the lower state, $E_\ell$, has a population of $N_\ell$ and a degeneracy of $g_\ell$.

The Einstein B coefficients, $B_{\ell u}$ and $B_{u\ell}$, describe the stimulated absorption and emission of photons in the presence of an external radiation field [169].

As indicated above, we assumed the model was optically thin; the local energy density was therefore sufficiently low that spontaneous emission was the primary radiation source. At far-infrared (FIR) and submillimetre wavelengths, the CO emission lines are caused by discrete changes in the angular momentum quantum number $J$ [168, 170]. For each transition $J_u \rightarrow J_\ell$, the intensity is given by

$$I_u = N_u A_{u\ell} \frac{hc\sigma_{u\ell}}{4\pi}, \qquad [\mathrm{W\,cm^{-2}\,str^{-1}}] \tag{7.3}$$

where $A_{u\ell}$ is the Einstein A coefficient for the rotational transition $J_u \rightarrow J_\ell$ (in $\mathrm{s^{-1}}$), $N_u$ is the population of the upper energy state (in $\mathrm{cm^{-2}}$), $\sigma_{u\ell}$ is the wavenumber of the emitted photon (in $\mathrm{cm^{-1}}$), $h$ is the Planck constant and $c$ is the speed of light (see Table A-1) [170, 171]. In thermal equilibrium, the population of the energy states is given by the Maxwell-Boltzmann distribution,

$$N_u = \frac{Ng_u}{Q_{\mathrm{rot}}} e^{-E_u/kT_{\mathrm{rot}}}, \qquad [\mathrm{cm^{-2}}] \tag{7.4}$$

where $N$ is the total column density of CO (in $\mathrm{cm^{-2}}$), $g_u = 2J_u + 1$ is the degeneracy of the energy level (a unitless value that desribes the spatial orientations of the angular momentum), $Q_{\mathrm{rot}}$ is the rotational partition function (unitless), $T_{\mathrm{rot}}$ is the excitation temperature (in K), $k$ is the Boltzmann constant (see Table A-1), and the energy level of the upper state is

$$E_u = J_u(J_u + 1)Bhc, \qquad [\mathrm{J}] \tag{7.5}$$

where $B$ is the rotational constant for CO (see Table A-1) [168, 169, 172, 173]. Given the above equation, the wavenumber of the emitted photon is

$$\sigma_{u\ell} = \frac{E_u - E_\ell}{hc} = 2BJ_u. \qquad [\mathrm{cm^{-1}}] \tag{7.6}$$

For a linear molecule such as CO [174, 175], the rotational partition function is given by

$$Q_{\mathrm{rot}}(T) = \frac{kT_{\mathrm{rot}}}{hcB}. \tag{7.7}$$

To calculate the intensity for each transition, we adopted an excitation temperature of 300 K and, as indicated in Section 7.1.1, a CO column density of $10^{15}$ molecules per square centimetre [159, 165].

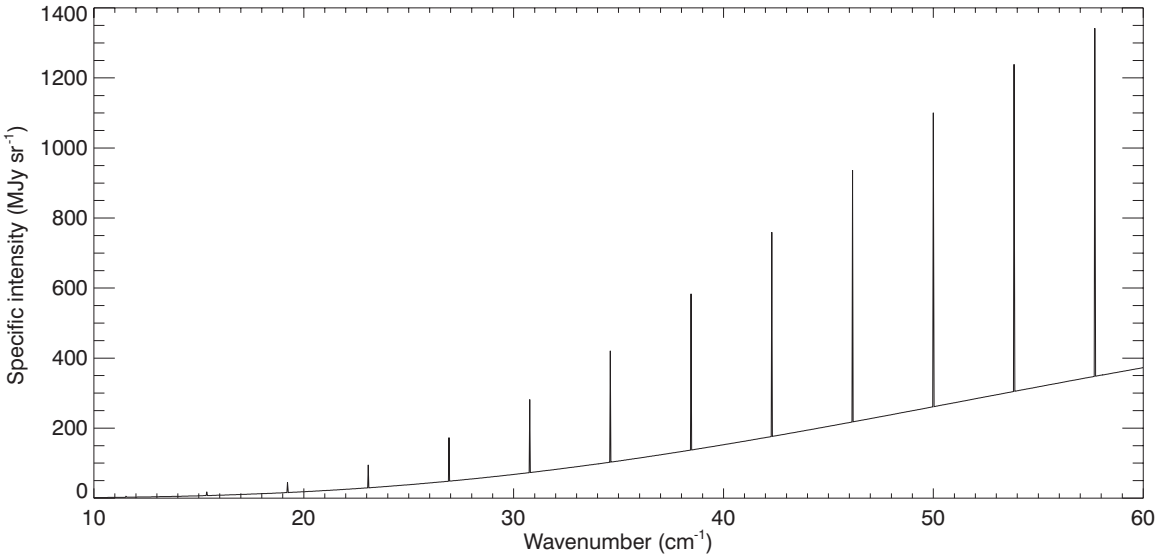


**Figure 7.3**: Example spectrum of the simulated molecular cloud. Located at a radius of 0.3 pc, the spectrum represents continuum emission at a dust temperature of 27.5 K with CO line emission at a temperature of 300 K.

The final value required to compute the line intensity (see Equation 7.3) is the Einstein A coefficient. The coefficients can be determined from spectral line characteristics listed in several online catalogs [176–178]. However, the multiple definitions of the Einstein A coefficient found in the databases frequently leads to confusion [169, 179, 180]. Appendix C compares two of the primary notations seen in the literature and compares the coefficients computed from these databases. As indicated in Appendix C-2, the 2004 edition of the High-resolution Transmission Molecular Absorption (HITRAN) database* explicitly lists the Einstein A coefficent [176, 181]. The CO line intensities were calculated using the Einstein A coefficients from HITRAN2004. Finally, the line intensity was converted to a specific intensity by dividing by the line width noted at the beginning of Section 7.1.

The line and continuum emission were summed to produce the total simulated emission from the entire cloud at each pixel. Figure 7.3 shows an example spectrum for a single SAS pixel at a radius of 0.3 pc. At that radius, the dust temperature was 27.5 K and emission lines were visible since that block was located inside the CO dust ring. With a simulated molecular cloud composed of spectra similiar to Figure 7.3, we proceeded with the SHIFTS simulation.

## 7.2 Simulated observations of a molecular cloud

As indicated in Section 1.3, one of the motivations for writing SHIFTS was to allow astronomers to explore the capabilities of the SPIRE spectrmeter. We explored these capabilities

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