

Simulated observations of young protoplanetary discs

Tom Douglas^{1*}, Paola Caselli¹, Aaron Boley², Richard Durisen³, Tom Hartquist¹, John Ilee¹

¹School of Physics and Astronomy, University of Leeds, Leeds LS2 9JT, UK

²Department of Astronomy, University of Florida, 211 Bryant Space Center, PO Box 112055, USA

³Department of Astronomy, Indiana University, 727 East 3rd Street, Swain West 319, Bloomington, IN 47405, USA

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ABSTRACT

The formation and earliest stages of protoplanetary discs are still lacking observational constraints. ALMA will soon revolutionize this field, so it is important to provide predictions and help the interpretation of future high sensitivity and high angular resolution observations. Here we present simulated ALMA observations of a relatively massive ($0.39 M_{\odot}$) self-gravitating disc embedded in a $10 M_{\odot}$ envelope with a structure similar to the pre-stellar core L1544. We focus on simple species and conclude that OCS is among the best tracers to measure the disc structure and kinematics.

Key words: circumstellar matter – infrared: stars.

1 INTRODUCTION

The formation and early evolution of protoplanetary discs around solar-type and low-mass protostars has little observational support, despite of the fast growing list of theoretical models on the dynamical evolution of star forming dense cores (e.g. Krasnopolsky et al. 2011; Machida et al. 2011; Braiding & Wardle 2012). The reason for this is that young protostars are surrounded by thick envelopes and power energetic outflows, thus observations of the young discs, predicted to have sizes of about 100 AU and masses as large as 10% the original core mass (e.g. Joos et al. 2012), are challenging. The use of sensitive interferometers is needed to achieve high angular resolution and spatially/spectrally disentangle the various (disc + envelope + outflow) components as well to filter out the extended emission tracing envelope material.

After the pioneer work of, e.g., Chandler et al. (1995), Brown et al. (2000), Looney et al. (2000), recent interferometric observations have discovered compact embedded discs in a sample of Class 0 (André et al. 2000) sources, finding masses between 0.4 and $>1 M_{\odot}$ (Jorgensen et al. 2007, 2009; Enoch et al. 2011). A 130 AU disc was discovered toward a Class 0 source in Perseus, using Jansky Very Large Array (JVLA) observations of NH₃ (Choi et al. 2007). Pineda et al. (2012) observed methyl formate with the Atacama Millimeter and sub-millimeter Array (ALMA) and found evidence of rotation toward one of the proto-binary Class 0 sources embedded in IRAS 16293-2422. These observations are consistent with an almost edge-on disc. Persson et al. (2012) observed H₂¹⁸O with ALMA toward the same

source and found evidence of relatively large ($\gtrsim 100$ K) excitation temperatures, as well as a HDO/H₂O abundance ratio close to that measured on Earth's oceans and Jupiter-family comets (Hartogh et al. 2011). When ALMA will be completed, it will be finally possible to spatially resolve these young discs and, for the first time, put stringent constraints on theoretical models. As full-operational ALMA is fast approaching, it is important to provide observational predictions based on dynamical models of young protoplanetary discs.

In this paper, we focus our attention to the young self-gravitating discs of Boley & Durisen (2008), where episodic heating induced by spiral shocks is present, as this may be a good representation of the earliest phases of protoplanetary discs and an alternative to the young "static" discs studied by, e.g. Visser et al. (2009, 2011). As shown by Ilee et al. (2011), the spiral shocks cause desorption of volatiles from dust icy mantles and trigger gas-phase chemical reactions with activation energies, which are inactive at lower temperatures. These processes produce clear chemical signatures of the disc dynamics. With the use of 3D radiative transfer modeling, we perform simulated ALMA observations of the disc studied by Ilee et al. (2011) and identify the best tracers of the physical structure of self-gravitating discs. The physical, chemical and radiative transfer models are described in Sect 2. Radiative transfer results are in Sect. 3, while ALMA simulated observations are in Sec. 4. Discussions and conclusions can be found in Sect. 5.

* E-mail: pytd@leeds.ac.uk

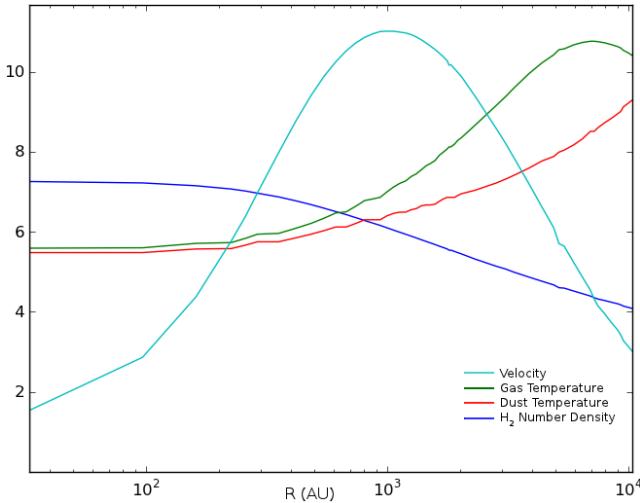


Figure 1. [NOTE: YOU NEED TO ADD LABELS AND UNITS TO THE AXES!!] Model of the pre-stellar core L1544 used as the envelope of the young protoplanetary disc in the hybrid model. Showing temperature (red) and dust (green) temperature in kelvin, log number density (blue) in cm^{-3} and inward velocity $\times 100$ (cyan) in m s^{-1} . Adapted from Keto & Caselli (2010) and Keto et al. (2012, in preparation).

2 DESCRIPTION OF THE MODEL

2.1 Physical and chemical structure

The physical model used to simulate the emission from a young protoplanetary disc is a hybrid model obtained from embedding a gravitationally unstable protoplanetary disc within an envelope with characteristics similar to the well-studied pre-stellar core L1544, as derived by Keto & Caselli (2010; hereafter KC2010). The KC2010 model follows the dynamical, chemical and thermal evolution of a contracting Bonnor-Ebert (Bonnor 1956; Ebert 1957) sphere with total mass of $10 M_{\odot}$, until it reaches the density, temperature and velocity profiles which best match observations. The pre-stellar core model adopted here contains slight modifications due to the inclusion of oxygen cooling in the outer regions of the cloud, where CO is mostly photodissociated (Keto et al., in preparation), and it is shown in Fig. 2.1. [NOTE: BESIDES THE PROBLEM WITH THE FIGURE NUMBER, YOU NEED TO READJUST FIGURES, AS THIS ONE IS THE FIRST ONE THAT YOU DESCRIBE, SO IT SHOULD BE NUMBER 1]

The pre-stellar core structure is maintained down to a radius of 80 AU, within which the young protoplanetary disc has been plugged in. The disc structure is derived by the hydrodynamic model of Boley(2007) and Boley (2009). The particular model considered here (as well as in Ilee et al. 2011) is a $0.39 M_{\odot}$ self-gravitating disc featuring prominent spiral arms. H_2 number densities in the disc range from 10^4 - 10^{13} cm^{-3} , and temperatures range from 30-400 K (figure 2.1). The dust and gas temperatures in the disc are assumed to be in equilibrium. The model is sampled over a regular grid of size $256 \times 256 \times 64$ with spatial resolution of 0.5 au in x, y and z. The gas/dust mass ratio was assumed to be 1/100 throughout both

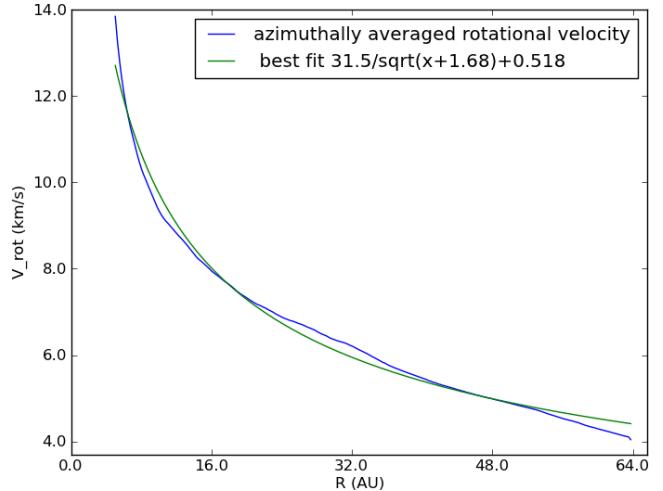


Figure 4. Azimuthally averaged rotational velocity in the disc mid-plane with best fit curve

sections model and the opacities were given by the model of dust grains with thick icy mantles and 10^6 yr coagulation from Ossenkopf and Henning (1994). The gas number density and temperature structure are displayed in Fig. XX.

Chemical abundances in the disc were taken from Ilee et. al (2011) which followed the changes of chemical abundances of trace particles moving through the disc as it evolved. The abundances of 125 species related by 1334 reactions were followed through the time evolution of the disc. These abundances were interpolated onto a 51^3 grid covering the disc with cells of size $2.2 \times 2.2 \times 0.22$ au. From Ilee et al. (2011) we selected the three species which appear to trace different regions of the disc : the inner 30 AU (OCS), the inner 60 AU (H_2CO) and the region between $\simeq 20$ and 60 AU (HCO^+) and one which traces the entirity of the disc (C^{18}O). As explained by Ilee et al. (2011), H_2CO and OCS mostly probe the central warm regions, where icy mantles evaporate, whereas HCO^+ preferentially traces the outer spiral pattern as in the central region it is destroyed by water molecules. The simple chemistry in the KC2010 model, adopted here as the envelope of the protoplanetary disc, does not provide detailed abundances of molecular species (besides CO and H_2O , see also Caselli et al. 2012). As discussed in the result section (Sec. 3), rough guesses have been made based on values measured toward similar objects.

2.2 The radiative transfer code

The radiative transfer program used, LIME (Brinch & Hogerheijde 2010), calculates line intensities based on a weighted sample of randomly chosen points in a continuous 3D model. The method of selecting these points is given in the grid-construction section. At each of these points, the density of the main collision partner (H_2), gas and dust temperatures, velocity, molecular abundances and turbulent velocity are taken from the model. These points are then smoothed by Lloyds algorithm (Lloyd 1982) in order to minimise the variation in distance between points whilst keeping the same underlying distribution. These points are

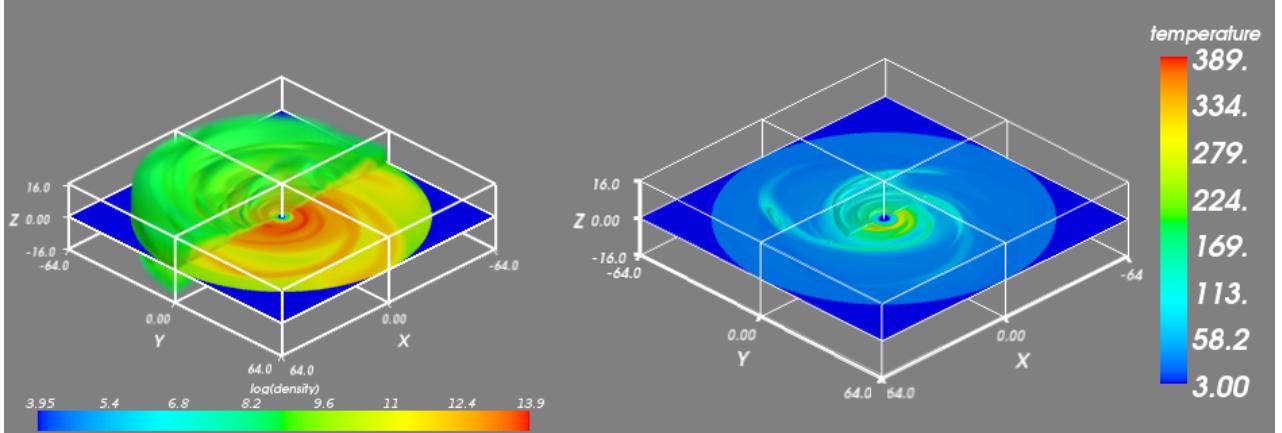


Figure 2. Left: A 3D plot of log number density (cm^{-3}) showing the spiral structure in the xy plane and scale height of the disc. Right: The 3D temperature structure of the disc; regions cooler than 40 degrees are not shown in 3D, demonstrating the narrow central region containing hot material.

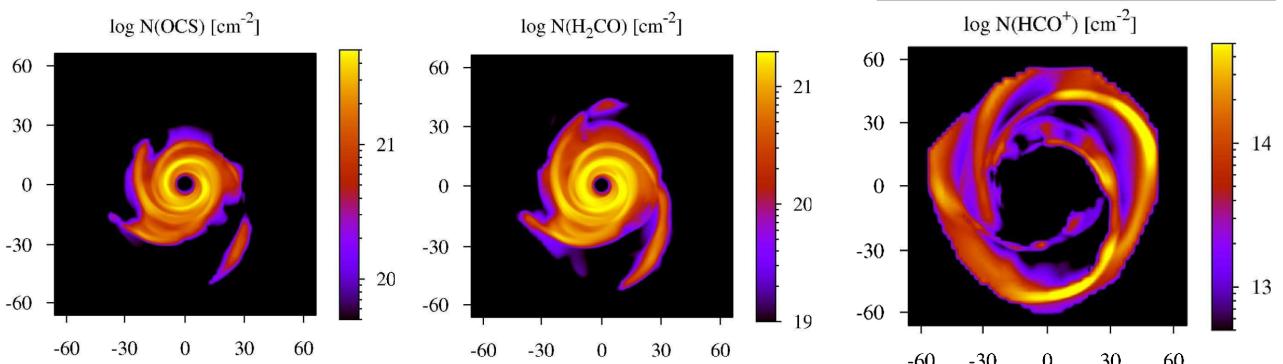


Figure 3. Column densities of OCS, H_2CO and HCO^+ used in the disc model. Figure adapted from Ilee et al. (2011) [SHOULD WE ALSO ADD C₁₈O COLUMN DENSITY AS WE WANT TO DISCUSS THAT LATER ??]

then connected by Delaunay triangulation ¹ and it is down these paths that photon propagation is restricted (figures 2.2). The level populations of the selected molecules are calculated at each of these points from collisional and radiative (de)excitation and the local radiation field is calculated. This is repeated 20 times with the populations of each level converging towards a single value. This number of iterations is sufficient for the signal to noise ratio of the level populations (as defined in Brinch & Hogerheijde 2010) to exceed 1000 in 99% of the points. [NOTE: WHY DO WE NEED TO REACH SUCH A HIGH S/N? — it isn't s/n in the usual sense, it's a measurement of how converged the model is, defined in brinch 2010 as change in populations this iteration / std-dev of change in pops over last 5 iterations] After 20 iterations of updating the level populations the model is ray-traced in order to produce synthetic brightness maps. In order to minimise the “blockyness” of the output images, resulting from the grid construction, the average of ten separate runs was taken (figure 2.2).

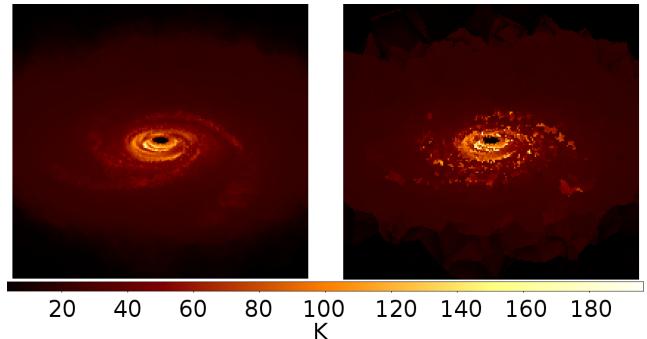


Figure 5. A plot showing the difference between a single LIME continuum image at 300 GHz (right) and the average of ten such images from different runs of the same model in LIME (left).

3 MODEL RESULTS

[NOTE: I SUGGEST TO:

1. SHOW THE MOMENT 0 AND 1 ONLY MAPS OF C₁₈O, OCS, H₂CO AND HCO⁺ + SPECTRA TOWARD THE CENTER AND +/- 30 AU (FOR EACH SPECIES, YOU CAN DO A 3-PANEL FIGURE SHOWING THE TWO MOMENTS AND A PANEL WITH THE 3

¹ In three dimensions this means that if four points are connected into a tetrahedron, the sphere circumscribing these four points contains no other points. It can be shown that this connection is unique for a given set of points.

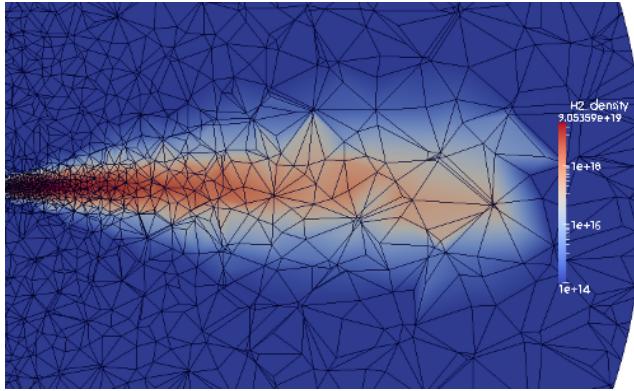


Figure 6. A plot of the points selected by the gridding process and the paths down which photons can propagate overlaid on a smoothed density model. The points are more concentrated at small radii and in the densest regions.

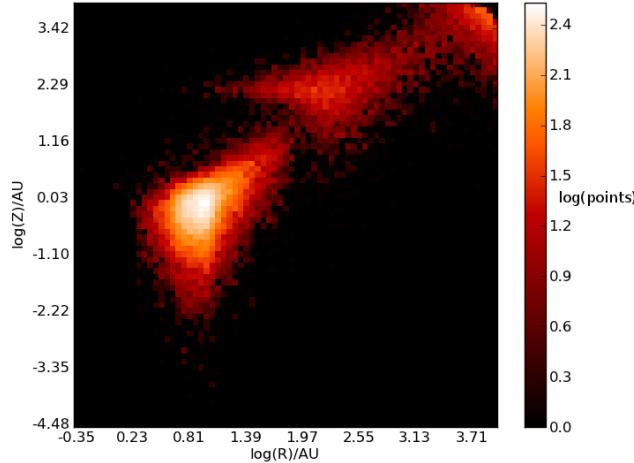


Figure 7. A 2D histogram of the point distribution throughout the model. The disc and envelope can be seen as two separate entities which have to be sampled using different point distributions

SPECTRA AT DIFFERENT LOCATIONS) + THE CONTINUUM MAP 3. SHOW THE SIMULATED ALMA OBSERVATIONS (SAME STYLE AS BEFORE) AND ALSO SHOW A SEPARATE FIGURE WITH THE PV DIAGRAMS OF ALL SPECIES.]

[NOTE: THE FOLLOWING PARAGRAPH IS NOT CLEAR AT ALL !!! PLEASE RE-WRITE MAKING SURE THAT THE SENTENCES MAKE SENSE AND THERE ARE NO TYPOS. PLEASE MAKE THE FIGURES AS SUGGESTED AND THEN RE-WRITE THIS PART.]

The results of these simulations for the molecules OCS, HCO^+ , H_2CO and isotopologues of CO are shown here, other molecules simulated but not shown include HCN, HNC, HNO, HCS^+ and CS. For the purpose of simulating observations the model was placed at roughly the distance of nearby low-mass star forming regions (100 pc) and is inclined at 30° to edge on. From these observations integrated intensity, intensity weighted velocity and position velocity diagrams through the centre of the model were

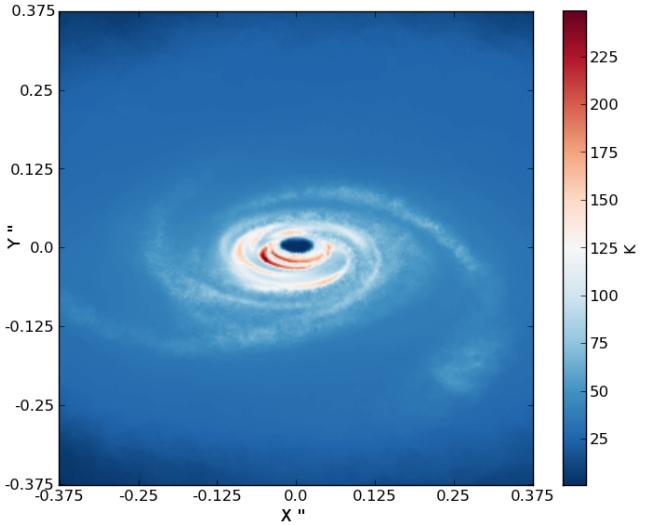


Figure 8. A 300 GHz continuum image of the model, created from the average of ten LIME runs.

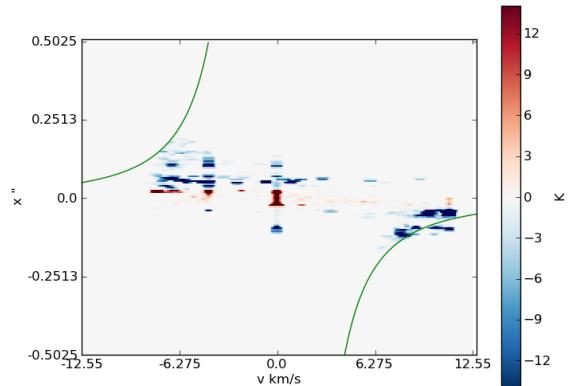


Figure 10. OCS 28-27 PV through centre

created. The simulations done are focused upon frequencies within ALMA band 7, selected to give the best trade off between resolution and sensitivity for early ALMA science **IS BAND 7 STILL THE BEST FOR US TO LOOK AT SEEING AS WE ARE NOW LOOKING AT ALMA FULL CAPABILITY RATHER THAN CYCLE1?** (Note the moment 1 and 0 maps were created by integrating between -12.5 to -0.5 km s^{-1} and $+0.5$ to $+12.5 \text{ km s}^{-1}$ to avoid being dominated by the contribution from the envelope, this can be seen in some PV diagrams as the strong absorption feature at all positions around zero velocity, moment 1 maps are shown with a cutoff of 1/1000 of the peak emission/absorption value)

After looking at a variety of lines which could be observed of ALMA band 6 or 7 (211-275 GHz and 275-373 GHz) we found that the OCS lines in alma band 7 (22-21 through 30-29) with upper energy levels between 161 and 271 K above the ground state provide a way to trace

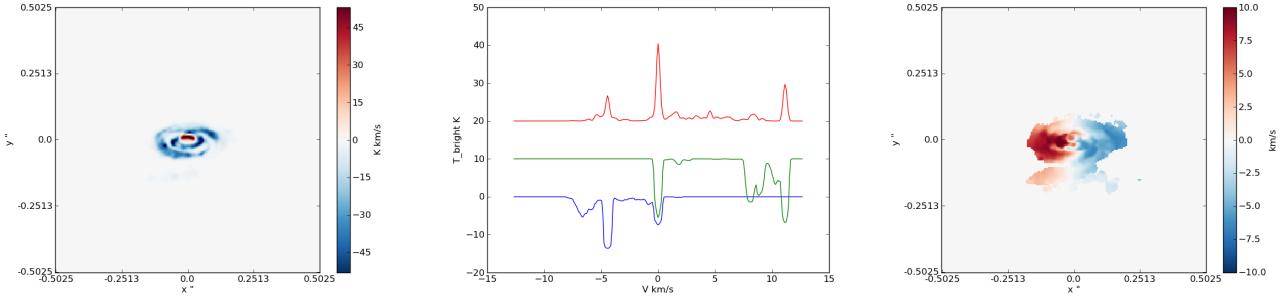


Figure 9. OCS 28-27 **Left:** Continuum subtracted integrated intensity map, **Centre:** Continuum subtracted spectra from $Y=0''$, $X=+0.1''$ (bottom), $X=-0.1''$ (centre) and $X=0''$ (top) spaced by 10 K for clarity, **Right:** Intensity weighted velocity map

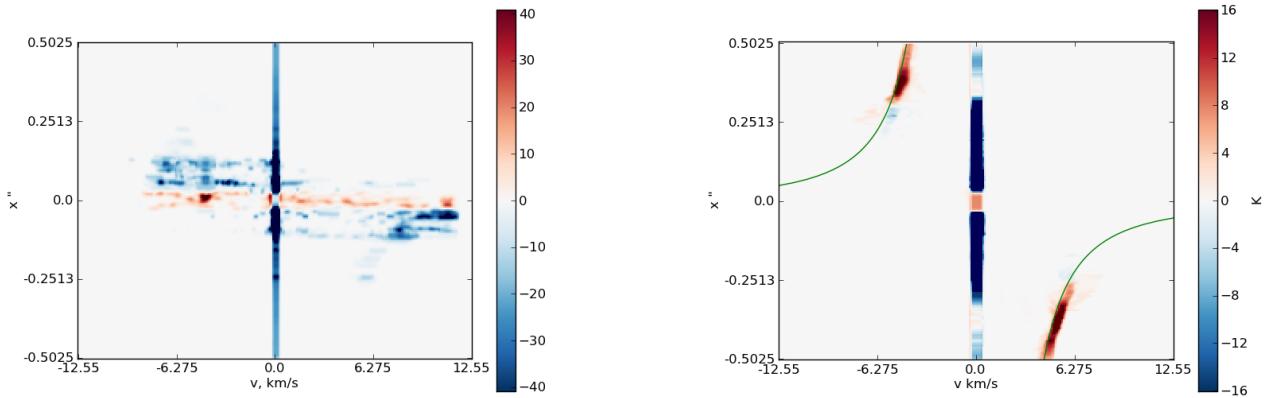


Figure 12. H₂CO 4₀4 - 3₀3 PV through centre

hot shocked gas in spiral arms without resolving structure. Figures ?? & ?? show the integrated intensity of the OCS $J=28-27$ line in the model described previously and one where the disc section of the model is an axis-symmetric model created by taking the azimuthal average of density, temperature and molecular abundance. The order of magnitude difference in the line intensity provides a method to detect hot dense gas without being able to resolve the spiral structure spatially.

More complex molecules such as H₂CO with many closely spaced spectral lines can be used to gain an estimate on the temperature of a region.

Some molecules such as HCO⁺ trace only the outer regions of the disc (Ilee 2011) and so can be used to look at the extended velocity and physical structure. In these colder less dense regions we see the molecular lines in emission rather than absorption. Figure ?? shows the rotation curve of the model as shown in figure 2.1 against the HCO⁺ $J=1-0$ line emission. It is clear that from observations such as these the rotation curve of a disc could be reconstructed.

In all the simulations except HCO⁺ we see molecular lines in absorption throughout the majority of the disc and in some cases a small amount of emission towards the centre. Molecular lines throughout the plane of the disc show up

Figure 14. HCO⁺ 1-0 pv through centre, with the rotation curve from figure 2.1 for comparison

in absorption against the continuum emission of the shock heated, dense midplane.

4 ALMA PREDICTIONS

In order to make predictions on the observability of the synthetic brightness maps created by LIME, CASA (common astronomy software applications) was used to simulate observing these with the completed ALMA in it's most extended configuration for a total time of four hours.

5 DISCUSSION AND CONCLUSIONS

In this paper we have performed radiative transfer simulations of a hybrid model comprising a $0.4 M_{\odot}$ self gravitating disc with radius 64 AU showing spiral density waves, surrounded by an envelope simulated as a collapsing $10 M_{\odot}$ BE-sphere. CASA simulations show that at a distance of 100 pc both spatial resolution of the spirals in such a disc and extraction of kinematic and temperature from molecular lines are possible in ALMA band 7. Our simulations show that many molecular species are predominantly seen in absorption towards the centre of self-gravitating protoplanetary discs. The quiescent nature of the envelope around such discs only obscures them within $\pm 0.5 km s^{-1}$.

One assumption made in this model is that the gas and dust

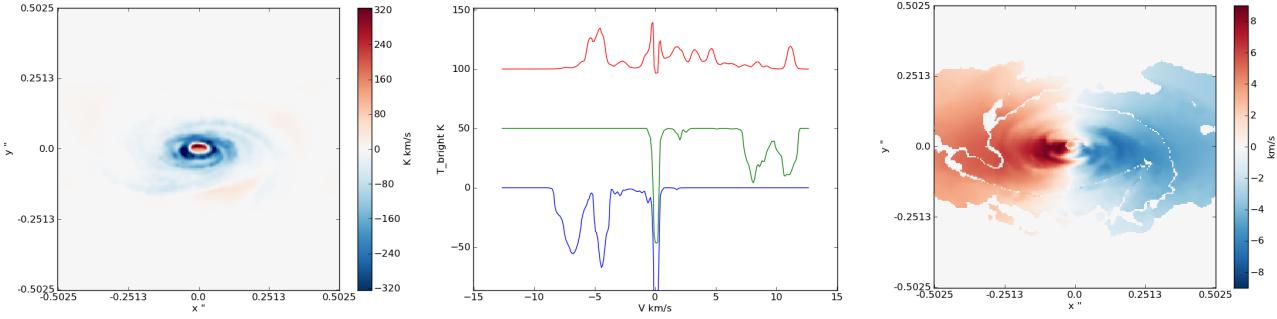


Figure 11. H₂CO 4₀ - 3₀ 3 **Left:** Continuum subtracted integrated intensity map, **Centre:** Continuum subtracted spectra from Y=0'', X=+0.1'' (bottom), X=-0.1'' (centre) and X=0'' (top) spaced by 50 K for clarity, **Right:** Intensity weighted velocity map

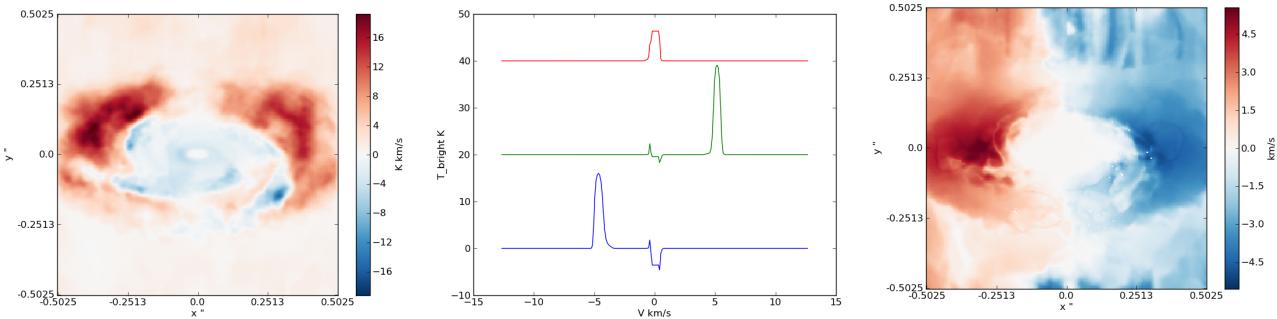


Figure 13. HCO⁺ 1-0 **Left:** Continuum subtracted integrated intensity map, **Centre:** Continuum subtracted spectra from Y=0'', X=+0.4'' (bottom), X=-0.4'' (centre) and X=0'' (top) spaced by 40 K for clarity, **Right:** Intensity weighted velocity map

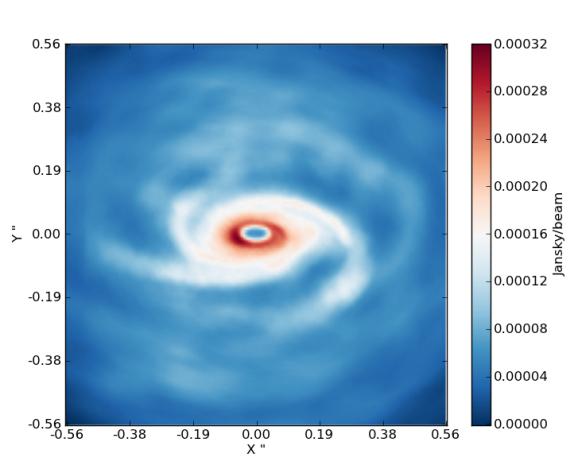


Figure 15. Continuum emission at 337GHz simulated for ALMA most extended configuration

are in thermal equilibrium. If they are not and the dust is significantly cooler than the gas then transitions may not show up in absorption.

In the model spirals shock heat the mid-plane layer and the colder more diffuse gas absorbs the continuum from it, this results in molecular lines being seen in absorption whenever lines of sight pass through the cold diffuse gas at larger heights on to the hot dense midplane of the disc. Rotation curves can be gathered from these observations even with spiral structure

Outflows could contaminate measurements of rotation

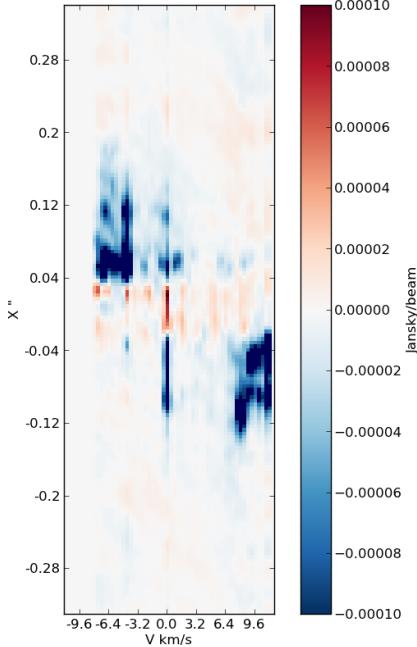


Figure 16. OCS 28-29 pv diagram simulated for ALMA most extended configuration

curves meaning that species which commonly trace outflows, such as CO and HCO⁺ are not going to be good tracers of disc rotation. However species such as OCS and C¹⁸O which are not commonly seen in outflows (Yildiz et al 2012,) can be used to trace disc rotation.

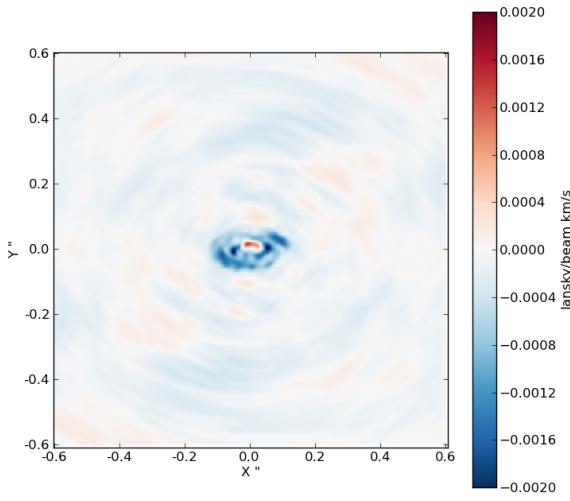


Figure 17. OCS 28-29 integrated intensity simulated for ALMA most extended configuration

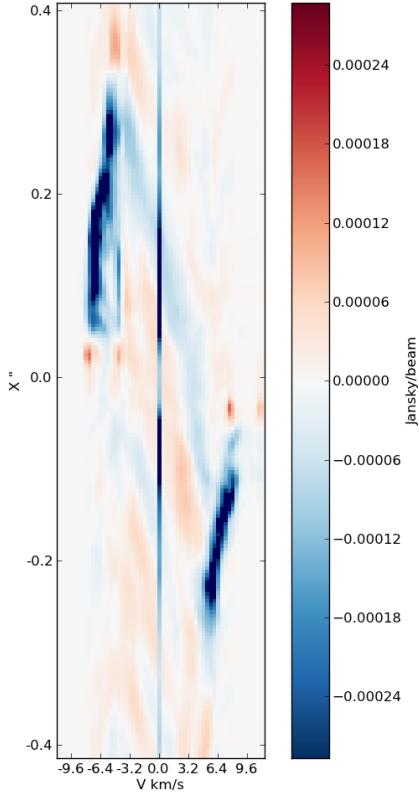


Figure 18. C17O 3-2 30 deg PV through centre simulated for ALMA most extended configuration

ACKNOWLEDGEMENTS

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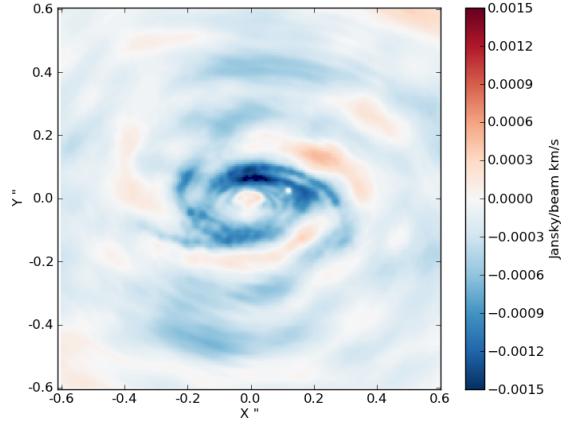


Figure 19. C17O 3-2 30 deg integrated intensity simulated for ALMA most extended configuration

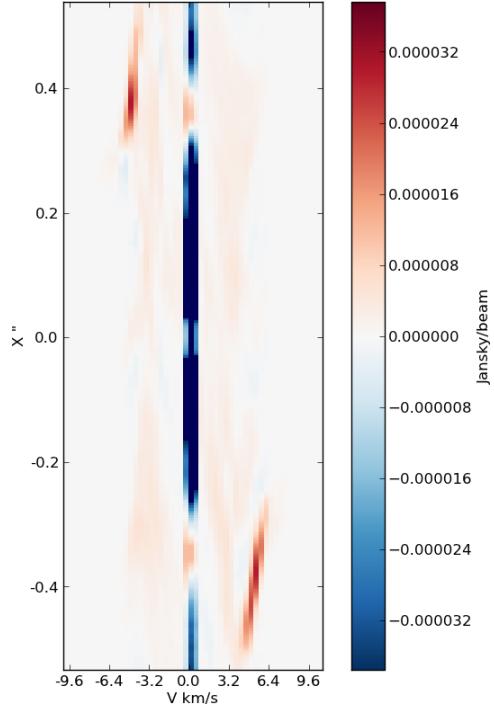


Figure 20. HCO⁺ 1-0 30 deg PV through centre simulated for ALMA most extended configuration

APPENDIX A: GRID CONSTRUCTION

In order to construct the grid, candidate points are randomly selected from the volume to be simulated. These candidates then have their density and molecular density compared against a reference point in order to decide if the point is to be used in the grid or not. [NOTE: THIS FIRST SENTENCE DOES NOT MAKE SENSE. PLEASE RE-WRITE IT AND MAKE SURE THAT IT IS CLEAR AND THERE ARE NO TYPOS.] Candidate grid points are selected at random in cylindrical co-ordinates, linearly spaced in z and ϕ and logarithmically spaced in r . For each point to be selected, a random number α is drawn from the semi-open set $[0, 1)$ as a threshold. After selection of random

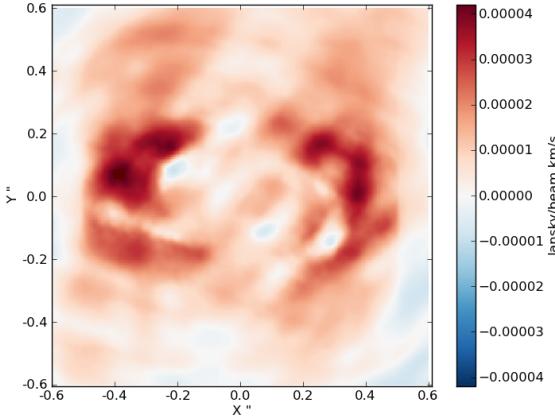


Figure 21. HCO^+ 1-0 30 deg integrated intensity simulated for ALMA most extended configuration

co-ordinates, the hydrogen density and molecular density at the candidate point (n and m , respectively) are compared against the densities of a reference point on the inner edge of the disc (n_0 and m_0). If $\alpha < \left(\frac{n}{n_0}\right)^{0.3}$ or $\alpha < \left(\frac{m}{m_0}\right)^{0.3}$ then the point is selected for use, otherwise another r , ϕ , z co-ordinate is selected and this becomes the candidate point. The function comparing the candidate point to the reference point and the candidate point distribution were selected empirically to sample all the scales while ensuring that the majority of points are located in the inner disc where the density is higher. 20% of these points are forced to be at radii greater than $\sqrt{R_{min}R_{max}}$ (where R_{min} and R_{max} are the inner and outer radius of the model) in order to stop too many of the selected points clustering in the high density disc and leaving the envelope undersampled. In addition to this method of selection, 5% of the points are linearly distributed in x , y and z with no bias with regards to density or abundance. This provides a minimum level of sampling for the large low density regions in the outer parts of the simulated volume. See figure 3 for an example of the points distribution in r , z .

APPENDIX B: OTHER INCLINATIONS

Figures showing different inclinations

This paper has been typeset from a T_EX/ L_AT_EX file prepared by the author.

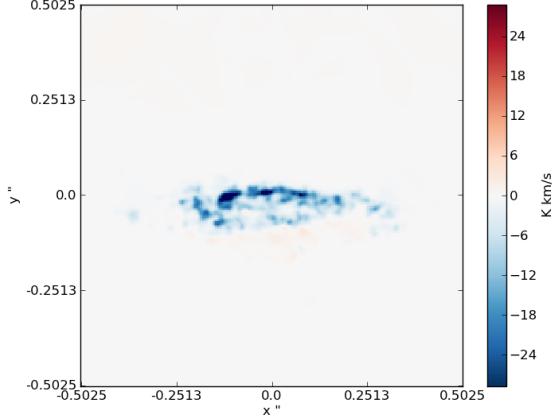


Figure B1. C18O 3-2 15 deg Continuum subtracted mom0

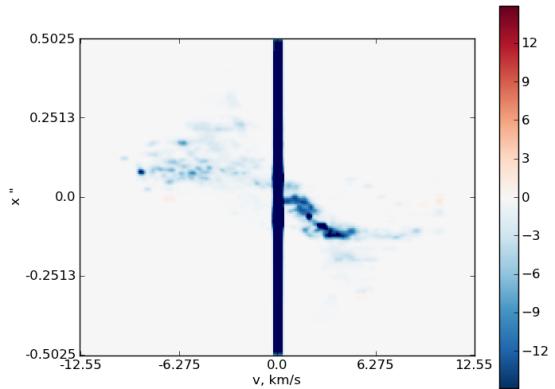


Figure B2. C18O 3-2 PV 15 deg through centre

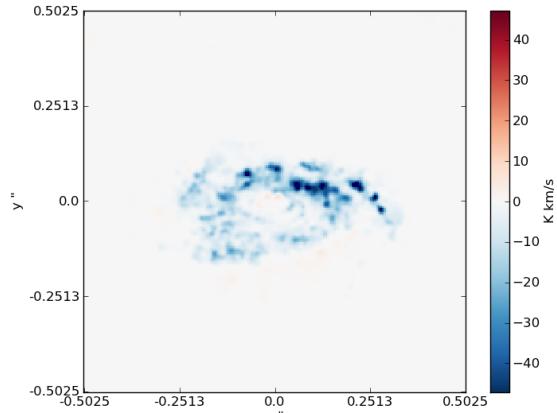


Figure B3. C18O 3-2 30 deg Continuum subtracted mom0

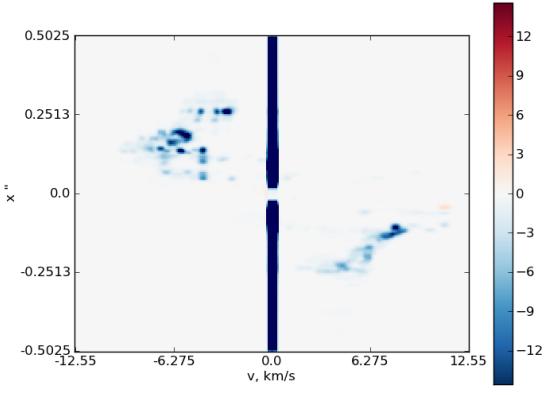


Figure B4. C18O 3-2 30 deg PV through centre

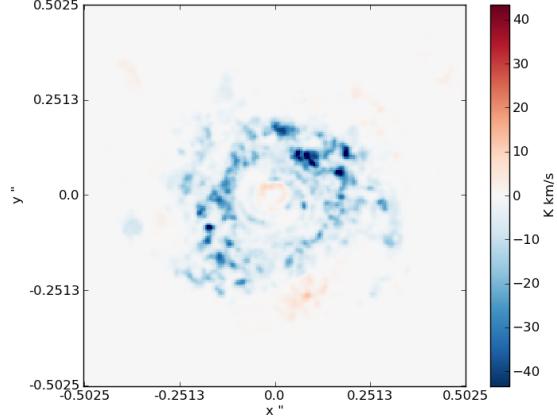


Figure B7. C18O 3-2 60 deg Continuum subtracted mom0

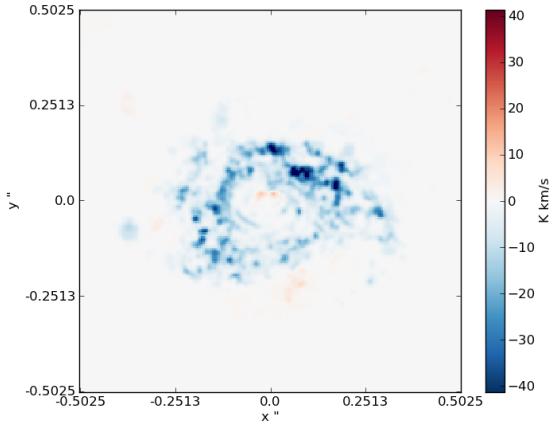


Figure B5. C18O 3-2 45 deg Continuum subtracted mom0

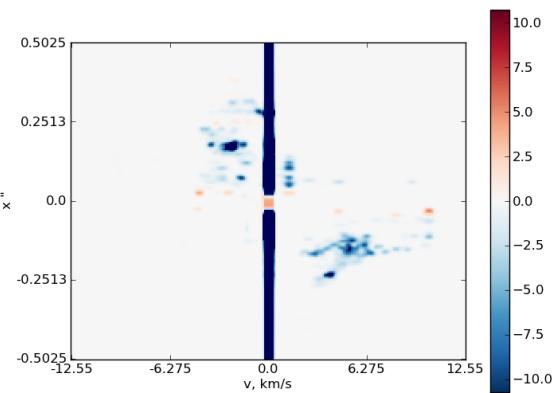


Figure B8. C18O 3-2 60 deg PV through centre

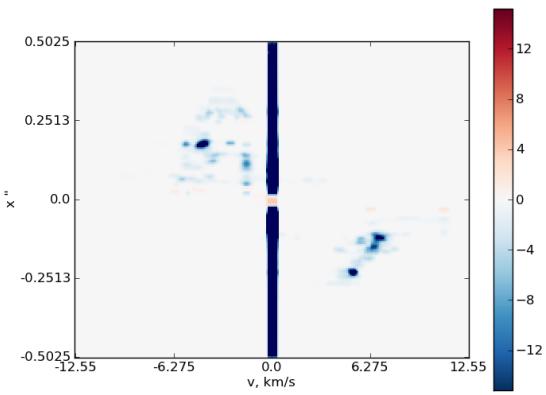


Figure B6. C18O 3-2 45 deg PV through centre

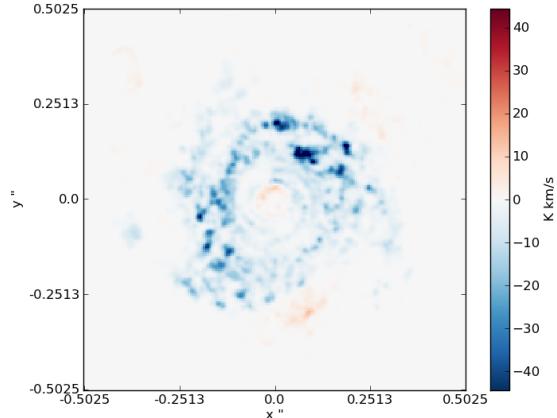


Figure B9. C18O 3-2 75 deg Continuum subtracted mom0

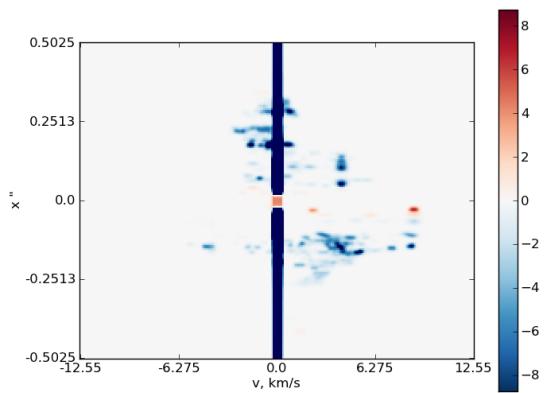


Figure B10. C₁₈O 3-2 75 deg PV through centre