SHAPEMOL: modelling gaseous nebulae with SHAPE in the molecular era of ALMA and HERSCHEL

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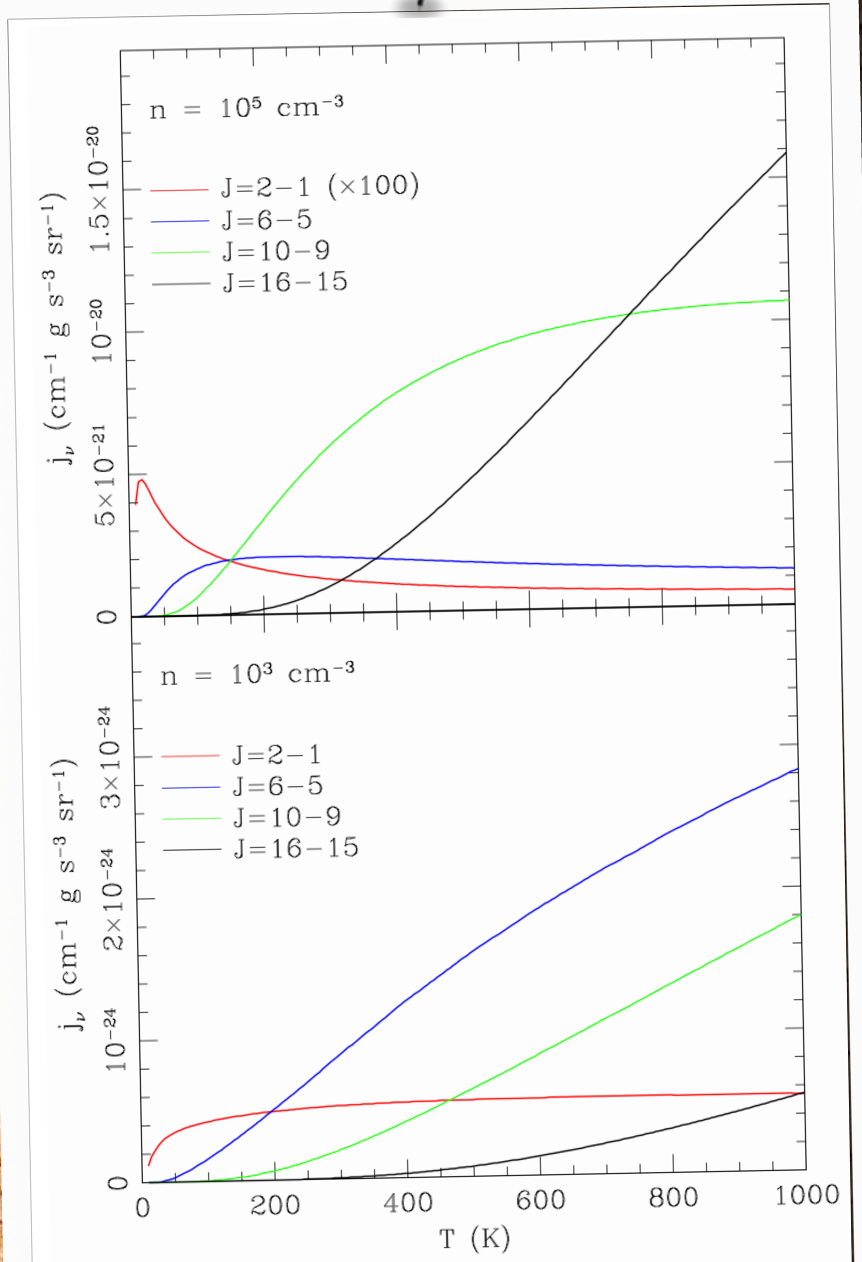
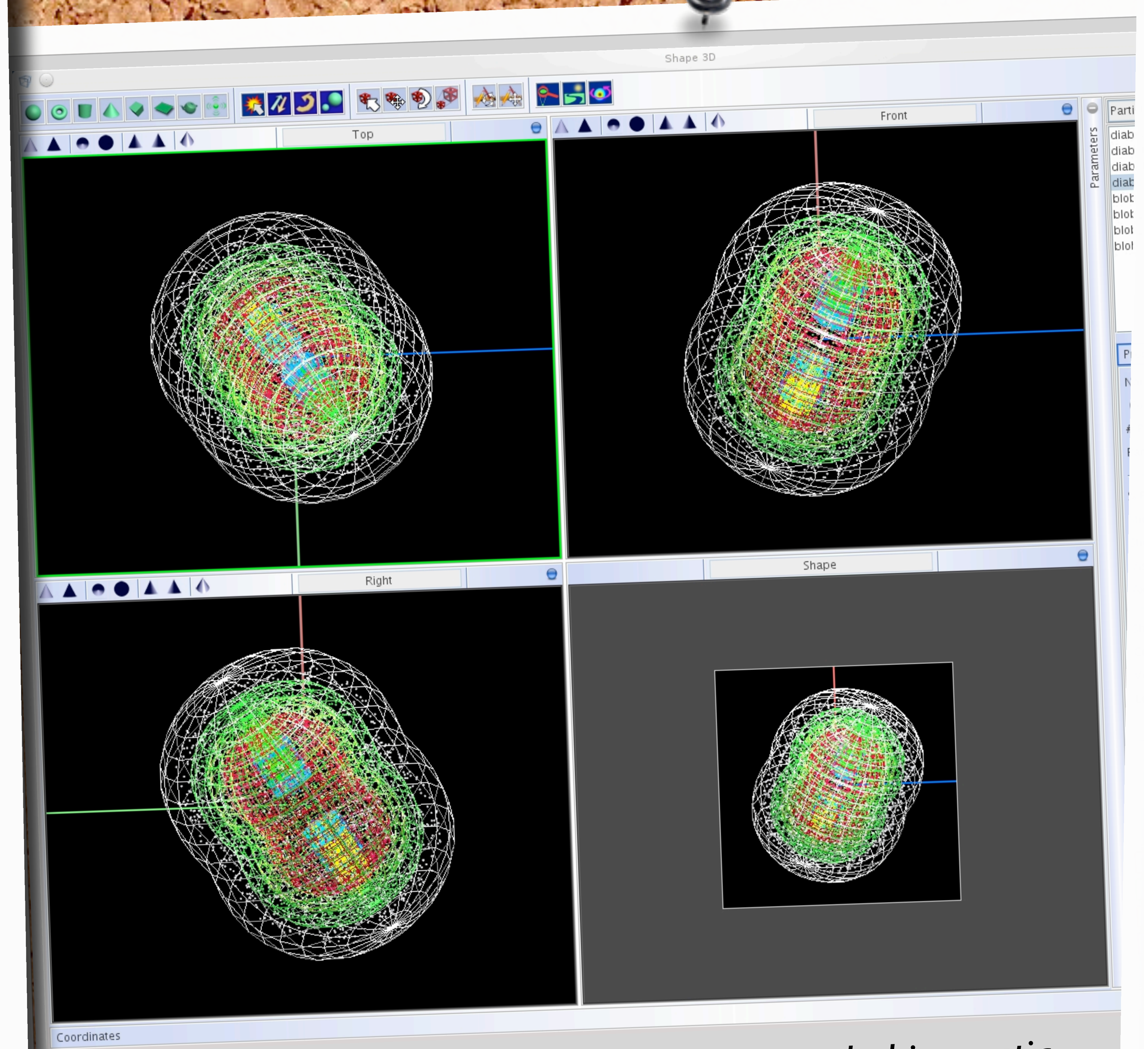
Introduction

Modern instrumentation in radioastronomy constitutes a valuable tool for studying the Universe: ALMA will reach unprecedented sensitivities and spatial resolution, while Herschel/HIFI has opened a new window (most of the sub-mm and far infrared ranges are only accessible from space) from where to probe molecular warm gas (~50-1000 K), complementing ground-based telescopes, which are essentially useless to accurately probe molecular gas with temperatures over ~100 K. On the other hand, the *SHAPE* software (*Steffen et al. 2010, IEEE Transactions on Visualization and Computer Graphics, April 2011 (vol. 17 no. 4), pp. 454-465*) has emerged in the last few years as the standard tool for determinging the morphology and velocity field of different kinds of gaseous nebulae (mainly planetary nebulae, protoplanetary nebulae and nebulae around massive stars, although it can also be applied to H II regions and molecular clouds) via spatio-kinematical modelling. Although *SHAPE* implements radiative transfer solving, it is only available for atomic species and not for molecules.

Being aware of the growing importance of the development of tools for assisting the analyses of molecular data from new era observatories, we introduce the computer code *SHAPEMOL*, a plug-in for *SHAPE* with which we intend to fill the so far empty molecular niche. *SHAPEMOL* enables spatio-kinematic modeling with accurate non-LTE calculations of line excitation and radiative transfer in molecular species. This code has been succesfully tested in the study of the excitation conditions of the molecular envelope of the young planetary nebula NGC 7027 using data from Herschel/HIFI and IRAM 30m (*Santander-García, Bujarrabal & Alcolea 2012, A&A, 545, 114*). Currently, it allows for radiative transfer solving in the ^{12}CO and ^{13}CO *J*=1-0 to *J*=17-16 lines. *SHAPEMOL*, used along *SHAPE*, allows one to easily generate synthetic maps to test against interferometric observations, as well as synthetic line profiles to match single-dish observations.



In the molecular regime, the k absorption and j emission coefficients (the latter shown for some ^{12}CO transitions) depend on the density n and temperature T in a heavily non-trivial way. Hence the need for SHAPEMOL!



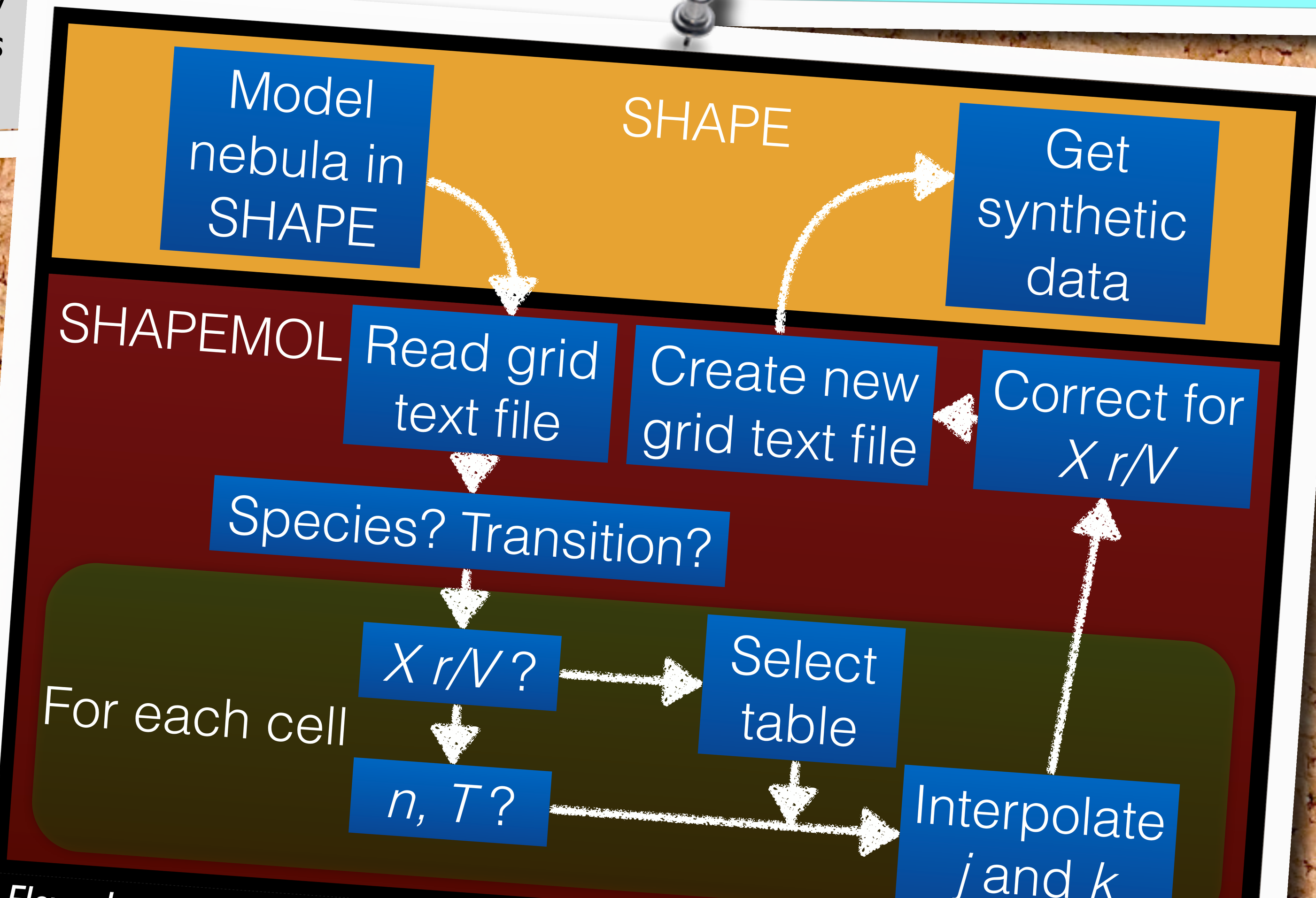
SHAPE is a user-friendly, powerful morphokinematic modelling and reconstruction tool. It allows for easy creation of synthetic images, maps and spectra of gaseous nebulae.

Modelling process: *SHAPE* and *SHAPEMOL*

We have used *SHAPE*'s version β4.51, specifically tailored for being used alongside our own *GDL/IDL*-based code, *SHAPEMOL**. A future version of *SHAPEMOL* will be fully integrated into *SHAPE*. The process is as follows:

1. We model the nebula in *SHAPE* and produce a text file with the position, velocity, density and temperature of each cell in the grid.
2. *SHAPEMOL* reads the text file. The user selects the desired molecular species and transition, the molecular abundance X and the local value of the microturbulence. *SHAPEMOL* then uses accurate non-LTE calculations of line excitation (based on the LVG approximation, e.g. *Castor 1970, A&A, 384, 603*) to compute the absorption and emission *k* and *j* coefficients of each individual cell in the grid.
3. *SHAPE* reads the text file produced by *SHAPEMOL* and performs full radiative transfer solving for the selected transition. After convolving the resulting datacube with the simulated telescope beam, it generates a 1-D spectrum to be compared directly with the observations.

***Interested in using SHAPEMOL? Contact the first author!**



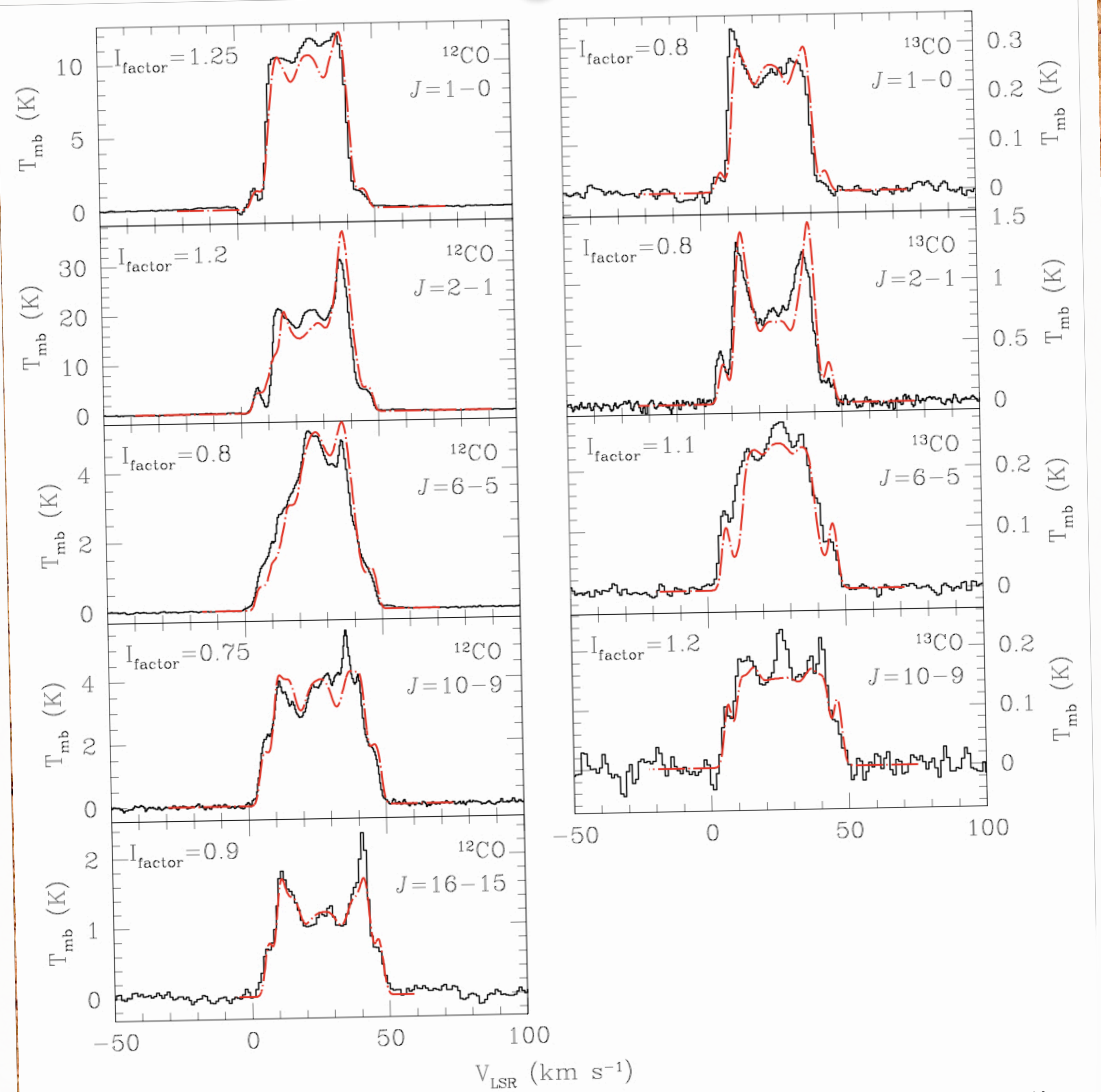
Flow chart describing the process performed by SHAPEMOL.

NGC 7027, a test case

We have built a relatively simple model of the molecular gas of NGC 7027. It consists of four nested, mildly bipolar shells with different conditions (thickness, CO abundance, constant density and temperature), and a pair of high-velocity polar blobs. Since our data lack any information on the geometry of the nebula, we have imposed similar distance, morphology and orientation to those found in other studies in low-excitation CO or H_2 (e.g. *Cox et al. 2002, A&A, 384, 603, Nakashima et al. 2010, AJ, 140, 490*). For each shell, we have assumed a velocity field composed of (a) a radial, constant component plus (b) a constant axial component which is triggered for distances to the nebular equator greater than 1 arcsec.

The resulting synthetic spectra of our model in the light of ^{12}CO *J*=1-0, 2-1, 6-5, 10-9 and 16-15 and ^{13}CO *J*=1-0, 2-1, 6-5 and 10-9 are shown here along with the observations.

The inner shell, located just beyond the photodissociation region (PDR), is rather different from the other three: its low-abundance, high-density, hot temperature (T~400K), and, furthermore, the fact that its velocity is 25% greater than the velocity of the middle and outer shells, are indicative of a front shock traveling outwards through the nebula, in a similar way as the low-velocity shock front found in CRL 618 (*Sánchez Contreras et al. 2004, ApJ, 617, 1142*, later confirmed by *Bujarrabal et al. 2010, A&A, 521, L3*), in which a bipolar cavity is expanding against the nebular halo. This shock front, along with the high-velocity blobs, is likely to have major implications on the shaping of the nebula, which is currently at work (see *Santander-García, Bujarrabal & Alcolea 2012, A&A, 545, 114*).



Resulting synthetic spectra (red) and observations (black) for 9 different ^{12}CO and ^{13}CO transitions in NGC 7027.