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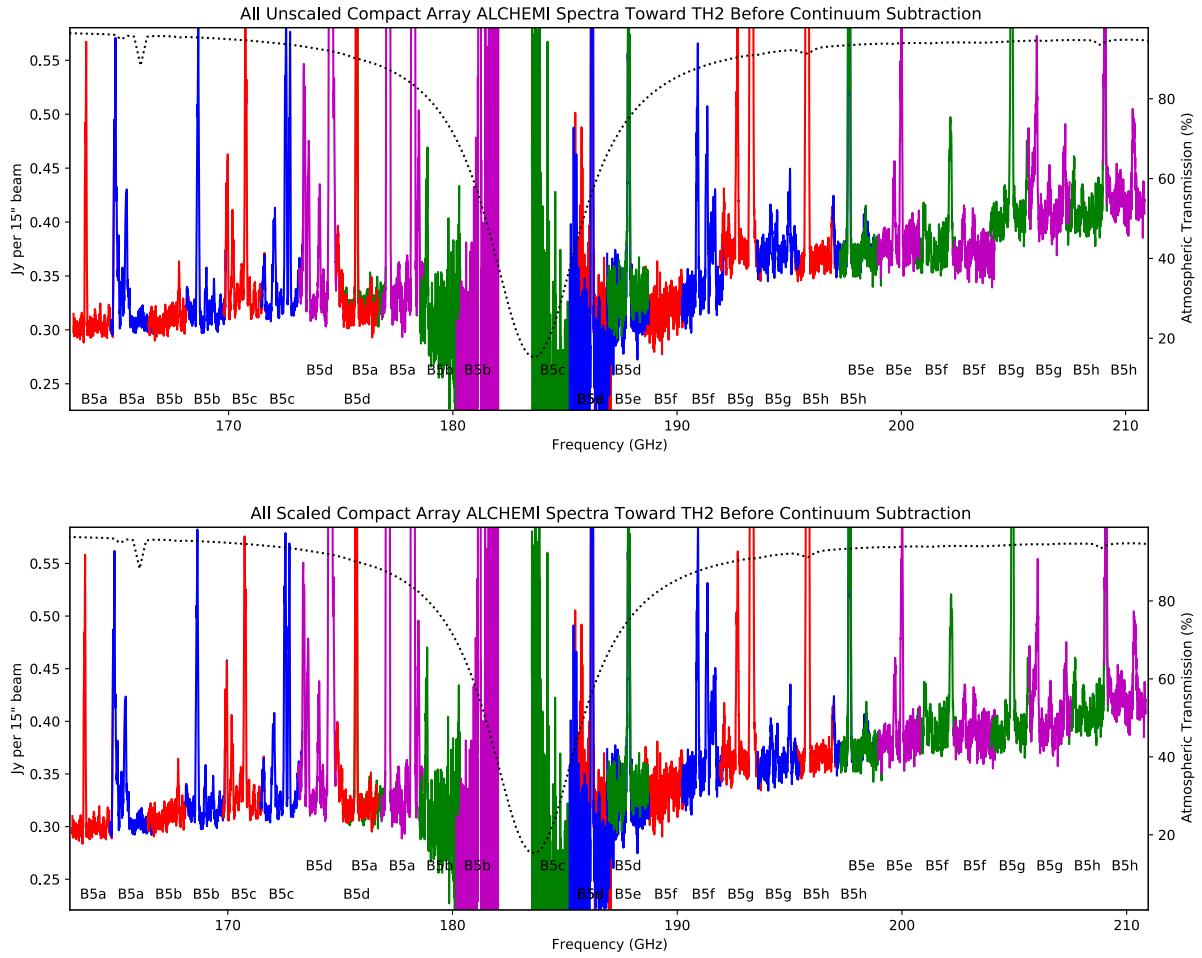


Fig. B.4. Same as Fig. B.2 but for Band 5 unscaled (top) and scaled (bottom).

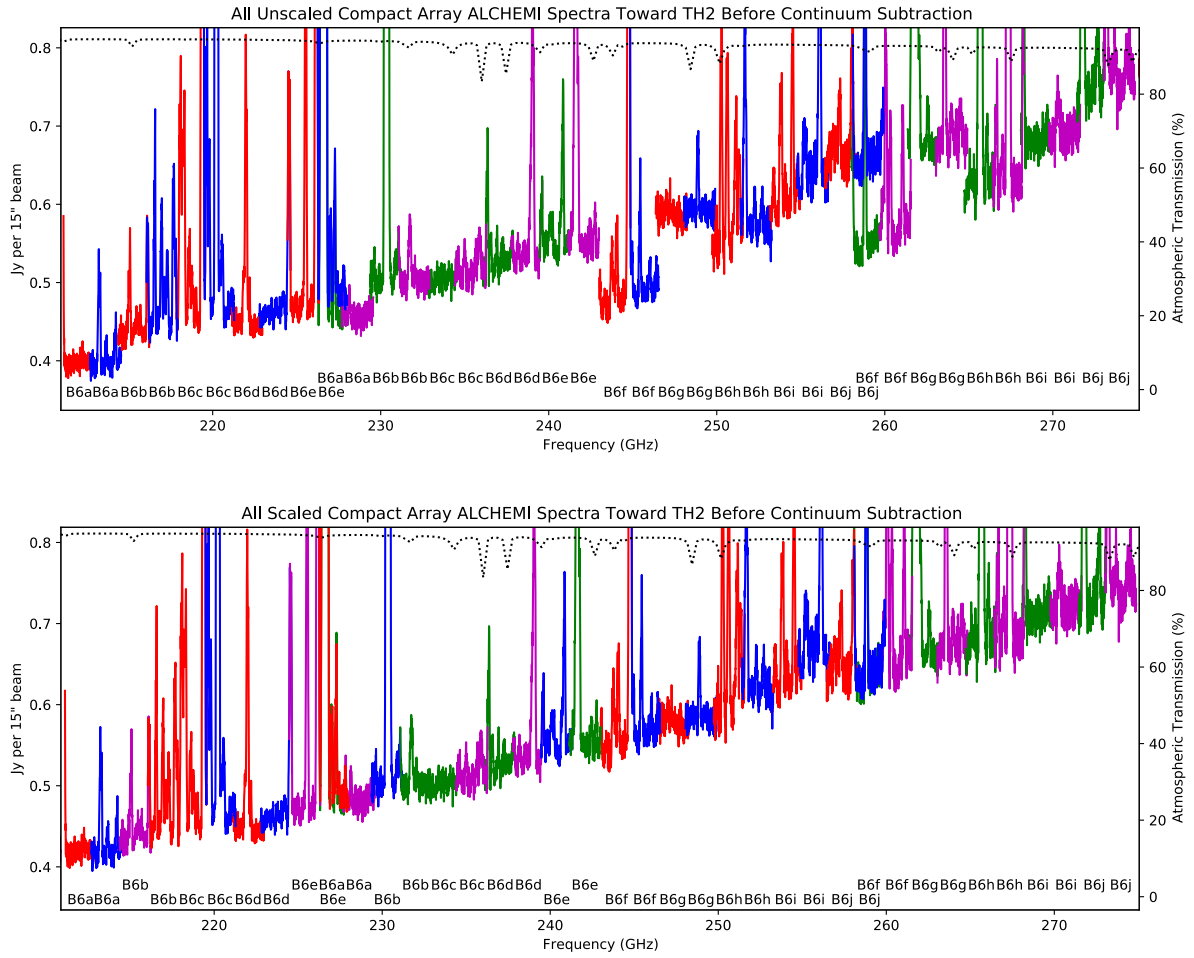


Fig. B.5. Same as Fig. B.2 but for Band 6 unscaled (top) and scaled (bottom).

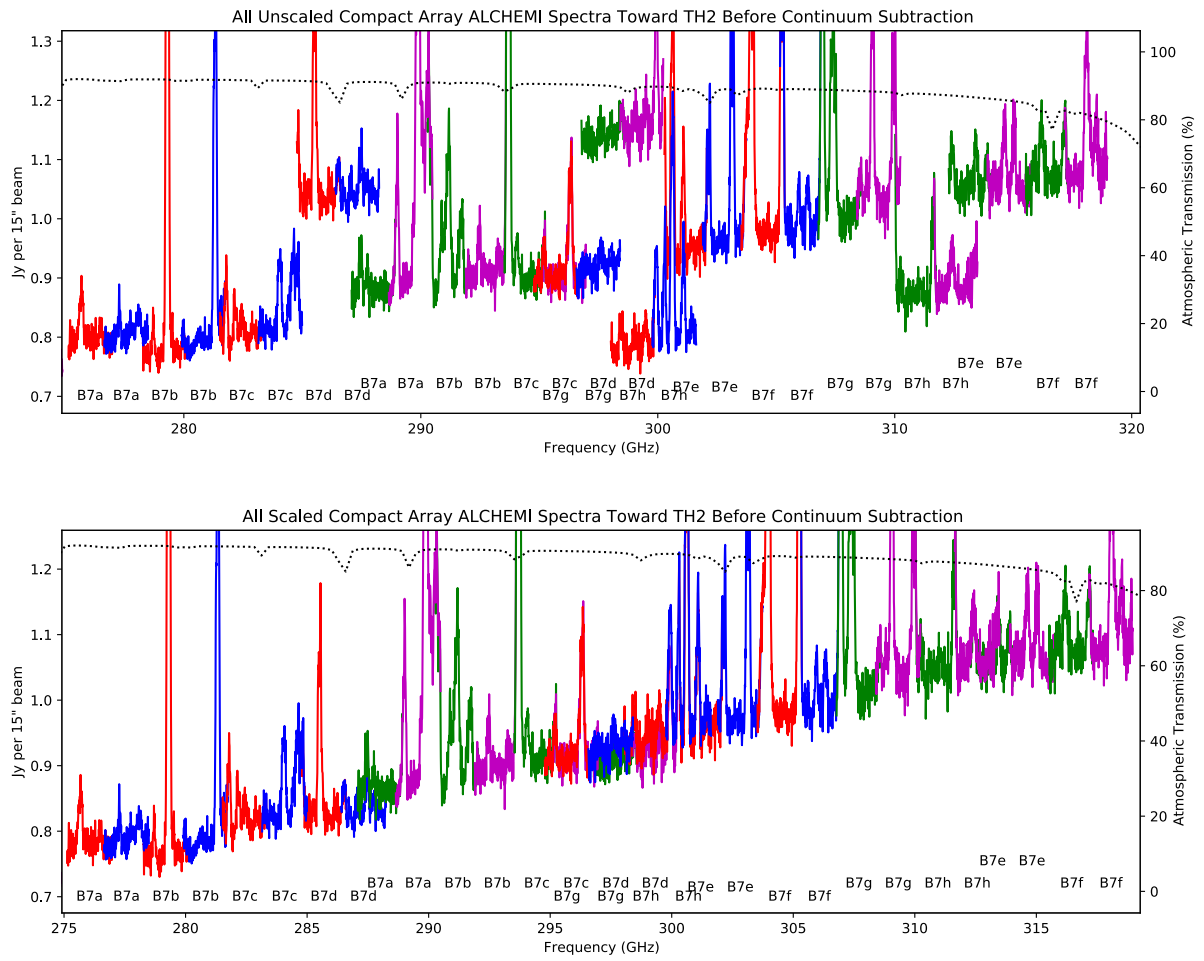


Fig. B.6. Same as Fig. B.2 but for the first-half of Band 7 unscaled (top) and scaled (bottom).

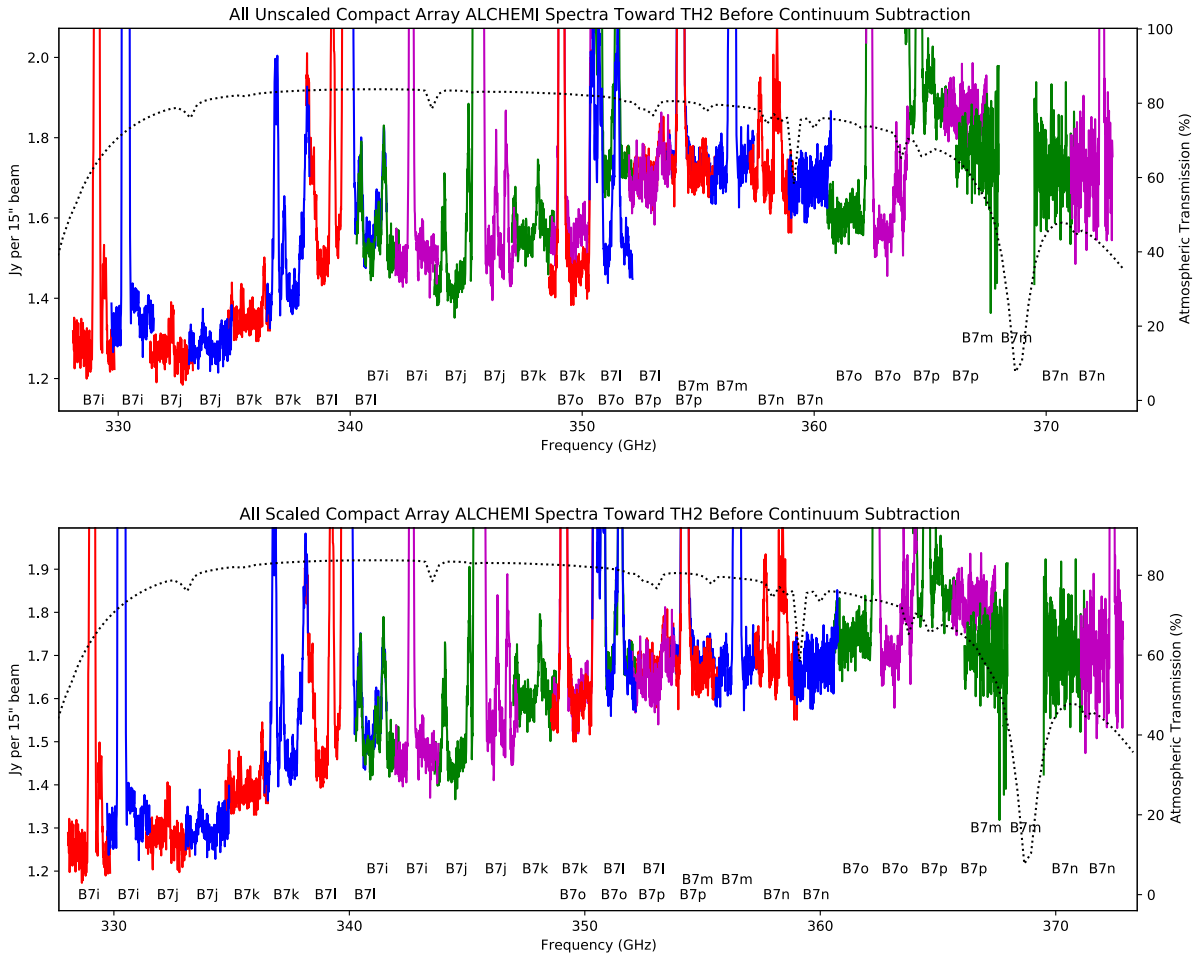


Fig. B.7. Same as Fig. B.2 but for the second half of Band 7 unscaled (top) and scaled (bottom).

Appendix C: ALCHEMI Flux Calibration

The ALMA flux calibration process includes a number of contributions to its uncertainty, including systematic errors within a given measurement calibrated with a single primary flux reference such as that due to:

1. The primary flux calibrator model used to set the absolute flux calibration scale.
2. The primary flux calibrator measurement used to define the reference point for the secondary flux calibrator flux.

as well as random uncertainties due to:

1. The bootstrapping from the primary to the secondary flux calibrator.
2. The bootstrapping from the secondary flux calibrator to the target source.
3. The lack of a proper elevation-dependent opacity correction during any of the bootstrapping steps.

Furthermore, even though extra mitigation measures can be done during an observation to account for items 4 and 5 above, there is nothing that can allow one to attain an absolute flux calibration error that is better than the error associated with the primary flux calibrator measurement and model.

Early in the process of imaging the ALCHEMI measurements, amplitude offsets between overlapping receiver tunings were noted (see Sect. 3.1 and Appendix B). The analysis of these offsets has given ALCHEMI the ability to correct for “at least one component” of the flux calibration uncertainty. This flux calibration alignment, though, does not allow for the determination of the absolute flux calibration reference. At best we have corrected the flux scales within our individual scheduling blocks to a common value. The ALCHEMI image cubes have been corrected for these flux rescaling factors, which we believe has corrected for noise introduced as part of the flux calibration process after the primary flux calibrator measurement.

In the following we address two levels of flux calibration uncertainty in the ALCHEMI data: Relative flux calibration, which represents the flux calibration uncertainty to be used when comparing fluxes within the ALCHEMI image cubes for a given set of imaging inputs (i.e., array, spatial, and spectral resolution); Absolute flux calibration, which represents the flux calibration uncertainty to be used when comparing fluxes derived from the ALCHEMI image cubes for comparison with other (non-ALCHEMI) measurements.

C.1. Relative Flux Calibration Uncertainty

The spectral flux normalization that we have applied to all ALCHEMI measurement sets has effectively normalized all ALCHEMI data to a common flux calibration scale for each array configuration⁵ measured in the ALCHEMI survey. This implies that we have normalized all ALCHEMI data measured with a given array configuration to the same relative flux calibration scale. This furthermore implies that comparison of spectral lines within the ALCHEMI survey can be compared using a relative flux calibration uncertainty.

The statistics of the amplitude scaling factors given in Table A.1 are provided in Table C.1. It is noteworthy that for our Band 3 measurements the 12mE configuration shows signif-

⁵ By array configuration we mean to differentiate among the Compact Array, either ACA (7m) or 12m Compact (12mC), the Extended Array (12m/12mE) and Combined (12m7m/12mE12mC) that were used for each spectral setup. Each of these observations consisted of a number of individual observations with slightly varying array configurations depending on the antenna availability at the time of the observation.

icant deviations from the average values of the scaling factors for that receiver band and configuration.

An estimate of the relative flux calibration uncertainty associated with a given receiver band and configuration can be derived from the scatter in the scaling factors (Table C.1) that we have applied to our measurement sets to normalize them to the same mean flux scale. The RMS values for the flux scale normalization factors for each Band and array configuration(s) (listed as Compact Array / Extended Array / Combined) are:

- Band 3: 2% / 12% / 12%
- Band 4: 1% / 2% / 2%
- Band 5: 2% / 2% / 2%
- Band 6: 5% / 1% / 5%
- Band 7: 8% / 3% / 9%

The relative flux calibration uncertainty for the ALCHEMI image cubes which are combinations of the Compact Array and Extended Array measurements will in reality be a complex combination of the relative flux calibration uncertainties, which itself depends upon the contribution of each array measurement to a given flux in the ALCHEMI survey. The contribution of each array to the combined measurement is dependent upon numerous factors such as relative visibility contributions and time-dependent variations between the individual array measurements. In the above, we conservatively estimate the relative flux calibration uncertainty for the combined values as the root-sum-square of the Compact Array and Extended Array scaling factor RMS values.

Be aware that the actual “flux uncertainty” to be used in a line-ratio analysis, for example, is not determined solely by the “flux calibration uncertainty” in complex sources such as NGC 253. The line flux one measures depends on how the imaging process (robust parameter, clean mask, clean depth, selfcal, etc.) has been performed and on the properties of the spectral line itself. The same imaging parameters can have different effects on different spectral lines. For example, when different spectral lines have distinct spatial extents or when one spectral line is bright and the other is faint because the brighter spectral line has a larger fraction of its flux cleaned. For these reasons, the real flux calibration uncertainty is likely to be larger than that assumed from an assessment of the quality of the flux calibration process alone.

C.2. Absolute Flux Calibration Uncertainty

The absolute flux calibration uncertainty starts with the relative flux calibration uncertainty and includes contributions due to the measurement, model, and application of the primary flux calibration source (see above). To estimate this additional contribution, we assume that the measurement of the relatively bright sources used as primary flux calibrators provide a negligible contribution to the primary flux calibration uncertainty. This uncertainty is then dominated by that associated with the primary flux calibrator model. Models used by ALMA within CASA are unlikely to be accurate to <5% (Butler 2012, priv. comm.). We use then the following recommendations for flux calibration accuracy, from the ALMA Proposer’s Guide for Cycle 5² (Section A.9.2 on “Flux Accuracy”), as an estimate of the primary flux calibrator model uncertainty:

- Bands 3, 4, 5: < 5%
- Bands 6, 7, 8: < 10%
- Bands 9 and 10: < 20%

The absolute flux calibration uncertainty, including the relative flux calibration uncertainty derived for the ALCHEMI image cubes, is given by the root-sum-squared of the relative

Table C.1. Statistics by bands and arrays of the relative flux scaling factors (a_i)

Band	Array	N_{obs}^a	Average \bar{a}_i	RMS σ_{a_i} (%)	$\min(a_i) / \max(a_i)$	$\max(a_i) - \min(a_i)$ (%)
B3	12mC	6	0.989	2.4	0.937 / 1.009	7
B3	12mE	6	1.000	12.4	0.789 / 1.123	34
B4	7m	7	1.000	1.3	0.980 / 1.021	4
B4	12m	7	1.000	1.7	0.968 / 1.026	6
B5	7m	8	1.000	2.3	0.955 / 1.033	8
B5 ^b	12m	8	0.911	2.3	0.856 / 1.147	29
B6	7m	10	0.974	4.7	0.867 / 1.027	16
B6	12m	10	1.003	1.2	0.990 / 1.034	4
B7	7m	16	1.006	8.1	0.833 / 1.257	42
B7	12m	16	1.001	2.5	0.956 / 1.044	9

Notes. ^(a)Total number of scheduling block measurements included in the subsequent statistics shown. ^(b)Excludes 12m Array SB B5f as the scaling factor for this SB appears to include amplitude calibration errors inherent in the delivered calibrated data products.

and primary flux standard model calibration uncertainties (listed as in Sect. C.1):

- Band 3: 5% / 13% / 13%
- Band 4: 5% / 5% / 5%
- Band 5: 5% / 5% / 5%
- Band 6: 11% / 10% / 11%
- Band 7: 13% / 10% / 13%

Therefore, for the sake of simplicity, we recommend the usage of a conservative 15% uncertainty for the absolute flux calibration within the ALCHEMI image cubes, at any frequency and configuration.

C.3. A Search for the ALCHEMI Flux Normalization Anomalies

We find that 11 of the 47 tunings (~23%) which comprise the ALCHEMI data set have amplitude scale factors which are larger than the ALMA amplitude calibration specification of 5%, with the two most discrepant tunings being 26% (Band 7) and 21% (Band 3). Table C.2 lists the measurement information for the 11 discrepant tunings.

In an attempt to determine the source(s) of the thirteen science goals with poor amplitude calibration, we have investigated how ALMA calibrates amplitude within the limits of the information provided to investigators. ALMA flux calibration is made within a given observation (or “execution block”) by measurement of a standard quasar selected from a list of monitored quasars, referred to as the “grid sources”. ALMA strives to measure these standard quasars at least once every 14 days at bands 3 and 7, and calibrates their fluxes to an absolute scale through reference measurements of primary flux calibrators (i.e., Uranus). The measured absolute fluxes for the grid source calibrators are available from the [ALMA calibrator archive](#). We have extracted the flux scaling information from the calibration pipeline weblog file “flux.csv” associated with each observing execution block (EB). This flux scaling information includes the “spectral index age” and time since the standardized flux for each calibrator was derived.

C.3.1. Possible Source of Error: Large Spectral Index Age (spixAge)

As the spectral index age (spixAge) is one of the factors used by [getALMAFlux](#) to extrapolate measured flux calibrator fluxes to

target frequencies, there was a concern that perhaps large spixAge factors were causing the large flux calibration errors. Using the spectral index age information extracted from the pipeline calibration process we show the correlation between spectral index age and amplitude scale factor in Figure C.1. There is no correlation between spixAge and the amount of the flux calibration error.

C.3.2. Possible Source of Error: Calibrator Catalog Band 3 Age

By inspecting the age of the absolutely calibrated Band 3 flux used by [getALMAFlux](#) (extracted from the flux.csv files associated with the pipeline calibration process), we find that there is no apparent correlation between the “Age”/“Band3Age” and large amplitude scaling factors. The “Age” or “Band3Age” is in almost all cases between 0 and 3 days for our most discrepant scale factor EBs. In one case it was 6 days, and another was 5 days, but neither of these were from our “worst cases”. Band 3 age does not appear to be a likely source for the discrepant amplitude scale factors.

C.3.3. Possible Source of Error: Flux Monitoring Time Gaps

Many, though not all, of the science goals (SGs) with discrepant amplitude scale factors occur just after a gap in the respective flux calibrator measurements. Specifically, for 8 of the 13 discrepant Band 3 SGs, there was a significant flux calibrator measurement time gap just before these SGs were observed, and this correlation between flux calibrator measurement time gap and discrepant scale factor does not exist for Band 6 (green) or Band 7 (black) SGs with discrepant amplitude scale factors. Although this may be an explanation for the excessive Band 3 flux calibration uncertainties, a time gap in the flux monitoring for our flux calibrators does not appear to be consistent for all SGs with discrepant flux calibration.

C.3.4. Possible Source of Error: Large Time Span Between System Temperature Measurements

By perusing the weblogs associated with the ALCHEMI measurements we know that the scaling from raw amplitude to a temperature scale (otherwise known as the “system temperature” measurement), was routinely made only every ~11 minutes

Table C.2. ALCHEMI tunings with discrepant amplitude calibration

SG ^a	Array	Flux Calibrators	SpixAge ^b	$100 \times \frac{\sigma_{gain}}{S_{gain}}$ ^c	a_i ^d
B7d	7m	J2258–2758,J0006–0623,J0522–3627	(3,-4,20),(-4,20),20	9.98	1.257
B3b	12mE	J2258–2758	142,144	0.86	0.789
B7h	7m	J2258–2758,J2253+1608,J0522–3627	(3,4),25,4	9.87	0.833
B6f	7m	J2253+1608	-1,0,6	1.98	0.867
B3d	12mE	J0006–0623	7	1.57	1.128
B3a	12mE	J0006–0623	-5,4	0.05,0.68	1.108
B3c	12mE	J0006–0623	-3,-6,0,1	0.48	1.107
B7o	7m	J2253+1608,J0522–3627	(7,0,2,3),2	2.06	0.922
B3f	12mE	J2258–2758,J2357–5311,J0006–0623	-27,-22,4	1.84	0.922
B6h	7m	J2258–2758	5,-3,0,-2	3.71,1.03,1.20,4.30	0.924
B3a	12mC	J0006–0623	23,27	0.24	0.937

Notes. ^(a)Refers to Science Goals within ALMA project nomenclature. ^(b)Number of days since the most recent ALMA-derived spectral index for a given calibrator. Multiple executions which used a given calibrator are grouped within parentheses. Negative values indicate spectral indices derived before a given calibrator measurement. Calibrator spectral indices are derived using measured Band 3 and Band 6 or Band 7 fluxes. ^(c)Normalized gain calibrator flux uncertainty averaged over all gain calibrator measurements for observation dates within five days. Multiple entries indicate multiple observation time ranges. Target for all gain calibration measurements was J0038–2459. ^(d)Amplitude scale factors are applied to the data as indicated by Equation 3.

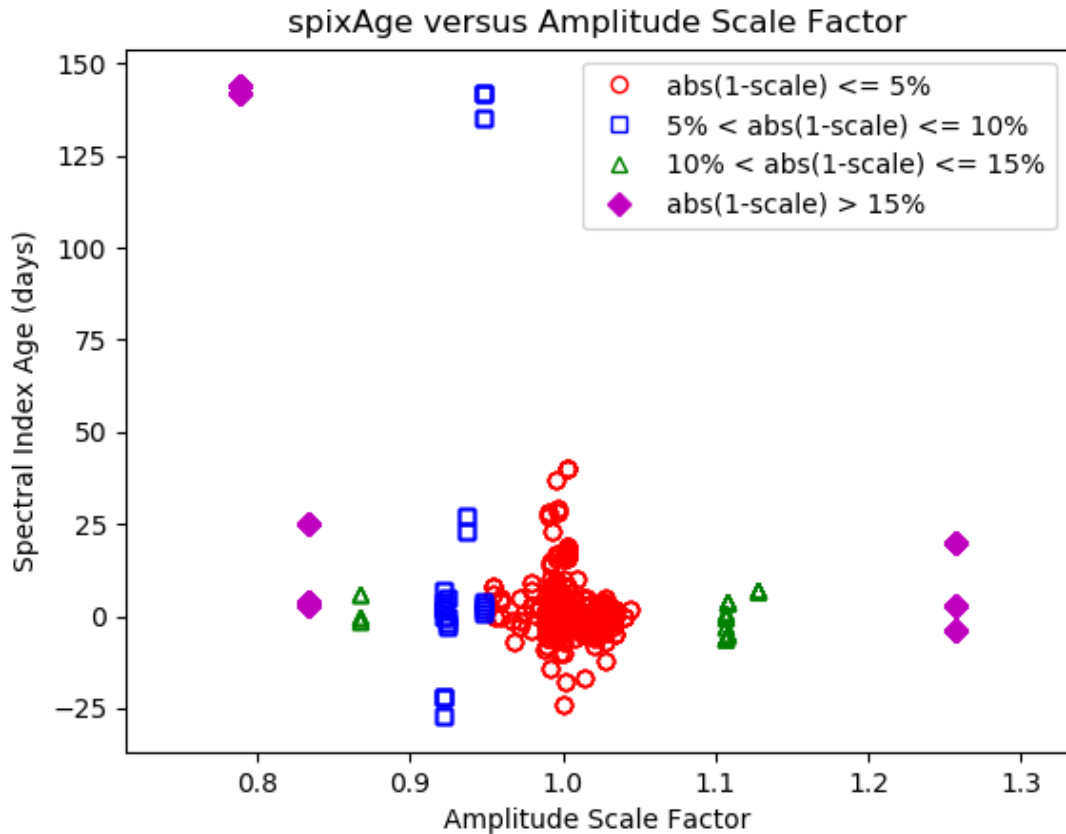


Fig. C.1. Correlation between spectral index age and amplitude scale factor for all ALCHEMI measurements. Coloring is used to designate ranges of amplitude scaling.

at Band 3 and every ~8 minutes at Band 7. As these system temperature measurements are required to track the changes in sky emission as a function of time, it could be that these basic amplitude scaling factors have not been sampled well enough in time, especially at the higher frequency bands. However this is an observatory trade-off between enhanced calibration accuracy and observing efficiency.

C.3.5. Possible Source of Error: Noisy Gain Calibrator Measurement

For the SG with the most discrepant flux calibration, B7d 7m (ngc253_d_07_7M) there may be an issue with gain calibrator phase stability. Three out of five execution blocks (EBs) for the scheduling block (SB) were taken on the same day

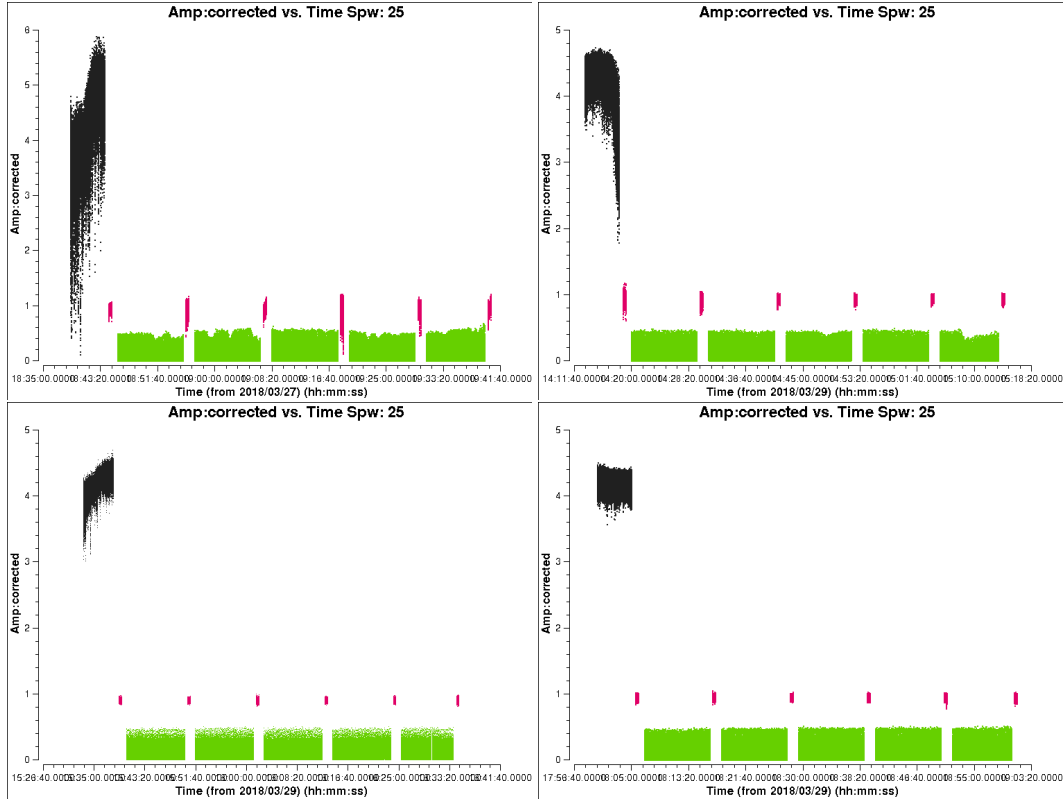


Fig. C.2. B3b 7m amplitude/bandpass calibrator flux versus time weblog plots for the four EBs in this SB.

(2018-01-21). J0038–2459 was observed as the gain calibrator for all the three EBs. Although the gain calibrator flux is expected to be stable over the three EBs, because the flux is very likely to be stable over the short time scale between these three EBs (about six hours), the derived flux densities in the pipeline calibration changed about 28% (peak-to-peak). The following is a summary of the pipeline-derived flux densities of the phase calibrator (reference: the weblog, stage 15).

# EB	start date/time (UT)	flux density (spw 16)
uid___A002_Xc96f17_X8658	2018-01-21 19:06:14	1024.0+-9.979 mJy
uid___A002_Xc96f17_X8ec1	2018-01-21 22:17:40	855.121+-12.804 mJy
uid___A002_Xc96f17_X92b9	2018-01-21 23:53:08	797.500+-5.496 mJy

It is possible that poor atmospheric phase stability is the cause of the large flux calibration uncertainty, as all the EBs were taken in the late afternoon to early evening, which is the part of the day when the atmospheric phase stability tends to be very the poorest. In fact, in the calibrated visibility amplitude vs time plot of the EB (weblog stage 17) one can see frequent amplitude drops in the Bandpass/Flux calibrator scan.

Another example of a correlation between poor phase stability and poor flux calibration is B3b 12mE (ngc253_b_03_TM1). As was the case for B7d 7m, the EBs for this SB were also affected by large phase fluctuations, and that they were also executed in daytime (late afternoon). Figure C.2 shows the pipeline plots of amplitude vs time for all the EBs for B3b 7m. Significant amplitude drops in the bandpass/amplitude calibrator (J2258–2758) can be seen especially

in EB uid___A002_Xcb1740_X94c9, and they could affect the flux scaling of the gain calibrator.

The following is a summary of the pipeline-derived flux density of gain calibrator J0038–2459 (reference: the weblog, stage 15).

spw=25	uid___A002_Xcb1740_X94c9	2018-03-27 18:36:03	955.851+-14.748 mJy
	uid___A002_Xcb339b_X600b	2018-03-29 14:10:14	938.721+-7.809 mJy
	uid___A002_Xcb339b_X633f	2018-03-29 15:30:21	903.452+-9.069 mJy
	uid___A002_Xcb339b_X68ab	2018-03-29 17:57:08	941.212+-1.904 mJy

The change of delivered flux density looks relatively large (5.8% in peak-to-peak) even though the EBs were taken within three days. This could be an explanation for the discrepant flux calibration (second worst of all SGs) for this SG.

In order to assess the effect of a large gain calibrator flux uncertainties on the derivation of our flux calibration uncertainty for all of the ALCHEMI SGs, we have extracted all derived gain calibrator fluxes and uncertainties from the ALCHEMI weblogs. We have derived a normalized gain calibration error for each SG by doing the following: Firstly, we calculate the weighted uncertainty (σ_{gain}) for all gain calibrator measurements; Secondly, we average normalized gain calibrator uncertainties ($\frac{\sigma_{gain}}{S_{gain}}$) over all spectral windows and measurements taken within 5 days of each other. This time window is expected to be shorter than any changes in the absolute flux of the gain calibrator; Finally, by using a normalized gain calibrator uncertainty, we are attempting to smooth-out any changes in gain calibrator flux measurement uncertainty due to differences in gain calibrator integration time.

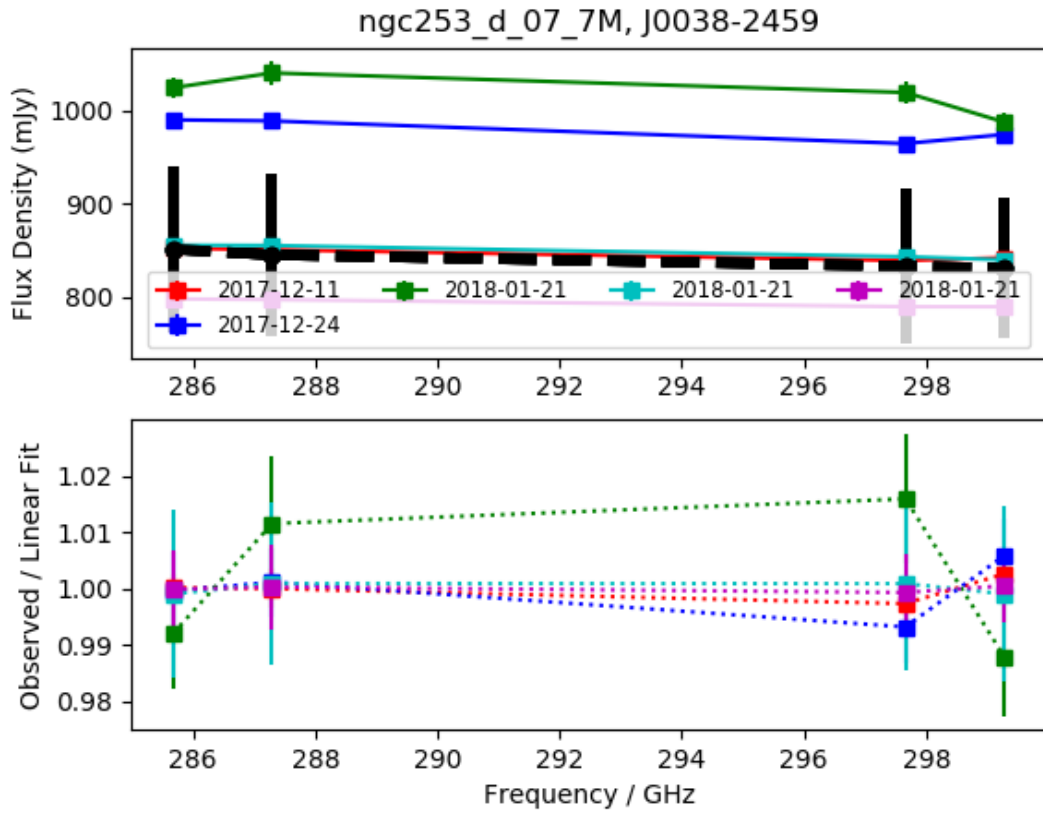


Fig. C.3. Sample gain calibration results for all EBs associated with B7d 7m. The bottom panel shows the residual from a linear fit for each measurement date to the measured flux densities displayed in the top panel.

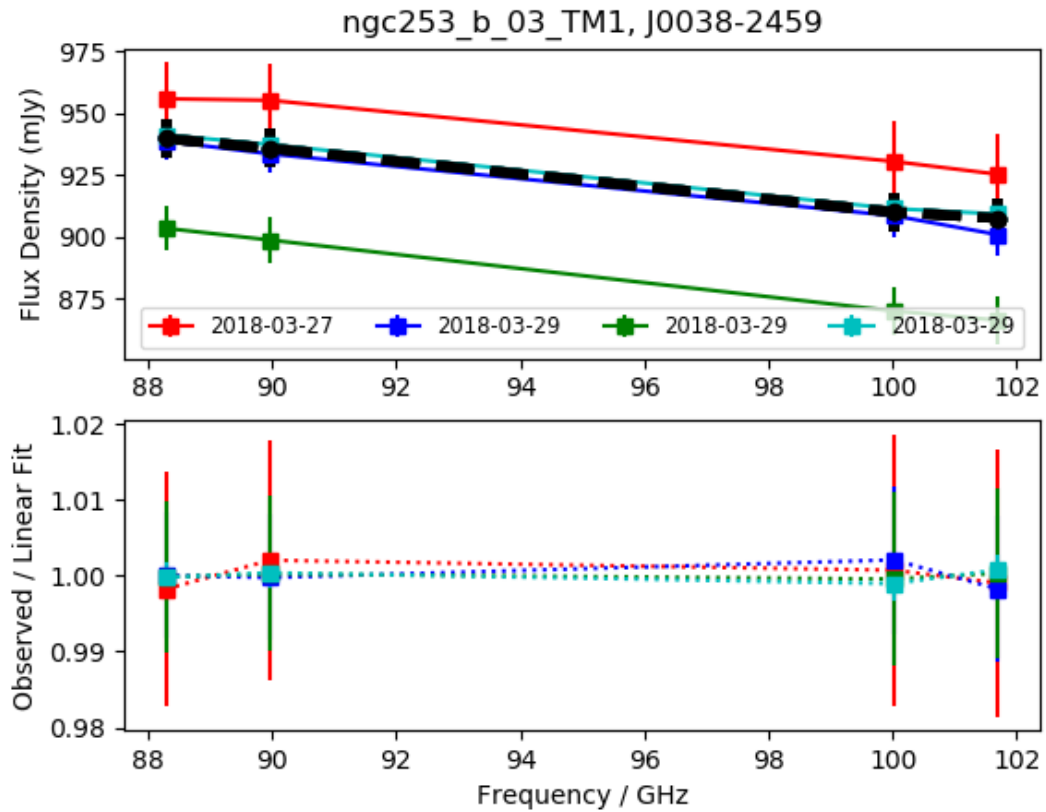


Fig. C.4. Sample gain calibration results for all EBs associated with B3b TM1. Same diagram style as used in Figure C.3.

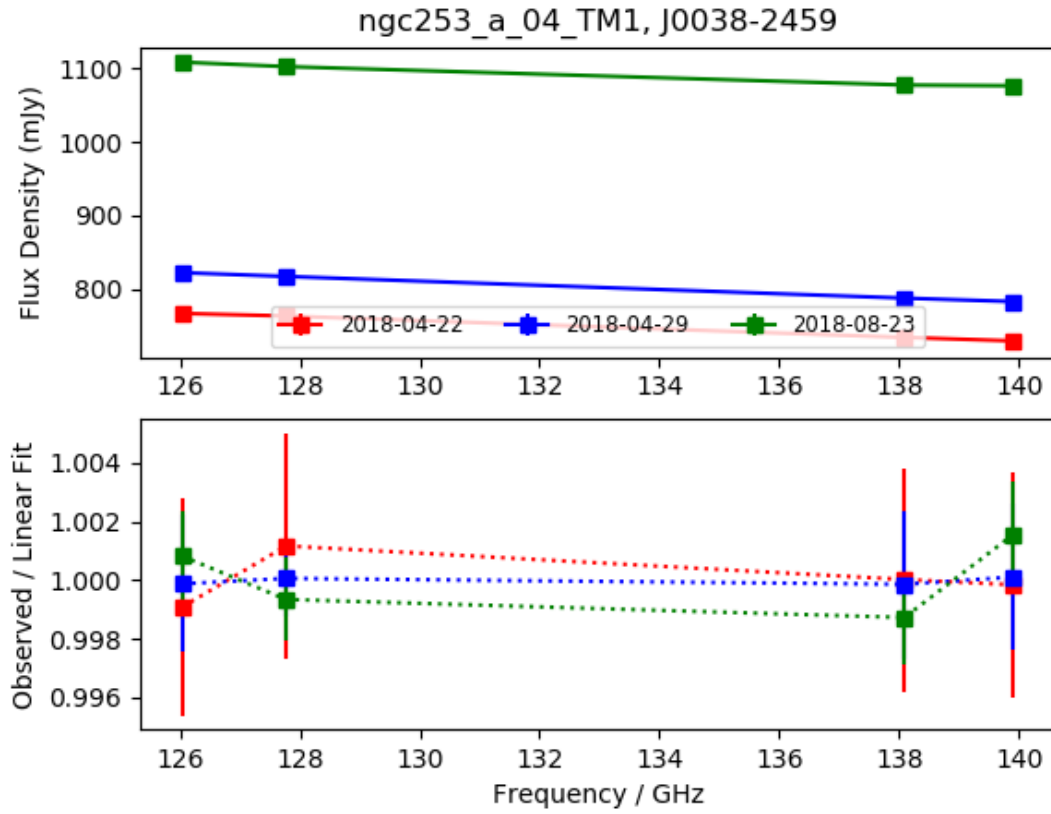


Fig. C.5. Sample gain calibration results for all EBs associated with B4a TM1. Same diagram style as used in Figure C.3.

Figures C.3, C.4, and C.5 show examples of gain calibrator measurements, with weighted uncertainties, and their associated weighted average as a function of frequency. Figure C.6 shows the correlation between normalized gain calibrator standard deviation (as a percentage) versus the associated amplitude calibration scale factor (calculated as a difference from a perfect amplitude scale factor of 1.0). Even though in a few cases large normalized gain calibration errors are associated with large amplitude scale factors, there is no systematic correlation between these measures.

C.4. Conclusion to Search for ALCHEMI Flux Normalization Anomalies

In Sections C.3.1 through C.3.5 we have investigated the possible sources of the discrepant flux calibration uncertainties derived for 13 of the ALCHEMI SBs. We find that with the exception of possible errors in T_{sys} measurement, which we are unable to properly analyze, none of the above potential sources of error appear to explain all of our discrepant amplitude calibration.

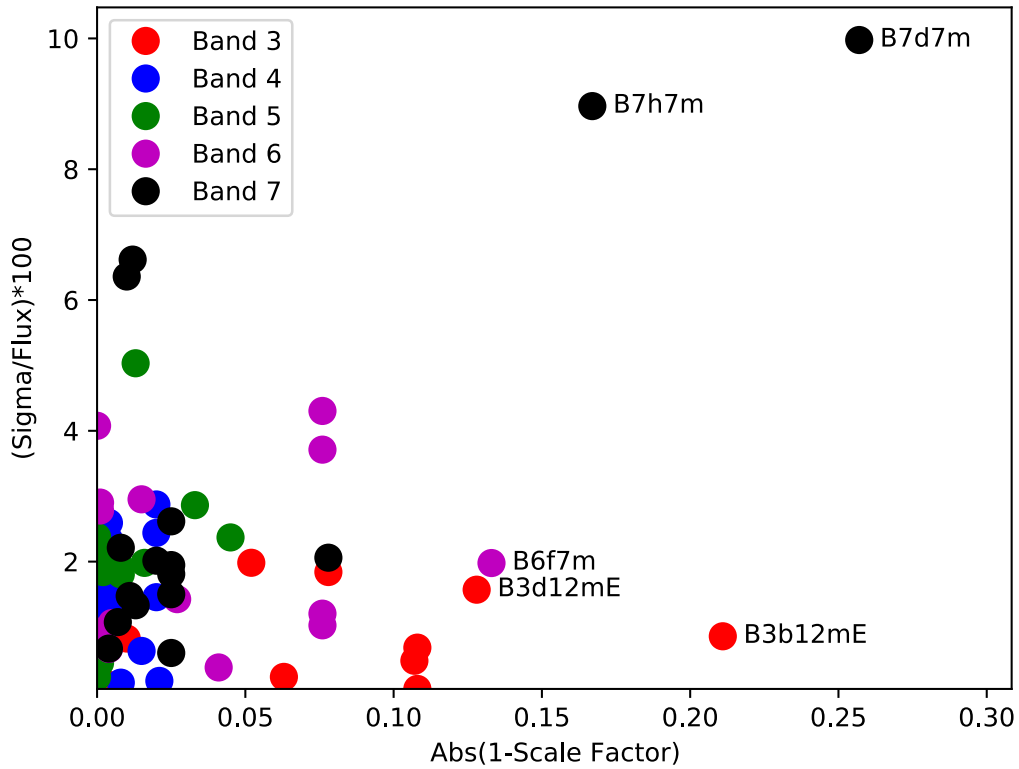


Fig. C.6. Correlation between normalized gain calibrator standard deviation (as a percentage) versus the associated amplitude calibration scale factor (calculated as a difference from a perfect amplitude scale factor of 1.0). Tunings with larger than 12% scale factors are annotated. See above description for calculation details.

Appendix D: Fitting details of individual species

Sect. 4.3.2 provided details on the procedure used to fit the modeled synthetic spectra to the low resolution ACA observations. In summary, the procedure consists on a human-supervised automatic fit, where the only intervention aims at ensuring convergence of the fit. Additional criteria used for the newly detected species (Sect. 4.4) are provided below in Sect. D.1. Thus, parameters were fixed or transitions were masked in the fit when convergence could not be achieved. The results are reported in Table. A.3. Here we note that in some cases, the large uncertainty in the fit to the temperature resulted in column density errors of the same order as the value fitted. Such is the case of H^{13}CN , despite being a clear detection with bright features, extra masking and fixing of the temperature was required to provide a reasonably narrow error on the column density (with only marginal change in the fitted column density value). However in most cases we decided to maintain such fits for the sake of consistency with the procedure applied to all species.

Although we know from previous studies that there is evidence for the presence of multiple components with different excitation temperatures (Aladro et al. 2011b), there are no really obvious deviations from the LTE fit. As an example the higher energy transitions of HC_3N appear to be underestimated, which could support the presence of a higher temperature component. Similarly H_2CO is not that well fitted under LTE, showing flat topped spectral features. For the sake of simplicity in the presentation of these data, we assumed a single LTE component for all species. A detailed analysis of the excitation of some of these species will be presented in future publications which will make use of the higher resolution ALCHEMI 12m Array data.

For the sake of completeness, a list of all transitions above a peak flux density of 15 mJy are presented in Table D.1. We note that these intensities correspond to those of the model fit to the observed spectra, and therefore parameters of velocity and width are those corresponding to the species as presented in Table A.3. As indicated in Sect. 4.3.2, no measurement or analysis of individual spectral features has been performed. For the reasons presented there, analysis has been performed per molecular species.

Below we provide some cases of transitions significantly deviating from LTE together with other special details on the fitting of individual species.

H_3O^+ : The fit to H_3O^+ emission has been performed only on the 307.2 GHz transition, which is one of the two transitions covered by our survey. Although the 307.2 GHz is blended with CH_3OH , this contribution is accounted for based on the CH_3OH fit to the whole survey. The 364.8 GHz transition, on the other hand, is the most obvious case of non-LTE emission, and is observed to be more than an order of magnitude brighter than predicted by LTE (Fig. F.11) The line ratio between these two transitions has been calculated based on the individual integrated intensity fit to each transition and not on the LTE intensities in Table. D.1. To explain the relatively large observed flux density ratio of $S_{364.8}/S_{307.2} = 6.8 \pm 1.0$ between the two transitions, non-LTE models from Phillips et al. (1992) suggest volume densities $< 10^7 \text{cm}^{-3}$ and effective excitation by dust emission. Together with the vibrational emission reported in Sect. 5.2, H_3O^+ is also probing the importance of infrared pumping in NGC 253 GMCs. However, the 396 GHz transition of H_3O^+ , not covered in our survey, is key to constrain the non-LTE physical conditions of the emitting gas. All other species below that show transitions not well fitted by the LTE approximations, are not as extreme as the case of H_3O^+ where, as mentioned

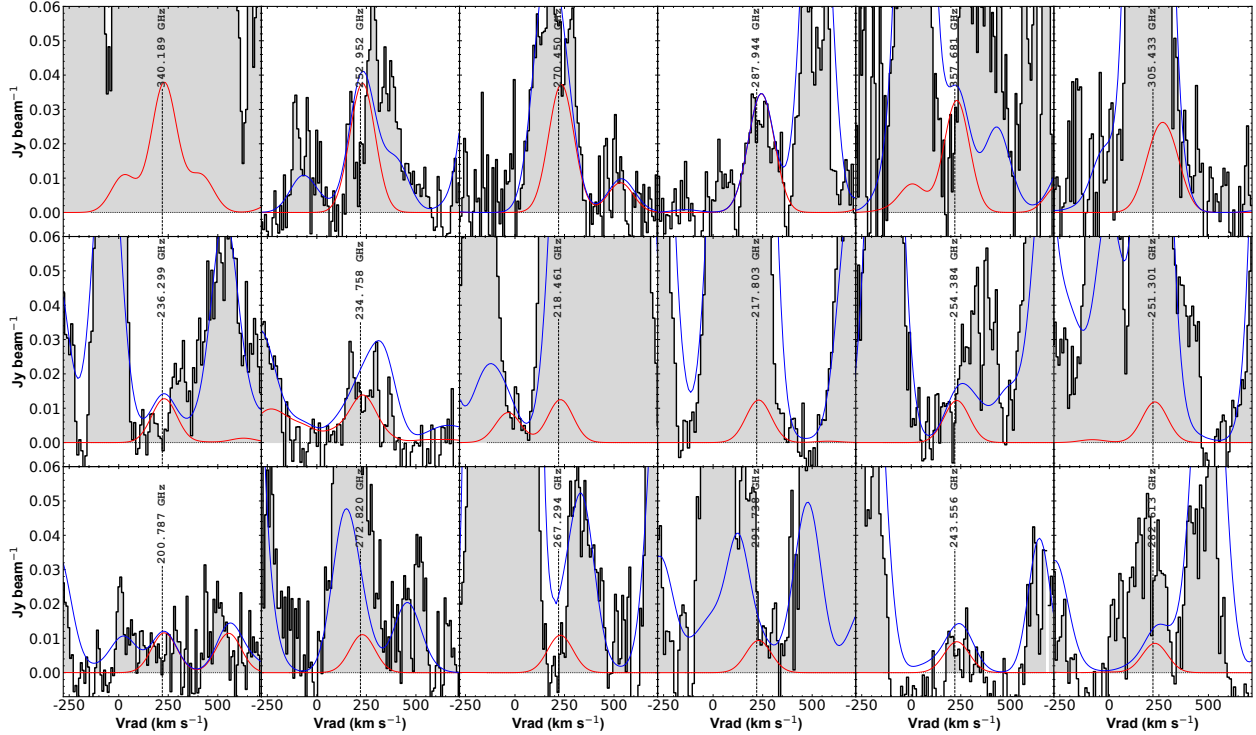


Fig. D.1. Modeled emission of $\text{C}_2\text{H}_5\text{OH}$ in red, overlaid over the observed spectrum (filled black histogram) and the global model including all molecular transitions in this study. Only the 18 brightest transitions or group of transitions according to the LTE model of $\text{C}_2\text{H}_5\text{OH}$ are displayed, ordered in descending order of brightness from left to right and top to bottom. The model generated with MADCUBA makes use of the spectroscopic parameters in JPL catalog entry 46004. The frequency of the brightest transition in each panel are displayed for reference.

above, the LTE approximation is underestimating the 364.8 GHz by more than an order of magnitude.

H_2S : The transition of H_2S at 216.71 GHz is approximately two times brighter than predicted by the LTE fit.

H_2CO : The transitions at 140.83 and 150.48 GHz are twice as bright as predicted by the LTE fit. A number of other transitions also deviate from the fit, but to a lesser extent. We note that we did not fit the ortho- and para- H_2CO separately, but we assumed the ortho-to-para ratio of 3.

HC_3N : All transitions above 270 GHz are brighter than the LTE fit estimate. This could be the signature of a warmer component and partially to the effect of varying opacity across the transitions.

HNCO : The brighter transitions of HNCO show an obvious double peak profile which is likely due to the distribution of this species at high resolution (Meier et al. 2015). This double peak profile, similarly observed in CH_3OH , is more apparent than in other species where the velocity components are more blended and the profile is a single peak. On the other hand, many of the fainter transitions of HNCO are overestimated by the LTE fit.

$\text{CH}_3^{13}\text{CCH}$: Despite being almost uniformly blended with other species, the fit of $\text{CH}_3^{13}\text{CCH}$ is consistent within the errors to that of the other two isotopologues, being ~ 0.1 dex above $\text{CH}_3\text{C}^{13}\text{CH}$ and ~ 0.4 dex above $^{13}\text{CH}_3\text{CCH}$. Although the uncertainties in the column density determination of the latter two isotopologues are of the same order as the value fitted, an independent fit to the three isotopologues are in good agreement, which supports the detection and fit to those species. Moreover, the ratio to the main isotopologue (Table 4) is consistent with what is observed with other species as discussed in Sect. 5.4.1).

CH_3OH : Two of the transitions of methanol, the $1_{1,0}-2_{0,2}$ at 205.79 GHz and $7_{1,7}-6_{1,6}$ at 335.58 GHz, show observed fluxes which are less than half of the LTE fit flux, while the $6_{1,5}-5_{1,4}$ at 292.7 GHz transition is about half of the LTE fit flux. Similar to what is observed in HNCO , the brighter transitions show a very clear double peak profile.

$^{13}\text{CH}_3\text{OH}$: There is only one transition of $^{13}\text{CH}_3\text{OH}$ which is bright enough and is not blended with other species. Therefore this is the only species in which the fit value should be considered with caution and probably an upper limit. This LTE fit has been discussed in Sect. 5.4.1.

CH_3CN : The $J = 7-6$ and $8-7$ groups of transitions at 128.7 and 147.1 GHz, respectively, show significantly brighter emission than that from the LTE fit, being up to a factor of two brighter on the former.

CH_2NH : While the $3_{1,1}-1_{0,1}$ transition at 166.85 GHz is not detected, though predicted by the LTE fit, the $2_{0,2}-1_{0,1}$ transition at 127.85 GHz is brighter than predicted.

D.1. Fitting details of newly detected species

On top of the fit criteria explained in Sect. 4.3.2 on detection of the brightest spectral features and requiring convergence of the fit, we enforced extra criteria to claim newly detected species. This is, at least one of the brightest (according to the LTE prediction) spectral features needs to be un-blended or marginally contaminated by emission from other species based on the LTE modeling to other transitions from the contaminant species. More importantly, all other blended transitions should be consistent with the residual spectra after subtraction of all other modeled species. In other words, any bright emission line predicted

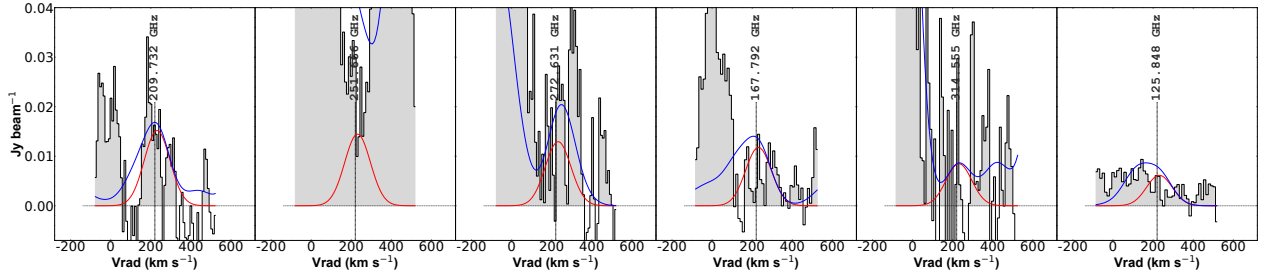


Fig. D.2. Same as Fig. D.1 showing the model of HOCN, using the spectroscopic parameters in CDMS catalog entry 43510.

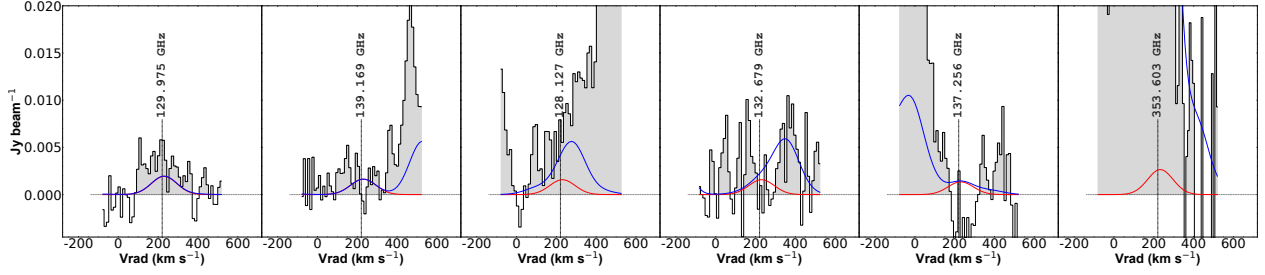


Fig. D.3. Same as Fig. D.1 showing the model of HC₃HO, using the spectroscopic parameters in JPL catalog entry 54007.

Table D.1. Intensities from the 744 transitions with > 15 mJy from the LTE model fit to the data

Formula	ν (GHz)	S (mJy)	Formula	ν (GHz)	S (mJy)	Formula	ν (GHz)	S (mJy)	Formula	ν (GHz)	S (mJy)
H β	126.794	24	HNCO	198.529	22	H α	256.302	86	He α	316.544	32
HC ₃ N	127.368	213	HNCO	198.529	25	CH ₃ C ₂ H	256.317	71	CH ₂ NH	317.405	64
CH ₃ CN	128.779	29	HNCO	198.529	28	CH ₃ C ₂ H	256.332	120	CH ₂ NH	317.405	78
SO	129.139	27	CH ₂ NH	199.823	34	CH ₃ C ₂ H	256.337	142	c-C ₃ H ₂	318.294	34
SiO	130.269	71	HC ₃ N	200.135	189	He α	256.406	27	CH ₃ OH	318.319	74
HNCO	131.886	59	H ₂ C ₂ N	201.144	31	²⁹ SiO	257.255	20	c-C ₃ H ₂	318.482	93
HNCO	131.886	49	CH ₃ CN	202.34	35	CH ₃ CN	257.508	39	c-C ₃ H ₂	318.79	30
HNCO	131.886	41	CH ₃ CN	202.356	77	CH ₃ CN	257.527	83	HC ₃ N, $\nu=7=1$	319.576	36
CH ₃ OH	132.891	15	H ₂ CS	202.924	39	HC ¹⁵ N	258.157	63	NH ₂ CN	321.93	19
C ₃ H ⁺	134.933	22	c-C ₃ H ₂	204.789	19	SO	258.256	150	CH ₃ OH	322.239	35
H β	135.249	26	CH ₃ C ₂ H	205.045	53	H ¹³ CN	259.012	105	C ₂ H ₅ OH	322.691	21
H α	135.286	50	CH ₃ C ₂ H	205.065	64	H ¹³ CN	259.012	152	C ₂ H ₂ OH	322.691	21
He α	135.341	15	CH ₃ C ₂ H	205.077	108	H ¹³ CN	259.012	71	CH ₃ NH ₂	323.462	16
HC ₃ N	136.464	231	CH ₃ C ₂ H	205.081	129	H β	260.033	46	¹³ CS	323.685	19
CH ₃ C ₂ H	136.705	21	H β	205.76	38	H ¹³ CO ⁺	260.255	339	CH ₃ C ₂ H	324.607	42
CH ₃ C ₂ H	136.718	27	CH ₃ OH	205.791	272	SiO	260.518	193	CH ₃ C ₂ H	324.638	49
CH ₃ C ₂ H	136.725	47	H ₂ CS	205.987	21	CH ₃ NH ₂	261.219	34	CH ₃ C ₂ H	324.657	81
CH ₃ C ₂ H	136.728	56	SO	206.176	98	HN ¹³ C	261.263	173	CH ₃ C ₂ H	324.663	97
SO	138.179	73	OCS	206.745	35	NH ₂ CN	261.594	20	CH ₃ NH ₂	325.531	50
¹³ CS	138.739	34	CH ₂ NH	207.38	15	CH ₃ OH	261.806	128	¹³ CN	325.943	30
H ₂ CO	140.84	135	NS	207.436	30	SO	261.844	264	¹³ CN	325.956	21
H ₂ C ₂ N	140.84	36	NS	207.835	39	C ₂ H	262.004	1153	¹³ CN	325.958	31
CH ₃ OH	143.866	33	NS	207.838	24	C ₂ H	262.006	876	¹³ CN	326.119	42
H β	144.474	28	C ₂ S	208.216	15	C ₂ H	262.065	837	¹³ CN	326.125	19
C ³⁴ S	144.617	92	H ₂ CS	209.2	41	C ₂ H	262.067	555	¹³ CN	326.142	57
c-C ₃ H ₂	145.09	48	HC ₃ N	209.23	167	C ₂ H	262.079	76	¹³ CN	326.143	33
CH ₃ OH	145.094	40	HOCN	209.732	15	C ₂ H	262.208	70	CH ₃ OH	326.631	15
CH ₃ OH	145.097	49	H α	210.502	74	HNCO	262.77	26	CH ₃ OH	326.961	15
CH ₃ OH	145.103	69	He α	210.588	23	HNCO	262.77	24	OCS	328.298	25
CH ₃ OH	145.126	15	H ₂ CO	211.211	410	HNCO	262.77	22	HC ₃ N, $\nu=7=1$	328.701	38
CH ₃ OH	145.132	26	CH ₃ OH	213.427	56	HNCO	263.749	117	CH ₃ NH ₂	329.199	51
HC ₃ N	145.561	243	HOCO ⁺	213.813	18	HNCO	263.749	108	C ¹⁸ O	329.331	4461
H ₂ CO	145.603	147	CH ₃ NH ₂	215.108	26	HNCO	263.749	99	HNCO	329.665	63
C ³³ S	145.756	19	SO	215.221	115	HC ₃ N	263.792	52	HNCO	329.665	58
OCS	145.947	17	c-C ₃ H ₂	216.279	155	CH ₃ NH ₂	264.172	32	HNCO	329.665	55
CH ₃ OH	146.368	34	H ₂ S	216.71	98	HNCO	264.694	26	¹³ CO	330.588	13300
CS	146.969	880	CH ₃ OH	216.946	19	HNCO	264.694	22	CH ₃ CN	331.046	23
H α	147.047	54	SiO	217.105	191	HNCO	264.694	24	CH ₃ CN	331.072	50
He α	147.107	17	¹³ CN	217.303	44	HC ₃ N, $\nu=7=1$	264.817	22	SO ₂	332.505	19

Table D.1. continued.

Formula	ν (GHz)	S (mJy)	Formula	ν (GHz)	S (mJy)	Formula	ν (GHz)	S (mJy)	Formula	ν (GHz)	S (mJy)
CH ₃ CN	147.163	19	¹³ CN	217.436	19	CH ₃ OH	265.29	27	CH ₂ NH	332.573	39
CH ₃ CN	147.175	42	¹³ CN	217.467	41	HCN,v2	265.853	47	CH ₂ NH	332.573	31
HOCO ⁺	149.676	27	c-C ₃ H ₂	217.822	69	HCN	265.886	6477	CH ₃ NH ₂	333.839	17
NO	150.176	23	c-C ₃ H ₂	217.822	207	CH ₂ NH	266.27	39	CH ₃ NH ₂	334.712	17
H ₂ CO	150.498	158	c-C ₃ H ₂	217.94	157	CH ₂ NH	266.27	30	CH ₃ OH	335.134	31
NO	150.547	23	c-C ₃ H ₂	218.16	52	H ¹⁵ NC	266.588	16	H β	335.207	55
c-C ₃ H ₂	150.852	126	H ₂ CO	218.222	369	CH ₃ OH	266.838	117	CH ₃ OH	335.582	136
HNCO	153.292	18	HC ₃ N	218.325	144	HCN,v2	267.199	48	C ¹⁷ O	337.061	617
HNCO	153.292	16	CH ₃ NH ₂	218.409	23	OCS	267.53	37	CH ₃ NH ₂	337.119	18
CH ₃ C ₂ H	153.791	30	CH ₃ OH	218.44	93	HCO ⁺	267.558	7021	C ³⁴ S	337.397	175
CH ₃ C ₂ H	153.805	37	NH ₂ CN	218.462	16	HOC ⁺	268.451	240	HC ₃ N,v7=1	337.825	40
CH ₃ C ₂ H	153.814	63	OCS	218.903	37	C ₂ H ₅ OH	270.444	18	H ₂ CS	338.081	49
CH ₃ C ₂ H	153.817	76	HNCO	218.981	29	C ₂ H ₅ OH	270.451	18	CH ₃ OH	338.124	147
HNCO	153.865	62	HNCO	218.981	26	H ₂ CS	270.521	56	c-C ₃ H ₂	338.204	100
HNCO	153.865	72	HNCO	218.981	24	HNC	271.981	3903	CH ₃ OH	338.345	197
HNCO	153.865	84	C ¹⁸ O	219.56	2380	HC ₃ N	272.885	40	CH ₃ OH	338.409	254
HNCO	154.415	16	HNCO	219.798	130	CH ₃ C ₂ H	273.373	58	CH ₃ OH	338.513	49
HNCO	154.415	19	HNCO	219.798	106	CH ₃ C ₂ H	273.399	68	CH ₃ OH	338.541	26
H β	154.557	29	HNCO	219.798	117	CH ₃ C ₂ H	273.415	114	CH ₃ OH	338.543	26
HC ₃ N	154.657	249	SO	219.949	217	CH ₃ C ₂ H	273.42	136	CH ₃ OH	338.56	15
c-C ₃ H ₂	155.518	26	¹³ CO	220.399	7383	HC ₃ N,v7=1	273.945	24	CH ₃ OH	338.583	28
CH ₃ OH	156.602	53	HNCO	220.585	29	H ₂ CS	274.521	29	CH ₃ OH	338.615	106
CH ₃ OH	156.829	15	HNCO	220.585	24	H ₂ ¹³ CO	274.762	35	CH ₃ OH	338.64	49
CH ₃ OH	157.049	28	HNCO	220.585	26	CH ₃ CN	275.894	36	CH ₃ OH	338.722	92
CH ₃ OH	157.179	44	CH ₃ CN	220.73	38	CH ₃ CN	275.916	78	CH ₃ OH	338.723	80
CH ₃ OH	157.246	60	CH ₃ CN	220.747	83	¹³ CS	277.455	37	SO	339.341	18
CH ₃ OH	157.271	50	H ₂ C ₂ N	221.254	20	CH ₃ OH	278.305	22	CN	339.447	52
CH ₃ OH	157.272	70	NH ₂ CN	221.361	17	CH ₃ OH	278.342	31	CN	339.476	74
CH ₃ OH	157.276	68	H β	222.012	40	H ₂ CS	278.886	58	CN	339.517	117
OCS	158.107	21	CH ₃ C ₂ H	222.129	58	N ₂ H ⁺	279.512	1339	CH ₃ NH ₂	339.724	56
SO	158.972	46	CH ₃ C ₂ H	222.15	69	OCS	279.685	36	³⁴ SO	339.858	16
H α	160.212	58	CH ₃ C ₂ H	222.163	117	H ₂ CO	281.527	544	CN	340.008	214
He α	160.277	18	CH ₃ C ₂ H	222.167	139	NH ₂ CN	281.708	20	CN	340.02	214
H ₂ C ₂ N	160.949	38	C ¹⁷ O	224.714	323	HC ₃ N	281.977	30	CN	340.032	1639
NS	161.298	19	C ₃ H ⁺	224.868	15	H β	282.333	49	CN	340.035	651
NS	161.697	26	CH ₂ NH	225.554	51	c-C ₃ H ₂	282.381	93	CN	340.035	1068
HC ₃ N	163.753	247	CH ₂ NH	225.556	17	HC ₃ N,v7=1	283.072	26	C ³³ S	340.053	33
CH ₃ OH	165.05	38	H ₂ CO	225.698	456	H ₂ ¹³ CO	283.442	26	CH ₃ OH	340.141	32
CH ₃ OH	165.061	53	CN	226.287	57	H α	284.251	94	C ₂ H ₅ OH	340.189	18
CH ₃ OH	165.099	55	CN	226.299	46	CH ₂ NH	284.253	27	C ₂ H ₅ OH	340.189	18
CH ₃ OH	165.19	48	CN	226.303	46	CH ₂ NH	284.254	152	CN	340.248	2129
CH ₃ OH	165.369	36	CN	226.315	110	CH ₂ NH	284.255	27	CN	340.248	1615
CH ₃ CN	165.556	25	CN	226.333	51	He α	284.366	29	CN	340.249	1201
CH ₃ CN	165.569	55	CN	226.342	53	HNCO	284.662	23	CN	340.262	155
H β	165.601	31	CN	226.36	265	HNCO	284.662	21	CN	340.265	154
CH ₃ OH	165.679	23	CN	226.617	60	HNCO	284.662	19	CH ₂ NH	340.353	16
H ₂ S	168.763	265	CN	226.632	461	c-C ₃ H ₂	284.805	50	CH ₂ NH	340.354	191
H ₂ CS	169.114	25	CN	226.66	1399	c-C ₃ H ₂	284.998	132	CH ₂ NH	340.355	16
CH ₃ OH	170.061	57	CN	226.664	458	CH ₃ OH	285.111	32	CH ₃ NH ₂	340.598	56
OCS	170.267	25	CN	226.679	565	HNCO	285.722	101	HC ¹⁸ O ⁺	340.633	69
HC ¹⁸ O ⁺	170.323	30	CN	226.874	1416	HNCO	285.722	93	SO	340.714	157
HCS ⁺	170.692	24	CN	226.875	2077	HNCO	285.722	86	CH ₃ OH	341.416	137
CH ₃ C ₂ H	170.876	39	CN	226.876	890	HNCO	286.747	23	CH ₃ C ₂ H	341.683	35
CH ₃ C ₂ H	170.893	47	CN	226.887	299	HNCO	286.747	19	CH ₃ C ₂ H	341.715	41
CH ₃ C ₂ H	170.902	80	CN	226.892	297	HNCO	286.747	21	CH ₃ C ₂ H	341.735	68
CH ₃ C ₂ H	170.906	96	HC ₃ N	227.419	122	CH ₃ OH	287.671	142	CH ₃ C ₂ H	341.741	81
HOCO ⁺	171.056	27	CH ₃ OH	229.759	25	C ₂ H ₅ OH	287.918	17	NH ₂ CN	342.038	17
HC ¹⁵ N	172.108	32	CH ₃ OH	230.027	29	C ₂ H ₅ OH	287.945	17	CS	342.883	1138
SO	172.181	68	CO	230.538	56226	C ³⁴ S	289.209	228	H ₂ CS	342.944	26
H ¹³ CN	172.677	15	OCS	231.061	38	CH ₃ OH	289.939	155	CH ₃ SH	343.048	15
H ¹³ CN	172.677	20	¹³ CS	231.221	53	CH ₃ OH	290.07	207	H ₂ ¹³ CO	343.326	32
H ¹³ CN	172.678	46	H α	231.901	80	CH ₃ OH	290.111	268	HC ¹⁵ N	344.2	55
H ¹³ CN	172.678	86	He α	231.995	25	CH ₃ OH	290.185	50	SO	344.311	145
H ¹³ CN	172.68	15	CH ₃ OH	234.683	19	CH ₃ OH	290.19	25	CH ₃ SH	345.021	15
HC ₃ N	172.849	239	CO ⁺	235.79	32	CH ₃ OH	290.191	25	H ¹³ CN	345.34	298
HCO	173.377	19	CO ⁺	236.063	57	CH ₃ OH	290.21	15	CO	345.796	112202
H ¹³ CO ⁺	173.507	194	HC ₃ N	236.513	102	CH ₃ OH	290.213	27	NS	345.823	20
SiO	173.688	141	H ₂ CS	236.727	50	CH ₃ OH	290.249	112	NS	345.824	15
HN ¹³ C	174.179	98	HC ₃ N,v7=1	237.432	16	CH ₃ OH	290.264	50	NS	346.221	17
H ₂ CS	174.345	27	NH ₂ CN	238.316	18	CH ₃ OH	290.307	81	SO	346.528	236
C ₂ H	174.663	658	CH ₃ CN	239.12	39	CH ₃ OH	290.308	94	HC ₃ N,v7=1	346.949	42

Table D.1. continued.

Formula	ν (GHz)	S (mJy)	Formula	ν (GHz)	S (mJy)	Formula	ν (GHz)	S (mJy)	Formula	ν (GHz)	S (mJy)
C ₂ H	174.668	446	CH ₃ CN	239.138	85	CH ₃ C ₂ H	290.452	54	H ¹³ CO ⁺	346.998	252
C ₂ H	174.722	382	CH ₃ C ₂ H	239.211	60	CH ₃ C ₂ H	290.48	63	SiO	347.331	100
C ₂ H	174.728	165	CH ₃ C ₂ H	239.234	72	CH ₃ C ₂ H	290.497	106	HN ¹³ C	348.34	130
C ₂ H	174.733	103	CH ₃ C ₂ H	239.248	121	CH ₃ C ₂ H	290.502	125	H ₂ CS	348.532	50
C ₂ H	174.807	90	CH ₃ C ₂ H	239.252	143	H ₂ CO	290.623	449	C ₂ H	349.337	934
He α	174.996	63	CH ₃ OH	239.746	119	HC ₃ N	291.068	22	C ₂ H	349.339	751
He α	175.067	20	H β	240.021	43	C ³³ S	291.486	45	C ₂ H	349.399	737
HNCO	175.189	24	H ₂ CS	240.266	27	OCS	291.84	34	C ₂ H	349.4	553
HNCO	175.189	18	HNCO	240.876	29	HC ₃ N,v7=1	292.199	29	CH ₃ CN	349.427	19
HNCO	175.189	21	HNCO	240.876	26	CH ₃ OH	292.673	144	CH ₃ CN	349.454	40
HNCO	175.844	106	HNCO	240.876	24	CH ₃ OH	293.464	35	CH ₃ OH	350.688	255
HNCO	175.844	82	C ³⁴ S	241.016	233	CS	293.912	1674	NO	350.689	373
HNCO	175.844	94	NH ₂ CN	241.479	19	CH ₃ CN	294.28	32	NO	350.691	274
HNCO	176.472	21	CH ₃ OH	241.7	133	CH ₃ CN	294.302	70	NO	350.695	199
HNCO	176.472	24	CH ₃ OH	241.767	175	SO	296.55	166	NO	350.73	24
HNCO	176.472	18	HNCO	241.774	128	NH ₂ CN	297.869	20	NO	350.737	24
HCN	177.26	423	HNCO	241.774	116	³⁴ SO	298.258	18	CH ₃ OH	350.905	728
HCN	177.26	557	HNCO	241.774	106	NS	299.7	32	NO	350.963	24
HCN	177.261	1175	CH ₃ OH	241.791	230	NS	299.701	23	NO	350.99	24
HCN	177.261	1987	CH ₃ OH	241.833	18	NS	300.099	27	NO	351.044	374
HCN	177.262	29	CH ₃ OH	241.833	18	HC ₃ N	300.16	16	NO	351.051	275
HCN	177.263	423	CH ₃ OH	241.842	40	c-C ₃ H ₂	300.192	52	NO	351.052	199
H β	177.723	33	CH ₃ OH	241.844	20	H ₂ S	300.506	189	SO ₂	351.257	15
HCO ⁺	178.375	3369	CH ₃ OH	241.879	94	H ₂ CO	300.837	567	c-C ₃ H ₂	351.523	64
SO	178.605	144	CH ₃ OH	241.888	40	SO	301.286	160	HNCO	351.633	45
HOC ⁺	178.972	108	CH ₃ OH	241.904	66	HC ₃ N,v7=1	301.325	31	HNCO	351.633	43
C ₃ H ⁺	179.903	25	CH ₃ OH	241.905	76	CH ₃ OH	302.37	157	HNCO	351.633	40
CH ₂ NH	180.627	39	HNCO	242.64	29	CH ₃ OH	303.367	496	H ₂ CO	351.769	426
CH ₃ OH	181.296	23	HNCO	242.64	24	SiO	303.927	154	c-C ₃ H ₂	351.782	20
HNC	181.325	2064	HNCO	242.64	26	OCS	303.993	31	c-C ₃ H ₂	351.966	56
CH ₃ OH	181.771	15	C ³³ S	242.914	47	SO	304.078	269	c-C ₃ H ₂	352.194	59
HC ₃ N	181.945	226	OCS	243.218	39	CH ₃ OH	304.208	635	He α	353.623	110
OCS	182.427	29	CH ₃ OH	243.916	122	H ₂ CS	304.306	55	CO ⁺	353.741	26
C ₂ S	182.553	15	H ₂ CS	244.048	52	C ₂ H ₅ OH	305.354	15	He α	353.767	34
CH ₃ CN	183.949	31	c-C ₃ H ₂	244.222	39	C ₂ H ₅ OH	305.434	15	H ₂ ¹³ CO	353.812	23
CH ₂ NH	183.957	20	CS	244.936	1886	CH ₃ OH	305.473	513	CO ⁺	354.014	37
CH ₂ NH	183.957	29	CH ₂ NH	245.126	35	¹³ CH ₃ OH	305.699	17	c-C ₃ H ₂	354.143	22
CH ₃ CN	183.963	67	HC ₃ N	245.606	83	CH ₂ NH	306.172	31	HCN,v2	354.46	149
c-C ₃ H ₂	184.33	61	HC ₃ N,v7=1	246.561	18	CH ₂ NH	306.172	47	HCN	354.505	6497
¹³ CS	184.982	54	CH ₃ OH	247.229	22	HNCO	306.554	18	CH ₃ NH ₂	354.844	24
N ₂ H ⁺	186.345	648	NO	250.437	138	HNCO	306.554	17	HC ₃ N,v7=1	356.072	44
CH ₃ C ₂ H	187.961	47	NO	250.441	87	HNCO	306.554	16	HCN,v2	356.256	151
CH ₃ C ₂ H	187.979	56	NO	250.449	51	CH ₃ OH	307.166	453	HCO ⁺	356.734	7789
CH ₃ C ₂ H	187.99	96	NO	250.475	16	H ₃ O ⁺	307.192	178	HC ₃ N,v7=2	356.937	15
CH ₃ C ₂ H	187.994	114	NO	250.483	16	H β	307.258	52	CH ₃ NH ₂	357.44	24
HC ₃ N	191.04	209	NO	250.708	16	¹³ CH ₃ OH	307.311	15	C ₂ H ₅ OH	357.681	16
H β	191.057	35	NO	250.753	16	CH ₃ C ₂ H	307.53	48	C ₂ H ₅ OH	357.682	16
CH ₂ NH	191.463	39	NO	250.796	138	CH ₃ C ₂ H	307.56	56	HOC ⁺	357.922	248
CH ₂ NH	191.463	56	NO	250.816	87	CH ₃ C ₂ H	307.577	94	CH ₃ OH	358.606	280
He α	191.657	68	NO	250.817	52	CH ₃ C ₂ H	307.583	112	CH ₃ C ₂ H	358.757	28
He α	191.735	21	c-C ₃ H ₂	251.314	193	HNCO	307.694	82	CH ₃ C ₂ H	358.791	33
CH ₃ OH	191.811	76	c-C ₃ H ₂	251.509	53	HNCO	307.694	76	CH ₃ C ₂ H	358.811	56
CH ₂ NH	192.212	27	CH ₃ OH	251.738	23	HNCO	307.694	71	CH ₃ C ₂ H	358.818	66
HOCO ⁺	192.435	24	CH ₃ OH	251.812	33	CH ₃ NH ₂	307.792	32	CH ₃ OH	361.852	25
C ³⁴ S	192.818	178	SO	251.826	145	H ₂ CS	308.748	29	NH ₂ CN	362.143	15
CH ₃ OH	193.415	87	CH ₃ OH	251.867	39	HNCO	308.798	18	HNC,v2=1	362.554	45
CH ₃ OH	193.442	112	CH ₃ OH	251.891	33	HNCO	308.798	17	HNC	362.63	3526
CH ₃ OH	193.454	151	CH ₃ OH	251.896	23	HNCO	308.798	16	H ₂ CO	362.736	329
CH ₃ OH	193.488	24	CH ₃ OH	251.9	39	CH ₃ OH	309.29	346	CH ₃ OH	363.74	101
c-C ₃ H ₂	193.489	55	CH ₃ OH	251.906	31	SO	309.502	16	HNC,v2=1	365.147	45
CH ₃ OH	193.507	61	CH ₃ OH	251.917	31	CH ₃ OH	310.193	213	HC ₃ N,v7=1	365.195	46
CH ₃ OH	193.511	24	C ₂ H ₅ OH	252.951	18	HC ₃ N,v7=1	310.451	33	HC ₃ N,v7=2	365.933	15
CH ₃ OH	193.511	38	C ₂ H ₅ OH	252.952	18	CH ₃ NH ₂	310.528	31	HC ₃ N,v7=2	366.235	15
CH ₃ OH	193.511	44	NS	253.57	33	CH ₃ OH	311.853	233	H ₂ ¹³ CO	366.27	32
C ³³ S	194.337	36	NS	253.971	33	CH ₃ CN	312.664	28	H β	366.653	59
OCS	194.586	32	CH ₃ OH	254.015	60	CH ₃ CN	312.688	60	CH ₂ NH	367.072	28
CH ₃ OH	195.147	79	CH ₂ NH	254.685	63	SO ₂	313.28	21	CH ₂ NH	367.072	33
C ₂ S	195.375	15	CH ₂ NH	254.685	83	CH ₃ OH	313.597	29	CH ₃ NH ₂	367.681	17
CS	195.954	1566	HC ₃ N	254.7	66	H ₂ CS	313.715	56	CH ₃ CN	367.834	31

Table D.1. continued.

Formula	ν (GHz)	S (mJy)	Formula	ν (GHz)	S (mJy)	Formula	ν (GHz)	S (mJy)	Formula	ν (GHz)	S (mJy)
HNCO	197.085	24	c-C ₃ H ₂	254.988	45	¹³ C ¹⁸ O	314.12	18	H ₂ S	369.101	460
HNCO	197.085	27	OCS	255.374	38	¹³ C ¹⁸ O	314.12	25	H ₂ S	369.127	32
HNCO	197.085	22	HC ¹⁸ O ⁺	255.48	67	CH ₃ OH	314.86	139	CH ₃ SH	369.394	17
HNCO	197.821	110	HC ₃ N, ν 7=1	255.689	20	CH ₃ OH	315.267	119	CH ₃ NH ₂	370.166	51
HNCO	197.821	123	HCS ⁺	256.028	28	OCS	316.146	28	H ₂ CS	371.844	40
HNCO	197.821	98	CH ₃ C ₂ H	256.293	60	H α	316.415	101	N ₂ H ⁺	372.673	1281

by the LTE model should be consistent with the observed spectra and no big outliers should be present. This may not be the case with previously reported species showing some out of equilibrium transitions reported above.

In this section we present details of the modeling of C₂H₅OH, HOCN and HC₃HO, since most relevant details regarding the newly detected isotopologues are discussed in Sect. 5.4. Figs. D.1, D.2, and D.3 show the fit results to these species where the spectral features are ordered by the brightness of the LTE modeled emission, thus showing only the brightest spectral features of each molecule.

We do not list the spectroscopic parameters of the detected transitions since these are directly extracted from the catalog entries indicated in the figures and more importantly these species have been previously identified in the Galactic ISM.

C₂H₅OH: All transitions above 3 mJy modeled emission were used to fit the emission of C₂H₅OH, where those falling within the spectral features of significantly brighter transitions were masked, adding up to a total of ~50 transitions considered. Among its brightest transitions only the transitions at 287.944 GHz (6_{4,2} – 5_{3,3}) and 287.917 GHz (6_{4,3} – 5_{3,2}) form an clearly unblended spectral feature. Other spectral lines at

252.952, 270.450, and 234.758 GHz, though partially blended, confirm the detection of C₂H₅OH, together with the fainter feature at 243.556 GHz also marginally blended as displayed in Fig. D.1. The identified transitions appear to show a double peak, similar to what is observed for CH₃OH, further supporting this detection.

HOCN: The brightest expected transition of HOCN in the whole frequency coverage of ALCHEMIS (10_{0,10} – 9_{0,9} at 209.732 GHz) is unambiguously detected and just marginally blended. The brightness of all other transitions drop quickly below the detection limit or are blended to other brighter species as shown in Fig. D.2. All spectral features shown in this figure, but for the one at 251.666 GHz were used in the fit.

HC₃HO: The two brightest transitions of HC₃HO (14_{0,14} – 13_{0,13} @ 129.975 GHz and 15_{0,15} – 14_{0,14} @ 139.169 GHz) appear unblended in our survey while most other transitions fall close to the noise level of our observations. We conservatively included transitions down to ~1 mJy in the fit to this species which may have resulted in an underestimate of the brightest transitions. A fit performed exclusively with the two brightest transitions would have resulted into a column density 80% higher yielding $N_{\text{HC}_3\text{HO}} = 10^{14.2} \pm 10^{13.6} \text{ cm}^{-2}$.

Appendix E: Extragalactic molecular census

Table E.1. Chronology of extragalactic detections.

Year	Molecule	Reference	Year	Molecule	Reference	Year	Molecule	Reference
1971	OH	1	2003	SO ₂	38	2013	C ₂	59
1974	H ₂ CO	2	2003	NO	38	2013	C ₃	59
1975	CO	3	2003	NS	38	2013	HCS ⁺	60
1975	¹³ CO	4	2003	³⁴ SO	38	2013	NH ₂ CHO	60
1977	H ₂ O	5	2004	HOC ⁺	39	2013	³⁰ SiO	60
1977	HCN	6	2004	NH	40	2014	H ₂ Cl ⁺	61
1978	H ₂	7	2004	OH ⁺	41,42	2014	H ₂ ³⁷ Cl ⁺	61
1979	NH ₃	8	2006	C ₂ S	43	2014	NH ₂	62
1979	HCO ⁺	9	2006	NH ₂ CN	44	2014	H ₂ ¹⁷ O	62
1980	CH	10	2006	HOCO ⁺	44	2014	¹³ CN	63
1985	CS	11	2006	c-C ₃ H	44	2015	ArH ⁺	64
1986	c-C ₃ H ₂	12	2006	DNC †	44	2015	³⁸ ArH ⁺	64
1987	CH ⁺	13,14	2006	N ₂ D ⁺ †	44	2015	HC ₃ N	65,66,75
1987	CH ₃ OH	15	2006	CH ₂ NH	44,45	2015	CH ₃ SH	67,68
1988	CN	16	2006	HC ¹⁸ O ⁺	44,46	2016	CF ⁺	69
1988	C ₂ H	16	2006	HC ¹⁷ O ⁺	46	2017	¹³ CH ⁺	70
1988	HNC	16	2006	H ¹⁵ NC	46,75	2017	SH ⁺	70
1988	HC ₃ N	16,17	2006	H ₂ ³⁴ S	46	2017	³⁴ SH ⁺	70
1989	HNCO	18,19	2006	H ₃ ⁺	47	2018	CH ₃ OCH ₃	71
1989	C ³⁴ S	20	2006	C ₄ H ₂	48	2018	CH ₃ OCHO	71
1991	C ¹⁸ O	21	2006	C ₆ H ₂	48	2019	HCl	72
1991	C ¹⁷ O	21	2006	C ₆ H ₆	48	2019	HCl	72
1991	SO	22,23	2008	H ₃ O ⁺	49	2020	O ₂ †	73
1991	N ₂ H ⁺	24	2009	C ³³ S	50	2020	l-C ₃ H ⁺	68
1991	SiO	24	2009	¹³ CH ₃ OH	51,52,75	2020	C ₃ N	68
1991	H ¹³ CO ⁺	24	2010	HF	53	2020	CH ₂ CHCN	68
1991	HN ¹³ C	24	2010	H ₂ O ⁺	53,54	2020	H ₂ CN	68
1991	H ¹³ CN	24	2010	¹³ C ¹⁸ O	55,56	2020	HCOOH	68,75
1991	CH ₃ CCH	25	2010	C ₆₀ †	57	2020	ND	74
1991	CH ₃ CN	25	2011	H ¹³ CCCN	58	2020	NH ₂ D	74
1993	¹³ CS	26	2011	HC ¹³ CCN	58	2020	HDO	74
1995	OCS	27	2011	HCC ¹³ CN	58	2021	H ₂ ¹³ CO	75
1995	HCO	28	2011	H ₂ ¹⁸ O	58	2021	C ₂ H ₅ OH	75
1996	DCO ⁺	29	2011	²⁹ SiO	58	2021	¹³ CCH	75
1996	DCN	29	2011	CH ₂ CO	58,45	2021	C ¹³ CH	75
1998	LiH †	30,31	2011	SO ⁺	45	2021	HOCN	75
1999	HC ¹⁵ N	32	2011	l-C ₃ H	45	2021	CH ₃ ¹³ CCH	75
1999	H ₂ S	33	2011	l-C ₃ H ₂	45	2021	CH ₃ C ¹³ CH	75
1999	H ₂ CS	33,34	2011	CH ₂ CN	45	2021	¹³ CH ₃ CCH	75
1999	C ₂ H ₂	35	2011	C ₄ H	45	2021	HC ₃ HO	75
2000	CO ⁺	36	2011	CH ₃ NH ₂	45	2021	Si ¹⁷ O †	75
2001	HD	37	2011	CH ₃ CHO	45			

Notes. Year of first detection of each individual molecular species, were first detections of isotopologues are also included. When first detection was tentative, confirmation is also included. (†) Species where only tentative detection have been reported.

References. (1) Weliachew (1971); (2) Gardner & Whiteoak (1974); (3) Rickard et al. (1975); (4) Solomon & de Zafra (1975); (5) Churchwell et al. (1977); (6) Rickard et al. (1977); (7) Thompson et al. (1978); (8) Martin & Ho (1979); (9) Stark & Wolff (1979); (10) Whiteoak et al. (1980); (11) Henkel & Bally (1985); (12) Seaquist & Bell (1986); (13) Magain & Gillet (1987); (14) Falgarone et al. (2017); (15) Henkel et al. (1987); (16) Henkel et al. (1988); (17) Mauersberger et al. (1990); (18) Nguyen-Q-Rieu et al. (1989); (19) Nguyen-Q-Rieu et al. (1991); (20) Mauersberger & Henkel (1989); (21) Sage et al. (1991); (22) Johansson (1991); (23) Petuchowski & Bennett (1992); (24) Mauersberger & Henkel (1991); (25) Mauersberger et al. (1991); (26) Henkel et al. (1993); (27) Mauersberger et al. (1995); (28) Sage & Ziurys (1995); (29) Chin et al. (1996); (30) Combes & Wiklind (1998); (31) Friedel et al. (2011); (32) Chin et al. (1999); (33) Heikkilä et al. (1999); (34) Martín et al. (2005); (35) van Loon et al. (1999); (36) Fuente et al. (2000); (37) Varshalovich et al. (2001); (38) Martín et al. (2003); (39) Usero et al. (2004); (40) González-Alfonso et al. (2004); (41) González-Alfonso et al. (2004); (42) van der Werf et al. (2010); (43) Martín et al. (2006); (44) Martín et al. (2006); (45) Muller et al. (2011); (46) Muller et al. (2006); (47) Geballe et al. (2006); (48) Bernard-Salas et al. (2006); (49) van der Tak et al. (2008); (50) Wang et al. (2009); (51) Martín et al. (2009a); (52) Muller et al. (2021); (53) van der Werf et al. (2010); (54) Weiß et al. (2010); (55) Martín et al. (2010); (56) Martín et al. (2019b); (57) García-Hernández et al. (2010); (58) Martín et al. (2011); (59) Welty et al. (2013); (60) Muller et al. (2013); (61) Muller et al. (2014a); (62) Muller et al. (2014b); (63) Takano et al. (2014); (64) Müller et al. (2015); (65) Aladro et al. (2015); (66) Costagliola et al. (2015); (67) Meier et al. (2015); (68) Tercero et al. (2020); (69) Muller et al. (2016); (70) Muller et al. (2017); (71) Sewilo et al. (2018); (72) Wallström et al. (2019); (73) Wang et al. (2020); (74) Muller et al. (2020); (75) This work.

The continuous growth of new species detected during the last two decades has resulted in various publications reporting up to date listings of the extragalactic molecular census including conference proceedings (Martín 2009; Martín et al. 2011), refereed publications (Martín et al. 2006, 2011; McGuire 2018), as well as online resources such as that hosted at CDMS⁶. Each of these reports have had different formats and criteria depending on the scope of the publication but all aiming to maintain updated information on first molecular extragalactic detections. Despite these available resources, given the legacy value of

ALCHEMI for the extragalactic molecular content, and the relevance of isotopologue detections in this work, which are not included in most of the references above, we provide here a detailed and updated extragalactic molecular census.

In this appendix we provide a comprehensive listing of all molecular species and isotopologues detected in the extragalactic ISM according to the chronology of detections (Table E.1) and grouped by the number of atoms in the molecule (Table E.2). Graphical representations of these lists can be found in Sect. 4.4.

Table E.2. Census of extragalactic molecular species and isotopologues detected.

2 atoms	3 atoms	4 atoms	5 atoms	6 atoms	7 atoms	> 7 atoms
ArH ⁺ , ³⁸ ArH ⁺	C ₂ H $\left\{ \begin{array}{l} {}^{13}\text{CCH} \\ \text{C}^{13}\text{CH} \end{array} \right.$	C ₂ H ₂	C ₄ H	C ₄ H ₂	CH ₂ CHCN	C ₂ H ₅ OH
C ₂	C ₂ S	C ₃ N	c-C ₃ H ₂	CH ₃ CN	CH ₃ CCH $\left\{ \begin{array}{l} {}^{13}\text{CH}_3\text{CCH} \\ \text{CH}_3^{13}\text{CCH} \\ \text{CH}_3\text{C}^{13}\text{CH} \end{array} \right.$	C ₆ H ₂
CF ⁺	C ₃	c-C ₃ H	l-C ₃ H ₂	CH ₃ OH, ¹³ CH ₃ OH	CH ₃ CHO	C ₆ H ₆
CH	H ₂ Cl ⁺ , H ₂ ³⁷ Cl ⁺	l-C ₃ H	CH ₂ CN	CH ₃ SH	CH ₃ NH ₂	C ₆₀ [†]
CH ⁺ , ¹³ CH ⁺	H ₂ O $\left\{ \begin{array}{l} \text{H}^{18}\text{O} \\ \text{H}^{17}\text{O} \\ \text{HDO} \end{array} \right.$	l-C ₃ H ⁺	CH ₂ CO	HC ₃ HO	HC ₃ N	CH ₃ OCH ₃
CN, ¹³ CN	H ₂ O ⁺	H ₂ CN	CH ₂ NH	NH ₂ CHO		
¹³ CO						
CO $\left\{ \begin{array}{l} \text{C}^{18}\text{O} \\ \text{C}^{17}\text{O} \\ {}^{13}\text{C}^{18}\text{O} \end{array} \right.$	H ₂ S, H ₂ ³⁴ S	H ₂ CO, H ₂ ¹³ CO	HC ₃ N $\left\{ \begin{array}{l} \text{H}^{13}\text{CCCN} \\ \text{HC}^{13}\text{CCN} \\ \text{HCC}^{13}\text{CN} \end{array} \right.$			CH ₃ OCHO
CO ⁺	H ₃ ⁺	H ₂ CS	HCOOH			
CS $\left\{ \begin{array}{l} {}^{13}\text{CS} \\ \text{C}^{34}\text{S} \\ \text{C}^{33}\text{S} \end{array} \right.$	HCN $\left\{ \begin{array}{l} \text{H}^{13}\text{CN} \\ \text{HC}^{15}\text{N} \\ \text{DCN}^\dagger \end{array} \right.$	H ₃ O ⁺	NH ₂ CN			
H ₂ , HD	HCO	HNCO				
HF	HCO ⁺ $\left\{ \begin{array}{l} \text{H}^{13}\text{CO}^+ \\ \text{HC}^{18}\text{O}^+ \\ \text{HC}^{17}\text{O}^+ \\ \text{DCO}^+ \end{array} \right.$	HOCN				
LiH [†]	HCS ⁺	HOCO ⁺				
NH, ND	HNC $\left\{ \begin{array}{l} \text{HN}^{13}\text{C} \\ \text{H}^{15}\text{NC} \\ \text{DNC} \end{array} \right.$	NH ₃ , NH ₂ D				
NO	HOC ⁺					
NS	N ₂ H ⁺ , N ₂ D ⁺ [†]					
O ₂ [†]	NH ₂					
OH	OCS					
OH ⁺	SH ⁺ , ³⁴ SH ⁺					
SiO $\left\{ \begin{array}{l} {}^{29}\text{SiO} \\ {}^{30}\text{SiO} \\ \text{Si}^{17}\text{O}^\dagger \end{array} \right.$	SO ₂					
SO, ³⁴ SO						
SO ⁺						

Notes. Species are alphabetically ordered in each column. ([†]) Species where only tentative detections have been reported. The table is updated from Martín et al. (2011) according to the list of detections in Table E.1, where references for each detection are provided.

⁶ <https://cdms.astro.uni-koeln.de/classic/molecules>

Appendix F: Full spectrum and model

Fig. F.1 presents the full spectrum analyzed in this article (gray histogram) with the best LTE model fit (red line) as well as the labels for each individual transition with flux density above 100 mJy according to the LTE model. Figs. F.2 to F.11 present a zoomed version of Fig. F.1 in 5 GHz windows and labeling transitions down to 2 mJy. We note that despite what was indicated

in Table A.1, the spectral window centered at 368.7 GHz could not be imaged with the 12 m data due to the poor atmospheric transmission. Despite the poorer quality of the data, this spectral window is included in Fig. F.11, which actually shows a bright spectral feature due to H₂S. The quality of the data can only be used to confirm the presence of the line but was not included in the fit.

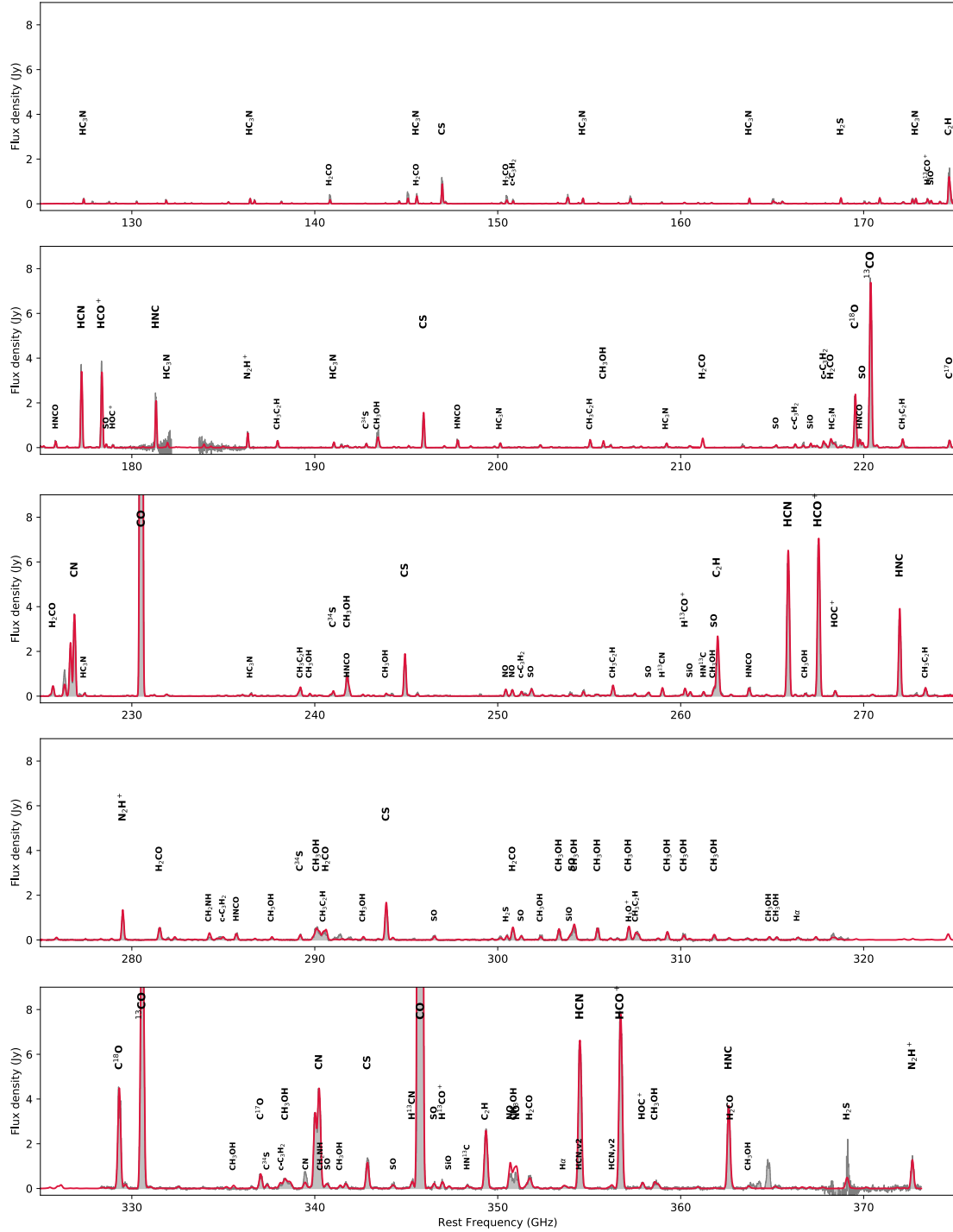


Fig. F.1. Full spectral coverage as in Fig.4 zoomed to 50 GHz frequency windows. The observed spectrum is shown in grey histogram and the model (Sect. 4.3.2) in red line. Only the brighter individual molecular transitions with intensities higher than 100 mJy are labeled with different y-axis position and character size depending on the modelled intensity for > 5, > 1, > 0.2, and > 0.1 Jy.

