

OBSERVATIONS OF UNIDENTIFIED LINES

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ABSTRACT. The three existing spectral surveys in the 3 mm window are compared. The NRAO and BTL surveys of SgrB2 are quite consistent, the NRAO and Onsala surveys of Ori(KL) less so. Lists of U-lines are assembled from the three surveys, and total 86 in Ori(KL), 66 in SgrB2, of which only 12 are common. Difficulties in selecting reliable lists of U lines are emphasized. Methods of identifying such lines include "direct," "hybrid," and "Shotgun" approaches; the probability of misidentification is analyzed for each. The "Shotgun" method is least reliable, although a few candidates should be followed up.

1. INTRODUCTION

A summary of the four spectral surveys carried out so far is given in Table 1. Here we discuss only the three 3 mm surveys. Typical sensitivities (5-sigma noise in T_R^*) are 0.15 K (Onsala), 0.1-0.15 K

TABLE 1. Summary of Surveys

Survey	Frequency Range	Dish	Beam	Efficiency	Sources
Onsala	72.2 - 91.1 GHz	20 m	47"	0.58	Ori(KL), IRC10216
NRAO	71.0 - 115.4	11 m	83"	0.64	Ori(KL), SgrB2
BTL	72.0 - 115.4	7 m	128"	0.77	SgrB2
CIT	215 - 247	10.4	30"	0.72	Ori(KL)

(NRAO), 0.2 K (BTL). There are gaps in the frequency coverage of the BTL survey, and the sensitivity varies considerably (0.05-0.35 K) over the survey.

2. CONSISTENCY OF THE SURVEYS

For several reasons, lists of U lines observed with different telescopes, sensitivities, and complex source structures, will not

necessarily appear very consistent. Selection criteria are important also, and are far from unambiguous.

2.1 NRAO vs. BTL Surveys (SgrB2)

NRAO sees 37 U lines. Three of these fall in gaps in the frequency covered by BTL. Another 11 to 20 would be too weak to be seen by BTL if they are emitted in regions unresolved by both NRAO and BTL beams. Thus BTL should see 14 to 23 of the NRAO U lines (of which two are "tentative"). BTL actually sees 12 of them.

BTL lists 22 U lines (Cummins et al. 1985). Three are easily identified. Another nine are too weak for NRAO assuming they arise in regions resolved by both telescopes. Thus NRAO should see ten of the BTL lines (one is "tentative"). NRAO actually sees seven of them.

Under fairly strong assumptions about the source size, we conclude that the BTL and NRAO surveys are quite consistent. All NRAO lines (observed double sideband) are verified by two LO settings and with two independent filter banks. BTL lines are observed single sideband; only one LO setting and one filter bank are used. Intensity ratios among the lines seen in both surveys vary dramatically, and indicate that some species are spatially compact, others extended. The relative calibration of the two surveys is in good agreement.

2.2 NRAO vs. Onsala Surveys (Ori(KL))

NRAO sees 17 U lines in the frequency range covered by Onsala. Six of these are too weak for Onsala assuming they are resolved by both telescopes. Thus Onsala should see 11 of the NRAO lines, but actually sees only three.

Onsala (Johannsson et al. 1984, 1985) sees 21 U lines, of which four are easily identified. Another 8 to 15 lines are too weak for NRAO if they are spatially unresolved by both telescopes. Thus NRAO should see between two and nine of the Onsala lines, but actually only detects one of them.

Even under strong assumptions about the source size in the various lines, the NRAO and Onsala surveys appear inconsistent. The actual lists of U lines are essentially orthogonal. At most 50% of the apparent inconsistency is removed by assuming the source size. Again, intensity ratios of lines seen in both surveys vary widely. Large ratios, which suggest spatial compactness, often occur for lines with rather large velocity widths, even though these are normally believed to be associated with compact core species. The Onsala survey is observed single sideband, and two independent LO settings are used for each line. The effects of moisture on the radome are unknown.

2.3 Other Contributors of U Lines

Lovas (1985) has compiled a catalogue of all observed millimeter-wave lines. In the 71-115 GHz range he lists 21 U lines for Ori(KL) of which six can be identified; of the remaining 15, two were contributed by Onsala, but not included by Johannsson et al. Eight of the 19 U

lines listed for SgrB2 can be identified; of the remaining 11, five were contributed by BTL but not included in Cummins *et al.* Opinions about the reality of lines appear to change with time. Most of the Lovas lines are weak, having been seen at sensitivity levels well below those of the spectral surveys. The Lovas U lines have been added to those of the surveys in the analysis given here.

Six very weak U lines have been seen in Ori(KL) at Quabbin by Ziurys (1985), at very high sensitivity (20 mK p-p). Large numbers of U lines undoubtedly exist at such levels.

3. PROBLEMS IN SELECTING U LINES

The extensive spectroscopic catalogue by Lovas (1984) should eliminate "obvious" identifications from previously published U lines.

"Doubtful" identifications are harder to avoid. Isotopic substitutions (H^{13}COOH , $\text{NH}_2^{13}\text{CHO}$, HNC^{18}O) are frequent possibilities, although the observed lines often seem too strong for the low opacities expected.

"Discredited" identifications (NaOH , HNO , COH^+) should be returned to the status of U lines. Most difficult are lines attributable to common species (e.g., NH_2CHO) but whose intensities are discrepant with excitation models (e.g., Cummins *et al.* 1985). Some of these identification problems wrongly remove U lines, others add them.

Limited sensitivity and spectral resolution create a major problem in selecting U lines. Only four species (CH_3OCHO , $(\text{CH}_3)_2\text{O}$, EtCN , VycN) have about 1000 transitions with $E/k \leq 100$ K in the 3 mm window, and thus fill 15% of the available spectrum in SgrB2 if all are excited. To deny the possibility that lines occurring at the frequencies of these species can arise from other species as well, seriously underestimates the actual number of U lines and decreases the ability to identify new species. The high sensitivity, high resolution Quabbin spectra illustrate graphically the complex blends that can occur, and the need for accurate intensities, in avoiding this problem.

Intrinsic lineshapes must be understood to identify U lines. A shoulder or asymmetry in the line of a known species could arise because of outflows or source structure in that species, or it could be a blended U line. Close blends will result in "anomalous" intensities. Possible new identifications which fall prey to these problems are NH_2 , several hf transitions of which appear as shoulders on lines of SO_2 and HDO at 241 GHz; and MgO , which appears as an enhanced intensity of one of the A/E doublet lines of CH_3OCHO at 240 GHz. NH_2D can, however, be distinguished from CH_3OCHO at 85.93 GHz, but only with sensitivity and spectral resolution much better than that of Johannsson *et al.*, who refuted the presence of NH_2D in Ori(KL) on the basis of inadequate sensitivity and resolution.

Finally, sideband deconvolution is a possible problem in the NRAO and CIT surveys. The NRAO survey observes multiple LO settings at most frequencies, so that confusion is minimized. The CIT survey applies a "clean" algorithm, the reliability of which has yet to be assessed. Even surveys using SSB filters but which do not "shift" the spectra (BTL) can suffer confusion because of limited rejection by the filter.

The problem of contamination by known species possessing many lines is by far the most serious in selecting U lines. Present surveys must be considered highly limited for this reason. Not only are greater sensitivity and spectral resolution needed, but perhaps interferometry as well, to provide needed spatial resolution.

4. THE LIST OF U LINES

Table 2 presents the list of 3 mm U lines derived from the three surveys. Symbols N, O, B, Q, L refer to NRAO, Onsala, BTL, Quabbin, and Lovas (1985) as the source. Intensities are given as T_R^* .

TABLE 2. The List of U Lines in the 3 mm Window

(a) SgrB2

T72626	N	0.17	SB ambiguity	T93870.2	B	(0.21)	NH ₂ CHO?
U76207	N,B	0.2	C ₃ H?	U95571	N	0.11	
T76648.6	B	0.09	VyCN?	U98266	L	0.04	³³ SO ₂ ?
U77978.5	B	0.13		U99289	N	0.18	wing of SO ₂
U79221	N,B	0.043,0.05		U99727	N,B	0.04	
U80240	N	0.08		U99867	B	0.08	
U80483	N	0.2,0.11		U100157	N	0.07	
U80491	N ^{}B}	0.09		U100197.2	N,B	0.1	
U80733	L	0.04	H ¹³ COOH?	U100758	N	0.08	
U81175	N	0.18		U100853	N	0.1	
U81506	N,B	0.19	NH ₂ ¹³ CHO?	T100910	N	0.07	SB ambiguity
T82080	N	0.17	SB ambiguity	U101000	L	0.05	
T82932	N	0.08		T101726	N	0.15	
U82967.3	N,B	0.18,0.16	(C ₃ H ₂)	T102217.2	B	(0.08)	NH ₂ CHO
T82980	N	0.07		U102812	B	0.04	
U83899	N,B?	0.12		U103216.6	B	0.04	
U84728	L	0.04	(C ₃ H ₂)	U103549	B	0.04	
U85230.6	N,B	0.07	H ¹⁵ NCO?	U103641.8	B	0.05	
T85315	N	0.07		U103715	N	0.25	
U85334	N,B?	0.18		U104200	N,B	0.1, 0.07	
U85339	N,B	0.5	(C ₃ H ₂)	U104589	L	0.15	EtCN?
U85904	N	0.2		U105537.5	N,B	0.03,0.02	
U86395.8	B	0.06		U108784	L	0.18	
U86416.9	B	0.05		U110240	N	0.8	¹³ CO? (also Ori)
U87246	N	0.13		U111828	L	0.04	
U89419	-	0.04	"COH ⁺ "	U113037	N	0.08	
U90212	L	0.04		U113062	N	0.1	
U90360	N	0.1		T113101	N	0.1	
U90841	L	0.08		T113115	N	0.08	
U90908	L	0.05		T113126	N	0.24	
T91430	N	0.07	SB ambiguity	T113160	N	0.12	
U93780	N	0.09		T113246	N	0.2	
U93844	L	0.06	EtCN?	U112481	N	0.55	

(b) Ori(KL)

T72498	N	0.10		U89649	Q	0.06	
T72705	N	0.12		T89936	O	0.20	
U72721	O	0.15		T89960	O	0.20	
U73839	O	0.30		T90763	O	0.20	
U74169	N	0.06		U90909	O	0.25	
U75051	N	0.18		T93650	N	0.1	
U75405	N	0.11		U93780	N	0.14	
U75656	O	0.12	CH ₃ SH	T95731	N	0.18	EtCN?
U75716	N	0.21		U98230	L	0.02	
T76152	O	0.10	C ₄ H?	U98240	L	0.03	
T76168	O	0.12		U98258	L	0.03	
T77983	O	0.20		U98334	L	0.02	
T77992	N	0.2		U98352	L	0.02	
U80482	N	0.14	C ₃ H ₂ ?	U99120	L	0.15	
T81674	N	0.05		U99269	N	0.05	
U83163	N	0.10		U100157	N	0.1	
U83236	N	0.08		T100134	Q	0.04	
U83804	N	0.04		U100224	Q	0.06	
T84308	O	0.10		U100498	L	0.05	HC ₉ N?
U84469	N	0.2		U101004	N	0.14	H ₂ CCO?
U84479	N	0.19		U101327	N	0.4	
T84496	N	0.12		U101375	N	0.3	
U84505	L	0.08	not in N	U101425	N	0.3	
U84970	O	0.20		U101786	N	0.05	
U85339	O,N	0.23,0.36		U103076	N	0.08	
U85506	O	0.10		U103516	N	0.08	
T86413	O	0.15		U103915	L	0.1	H56γ?
T86418	O	0.20		U105540	O	0.05	
U86823	N	0.1	EtCN?	U105590	O	0.15	
U86864	L	0.08	EtOH?	U105746	N	0.18	
T86980	O	0.10		U106009	N	0.1	
U88411	N	0.12	H52β?	U106365	N	0.1	
U88471	Q	0.05		T106942	N	0.07	
U88503	Q	0.05		U109738	L	0.02	
U88527	Q	0.04		U109770	L	0.03	
U88583	Q	0.03		U110240	N	0.16	
U88742	L	0.03		U110487	N	0.1	
U88749	L	0.03		U110770	L	0.04	
U88770	L	0.03		U113062	N	0.12	
U88861	L	0.15		U113211	N	0.2	
T88874	N	0.15		U114006	N	0.09	
U89540	Q	0.02		T114336	N	0.08	
U89643	Q	0.04		T114841	N	0.08	

Although not all apparent discrepancies between existing surveys appear explained by differing source/telescope matches, we have added the U line lists of the three 3 mm surveys, most of the U lines from Lovas (1985), and the new U lines from Quabbin. The final list gives 86 lines in Ori(KL), 66 in SgrB2, of which only 12 are common. Thus

there are 140 U lines in the two sources. There are additional U lines in IRC10216, W51, TMC-1 etc., which are unique to these sources.

It is unlikely that distinct chemistries are implied by the different U lines in different sources. Of 65 currently identified molecular species in space, seven are seen solely in diffuse clouds (optical) or circumstellar shells, and eight are seen only in cold dark clouds. Of the remaining 50 species seen in SgrB2 and Ori(KL) (as well as other warm sources), all occur in SgrB2, and at least 43 occur in Ori(KL). Excitation differences in the two sources more likely explain differences in U lines (as well as known lines) than does a distinct chemistry.

5. BASIC FACTS ABOUT U LINES

Statistical tests show that U lines are randomly distributed in frequency. To current sensitivity limits, the intensity distribution of U lines, and of all lines, is reasonably approximated by $N(I) = N(C) \exp[-a(I-C)]$ where C refers to the confusion limit ($a = \text{constant}$). By actual count (3 mm window) $N(I > S) = 550$ for lines more intense than the current sensitivity limit $S \approx 0.06$ K. Total confusion will occur in SgrB2 ($\Delta v \approx 8$ km/s) for $N(I > C) \approx 44300 \text{ MHz}/8 \text{ MHz} = 5500$, i.e., about 10^4 lines in the 3 mm window (44300 MHz wide).

For the assumed exponential intensity distribution, integration gives $N(I > S) = a^{-1}N(C)\exp[-a(S-C)]$ and the probability of finding a line at a given frequency at any intensity as $\theta(I > S) = N(I > S) \Delta v / (v_1 - v_2)$ where $v_1 - v_2 = 44300 \text{ MHz}$. The probability of finding a line at a given frequency with intensity in the range I, I + dI is $\theta(I) = N(C)\exp[-a(I-C)] \Delta v / (v_1 - v_2)$. These probabilities $\theta(I > S)$, $\theta(I)$ of finding a line purely by chance at a given frequency are central to determining the reliability of identification of U lines. Values of θ for various philosophies in selection of U lines are given in Table 3 for the case of SgrB2 ($\Delta v = 8$ km/s).

TABLE 3. Probabilities for Accidental Occurrence of Lines

Line Selection	Velocity	Intensity	θ
U lines only	exact	any	$\theta(I > S) \approx 0.012$
U + "CH ₃ OCHO"	exact	any	$\theta(I > S) \approx 0.10$
U + "CH ₃ OCHO"	$\Delta v = 10 \text{ km/s}$	any	$\theta(I > S) \approx 0.15$
U + "CH ₃ OCHO"	$\Delta v = 10 \text{ km/s}$	correct	$\theta(I) \sim 0.10$

Here, "CH₃OCHO" means one allows weaker transitions of the common contaminants (CH₃OCHO, (CH₃)₂O, EtCN, VyCN) as U lines, under the assumption that U lines could at least be blended with them. The fact that $\theta(I)$ is comparable with $\theta(I > S)$ is because nearly all U lines of

interest are at the low intensity range where their number density is highest.

Before discussing methods of identifying U lines, we briefly review some simple statistics. Assume we have precisely measured frequencies for a candidate species containing n available transitions in the 3 mm window. Since U lines are randomly distributed in frequency, the probability p of accidental matchup of any m transitions ($m < n$) with corresponding U lines is the binomial function $B(n, m, \theta)$. If we demand that all M expected transitions are matched, then $p = \theta^M$. If we match all M expected transitions and demand that none others are matched, then $p = \theta^M(1-\theta)^{n-M}$. Of course, $B(n, m, \theta) > \theta^M > \theta^M(1-\theta)^{n-M}$.

6. METHODS OF IDENTIFICATION

Three methods are discussed. The difference is in the selection of a candidate species. Let ζ be the probability that the candidate is wrongly selected, i.e., is not an observable interstellar species. p is the probability that m transitions of any candidate species will match U lines purely by chance, hence falsely indicating the presence of that species. The net probability of a misidentification is then $P = \zeta + (1-\zeta)p$.

6.1 Direct Method

One simply selects a candidate, obtains laboratory frequencies (without extrapolation) and compares it with U line lists. ζ is not specifiable in this case, but certainly if few or no matchups occur, ζ should be assumed unity and the candidate abandoned. This method has given untenable identifications in a few cases (COH^+ , HNO , NaOH), because only one line was matched, so that $P = p = \theta \approx 0.15$, unacceptably high.

6.2 Hybrid Method

This method, applied by Thaddeus and co-workers for several species (HCS^+ , HCO^+ , C_3H , C_3H_2) starts with a "bright idea" for the selection of a candidate, using close chemical reasoning based on current knowledge of interstellar chemistry. Such candidates lack laboratory data so approximate ab initio frequencies are obtained and matched roughly with M U lines. If $M = 0$, the candidate is rejected. M may be only 1 or 2 at this stage, but the matchups are used to refine the molecular constants and predict new frequencies, which are then matched. Being iterative, and containing many consistency checks (the presence of doublets in C_3H , C_3H_2 ; agreement with previously estimated bond lengths, chemical principles), ζ is likely very small for this method, although it is not formally specifiable. In all cases to date, measured laboratory frequencies have been obtained subsequent to the analysis, making $\zeta \approx 0$ except for the small chance that the verified molecular constants belong to some species other than the one claimed. In most cases this can be virtually ruled out by laboratory tests.

6.3 Shotgun Method

This method, applied by Turner (1979, 1983) calculates pseudo-accurate frequencies for ~ 1000 species based on molecular constants determined by microwave spectroscopy. The frequencies are only pseudo-accurate in principle because the calculations (accurate to 8th order in the angular momentum operators) extrapolate to the 3 mm range from constants often derived from measures in the 40 GHz range or lower. Molecular constants may therefore be insufficiently accurate for present purposes, and accuracies within ± 3 MHz cannot always be guaranteed in the 3 mm window. The calculated spectra are then matched with the U line list. The probability that many species will be found with large numbers of matchups m is found to be significant. Based

purely on chance, the expectation value is that $\epsilon(m) = \sum_{i=1}^{\eta} N(n_i)B(n_i, m, \theta)$

molecules will have m matchups, where η is the total number of species analyzed, and the i th species has n_i available transitions in the 3 mm window (Turner 1983). $\epsilon(m)$ is sufficiently large, for m as high as 10, that one must now select "reasonable" species from among them, based on additional (subjective) criteria. For example, 1,3,4-thiadiazole (a 6-member ring containing S, and having $m = 14$) is rejected on grounds that it is "chemically unlikely." In the Shotgun process, $\zeta \equiv \epsilon(m)/\eta$ is significant purely by reason of the statistical nature of the selection process. It is further enhanced by the potentially unreliable spectroscopy.

There are two fundamental flaws in the Shotgun method. One is contained in the properties of $\epsilon(m)$. For small n_i and hence small m , the method is useless because $\epsilon(m)$ is weighted upward by the large number of species with large n_i for which, from the properties of $B(n_i, m, \theta)$, m is expected to be large. For large m and not too large n_i , the method is perhaps promising, because $\epsilon(m)$ is not weighted so much by other species. These statements are equivalent to saying that missing (unobserved) transitions in the Shotgun cast serious doubt on the species in question. The other serious shortcoming is that the selection process is intrinsically not a "bright idea." By giving too many promising candidates and forcing a selection on other (arbitrary) grounds, one tends to select only species which are obvious extrapolations from already identified species, but these are large molecules (the entire process is predicated on the large, stable species traditionally studied by microwave spectroscopy), and the formation process for large species in the ISM is unknown. Thus the final selection is really just a wild guess, not subject to much chemical reasoning.

7. POSSIBLE INTERSTELLAR CANDIDATES

The BTL and Onsala surveys, as well as Lovas' compendium which has allowed identification of many lines, causes the current U line list (Table 2) to differ appreciably from that used by Turner (1983). In

Table 4 we discuss the impact of these changes on the species predicted by the Shotgun in 1983. n_f is the number of favorable transitions ($E/k < 100$ K, adequate dipole moment) in the 3 mm window, m_f the number that match U lines. Under m_f , "new" refers to the U line list of Table 2, and "new*" to that list plus lines attributable to CH_3OCHO . B is the binomial function and $P = \zeta + (1-\zeta)B$, where $\zeta \equiv \epsilon(m)/\eta$ is taken from Turner (1983). Q is the quality of spectroscopy used in the Shotgun species. "1" means "good," with reasonable chance that calculated 3 mm frequencies are sufficiently accurate. A value of 3 means almost no chance that calculated frequencies are accurate enough. Four of the six candidates from 1983 have survived the upheaval in the U line list, but three of these have a much larger value of ζ than given by $\epsilon(m)/\eta$ in view of their doubtful spectroscopy. Thus P is strongly underestimated for these. OCCCS failed because recent accurate spectroscopy has shown that the older constants were highly inaccurate. As a formal comparison, the much-publicized C_3H_2 has three missing transitions among the ten that should be seen in SgrB2 (including the lowest-energy para transition), but values of B and P are still extremely low, so that misidentification due to chance is very unlikely.

TABLE 4. Shotgun Candidates

Species		n_f	m_f		B	P	Q	
			1983	new				new*
Transacrolein	$\text{CH}_2\text{CH}-\text{HCO}$	14	4	5	5	0.020	0.035	1
Vinyl isocyanide	$\text{CH}_2\text{CH}-\text{NCO}$	21	6	5	6	0.054	0.061	2
Crotonitrile	$\text{CH}_3\text{CH}=\text{CHCN}$	30	9	6	9	0.014	0.015	3
Isopropyl cyanide	$(\text{CH}_3)_2\text{CHCN}$	18	5	3	6	0.019	0.026	3
Me vinyl ether	$\text{CH}_3\text{OCH}_2\text{CH}$	12	4	1	2	not viable		2
Tricarbon oxide sulfide	OCCCS	22	5	2	2	not viable		3
[New Candidates]								
Allyl cyanide (cis)	$\text{CH}_2=\text{CH}-\text{CH}_2\text{CN}$	36	-	6	9	0.021	0.023	3
		(gauche)	36	-	6	7	0.039	0.041
Propyleneimine (cis)	$\text{H}_2\text{C}-\text{CH}-\text{CH}_3$	14	-	4	6	0.003	0.004	3
		(trans)	$\begin{array}{c} \diagdown \\ \text{N} \\ \diagup \end{array}$	14	-	5	6	0.003
[Comparison]								
Cyclopropenylidene	C_3H_2	10	-	7	7	9(-6)	9(-6)	-

8. CONCLUSIONS

It is difficult to select a reliable list of U lines. Surveys are not apparently consistent, owing to different telescope/source matching, and also apparently to intrinsic lack of reliability at threshold sensitivity limits. Further, contamination by identified species is important but hard to assess. Current practices (eliminating all lines of CH₃OCHO etc.) are overly conservative. The more species that are identified and the more lines they remove from further consideration (under current practices), the fewer lines remain that can in principle be identified. It has been estimated that ~150 species will cover all of frequency space in the 3 mm window so that nothing more can be identified. Obviously there are more than 150 interstellar species. At some point we must therefore consider blending and intensity modelling. Better observations are mandatory. At present, intensity information seems poorly understood. For example, the straight line typically found in plotting $\log(W/vS\mu^2)$ vs. E_u (W is the integrated intensity, E_u the upper level energy) for all observed transitions of a given species implies quasi-thermalization of that species but at a temperature $T_{rot} < T_{kin}$. Such a condition should not in fact produce a straight line at all (cf. Cummins *et al.* 1985).

It is increasingly difficult to identify lines. More lines are required to secure an identification as the sensitivity increases, because θ increases. Intensity modelling is therefore increasingly important in identifications. Whichever of the three methods for selection of a candidate is adopted, the final uncertainty in the identification is at least $P = p = B(n,m,\theta)$. Thus the final step should always be to obtain highly sensitive spectra of each matched line. By thus minimizing potential blends, θ is reduced because both the precise line frequency and intensity are better specified.

Among the methods discussed for identification, the Shotgun method is no longer recommended. Its reliability decreases as the number of observed lines in the 3 mm window increases. Also, its intrinsic information is limited to molecules traditionally studied in the laboratory, species not well related to those of greatest potential interest in astrochemistry.

9. REFERENCES

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DISCUSSION

IRVINE: In comparing the existing spectral surveys it is important to point out that there is excellent agreement between the Onsala survey of Orion KL at 3 mm and the CALTECH survey at 1 mm, both in terms of the abundances of molecular species and in terms of the relatively small number of unidentified lines (after recent laboratory work on species like methanol and $^{13}\text{CH}_3\text{OH}$, e.g. at Duke University).

TURNER: I do not see the relevance of the statement that the Onsala and CIT surveys "agree" in terms of abundances predicted by each. First, reliable abundances must be derived using all available data together, not separately. Second, these abundances refer to relatively strong lines of a few well known species. There is little or no agreement for species involving weak lines. U lines are nearly always weak, near the sensitivity limits of all surveys.

As for the small number of U lines seen by Onsala, this seems to be a result of at least two factors: (1) the 71-91 GHz range covered by Onsala is not very representative - the 71-80 GHz part is well known to have relatively few U lines. The larger number of U lines I claim comes at least in part from the full 71-115 GHz range covered by NRAO. (2) Onsala is not as sensitive as NRAO to spatially extended emission. That this may well be an important factor is indicated also by the fact that the Nobeyama survey of Ori KL showed only 4 U lines in the 3 mm window; Nobeyama is even less sensitive to extended emission than Onsala. I emphasize that telescope parameters are highly important in determining the number of U lines seen in various surveys.

GUELIN: Another complication in the interpretation of the spectra of some sources (e.g. SgrB2) is that line profiles may be complex due to self-absorption. For example, U85334 that you observe in SgrB2 close to the 85339 line of C_3H_2 is very probably the high velocity wing of this line.

TURNER: I agree that this is an additional problem. In the particular case you have drawn attention to, the self-absorption would have to be unusually deep and narrow, which is why I isolated U85334 as a bonafide U line.

WALMSLEY: What seems to have come out of the Onsala and CALTECH surveys is that there are surprisingly very few unidentified features. This suggests that abundances decrease rapidly with increasing complexity. Do you agree?

TURNER: I think the impression of relatively few U lines as suggested by the Onsala group is overstated. As mentioned in this talk, my combined U line list numbers 140 lines in SgrB2 and Ori KL, many times the number quoted by Onsala. Not only does the NRAO survey see many U lines not observed by Onsala, but also the restricted spectral range covered by Onsala (71-91 GHz) is relatively sparse in U lines compared to the 91-115 GHz region. I cannot comment on the CIT survey, since NRAO has not done one in the 1.3 mm region, but sample spectra I have observed

in the 240-270 GHz range (above the range covered by CIT) seem to suggest many U lines.

Apart from these remarks, I don't agree that abundance decreases sharply with molecular complexity. Molecules such as CH_3OCHO , EtCN , $(\text{CH}_3)_2\text{O}$, CH_2CHCN produce a thousand transitions among them with energy $\leq 100\text{K}$ in the 3 mm window alone. Their abundances ($10^{14} - 10^{15} \text{ cm}^{-2}$) are certainly not falling off rapidly compared to those of many simpler species.