ON THE IDENTIFICATION OF MM-WAVELENGTH U-LINES

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During the past five years, a total of about 180 U-lines has been observed by the author and others in the 70-115 GHz region in the prominent molecular clouds Sgr B2 and Ori (KL). A program to identify the carriers of these lines has been undertaken. A computer code, incorporating nine different centrifugal distortion Hamiltonians, generates spectra of asymmetric rotors from given rotational and centrigugal-distortion constants. Spectra have been computed for ∿550 molecules that are considered potentially interesting astrophysically. Molecules were selected from Landolt-Bornstein Volumes IV (1967) and VI (1974) on Molecular Constants, and from the spectroscopic literature (1973 - present).

A calculated transition frequency is declared "matched" to a U-line if the frequencies agree within ± 3 MHz. The criteria applied in deciding whether a given molecule is a good candidate for interstellar identifications are

(1) that there be at least three matching transitions,
(2) that there be at least two matching transitions having quantum number $K_{-1} \leq 1$ and corresponding to the largest dipole moment component,
(3) that the energies of all matching transitions be sufficiently low (matching transitions with very low J values are weighted highly in deciding the merits of a candidate),
(4) that the microwave spectroscopy be "reliable". All calculations are checked against measured frequencies (typically in the 20-40 GHz region), and agreement is demanded with an accuracy sufficient to justify an extrapolation from the 20-40 GHz region to the 70-115 GHz region.

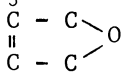
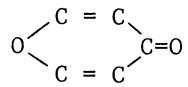
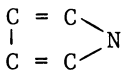
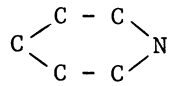
Molecules that satisfy these criteria and that are therefore judged to be reasonable interstellar candidates appear in the table below. The list in the table has been arbitrarily truncated; many other molecules have statistics as favorable as some that appear, but are subjectively judged less likely (e.g., 1,3,4 thiadiazole, a 5-member ring containing sulfur). Additional comments follow.

B. H. Andrew (ed.), Interstellar Molecules, 45–46.

(1) "Overlap" refers to two or more transitions having the same frequency within the ± 3 MHz tolerance. When overlap occurs, the group of transitions involved is counted as only one transition. "Yes(n)" means n groups are overlapped, which amounts to a minimum of 2n, but more usually 4n transitions counted as n matches.

(2) The probability of accidental matchups has been estimated, and implies that perhaps 25% of the entries in the table occur due to chance.

(3) Candidates are not rejected on the basis that one, or even two, calculated transitions were not observed to the sensitivity limit (0.1 K) of the survey. "Control" molecules such as ethyl cyanide and methyl formate were not seen in two or more transitions, while their statistics in the format of the table would read 9 6 5 N and 5 3 2 N, respectively.

Molecule		Number of Matches: Total	$K_{-1} \leq 1$	$K_{-1} \leq 1$ & μ_{max}	Overlap
nitrosyl cyanide	NOCN	3	3	1	N
1-penten-3-yne	CH_3-CC-CH=CH_2	7	4	4	N
formic anhydride	HCO-O-HCO	8	3	3	N
propyl cyanide (gau.)	$CH_3CH_2CH_2CN$	7	5	3	N
(trans)	$CH_3CH_2CH_2CN$	5	3	2	N
crotonitrile (cis)	CH_3-CH=CHCN	8	5	3	N
(tr A)	CH_3-CH=CHCN	6	3	2	N
(tr E)	CH_3-CH=CHCN	4	2	2	N
cyanoallene	CH_2=C=CHCN	4	2	2	N
ethoxyethyne	CH_3CH_2OCCH	6	5	5	N
methyl vinyl ether	$CH_3OCH=CH_2$	4	3	3	N
glyoxal	HCO-HCO	3	2	2	N
vinyl formate	HCO-O-$CHCH_2$	6	3	3	N
crotonaldehyde (A)	$CH_3CH=CH-CHO$	5	4	3	N
(E)	$CH_3CH=CH-CHO$	4	4	2	N
2,5 dihydrofuran		4	4	4	Y(4)
4-pyrone		5	4	4	Y(5)
pyrrole		3	2	2	Y(3)
piperidine		4	3	3	Y(3)

In light of the above comments, the entries in the table should not be regarded as definitive identifications. Additional observations are planned to further test these and other species. The ultimate degree of success of this approach to the identification of U-lines may rest on laboratory verifications. Work is currently underway in this area by several groups.

At a level of 0.1 K there is about one U-line every 170 MHz in the 3-mm wavelength region. Accidental matchups of lines can be expected. Viable identifications of new interstellar molecules must now rest on many more matching transitions than was once considered adequate.

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