

Table A.1. Observed line parameters for CH₂CCHCCH in TMC-1.

JK_aK_c	ν_{obs}^a (MHz)	$\int T_A^* dv^b$ (mK km s ⁻¹)	Δv^c (km s ⁻¹)	T_A^* (mK)
7 _{1,7} – 6 _{1,6}	34472.262(10)	2.4±0.4	0.60±0.05	3.7±0.3 ^d
7 _{0,7} – 6 _{0,6}	35126.923(10)	4.0±0.5	0.77±0.05	4.8±0.3
7 _{2,6} – 6 _{2,5}	35195.532(10)	1.6±0.4	0.63±0.07	2.4±0.3
7 _{3,5} – 6 _{3,4}	35222.531(10)	1.0±0.4	0.70±0.20	1.3±0.3
7 _{3,4} – 6 _{3,3}	35223.195(10)	0.7±0.3	0.60±0.17	1.0±0.3
7 _{2,5} – 6 _{2,4}	35269.664(10)	2.2±0.5	0.74±0.08	2.7±0.3
7 _{1,6} – 6 _{1,5}	35897.418(10)	3.6±0.5	0.73±0.05	4.7±0.3
8 _{1,8} – 7 _{1,7}	39390.116(10)	4.3±0.4	0.77±0.04	5.3±0.3
8 _{0,8} – 7 _{0,7}	40118.252(10)	4.7±0.4	0.72±0.05	6.1±0.3
8 _{2,7} – 7 _{2,6}	40218.511(20)	0.8±0.4	0.50±0.20	1.6±0.3 ^e
8 _{2,6} – 7 _{2,5}	40329.448(10)	2.6±0.6	0.75±0.09	3.2±0.4
8 _{1,7} – 7 _{1,6}	41018.002(10)	2.7±0.5	0.55±0.06	4.6±0.4
9 _{1,9} – 8 _{1,8}	44305.369(10)	2.8±0.5	0.61±0.07	4.3±0.5
9 _{0,9} – 8 _{0,8}	45099.094(20)	4.4±1.0	0.57±0.02	8.0±2.0 ^f
9 _{2,8} – 8 _{2,7}	45239.452(10)	3.2±0.8	0.73±0.10	4.1±0.6
9 _{3,7} – 8 _{3,6}	45291.918(10)			^g
9 _{3,6} – 8 _{3,5}	45294.382(20)	1.3±0.5	0.69±0.17	1.9±0.5
9 _{2,7} – 8 _{2,6}	45397.522(20)	1.5±0.5	0.52±0.15	1.8±0.6 ^h
9 _{1,8} – 8 _{1,7}	46135.431(10)	2.3±0.5	0.60±0.07	4.7±0.6
10 _{1,10} – 9 _{1,9}	49217.784(10)	3.2±0.7	0.65±0.10	4.9±0.6

Notes.

- (^a) Observed frequency assuming a v_{LSR} of 5.83 km s⁻¹.
(^b) Integrated line intensity in mK km s⁻¹.
(^c) Linewidth at half intensity derived by fitting a Gaussian function to the observed line profile (in km s⁻¹).
(^d) Blended with a negative feature produced in the folding of the frequency switching observing procedure.
(^e) Blended with two negative features produced in the frequency switching folding. The intensity is uncertain
(^f) Heavily blended with HCCCH₂CN. Frequency difference between both lines lower than 20 kHz. We estimate that the contribution of this contaminating feature, by comparison with other similar lines of this species, is ~50%
(^g) Fully blended with a negative feature produced in the frequency switching folding. The fit is unreliable.
(^h) Blended with two lines from other species. The separation between them still allows for a reasonable fit to the line parameters.

Appendix A: Line parameters of H₂CCHCCH and CH₃C₄H

Line parameters for the different molecules studied in this work were obtained by fitting a Gaussian line profile to the observed data. A window of ± 20 km s⁻¹ around the v_{LSR} of the source was considered for each transition. The derived line parameters for H₂CCCHCCH are given in Table A.1. Those of CH₃C₄H are provided in Table A.2.

Appendix B: Observed and calculated frequencies for H₂CCHCCH

In this section, we provide the full list of observed and calculated frequencies for allyl cyanide. The laboratory data come from McCarthy et al. (2020). All lines were weighted in the fit as $1/\sigma^2$. Laboratory data have an accuracy of 2 kHz, while the corresponding uncertainty for the rotational transitions measured in TMC-1 is 10 kHz, with the exception of four lines showing some partial blending with other features for which we assigned an uncertainty of 20 kHz.

Table A.2. Observed line parameters for CH₃C₄H in TMC-1.

J_u	K	ν (MHz)	$\int T_A^* dv^a$ (mK km s ⁻¹)	v_{LSR}^b (km s ⁻¹)	Δv^c (km s ⁻¹)	T_A^* ^d (mK)
8	2	32570.504	2.1 ± 0.5	5.80 ± 0.05	0.82 ± 0.11	2.4 ± 0.3
8	1	32571.457	30.8 ± 0.7	5.80 ± 0.02	0.74 ± 0.01	39.3 ± 0.3
8	0	32571.775	33.6 ± 0.7	5.80 ± 0.02	0.73 ± 0.01	42.8 ± 0.3
9	2	36641.764	2.8 ± 0.5	5.81 ± 0.03	0.79 ± 0.07	3.4 ± 0.3
9	1	36642.836	32.0 ± 0.7	5.79 ± 0.04	0.69 ± 0.01	43.8 ± 0.3
9	0	36643.194	33.9 ± 0.7	5.80 ± 0.02	0.69 ± 0.01	46.3 ± 0.3
10	2	40713.005	2.0 ± 0.5	5.78 ± 0.03	0.47 ± 0.08	3.9 ± 0.4
10	1	40714.197	31.9 ± 0.7	5.81 ± 0.02	0.57 ± 0.01	53.0 ± 0.4
10	0	40714.594	34.2 ± 0.7	5.80 ± 0.02	0.58 ± 0.01	55.2 ± 0.4
11	2	44784.226	2.2 ± 0.7	5.89 ± 0.05	0.61 ± 0.10	3.4 ± 0.5
11	1	44785.536	30.0 ± 0.8	5.79 ± 0.02	0.63 ± 0.01	44.5 ± 0.5
11	0	44785.973	30.9 ± 0.8	5.80 ± 0.02	0.60 ± 0.02	48.6 ± 0.5
12	2	48855.424	1.9 ± 0.6	5.85 ± 0.04	0.44 ± 0.07	4.1 ± 0.6
12	1	48856.853	23.8 ± 0.8	5.80 ± 0.02	0.57 ± 0.01	39.1 ± 0.6
12	0	48857.330	27.1 ± 0.8	5.80 ± 0.02	0.58 ± 0.01	44.2 ± 0.6

Notes. (^a) Observed frequency assuming a v_{LSR} of 5.83 km s⁻¹.

(^b) Local standard of rest velocity of the line in km s⁻¹.

(^c) Integrated line intensity in mK km s⁻¹.

(^d) Linewidth at half intensity derived by fitting a Gaussian function to the observed line profile (in km s⁻¹).

Table B.1. Observed frequencies for H₂CCCHCCH in the laboratory and in TMC-1.

Transition	ν (MHz)	Unc. (MHz)	ν_{cal} (MHz)	Unc. (MHz)	$\nu(obs - cal)$ (MHz)	
2 _{1,2} – 1 _{1,1}	9854.409	0.002	9854.4102	0.0004	-0.0012	A
2 _{0,2} – 1 _{0,1}	10056.532	0.002	10056.5335	0.0003	-0.0015	A
2 _{1,1} – 1 _{1,0}	10261.996	0.002	10261.9977	0.0005	-0.0017	A
3 _{1,3} – 2 _{1,2}	14780.736	0.002	14780.7355	0.0006	0.0005	A
3 _{0,3} – 2 _{0,2}	15081.411	0.002	15081.4106	0.0004	0.0004	A
3 _{2,2} – 2 _{2,1}	15088.775	0.002	15088.7753	0.0005	-0.0003	A
3 _{1,2} – 2 _{1,1}	15392.077	0.002	15392.0770	0.0007	0.0000	A
4 _{1,4} – 3 _{1,3}	19706.013	0.002	19706.0129	0.0007	0.0001	A
4 _{0,4} – 3 _{0,3}	20102.224	0.002	20102.2239	0.0006	0.0001	A
4 _{2,3} – 3 _{2,2}	20117.206	0.002	20117.2044	0.0006	0.0016	A
4 _{2,2} – 3 _{2,1}	20130.481	0.002	20130.4822	0.0006	-0.0012	A
4 _{1,3} – 3 _{1,2}	20521.046	0.002	20521.0456	0.0008	0.0004	A
5 _{1,5} – 4 _{1,4}	24629.906	0.002	24629.9066	0.0007	-0.0006	A
5 _{2,4} – 4 _{2,3}	25144.638	0.002	25144.6375	0.0007	0.0005	A
7 _{1,7} – 6 _{1,6}	34472.262	0.010	34472.2569	0.0013	0.0051	B
7 _{0,7} – 6 _{0,6}	35126.923	0.010	35126.9230	0.0020	0.0000	B
7 _{2,6} – 6 _{2,5}	35195.532	0.010	35195.5240	0.0011	0.0080	B
7 _{3,5} – 6 _{3,4}	35222.531	0.010	35222.5236	0.0025	0.0074	B
7 _{3,4} – 6 _{3,3}	35223.195	0.010	35223.2044	0.0024	-0.0094	B
7 _{2,5} – 6 _{2,4}	35269.664	0.010	35269.6575	0.0024	0.0065	B
7 _{1,6} – 6 _{1,5}	35897.418	0.010	35897.4116	0.0019	0.0064	B
8 _{1,8} – 7 _{1,7}	39390.116	0.010	39390.1081	0.0021	0.0079	B
8 _{0,8} – 7 _{0,7}	40118.252	0.010	40118.2535	0.0030	-0.0015	B
8 _{2,7} – 7 _{2,6}	40218.511	0.020	40218.4833	0.0016	0.0277	B
8 _{2,6} – 7 _{2,5}	40329.448	0.010	40329.4495	0.0038	-0.0015	B
8 _{1,7} – 7 _{1,6}	41018.002	0.010	41017.9994	0.0029	0.0026	B
9 _{1,9} – 8 _{1,8}	44305.369	0.010	44305.3697	0.0031	-0.0007	B
9 _{0,9} – 8 _{0,8}	45099.094	0.020	45099.0983	0.0044	-0.0043	B
9 _{2,8} – 8 _{2,7}	45239.452	0.010	45239.4588	0.0023	-0.0068	B
9 _{3,6} – 8 _{3,5}	45294.382	0.020	45294.4077	0.0034	-0.0257	B
9 _{2,7} – 8 _{2,6}	45397.522	0.020	45397.5168	0.0055	0.0052	B
9 _{1,8} – 8 _{1,7}	46135.431	0.010	46135.4358	0.0043	-0.0048	B
10 _{1,10} – 9 _{1,9}	49217.784	0.010	49217.7869	0.0045	-0.0029	B

Notes.^(A) Observed frequencies in the laboratory are from McCarthy et al. (2020).^(B) Frequencies observed in TMC-1 adopting a v_{LSR} of 5.83 km s⁻¹.^(b) Observed minus calculated frequencies in MHz.