#	TAG	MOLECULE	Min.Meas.(MHz)	Max Meas.(MHz)	Max Pred.(MHz)	J Max meas. *(or N)*	J Min meas. *(or N)*	K Max meas. (or Ka)	K Min meas. (or Ka)	Last M. (entry)	Database	lowest v level cm-1	QNF	Extra info spectro	extra info astro	Species name
														priority to measurements		
2	**13002**	**CH (v=0,1)**	701	4250352	14289108	5	1			2007 (2010)	JPL	2733	224	The latest JPL entry includes predictions for v = 1, but otherwise appears highly similar to that previously created in CDMS (13502) which gives predictions (for v=0 only) up to higher frequency (14.3 THz). Keywords: lamda-doubling, spin-rotation, LMR, infrared, not particularly rigid.	Detected (in list CDMS).	Methylidyne
2	**13503**	**CH^+ (ion)**	835137	835137	7398193	1	0			2010	CDMS	2753.6	101	* A combined fit of all available data of all isotopic species has been carried out. Note that the rotational transition measured is at different frequnency to that of previous entries. Additional rovibrational transitions between the electronic X and A states of four isotopologs were also used. There are two lines in the range of HIFI. Predictions should be viewed with some caution; considerable caution is advised for transitions beyond J" = 10. Keyword: ab-initio dipole moment		Methylidynium
2	14003	^{13}CH	7091	536132	14789069	2	1			2008 (2009)	JPL		255	$X\ ^2\Pi$ states, keywords: Hunds case(b), fine, hyperfine		13 C-Methylidyne
2	14004	CD	439255	916954	1862237	2	1			2008 (2009)	JPL		234	$X\ ^2\Pi$ states, keywords: Hunds case(b), fine, hyperfine		Methylidyne, deuterated
2	14502	**$^{13}CH^+$**			14033285					2010	CDMS		101	New entry. See parent 13503. The hyperfine splitting caused by the 13C nucleus may be relevant in quiescent sources for low values of J. A separate hyperfine calculation is provide on CDMS for J" up to 2.		
2	14503	**CD^+**	453521	453521	9479353	1	0			2010	CDMS		101	New entry. Combined isotopic fit. See parent 13503.		Methylidynium, $^1\Sigma^+$, deuterated isotopolog
2	**15501**	**NH**	946380	4874132	16488902	6	0			2004	CDMS	3125.6	134	measured sufficiently for HSO	IRC+10216; SgrB2: see CDMS	
2	15502	$^{13}CD^+$			8994188					2010	CDMS		101	New entry. Combined isotopic fit.See parent 13503.		Methylidynium, $^1\Sigma^+$, deuterated ^{13}C isotopolog
2	15503	$^{14}CH^+$			10392368					2010	CDMS		101	New entry. Combined isotopic fit.See parent 13503.		
2	15504	CT^+			5412134					2010	CDMS		101	New entry. Combined isotopic fit.See parent 13503.		
2	**16502**	**ND**	491907	1076738	8669055	2	0			2004	CDMS		104			
2	**17001**	**OH**	89	3789214	39855077	10	1			1986	JPL	3568.0	1905	Measured sufficiently for HSO. Intensities decrease rapidly above 100GHz and start to increase again around 1THz, lines at high energy in HSO range except 1.8 THz		
2	17005	OH v=1,2	1371	49662	29936152	7	1			1999	JPL		1905			
2	**17501**	**OH^+ (ion) *** $^21_{2+}$**	909045.2000	1033118.6000	13170659	1	0			2003	CDMS		**113**	2006 QNF corrected		
2	**20002**	**HF**	1232476.2700	6131968.4000	9732646.5590	5	0			1987	JPL		101	few lines	Sgr B2. See CDMS.	
2	21002	DF ?									JPL					
2	**26504**	**CN**	112101.656	(340247.770) 1020030 =>	4486683.1047	*9 =>*	*0*			2005	CDMS	2042.4	154	Measurements higher than indicated. Fine and hyperfine structure. Measurements available up till at least 1.02 THz that do not resolve hyperfine structure. However, for higher frequencies predictions with hyperfine structure are given rather than the measurements. Also unpublished work by Gottlieb (2005).		
2	27505	^{13}CN	108412.8620	217483.6060	4302620.3723	3	1			2005	CDMS		144	Data of all four stable isotopic species have been treated in one overall fit. Measured data for 13CN seems only available at low freq (check references).		
2	27506	$C^{15}N$	109689.6100	219934.8200	4350828.7129	3	1			2005	CDMS		123	Few lines measured. Data of all four stable isotopic species have been treated in one global fit. Rotational data on 12C15N is available only through interstellar observation		
2	**28503**	**CO**	115271	4340138	10329359	37	0			2000	CDMS	2143.2		measured sufficiently for HSO		
2	28505	$C^{13}N^{15}$			4166621					2005	CDMS		154			
2	**28513**	**CO+**	117692	589872	4096493	5	0			2009	CDMS		112	Unlike older JPL entry a value for the dipole moment is used and new data included in fit. Predictions beyond 1.5 THz should be viewed with some caution.	Typical PDR molecule. M17SW, NGC 7027, NGC 7023, IRAS 16293–2422. (CDMS)	Carbon monoxide cation
2	29	**SiH**									**No Entry**	me		Not in JPL/CDMS. predictions from LMR spectra available: Astrophys. J. 292 188-191 1985, Brown, Curl, Evenson, rotational spectrum starts at 625	Orion KL? See CDMS.	
2	29501	**^{13}CO ***	771184	3287972	7183021	30	6			2000 (2006)	CDMS		101	Seperate hyperfine calculation for low J available (CDMS). Lower freq measurements given on JPL.		
2	29503	**$C^{17}O$**	112358	898522	4449864	11	1			2003	CDMS		112			
2	**30008**	**NO**	0,6	464039	2993522	0.5	8.5			1978	JPL		814			
2	30502	**$C^{18}O$**	109782	1972210	6443872	18	0			2001	CDMS		101			
2	30503	**$^{13}C^{17}O$**	107288	965142	4250981	11	1			2003	CDMS		112			
2	31502	**$^{13}C^{18}O$**	104711	941966	6931121	9	0			2000	CDMS		112			
2	**31507**	**CF+ v = 0,1**	205170	512846	3857077	5	1			2010	CDMS	1766.3592 ?	1202	In this entry new recent measurements are used in a combined fit with ^{13}CF. Predictions should be viewed with caution above 1.5 THz and overall for the excited state. Keyword: partition funcntion. See CDMS.	Detection toward the PDR Orion-Bar see CDMS.	
2	**32001**	**O_2**	50474	2502324	11157474					2010	JPL (CDMS)	done	102	Or see CDMS 32508. Combined CDMS/JPL entry contains new data by Drouin et al 2010. Predictions should be viewed with caution above 4 THz.	rho-ophiuchi cloud see CDMS	Molecular oxygen

2	32002	O_2 v = 1	57726	62583	9816611	14	3			1987	JPL	1556.2	102			
2	32509	$^{13}CF^+$ v = 0,1	195494	586351	3865964	6	1			2010	CDMS		1202	Combined fit with parent see 31507. Keyword: dipole moment see CDMS.		Fluoromethylidynium, $X^1\Sigma^+$, ^{13}C
2	33003	**SH (v = 0, 1)**	100	7373958	9969260	14	1			1996	JPL		1325	Measurements lacking in HIFI operating range above 1 THz. Predicted errors around a few MHz in HSO range, lines at high energy except above 1.38 THz and below 447 MHz		
2	34001	$O^{18}O$	52413	1222204	9953715					2009 (2010)	JPL		102	Combined JPL/CDMS catalog entry. Keyword : intensity of magnetic dipole transitions		Molecular oxygen, singly substituted 18O isotope
2	34005	SD	13,6	1042864	9851932	6	1			1996 (1997)	JPL		234			
2	**36001**	**HCl**	625901	6196759	9759412	12	1			1987	JPL	2883.9	112		Dense interstellar cloud OMC-1. Sgr B2. See CDMS.	
2	36002	$^{18}O_2$	50981	1611544	9996308					2009 (2010)	JPL		102	Combined JPL/CDMS catalog entry. Keyword : intensity of magnetic dipole transitions		Molecular oxygen, double substituted 18O isotope
2	37001	DCl	323282	646504	8404310	2	0			1971 (1990)	JPL		112			
2	**38001**	**$H^{37}Cl$**	624964.3740	6187546.5500	9745148.8322	10	0			1987 (1989)	JPL		112			
2	40501	**SiC (v = 0)**	157949.1010	460028.0950	2015969.9412	11	3			1990	CDMS	953.2	203			
2	**42505**	**SiN**	87045.3570	741702.6260	1779777.0401	17	1			2006	CDMS	1138.4	133	The prediction contains 14N hyperfine splitting throughout even though it will be negligible in the submillimeter region. Calculations of frequencies with predicted uncertzainties much larger than 100 kHz should be viewed with some caution. The dipole moment is ab initio.	IRC+10216, Sgr B2(M), L15-L18 see CDMS	
2	**43501**	**CP**	95164.1580	1048418.6100	2598373.3372	23	1			1999	CDMS	1226.1	123		IRC+10216 see CDMS	Phosphaethynyl Radical
2	**44501**	**CS (v = 0 - 4)**	47570	1068287.1000	4694999.4530	22	0			2005 (2008)	CDMS	1272.2	1202	Global fit involving several isotopic species. Lines in vibrtationally exicted states are also given. The entry has recently been extended up to v=4. Transition frequencies with uncertainties larger than 100 kHz have not been merged. Keywords: partition function.	Detected up to v=3.	
2	**44505**	**SiO (v = 0 - 6)**	42519.3400	344916.2470	2589012.5819	8	0			1998	CDMS	1229.6	1202	Global isotopic invariant fit. Apparently only low freq measuremets (check refs) extrapolation to high freq and high v may have errors larger than those suggested in the predictions		
2	**45013**	**PN (v = 0 - 4)**	46656.3240	375856.3100	3289464.6075	9	0			1995	JPL		1203			
2	**45501**	**^{13}CS (v = 0, 1) ***	45922.0367	1015929.4150	4440300.5913	22	0			2003	CDMS		1202	Global fit involving several isotopic species. Lines in v = 1 are also given. A separate hyperfine calculation is available in CDMS. Transition frequencies with uncertainties larger than 100 kHz have not been merged. Keywords: ^{13}C spin-rotation hyperfine, partition function.	Detected in v=0	
2	**45502**	**$C^{33}S$ (v = 0, 1)**	289382.4250	1067228.5000	4657510.5427	22	0			2003	CDMS		1202	Global fit involving several isotopic species. Lines in v =1 are also given. A separate hyperfine calculation is available in CDMS up to J =5. Transition frequencies with uncertainties larger than 100 kHz have not been merged. Keywords: partition function.	Detected in v=0	
2	**45504**	**^{29}SiO (v = 0 - 3)**	42879.4200		1989338.7103	1	0			1998	CDMS		1202	Global isotopic invariant fit. One line only for this isotope ? - see main		
2	**46009**	**AlF**	32970.592	461329.74	3113107.6834	17	2			1974	JPL	792.7	112			
2	**46010**	**NS**	69002.8900	348515.8890	9070616.6252	7.5	0.5			1982	JPL		814			
2	**46501**	**$C^{34}S$**	47860.4681	1058904.1750	4622307.7012	22	0			2003	CDMS		1202	Global fit involving several isotopic species. Lines in v =1 are also given. Transition frequencies with uncertainties larger than 100 kHz have not been merged. Keywords: partition function.		
2	**46502**	**^{30}SiO (v = 0 - 3)**	42373.3400		1993420.4522	1	0			1998	CDMS		1202	Global isotopic invariant fit. one line only for this isotope ? - see main		
2	46503	$Si^{18}O$	40352.8020	443744.2520	1991223.6407	11	0			1998 (2000)	CDMS		1202			
2	46508	$^{13}C^{33}S$ *	275028.7950	915741.3800	3379131.6535	20	5			2003	CDMS		1202* (101)	*QNF inapropriate for main entry since vibrational QN is not given and should be 101. Global fit involving several isotopic species. A separate hyperfine calculation for ^{33}S is available in CDMS up to J =5. ^{13}C hyperfine splitting has NOT been considered. Keywords: partition function, ^{33}S hyperfine.	not yet detected	
2	**47006**	**PO**	64973.9510	980644.0000	2630371.2929					1983 (1997)	JPL		224	**The dipole is unknown so a unit dipole (1.0 Debye) was used in the calculations.** Hence intensities are not absolute. See other notes on JPL.	Oxygen rich circumstellar envelope VY Canis Majoris	
2	**47501**	**$^{13}C^{34}S$?**	45463.4240	953456.9850	3351634.5578	21	0			2004	CDMS		101	Global fit involving several isotopic species.	Possibly detected?	
2	48009	$N^{34}S$	6774.7500	114132.9700	9080242.0676	2.5	0.5			1982	JPL		814			
2	**48010**	**SO^+**	69408.3710	349433.3770	2290314.8719	8	1			1992	JPL		213			
2	**48501**	**SO (v = 0)**	13043.8070	1882560.1500	3759513.7368	45	0			1997	CDMS	done	102			
2	48502	SO v = 1	12752.2180	1023164.1430	2409014.8478	25	1			1998	CDMS	1138.0	102			
2	**48503**	**$C^{36}S$**	47508.8190	996292.3050	3499683.5060	21	0			2003	CDMS		1202*	*QNF corresponds to uncorrected global fit, the vibrational QN is superfluou and identifes the isotopologue. Global fit involving several isotopic species. Transition frequencies with uncertainties larger than 100 kHz have not been merged. Keywords: partition function.	Detected	
2	49501	^{33}SO	98474.6020	1021035.9900	2569279.0619	25	2			1996	CDMS		113			
2	49502	$S^{17}O$	61161.1500	620587.3070	2454351.8200	16	1			1996	CDMS		113			
2	49508	$^{13}C^{36}S$			3301037.8166					2003 (2004)	CDMS		1202* (101)	*QNF inapropriate for main entry since vibrational QN is not given and should be 101. Global fit involving several isotopic species. Because of the global nature of the fit, predictions could be made for this isotopologue even though no transition frequencies have been recorded. 13C hyperfine splitting has NOT been considered. Keywords: partition function.	Not detected	
2	**50501**	**^{34}SO**	12524.8710	1053242.4800	3184869.4845	26	0			1996	CDMS		102			

2	50502	$S^{18}O$	11134.2380	1034288.3120	2773455.3607	26	1			1996	CDMS		102			
2	52502	^{36}SO	104518.1030	952167.2770	2636098.0740	24	1			1996	CDMS		102			
2	**58502**	**NaCl (v = 0, 1)**	104189.7400	929326.9381	1633276.9968	73	7			2002	CDMS	361.1	1202			
2	60502	**$Na^{37}Cl$ (v = 0,**	113858.0300	928804.7309	1512312.8869	74	8			2002	CDMS		1202			
2	60506	**SiS v = 0 à 5**	17713.1040	922732.5790	2774259.4975	51	0			2007	CDMS		1202	rotational transitions including those in vibrationally excited states	IRC+10216 up to v=3, Sgr B2 ?, massiva star forming see CDMS	Silicon monosulfide
2	***61506***	***^{29}SiS v=0*** à 2	53463.3480	888189.9940	2579245.2911	50	2			2007	CDMS		1202	rotational transitions including those in vibrationally excited states	IRC+10216 see CDMS	
2	***61508***	***$Si^{33}S$ v =0*** à 1	339910.9610	571989.1850	2392393.5153	32	18			2007	CDMS		1202		IRC+10216 see CDMS	
2	62005	**AlCl**	14571.0739	14582.5121	1290084.7325	4	2			1993	JPL	477.4	132	Measured only J 0-1		
2	***62508***	***$Si^{34}S$ v = 0*** à 2	17488.2470	897547.8020	2556263.1530	51	0			2007	CDMS		1202	rotational transitions including those in vibrationally excited states	IRC+10216 see CDMS	
2	***62510***	***^{30}SiS v = 0*** à 2	17343.2990	924758.1800	2551612.8818	53	0			2007	CDMS		1202	rotational transitions including those in vibrationally excited states	IRC+10216 see CDMS	
2	62512	$^{29}Si^{33}S$			2151942.8057					2007	CDMS		101			
2	***63504***	***$^{29}Si^{34}S$ v=0*** à 1			2236770.3646					2007	CDMS		1202	rotational transitions including those in vibrationally excited states	IRC+10216 see CDMS	
2	63505	$^{30}Si^{33}S$			2130877.3038					2007	CDMS		101			
2	***64513***	***$^{30}Si^{34}S$ v=0*** à 1			2229342.3129					2007	CDMS		1202	rotational transitions including those in vibrationally excited states	IRC+10216 see CDMS	
2	***64514***	***$Si^{36}S$***	17214.9750	34429.8160	2126137.5509	2	0			2007	CDMS		101	2 lines measured	IRC+10216 see CDMS	
2	65507	$^{29}Si^{36}S$			1990088.3869					2007	CDMS		101			
2	66505	$^{30}Si^{36}S$	16570.6670	33141.2130	1969812.5546	2	0			2007	CDMS		101	2 lines measured		
2	72	**FeO**									no entry				Sgr B2 ? See CDMS	
2	**74505**	**KCl (v = 0, 1)**	99316.4400	928482.6368	1109074.1616	124	12			2004	CDMS	278	1202			
2	76504	$K^{37}Cl$ (v = 0, 1)	140997	924523	1078781	128	58			2004	CDMS		1202			
2	76505	^{41}KCl (v = 0, 1)	305265	907658	1084530	124	40			2004	CDMS		1202			
3	**4001**	**H_2D^+** **	155987	3453653	7546880	3	0	2	0	2010	JPL	2206.3	303	The new entry contains higher frequency data and uses IR combination differences. See JPL webpage for details. Ortho and para should be treated	First detection by Stark et al. 1999. 372 GHz ortho recently measured by Caselli et al. A&A Lett in prestellar core L1544. Tracer of massive very cold	
3	4581	**p-H_2D^+**									Vastel					
3	4591	**o-H_2D^+**									Vastel					
3	5501	**HD_2^+**	691660	1476605	15423940	2	0	2	0	2005	CDMS		303	large frequency uncertainty except on 3 lines measured. Ortho and para should be treated separately at low T. Ortho and para should be treated separately at low T ; available through links in the documentation file.	C. Vastel, T. G. Phillips, and H. Yoshida, Detection of D2H+ in the Dense Interstellar Medium Astrophys. J. 606, L127–L130 (2004).Models predict as abundant as H2D+	
3	5581	**p-HD_2^+**									Vastel					
3	5591	**o-HD_2^+**									Vastel					
3	14501	**CH_2**	68371	194253	13068464	6	0	5	0	2005	CDMS		2306	Ortho and para should be treated separately at low T ; available through links in the documentation file.	Toward Orion KL and W51. Toward Sgr B2 and W49 N(ISO Long Wavelength Spectrometer) see CDMS	
3	16501	**NH_2**			18207485	??	??			2001	CDMS		7416	Ortho and para should be treated separately at low T ; available through links in the documentation file. Measured lines do not seem to be indicated. Weak lines have large uncertainties, strong lines are OK. Hyperifine splitting.	Sgr B2 (N) and (M) see CDMS.	
3	**18003**	**H_2O** **	22235.0800	29683654.0339	29780343.4589	22	0	17	0	2005	JPL		1404		(first detection?) ortho observed in Orion, SgrB2, and W49 displaying maser activity: A. C. Cheung, D. M. Rank, C. H. Townes, D. D. Thornton, and W. J. Welch, Detection of Water in Interstellar Regions by its Microwave Radiation, Nature 221, 626–628 (1969).	
3	**18083**	**p-H_2O**									Vastel					
3	**18093**	**o-H_2O**									Vastel					
3	**18005**	**H_2O: v2, 2v2, v1, v3**	2159.9800	14997241.2259	14997828.7465	22	0	22	0	2005	JPL		1404	first 4 vibrations	v2 = 1 excited vibrational state detected in emission first towards VY CMa and W Hya: K. M. Menten and G. J. Melnick, Hot Water around Late-Type Stars – Detection of Two Millimeter Wave Emission Lines from the v2 Vibrationally Excited State Astrophys. J. 341, L91–L94 (1989).	
3	**19002**	**HDO**	486.5280	1950538.6900	9994626.2850	13	0	7	0	1985 (1989)	JPL		303		Reported first by B. E. Turner, N. Fourikis, M. Morris, P. Palmer, and B. Zuckerman, Microwave Detection of Interstellar HDO Astrophys. J. 198, L125–L128 (1975).	
3	**19003**	**$H_2{}^{17}O$**	13535.5140	748458.2540	9974156.2503	6	1	6	0	1975	JPL				Detected in emission toward Orion KL, Å. Hjalmarson,et al, Recent Astronomy Highlights from the Odin Satellite Adv. Space Res. 36, 1031–1047 (2005).	
3	**19004**	**H_3O^+ GS, v2=1**	307192	1807825	9897705					2010	JPL		1303	Rovibrational transitions. The two inversion states of the ground state, □v1 = 1, v2 = 1, □v3 = 1, □v4 = 1 states are included in this calculation. The vibrational labelling is given on the JPL webpage.	orion-KL, OMC-1, Sgr B2, orion BN, IRc2 (e.g. see CDMS)	Hydronium ion
3	**(19005)**	**H_3O^+ GS, v1, v3, v4 =1**	4579664							2010	JPL		1303	Not included in template since first line is already at 4 THz. First entry has minor sorting problem for frequencies.		
3	**20003**	**$H_2{}^{18}O$**	5625.1470	745320.2000	9995653.5393	7	1	7	0	1985	JPL				spec.	
3	**20081**	**p-D_2O**									Vastel			Vastel ortho/para (or see below)	See below	
3	**20091**	**o-D_2O**									Vastel			Vastel ortho/para (or see below)	See below	

3	**20502**	**D_2O**	10947.1339	5144901.4490 =>	29343954.9241	17	0	10	0	2007	CDMS		303	Or use 20081, 20091 (Vastel). ortho/para See extensive notes on CDMS webpage. S. Brünken, H. S. P. Müller, C. Endres, F. Lewen, and T. Giesen, B. Drouin, J. C. Pearson, and H. Mäder, 2007, Phys. Chem. Chem. Phys. 9, 2103. The dataset contains extensive v2 = 0 and 1 pure rotational data both with microwave and with infrared accuracy as well as extensive rovibrational transitions between these states. At lower temperatures, it may be necessary t distinguish between ortho-D2O and para-D2O.**In CASSIS seperate ortho/para calculations are available (tag 18083, 18093).**	detected in emission and absorption toward IRAS 16293-2422, a low-mass protostellar binary system: H. M. Butner, S. B. Charnley, C. Ceccarelli, S. D. Rodgers, J. R. Pardo, B. Parise, J. Cernicharo, and G. R. Davis, Discovery of Interstellar Heavy Water Astrophys. J. 659, L137–L140 (2007).	fully deuterated water
3	21001	$HD^{18}O$	5902.3800	241680.3800	9980036.1603	12	1	5	0	1978 (1991)	JPL		303			
3	**25501**	**CCH (v = 0)**	87284	960308	2953199	11	1			2009	CDMS	done	123	The present entry is based on new rest frequencies for the N = 1 – 0 and 2 – 1 transitions obtained from astronomical observations. Predictions should be reliable to around 1.5 THz. Keywords: vibrational partition function	IRC+10216 & TMC-1. Cold dark clouds, various. (AW)	Ethynyl
3	25503	CCH v2 = 1	170885.8410	348974.5230	2176757.3925	5	1	1	-1	1987 (2004)	CDMS	371.6	224	Because of the limited amount of data, predictions to higher frequencies should be viewed with some caution. Measurements at higher frequency needed ? (litterature not yet verified)+Y91		Ethynyl, $v_2 = 1$, Π_i
3	**26501**	**CCD**	72107.7000	360674.1700	1440578.4948	5	0			1985	CDMS		133		**DETECTED**	
3	26502	^{13}CCH	84119.3290	336656.4460	2097765.4760	5	1			1995	CDMS		154			
3	26503	$C^{13}CH$	85229.3260	341081.2830	2125248.0045	5	1			2010	CDMS		154	Newest entry includes in the fit rest frequencies for the N = 1 – 0 transition from astronomical observations		
3	**27501**	**HCN (v = 0) ***	5317.163479	1946190.8800	7725593.2476	22	5	0	0	2002	CDMS	done	1303	The main entry in CDMS does not give the hyperfine components. These can be obtained from a link on the information page. Done OK for HSO.	HCN is abundant in all kinds of environments, from dark clouds to star-forming regions and circumstellar envelopes. The detection was reported in detail by D. Buhl and L. E. Snyder, Astrophys. J. 163, L47–L52 (1971). The detection of H13CN was also reported. (HM)	
3	**27502**	**HNC (v = 0)**	90663.5680	1990360.6080	4219978.3546	22	0	0	0	2000	CDMS	done	1303	14N quadrupole structure unresolved. Done OK for HSO.		
3	27503	HCN v2 = 1 *	20181.4000	1955679.8250	6362708.3824	34	6	1	-1	2003 (2007)	CDMS	**1303**	**1303**	2006 QNF corrected. Separate hyperfine calculation. See v = 0.	Maser IRC+10216; Proto-Planetary Nebula CRL 618: See CDMS.	
3	27504	HNC v2 = 1	271924.1560	1989946.0770	4246855.0695	22	2	1	-1	2001 (2005)	CDMS	698	1303			
3	***27507***	***HCN v2 = 2***	89087.6900	1959441.1500	4166613.0671	22	0			2003 (2007)	CDMS		202		Maser IRC+10216 see CDMS	
3	27508	HCN v2 = 3	9242.2000	1968687.8130	4179641.0621	22	4			2003 (2007)	CDMS		202			
3	***27509***	***HCN v3 = 1 (CN stretch)***	88027.2800	967838.0990	4186792.4731	11	0			2003 (2007)	CDMS	2096.8	101		IRC+10216 including maser see CDMS	
3	***27510***	***HCN v1 = 1 (HC stretch)***	88006.6900	879724.0200	4186225.5956	10	0			2003 (2007)	CDMS	3311.5	101		IRC+10216 see CDMS	
3	**28515**	**$HN^{13}C$**	87090	174179	2171432	2	0			2001 (2009)	CDMS		101	At low J, the 14N, H, and 13C hyperfine splitting has been resolved in part in astronomical observations. Therefore, a separate hyperfine calculation up to J" = 2 is provided. Little mwave data(2 lines) but rovibrational data included in fit.Keyword: partion function(hyperfine splitting)		
3	28006	$H^{15}NC$	88865.7150	177729.0940	2918588.6767	2	0			1976 (1979)	JPL		101	two lines measured		
3	**28501**	**$H^{13}CN$ v=0**	517969.8210	1981790.0100	7295370.6353	23	5			2006 (2005)	CDMS	done	101		**see parent species**	
3	**28506**	**$HC^{15}N$ v = 0**	774257.6510	1975268.4380	6073980.1392	23	8			2005	CDMS		101		see CDMS	
3	28507	$HC^{15}N$ v2 = 1	8897.3650	1984698.2080	5773642.1934	23	1			2005	CDMS		202			
3	**28508**	**DNC**	228910	1979120	2959674	26	2			**2009**	CDMS		101	The 2009 entry contains new low-J data including resolved 14N and D hyperfine structure. A separate hyperfine calculation up to J" = 2 is provided. The predictions should be reliable up to 2.5 THz. Keywords: dipole moment, hyperfine partition function.	**DETECTED**	Deuterium isocyanide.
3	**28509**	**DCN v = 0 ***	506825.2550	1950663.1530	4574481.6951	27	6			2004 **(2006)**	CDMS	done		Prevision seems good enough for HIFI but limited number of lines measured A separate hyperfine calculation is provided from the information page. See notes on this page concerning the partition function.	**Orion nebula; PDR orion bar: see CDMS.**	
3	28510	DCN v2 = 1	20454.4000	946650.8940	4298895.2418	13	1			2004 **(2006)**	CDMS	check	1303	OK for HIFI. Prevision seems good enough for HIFI but limited number of lines measured. See notes on this page concerning the partition function.		
3	28511	$H^{13}CN$ v2 = 1	9018.8940	1990948.0360	7085460.1505	23	1			2005 **(2006)**	CDMS	check	202	OK for HIFI.The two vibrational states v = 0 and v2 = 1 have been treated together. Prevision seems good enough for HIFI but limited number of lines measured. (Very) weak lines badly predicted.		
3	(29002) not in templat	**HCO^+ v=0** v1=1,v2=1,2,v3=1	89188.5230	1163608.7748	3560637.3006	13	0			2007	JPL (or see CDMS)		1303	slightly less recent than CDMS (29507 & 29508) but includes simutlaneous fitting of vibrational states		
3	**29004**	**HCO**	86670.7600	352978.0600	2991424.2008	12	1	3	0	1983	JPL	1080.8	325	Inspection of database indicates measurements needed at higher frequency. Check references.		
3	**29504**	**HOC^+ (v2 = 0)**	89487.4140	805056.3990	3551189.0041	9	0	0	0	2000	CDMS		1303			Hydroxymethylidynium
3	29505	HOC^+ v2 = 1	536075.1000	813217.8120	3372831.5157	9	5			2000	CDMS		1303			
3	**29506**	**N_2H^+ (v = 0) ***	465824	745209	4342766	**8**	4			2009	CDMS		101	The full experimental data set has apparently not been merged. Hence the range of measured frequencies and QNs is probably larger than indicated. Check litterature quoted on CDMS. A separate hyperfine (14N) calculation i provided for J"≤ 4. With respect to the Feb. 2006 entry, improved rest frequencies for the strongest 14N hyperfine have been added. Keywords: partition function, H parameter estimation, 14N hyperfine.	P. Caselli, P. C. Myers, and P. Thaddeus, 1995, Astrophys. J. 455, L77.	Diazenylium

3	**29507**	**HCO^+ (v = 0)**	89188.5247	1158727.2266	4070444.5862	13	0			2007	CDMS **(or see JPL)**	829.7 (v2)	101	Combined fit of v2 = 0 and 1. See notes on CDMS webpage for all sources of data and details of fit. In particular: 1) F. Tinti, L. Bizzocchi, C. Degli Espost and L. Dore, 2007, Astrophys. J., 669:L113–L116, 2007. V. Lattanzi, A. Walters, B. J. Drouin, and J. C. Pearson, 2007, Astrophys. J., 662, 771. Predictions beyond 2 THz should be viewed with caution. The partition function takes into account both vibrational states; individual contributions are given in parentheses.		Oxomethylium, formyl cation
3	29508	HCO^+ v2 = 1								2007	CDMS		202	as above		
3	29509	N_2H^+ (v2 = 1)	? =>	? =>	? =>	? =>	? =>			2005 **(2006)**	CDMS			Measurements not indicated.The predictions are assumed to be reliable to at least 1.2 THz. Dipole moment of v = 0 used. See notes on info page for partition function and H constant.		
3	29510	$D^{13}CN$ *	427003.7370	711530.6410	4497346.8877	28	5			2004 **(2006)**	CDMS		101	OK for HIFI. The dipole moment was assumed to agree with that of DCN. The 14N hyperfine splitting can be resolved for low values of J; a separate hyperfine calculation is provided. Prevision seems good enough for HIFI but limited number of lines measured.		
3	29511	$DC^{15}N$	632897.7800	1964739.1460	4173683.8402	28	8			2005 **(2006)**	CDMS		101	OK for HIFIS. everal transitions have resolved the D or 15N hyperfine structure to a varying degree. The dipole moment was assumed to agree with that of DCN. Prevision seems good enough for HIFI but limited number of lines measured. Hyperfine struture not used for partition function		
3	29512	$H^{13}C^{15}N$ v=0	83727.5770	2005151.1810	5754472.9619	24	0			2004 (2006)	CDMS		101			
3	29513	$H^{13}C^{15}N$ v2=1	167411.1710	2004616.4500	5459047.2114	24	1			2004 (2006)	CDMS		202			
3	**30002**	**$H^{13}CO^+$**	86754.2884	1127120.8128	3450112.8615	13	0			2007	JPL		101	Both JPL and CDMS (30504) incoporate the most recent data of V. Lattanzi, A. Walters, B. J. Drouin and J.C. Pearson, 2007, Astrophys. J. 662. For the hyperfine structure at low J see CDMS webpage.	(1) E. M. Gregersen and N. J. Evans II, 2001, Astrophys. J., 553, 1042. (2) J. Schmid-Burgk, D. Muders, H. S. P. Müller, and B. Brupbacher-Gatehouse; 2004, Astron. Astrophys., 419 949.	
3	**30003**	**DCO^+**	72039,0	1151718	2952515	16	0			2007	JPL (or use CDMS)		1304			
3	30010	$HO^{13}C^+$	85752.7140	85752.7140	3400688.1444	1	0			1982 (1996)	JPL		101	1 line measured		
3	**30505**	**$HC^{17}O^+$**	261164.9200	348211.1530	3973833.8135	4	2			2001 (2004)	CDMS		101	(1) L. Dore, C. Puzzarini, and G. Cazzoli, 2001, Can. J. Phys., 79, 359.	see lab entry <=	
3	30506	DOC^+	152769.7930	839752.7080	3628272.6534	11	1			2000	CDMS		101			
3	30507	^{15}NNH+	90263.8330	90263.8330	2251403.6714	1	0			1990 (2005)	CDMS		101	**1 line measured**		
3	30508	$N^{15}NH+$			2274888.3860					1990 (2005)	CDMS		101			
3	**30509**	**N_2D^+ ***	385516	693806	3824865.5487	9	3			2009	CDMS		101	The full experimental data set has apparently not been merged. Hence the range of measured frequencies and QNs is probably larger than indicated. Check litterature quoted on CDMS. A separate hyperfine (^{14}N) calculation is provided for J"≤ 4. With respect to the Feb. 2006 entry, improved rest frequencies for the strongest ^{14}N hyperfine of J" = 0-2 have been added. Keywords: partition function, H parameter estimation; ^{14}N hyperfine.	L. Dore, P. Caselli, S. Beninati, T. Bourke, P. C. Myers, and G. Cazzoli, 2004, Astron. Astrophys. 413, 1177.	
3	(30510 not in template)	**DCO^+ ***								2009	CDMS =>		101	Or use JPL. CDMS web page gives separate hyperfine fitThe 2009 entry uses newly published astronomical observations for the J = 1 – 0 transition.	**see JPL entry**	
3	30511	$D^{13}C^{15}N$	276237.0150	1997724.0780	4098882.1358	29	0			2004 **(2006)**	CDMS		101	OK for HIFI. No hyperfine splitting and no excited vibrational states were considered in the calculation of the partition function. The dipole moment was assumed to agree with that of DCN. Prevision seems good enough for HIFI but limited number of lines measured.		
3	31004	$H^{18}OC^+$	86611.5600	86611.5600	3435041.9844	1	0			1982	JPL		101	1 line measured		
3	**31005**	**HNO**	18831.7300	498027.5870	9951970.4018	15	0	13	0	1984	JPL		304			
3	31007	$D^{13}CO^+$	70733.2180	1130859.8531	2815678.7226	16	0			2007	JPL		101	Or use CDMS. See notes on JPL and CDMS webpages and entry for parent species		
3	**31506**	**$HC^{18}O^+$**								2004	CDMS					
3	31508 (not in template)	$D^{13}CO^+$								2007	CDMS (or use JPL)					
3	32007	DNO	25823.3600	365690.3650	9526278.0916	12	0	11	0	1984	JPL		304			
3	32505	$DC^{18}O^+$	137653.5239	688073.0967	3214014.5887	8	1			2005	CDMS		101			
3	**34082**	**p-H_2S**									Vastel					
3	**34092**	**o-H_2S**									Vastel					
3	**34502**	**H_2S **	35028	7787379	16623204		0		0	1995 (2008)	CDMS		303	The predictions should be reliable as long as the uncertainties do not exceed much more than 5 MHz. Keywords FIR, ortho/para. In CASSIS seperate ortho/para calculations are available based on the previous JPL entry, see 34082, 34092.	Star-forming regions, circumstellar envelope of OH231.8+4.2, cold dark clouds L134N and TMC-1	hydrogen sulfide
3	**35502**	**HDS**	5161	628018	10243336					1971 / 1985* (2008)	CDMS		303	The predictions should be reliable as long as the uncertainties do not exceed much more than 5 MHz. Keywords FIR* (not merged).	Detected in G 34.3+0.15.1.	Hydrogen sulfide - mono-deuterated

3	35503	$H_2{}^{33}S$ **	168304	1071059	12063398					1995 (2008)	CDMS		314	The predictions should be reliable as long as the uncertainties do not exceed much more than 5 MHz. Keywords: ortho/para, hperfine, FIR transitions included in fit	not yet detected	Hydrogen sulfide - 33S isotopologue
3	**36082**	**p-D_2S**									Vastel					
3	**36092**	**o-D_2S**									Vastel					
3	**36502**	**C_3 ν_2**	1890558	2083626	3471933					2003 (2006)	CDMS	63.4 (this)	1303	Rovibrational transitions. Lines in THz region.	IRC +10216 Hinkle, K. H., Keady, J. J., & Bernath, P. F. 1988, Science, 241, 1319. SgR B2: KAO Boreiko, R. T., & Betz, A. L. 1996, ApJ, 464, L83; ISO Cernicharo, J., Goicoechea, J. R., & Caux, E. 2000, ApJ, 534, L199 etc. (AW)	Hydrogen sulfide, mono-deuterated species with 34S
3	**36503**	**D_2S** **	91359	672337	6938464					1971 / 1985* (2008)	CDMS		303	The predictions should be reliable as long as the uncertainties do not exceed much more than 5 MHz. In CASSIS seperate ortho/para calculations are available based on the previous JPL entry (tag 36082, 36092 below). Keywords: ortho/para, FIR*.	Detected toward two dense, cold clouds Barnard 1 and NGC 1333 IRAS 4A	Hydrogen sulfide - doubly-deuterated
3	**36504**	**$H_2{}^{34}S$** **	89756	1072501	13321849					1995 (2008)	CDMS		303	The predictions should be reliable as long as the uncertainties do not exceed much more than 5 MHz. Keywords: ortho/para, hyperfine	detected	Hydrogen sulfide - 34S isotopolog
3	37503	$HD^{34}S$	10802	52979	9071993					1951* (2008)	CDMS		303	*FIR transitions measured in 1985 have not been merged. The predictions should be reliable as long as the uncertainties do not exceed 3 MHz; transitions with predicted uncertainties larger than 5 MHz should be viewed with great caution.	no detection	
3	38507	$D_2{}^{34}S$ **								1985 (2008)	CDMS		303	No transition frequencies are available currently that have been measured wit microwave accuracy. It is recommended to view all predictions with some caution. Nevertheless, predictions with calculated uncertainties of less than 5 MHz and with quantum numbers smaller than 5 should be quite reasonable. Keywords: ortho/para	no detection	Hydrogen sulfide, doubly-deuterated species with 34S
3	39507	$H_2{}^{37}Cl+$	188433	484231	3993958	(4)	(1)	3	0	2001 (2010)	CDMS		314	Predictions with uncertainties much larger than 1 MHz should be viewed wit caution. Keywords: ortho/para, IR included in fit, dipole moment - see CDMS		Chloronium, X^1A_1, 37Cl isotopolog
3	**40006**	**C_2O**	9647	184794	1631159	9	0			1995	JPL		102		TMC-1 see CDMS	
3	**43003**	**AlO**	76553	382723	2120599	10	1			1990	JPL		123			
3	**44004**	**N_2O**	25123.2485	552487.0360	1527725.5937	22	0			1978	JPL		101		VY CANIS MAJORIS in 2009 (CDMS)	
3	44009	N_2O v2 = 1	75399.2600	1655744.2027	1854703.6425	**65**	2			2005 **(2006)**	JPL	589.6 ?	202	Seems OK for HSO. Hyperfine splittings are not calculated. The ground state dipole moment and partition function were used for the prediction.		
3	**44011**	**AlOH**	157390	377596	2229590	**12**	4			1993 (1996)	JPL		112		VY CANIS MAJORIS in 2010 (CDMS)	
3	44012	N_2O v2 = 2	25177.6500	554025.9980	1657775.5519	22	0	2	-2	1996	JPL		202			
3	***44502***	***HCP***	199749.4200	798364.7210	2573785.3070	20	4			2005 (2007)	CDMS		101		M. Agúndez, J. Cernicharo, and M. Guélin, Discovery of Phosphaethyne (HCP) in Space: Phosphorus Chemistry in Circumstellar EnvelopesAstrophys. J. 662, L91–L94 (2007).	
3	44503	HCP v2 = 1	159716.7300	799879.5100	1635253.5229	20	3			2001 (2000)	CDMS		202			
3	45007	$N^{15}NO$	25121.5500	1627093.5332	2588839.1026	65	0			2005	JPL			**New data by Drouin and Maiwald JMS 2005**		
3	45008	^{15}NNO	24274.6000	1620498.4356	2549724.4743	67	0			2005	JPL			**New data by Drouin and Maiwald JMS 2005**		
3	45503	DCP	33968.7300	1253948.4500	2192316.1309	37	0			2001 (2000)	CDMS		101			
3	**45506**	**HCS^+**	85347.8900	937918.3930	2833369.4633	22	1			2003	CDMS		101		Ori KL & Sgr B2 see CDMS	Thiomethylium, thioformyl cation
3	45510	$H^{13}CP$	153109.4990	459208.7550	2354750.1772	12	3			1996 (2007)	CDMS		101			
3	46007	$N_2{}^{18}O$	379413.9680	1630322.0418	2074014.4609	**69**	15			2005	JPL		101	**OK for HSO. New data by Drouin and Maiwald JMS 2005**		
3	46504	$H^{13}CS^+$	81777.3620	367943.1020	2556215.9349	9	1			2003	CDMS		101			
3	46505	DCS+	72072.5800	935925.5900	2396956.1750	26	1			2003	CDMS		101			
3	47502	$HC^{34}S^+$	125947.2380	880874.5050	2583138.4533	21	2			2003	CDMS		101			
3	**49510**	**NaCN**	10962.9463	39369.7637	999919.6853	13	0	2	0	1984 (2007)	CDMS		303		IRC+10216 and the PPN CRL 2688 see CDMS.	sodium (isocyanide)
3	**50009**	**MgCN**	101877.5560	376460.8690	997996.7757	38	9			1997	JPL		112			
3	**50504**	**MgNC v = 0**	11922.9251	369455.9730	1143910.3592	32	1			1998	CDMS		133			
3	50505	MgNC v2 = 1	325364.0840	375031.8710	722368.1654	32	26	1	-1	1998	CDMS		213			
3	50513	$Na^{13}CN$	10908.6373	30590.6388	999208.4267	13	0	2	0	1984 (2007)	CDMS		303			
3	**52527**	**c-SiC_2**	23600.2420	369498.2160	1970969.8789	17	3	0	0	1989 (2008)	CDMS		303	Dataset appears is as for JPL, but new analysis Since the data set is very sma predictions above 500 GHz or with predicted uncertainties larger than 0.5 MHz should be viewed with great caution. See notes on CDMS.		
3	52528	c-SiC_2 v3=1								1994 (2008)	CDMS		303			
3	52529	c-SiC_2 v3=2								1994 (2008)	CDMS		303			
3	***53501***	***AlNC***	131642.1890	-	1008129.0599	32	10			1997	CDMS		101		IRC+10216 see CDMS	
3	53509	c-$Si^{13}CC$								2008	CDMS		303		1) J. Cernicharo, M. Guélin, C. Kahane, M. Bogey, C. Demuynck, and J. L. Destombes, 1991, Astron. Astrophys., 246, 213. (2) J. H. He, D.-V. Trung, S. Kwok, H. S. P. Müller, T. Hasegawa, T. C. Peng, and Y. C. Huang, 2008, Astrophys. J. Suppl. Ser., accepted.	
3	53510	c-$^{29}SiC_2$								2008	CDMS		303		See above	

3	***54501***	***SiCN***	16584.9660	1092406.7201	338470.7840	31	1	1	-1	2001	CDMS		234		IRC+10216 see CDMS	
3	***54502***	***SiNC***	19138.8960	339593.7480	1259295.7709	27	1	1	-1	2001	CDMS		234		IRC+10216 see CDMS	
3	54505	c-$^{30}SiC_2$								2008	CDMS		303	see notes on CDMS	See 53509 above	
3	**55503**	**CCP**	120854	413287	1249841	32	9			2008	CDMS		224	Predictions with uncertainties larger than 0.5 MHz should be viewed with caution. Predictions for the higher-lying Π3/2 spin component should be viewed with **great** caution	IRC+10216: Halfen et al., Astrophys. J. 677, L101–L104 (2008)	Phosphapropynylidyne
3	56512	^{13}CCP	17793	30610	1179804	3	1			2009	CDMS		255	Predictions with uncertainties larger than 0.5 MHz should be viewed with caution. Moreover, all predictions for the higher-lying Π3/2 spin component should be viewed with great caution. Keyword: dipole momer		Phosphapropynylidyne, 13C on C1
3	56513	C^{13}CP	18544	31852	1227551	3	1			2009	CDMS		255	Predictions with uncertainties larger than 0.5 MHz should be viewed with caution. Moreover, all predictions for the higher-lying Π3/2 spin component should be viewed with great caution. Keyword: dipole momer		Phosphapropynylidyne, 13C on C2
3	**56502**	**C_2S**	11119.4460	285490.5060	1275906.9974	23	0			1992	CDMS		102			
3	**60503**	**OCS v = 0**	12162.9790	1090870.4590	1199079.2725	90	0			2005	CDMS		101	Recently updated. Reliable predictions are possible beyond the quoted Jmax of 99. See CDMS info on partition function and dipole moment.		
3	60504	OCS v2 = 1	12.7229	1117399.2370	1201716.5133	92	1	1	-1	1989	CDMS		202			
3	61502	O^{13}CS	12123.8420	315128.7740	1195219.5830	26	0			1988	CDMS		101			
3	61503	OC^{33}S	72057.8360	504036.3800	1172175.8523	42	5			1992	CDMS		101			
3	61504	^{17}OCS	70603.0220	493869.5540	1160262.6094	42	5			1990	CDMS		101			
3	62505	OC^{34}S	11865.6620	805302.9730	1169877.5912	68	0			1980	CDMS		101			
3	62506	^{18}OCS	11409.7080	501641.3840	1125161.1725	44	0			1987	CDMS		101			
3	62507	O^{13}C^{33}S	299149.1150	502328.1950	1168205.6583	42	24			1981	CDMS		101			
3	63502	O^{13}C^{34}S	11823.4608	496218.7360	1165715.0897	42	0			1990	CDMS		101			
3	63503	^{18}O^{13}CS	11382.1272	681950.6810	1122438.5186	60	0			2003	CDMS		101			
3	**64502**	**SO_2 v = 0**	4546.0180	3198148.1800	7970283.8563	91	1	84	0	1998	CDMS		303			
3	64503	SO_2 v2 = 1	5086.2522	1987667.4430	6052881.1218	81	0	75	0	1993	CDMS		303			
3	64510	OC^{36}S	11599.3720	486821.8280	1143721.6689	42	0			1987	CDMS		101			
3	64511	^{18}OC^{34}S	11119.9360	488909.7950	1096685.7050	44	0			1987	CDMS		101			
3	65501	$^{33}SO_2$	9592.3000	947591.7940	3449539.8070	48	1	39	0	2000	CDMS		314			
3	65502	SO^{17}O	7994.2000	833541.6490	2998057.2338	65	1	59	0	2000 (2007)	CDMS		304			
3	66501	$^{34}SO_2$	9650.6300	1067499.4960	6829231.0771	56	0	49	0	1998	CDMS		303			
3	66502	SO^{18}O	8360.6000	1062417.1030	3734294.0660	60	0	59	0	1998	CDMS		303			
4	**16503**	**CH_2D^+ ?!x**								2004	CDMS		1404	pure rot spectrum not meas		
4	**17002**	**NH_3**			39234952					2009	JPL		7336	The two inversion states of the ground state and the v2 = 1 state (see below) are included in the same calculation but this entry is a prediction of the ground state rotation-inversion transitions only.. See extensive notes on JPL website, including for constant coding. Measurements are not indicated but the dataset is discussed on the website and includes hyperfine, infrared and far-infrared.	Sgr B2 etc. see CDMS	
4	**17004**	**NH_3 v2 = 1**			39523460					2009	JPL		7336	The two inversion states of the ground state (see above) and the v2 = 1 state are included in the same calculation but this entry is a prediction of the v2 = 1 rotation-inversion transitions only. See extensive notes on JPL website, including for constant coding. Measurements are not indicated but the dataset is discussed on the website and includes hyperfine, infrared and far-infrared.	Towards Orion KL: see CDMS	
4	**18002**	**$^{15}NH_3$**			2991056					1981	JPL		1303		Orion Molecular Cloud (OMC-1): see CDMS.	
4	**18501**	**NH_2D**	7561.9200	854515.3000	10139983.9143	0	20			2004	CDMS		1404	Ortho and para should be treated separately at low T ; available through links	Sgr B2, Orion KL and Orion Nebula see CDMS	
4	**19004**	**H_3O^+, GS v2=1**	307192	3077891	9897705					2008 (2010)	JPL		1303	The two inversion states of the ground state, v1 = 1, v 2 = 1, v3 = 1, v4 = 1 states are included in this calculation. Vibrational assginements are explained on JPL helpfile. Keywords: inversion, vibrational states, estimated dipole moments (intensities) for v3 & v4.	Orion KL, OMC-1, SgrB2, Orion BN-IRc2	Hydronium ion
4	(19005)	H_3O^+ v1, v3, v 4 = 1	4579664							2008 (2010)	JPL			Outside HIFI range not in template. Combined analysis of vibrational states see 19004 above. Note a0=-10, b1=-21 etc.		
4	**19501**	**NHD_2**	5364	2578357	9234493					2007	CDMS		1404	Keywords: tunneling, ortho/para	L134N dark cloud (also known as L183): see CDMS	
4	**19504**	**$^{15}NH_2D$**	151616	656561	9613923					2008	CDMS		1404	Keywords: tunneling, ortho/para	Barnard-1b, NGC1333-DCO+, and L1689N in 2009. (see CDMS)	Ammonia, singly deuterated isotopolog with 15N
4	**20501**	**ND_3**	1302.3840	618124.8600	7298137.8546	19	0			1994 (2002)	CDMS		1303		NGC 1333 and in the Barnard 1 Cloud: see CDMS	
4	20503	H_2DO^{+**}	211108.8010	716959.3920	2476578.2338	0	0	4	3	2008 (2007)	CDMS		1404	See info on CDMS website for tunneling ortho/para and other important info. All predictions should be viewed with caution. Transitions with J ≤ 5 and Ka ≤ 3 may be reasonably well predicted.		
4	20504	$^{15}NH_2D$	172154	649587	7630603					2008	CDMS		1404	Extensive far-infrared data has not been merged. Predictions for low energy transitions should be good. Predictions with calculated uncertainties below 1 MHz should be reliable. Keywords: tunneling, ortho/para		
4	26002	C_2H_2 GS, v4, 2v4, v5, 2v5, v4+v5			7252450.9046					1991 (2007)	CDMS		1303	CHECK WHY FREQUENCIES DIFFERENT FROM CDMS ENTRYIdetected by rotation vibration spectrum,		
4	27511	HCCD	178347	653774	2369330	2		11		2008	CDMS		101	Predictions should be reliable up to at least 1.5 THz.	Not yet detected	Acetylene, ethyne, monodeuterated
4	28010	DCCD	365	18482876	19868994					2009	JPL		1303	Rovibrotational transitions between various vibrational states: GS, v4, 2v4, v5, 2v5, 3v5, v4 + v5, 2v4 + v5. Vibrational designations given on JPL webpage. Keyword: vibrational transition moment: uncertainty in intensities		Acetylene, ethyne: deuterated
4	**28502**	**H_2CN**	73342	368301	1994905.3766	5	0	5	0	1992	CDMS	954	6315	At low temperatures, it may be necessary to discern between ortho-H2CN and para-H2CN. hyperfine splitting		

4	**28504**	**$HCNH^+$**	148221	740922	3681460.9728	9	1			2007 (2006)	CDMS	645.9	101	With respect to the Aug 2006 entry, an H value was used in the fit. It was taken from (3) P. Botschwina, 1986, Chem. Phys. Lett. 124, 382.J" = 2 and 5 lines omitted from the fit. Predictions should be reliable up to about 1.3 THz. Uncertainities of around 1MHz quoted at 2 THz.The 14N hyperfine structure is resolvable in cold astronomical sources. Hyperfine structure has not been considered in the calculation of the partition function. See detailed notes on CDMS webpage.		
4	29502	$HCND^+$	190230	443831	3153024.6756	7	2			1998 (2001)	CDMS		101			
4	29514	$H^{13}CNH^+$	see=>	see =>	3232149.3040	na =>	na=>			2007 (1986)	CDMS			The predictions are based on infrared transitions only. Transitions uo to 1 THz may be found within 3 to 5 times the predicted uncertainties.		
4	**30501**	**H_2CO ****								2005	CDMS		303	Cassis separate ortho para entries see below.		Formaldehyde,
4	**30581**	**p-H_2CO**									Vastel					
4	**30591**	**o-H_2CO**									Vastel					
4	31501	HDCO	14.7000	1621678.5090	3499499.6013	37	0	33	0	1999	CDMS		303			
4	31503	$H_2{}^{13}CO$								2000	CDMS					
4	**32502**	**D_2CO ****	0	1853306	3499576	43	1	35	0	1999	CDMS		303	Cassis separate ortho para entries see below.	**DETECTED**	
4	32582	p-D_2CO									Vastel					
4	32592	o-D_2CO									Vastel					
4	32503	$H_2C^{18}O$								2000	CDMS					
4	32507	$HD^{13}CO$	14800	262950	997957					1978 (2008)	CDMS		303	Because of the very small data set, predictions probably only reliable if they have ΔJ = 1, ΔKa = 0, and uncertainties of 1 MHz at most. The small b-dipol moment component of about 0.2 D has been omitted because these transitions can not be predicted with confidence at present.	Parent isotopologue detected	Formaldehyde, singly deuterated isotopologue with 13C
4	33506	$D_2{}^{13}CO$	16015	288555	3498448					1978* (2008)	CDMS		303	* Also contains FIR data measured in 2005 and that dominates the dataset. Because of this data the predictions should be adequate throughout not only for astronomical observations but also for laboratory spectroscopy. Transition frequencies with very small predicted uncertainties may deviate from their predicted positions by slightly more than three times the uncertainties. Keywords: ortho/para.	Parent isotopologue detected	Formaldehyde, doubly deuterated isotopologue with 13C
4	**34501**	**PH_3 ?**								2006 (2008)	CDMS		202	Full set of measured transitions probably not given in catalogu see references At low temperatures, it may be necessary to discern between A-PH_3 (K = 3n) and E-PH_3 (K = 3n ± 1). The nuclear spin-weight ratio is 2 : 1 for A-PH3 with K > 0 and all other states, respectively. Note: The A_1/A_2 splitting may be resolvable in astronomical observations. The $J = 1_1$ level is the lowest E state leve at 8.3711 cm^{-1} above ground.	Tentative detection in 2008 in IRC+10216 And CRL 2688 (HM).	Phosphine
4	**37003**	**c-C3H**	14686	441572	1617188					1994 (1995)	JPL		325			Cyclopropynylidyne
4	**37501**	**l-C_3H v = 0, v4 = 1**	2683	571024	3398041		0			2009	CDMS		1325	Linear molecule with symetric top coding because of additional contirbution to angular momentum. Lines correspond to vibrational ground state (v=0); v4 = 1, $^2\Sigma^u$ (v=1); and transitions between the two. Predictions for the rovibrational transitions between the lower lying $^2\Pi_{1/2}$ state and the $^2\Sigma^u$ state, which occur around 1 THz, should be viewed with some caution; the same applies to all transitions having predicted uncertainties much larger than 1 MHz. Keywords: vibrationally excited, vibrational transitions, Renner Teller, coriolis interaction, transition dipole moment.	N. Kaifu, M. Ohishi, K. Kawaguchi, S. Saito, S. Yamamoto, T. Miyaji, K. Miyazawa, S.-I. Ishikawa, C. Noumara, S. Harasawa, M. Okuda, and H. Suzuki, 2004, Publ. Astron. Soc. Japan 56, 69.	Propynylidyne,
4	38004	c-$CC^{13}CH$								1994 (1995)	JPL		356			
4	38005	c-$^{13}CCCH$								1994 (1995)	JPL		356			
4	38006	c-C3D								1992 (1995)	JPL		335			
4	38503	l-C_3D *	99657.7910	304013.0100	1492411.3585	15	5			2005 (2009)	CDMS		1314	Linear molecule with symetric top coding because of additional contirbution to angular momentum. Lines correspond to vibrational ground state (v=0); v4 = 1, 2Σμ (v=1); and transitions between the two. A separate hyperfine calculation is provided on CDMS up to N = 5. Since no rovibrational transitions have been observed thus far predictions of this type of transitions should be viewed with caution; the same applies to all transitions having predicted uncertainties much larger than 1 MHz. Keywords: partition function, hyperfine (D), vibrationally excited, vibrational transitions, Renner Teller, transition dipole moment.	not detected	
4	38504	$^{13}CCCH$ v = 0, v4 = 1	157303.5990	326689.5490	990189.8659	16	1	1	-1	2004	CDMS		1356	see parent isotopologue & CDMS	not detected	
4	38505	$C^{13}CCH$ v = 0, v4 =	163466.7300	331408.1350	985276.9385	16	1	1	-1	2004	CDMS		1356	see parent isotopologue & CDMS	not detected	
4	38506	$CC^{13}CH$ v = 0, v4 =	158631.4000	329287.7170	997976.5260	16	1	1	-1	2004	CDMS		1356	see parent isotopologue & CDMS	not detected	
4	**39501**	**HCCN**	6686.7620	197801.1030	1488932.4592	9	0			1993	CDMS		114		IRC+10216, Sgr B2, and Orion A: see CDMS	cyanomethylene radica
4	**43509**	**HCNO**	22938	275227	2052001	0	12			1971 (2009)	CDMS		101	Keywords: hyperfine(<69 GHz), quasi-linear, partition function	Detected in dark clouds in 2009. Protostar L1527. Also in L1527, L1544, L183. Not found in TMC (CDMS).	Fulminic acid, hydrogen fulminate

4	**43510**	**HOCN**	167792	357985	1496945	17	7	4	0	2009	CDMS		303	Predictions with uncertainties exceeding 0.5 MHz and with Ka = 3 and 4 should be viewed with caution, all higher Ka transitions with great caution. 14N hyperfine splitting may be resolved for low values of J. Therefore, a separate hyperfine calculation is provided (CDMS) for J'≤ 8 and Ka ≤ 1. The Ka = 1 hfs splitting should be viewed with caution. Keywords: omitted b-type transitions.	Tentatively detected in SgRB2(OH) (CDMS)	Cyanic acid, hydrogen cyanate
4	**43511**	**HNCO**	11191	1079147	4993777					2007 (2009)	CDMS		303	The FIR transitions from (3) (with uncertainties of 3 MHz or more) have not been merged. The predictions should be reliable throughout. 14N hyperfine splitting may be resolved for low values of J & a separate hyperfine calculation is provided for a-type transitions with J≤ 7 and Ka ≤ 1. Keywords:partition function, dipole moment (see CDMS).	SgRB2 (OH). Dark clouds such as TMC1. (CDMS)	Isocyanic acid, hydrogen isocyanate
4	44006	DNCO	8422.9600	246100.6550	2996027.5329	31	0			1975	JPL		304			
4	44007	$H^{15}NCO$	8378.5300	106985.7500	2988712.5397	40	3	40	0	1975	JPL		303			
4	44008	$HN^{13}CO$	8839.1600	198536.0000	2998388.6396	39	0	39	0	1975	JPL		304			
4	44513	DCNO	41169	329301	1842318	16	1			1971 (2009)	CDMS		101	The predictions are reliable up to about 1000 GHz. Keywords: quasi-linear, partition function	Not yet detected	Fulminic acid, deuterated isotopolog; deuterium fulminate
4	44514	$H^{13}CNO$	110913	399202	1919510	18	4			1990 (2009)	CDMS		101	The predictions should be reliable up to about 1200 GHz. Keywords: quasi-linear, partition function	Not yet detected	Fulminic acid, hydrogen fulminate; isotopolog with 13C
4	44514	$HC^{15}NO$	91744	435674	1939131	19	3			1995 (2009)	CDMS		101	The predictions should be reliable up to about 1200 GHz. Keywords: quasi-linear, partition function	Not detected	Fulminic acid, hydrogen fulminate; isotopolog with 15N
4	45006	$HNC^{18}O$	8030.8500	208670.1600	2990826.7433	45		45	0	1975	JPL		304			
4	**45010**	**$HOCO^+$**	124932.4450	425864.0189	9993730.1796	29	5	29	0	1988	JPL		303		SgrB2, Sgr A, low mass protostar IRAS 04368+2557 in L1527: see CDMS	Oxyhydroxymethylium, protonated carbon dioxide
4	46011	DOCO+	120429.3210	403850.5450	2312046.1620	20	5	6	0	1988 (1995)	JPL		303			
4	46012	$HO^{13}CO^+$	340695.6800	406119.6630	9982276.4773	19	15	19	0	1988	JPL		303			
4	**46509**	**H_2CS ****	1046.4866	927286.0370	3752898.4549					**2008**	CDMS		303	With respect to the 2006 entry, ground state combination differences were taken from D. J. Clouthieret et al. J. Chem. Phys. 101 7300. Additional millimeter and submillimeter transitions were published by A. Maeda et al. 2008, Astrophys. J. Suppl. Ser., accepted. Predictions with uncertainties of less than 1 MHz should be sufficiently reliable. (HM). See other information on CDMS. Separate ortho/para may be necessary at low T.		
4	**47504**	**HDCS**	91171.0670	378785.3600	1830368.9927	12	0	7	0	1997 (2004)	CDMS		303	The dipole moment was derived from that of that main isotopomer. There is a small b-dipole moment component of about 0.1D. However, since no b-type transitions have been observed, no reliable predictions can be made for this type of transitions.	**DETECTED**	
4	47505	$H_2{}^{13}CS$ **	967.5870	67024.9600	1963950.5906	8	0	1	0	1993 **(2006)**	CDMS		303	Separate ortho/para may be necessary at low T. See notes on precision of predictionsHigher order distortion parameters were estimated based on H2CS data and were kept fixed in the fit. The dataset is considerably smaller than that of the main isotopic species. Nevertheless, transitions with ΔJ = 1 and Ka = 0 and 1 should be fairly reliable up to 150 GHz. Transitions with higher values of Ka should be viewed with increasing caution. The dipole moment of the main isotopic species is used.		
4	47506	$H_2C^{33}S$ **	1020.7220	37010.1330	1499558.3409	8	0	1	0	1987 **(2006)**	CDMS		314	Hyperfinc structure given in predictions. Separate ortho/para may be necessary at low T. See notes on precision of predictions. Higher order distortion parameters were estimated based on interpolation between H2C34S and H2CS values and were kept fixed in the fit. The H2C33S dataset is much smaller than that of the main isotopic species. Nevertheless, transitions with ΔJ = 1 and Ka = 0 and possibly 1 should be fairly reliable up to about 100 GHz, possibly higher. Transitions with higher values of Ka should be viewed with increasing caution.		
4	**48507**	**D_2CS ****	7924.4600	145461.9650	998509.4504	40	0	5	0	2005 **(2006)**	CDMS		303	Separate ortho/para may be necessary at low T. The dipole moment was assumed to agree with that of the main isotopic species	N. Marcelino, J. Cernicharo, E. Roueff, M. Gerin, and R. Mauersberger, 2005 Astrophys. J. 620, 308.	
4	48508	$H_2C^{34}S$ **	21230.1500	68539.9400	1974065.8449	8	0	1	0	1993 **(2006)**	CDMS		303	Separate ortho/para may be necessary at low T. See notes on precision of predictions Higher order distortion parameters were estimated based on H2CS data and were kept fixed in the fit. The H2C34S dataset is considerably smaller than that of the main isotopic species. Nevertheless, transitions with ΔJ = 1 and Ka = 0 and 1 should be reliable up to 200 GHz or even higher. Transitions with higher values of Ka should be viewed with increasing caution. The dipole moment of the main isotopic species was used.		
4	**50511**	**C_3N v = 0**	9885.8900	197890.1010	976720.9482	21	1			1983	CDMS		133	July 2007. Corrected intensity in C3N, v = 0; the partition function had considered the lowest excited vibrational state, however, the old predictions did not.		
4	50512	C_3N v_5 = 1	188517.3650	278447.4260	981444.5819	28	18	1	-1	1989	CDMS		213	See notes on CDMS concerning hyperfine structure etc.		
4	**50514**	**C_3N^- (anion) ***	97029	504182	957962	52	9			2010	CDMS		101	Latest entry includes new measurements.A separate hyperfine calculation is provided up to J" = 4. (http://www.ph1.uni-koeln.de/cdms/catalog/archive/C3N-/c050514_hfs.cat). Keywords ^{14}N hyperfine, spin multiplicity, partition function	IRC+10216: Thaddeus et al.,Astrophys. J. 677, 1132–1139 (2008). Searched for, but not found in TMC-1.	Cyanoethynylide Ion
4	51511	$^{13}CCCN$	19073.6040	276671.5560	714512.9661	29	0			2003	CDMS		144			
4	51512	$C^{13}CCN$	9829.3690	186975.8250	736775.6040	19	0			2003	CDMS		144			
4	51513	$CC^{13}CN$	9847.7130	266119.7610	738104.4944	27	0			2003	CDMS		144			
4	51514	$C_3{}^{15}N$	9593.4860	268815.7720	719001.5987	28	0			2003	CDMS		123			
4	**52501**	**C_3O**	9621	739493	1102022	77	0			2008	CDMS	120	101	Keyword: Partition function	Detected	Oxopropadienylidene
4	52530	C_3O v5 = 1	19367	589876	1079671	61	1			2008	CDMS	120*	202	Keyword: Partition function	Not detected	Oxopropadienylidene, v5 = 1

4	53516	^{13}CCCO	27796.9600	46328.0380	905428.2292	5	2			1985 (2009)	CDMS		101	Predictions should be reliable up to about 120 GHz only because of the very small data set.	Not detected	Oxopropadienylidene, 13C on C1
4	53517	C^{13}CCO	28705.4110	57410.4210	915960.4753	6	2			1985 (2009)	CDMS		101	see above	Not detected	Oxopropadienylidene, 13C on C2
4	53518	CC^{13}CO	28787.8950	57575.2840	918584.7636	6	2			1985 (2009)	CDMS		101	see above	Not detected	Oxopropadienylidene, 13C on C3
4	54511	$C_3{}^{18}O$	36578.1640	182869.5470	866440.0273	20	2			1985 (2009)	CDMS		101	Predictions should be reliable up to about 300 to 400 GHz.	Not detected	Oxopropadienyliden; 18O isotopolog
4	**59503**	**HNCS a type**	35135	1064196	1158499	91	2		0	1995	CDMS		303		Sgr B2(OH) & Sgr B2(N)	Isothiocyanic acid
4	**59504**	**HNCS b type**	944663	1053985	4764344	30	20	1	0	1995	CDMS		303	6 lines measured		Isothiocyanic acid
4	**59505**	**HSCN**	79863	345650	1121747	30	6	15	0	2009	CDMS		303	Predictions of transitions with Ka≥ 7 and with uncertainties exceeding 0.5 MHz should be viewed with caution. 14N hyperfine splitting may be resolved for low values of J &, a separate hyperfine calculation is provided for J≤ 10 and Ka ≤ 1. Keywords: spin multiplicity of 14N, unpredicted b-type transitions	SgrB2(N) in 2009.	Thiocyanic acid. Hydrogen thiocyanate
4	**64501**	**c-SiC$_3$**	1169.7670	285513.3020	997987.7727	26	0	26	0	1999	CDMS		303			
4	**64505**	**l-SiC$_3$**	10990.8460	274643.7860	543059.9867	50	1			2000	CDMS		102			
4	**68503**	**C$_3$S**	5780.7590	294699.8400	571427.2405	51	0			1992	CDMS		101			
4	69502	C^{13}CCS	11445	17168	565698	3	1			1992	CDMS		101	2 lines measured		
4	69503	^{13}CCCS	5566	16698	550238	3	0			1992	CDMS		101	3 lines measured		
4	70502	$C_3{}^{34}S$	5640	293198	557603	52	0			1992 (2001)	CDMS		101			
5	17003	CH_3D	232644	1626393	4828251	7	0	6	0	2009	JPL		202	Combined entry with CDMS (17503). The latest entry combines new THz data by Drouin et al. Keywords: IR ground state combination differences, distortion corrections (caution Intensities J>8), separate A & E species at low temperatures.	No detection.	Methane; monodeuterated isotopolog
5	18006	$^{13}CH_3D$	464838	1625012	4824332	7	1	6	0	2009	JPL		202	Combined entry with CDMS (18504). The latest entry combines new THz data by Drouin et al. Keywords: IR ground state combination differences, approximations to 12C, distortion corrections (caution Intensities J>8).	No detection	Methane; 13C and D substitution
5	**29003**	**CH$_2$NH (H$_2$CNH)**	5288	110899	2997263	(33)	(0)	6	0	1973 (1981)	JPL	1061	304	14 N HFS	1st (Sgr B2) P. D. Godfrey, R. D. Brown, B. J. Robinson, and M. W. Sinclair, Discovery of Interstellar Methanimine (Formaldimine) Astrophys. Lett. 13, 119–121 (1973). One transition, 110 –111 near 5290 MHz, with 14N hyperfine pattern. Abundant also in other hot core sources; e.g.: J. E. Dickens, W. M. Irvine, C. H. De Vries, and M. Ohishi, Hydrogenation of Interstellar Molecules: A Survey for Methylenimine (CH2NH) ApJ. 479, 307–312 (1997). (HM)	Methanimine. Methylenimine.
5	**30005**	**^{13}CH$_2$NH**	62454	129950	2974174	4	0	1	0	1977 (1980)	JPL		303		S.E. Cummins, R.A. Linke, and P. Thaddeus, A Survey of the Millimeter-Wave Spectrum of Sagittarius B2, ApJ. Suppl. Ser. 60, 819–878 (1986).	13C see above
5	30006	$CH_2{}^{15}NH$	62424.6400	129897.0200	2993001.6763	4	0	1	0	1977 (1980)	JPL		303			
5	30007	CH_2ND	30646.3200	128302.4900	2988534.9242	13	0	3	0	1977 (1981)	JPL		304			
5	**31504**	**H$_2$COH$^+$**	121864.5260	384683.2560	1997560.0253	11	1	10	0	1995	CDMS		303		Detected toward Sgr B2, Orion KL, W51, and possibly in NGC 7538 and DR21(OH). It was not found toward several dark clouds. The account was reported by M. Ohishi et al. Astrophys. J. 471, L61–L64 (1996). (HM see CDMS)	Protonated formaldehyde
5	32506	$H_2{}^{13}COH^+$	118779.5050	223978.8810	2494937.7240	6	1	2	0	1997 (2006)	CDMS		303			
5	**38002**	**c-C$_3$H$_2$**	18343.1430	410296.0840	4974063.8403	35	1	27	0	1993	JPL		1404		TMC-1. Laboratory and astronomical identification of cyclopropenylidene, C3H2, Thaddeus, P.; Vrtilek, J. M.; Gottlieb, C. A., ApJ Lett, (2) 299, L63-L66 (1985). (AW)	
5	**38501**	**l-C$_3$H$_2$**	145420.8200	370597.0940	1192403.1429	18	6	18	0	1990 (2002)	CDMS		303	The predictions, in particular at higher J or Ka, should be viewed with some caution.The dipole moment is from a quantum chemical calculation. At low temperatures, it may be necessary to discern between ortho and para. (HM)		Propadienylidene
5	39001	c-H^{13}CCCH	119816.2000	246958.4870	4520733.5967	24	2			1987 (1996)	JPL		303			
5	39002	c-HC^{13}CCH	142698.1700	245932.6860	3316794.2352					1987 (1996)	JPL		303			
5	39003	c-C_3HD	118648.1170	296782.7070	4482246.8043					1987 (1996)	JPL		303			
5	39502	l-^{13}CCCH$_2$	20004.4920	363090.6300	1044855.6529	18	0			2002	CDMS		314			
5	39503	l-C^{13}CCH$_2$	20785.1530	356428.6380	1044242.1767					2002	CDMS		314			
5	39504	l-CC^{13}CH$_2$	20194.4420	386906.7250	1040700.4215					2002	CDMS		314			
5	**40505**	**H$_2$CCN ***	219267.2440	284215.0700	1486204.5572	*14*	*10*	6	1	2004 (2005)	CDMS		314 (6315)	1H/14N hfs info N<10 ortho/para. Main entry includes 4 quantum numbers: N, Ka, Kc, and J + 1/2; separate hyperfine calculation for low freqs see CDMS info page for access and info on partition function etc.	1st: W. M. Irvine et al, Identification of the Interstellar Cyanomethyl Radical (CH2CN) in the Molecular Clouds TMC-1 and Sagittarius B2, Ap. J. 334, L107–L111 (1988). Lines observed but not identified: S. E. Cummins, R. A. Linke, and P. Thaddeus, A survey of the millimeter-wave spectrum of Sagittarius B2, Ap J. 576, 819–878 (1986). (HM)	Cyanomethyl radical
5	**42003**	**NH$_2$CN**	7383.5960	476409.9280	7299967.4835	65	0	62	0	1988	JPL		1404		SgrB2. Microwave detection of interstellar cyanamide, Turner, B. E.; Liszt, H S.; Kaifu, N.; Kisliakov, A. G., ApJ 201 (2), L149-L152 (1975). (AW)	Cyanamide

5	**42501**	**H_2CCO**	377.4158	783725.3470	1770462.7337	41	0	41	0	2003	CDMS		303	At low temperatures, it may be necessary to discern between ortho-H2C2O and para-H2C2O.	First identified toward Sgr B2 by B. E. Turner, Microwave Detection of Interstellar Ketene Astrophys. J. 213, L75–L79 (1977). Also detected, e.g., in Orion and in TMC-1. (HM)	Ethenone. Aka ketene
5	43505	$H_2C^{13}CO$	1132.2420	363595.5370	1455601.2167	18	0	17	0	2003	CDMS		303			
5	43506	$H_2{}^{13}CCO$	19457.5620	352051.0290	1429113.1762	18	0	17	0	2003	CDMS		303			
5	43507	HDC_2O	7901.0800	323720.9250	1275654.7783	26 $	0	8	0	2005 **(2006)**	CDMS		303	$ for DJ=0 otherwise 17 See notes on fit. Some higher order centrifugal distortion constants were kept fixed to values estimated from the main isotopomer. The dipole moment was assumed to be the same as for the main isotopomer		Singly deuterated ethenone (ketene)
5	44508	$H_2CC^{18}O$	18702.8430	383446.7640	1344659.5916						CDMS					
5	44509	D_2C_2O	3408.7500	340554.6310	1242850.6773	26 $	0	10	0	2005 **(2006)**	CDMS		303	$ for DJ=0 otherwise 19. At low T ortho/para. See notes on fit => Some higher order centrifugal distortion constants were kept fixed to values estimated from the main isotopomer. The dipole moment was assumed to be the same as for the main isotopomer		Doubly deuterated ethenone (ketone)
5	**46506**	**t-HCOOH**	0.0891	991288.3950	3665062.3438	56	2	51	0	2002	CDMS		303		Formic acid, HC(O)OH, seems to be a fairly typical hot core molecule that is quite abundant. A first transition of this molecule was detected toward Sgr B2 The detection of formic acid in a dark cloud was also reported. (HM) See CDMS.	Formic aicd - trans isomer
5	46507	c-HCOOH	16350.1500	991277.5900	4656249.8071	47	0	47	0	2002	CDMS		303	1365 cm-1 higher in energy than trans conformer,	No detection but the trans- isomer has been detected.	Formic acid - cis isomer
5	47002	t-H^{13}COOH	8060	1181298	1899983		0		0	2008	JPL		303	New measurements of submillimeter lines Lattanzi et al. 2008 ApJS..176..536.		Formic acid (trans) - 13C isotope
5	47003	t-DCOOH	8559	1177023	1899973		0		0	2008	JPL		303	New measurements of submillimeter lines Lattanzi et al. 2008 ApJS..176..536.		Formic acid (trans) - D isotope on C atom
5	47004	t-HCOOD	8831	1195662	1899984		0		0	2008	JPL		303	New measurements of submillimeter lines Lattanzi et al. 2008 ApJS..176..536.		Formic acid (trans) - deuteratium isotope on O atom
5	47008	c-DCOOH	15643	1148642	1899998					2008	JPL		303	New measurements of submillimeter lines Lattanzi et al. 2008 ApJS..176..536.		Formic acid (cis) - deuteratium isotope on C atom
5	47009	c-HCOOD	19004	1195397	1899885					2008	JPL		303	New measurements of submillimeter lines Lattanzi et al. 2008 ApJS..176..536.		Formic acid (trans) - deuteratium isotope on C atom
5	47010	c-H^{13}COOH	14471	1093963	1899886					2008	JPL		303	New measurements of submillimeter lines Lattanzi et al. 2008		Formic acid (cis) - 13C isotope
5	47503	t-H^{13}COOH	8060.4500	991971.1290	3102446.6531	51	0	45	0	2002	CDMS		303			
5	**49503**	**C_4H v = 0**	9493.0600	199850.7870	938976.5496	22	1			1995	CDMS		123		IRC+10216, TMC-1, diffuse medium, PDRs: see CDMS	
5	***49504***	***C_4H v7 = 1***	227824.2870	295416.6560	940843.1357	32	23	1	-1	1987	CDMS		213		IRC+10216 see CDMS	
5	***49505***	***C_4H v7 = 2^0***	229466.0260	296410.8560	943295.8623	32	23			1987	CDMS		112		IRC+10216 see CDMS	
5	***49506***	***C_4H v7 = 2^2***	228787.4780	296478.2080	942681.0268	32	23	2	2	1987	CDMS		213	$v_7 = 2^2$	IRC+10216 see CDMS	
5	**49509**	**C_4H^-**	9309	502364	873179	54	0			2008(2009)	CDMS		101	negative ion $X\,^1\Sigma+$	IRC +10216, toward the Low-Mass Protostar IRAS 04368+2557 in L1527: see CDMS	Butadiynylide ion
5	**50506**	**C_4D**	88308.0340	282577.1670	871799.5818	32	9			2005	CDMS		112		TMC-1 see CDMS	
5	***50507***	***$^{13}CCCCH$***	9166.2450	275602.9650	824738.4306	29	1			1995	CDMS		154		IRC+10216 see CDMS and check publication to know which 13C species	
5	***50508***	***$C^{13}CCH$***	9448.1650	284004.6390	849840.0313	31	1			1995	CDMS		154		IRC+10216 see CDMS and check publication to know which 13C species	
5	***50509***	***$CC^{13}CH$***	9462.6150	303386.2790	851130.3928	33	1			1995	CDMS		154		IRC+10216 see CDMS and check publication to know which 13C species	
5	***50510***	***$CCC^{13}CH$***	9208.7700	267608.3040	828438.0098	29	1			1995	CDMS		154		IRC+10216 see CDMS and check publication to know which 13C species	
5	*50515*	*C_4D^-*	25944	34592	397604	4	2			2008	CDMS		101	negative ion $X\,^1\Sigma+$. Only two measured lines? Predictions may be reliable up to around 150 GHz.	Parent isotopolog (49509) has been detected.	Butadiynylide ion, deuterated species
5	**51004**	**HCCNC**	9935.2000	327787.1860	991053.6033	33	1			1992	JPL		102		TMC1, IRC+10216.Detection of isocyanoacetylene HCCNC in TMC-1, Kawaguchi et al, ApJ(2) Lett. 386, L51-L53 (1992). Detection of HCCNC from IRC+10216, Gensheimer, P. D., Ap. J. Lett. 479, L75 (1997). (AW)	Ethyl isocyanide
5	51005	HCCNC v7 state	49793.1590	329088.2610	984982.7858	34	4	1	-1	1992	JPL		202			see above
5	51006	HCCNC v6 state	49761.8290	249000.1210	983834.0023	25	4	1	-1	1992	JPL		202			see above
5	51007	HCCNC v5 state	49688.3820	248559.9040	985342.5941	25	4	1	-1	1992	JPL		202			see above
5	51008	HNCCC	9336.1300	46683.1000	931415.1922	5	0			1993 (1995)	JPL		102		First detection not yet found in literature check refs.	3-Imino-1,2-propa-dienylidene
5	**51501**	**HC_3N (0,0,0,0)**	9098.1152	808199.2820	1864103.0738	89	0			2000	CDMS		101		SgrB2, Orion KL, TMC1, IRC+10216, CRL618 (inc vib), ext galaxies? Detection of Interstellar Cyanoacetylene, Turner, B. E., Ap.J., 163, L35 (1971). Vibrational states in CRL618 e.g. Observational Evidence of the Formation of Cyanopolyynes in CRL 618 through the Polymerization of HCN Pardo, Juan R.; Cernicharo, José; Goicoechea, Javier R., ApJ., 628(1), 275-282 (2005) Vibrationally excited HC_3N toward hot cores, Wyrowski, F.; Schilke, P.; Walmsley, C. M., Astron. Astrophys. 341, 882-895 (1999)	Cyanoacetylene, Propynenitrile
5	**51502**	**HC_3N (0,0,0,1)**	39.2313	811266.5005	1496775.3987	89	2	1	-1	2000	CDMS		202		CRL 618	
5	**51503**	**HC_3N (0,0,0,2)**			1295034.3570					2000	CDMS		202		CRL 618	
5	**51504**	**HC_3N (0,0,1,0)**	27339.1500	810134.6222	1459120.0447	89	2	1	-1	2000	CDMS		202		CRL 618	
5	**51506**	**HC_3N (1,0,0,0)**	9085.6350	806962.0643	1247697.8863	89	0	1	-1	2000	CDMS		202		CRL 618	
5	**51507**	**HC_3N v4 = v7 = 1**	72872.8030	791969.2169	1135502.9280	87	7	1	-1	2000	CDMS		202		CRL 618	
5	**51508**	**HC_3N v5 = 1, v7 = 3**	36395.8000	808697.7686	1081479.0324	89	3	3	-3	2000	CDMS		303		CRL 618	
5	51509	HC_3N v4 = 1, v7 = 2 / v5 = 2^{0e}	128067.2700	709201.8560	1028928.5985	78	13	2	-2	2000	CDMS		303			

5	**52508**	**DC_3N**	50658.5980	211050.8420	808947.6258	25	5			1983 (2005)	CDMS		101		**DETECTED.** In spectral survey Caux et al IRAS16293 low energy lines seem present	
5	52509	$H^{13}CCCN$	8816.9010	616482.1720	1045775.9010	70	0			2001 (2004)	CDMS		101			
5	52510	$HC^{13}CCN$	9059.5430	615366.8550	1083406.9076	68	0			2001 (2004)	CDMS		101			
5	52511	$HCC^{13}CN$	9060.4030	615426.0480	1083510.0567	68	0			2001 (2004)	CDMS		101			
5	52512	$HCCC^{15}N$	8833.5450	608840.1300	1047745.2529	69	0			2004	CDMS		101			
5	52513	DC_3N v7 = 1	67703.9470	296540.4300	786630.8155	35	7			1988 (2005)	CDMS		202			
5	**52514**	**$H^{13}CCCN$ v7 = 1**	123737.9720	618843.6290	874177.6994	70	13			2001 (2005)	CDMS		202		CRL618 (AW)	
5	**52515**	**$HC^{13}CCN$ v7 = 1**	118218.8110	617682.5510	898105.0108	68	12			2001 (2005)	CDMS		202		CRL618 (AW)	
5	**52516**	**$HCC^{13}CN$ v7 = 1**	136226.2140	608696.9820	898218.0566	67	14			2001 (2005)	CDMS		202		CRL618 (AW)	
5	52517	$HCCC^{15}N$ v7 = 1	123968.6160	796520.4180	875809.8060	90	13			2004 (2005)	CDMS		202			
5	**52518**	**$H^{13}CCCN$ v7 = 2**	124211.9189	620903.2583	796090.6327	70	13			2001 (2005)	CDMS		202		CRL618 (AW)	
5	**52519**	**$HC^{13}CCN$ v7 = 2**	118491.7460	610032.7530	810594.8104	67	12			2001 (2005)	CDMS		202		CRL618 (AW)	
5	**52520**	**$HCC^{13}CN$ v7 = 2**	118512.1167	610707.5674	808821.8786	67	12			2001 (2005)	CDMS		202		CRL618 (AW)	
5	**52521**	**$H^{13}CCCN$ v6 = 1**	123634.4141	617957.9346	872960.5047	70	13			2001 (2006)	CDMS		202		CRL618 (AW)	
5	**52522**	**$HC^{13}CCN$ v6 = 1**	127031.1551	616832.6728	896905.7816	68	13			2001 (2006)	CDMS		202		CRL618 (AW)	
5	**52523**	**$HCC^{13}CN$ v6 = 1**	127040.3336	607829.7373	896977.3103	67	13			2001 (2006)	CDMS		202		CRL618 (AW)	
5	52524	$H^{13}CCCN$ v5 = 1 / v7 = 3	35268.8200	176421.3350	711443.8913	20	3			2001 (2006)	CDMS		1303			
5	52525	$HC^{13}CCN$ v5 = 1 / v7 = 3	36240.3600	172223.0700	721810.0794	19	3			2001 (2006)	CDMS		1303			
5	52526	$HCC^{13}CN$ v5 = 1 / v7 = 3	36243.8400	621586.0645	895427.7291	68	3			2001 (2006)	CDMS		1303			
5	**55501**	**HC(O)CN ***	122743.8270	437076.0670	1998978.0148					1995 (2006)	CDMS		303	Separate calculation with hyperfine structure available up to 300 GHz with J up to 25. Predictions of transitions with very high quantum numbers or at rather high frequencies should be viewed with caution. Transition frequencies with predicted uncertainties of less than 1 MHz should be reliable. (HM) see other information on CDMS including partition function.	Sgr B2 (2008) see CDMS.	formyl cyanide, cyanoformaldehyde
5	**76009**	**C_4Si**	128819.5490	147216.3280	699668.4491	48	41			1989	JPL		101	6 lines measured		
6	**32003**	**CH_3OH (vt = 0,1,2)**	not merged	not merged	5999954	30 see JPL		13 see JPL		2008 (2010)	JPL		1304	New entry to 6THz for Herschel. See extensive notes on JPL. Measured lines have not been merged. The quantum numbers are J, (sign)K , (parity), ɣ. Note a=-10, B=-20 e.g. a2 = -12. The parities + and - refer to A^+ and A^- states; while states with no parity designation refer to E symmetry. A signed value of K_a is used to differentiate $^+E_1$ from $^-E_2$ states. . Keywords: internal rotation, torsion-rotation interaction, centifugal distortion, rho axis method, FTIR transitions included, intensity (see details on JPL and CDMS)		
6	33502	**$^{13}CH_3OH$ (vt = 0,1)**	9153.500	680000.172	999158.832	20	0			1997	CDMS		999(?)			
6	33	**CH_3OD**									no entry				**DETECTED**	
6	33	**CH_2DOH**									no entry				**DETECTED**	
6	34	**CHD_2OH**									no entry				**DETECTED**	
6	35	**CD_3OH**									no entry				**DETECTED**	
6	**41001**	**CH_3CN (vt =**	8208	1482121	1831361	82	0			1996	JPL		1304	Only for v=1 see new entry for v=0 below	TMC1, CRL618	Methyl cyanide
6	**41009**	**CH_3NC**	40210	140733	1972037	7	1	6	0	1970	JPL		202			
6	**41010**	**CH_3CN (v8 = 1)**	8208	1394532	1831361	*76*	*0*	13	0	1996 (1997 / 2010?)	JPL	this is	1304	See JPL website for coding of v. Keywords: approximation of some constants and dipole moment (see JPL)	Orion (listed on CDMS)	Methyl cyanide, acetonitrile, cyanomethane: lowest vibrational state.
6	**41503**	**H_2CCNH (CH_2CNH) ?**	? =>	? =>	? =>					1984 (2006)	CDMS		303 (1405)	Freq of meas not indicated check refs. Because of the small data set, predictions of transitions with uncertainties exceeding 300 kHz should be viewed with some caution, those with uncertainties larger than 1 MHz should be viewed with great caution. 4N HFS + tunneling info.	SGRB2(N, LMH)	Etheneimine. Ketenimine

6	**41505**	**CH_3CN**	331014	1626658	1806588	89	18	21	0	2009	CDMS		202	Joint CDMS/JPL.Or see JPL 41001. New entry contains high frequency measurements. Separate hyperfine calculations available up to J" = 9 (184 GHz). Keywords 14N hyperfine, A & E states	Sgr(B), SgR(A) ?, dark clouds, IRAS 16293-2422, IRC+10216,	Methyl cyanide, acetonitrile, cyanomethane
6	**42508**	**$^{13}CH_3CN$**	71464	1192700	1754708	67	3	15	0	2009	CDMS		202	Joint CDMS/JPL. Or see JPL 42006. New entry contains high frequency measurements. Separate hyperfine calculations available up to J" = 5 (108 GHz). Keywords 14N hyperfine, A & E states	Orion A	Methyl cyanide, acetonitrile, cyanomethane: 13C substitution
6	**42509**	**$CH_3{}^{13}CN$**	91939	1191056	1805678	64	4	15	0	2009	CDMS		202	Joint CDMS/JPL. Or see JPL 42007. New entry contains high frequency measurements. Separate hyperfine calculations available up to J" = 5 (111 GHz). Keywords 14N hyperfine, A & E states	SgRB2, Orion A	Methyl cyanide, acetonitrile, cyanomethane: 13C substitution
6	**42510**	**$CH_3C^{15}N$**	17844	1191252	1682984	67	0	12	0	2009	CDMS		202	Joint CDMS/JPL. Or see JPL 42001. Keywords: A & E states	SgRB2(N)	Methyl cyanide, acetonitrile, cyanomethane: 15N substitution.
6	**42511**	**CH_2DCN**	34584	1196285	1510292	69	1	10	0	2009	CDMS		303	Joint CDMS/JPL. Or see JPL 42008. Keyword:; small b-dipole transition (caution for predictions)	Irc2 Orion	deuterated acetronitrile
6	43513	$^{13}CH_3{}^{13}CN$	249849	1138866	1683729	64	13	9	0	2009	CDMS		202	Joint CDMS/JPL. Or see JPL 43005. New entry contains high frequency measurements. Separate hyperfine calculations available up to J" = 5 (108 GHz). Keywords 14N hyperfine, A & E states,main isototope approximations.	not yet detectd	Methyl cyanide, acetonitrile, cyanomethane: double 13C substitution.
6	**45003**	**NH_2CHO**	1538	84807	1930619	30	0	25	0	1973	JPL		304			
6	**50503**	**l-C_4H_2**	8931	367531	805098	41	0	3	0	2002	CDMS		303	Missing from previous entry of this table. Predictions unreliable for Ka>3 and not given. Keywords: calculated dipole moment, treat ortho and para separately at low temperature	Detected (CDMS list)	butatrienylidene
6	**52503**	**HC_3NH^+**	8658	34631	294300	5	0	67		2000	CDMS		102			
6	**54504**	**c-H_2C_3O**	9161.6100	246319.8100	1235569.5519	27	0	12	0	1990 (2002)	CDMS		303		Sgr B2(N) laregly in absorption; see CDMS.	cyclopropenone
6	**54510**	**HCCCHO (HC_2CHO)**	15146	187063	2642979	20	1	10	0	1973 (2008)	CDMS		303	The latest entry from CDMS also includes ground state combination differences. Otherwise data is for previous JPL entry. Predictions with uncertainties larger than 1 MHz should be viewed with caution.	W. M. Irvine et al., New Interstellar Polyatomic Molecule – Detection of Propynal in the Cold Cloud TMC-1, Astrophys. J. 335, L89–L93 (1988). And Sgr B2(N) (CDMS).	Propynal. Propiolic aldehyde.
6	**61505**	**C_5H**	7152.1720	284026.8140	669999.1983	59	1			2005 **(2006)**	CDMS		224	Also see JPL predictions to higher frequency. Predictions for the hyperfine splitting in the higher lying 2Π3/2 spin component as well as those for transitions above 400 GHz should be viewed with caution. Dipole moment ab initio.	IRC +10216, TMC-1: see CDMS	Pentadiynylidyne
6	**63501**	**l-HC_4N ***			455421.8628					1999 (2004	CDMS		102	Measurements not indicated in database - check J. Tang, Y. Sumiyoshi, and Y. Endo, 1999, Chem. Phys. Lett. 315, 69. See CDMS for hyperfine structure and info on the partition function.	IRC +10216 see CDMS	Cyanoethynylmethylene
6	**74501**	**C_5N**	5604.2490	16842.3053	269238.1937	6	2			1997	CDMS		133		TMC-1 & IRC+10216 ? See CDMS.	Cyanobutadiynyl ion
6	**74513**	**C_5N^- ***	22221	111099	529646.0620	40	7			(2008)	CDMS		101	$X^1\Sigma^+$ No laboratory data are available at present but very accurate ab initio calculations, provide reliable spectroscopic parameters. The predictions are probably reliable up to 200, maybe even 300 GHz. A separate hyperfine calculation is available on CDMS. Keywords: ^{14}N hyperfine, partition function	Detection in IRC+10216, Cernicharo et al, 2008, ApJ 688, Issue 2, pp. L83-L86.	Cyanobutadiynylide
7	**31008**	**CH_3NH_2**	3015	4118281	5588227					2005 (2009)	**JPL**		1303	NEW ENTRY in 2009. The vibrational designations are: 0 for the A species; 1 for A_2 ; 2 for B_1 ; 3 for B_2 ; 4 for E_1 , l = 1; 5 for E_1 , l = -1; 6 for E_2 , l = 1; 7 for E_2 , l = -1.	N. Kaifu, K. Nagane, K. Akabane, T. Iguchi, K. Takagi, Detection of interstellar methylamine, ApJ. 191 L135-L137 (1974)	methylamine
7	**40502**	**CH_3CCH**	153673.4387	1192389.4880	1881099.8961	70	8	21	0	2008	CDMS		1303			Propyne. Methyl acetylene.
7	40504	CH_3CCH v10 = 1	17139.5880	924549.0600	1619465.0522	54	0			2003	CDMS		1303		The v10 = 1 state of propyne is the lowest excited, doubly degenerate bending state of this molecule. It corresponds to v8 = 1 of CH3CN, which has been detected in the ISM. (HM)	see above
7	40507	CH_3CCH v10			11287797.5623					2004 (2005)	CDMS		1303			see above
7	40508	CH_3CCH v9			20394671.3068					2004 (2005)	CDMS		1303			see above
7	41002	$CH_3C^{13}CH$	33160.3500	215522.1700	1322766.7664	13	1	7	0	1977	JPL		202			see above
7	41003	$CH_3{}^{13}CCH$	34168.4700	239152.9400	1343825.4935	14	1	10	0	1977	JPL		202			see above
7	**41501**	**CH_3CCD**	15576.3292	451489.5040	994474.6254	29	0	18	0	1993 (2002)	CDMS		202		**DETECTED**	see above
7	**41502**	**CH_2DCCH**	4686.8880	470746.9290	999981.6228	29	0	12	0	1993 (2002)	CDMS		303		**DETECTED**	see above
7	41004	$^{13}CH_3CCH$	33252.2200	149630.2600	1324329.5694	9	1	6	0	1977	JPL		202			see above
7	42	**CHD_2CCH**									no entry				**DETECTED**	
7	**44003**	**CH_3CHO A&E vt=0,1,2**	5778	417240	899946	26	1			1996 (2008)	JPL		1404	New simultaneous fit combining A & E species ground, 1st & 2nd torsional states. Data fits to experimental precision, however much of the frequency data above 300 GHz is of 1 MHz precision or worse. Gs: A-0; E-1,2. Vt=1: A 3; E-4,5. Vt=2: A-6; E-7,8. Keywords: internal rotation,ρ axis method, torsions, partition function.		acetaldehyde
7	**44504**	**c-C_2H_4O**	23061	357422	1499649	49	0	35	0	1998	CDMS		303			
7	**53001**	**C_2H_3CN v=0 ; v11=1 ; v15=1**	5844	1158221	1999994	125	0			2009	JPL	239 (v11) 340 (v15)	1405	New entry includes recent measurements and analyis, including higher frequency data. Also for the ground vibrational state 14N quadrupole splittings have been fitted where they have been resolved experimentally. Coding of vibrations: 0 = ground state; 1 = in plane CCN bend v11 = 1; 2 = CCN out of plane bend, v15 = 1. See detailed notes on JPL webpage. Keywords: .parttiton function, dipole moment, perturbations from interaction of vibrational states- See detailed notes on JPL webpage	SgrB2, TMC-1, IRC+10216. Vibrational states: SgrB2(N), orion KL. See CDMS.	Vinyl cyanide, acrylonitrile, propenenitrile
7	54001	$CH_2CH^{13}CN$	18432	29007	348699	3	1	3	0	1959	JPL		303			

7	54002	$CH_2{}^{13}CHCN$	18405.3300	28996.4500	177319.9110	3	1	3	0	1959	JPL		303			
7	54003	**$^{13}CH_2CHCN$**	18032.4600	28364.8000	179667.3544	3	1	3	0	1959	JPL		303		SgrB2. See CDMS.	
7	54004	CH_2CDCN	9382	207365	799773					1996	JPL		303	omitted in last version of table		acyrlonitrile D(2) substitution
7	54008	$CH_2CHC^{15}N$	9206	529803	699755		0		0	2009	JPL		303	keyword : ge dipole moment used		Acrylonitrile, 15N isotope
7	**73502**	**C_6H^-**	8261	187212	440066	68	2			2006	CDMS		101	**negative ion**	TMC-1 & IRC+10216: see CDMS	
7	**73501**	**C_6H ***	70690.3900	219086.4040	550231.7018	79	25	1	-1	2005	CDMS		213		TMC-1 & IRC+10216: Low-Mass Protostar IRAS 04368+2557 in L1527; see CDMS. Vibrationally excited also detected Cernicaro et al submitted to ApJS (AW)	Hexatriynyl,
7	74506	$^{13}CC_5H$	12122.2660	20211.1760	268214.6511	7	3			2005	CDMS		255			
7	74507	$C^{13}CC_4H$	12339.7460	20569.9450	271823.1188	7	3			2005	CDMS		255			
7	74508	$C_2{}^{13}CC_3H$	12460.0810	20768.3810	275602.3788	7	3			2005	CDMS		255			
7	74509	$C_3{}^{13}CC_2H$	12464.2210	20776.8630	275725.5064	7	3			2005	CDMS		255			
7	74510	$C_4{}^{13}CCH$	12353.5310	20591.2700	272092.2864	7	3			2005	CDMS		255			
7	74511	$C_5{}^{13}CH$	12153.6110	20258.3660	268844.2142	7	3			2005	CDMS		255			
7	**75503**	**HC_5N v = 0**	26626.5430	457367.0890	528924.3648	172	9			2004	CDMS		101		observed with vibrational states in CRL618 (Cernicaro et al), Orion-KL (AW)	
7	**75504**	**HC_5N v11 = 1**	24003.5180	269476.1590	298791.3594	101	8	1	-1	2004	CDMS		202		CRL618 (AW)	
7	**75505**	**HC_5N v11 = 2**	26737.8400	229992.4040	264749.0429	86	9	2	-2	2004	CDMS		202		CRL618 (AW)	
7	**75506**	**HC_5N v10 = 1**	29348.6200	269348.0220	298650.6430	101	10	1	-1	2004	CDMS		202		CRL618 (AW)	
7	**75507**	**HC_5N v11 = 3**	29447.5000	230454.9270	265258.1412	86	10	3	-3	2004	CDMS		202		CRL618 (AW)	
7	75508	HC_5N v11 = 4	37587.9500	231059.7870	265954.7095	86	25	4	-4	2004	CDMS		202			
7	75509	HC_5N v9 = 1	29320.5800	269158.7170	298441.1664	101	10	1	-4	2004	CDMS		202		may be detected?	
7	(55510)	HC_5N v7								2005	CDMS		1303	High frequency data corresponding to rovibrational transitions. Not included in ISM template.		
7	**76506**	**DC_5N**								2004	CDMS		101		TMC-1 (AW)	
7	**76507**	**$H^{13}CC_4N$**								2004	CDMS		101		TMC-1 (AW)	
7	**76508**	**$HC^{13}CC_3N$**								2004	CDMS		101		TMC-1 (AW)	
7	**76509**	**$HC_2{}^{13}CC_2N$**								2004	CDMS		101		TMC-1 (AW)	
7	**76510**	**$HC_3{}^{13}CCN$**								2004	CDMS		101		TMC-1 (AW)	
7	**76511**	**$HC_4{}^{13}CN$**								2004	CDMS		101		TMC-1 (AW)	
7	76512	$HC_5{}^{15}N$								2004	CDMS		101			
8	**56008**	**C_2H_3CHO ?**	8750.9420	178303.3146	1999004.0514	29	0	27	0	1975	JPL		1404		Very recently, the detection has been reported towards Sgr B2(N): J. M. Hollis, P. R. Jewell, F. J. Lovas, A. Remijan, and H. Møllendal, Green Bank Telescope Detection of New Interstellar Aldehydes: Propenal and Propanal Astrophys. J. 610, L21–L24 (2004). Only two lines have been detected so far thus the detection should be viewed with some caution. (HM)	2-Propenal. s-trans and s-cis Acrolein
8	**56507**	**H_2NCH_2CN**	115977.8530	289828.0460	1356618.5503					2008	CDMS		303	Predictions of b-type transitions beyond Ka = 3 – 2 as well as those having uncertainties larger than 1 MHz should be viewed with caution. The 14N hyperfine splitting can be resolved for low values of J. (HM). Therefore, a separate hyperfine calculation is provided on CDMS up to 40 GHz. See CDMS for other info (AW). http://www.astro.uni-koeln.de/cgi-bin/cdmsinfo?file=e056507.cat	A. Belloche, K. M. Menten, C. Comito, H. S. P. Müller, P. Schilke, J. Ott, S. Thorwirth, and C. Hieret, Detection of Aminoacetonitrile in Sgr B2(N) Astron Astrophys., accepted (2008). (HM) http://www.astro.uni-koeln.de/site/vorhersagen/molecules/ism/AAN.html	Aminoacetonitrile
8	60	**CH_3COOH**									**No entry**			In the previous version of this table the wrong tag (and wrong molecular mass) was erroneously associated to this species. In fact there is no entry in the databases but published data is available (also for the triply deuterated species). New measurements are being taken at JPL. (AW)	D. M. Mehringer, L. E. Snyder, Y. Miao, and F. J. Lovas, Detection and Confirmation of Interstellar Acetic Acid ApJ. 480, L71–L74 (1997). A. Remijan, L. E. Snyder, S.-Y. Liu, D. Mehringer, and Y.-J. Kuan, Acetic Acid in the Hot Cores of **Sagitarrius B2(N)** and **W51** Astrophys. J. 576, 264–273 (2002). (HM)	Acetic Acid
8	**60003**	**CH_3OCHO A & E vt=0 & 1**	8570	668060	1698657	62	0	>55	0	2009	JPL		1404	New simultaneous fit combining A & E species and ground and first torsional states. Gs: A-0; E-1,2. Vt=1: A-3; E-4,5. See V. Ilyushin et al., J. Mol. Spectrosc. 255 (2009) 32-38 and references therein. Keywords: internal rotationρ axis method, torsions, partition function.	A typical **hot core** molecule. It is very abundant in **massive star-forming regions**. It was detected first in **Sgr B2** Brown, R. D.et al. ApJ,197, 1975, L29-L31. **Orion KL** (Schilke et al. 1997 ; Blake et al. 1987) and **Sgr B2(N)** (Snyder, Kuan, & Miao 1994 ; Miao et al. 1995). Around the **Low-mass Protostar IRAS 16293-2422S**. Cazaux, A. G. G. M. Tielens, C. Ceccarelli, A. Castets, V. Wakelam, E. Caux, B. Parise, D. Teyssier, Astrophys. J. 593, L51–L55 (2003). (HM&AW)	Methyl formate. Methyl methanoate
8	**60501**	**$CH_2(OH)CHO$**	7805.8300	356136.8000	1199884.6122	66	0	53	0	2001	CDMS		303		**Sgr B2(N).** 1st: J. M. Hollis, F. J. Lovas, and P. R. Jewell, Interstellar Glycolaldehyde: The First Sugar Astrophys. J. 540, L107–L110 (2000). (HM) See detailed notes on CDMS webpage for other references.	Hydroxyethanal. Glycolaldehyde
8	**65503**	**CH_3C_3N**	70151.5990	289074.9040	408652.6016	70	16	15	0	1985	CDMS		202		TMC1. The detection of interstellar methylcyanoacetylene, Broten, N. W.; MacLeod, J. M.; Avery, L. W.; Friberg, P.; Hjalmarson, A.; Hoglund, B.; Irvine, W. M. ApJ Lett (2) 276, 1984, L25-L29. 984 (AW)	Methylcyanoacetylene
8	**65506**	**CH_2CCHCN ***	9099.2100	177605.8340	499984.7007	15	1	1	0	**1986 (2006)**	CDMS		303	Low energy lines at low frequency only measured. 14N hyperfine structure (given from link on info page below 50GHz). Since Ka = l↔ 0 were the only b-type transitions observed, predictions for this type of transitions should be viewed with caution at higher Ka. All predictions above about 350 GHz should be viewed with caution.	F. J. Lovas, A. J. Remijan, J. M. Hollis, P. R. Jewell, and L. E. Snyder, Hyperfine Structure Identification of Interstellar Cyanoallene toward **TMC-1**, Astrophys. J. 637, L37–L40 (2006). (HM)	2,3-Butadienenitrile. Cyanoallene.
8	**74502**	**l-C_6H_2**	8068.3190	18849.3980	80780.0962	7	2	7	0	1997	CDMS		303	Transitions with Ka = 2 or higher have not been observed and are likely not reliably predictable at present. ortho/para.	First Astronomical Detection of the Cumulene Carbon Chain Molecule H2C6 in TMC-1 Langer, W. D.; Velusamy, T.; Kuiper, T. B. H.; Peng, R.; McCarthy, M. C.; Travers, M. J.; Kovacs, A.; Gottlieb, C. A.; Thaddeus, P. ApJ Lett480, L63 (1997) (AW)	Hexapentaenylidene
8	***85501***	***C_7H***	7869.4290	195386.4420	263084.9916	112	4	1	-1	1997	CDMS		224	Eight New Carbon Chain Molecules, McCarthy, M. C.; Travers, M. J.; Kovacs, A.; Gottlieb, C. A.; Thaddeus, P. ApJ 113, 105 (1997) (AW)	t appears as if this is the only CnH radical that has been detected toward IRC +10216 and not toward TMC-1 (HM) see CDMS.	

9	42	**CH_2CHCH_3**									NoEntry				TMC-1 (2007) see CDMS	Propene. Propylene.
9	**46004**	**C_2H_5OH trans & gauche**	9388	1643967	1999916	76	0	0	0	2008	JPL		1404	v = 0 - gauche - ; v =1 - gauche + ; v = 2 trans. Any K higher than 26 will be wrong by significantly more than the calculated valueKeywords: trans & gauche, fixed frame axis method intensities	SgrB2, Orion. Detection of interstellar trans-ethyl alcohol Zuckerman, B.; Turner, B. E.; Johnson, D. R.; Lovas, F. J.; Fourikis, N.; Palmer, P.; Morris, M.; Lilley, A. E.; Ball, J. A.; Clark, F. O. Ap J., 96, 1975, pt. 2, L99-L102. The Detection and Mapping Observations of C2H5OH in Orion Kleinmann-Low, Ohishi, Masatoshi; Ishikawa, Shin-Ichi; Yamamoto, Satoshi; Saito, Shuji; Amano, Takayoshi, Ap J Lett (1995) 446, L43 (AW)	Ethanol. Ethyl alcohol
9	**46008**	**CH_3OCH_3 (DME)**	9118	386800	2173649	24	1	20	0	1979	JPL		1404	The v designations of 0, 1, 2, 3 represent the AA, EE, EA, and AE states, respectively. New data is available and should appear soon (probably on CDMS).	Orion, IRAS16293, CRL618. Radio Detection of Interstellar Dimethyl Ether, Snyder, L. E.; Buhl, D.; Schwartz, P. R.; Clark, F. O.; Johnson, D. R.; Lovas, F. J.; Giguere, P. T. Ap. J. 191, L79 (1974) (AW)	Dimethyl ether
9	**55001**	**CH_3CH_2CN ***	8949	1160436	3370834		0		0	2009	JPL	see below	303	This entry contains new measurments at higher frequency. No entry for torsions and bending? See below. The methyl torsion and the 14N hyper ne have been resolved in ethyl cyanide, but the effects are small and may not be important for mm-wave astronomy. Separate hyperfine calculationare available on CDMS. Keywords: dipole moment, partition function - see notes on JPL.	**A fairly prototypical hot core molecule**: **OMC-, Sgr B2.** has also been detected toward **low-mass star-forming regions** (**IRAS 16293-2422)** see CDMS.	Propionitrile. Ethyl cyanide. Propanenitrile
9	55	**CH_3CH_2CN vb=1**									**NoEntry**	206.5		No entry in databases for excited bending and torsional states that are seen in astro spectra ? Measurements by Pearson et al do not seem to be in litterature	Two lowest vibrational states vb = 1 (in plane CCN bend) and vt = 1 (torsion) detected toward **Sgr B2(N-LMH)** see CDMS.	
9	55	**CH_3CH_2CN vt=1**									**NoEntry**	217.5		see above	See above.	
9	**56504**	**$CH_3CH_2{}^{13}CN$ ***	8039	358265	2190003					2007	CDMS		303	The observed transitions were taken from K. Demyk et al (see astro).The 14N hyperfine splitting is often negligible, however, it may be resolved for low values of J and a separate hyperfine calculation is provided on CDMS for J≤ 10 and frequencies below 92 GHz. (HM) See also CDMS webpage.	**Orion IRc2** see CDMS.	Ethyl cyanide, propionitrile, 13C on C1
9	**56505**	**$CH_3{}^{13}CH_2CN$ ***	8905.0440	359108.3500	2174022.4131					2007	CDMS		303	see above	see above	Ethyl cyanide, propionitrile, 13C on C2
9	**56506**	**$^{13}CH_3CH_2CN$ ***	8731.7870	358240.1570	2176611.4249					2007	CDMS		303	see above	see above	Ethyl cyanide, propionitrile, 13C on C3
9	**56508**	**$CH_3CH_2C^{15}N$**	8439.6160	650899.0230	1896689.1384					2009	CDMS		303	New measurements published in 2009. Predictions with uncertainties exceeding 0.5 MHz should be viewed with caution.	First detected in Orion. Margulès et al. 2009 A&A 493 565-569	Ethyl cyanide, propionitrile, 15N isotopologue
9	56509	CH_3CHDCN	8145.6380	644317.8230	1792874.3117					2009	CDMS		303	New measurements published in 2009. Predictions with uncertainties exceeding 0.5 MHz should be viewed with caution.	Searched for but not detected in Orion.	Ethyl cyanide, propionitrile, monodeuterated at C2
9	56510	$CH_2D^{ip}CH_2CN$	8425.9390	630673.6520	1893610.9328					2009	CDMS		303	New measurements published in 2009. Predictions with uncertainties exceeding 0.5 MHz should be viewed with caution.	Searched for but not detected in Orion.	Ethyl cyanide, propionitrile, monodeuterated at C3, in plane
9	56511	$CH_2D^{op}CH_2CN$	8505.1600	642501.3460	1810555.3666					2009	CDMS		303	New measurements published in 2009. Predictions with uncertainties exceeding 0.5 MHz should be viewed with caution.	Searched for but not detected in Orion.	Ethyl cyanide, propionitrile, monodeuterated at C3, out of plane
9	**59**	**$CH_3C(O)NH_2$**	8425.1200								**NoEntry**				**Sgr B2.** J. M. Hollis, F. J. Lovas, A. R. Remijan, P. R. Jewell, V. V. Ilyushin, and I. Kleiner, Detection of Acetamide (CH3CONH2): the Largest Interstellar Molecule with a Peptide Bond Astrophys. J. 643, L25–L28 (2006). (HM)	Acetamide
9	**64507**	**CH_3C_4H**	8142.9700	512315.8030	662155.7127	126	0	15	0	2008	CDMS		202	Latest entry contains new data. At low temperature it may be necessary to consider A & E species (HM). Edited information from CDMS. For details see CDMS webpage. Note that low freqeucney data is not indicated as inlcuded in fit but may be found in litterature (AW).	1st two : J. M. MacLeod, L. W. Avery, N. W. Broten, The detection of interstellar methyldiacetylene (CH3C4H) Astrophys. J. 282, L89–L92 (1984); C. M. Walmsley, P. R. Jewell, L. E. Snyder, and G. Winnewisser, Detection of interstellar methyldiacetylene (CH3C4H) in the dark dust cloud TMC 1 Astron. Astrophys. 184, L11–L14 (1984).	1,3-pentadiyne. Methyldiacetylene
9	**97501**	**C_8H**	9973.3560	99331.7500	164813.3966	85	8	1	-1	1996	CDMS		224		IRC+10216 and TMC-1: see CDMS	octatetraynyl radical
9	**97502**	**C_8H^-**	9333.4340	18666.8140	287911.6892	16	7			2007	CDMS		101		IRC+10216 and TMC-1: see CDMS	Octatetraynylide anion
9	**99501**	**HC_7N** v = 0	27071.8150	226597.5130	259244.4689	201	23			2004	CDMS		101			
9	**99502**	**HC_7N v15 = 1**	81363.0380	114125.3620	135585.6761	101	71	1	-1	2004	CDMS		202	CRL 618 (AW)		
9	99503	HC_7N v15 = 2	81442.8860	114316.4780	135821.9602	101	71	2	-2	2004	CDMS		202			
10	**58003**	**$(CH_3)_2CO$**			999993					2002 (2008)	JPL		1404	New entry 2008. Measured lines not merged or indicated - check publications. Code for (v',v) : (0,0) AA ; (01) EE ; (2,1) EA ; (1,1) AE. Keywords: double internal rotor, torsional sublevels, K dependence, IAM, partition function	**Sgr B2**: (1st) F. Combes, et al.. Astrophys. 180, L13–L16 (1987) **Orion KL Hot Core**: D. N. Friedel et al, Astrophys. J. 632, L95–L98 (2005); includes **a few torsional lines**	Propanone. Acetone
10	**58505**	**s-CH_3CH_2CHO**	8114	285407	1488518					1987 (2008)	CDMS		303	Lowest energy conformer. Predictions with uncertainties larger than 0.5 MHz should be viewed with caution. Keywords: conformers, internal rotation, torsion, partition function.	The detection has been reported towards Sgr B2(N) and appears secure: J. M. Hollis, P. R. Jewell, F. J. Lovas, A. Remijan, and H. Møllendal, Green Bank Telescope Detection of New Interstellar Aldehydes: Propenal and Propanal Astrophys. J. 610, L21–L24 (2004). (HM)	syn-Propanal (sometimes called cis-) Propionaldehyde.
10	**62503**	**aGg'-$(CH_2OH)_2$**	8603.5200	366237.5200	599994.3011	51	0	32	0	2003	CDMS		1404	Lowest state conformer. Predictions should be quite reliable if J≤ 40 and Ka ≤ 15. Spin-statistics have been taken into account. OH tunneling.	**Sgr B2(N-LMH)** J. M. Hollis et al. Astrophys. J. 571, L59–L62 (2002). And others see CDMS. **Comet C/1995 O1 (Hale-Bopp)** J. Crovisier et al., Astron. Astrophys. 418, L35–L38 (2004). (HM)	Ethylene glycol. Ethandiol

10	62504	gGg'-$(CH_2OH)_2$	10159.8800	506589.3650	599929.4970	40	0	40	0	2004	CDMS		1404	About 200 cm–1 higher in energy. The partition function was with the 000 level of state 0 set to zero ! Therefore, one has to consider the energy difference of about 200 cm–1 for proper intensity calculations if thermal equilibration has been achieved. Predictions should be quite reliable if ± 40 and Ka <= 6 or if Ka ≤ J ≤ 12. Spin-statistics have been taken into account. OH tunneling.	See above.	See above
10	**89501**	**CH_3C_5N**	6224.1750	38901.4500	202213.5245	26	3	6	0	1998	CDMS		203		1st (tentative): L. E. Snyder, T. L. Wilson, C. Henkel, P. R. Jewell, and C. M. Walmsley, Detection of Interstellar Methylcyanodiacetylene in the Dark Dust Cloud TMC 1 Bull. Am. Atron. Soc. 16, 959 (1984). Later confirmed see CDMS.	Cyanopentadiyne. Methylcyanodiacetylene
11	**74514**	**C_2H_5OCHO**	10642	377217	999995					2009	CDMS		1404	Predictions of transitions with uncertainties larger than 1 MHz should be viewed with **grea**t caution. Keywords: anti & gauche conformers, perturbation by low lying v state, partition function.	SgrB2(N) : A.Belloche et al., Astron. Astrophys. Accepted	ethyl formate, ethyl methanoate
11	**88502**	**CH_3C_6H**	28010.8800	38911.6400	202262.5884	25	17	9	0	2002	CDMS		202	At low temperatures, it may be necessary to discern between A-CH3C6H and E-CH3C6H.	A. R. Remijan, J. M. Hollis, L. E. Snyder, P. R. Jewell, and F. J. Lovas, Methyltriacetylene (CH3C6H) toward**TMC-1**: Presently the Largest Detected Symmetric Top Astrophys. J. 643, L37–L40 (2006). (HM)	1,3,5-Heptatriyne. Methyltriacetylene.
11	**123501**	**HC_9N**	? =>	? =>	99920					2004	CDMS		101	Expt lines not indicated check publi. Lines > 100 GHz ?14N HFS info The experimental lines are from (1) M. C. McCarthy, E. S. Levine, A. J. Apponi, and P. Thaddeus, 2000, J. Mol. Spectrosc. 203, 75.	N. W. Broten, T. Oka, L. W. Avery, J. M. MacLeod, and H. W. Kroto, The Detection of HC9N in Interstellar Space Astrophys. J. 223, L105–L107 (1978) (HM). In **Heile's Cloud 2 (dark intersellar cloud?)** (AW)	Cyanooctatetrayne. Cyanotetraacetylene
12	**60**	**$C_2H_5OCH_3$? (EME)**									**NoEntry**				Possible detection**W51e2.** G. W. Fuchs, U. Fuchs, T. F. Giesen, and F. Wyrowski, Trans-Ethyl Methyl Ether in Space A new Look at a Complex Molecule in Selected Hot Core Regions Astron. Astrophys. 444, 521–530 (2005) (HM)	Ethyl Methyl Ether
12	**69505**	**n-C_3H_7CN**	4813	283195	999938					1988 (2009)	CDMS		1404	Predictions of transitions with uncertainties larger than 1 MHz should be viewed with caution. Keywords: anti-anti & anti-gauche conformers, ^{14}N hyperfine, CH_3 internal rotation (low freq transitions), partition function.	SgrB2(N) : A.Belloche et al., Astron. Astrophys. Accepted	n-propyl cyanide, n-butyronitrile
13	147501	**$HC_{11}N$**	6086.2590	14539.3340	50715.6348	43	17			1996	CDMS		101		TMC-1 see CDMS.	
15	171501	$HC_{13}N$?								2003	CDMS			not yet seen but next in series		

§ tailed checks of literature are being m

onnally excited states given even if no detection

**Number of atoms.**

***** **For hyperfine splitting click on the documentation link of the molecule on CDMS web page.**

****** **Treat ortho and para separately; tables created by C. Vastel.**

******* first transtion about 1 THz or higher

! predictions may have substantial uncertainties

x not yet included in template

? detection not sure

QNF **Use this code to know the real quantum numbers format used for each molecule. The code format can be found at:**

NR not in range of our spectral survey

NI not identified in our spectral survey