

# INTERSTELLAR MOLECULES

Frank J. Lovas and Lewis E. Snyder

A number of molecules have been detected in the interstellar medium, in circumstellar envelopes around evolved stars, and comae and tails of comets through observation of their microwave, infrared, or optical spectra. The following list gives the molecules and the particular isotopic species that have been reported thus far. Molecules are listed by molecular formula in the Hill order. Molecules are listed by molecular formula in the Hill order. All species not footnoted otherwise are observed in interstellar clouds, while some are also found in comets and circumstellar clouds. The list was last updated in November 2005 and lists 147 molecules (263 isotopic forms).

Molecular formula	Name	Isotopic species
AlCl	Aluminum monochloride	AlCl <sup>a</sup>
		Al <sup>37</sup> Cl <sup>a</sup>
AlF	Aluminum monofluoride	AlF <sup>a</sup>
AlN	Aluminum isocyanide	AlNC <sup>a</sup>
CF <sup>+</sup>	Fluoromethyldynium ion	CF <sup>+</sup>
CH	Methyldiyne	CH
CH <sup>+</sup>	Methyliumylidene	CH <sup>+</sup>
CHN	Hydrogen cyanide	HCN
		H <sup>13</sup> CN
		HC <sup>15</sup> N
		DCN
CHN	Hydrogen isocyanide	HNC
		H <sup>15</sup> NC
		HN <sup>13</sup> C
		DNC
		D <sup>15</sup> NC
		HNCO
CHNO	Isocyanic acid	DNCO
CHNS	Isothiocyanic acid	HNCS
CHO	Oxomethyl	HCO
CHO <sup>+</sup>	Oxomethylium	HCO <sup>+</sup>
		H <sup>13</sup> CO <sup>+</sup>
		HC <sup>17</sup> O <sup>+</sup>
		HC <sup>18</sup> O <sup>+</sup>
		DCO <sup>+</sup>
		D <sup>13</sup> CO <sup>+</sup>
		HOC <sup>+</sup>
CHO <sup>+</sup>	Hydroxymethyldiyne	HOCO <sup>+</sup>
CHO <sub>2</sub> <sup>+</sup>	Hydroxyoxomethylium	HOCO <sup>+</sup>
CHS <sup>+</sup>	Thiooxomethylium	HCS <sup>+</sup>
CH <sub>2</sub>	Methylene	CH <sub>2</sub>
CH <sub>2</sub> N <sup>+</sup>	Iminomethylium	HCNH <sup>+</sup>
CH <sub>2</sub> N	Methylene amidogen	CH <sub>2</sub> N
CH <sub>2</sub> N <sub>2</sub>	Cyanamide	NH <sub>2</sub> CN
CH <sub>2</sub> O	Formaldehyde	H <sub>2</sub> CO
		H <sub>2</sub> <sup>13</sup> CO
		H <sub>2</sub> C <sup>18</sup> O
		HDCO
		D <sub>2</sub> CO
		HCOOH
		H <sup>13</sup> COOH
HCOOD		
D <sub>2</sub> CO	Formic acid	D <sub>2</sub> CO
CH <sub>2</sub> O <sub>2</sub>	Formic acid	HCOOH
		H <sup>13</sup> COOH
		HCOOD
		D <sub>2</sub> CO
CH <sub>2</sub> S	Thioformaldehyde	H <sub>2</sub> CS
		H <sub>2</sub> <sup>13</sup> CS

## References

1. Lovas, F. J., "Recommended Rest Frequencies for Observed Interstellar Molecule Microwave Transitions - 1991 Revision," *J. Phys. Chem. Ref. Data*, 21, 181-272, 1992.
2. Snyder, L. E., "Cometary Molecules," Internat. Astron. Union Symposium No. 150, *Astrochemistry of Cosmic Phenomena*, Ed. P.D. Singh, Kluwer Academic Publishers, Dordrecht, The Netherlands, pp. 427-434 (1992).

Molecular formula	Name	Isotopic species
H <sub>2</sub> C <sup>34</sup> S	Methyl	H <sub>2</sub> C <sup>34</sup> S
		HD <sub>2</sub> CS
		D <sub>2</sub> CS
		CH <sub>3</sub> <sup>a</sup>
CH <sub>3</sub> N	Methanimine	CH <sub>2</sub> NH
CH <sub>3</sub> NO	Formamide	<sup>13</sup> CH <sub>2</sub> NH
		NH <sub>2</sub> CHO
CH <sub>3</sub> O <sup>+</sup>	Hydroxy methylium ion	NH <sub>2</sub> <sup>13</sup> CHO
		H <sub>2</sub> COH <sup>+</sup>
CH <sub>4</sub>	Methane	CH <sub>4</sub>
CH <sub>4</sub> O	Methanol	CH <sub>3</sub> OH
		<sup>13</sup> CH <sub>3</sub> OH
		CH <sub>3</sub> <sup>18</sup> OH
		CH <sub>2</sub> DOH
		CH <sub>3</sub> OD
		CHD <sub>2</sub> OH
		CD <sub>3</sub> OH
CH <sub>4</sub> S	Methanethiol	CH <sub>3</sub> SH
CH <sub>3</sub> N	Methylamine	CH <sub>3</sub> NH <sub>2</sub>
CMgN	Magnesium cyanide	MgCN <sup>a</sup>
CMgN	Magnesium isocyanide	<sup>24</sup> MgNC <sup>a</sup>
		<sup>25</sup> MgNC <sup>a</sup>
		<sup>26</sup> MgNC <sup>a</sup>
CN	Cyanide radical	CN
		<sup>13</sup> CN
		C <sup>15</sup> N
CN <sup>+</sup>	Cyanide radical ion	CN <sup>+</sup> <sup>b</sup>
CNNa	Sodium cyanide	NaCN <sup>a</sup>
CNSi	Silicon cyanide	SiNC <sup>a</sup>
CNSi	Silicon isocyanide	SiNC <sup>a</sup>
CN <sub>2</sub>	Cyanoimidogen	NCN <sup>b</sup>
CO	Carbon monoxide	CO
		<sup>13</sup> CO
		C <sup>17</sup> O
		C <sup>18</sup> O
CO <sup>+</sup>	Carbon monoxide ion	<sup>13</sup> C <sup>18</sup> O
		CO <sup>+</sup>
COS	Carbon oxysulfide	OCS
		OC <sup>34</sup> S
		O <sup>13</sup> CS
CO <sub>2</sub>	Carbon dioxide	<sup>18</sup> OCS
		CO <sub>2</sub>
CO <sub>2</sub> <sup>+</sup>	Carbon dioxide ion	CO <sub>2</sub> <sup>+</sup> <sup>b</sup>
CP	Carbon phosphide	CP <sup>a</sup>

Molecular formula	Name	Isotopic species	Molecular formula	Name	Isotopic species
CS	Carbon monosulfide	CS C <sup>33</sup> S C <sup>34</sup> S C <sup>36</sup> S <sup>13</sup> CS <sup>13</sup> C <sup>34</sup> S	C <sub>3</sub> H <sub>3</sub> N	Acrylonitrile (vinyl cyanide)	CH <sub>2</sub> CHCN
CSi	Silicon carbide	SiC <sup>a</sup>	C <sub>3</sub> H <sub>4</sub>	Propyne	CH <sub>3</sub> CCH CH <sub>2</sub> C <sup>13</sup> CH <sup>13</sup> CH <sub>3</sub> CCH CH <sub>2</sub> DCCH CH <sub>3</sub> CCD
C <sub>2</sub>	Dicarbon	C <sub>2</sub>	C <sub>3</sub> H <sub>5</sub> O	Propenal	CH <sub>2</sub> CHCHO
C <sub>2</sub> H	Ethynyl	C <sub>2</sub> H <sup>13</sup> CCH C <sup>13</sup> CH C <sub>2</sub> D HCCN HCCH CH <sub>2</sub> CN H <sub>2</sub> CCO CH <sub>3</sub> CN <sup>13</sup> CH <sub>3</sub> CN CH <sub>3</sub> <sup>13</sup> CN CH <sub>3</sub> C <sup>15</sup> N CH <sub>2</sub> DCN	C <sub>3</sub> H <sub>5</sub> N	Propanenitrile (ethyl cyanide)	CH <sub>3</sub> CH <sub>2</sub> CN
C <sub>2</sub> HN	Cyanomethylene	HCCN	C <sub>3</sub> H <sub>6</sub> O	Acetone	(CH <sub>3</sub> ) <sub>2</sub> CO
C <sub>2</sub> H <sub>2</sub>	Acetylene	HCCH	C <sub>3</sub> H <sub>6</sub> O	Propenal	CH <sub>3</sub> CH <sub>2</sub> CHO
C <sub>2</sub> H <sub>2</sub> N	Cyanomethyl	CH <sub>2</sub> CN	C <sub>3</sub> N	Cyanoethynyl	CCCN
C <sub>2</sub> H <sub>2</sub> O	Ketene	H <sub>2</sub> CCO	C <sub>3</sub> O	1,2-Propadienyldiene, 3-oxo	CCCO
C <sub>2</sub> H <sub>3</sub> N	Acetonitrile	CH <sub>3</sub> CN <sup>13</sup> CH <sub>3</sub> CN CH <sub>3</sub> <sup>13</sup> CN CH <sub>3</sub> C <sup>15</sup> N CH <sub>2</sub> DCN	C <sub>3</sub> S	1,2-Propadienyldiene, 3-thioxo	CCCS
C <sub>2</sub> H <sub>3</sub> N	Isocyanomethane	CH <sub>3</sub> NC	C <sub>3</sub> Si	Silicon tricarbon	SiC <sub>3</sub>
C <sub>2</sub> H <sub>4</sub>	Ethylene	H <sub>2</sub> CCH <sub>2</sub>	C <sub>4</sub> H	1,3-Butadiynyl radical	HCCCC H <sup>13</sup> CCCC HC <sup>13</sup> CCC HCC <sup>13</sup> CC HCCC <sup>13</sup> C DCCCC HCCCCN
C <sub>2</sub> H <sub>4</sub> O	Acetaldehyde	CH <sub>3</sub> CHO	C <sub>4</sub> HN	3-Cyano-1,2-propadienyldiene	HCCCCN
C <sub>2</sub> H <sub>4</sub> O	Ethylene oxide	<i>c</i> -C <sub>2</sub> H <sub>4</sub> O <sup>c</sup>	C <sub>4</sub> H <sub>2</sub>	Butatrienyldiene	H <sub>2</sub> CCCC
C <sub>2</sub> H <sub>4</sub> O	Ethanol	CH <sub>2</sub> CHOH	C <sub>4</sub> H <sub>2</sub>	1,3-Butadiyne	HCCCCH <sup>a</sup>
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Methyl formate	CH <sub>3</sub> OCHO	C <sub>4</sub> H <sub>3</sub> N	2-Butynenitrile	CH <sub>3</sub> CCCN
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Acetic acid	CH <sub>3</sub> COOH	C <sub>4</sub> H <sub>3</sub> N	Cyanoallene	CH <sub>2</sub> CCHCN
C <sub>2</sub> H <sub>4</sub> O <sub>2</sub>	Glycolaldehyde	CH <sub>2</sub> OHCHO	C <sub>4</sub> Si	Silicon tetracarbide	SiC <sub>4</sub> <sup>a</sup>
C <sub>2</sub> H <sub>6</sub>	Ethane	CH <sub>3</sub> CH <sub>3</sub> <sup>b</sup>	C <sub>5</sub>	Pentacarbon	C <sub>5</sub> <sup>a</sup>
C <sub>2</sub> H <sub>6</sub> O	<i>trans</i> -Ethanol	<i>t</i> -CH <sub>3</sub> CH <sub>2</sub> OH	C <sub>5</sub> H	2,4-Pentadienyldiyne	HCCCCC
C <sub>2</sub> H <sub>6</sub> O	<i>gauche</i> -Ethanol	<i>g</i> -CH <sub>3</sub> CH <sub>2</sub> OH	C <sub>5</sub> HN	2,4-Pentadienenitrile	HCCCCCN H <sup>13</sup> CCCCCN HCC <sup>13</sup> CCCCN HCC <sup>13</sup> CCCN HCCC <sup>13</sup> CCN HCCCC <sup>13</sup> CN DCCCCCN
C <sub>2</sub> H <sub>6</sub> O	Dimethyl ether	CH <sub>3</sub> OCH <sub>3</sub>	C <sub>5</sub> H <sub>4</sub>	1,3-Pentadiyne	CH <sub>3</sub> C <sub>4</sub> H
C <sub>2</sub> H <sub>6</sub> O <sub>2</sub>	Ethylene glycol	HOCH <sub>2</sub> CH <sub>2</sub> OH	C <sub>5</sub> N	1,3-Butadiynylum, 4-cyano	C <sub>5</sub> N
C <sub>2</sub> O	Oxoethenyldiene	CCO	C <sub>6</sub> H	1,3,5-Hexatriynyl	HCCCCCC
C <sub>2</sub> S	Thioxoethenyldiene	CCS CC <sup>34</sup> S	C <sub>6</sub> H <sub>2</sub>	1,3,5-Hexatriyne	HCCCCCCC <sup>b</sup>
C <sub>2</sub> Si	Silicon dicarbide	<i>c</i> -SiC <sub>2</sub> <i>c</i> - <sup>29</sup> SiC <sub>2</sub> <i>c</i> - <sup>30</sup> SiC <sub>2</sub> <i>c</i> -Si <sup>13</sup> CC	C <sub>6</sub> H <sub>2</sub>	1,2,3,4,5-Hexapentaenyldiene	H <sub>2</sub> CCCCC
C <sub>3</sub>	Tricarbon	C <sub>3</sub>	C <sub>6</sub> H <sub>3</sub> N	Methylcyanodiacetylene	CH <sub>3</sub> C <sub>4</sub> CN
C <sub>3</sub> H	Cyclopropenyldiyne	<i>c</i> -C <sub>3</sub> H	C <sub>6</sub> H <sub>6</sub>	Benzene	C <sub>6</sub> H <sub>6</sub>
C <sub>3</sub> H	Propenyldiyne	<i>l</i> -C <sub>3</sub> H	C <sub>7</sub> H	2,4,6-Heptatrienyldiyne	HCCCCCCC
C <sub>3</sub> HN	Cyanoacetylene	HCCCN H <sup>13</sup> CCCN HC <sup>13</sup> CCN HCC <sup>13</sup> CN HCCC <sup>15</sup> N DCCCN	C <sub>7</sub> HN	2,4,6-Heptatrienenitrile	HC <sub>7</sub> N
C <sub>3</sub> HN	Isocyanoacetylene	HCCNC	C <sub>8</sub> H	1,3,5,7-Octatetraynyl	HC <sub>8</sub>
C <sub>3</sub> HN	1,2-Propadienyldiene, 3-imino	HNCCC	C <sub>9</sub> HN	2,4,6,8-Nonatetraynenitrile	HC <sub>9</sub> N
C <sub>3</sub> H <sub>2</sub>	Cyclopropenyldiene	<i>c</i> -C <sub>3</sub> H <sub>2</sub> <i>c</i> -H <sup>13</sup> CCCH <i>c</i> -HC <sup>13</sup> CCH <i>c</i> -C <sub>3</sub> HD <i>l</i> -H <sub>2</sub> CCC	C <sub>11</sub> HN	2,4,6,8,10-Undecapentaynenitrile	HC <sub>11</sub> N
C <sub>3</sub> H <sub>2</sub>	Propadienyldiene	<i>l</i> -H <sub>2</sub> CCC	ClH	Hydrogen chloride	H <sup>35</sup> Cl H <sup>37</sup> Cl
C <sub>3</sub> H <sub>2</sub> N <sup>+</sup>	Protonated cyanoacetylene	HCCCNH <sup>+</sup>	ClK	Potassium chloride	K <sup>35</sup> Cl <sup>a</sup> K <sup>37</sup> Cl <sup>a</sup>
C <sub>3</sub> H <sub>2</sub> O	2-Propynal	HCCCHO	ClNa	Sodium chloride	Na <sup>35</sup> Cl <sup>a</sup> Na <sup>37</sup> Cl <sup>a</sup>
C <sub>3</sub> H <sub>2</sub> O	Cyclopropenone	<i>c</i> -C <sub>3</sub> H <sub>2</sub> O	FH	Hydrogen fluoride	HF
			FeO	Iron monoxide	FeO
			HLi	Lithium hydride	<sup>7</sup> LiH

Molecular formula	Name	Isotopic species	Molecular formula	Name	Isotopic species
HN	Imidogen	HN	H <sub>4</sub> Si	Silane	SiH <sub>4</sub> <sup>a</sup>
HNO	Nitrosyl hydride	HNO	NO	Nitric oxide	NO
HN <sub>2</sub> <sup>+</sup>	Hydrodinitrogen(1+)	N <sub>2</sub> H <sup>+</sup>	NP	Phosphorus nitride	NP
		<sup>15</sup> NNH <sup>+</sup>	NS	Nitrogen sulfide	NS
		N <sup>15</sup> NH <sup>+</sup>			N <sup>134</sup> S
HO	Hydroxyl	N <sub>2</sub> D <sup>+</sup>	NSi	Silicon nitride	SiN
		OH	N <sub>2</sub>	Nitrogen	N <sub>2</sub>
		<sup>17</sup> OH	N <sub>2</sub> <sup>+</sup>	Nitrogen ion	N <sub>2</sub> <sup>+</sup> <sup>b</sup>
		<sup>18</sup> OH	N <sub>2</sub> O	Nitrous oxide	N <sub>2</sub> O
HO <sup>+</sup>	Oxoniumylidene	HO <sup>+</sup> <sup>b</sup>	OS	Sulfur monoxide	SO
HS	Mercapto	SH			<sup>34</sup> SO
H <sub>2</sub>	Hydrogen	H <sub>2</sub>			<sup>33</sup> SO
H <sub>2</sub> N	Amidogen	NH <sub>2</sub>			S <sup>18</sup> O
H <sub>2</sub> O	Water	H <sub>2</sub> O	OS <sup>+</sup>	Sulfur monoxide ion	SO <sup>+</sup>
		H <sub>2</sub> <sup>18</sup> O	OSi	Silicon monoxide	SiO
		HDO			Si <sup>18</sup> O
H <sub>2</sub> O <sup>+</sup>	Oxoniumyl	H <sub>2</sub> O <sup>+</sup> <sup>b</sup>			<sup>29</sup> SiO
H <sub>2</sub> S	Hydrogen sulfide	H <sub>2</sub> S			<sup>30</sup> SiO
		H <sub>2</sub> <sup>34</sup> S	O <sub>2</sub> S	Sulfur dioxide	SO <sub>2</sub>
		HDS			<sup>33</sup> SO <sub>2</sub>
		D <sub>2</sub> S			<sup>34</sup> SO <sub>2</sub>
H <sub>3</sub> <sup>+</sup>	Trihydrogen ion	H <sub>3</sub> <sup>+</sup>			OS <sup>18</sup> O
		H <sub>2</sub> D <sup>+</sup>	SSi	Silicon monosulfide	SiS
		D <sub>2</sub> H <sup>+</sup>			Si <sup>33</sup> S
H <sub>3</sub> N	Ammonia	NH <sub>3</sub>			Si <sup>34</sup> S
		<sup>15</sup> NH <sub>3</sub>			<sup>29</sup> SiS
		NH <sub>2</sub> D			<sup>30</sup> SiS
		NHD <sub>2</sub>			Si <sup>36</sup> S
		ND <sub>3</sub>	S <sub>2</sub>	Disulfur	S <sub>2</sub> <sup>b</sup>
H <sub>3</sub> O <sup>+</sup>	Oxonium hydride	H <sub>3</sub> O <sup>+</sup>			

*l*- before the isotopic species indicates a linear configuration, while *c*- indicates a cyclic molecule.

<sup>a</sup> Reported only in circumstellar clouds.

<sup>b</sup> Reported only in comets.