

Description of the abundance for each molecule and isotopologue codes

Molecule	Molecule Code	Isotope Code	Formula	Abundance	Since GEISA version
H ₂ O	1	161	H ¹⁶ OH	0.997317	2003
		181	H ¹⁷ OH	0.002000	2003
		171	H ¹⁸ OH	3.718840 × 10 ⁻⁴	2003
		262	D ₂ ¹⁶ O	2.419700 × 10 ⁻⁸	2003
		282	D ₂ ¹⁸ O	4.852080 × 10 ⁻¹¹	2011
		272	D ₂ ¹⁷ O	9.022841 × 10 ⁻¹²	2020
CO ₂	2	626	¹⁶ O ¹² C ¹⁶ O	0.9842	2003
		636	¹⁶ O ¹³ C ¹⁶ O	1.106 x 10 ⁻²	2003
		628	¹⁶ O ¹² C ¹⁸ O	3.947 x 10 ⁻³	2003
		627	¹⁶ O ¹² C ¹⁷ O	7.339 x 10 ⁻⁴	2003
		638	¹⁶ O ¹³ C ¹⁸ O	4.434 x 10 ⁻⁵	2003
		637	¹⁶ O ¹³ C ¹⁷ O	8.246 x 10 ⁻⁶	2003
		828	¹⁸ O ¹² C ¹⁸ O	3.957 x 10 ⁻⁶	2003
		728	¹⁷ O ¹² C ¹⁸ O	1.472 x 10 ⁻⁶	2011
		727	¹⁷ O ¹² C ¹⁷ O	1.430 x 10 ⁻⁷	2011
		838	¹⁸ O ¹³ C ¹⁸ O	4.446 x 10 ⁻⁸	2003
		738	¹⁷ O ¹³ C ¹⁸ O	1.654 x 10 ⁻⁸	2011
		737	¹⁷ O ¹³ C ¹⁷ O	1.55 x 10 ⁻⁹	2003
O ₃	3	666	¹⁶ O ¹⁶ O ¹⁶ O	0.992901	2011
		668	¹⁶ O ¹⁶ O ¹⁸ O	0.003982	2003
		686	¹⁶ O ¹⁸ O ¹⁶ O	0.001991	2003
		667	¹⁶ O ¹⁶ O ¹⁷ O	7.404750 × 10 ⁻⁴	2003
		676	¹⁶ O ¹⁷ O ¹⁶ O	3.702370 × 10 ⁻⁴	2003
N ₂ O	4	446	¹⁴ N ¹⁴ N ¹⁶ O	0.990333	2003
		447	¹⁴ N ¹⁴ N ¹⁷ O	3.692800 × 10 ⁻⁴	2003
		448	¹⁴ N ¹⁴ N ¹⁸ O	0.001986	2003
		456	¹⁴ N ¹⁵ N ¹⁶ O	0.003641	2003
		546	¹⁵ N ¹⁴ N ¹⁶ O	0.003641	2003
		458	¹⁴ N ¹⁴ N ¹⁸ O	7.300807 × 10 ⁻⁴	2011
		548	¹⁵ N ¹⁴ N ¹⁸ O	7.300807 × 10 ⁻⁴	2011
		556	¹⁵ N ¹⁵ N ¹⁶ O	1.338574 × 10 ⁻⁵	2011

Molecule	Molecule Code	Isotope Code	Formula	Abundance	Since GEISA version
CO	5	26	$^{12}\text{C}^{16}\text{O}$	0.986544	2003
		36	$^{13}\text{C}^{16}\text{O}$	0.011084	2003
		28	$^{12}\text{C}^{18}\text{O}$	0.001978	2003
		27	$^{12}\text{C}^{17}\text{O}$	3.678670×10^{-4}	2003
		38	$^{13}\text{C}^{18}\text{O}$	2.222500×10^{-5}	2003
		37	$^{13}\text{C}^{17}\text{O}$	4.132920×10^{-6}	2003
CH ₄	6	211	$^{12}\text{CH}_4$	0.988274	2003
		311	$^{13}\text{CH}_4$	0.011103	2003
O ₂	7	66	$^{16}\text{O}^{16}\text{O}$	0.995262	2003
		68	$^{16}\text{O}^{18}\text{O}$	0.003991	2003
		67	$^{16}\text{O}^{17}\text{O}$	7.422350×10^{-4}	2003
NO	8	46	$^{14}\text{N}^{16}\text{O}$	0.993974	2003
		56	$^{15}\text{N}^{16}\text{O}$	0.003654	2003
		48	$^{14}\text{N}^{18}\text{O}$	0.001993	2003
SO ₂	9	626	$^{32}\text{S}^{16}\text{O}_2$	0.945678	2003
		646	$^{34}\text{S}^{16}\text{O}_2$	0.041950	2003
NO ₂	10	646	$^{14}\text{N}^{16}\text{O}_2$	0.991616	2003
NH ₃	11	411	$^{14}\text{NH}_3$	0.995872	2003
		511	$^{15}\text{NH}_3$	0.003661	2003
PH ₃	12	131	$^{31}\text{PH}_3$	0.999533	2003
HNO ₃	13	146	$\text{H}^{14}\text{N}^{16}\text{O}$	0.989110	2003
		156	$\text{H}^{15}\text{N}^{16}\text{O}$	0.003636	2011
OH	14	61	^{16}OH	0.997473	2003
		81	^{18}OH	0.002000	2003
		62	^{16}OD	1.553710×10^{-4}	2003
HF	15	19	H^{19}F	0.999844	2003
HCl	16	15	H^{35}Cl	0.757587	2003
		17	H^{37}Cl	0.242257	2003
HBr	17	19	H^{79}Br	0.506781	2003
		11	H^{81}Br	0.493063	2003
HI	18	17	H^{127}I	0.999844	2003
ClO	19	56	$^{35}\text{Cl}^{16}\text{O}$	0.755908	2003
		76	$^{37}\text{Cl}^{16}\text{O}$	0.241720	2003
OCS	20	622	$^{16}\text{O}^{12}\text{C}^{32}\text{S}$	0.937395	2003
		624	$^{16}\text{O}^{12}\text{C}^{34}\text{S}$	0.041583	2003
		632	$^{16}\text{O}^{13}\text{C}^{32}\text{S}$	0.010531	2003
		623	$^{16}\text{O}^{12}\text{C}^{33}\text{S}$	0.007399	2003
		822	$^{18}\text{O}^{12}\text{C}^{32}\text{S}$	0.001880	2003
		634	$^{16}\text{O}^{13}\text{C}^{34}\text{S}$	4.671757×10^{-4}	2003
H ₂ CO	21	126	$\text{H}_2^{12}\text{C}^{16}\text{O}$	0.986237	2003
		136	$\text{H}_2^{13}\text{C}^{16}\text{O}$	0.011080	2003
		128	$\text{H}_2^{12}\text{C}^{18}\text{O}$	0.001978	2003

Molecule	Molecule Code	Isotope Code	Formula	Abundance	Since GEISA version
C ₂ H ₆	22	226	¹² C ₂ H ₆	0.976990	2003
		236	¹² C ¹³ CH ₆	0.021953	2003
CH ₃ D	23	212	¹² CH ₃ D	6.157510 × 10 ⁻⁴	2003
		312	¹³ CH ₃ D	6.917850 × 10 ⁻⁶	2011
C ₂ H ₂	24	221	¹² C ₂ H ₂	0.977599	2003
		231	¹² C ¹³ CH ₂	0.021966	2003
C ₂ H ₄	25	211	¹² C ₂ H ₄	0.977294	2003
		311	¹² C ¹³ CH ₄	0.021959	2003
GeH ₄	26	411	⁷⁴ GeH ₄	1.000000	2003
HCN	27	124	H ¹² C ¹⁴ N	0.985114	2003
		134	H ¹³ C ¹⁴ N	0.011068	2003
		125	H ¹² C ¹⁵ N	0.003622	2003
		224	D ¹² C ¹⁴ N	1.534456 × 10 ⁻⁴	2011
C ₃ H ₈	28	221	¹² C ₃ H ₈	0.965835	2003
C ₂ N ₂	29	224	¹² C ₂ ¹⁴ N ₂	0.970752	2003
C ₄ H ₂	30	211	¹² C ₄ H ₂	0.955998	2003
HC ₃ N	31	124	H ¹² C ₃ ¹⁴ N	0.963346	2003
HOCl	32	165	H ¹⁶ O ³⁵ Cl	0.755790	2003
		167	H ¹⁶ O ³⁷ Cl	0.241683	2003
N ₂	33	44	¹⁴ N ¹⁴ N	0.992687	2003
CH ₃ Cl	34	215	¹² CH ₃ ³⁵ Cl	0.748937	2003
		217	¹² CH ₃ ³⁷ Cl	0.239491	2003
H ₂ O ₂	35	166	H ₂ ¹⁶ O ¹⁶ O	0.994952	2003
H ₂ S	36	121	H ₂ ³² S	0.949884	2003
		141	H ₂ ³⁴ S	0.042137	2003
		131	H ₂ ³³ S	0.007498	2003
HCOOH	37	261	H ¹² C ¹⁶ O ¹⁶ OH	0.983898	2003
COF ₂	38	269	¹² C ¹⁶ O ¹⁹ F ₂	0.986544	2003
SF ₆	39	29	³² S ¹⁹ F ₆	0.950180	2003
C ₃ H ₄	40	341	¹² C ₃ H ₆	0.966587	2003
HO ₂	41	166	H ¹⁶ O ₂	0.995107	2003
ClONO ₂	42	564	¹⁵ Cl ¹⁶ O ¹⁴ N ¹⁶ O ₂	0.749570	2003
		764	¹⁷ Cl ¹⁶ O ¹⁴ N ¹⁶ O ₂	0.239694	2003
CH ₃ Br	43	79	¹² CH ₃ ⁷⁹ Br	0.500995	2011
		81	¹² CH ₃ ⁸¹ Br	0.487433	2011
CH ₃ OH	44	216	¹² CH ₃ ¹⁶ OH	0.985930	2011
NO ⁺	45	46	¹⁴ N ¹⁶ O ⁺	0.993974	2011
HNC	46	142	H ¹⁴ N ¹² C	0.985114	2011
C ₆ H ₆	47	266	¹² C ₆ H ₆	0.934291	2011
C ₂ HD	48	122	¹² C ₂ HD	3.045500 × 10 ⁻⁴	2011
CF ₄	49	291	¹² C ¹⁵ F ₄	0.988890	2011
CH ₃ CN	50	234	¹² CH ₃ ¹² C ¹⁴ N	0.973866	2011

Molecule	Molecule Code	Isotope Code	Formula	Abundance	Since GEISA version
HDO	51	162	H ¹⁶ OD	3.106930 × 10 ⁻⁴	2015
		182	H ¹⁸ OD	6.230030 × 10 ⁻⁷	2015
		172	H ¹⁷ OD	1.158530 × 10 ⁻⁷	2015
SO ₃	52	26	³² S ¹⁶ O ₃	0.943400	2015
HONO	53	1	H ¹⁶ O ¹⁵ N ¹⁶ O	0.9937102	2020
COFCl	54	265	¹² C ¹⁶ OF ³⁵ Cl	1.000000	2020
		267	¹² C ¹⁶ OF ³⁷ Cl	1.000000	2020
CH ₃ I	55	1	¹² CH ₃ I	1.000000	2020
CH ₃ F	56	1	¹² CH ₃ F	1.000000	2020
RuO ₄	57	102	¹⁰² RuO ₄	1.000000	2020
		104	¹⁰⁴ RuO ₄	1.000000	2020
		101	¹⁰¹ RuO ₄	1.000000	2020
		99	⁹⁹ RuO ₄	1.000000	2020
		100	¹⁰⁰ RuO ₄	1.000000	2020
		97	⁹⁷ RuO ₄	1.000000	2020
		98	⁹⁸ RuO ₄	1.000000	2020
		106	¹⁰⁶ RuO ₄	1.000000	2020
		103	¹⁰³ RuO ₄	1.000000	2020