

Summary of molecule and isotope codes in GEISA-03

Molecule	Molecule Code	Isotope Code	Formula
H₂O	1	161	H ¹⁶ OH
		162	H ¹⁶ OD
		171	H ¹⁷ OH
		181	H ¹⁸ OH
		182	H ¹⁸ OD
CO₂	2	626	¹⁶ O ¹² C ¹⁶ O
		627	¹⁶ O ¹² C ¹⁷ O
		628	¹⁶ O ¹² C ¹⁸ O
		636	¹⁶ O ¹³ C ¹⁶ O
		637	¹⁶ O ¹³ C ¹⁷ O
		638	¹⁶ O ¹³ C ¹⁸ O
		728	¹⁷ O ¹² C ¹⁸ O
		828	¹⁸ O ¹² C ¹⁸ O
838	¹⁸ O ¹³ C ¹⁸ O		
O₃	3	666	¹⁶ O ¹⁶ O ¹⁶ O
		668	¹⁶ O ¹⁶ O ¹⁸ O
		686	¹⁶ O ¹⁸ O ¹⁶ O
		667	¹⁶ O ¹⁶ O ¹⁷ O
		676	¹⁶ O ¹⁷ O ¹⁶ O
N₂O	4	446	¹⁴ N ¹⁴ N ¹⁶ O
		447	¹⁴ N ¹⁴ N ¹⁷ O
		448	¹⁴ N ¹⁴ N ¹⁸ O
		456	¹⁴ N ¹⁵ N ¹⁶ O
		546	¹⁵ N ¹⁴ N ¹⁶ O
CO	5	26	¹² C ¹⁶ O
		27	¹² C ¹⁷ O
		28	¹² C ¹⁸ O
		36	¹³ C ¹⁶ O
		37	¹³ C ¹⁷ O
		38	¹³ C ¹⁸ O
CH₄	6	211	¹² CH ₄
		311	¹³ CH ₄
O₂	7	66	¹⁶ O ¹⁶ O
		67	¹⁶ O ¹⁷ O
		68	¹⁶ O ¹⁸ O

Table 2. (contd.)

Molecule	Molecule Code	Isotope Code	Formula
NO	8	46	$^{14}\text{N}^{16}\text{O}$
		48	$^{14}\text{N}^{18}\text{O}$
		56	$^{15}\text{N}^{16}\text{O}$
SO₂	9	626	$^{32}\text{S}^{16}\text{O}_2$
		646	$^{34}\text{S}^{16}\text{O}_2$
NO₂	10	646	$^{14}\text{N}^{16}\text{O}_2$
NH₃	11	411	$^{14}\text{NH}_3$
		511	$^{15}\text{NH}_3$
PH₃	12	131	$^{31}\text{PH}_3$
HNO₃	13	146	$\text{H}^{14}\text{N}^{16}\text{O}$
OH	14	61	^{16}OH
		62	^{16}OD
		81	^{18}OH
HF	15	19	H^{19}F
HCl	16	15	H^{35}Cl
		17	H^{37}Cl
HBr	17	11	H^{81}Br
		19	H^{79}Br
HI	18	17	H^{127}I
ClO	19	56	$^{35}\text{Cl}^{16}\text{O}$
		76	$^{37}\text{Cl}^{16}\text{O}$
OCS	20	622	$^{16}\text{O}^{12}\text{C}^{32}\text{S}$
		623	$^{16}\text{O}^{12}\text{C}^{33}\text{S}$
		624	$^{16}\text{O}^{12}\text{C}^{34}\text{S}$
		632	$^{16}\text{O}^{13}\text{C}^{32}\text{S}$
		634	$^{16}\text{O}^{13}\text{C}^{34}\text{S}$
		822	$^{18}\text{O}^{12}\text{C}^{32}\text{S}$
H₂CO	21	126	$\text{H}_2^{12}\text{C}^{16}\text{O}$
		128	$\text{H}_2^{12}\text{C}^{18}\text{O}$
		136	$\text{H}_2^{13}\text{C}^{16}\text{O}$
C₂H₆	22	226	$^{12}\text{C}_2\text{H}_6$
		236	$^{12}\text{C}^{13}\text{CH}_6$
CH₃D	23	212	$^{12}\text{CH}_3\text{D}$
C₂H₂	24	221	$^{12}\text{C}_2\text{H}_2$
		231	$^{12}\text{C}^{13}\text{CH}_2$

Table 2. (contd.)

Molecule	Molecule Code	Isotope Code	Formula
C₂H₄	25	211	¹² C ₂ H ₄
		311	¹² C ¹³ CH ₄
GeH₄	26	411	⁷⁴ GeH ₄
HCN	27	124	H ¹² C ¹⁴ N
		125	H ¹³ C ¹⁵ N
		134	H ¹³ C ¹⁴ N
C₃H₈	28	221	¹² C ₃ H ₈
C₂N₂	29	224	¹² C ₂ ¹⁴ N ₂
C₄H₂	30	211	¹² C ₄ H ₂
HC₃N	31	124	H ¹² C ₃ ¹⁴ N
HOCl	32	165	H ¹⁶ O ³⁵ Cl
		167	H ¹⁶ O ³⁷ Cl
N₂	33	44	¹⁴ N ¹⁴ N
CH₃Cl	34	215	¹² CH ₃ ³⁵ Cl
		217	¹² CH ₃ ³⁷ Cl
H₂O₂	35	166	H ₂ ¹⁶ O ¹⁶ O
H₂S	36	121	H ₂ ³² S
		131	H ₂ ³³ S
		141	H ₂ ³⁴ S
HCOOH	37	261	H ¹² C ¹⁶ O ¹⁶ OH
COF₂	38	269	¹² C ¹⁶ O ¹⁹ F ₂
SF₆	39	29	³² S ¹⁹ F ₆
C₃H₄	40	341	¹² C ₃ H ₄
HO₂	41	166	H ¹⁶ O ₂
ClONO₂	42	564	¹⁵ Cl ¹⁶ O ¹⁴ N ¹⁶ O ₂
		764	¹⁷ Cl ¹⁶ O ¹⁴ N ¹⁶ O ₂