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Isotopologue Metadata



Download this data in text format as [molparam.txt](#).

1: H₂O

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	Q(296 K)	Q (full range)	<i>g_i</i>
1	1	H ₂ ¹⁶ O	161	0.997317	18.010565	174.58	q1.txt	1
2	2	H ₂ ¹⁸ O	181	0.002000	20.014811	176.05	q2.txt	1
3	3	H ₂ ¹⁷ O	171	3.718840 × 10 ⁻⁴	19.01478	1052.14	q3.txt	6
4	4	HD ¹⁶ O	162	3.106930 × 10 ⁻⁴	19.01674	864.74	q4.txt	6
5	5	HD ¹⁸ O	182	6.230030 × 10 ⁻⁷	21.020985	875.57	q5.txt	6

6	6	HD ¹⁷ O	172	1.158530×10^{-7}	20.020956	5226.79	q6.txt	36
129	7	D ₂ ¹⁶ O	262	2.419700×10^{-8}	20.022915	1027.80	q129.txt	1

2: CO₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
7	1	¹² C ¹⁶ O ₂	626	0.984204	43.98983	286.09	q7.txt	1
8	2	¹³ C ¹⁶ O ₂	636	0.011057	44.993185	576.64	q8.txt	2
9	3	¹⁶ O ¹² C ¹⁸ O	628	0.003947	45.994076	607.81	q9.txt	1
10	4	¹⁶ O ¹² C ¹⁷ O	627	7.339890×10^{-4}	44.994045	3542.61	q10.txt	6
11	5	¹⁶ O ¹³ C ¹⁸ O	638	4.434460×10^{-5}	46.997431	1225.46	q11.txt	2
12	6	¹⁶ O ¹³ C ¹⁷ O	637	8.246230×10^{-6}	45.9974	7141.32	q12.txt	12
13	7	¹² C ¹⁸ O ₂	828	3.957340×10^{-6}	47.998322	323.42	q13.txt	1
14	8	¹⁷ O ¹² C ¹⁸ O	827	1.471800×10^{-6}	46.998291	3766.58	q14.txt	6
121	9	¹² C ¹⁷ O ₂	727	1.368470×10^{-7}	45.998262	10971.57	q121.txt	1
15	0	¹³ C ¹⁸ O ₂	838	4.446000×10^{-8}	49.001675	652.24	q15.txt	2
120	11	¹⁸ O ¹³ C ¹⁷ O	837	1.653540×10^{-8}	48.001646	7595.04	q120.txt	12
122	12	¹³ C ¹⁷ O ₂	737	1.537500×10^{-9}	47.0016182378	22120.47	q122.txt	2

3: O₃

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
16	1	¹⁶ O ₃	666	0.992901	47.984745	3483.71	q16.txt	1
17	2	¹⁶ O ¹⁶ O ¹⁸ O	668	0.003982	49.988991	7465.68	q17.txt	1
18	3	¹⁶ O ¹⁸ O ¹⁶ O	686	0.001991	49.988991	3647.08	q18.txt	1
19	4	¹⁶ O ¹⁶ O ¹⁷ O	667	7.404750×10^{-4}	48.98896	43330.85	q19.txt	6
20	5	¹⁶ O ¹⁷ O ¹⁶ O	676	3.702370×10^{-4}	48.98896	21404.96	q20.txt	6

4: N₂O

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
21	1	¹⁴ N ₂ ¹⁶ O	446	0.990333	44.001062	4984.90	q21.txt	9
22	2	¹⁴ N ¹⁵ N ¹⁶ O	456	0.003641	44.998096	3362.01	q22.txt	6

23	3	¹⁵ N ¹⁴ N ¹⁶ O	546	0.003641	44.998096	3458.58	q23.txt	6
24	4	¹⁴ N ₂ ¹⁸ O	448	0.001986	46.005308	5314.74	q24.txt	9
25	5	¹⁴ N ₂ ¹⁷ O	447	3.692800×10^{-4}	45.005278	30971.79	q25.txt	54

5: CO

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
26	1	¹² C ¹⁶ O	26	0.986544	27.994915	107.42	q26.txt	1
27	2	¹³ C ¹⁶ O	36	0.011084	28.99827	224.69	q27.txt	2
28	3	¹² C ¹⁸ O	28	0.001978	29.999161	112.77	q28.txt	1
29	4	¹² C ¹⁷ O	27	3.678670×10^{-4}	28.99913	661.17	q29.txt	6
30	5	¹³ C ¹⁸ O	38	2.222500×10^{-5}	31.002516	236.44	q30.txt	2
31	6	¹³ C ¹⁷ O	37	4.132920×10^{-6}	30.002485	1384.66	q31.txt	12

6: CH₄

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
32	1	¹² CH ₄	211	0.988274	16.0313	590.48	q32.txt	1
33	2	¹³ CH ₄	311	0.011103	17.034655	1180.82	q33.txt	2
34	3	¹² CH ₃ D	212	6.157510×10^{-4}	17.037475	4794.73	q34.txt	3
35	4	¹³ CH ₃ D	312	6.917850×10^{-6}	18.04083	9599.16	q35.txt	6

7: O₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
36	1	¹⁶ O ₂	66	0.995262	31.98983	215.73	q36.txt	1
37	2	¹⁶ O ¹⁸ O	68	0.003991	33.994076	455.23	q37.txt	1
38	3	¹⁶ O ¹⁷ O	67	7.422350×10^{-4}	32.994045	2658.12	q38.txt	6

8: NO

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
39	1	¹⁴ N ¹⁶ O	46	0.993974	29.997989	1142.13	q39.txt	3
40	2	¹⁵ N ¹⁶ O	56	0.003654	30.995023	789.26	q40.txt	2

41	3	¹⁴ N ¹⁸ O	48	0.001993	32.002234	1204.44	q41.txt	3
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9: SO₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	Q(296 K)	Q (full range)	<i>g_i</i>
42	1	³² S ¹⁶ O ₂	626	0.945678	63.961901	6340.30	q42.txt	1
43	2	³⁴ S ¹⁶ O ₂	646	0.041950	65.957695	6368.98	q43.txt	1

10: NO₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	Q(296 K)	Q (full range)	<i>g_i</i>
44	1	¹⁴ N ¹⁶ O ₂	646	0.991616	45.992904	13577.48	q44.txt	3

11: NH₃

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	Q(296 K)	Q (full range)	<i>g_i</i>
45	1	¹⁴ NH ₃	4111	0.995872	17.026549	1725.22	q45.txt	3
46	2	¹⁵ NH ₃	5111	0.003661	18.023583	1153.30	q46.txt	2

12: HNO₃

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	Q(296 K)	Q (full range)	<i>g_i</i>
47	1	H ¹⁴ N ¹⁶ O ₃	146	0.989110	62.995644	2.14 × 10 ⁵	q47.txt	6
117	2	H ¹⁵ N ¹⁶ O ₃	156	0.003636	63.99268	1.43 × 10 ⁵	q117.txt	4

13: OH

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	Q(296 K)	Q (full range)	<i>g_i</i>
48	1	¹⁶ OH	61	0.997473	17.00274	80.35	q48.txt	2
49	2	¹⁸ OH	81	0.002000	19.006986	80.88	q49.txt	2
50	3	¹⁶ OD	62	1.553710 × 10 ⁻⁴	18.008915	209.32	q50.txt	3

14: HF

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	Q(296 K)	Q (full range)	<i>g_i</i>
51	1	H ¹⁹ F	19	0.999844	20.006229	41.47	q51.txt	4

110	2	D ¹⁹ F	29	1.557410 × 10 ⁻⁴	21.012404	115.91	q110.txt	6
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15: HCl

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
52	1	H ³⁵ Cl	15	0.757587	35.976678	160.65	q52.txt	8
53	2	H ³⁷ Cl	17	0.242257	37.973729	160.89	q53.txt	8
107	3	D ³⁵ Cl	25	1.180050 × 10 ⁻⁴	36.982853	462.78	q107.txt	12
108	4	D ³⁷ Cl	27	3.773500 × 10 ⁻⁵	38.979904	464.13	q108.txt	12

16: HBr

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
54	1	H ⁷⁹ Br	19	0.506781	79.92616	200.17	q54.txt	8
55	2	H ⁸¹ Br	11	0.493063	81.924115	200.23	q55.txt	8
111	3	D ⁷⁹ Br	29	7.893840 × 10 ⁻⁵	80.932336	586.40	q111.txt	12
112	4	D ⁸¹ Br	21	7.680160 × 10 ⁻⁵	82.930289	586.76	q112.txt	12

17: HI

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
56	1	H ¹²⁷ I	17	0.999844	127.912297	388.99	q56.txt	12
113	2	D ¹²⁷ I	27	1.557410 × 10 ⁻⁴	128.918472	1147.06	q113.txt	18

18: ClO

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
57	1	³⁵ Cl ¹⁶ O	56	0.755908	50.963768	3274.61	q57.txt	4
58	2	³⁷ Cl ¹⁶ O	76	0.241720	52.960819	3332.29	q58.txt	4

19: OCS

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
59	1	¹⁶ O ¹² C ³² S	622	0.937395	59.966986	1221.01	q59.txt	1
60	2	¹⁶ O ¹² C ³⁴ S	624	0.041583	61.96278	1253.48	q60.txt	1

61	3	$^{16}\text{O}^{13}\text{C}^{32}\text{S}$	632	0.010531	60.970341	2484.15	q61.txt	2
62	4	$^{16}\text{O}^{12}\text{C}^{33}\text{S}$	623	0.007399	60.966371	4950.11	q62.txt	4
63	5	$^{18}\text{O}^{12}\text{C}^{32}\text{S}$	822	0.001880	61.971231	1313.78	q63.txt	1

20: H₂CO

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	<i>Q</i> (full range)	<i>g_i</i>
64	1	H ₂ ¹² C ¹⁶ O	126	0.986237	30.010565	2844.53	q64.txt	1
65	2	H ₂ ¹³ C ¹⁶ O	136	0.011080	31.01392	5837.69	q65.txt	2
66	3	H ₂ ¹² C ¹⁸ O	128	0.001978	32.014811	2986.44	q66.txt	1

21: HOCl

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	<i>Q</i> (full range)	<i>g_i</i>
67	1	H ¹⁶ O ³⁵ Cl	165	0.755790	51.971593	19274.79	q67.txt	8
68	2	H ¹⁶ O ³⁷ Cl	167	0.241683	53.968644	19616.20	q68.txt	8

22: N₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	<i>Q</i> (full range)	<i>g_i</i>
69	1	¹⁴ N ₂	44	0.992687	28.006148	467.10	q69.txt	1
118	2	¹⁴ N ¹⁵ N	45	0.007478	29.003182	644.10	q118.txt	6

23: HCN

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	<i>Q</i> (full range)	<i>g_i</i>
70	1	H ¹² C ¹⁴ N	124	0.985114	27.010899	892.20	q70.txt	6
71	2	H ¹³ C ¹⁴ N	134	0.011068	28.014254	1830.97	q71.txt	12
72	3	H ¹² C ¹⁵ N	125	0.003622	28.007933	615.28	q72.txt	4

24: CH₃Cl

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	<i>Q</i> (full range)	<i>g_i</i>
73	1	¹² CH ₃ ³⁵ Cl	215	0.748937	49.992328	57916.12	q73.txt	4
74	2	¹² CH ₃ ³⁷ Cl	217	0.239491	51.989379	58833.90	q74.txt	4

25: H₂O₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
75	1	H ₂ ¹⁶ O ₂	1661	0.994952	34.00548	9847.99	q75.txt	1

26: C₂H₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
76	1	¹² C ₂ H ₂	1221	0.977599	26.01565	412.45	q76.txt	1
77	2	H ¹² C ¹³ CH	1231	0.021966	27.019005	1656.18	q77.txt	8
105	3	H ¹² C ¹² CD	1222	3.045500 × 10 ⁻⁴	27.021825	1581.84	q105.txt	6

27: C₂H₆

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
78	1	¹² C ₂ H ₆	1221	0.976990	30.04695	70882.52	q78.txt	1
106	2	¹² CH ₃ ¹³ CH ₃	1231	0.021953	31.050305	36191.80	q106.txt	2

28: PH₃

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
79	1	³¹ PH ₃	1111	0.999533	33.997238	3249.44	q79.txt	2

29: COF₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
80	1	¹² C ¹⁶ O ¹⁹ F ₂	269	0.986544	65.991722	70028.43	q80.txt	1
119	2	¹³ C ¹⁶ O ¹⁹ F ₂	369	0.011083	66.995083	1.40 × 10 ⁵	q119.txt	2

30: SF₆

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
126	1	³² S ¹⁹ F ₆	29	0.950180	145.962492	1.62 × 10 ⁶	q126.txt	1

31: H₂S

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
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81	1	H ₂ ³² S	121	0.949884	33.987721	505.79	q81.txt	1
82	2	H ₂ ³⁴ S	141	0.042137	35.983515	504.35	q82.txt	1
83	3	H ₂ ³³ S	131	0.007498	34.987105	2014.94	q83.txt	4

32: HCOOH

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
84	1	H ¹² C ¹⁶ O ¹⁶ OH	126	0.983898	46.00548	39132.76	q84.txt	4

33: HO₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
85	1	H ¹⁶ O ₂	166	0.995107	32.997655	4300.39	q85.txt	2

34: O

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
86	1	¹⁶ O	6	0.997628	15.994915	6.72		1

35: ClONO₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
127	1	³⁵ Cl ¹⁶ O ¹⁴ N ¹⁶ O ₂	5646	0.749570	96.956672	4.79 × 10 ⁶	q127.txt	12
128	2	³⁷ Cl ¹⁶ O ¹⁴ N ¹⁶ O ₂	7646	0.239694	98.953723	4.91 × 10 ⁶	q128.txt	12

36: NO⁺

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
87	1	¹⁴ N ¹⁶ O ⁺	46	0.993974	29.997989	311.69	q87.txt	3

37: HOBr

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
88	1	H ¹⁶ O ⁷⁹ Br	169	0.505579	95.921076	28339.38	q88.txt	8
89	2	H ¹⁶ O ⁸¹ Br	161	0.491894	97.919027	28237.98	q89.txt	8

38: C₂H₄

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹ ₁	Q(296 K)	Q (full range)	<i>g_i</i>
90	1	¹² C ₂ H ₄	221	0.977294	28.0313	11041.54	q90.txt	1
91	2	¹² CH ₂ ¹³ CH ₂	231	0.021959	29.034655	45196.89	q91.txt	2

39: CH₃OH

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	Q(296 K)	Q (full range)	<i>g_i</i>
92	1	¹² CH ₃ ¹⁶ OH	2161	0.985930	32.026215	70569.92	q92.txt	2

40: CH₃Br

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	Q(296 K)	Q (full range)	<i>g_i</i>
93	1	¹² CH ₃ ⁷⁹ Br	219	0.500995	93.941811	83051.98	q93.txt	4
94	2	¹² CH ₃ ⁸¹ Br	211	0.487433	95.939764	83395.21	q94.txt	4

41: CH₃CN

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹ ₁	Q(296 K)	Q (full range)	<i>g_i</i>
95	1	¹² CH ₃ ¹² C ¹⁴ N	2124	0.973866	41.026549	88672.19	q95.txt	3

42: CF₄

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	Q(296 K)	Q (full range)	<i>g_i</i>
96	1	¹² C ¹⁹ F ₄	29	0.988890	87.993616	1.21 × 10 ⁵	q96.txt	1

43: C₄H₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	Q(296 K)	Q (full range)	<i>g_i</i>
116	1	¹² C ₄ H ₂	2211	0.955998	50.01565	9818.97	q116.txt	1

44: HC₃N

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	Q(296 K)	Q (full range)	<i>g_i</i>
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109	1	H ¹² C ₃ ¹⁴ N	1224	0.963346	51.010899	24786.84	q109.txt	6
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45: H₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
103	1	H ₂	11	0.999688	2.01565	7.67	q103.txt	1
115	2	HD	12	3.114320 × 10 ⁻⁴	3.021825	29.87	q115.txt	6

46: CS

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
97	1	¹² C ³² S	22	0.939624	43.971036	253.62	q97.txt	1
98	2	¹² C ³⁴ S	24	0.041682	45.966787	257.77	q98.txt	1
99	3	¹³ C ³² S	32	0.010556	44.974368	537.50	q99.txt	2
100	4	¹² C ³³ S	23	0.007417	44.970399	1022.97	q100.txt	4

47: SO₃

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
114	1	³² S ¹⁶ O ₃	26	0.943400	79.95682	7783.30	q114.txt	1

48: C₂N₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
123	1	¹² C ₂ ¹⁴ N ₂	4224	0.970752	52.006148	15582.44	q123.txt	1

49: COCl₂

global ID	local ID	Formula	AFGL code	Abundance	Molar Mass /g·mol ⁻¹	<i>Q</i> (296 K)	Q (full range)	<i>g_i</i>
124	1	¹² C ¹⁶ O ³⁵ Cl ₂	2655	0.566392	97.9326199796	1.48 × 10 ⁶	q124.txt	1
125	2	¹² C ¹⁶ O ³⁵ Cl ³⁷ Cl	2657	0.362235	99.9296698896	3.04 × 10 ⁶	q125.txt	16