

Table S1. List of parent ions and fragmentation products for (A) CO₂, (B) low-mass organics, (C-D) PH₃ and H₂S, (E) NH₄⁺, (F) H_xSO_y fragments, (G) HNO₂ and HNO₃, and (H) H³⁵Cl/H³⁷Cl.

(A) carbon dioxide					
LMNS amu	count	formula	parent & fragment ions	expected amu	Δamu
44.991	21504	¹³ CO ₂ ⁺	(M+1) ⁺	44.993355	0.002
43.991	1769472	CO ₂ ⁺	M ⁺	43.990000	0.001
28.997	6656	¹³ CO ⁺	[(M+1)-O] ⁺	28.998355	0.001
27.995	512000	CO ⁺	[M-O] ⁺	27.995000	0.000
22.496	560	¹³ CO ₂ ⁺⁺	(M+1) ⁺⁺	22.496677	0.001
15.995	335872	O ⁺	[M-O-C] ⁺	15.995000	0.000
12	344064	¹² C ⁺	[M-2O] ⁺	12.000000	0.000
(B) low-mass organics					
LMNS amu	count	formula	parent & fragment ions	expected amu	Δamu
78.053	16	C ₆ H ₆ ⁺	Benzene: M ⁺	78.046950	0.001
77.04	2	C ₆ H ₅ ⁺	Benzene F1: [M-H] ⁺	77.039125	0.000
40.029	80	C ₃ H ₄ ⁺	Propyne: M ⁺	40.031300	0.000
30.046	208	C ₂ H ₆ ⁺	Ethane: M ⁺	30.046950	0.000
29.039	992	C ₂ H ₅ ⁺	Ethane F1: [M-H] ⁺	29.039125	0.000
28.032	122880	C ₂ H ₄ ⁺	Ethene: M ⁺ Ethane F2: [M-2H] ⁺	28.031300	0.000
27.023	124	C ₂ H ₃ ⁺	Ethene F1: [M-H] ⁺ Ethane F3: [M-3H] ⁺	27.023475	0.002
26.014	122	C ₂ H ₂ ⁺	Ethene F2: [M-2H] ⁺ Ethane F4: [M-4H] ⁺ Ethyne: M ⁺	26.015650	0.000
16.031	39936	CH ₄ ⁺	Methane: M ⁺	16.031300	0.003
15.023	22528	CH ₃ ⁺	Methane F1: [M-H] ⁺ Ethane F5: [M-3H-C] ⁺	15.023475	0.000
(C) phosphine					
LMNS amu	count	formula	parent & fragment ions	expected amu	Δamu
35.005	12	³¹ P ⁺	(M+1) ⁺	35.003659	0.001
33.992	19	³¹ P ⁺	M ⁺	33.997382	0.005
32.985	18	³¹ P ⁺	[M-H] ⁺	32.989557	0.005
30.973	11	P ⁺	[M-3H] ⁺	30.973907	0.001
(D) hydrogen sulfide					
LMNS amu	count	formula	parent & fragment ions	expected amu	Δamu
33.992	19	H ₂ S ⁺	M ⁺	33.9877212	0.004
32.985	18	HS ⁺	[M-H] ⁺	32.9798962	0.005
31.972	335	³² S ⁺	[M-2H] ⁺	31.9720712	0.000

(E) ammonium					
LMNS amu	count	formula	parent & fragment ions	expected amu	Δ amu
18.034	66	NH ₄ ⁺	M ⁺	18.034374	0.000
16.018	40960	⁺ NH ₂	[M-2H] ⁺	16.018724	0.001
15.013	7680	⁺ NH	[M-3H] ⁺	15.010899	0.002
14	19456	¹⁴ N ⁺	[M-4H] ⁺	14.003074	0.003
(F) sulfuric acid/sulfate fragments					
LMNS amu	count	formula	parent & fragment ions	expected amu	Δ amu
79.958	0	SO ₃ ⁺	[M-18] ⁺	64.969896	0.010
65.961	1	³⁴ SO ₂ ⁺	[(M+2)-34] ⁺	63.962071	0.000
64.96	3	HSO ₂ ⁺	[M-33] ⁺	50.970692	0.002
63.962	5	SO ₂ ⁺	[M-34] ⁺	49.962867	0.005
50.969	0	H ³⁴ SO ⁺	[(M+2)-49] ⁺	48.974896	0.001
49.968	3	³⁴ SO ⁺	[(M+2)-50] ⁺	47.967071	0.001
48.974	2	HSO ⁺	[M-49] ⁺	33.967867	0.002
47.966	10	SO ⁺	[M-50] ⁺	31.972071	0.000
(G) nitrous and nitric acids					
LMNS amu	count	formula	parent & fragment ions	expected amu	Δ amu
47	94	HNO ₂ ⁺	Nitrous Acid: M ⁺	47.000899	0.001
31.006	26	HNO ⁺	Nitrous Acid: [M-16] ⁺	31.005899	0.000
29.997	270	NO ⁺	Nitric Acid: [M-33] ⁺ Nitrous Acid: [M-17] ⁺	29.998074	0.001
17.002	296	⁺ OH	Nitric Acid: [M-46] ⁺ Nitrous Acid: [M-30] ⁺	17.002825	0.001
15.995	335872	O ⁺	Nitric Acid: [M-47] ⁺ Nitrous Acid: [M-31] ⁺	15.995000	0.000
14	19456	¹⁴ N ⁺	Nitric Acid: [M-49] ⁺ Nitrous Acid: [M-33] ⁺	14.003074	0.003
62.994	1	HNO ₃ ⁺	Nitric Acid: M ⁺	62.995899	0.002
(H) hydrochloric acid					
LMNS amu	count	formula	parent & fragment ions	expected amu	Δ amu
37.968	152	H ³⁷ Cl ⁺	(M+2) ⁺	37.973728	0.006
36.966	9	³⁷ Cl ⁺	[(M+2)-H] ⁺	36.965903	0.000
35.981	704	HCl ⁺	M ⁺	35.976678	0.004
34.972	15	³⁵ Cl ⁺	[M-H] ⁺	34.968853	0.003
1.008	3520	H ⁺	[M-Cl] ⁺ , [(M+2)-Cl] ⁺	1.007825	0.000

Table S2. List of assignments, including alternatives, for the LMNS mass data from 51.3 km.

(a) Bold , resolving power (RP) outside of estimated LMNS resolution. (b) Difference in mass between successive mass pairs. (c) Normal typeface, tentative assignment; <i>italics</i> , putative assignment. (d) <i>Italics</i> = $\Delta\text{amu} > 0.006$ amu.															
#	RP ^a	Δm^b	amu	count	assignment ^c	expected amu	Δamu^d	alternative ^c	amu	Δ^d	alt. ^c	amu	Δ^d	composite mass	Δamu
1			1.008	3520	H	1.007825	0.000								
2	2	1.008	2.016	22016	H₂	2.014102	0.002								
3	3	0.934	2.950	23											
4	60	0.050	3.000	26	³He	3.016029	<i>0.016</i>	H ₃	3.023475	<i>0.023</i>					
5	61	0.050	3.050	29	HD	3.021927	<i>0.028</i>								
6	5	0.750	3.800	12											
7	26	0.150	3.950	13312											
8	80	0.050	4.000	34816	⁴He	4.002603	0.003								
9	81	0.050	4.050	32256	D₂	4.028204	0.022								
10	2	5.000	9.050	70											
11	11	0.950	10.000	66	B	10.012937	<i>0.013</i>								
12	201	0.050	10.050	70											
13	12	0.900	10.950	76											
14	220	0.050	11.000	96											
15	221	0.050	11.050	78											
16	13	0.950	12.000	344064	¹²C	12.000000	0.000								
17	7	2.000	14.000	19456	¹⁴N	14.003074	0.003	CH ₂	14.01565	<i>0.016</i>					
18	15	1.000	15.000	20992	¹⁵N	15.000109	0.000								
19	1155	0.013	15.013	7680	NH	15.010899	0.002								
20	3004	0.005	15.018	16896	NH / CH₃										
21	3005	0.005	15.023	22528	CH₃	15.023475	0.000								
22	3006	0.005	15.028	22016	CH₃										
23	3007	0.005	15.033	12800	CH₃										
24	17	0.962	15.995	335872	O	15.995000	0.000								
25	696	0.023	16.018	40960	NH₂	16.018724	0.001								
26	1233	0.013	16.031	39936	CH₄	16.031300	0.000	¹³ CH ₃	16.02683	0.004					
27	18	0.971	17.002	296	OH	17.002825	0.001								
28	709	0.024	17.026	244	NH₃ / NHD / ¹³CH₄	17.026549	0.001	¹³ CH ₄	17.034655	<i>0.009</i>	NHD	17.025001	0.001	17.028735	0.003

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29	19	0.959	17.985	336	³⁶ Ar ⁺⁺	17.983773	0.001				OD	18.009102	0.024		
30	720	0.025	18.010	1088	H ₂ O	18.010650	0.001	¹⁸ O	17.99916	0.011					
31	751	0.024	18.034	66	NH ₄ / NH ₂ D	18.034374	0.000	NH ₂ D	18.032826	0.001					
32	20	0.953	18.987	34	³⁸ Ar ⁺⁺	18.981366	0.006								
33	1727	0.011	18.998	18	F	18.998403	0.000								
34	2112	0.009	19.007	5	¹⁸ OH	19.006985	0.000	HDO	19.016927	0.010					
35	21	0.974	19.981	480	⁴⁰ Ar ⁺⁺	19.981192	0.000								
36	1817	0.011	19.992	384	²⁰ Ne	19.992440	0.000								
37	1429	0.014	20.006	112	HF	20.006228	0.000								
38	2224	0.009	20.015	30	H ₂ ¹⁸ O	20.014810	0.000	D ₂ O	20.023204	0.008					
39	21	0.978	20.993	10	²¹ Ne	20.993847	0.001								
40	22	0.998	21.991	45056	²² Ne	21.991385	0.000								
41	5499	0.004	21.995	47104	²² Ne / CO ₂ ⁺⁺			CO ₂ ⁺⁺	21.995	0.000					
42	45	0.501	22.496	560	¹³ CO ₂ ⁺⁺	22.496677	0.001								
43	7	3.506	26.002	112	CN	26.003074	0.001								
44	2168	0.012	26.014	122	C ₂ H ₂	26.015650	0.002								
45	27	0.996	27.010	102	HCN	27.010899	0.001								
46	2079	0.013	27.023	124	C ₂ H ₃	27.023475	0.000								
47	29	0.965	27.988	507904	CO(a)										
48	3999	0.007	27.995	606208	CO(b)	27.995000	0.000								
49	5600	0.005	28.000	655360	N ₂ (a) / CO(c)										
50	5601	0.005	28.005	671744	N ₂ (b)	28.006148	0.001								
51	4002	0.007	28.012	499712	N ₂ (c)										
52	1402	0.020	28.032	122880	C ₂ H ₄	28.031300	0.001	DCN	28.017176	0.015	CH ₂ N	28.018724	0.013		
53	30	0.965	28.997	6656	¹³ CO(a)	28.998355	0.001								
54	4834	0.006	29.003	7040	¹³ CO(b) / ¹⁴ N ¹⁵ N			¹⁴ N ¹⁵ N	29.003183	0.000					
55	807	0.036	29.039	992	C ₂ H ₅	29.039125	0.000								
56	31	0.958	29.997	1024	C ¹⁸ O	29.999160	0.002	NO	29.998074	0.001					
57	613	0.049	30.046	208	C ₂ H ₆	30.046950	0.001								
58	33	0.927	30.973	11	P	30.973907	0.001								
59	940	0.033	31.006	26	HNO	31.005899	0.000	CF	30.998403	0.008					

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60	33	0.966	31.972	128	³² S	31.972071	0.000								
61	1777	0.018	31.990	320	O ₂	31.990000	0.000	PH	31.981732	0.008					
62	33	0.995	32.985	18	PH ₂	32.989557	0.005	HS	32.979896	0.005	PD	32.988009	0.003		
63	35	0.981	33.966	15	³⁴ S	33.967867	0.002								
64	1307	0.026	33.992	19	PH ₃	33.997382	0.005	H ₂ S	33.987721	0.004	PHD	33.995834	0.004		
65	2616	0.013	34.005	21	H ₂ O ₂	34.005650	0.001								
66	36	0.967	34.972	15	³⁵ Cl	34.968853	0.003								
67	1061	0.033	35.005	12	PH ₂ D	35.003659	0.001	HDS	34.993998	0.011					
68	37	0.961	35.966	656	³⁶ Ar	35.967545	0.002								
69	2399	0.015	35.981	704	HCl	35.976678	0.004								
70	38	0.985	36.966	9	³⁷ Cl	36.965903	0.000								
71	38	1.002	37.968	152	H ³⁷ Cl / ³⁸ Ar	37.973728	0.006	³⁸ Ar	37.962732	0.005					
72	20	1.982	39.950	1376	⁴⁰ Ar(a)										
73	4995	0.008	39.958	1504	⁴⁰ Ar(b)										
74	5709	0.007	39.965	1664	⁴⁰ Ar(c)	39.962383	0.003								
75	5710	0.007	39.972	1696	⁴⁰ Ar(d)										
76	702	0.057	40.029	80	C ₃ H ₄	40.031300	0.002								
77	11	3.962	43.991	1769472	CO ₂	43.990000	0.001	N ₂ O	44.001148	0.010					
78	45	1.000	44.991	21504	¹³ CO ₂	44.993355	0.002	CO ₂ H	44.997825	0.007					
79	146	0.311	45.302	108	¹³⁶ Xe ⁺⁺⁺	45.302406	0.000								
80	66	0.693	45.995	7936	CO ¹⁸ O	45.994160	0.001	NO ₂	45.993074	0.002	HCOOH	46.00565	0.011		
81	47	1.005	47.000	94	HNO ₂	47.000899	0.001	¹⁵ NO ₂	46.990109	0.010					
82	50	0.966	47.966	10	SO	47.967071	0.001								
83	49	1.008	48.974	2	HSO	48.974896	0.001								
84	50	0.994	49.968	3	³⁴ SO	49.962867	0.005								
85	51	1.001	50.969	2	ClO / H ³⁴ SO (trace)	50.963852 68	0.005	H ³⁴ SO (trace)	50.970692	0.002					
86	51	1.011	51.980	0											
87	27	2.024	54.004	0											
88	10	5.962	59.966	1	COS	59.967071	0.001								
89	61	1.002	60.968	0											
90	61	1.009	61.977	0											
91	62	1.017	62.994	1	HNO ₃	62.995899	0.002								

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