

PALMS file hints
created 200410 21 by Dan Murphy

Some negative peaks to look at:

- 12, 24 : C and C2 fragments from organics
- 19 : fluorine. Rare but unique.
- 26 : CN-
- 35, 37 : chlorine isotopes. 35 is the larger isotope and very unique.
- 43 : AlO in mineral particles, C2H3O in organics
- 45 : usually CO2H from oxygenated organics
- 46, 62 : usually NO2 and NO3 from nitrate
- 60, 76 : usually SiO2 and SiO3 from minerals
- 79 : Phosphorus or bromine (PO3- or Br-)
- 89 : oxalate
- 93 : almost always NaCl.Cl from salt
- 97 : the main negative sulfate peak HSO4-
- 115 : Sometimes sodium nitrate (NaNO3.NO-)
- 195 : Sulfuric acid cluster ion (H2SO4.HSO4)

97+195 is a quick look at sulfate
24+26+45 is a very quick look at organic

Some positive peaks to look at:

- 7 : Li. Not abundant but unique
- 12 : C
- 18 : NH4 and H2O. May be able to use 19 (H3O+) to separate
- 23 : Sodium. Very unique.
- 24 : C2 in organics, Mg in sea salt or meteoric material
- 28 : CO in organics, Si in minerals
- 30 : Usually NO+ from nitrate and probably most any nitrogen species.
Ammonium makes mass 30, but with lower efficiency than nitrate.
- 39 : usually K
- 40 : usually Ca if it is a big fraction of the ion current
- 56 : Fe and CaO. Tell them apart using the 54Fe isotope
- 48 : As a common small peak SO+ from sulfate.
As a rare big peak 48Ti. Excluding rare clusters helps here.
- 81 : Often NaCl.Na from sea salt.
- 99 : As a small peak protonated sulfuric acid.
- 165 : Na2H2SO4.Na: from sodium sulfate
- 208 : Almost always Pb.

***** Cluster Analysis Hints *****

***** Positive clusters *****

#spectra % notes

0	0	not in positive cluster (e.g. negative spectrum)
1	0	null
2	152258 48.6	organic & sulfate with some 30
3	79059	25.3 strong biomass burning, perhaps with sulfate
4	37445	12.0 organic & sulfate with more 18 and 30 than cat #2
5	13974	4.5 biomass burning with larger K than #3, a few large K not biomass
6	9407	3.0 sea salt and similar
7	6236	2.0 large NO+ peak, often low ion intensity (wet??)
8	4108	1.31 organic and sulfate with large 24, 36. Modified EC???
9	2825	0.90 Al mineral
10	2192	0.70 Ca mineral
11	1519	0.49 Si mineral, some other large 28
12	1340	0.43 large Fe Includes some meteoric and some mineral
13	480 0.15	large 80, probably pyridine
14	468 0.15	large vanadium peak
15	411 0.13	large Pb and Zn
16	341 0.11	Na, K with 108
17	151 0.05	large K mineral or salt
18	127 0.04	elemental carbon
19	91 0.03	44, 58, 70, 86, may include some amines
20	82 0.03	Mg and other large 24
21	78 0.02	large Sn peak
22	69 0.01	large K with 30
23	23 0.01	Sr with K
24	47 0.01	Na and K that didn't fit sea salt
25	45 0.01	56 and 44
26	43 0.01	K and elemental carbon with n+1 peaks
27	41 0.01	Titanium
28	38 0.01	masses 73 and 147
29	28 0.01	masses 30 and 80
30	24 0.01	C, Sb, and Pb
31	22 0.01	large Cu peak
32	21 0.01	masses 44 and 84
33	10 0.00	mass 47
34	8 0.00	K with masses 124 and 140
35	4 0.00	masses 29, 91, 77, 65, ...
36	4 0.00	large arsenic peak and/or rhenium
37	3 0.00	large tungsten peak
38	2 0.00	large silver peak
39	1 0.00	Co and Mo
40	1 0.00	mass 31
41	1 0.00	mass 121
42	1 0.00	mass 86

***** Negative clusters *****

#spectra % notes

0	0	not in negative cluster (e.g. positive spectrum)
1	0	null

2	159036	58.2	sulfate with organic
3	44661	16.3	organic with sulfate
4	34006	12.4	sulfate
5	15749	5.8	sulfate with sulfuric acid cluster ion
6	6298	2.3	sulfate with organic with organic acids, other oxygenates
7	5495	2.0	chlorine, mostly sea salt, often processed
8	2759	1.01	O- & organic and sulfate
9	1545	0.56	nitrate
10	1086	0.40	large mass 26 (CN-)
11	842	0.31	mineral (SiO ₃ , more)
12	291	0.11	sodium nitrate peaks
13	206	0.07	sodium sulfate peaks
14	206	0.07	OH-, Cl, organics
15	198	0.07	large H- peak
16	175	0.06	large O- and OH-
17	133	0.05	elemental carbon and elemental carbon with n+1 (eg C ₂ H-)
18	109	0.04	phosphorus peaks
19	102	0.04	mass 29 and 97
20	94	0.03	elemental carbon with sulfate
21	82	0.03	sea salt cluster ions
22	67	0.02	mass 42, 26 with nitrate and sulfate
23	59	0.02	nitrate-mineral
24	54	0.02	mass 88 (FeO ₂ -) with various
25	45	0.01	CN- with masses 66, 177, others
26	41	0.01	mixed sulfate, Cl, nitrate
27	32	0.01	mass 43
28	25	0.01	fluorine, O-, OH-, ...
29	7	0.00	probably processed elemental carbon
30	1	0.00	masses 60 and 89
31	1	0.00	masses 74 and 58
32	1	0.00	large bromine peak
33	1	0.00	large mass 120