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Basic Instructions for bulk upload:

There are 3 types of bulk uploads: Sample, Chemical Analysis, and Images. These must be done from a Microsoft Excel spreadsheet (.xls file). Only the first worksheet in a .xls workbook file (first tab at bottom left) will be uploaded, so be certain that the first sheet contains the data you want uploaded for the correct type of upload.

General Advice on file organization:

There are many functional ways to do this, but I like to keep all files (images, analyses, plots, etc) associated with a particular sample in a single folder. Nested folders are OK, but I have found over the years that it gets to be very confusing where data on a sample is spread among many different folders ("...now where did I put that X-ray map???").

So a file system might be organized like this:

- Sample
 - Sample information
 - Sample photograph
 - P-T conditions
 - Plots etc.
 - Summary information
 - o Subsample1
 - Maps
 - Image
 - Mnz
 - Data
 - (Each of these can be in folders or not)
 - o Subsample2
 - Maps
 - Images
 - Data
 - Etc.

This type of file structure is not necessary so long as the appropriate subsample is indicated in the respective spreadsheet (see below for specifics). The important thing is to keep the chain of evidence intact – that is, you know where every image, analysis, etc. comes from.

What is a subsample?

MetPetDB differentiates among subsamples. These are parts of a sample (hand sample) that are used for different purposes. A thin section is a subsample. A polished thin section for microprobe work is another subsample. Multiple polished thin sections are multiple subsamples. A rock chip mounted in epoxy for analysis or ground to a powder for bulk analysis is another subsample. It is important to keep track of which subsample is associated with each piece of data and one way to do this is to keep subsample-specific information inside individual folders. In order to create a subsample, you must find the main sample in "my samples" and below the listed attributes is a link called "Add Subsample". A subsample type must be specified from this list: Thin Section, Polished Thin Section, Rock Chip, or Mineral Separate.

Subsamples may also be created during chemical analysis bulk upload by providing a subsample name and the type of subsample for each new subsample. See Chemical Analysis Bulk Upload.

Required format for bulk uploads: Sample Upload

An upload worksheet contains data arranged in columns, each with an appropriate header. The following is a list of accepted headers, with notes as to which fields are required for every uploaded sample. The first row is reserved for the column headers. Each additional row should contain data for each sample to be uploaded. Only some fields are required in order to upload your data, as indicated below, but we encourage you to be thorough to maintain a database that is as versatile as possible. See example spreadsheet for more information.

All uploaded samples will initially be private. They may then be made public once they are in My Samples. You are encouraged to check your uploaded data before making it public, as once it is public, it cannot be edited or deleted except by a system administrator, and then only to correct errors (this ensures that public data used by everyone does not change).

Sample Ownership

Every sample must have an owner, who controls access privileges for the sample. Published data has the owner "Public" and can only be modified by the system administrator to correct errors. Also note that all sample numbers owned by an individual must be unique, as these are identifiers to MetPetDB. Ownership is assigned to the user at upload or sample entry into the database.

Some thought should be given to how you will access samples that you did not upload. Most petrologists have personal samples, and many have samples that students have collected and left behind. As samples can only belong to the user who uploaded them, it is important to clarify who should have access to these samples as part of a project. Note first that there is a separate header for "Collector" so that samples collected by a student can always be identified. Also, one can specify additional collection information as a "Comment" (e.g. Sample collected by John Doe for his PhD thesis").

The important point about a sample owner is that the owner controls access privileges. For example, if your student now works on Wall Street and you wish to continue to work on her samples, you may as long as the samples are included in a project to which you have access.

List of headers:

REQUIRED FIELDS

SAMPLE NUMBER

Each sample name must be unique to the sample owner. That is, there may be more than one sample with a specific number (e.g. 93-24) but only one sample with a particular owner can have this number.

ROCK TYPE - PRIMARY

This is not an exercise in taxonomy. However, every rock in the database must have a name. The "Rock Type - Primary" must be from list of rock types (see <u>Appendix A</u>). Additionally, multiple rock names are not only permitted, but encouraged (simply add an additional rock names as "Rock Type – Supplemental" – see below). However, a single rock type is required. The list in Appendix A is largely from the British Geological Survey's recommendations.

LATITUDE

Must be between -90 and 90 (negative for south). Units are decimal degrees (DD.DDDD). For notes on converting to decimal degrees see <u>Appendix B</u>. Note that five (5) decimal places corresponds to roughly 1 meter spatial resolution.

LONGITUDE

Must be between -180 and 180 (negative for west). Units are decimal degrees (DD.DDDD). For notes on converting to decimal degrees see <u>Appendix B</u>.

REFERENCE – required for published data.

Data that are published require a reference to the publication. MetPetDB uses the year and the GeoRef assension number (the same as NAVDAT), which can be found from a GeoRef search. For example, "1983-018415".

OPTIONAL FIELDS

LATITUDE ERROR

Units are in meters Latitude and longitude errors are an optional field for samples that are not well located.

LONGITUDE ERROR

Units are in meters Latitude and longitude errors are an optional field for samples that are not well located.

IGSN

IGSN (International Geological Sample Numbers) are unique identifiers that are created by SESAR (System for Earth SAmple Registration http://www.geosamples.org/). You must register your samples to obtain an IGSN. If you have an IGSN you can enter it here. We plan to have a tool for automatic sample registration through MetPetDB in the future.

REGION

This is the region from which the sample was collected. It can be any text you choose and there can be any number of regions. Regions can be geographic (e.g. Alps, Valhalla Complex, Raging River Valley, Pine Island) or political (e.g. Vermont, Cooke County).

When specifying multiple regions, put each distinct region in a separate spreadsheet column. Each column should be headed by the word "Region".

Also: you may want to look through the database to see if your region already exists.

COUNTRY

Where sample was collected. Pretty obvious, except where countries change names or the boundaries change. For consistency, input the country of collection at the time the sample was collected.

ALIAS (alternate sample number)

In some cases the same rock sample has been referred to by different sample numbers. These are sample aliases. There can be any number of aliases.

COLLECTOR

The name of the person who collected the sample. Preferred format: Lastname, First name middle initial.

DATE OF COLLECTION

Must be a date in MM-DD-YYYY, YYYY-MM-DD or a shortened version (i.e. YYYY, or, YYYY-MM).

PRESENT SAMPLE LOCATION

Institution, department, or lab where the sample currently resides (in case someone wishes to find the sample).

GRADE

This is the grade of metamorphism. The grade must be from the list of metamorphic grades in <u>Appendix C.</u> Alternate descriptions of the metamorphic grade are encouraged, and should included as "Comments".

ROCK TYPE - SUPPLEMENTAL

Additional rock type beyond the primary rock type or name. There may be as many supplemental rock types as you want, and you may use any name you like.

COMMENT

There may be any number of comment columns. You can input alternate rock names or alternate descriptions of the metamorphic grade (or anything else) as comments.

For organization purposes, it is probably best to put separate types of information in separate comment columns, rather than strung together in a single comment. The key to using the comment field is to put in information that will describe the sample, and will help others find it in a search.

MINERALS PRESENT and MINERAL MODES

A list of minerals present in the sample and, if available, the modes of the minerals are very useful information. For an individual spreadsheet, the format is to

- (1) Put the name of a specific mineral as the column header. Headers must be from LIST OF MINERALS (see <u>Appendix D</u>).
- (2) If the mineral is present but the mode is unknown, put "x" in the field
- (3) If the mineral is present and the mode is known, put the mode in the field (note: modes typically sum to 100%).
- (4) If the mineral is not present, leave the field blank.

For example, for a suite of schists, this part of the spreadsheet might look like this:

Quartz	Plagioclase	Muscovite	Biotite	Garnet	Chlorite	Ilmenite	Zircon	Staurolite	Kyanite
X	X	X	X	X		X		X	
30	5	30	20	10		1			
X		X	X	20	X	<1	?	X	
X	X	X	X	X			X	X	X

Any text or number field is permissible and signifies a mineral is present.

Common usage included

- (1) A number (= mode)
- (2) $\langle or \rangle$ a number
- (3) x = present
- (4) ? = may be present
- (5) t = present in trace amounts

Required format for bulk uploads: Chemical Analysis Upload

Chemical analyses are referenced to a sample number and a subsample, which are required (see <u>What is a Subsample?</u>). The sample and subsample must be uploaded/added first, before chemical analyses can be uploaded. An upload worksheet contains data arranged in columns, each with an appropriate header. The following is a list of accepted headers, with notes as to which fields are required for every uploaded analysis.

The first row is reserved for the column headers. The second row is reserved for units (chemical analysis and precision). Each additional row should contain data for each analysis to be uploaded. Only some fields are required in order to upload your data, as indicated below, but we encourage you to be thorough to maintain a database that is as versatile as possible. See example spreadsheet for more information.

Please note that chemical analyses must be in weight percent, ppm, or ppb, and molar percents will be calculated by the database with a user specified method (coming soon).

All uploaded chemical analyses will initially be private. They may then be made public once they are in My Samples. You are encouraged to check your uploaded data before making it public, as once it is public, it cannot be modified except by a system administrator, and then only to correct errors.

List of headers:

REQUIRED FIELDS

SAMPLE NUMBER

Must correlate to existing sample in database. For information on uploading samples to the database see above.

SUBSAMPLE

Must correlate to existing subsample of the given sample number. See <u>What is a Subsample?</u> If a subsample has not yet been created, you may create one here, but you must provide a subsample type (see below).

MINERAL

This must be in agreement with minerals or mineral modes listed as present for the sample. If the analysis is a whole rock analysis, this field should read "whole rock".

METHOD

Method of analysis, i.e. EMP, LA-ICPMS, SIMS, etc.

SUBSAMPLE TYPE – required to create subsamples at bulk upload

In order to create a subsample during bulk upload of chemical analysis, you must specify a type for the new subsample. Subsample types accepted: Thin section, Polished thin section, Rock Chip, or Mineral separate. Subsample type only needs to be specified for the first chemical analysis for a particular subsample in a list. For example, if you have 5 garnet analyses on a new polished thin section that you want to upload, you only need to enter "polished thin section" in the subsample type column for the first (topmost) analysis.

REFERENCE – required for published data.

Data that are published require a reference to the publication. MetPetDB uses the GeoRef assension number (the same as NAVDAT), which can be found from a GeoRef search.

OPTIONAL FIELDS

ANALYTICAL FACILITY

The analytical facility where analysis was performed. This can be the name of an institution or department.

ANALYSIS DATE

Must be a date in MM-DD-YYYY, YYYY-MM-DD or any shortened version (i.e. YYYY, or, YYYY-MM).

ANALYST

The name of the person who analyzed the sample. Preferred format: Lastname, First initial.

REFERENCE IMAGE

The filename of image on which the analysis location is referenced. The goal here is to allow the user to easily find an image showing the context of a chemical analysis, so please be sure to upload the reference image.

POINT

The analysis number. It should be unique to the subsample to allow differentiation between different points for a particular subsample.

X POS

The Cartesian X-coordinate for the location of the point on the reference image. This should be in pixels measured up from the lowermost pixel in the image (X POS = 0)

Y POS

The Cartesian Y-coordinate for the location of the point on the reference image. This should be in pixels measured over from the leftmost pixel in the image (Y POS = 0).

X STAGE

The stage X-coordinate recorded by a microscope or microprobe. These are in microns.

Y STAGE

The stage Y-coordinate recorded by a microscope or microprobe. These are in microns.

ELEMENTS/SPECIES - at least one required

Headers should be different elements /species (e.g. CaO, SiO2, Mg).

UNITS – must be in second row and in proper format, (e.g. wt%, ppm) - see Appendix E.

Non numerical values can be used to indicate information about an analysis as in the table below:

Values for Elements/Species can be numeric or these abbreviations:

n.d. = not determined

(blank) = not determined

n.a. = not determined (literally not analyzed)

- = not determined

b.d. = below detection

b.d.l. = below detection limit

< (a value) = less than the specified value

PRECISION

Uncertainty of measurement (relative or absolute). Each precision column must refer to the preceding column of Elements/Species concentrations.

UNITS – must be in second row and in proper format, including –abs or -rel for absolute vs. relative, see <u>Appendix E</u>.

TOTAL

The total weight percent of measured elements/species for this point. This indicates the completeness of the analysis to a user.

COMMENT

There may be any number of comment columns. You can input any type of description of the analytical strategy.

For organization purposes, it is probably best to put separate types of information in separate comment columns, rather than strung together in a single comment. The key to using the comment field is to put in information that will describe the analysis, and will help others find it in a search.

Required format for bulk uploads: Image Upload

Image upload is performed .zip image folder upload which includes a metadata spreadsheet on the main directory of the .zip folder. Images are referenced to a sample number and a subsample, which are required (see What is a Subsample?). The sample and subsample must be upoloaded/added first, before images can be uploaded.

Preparing .zip folder of images:

Images for database subsamples should be compiled to a single compressed folder to be uploaded in .zip format. The compressed folder must not contain subdirectories, and all image files must have unique file names that are also unique to their respective subsample's list of image files. Filenames should be catalogued in the accompanying image upload spreadsheet. Acceptable formats are: .jpg , .gif , .tif , and .png. The current size limit is 50 megabytes per image.

Note that the Image Upload Spreadsheet (.xls file) must be on the main directory of the image .zip folder!

The Image Upload Spreadsheet:

Be sure the image data are on the first worksheet of the upload spreadsheet. An upload spreadsheet contains data arranged in columns, each with an appropriate header. The following is a list of accepted headers, with notes as to which fields are required for every uploaded image. The first row is reserved for the column headers. Each additional row should contain data for each image to be uploaded. Only some fields are required in order to upload your images, as indicated below, but we encourage you to be thorough to maintain a database that is as versatile as possible. See example spreadsheet for more information.

All uploaded samples will initially be private. They may then be made public once they are in My Samples. You are encouraged to check your uploaded data before making it public, as once it is public, it cannot be edited or deleted, except by the system administrator.

List of headers:

REOUIRED FIELDS

SAMPLE NUMBER

Must correlate to existing sample in database. For information on uploading samples to the database see above.

FILE (or PATH)

The complete filename of the image as it appears in the zipped folder, including a .xxx extension indicating the file format (e.g. samp1_polish_scan.jpg). Path notation may be used for subdirectories, using colons between each subdirectory (e.g.: zipfolder:08-1xraymaps:08-1Femap.jpg)

IMAGE TYPE

Must be from list of acceptable image types. Below is a table of acceptable image types and comments for each one. Note that abbreviations may be used for certain image types.

Image Type	Abbreviation	Comments		
Map	MAP	Map (geologic or otherwise) with sample locations		
Cross Section	XC	Geologic cross section with sample locations		
Field Photo	FP	Field photo of outcrop or sample location		
Photograph	РНОТО	General sample imagery		
Thin Section Scan	TSS	Special image of entire thin section		
Photomicrograph-Transmitted	TPPL			
Plane Polarized				
Photomicrograph-Transmitted	TXPL			
Crossed Polars				
Photomicrograph-Reflected Plane	RPPL			
Polarized				
Photomicrograph-Reflected	RXPL			
Crossed Polars				
Secondary Electron Image	SE			
Back-Scattered Electron Image	BSE			
Cathodoluminescence Image	CL			
X-ray Map	XRM	Element name is required for X-ray maps		

ELEMENT -required x-ray maps

The element or species that was measured to create an x-ray map.

OPTIONAL FIELDS

SUBSAMPLE

Must correlate to existing subsample of the given sample number. See <u>What is a Subsample?</u> If a subsample has not yet been created, you must go back and create one with an appropriate name.

SCALE

Full width of image measured along the actual sample in milimeters. For example, a horizontal scan of a full standard thin section should have a scale of ~46 mm.

PARENT IMAGE

The filename for another image on which this image can be located (including extension). This gives the user further context information for a small scale image.

LOCATION ON PARENT

A description of the location of this image on a larger scale parent image so that a user may find the location of this image and further structural/textural context for your data.

COLLECTOR

The person who collected the image, as this may not be the sample owner. Preferred format: Lastname, First initial.

DWELL TIME

Value in milliseconds for x-ray maps.

CURRENT

Value in nanoAmps for x-ray maps.

VOLTAGE

Value in kilovolts for x-ray maps.

COMMENT

There may be any number of comment columns. You can input any type of description of the analytical strategy.

For organization purposes, it is probably best to put separate types of information in separate comment columns, rather than strung together in a single comment. The key to using the comment field is to put in information that will describe the image, and will help others find it in a search.

Appendix A. List of Rock Types:

Slate

Phyllite

Schist

Gneiss

Migmatite

Anatectite

Marble

Calc-silicate

Greenschist

Amphibolite

Blueschist

Eclogite

Granofels

Hornfels

Skarn

Quartzite

Jadeitite

Glaucophanite

Serpentinite

Garnetite

Pyroxenite

Cordierite-Anthophyllite

Metapelite

Metaigneous

Metaarkose

Metagreywacke

Metabasite

Metacarbonate

Metagranite

Cataclasite

Mylonite

Latitude and Longitude

Values should be entered in DD.DDDDD format. Five units after the decimal point provides a spatial accuracy of approximately 1 m (at the equator). Conversion from DD M.MMM or DD MM SS to DD.DDDDD is simple and can be done in a spreadsheet by recognizing that there are 60 S in one M and 60 M in on D.

Note that there is an optional error for latitude and longitude. If the sample is poorly located (worse than 1 meter) then an error should be specified.

With modern GPS, sample location is routine and most field geologists now locate samples with latitude and longitude routinely. For older data the latitude and longitude must be determined in some fashion. Here are several possible ways, depending on what information is currently available.

Location in UTM coordinates

If UTM coordinates are available for a sample, the conversion to DD.DDDDD can be done on a spreadsheet, but it is not trivial. The reader is referred Steven Dutch's excellent web site at http://www.uwgb.edu/dutchs/UsefulData/UTMFormulas.HTM
Fortunately, Steven has supplied a spreadsheet for these conversions.

Locations on topomaps

If samples are located only on paper copies of topographic maps then there are a couple of options, depending on what type of software you currently have or how much money you wish to spend.

- 1. You can try to read the latitude and longitude directly off of the topo map. This is time-consuming and not very accurate. It is typically more accurate and faster to read the UTM coordinates and do the conversion to DD.DDD (see above). Alternatively, one of the approaches below should work still better.
- 2. Use the web site http://www.topozone.com/. Topozone.com has all US topographic maps. If you can find your sample location on the appropriate map, you can read off the latitude and longitude on the screen (be sure you have the correct format DD.DDDDD and the correct map datum (NAD83/WGS84) specified). You can copy and paste individual lat-long values. This service used to be free, but now requires a subscription to https://www.trails.com/.
- 3. If you have good GPS software on your computer with stored topographic maps you should be able to find your sample location on the topographic map and store it as a waypoint. Waypoint files are usually ASCII (text) and can be copied into a spreadsheet. I have used MacGPS Pro (for Macintosh only) with good success.

You can find your sample location on Google Earth and read off the latitude and longitude. I don't know what the accuracy of this approach might be, but it is relatively straightforward if you can find your sample location. This method requires retyping each lat-long values.

Appendix C. List of Metamorphic Grades

Zeolite

Prehnite-pumpellyite

Greenschist

Amphibolite

Epidote amphibolite

Granulite

Blueschist

Eclogite

Hornfels

Chlorite zone

Biotite zone

Garnet zone

Staurolite zone

Staurolite-kyanite zone

Kyanite zone

Sillimanite zone

Andalusite zone

Sillimanite-K feldspar zone

Garnet-cordierite zone

Migmatite zone

Ultra high pressure

Ultra high temperature

Appendix D:

Clay

Clinoamphibole

List of minerals (alphabetical):

Acmite Clinoenstatite Larnite Actinolite Clinopyroxene Lawsonite Aegirine Clinozoisite Lepidocrocite Clintonite Aenigmatite Lepidolite Albite Coesite Leucite Alkali Feldspar Cordierite Limonite Allanite Corumdum Magnesite Cristobalite Almandine Magnetite Amphibole Cummingtonite Margarite Analcite Diamond Melilite Anatase Diaspore Merwinite Andalusite Diopside Mica Andesine Dolomite Monazite Montmorillonite Anhydrite Ekermannite

Ankerite Enstatite Mullite Annite **Epidote** Muscovite Anorthite Feldspar Na Pyroxene Ferrosilite Native Elements Anthophyllite Apatite Galena Nepheline Apophyllite Garnet Oligoclase Gedrite Arfvedsonite Olivine Astrophyllite Ghanite Omphacite

Augite Gibbsite Ortho- and Ring Silicates

Axinite Glauconite Orthoclase
Baryte Glaucophane Orthopyroxene

Goethite Oxides Beryl **Biotite** Graphite Paragonite Grossular Boehmite Pectolite **Brookite** Gunerite Periclase Brucite Gypsum Perovskite Bustamite Hedenbergite Phengite Ca Pyroxene Hematite Phlogopite Calcite Hercynite Phosphates Carbon Hornblende Piemontite Carbonates Huite Plagioclase Cassiterite Hydoxides Prehnite Celestine Illite Pryoxmangite Celsian Ilmenite Pumpellyite Jadeite Chain Silicates Pyrite Chalcopyrite Kaersutite Pyrope Kalsilite Chlorite Pyrophyllite Chloritoid Kaolinite Pyroxene Chromite Katophorite Pyrrhotite

Kyanite

Labradorite

Quartz

Rankinite

Rhodocrosite Smectite Tectosilicates Sodalite Tilleyite Rhodonite Richterite Spessartine Topaz Riebeckite Sphalerite Tourmaline Rutile Sphene Tremolite Sanadine Spinel(1) Tridymite Sapphirine Spinel(2) Vermiculite Scapolite Spodumene Vesuvanite Sericite Spurrite Wollastonite Serpentine Staurolite Wonesite **Sheet Silicates** Stilpnomelane Xenotime Siderite Sulphates Zeolite Sulphides Zircon Silica Sillimanite Talc Zoisite

List of Minerals (categorized):

Mica:

	Wonesite	Clinoenstatite	
Tectosilicates:	Margarite	Omphacite	
Nepheline	Glauconite	Na Pyroxene:	
Scapolite	Lepidolite	Jadeite	
Silica:	Muscovite:	Acmite	
Coesite	Phengite	Aegirine	
Quartz	Sericite		
Tridymite	Clintonite	Spodumene	
Cristobalite	Biotite:	Orthopyroxene: Enstatite	
Analcite		Ferrosilite	
Sodalite	Phlogopite		
Kalsilite	Annite	Amphibole:	
Leucite	Paragonite	Orthoamphibole:	
	Astrophyllite	Gedrite	
Zeolite	Chlorite	Anthophyllite	
Feldspar:	Clay:	Clinoamphibole:	
Celsian	Vermiculite	Hornblende	
Alkali Feldspar:	Smectite	Kaersutite	
Orthoclase	Kaolinite	Glaucophane	
Sanadine	Montmorillonite	Cummingtonite	
Plagioclase:	Illite	Tremolite	
Anorthite	Stilpnomelane	Richterite	
Oligoclase	Pyrophyllite	Katophorite	
Labradorite	Serpentine	Ekermannite	
Albite	Chain Silicates:	Riebeckite	
Andesine	Pyroxene:	Arfvedsonite	
Sheet Silicates:	Clinopyroxene:	Gunerite	
Talc	Ca Pyroxene:	Actinolite	
Apophyllite	Diopside	Aenigmatite	
Prehnite	Hedenbergite	Rhodonite	
) C			

Augite

Bustamite

Pryoxmangite Cassiterite Sapphirine Corumdum Wollastonite Periclase Pectolite **Brookite** Ortho- and Ring Silicates: Perovskite Rankinite Hematite Andalusite Rutile Lawsonite Hydoxides: Chloritoid Diaspore Huite Gibbsite Garnet: Lepidocrocite Almandine Goethite Grossular Brucite Boehmite Pyrope Limonite Spessartine Sulphides: Epidote Group: Pyrrhotite **Epidote** Chalcopyrite Clinozoisite Piemontite Pyrite Allanite

Sphalerite Galena Zoisite Sulphates: Vesuvanite Gypsum Axinite Anhydrite Melilite Baryte Sillimanite Celestine Spurrite Carbonates: Sphene Siderite Tillevite Dolomite Tourmaline Magnesite Zircon Ankerite Mullite Calcite Merwinite Rhodocrosite Topaz Phosphates: Kyanite

Larnite Monazite
Pumpellyite Native Elements:
Staurolite Carbon:

Apatite

Xenotime

Olivine Graphite
Oxides: Diamond
Anatase

Ilmenite
Spinel(1):
Chromite
Spinel(2)
Hercynite
Ghanite
Magnetite

Beryl

Cordierite

Appendix E. Acceptable Units

For Elements/Species:

wt% - weight percent ppm – parts per million ppb – parts per billion

For Precision:

wt%-abs - weight percent absolute ppm-abs - parts per million absolute ppb-abs - parts per billion absolute %-rel - percent relative