The pmob (PaleoMagnetic OBject) format: DEVELOPMENT VERSION 0.0.0.9011

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Introduction to EGU presentation.

With the ideas below, we would like to initiate data exchangeability in paleomagnetism based on the open-source programming language R. We are aware that numerous laboratories developed individual and valuable software solutions for various issues, but the lack in comparability of their results is often an issue. To make best use of these data formats they need to be exchangeable. Therefore, we consider creating a common data format called pmob (standing for PaleoMagnetic OBject), to and from which individual formats can be transformed without in-depth programming knowledge.

We would appreciate feedback on the document and thoughts below.

Foreword

The pmob format is aimed at interchanging into each other the existing formats used to store paleomagnetic data. It consists of a data table that is based on the data types found in several formats in the literature. Data in pmob are organised as columns identified by an abbreviated name as header. This format leaves the possibility to any user to include additional information (in the form of new columns) if needed.

The format of pmob is under discussion, and will evolve with time. Thus, anyone is invited to suggest changes to this format, and all inputs will be appreciated.

IF YOU WORK ON THIS DOCUMENT PLEASE INDICATE THAT IT IS A MODIFIED VERSION BY ADDING 1 TO THE LAST VERSION NUMBER (0.0.0.9XXX +1) AND GIVING YOUR INITIALS.

The pmob headers will be strictly and thoroughly defined: units and accepted values need to be provided to make it an unambiguous database format. This format also reduces redundant information. For instance, the angle around a circle is defined by angular values in the [0,360[real number interval, with 360 excluded as it is equivalent to an angle of 0.

It should be noted that the pmob format does not ambition to set a strict standard for all measurements. On the contrary, it aims to allow the conversion between different data reporting standards, taking into account that measurements and data analysis may have been done differently. Whether a practice is acceptable or not will not be discussed here: it is up to the user and to the community to have critical appreciation.

Points still in development:

- Decide on the amount of precision for normal and scientific numeric values, or precise case by case? EXCEPTION OF DECIMAL DEGREES: what is the amount of precision required? This value has to be set by default (but can be changed by the user) due to the difficulty of working with decimal numbers (see discussion below)

- Decide on fold plunge convention (see mainly Fig. 2): dip and azimuth are used for standardisation reasons, but trend (dip direction) and plunge (dip angle) can also be used

- Check cross platform validity of CSV file format

- Information of measurements of continuous cores: the volume should be known, but what parameters are usually provided to compute it? Provide complete overview of parameters

- How can we document the noise level? Is it different for each x, y and z coordinates? Should we document it for multiple parameters? Is it available in other formats?

DISCUSSION:

Should we add specific headers for the instrumental parameters to interpret long core data? If yes, what are the pertinent ones that need to be transferred between data formats? How is the sensor length in 2G measurements taken into account?

Implementation

The idea of pmob is to define functions converting to and from pmob, which would allow conversion using a few lines of code:

```
library(inteRmag) # Importation of package
setwd("C:/Users/Chris/Desktop/pmob") # Defining the file directory
pmob_1 <- magic_to_pmob("magic_contribution_16645.txt") # Importing MagIC file into pmob
pmob_to_ppl(pmob = pmob_1, name = "contribution_16645.ppl")# Exporting pmob file to PuffinPlot format</pre>
```

To make the conversion functions, two cases of general formatting need to be considered:

- When the data format present itself as a simple data table: the user is only required to attribute the right data to the right header, with some unit conversion if necessary. This is easy to do even for people using R for the first time, by applying table reading functions, such as. read.table(), and setting a data table in R using the data.frame() function.

- When the data format is more complicated, for instance when several tables, each standing for a different sample, are separated by a specific text pattern (e.g. '9999' in the Utrecht format, which is followed by a line describing the next sample, see Figure 1): in that case string matching will be implemented (identifying the '9999' and the pattern of the sample-describing line in our example shown in Figure 1), which is slightly more advanced.

Each of the R functions come with a help page, which can be called in R typing an interrogation point before the name of the function (e.g. ?magic_to_pmob). The implementation of the conversion functions can be carried out by anyone willing to learn the R coding bases, and will be performed by the pmob core team at the request of users that are unfamiliar with R. However, such functions need to be established only once for each format. Then, the only knowledge required is the application of the 4 lines of code shown above.

Guillaume, 2G Rennes "BOSP01","", 0.00, 90.00, 10.00, 0.00, 0.00 20, 16.9058, 1.56502, 1.40897, 0, CO, 0.000000 90, 15.6682, 1.94619, -0.136054, 0, CO, 0.000000 120, 17.5964, 3.48161, -1.82780, 0, CO, 0.000000 160 , 26.7982 , 8.65471 , -0.105740 , 0 , C0 , 0.000000 200, 27.6951, 9.25560, -1.46637, 0, CO, 0.000000 250 , 21.0762 , 6.77309 , -0.699910 , 0 , C0 , 0.000000 300, 17.3274, 8.44843, 0.265561, 0, CO, 0.000000 350 , 11.3722 , 5.52108 , 2.14170 , 1 ,C0, 0.000000 400, 13.0942, 9.21076, 3.62870, 0, CO, 0.000000 450 , 9.16592 , 2.15247 , 1.28789 , 1 ,C0, 0.000000 475, 11.2108, 7.87892, -0.703139, 0, CO, 0.000000 500 , 5.43318 , 8.57668 , 1.20538 , 1 ,C0, 0.000000 525, 4.54081, 11.1121, -0.640448, 0, CO, 0.000000 550 . -1.17040 , 4.25202 , 4.34170 , 1 ,C0, 0.000000 575, -2.27444, 7.22332, 4.46099, 1, CO, 0.000000 9999 "BOSP02","", 0.00, 90.00, 10.00, 0.00, 0.00 20, -4.01525, 9.44395, -1.69955, 1, CO, 0.000000 90, 6.00628, 13.3991, -0.796233, 1, C0, 0.000000 120 , 7.84305 , 15.6861 , 1.23408 , 1 , CO, 0.000000 160, 16.5830, 21.5157, 0.901345, 0, C0, 0.000000 200, 15.1928, 23.3453, 1.50942, 0,C0, 0.000000 250, 12.2960, 25.9731, 2.86726, 0, CO, 0.000000 300, 11.8744, 20.8341, 1.63946, 0, CO, 0.000000 350, 6.82063, 16.3498, 4.19821, 0, CO, 0.000000 400 , 10.3139 , 17.2108 , 3.94170 , 1 ,C0, 0.000000 450 , 8.13004 , 13.1928 , 2.46996 , 1 , CO , 0.000000 475 , 7.06637 , 12.1614 , 3.25919 , 1 ,C0, 0.000000 500, 5.27803, 8.48789, 0.997309, 1, CO, 0.000000 525, 3.82691, 8.62422, -1.75426, 1, C0, 0.000000 550, 3.04753, 4.00090, 0.916592, 1, CO, 0.000000 575, 3.02780, -1.53991, -1.62780, 1, CO, 0.000000 9999

Figure 1: example of the Utrecht format

Units

Units follow the SI (International System of Units): kg, m, s, A and K are used. Angles, longitude and latitude are represented by decimal degrees. Time is represented by separate columns for year, month, day, minute and second. Unit conversion functions are (or will be) provided. Especially with the CGS (centimetre–gram–second) unit system. CGS eases calculations when dealing with magnetism (as certain constants are simplified to be unity, see Tauxe 2010), and is therefore still largely used in paleomagnetism. Visualisation tools, when coded within the framework of pmob, should allow for the option of SI or CGS units. However, the strict pmob object will remain in SI units.

Sample coordinate system

As shown in Figure 3, the pmob format uses the sample coordinate system defined in Tauxe (2010). The orientation in the field and in the measurement device as they are defined in pmob are derived from this coordinate system. Data using other coordinate systems, when converted into pmob, will see their coordinate system be converted accordingly. Equally, when conversion is done in the other sense, the sample coordinate system will be converted back into the sample coordinate system of the original data format.

Exporting pmob as a file and the problem of decimals

The pmob format is (or at least will be) associated with specific file writing and reading functions to save and load back the data. The file is exported in the CSV format (Comma-Separated Values), which can be encoded by different character standards (e.g. ASCII or UTF-8). In accordance with the CSV format, commas (",") act as column separators, and points (".") as decimal separator. Line breaks are signalled by the carriage return (CR) and line feed (LF) characters following each other in that order. For information CR and LF are respectively coded in ASCII by the characters 13 (0×0D) and 10 (0×0A), and in several programming languages (R included) by \r and \n. Alphanumeric values and headers (i.e. objects of character class in R) are quoted (i.e. surrounded with ""). Boolean values (TRUE/FALSE) are noted TRUE and FALSE, unquoted. Not available values are noted NA, unquoted. Integers are written as such, unquoted. Numeric values are separated into normal numeric values and scientific numeric values. Normal numeric values are characterised by digits on both sides of the decimal point (e.g. 135.99), while scientific numeric values are made of a single digit before the decimal point, numerous digits following the decimal point, the letter e and digits indicating the factor of 10 (e.g. 1.3599e2). Normal numeric values are used for the depth, temperatures, treatment fields in Tesla, the lowest time units and for all the angles including longitude and latitude. Scientific numeric values are used for the magnetic moments, magnetizations, magnetic susceptibilities, mass, volume and area. In the R environment, the precision of these numbers is limited by the computational imprecision (see next paragraph), which is negligible for calculations. However, when writing the data down in the CSV file, this precision is determined by the amount of digits that are written down. For convenience of programming, by default we fix the precision of normal numerical values to three digits after the decimal point, and the precision

Numeric values (numbers having decimals) in R can pose a problem, as they are stored in the computer as fractions. Roughly put, this means that the number has an imprecision of a scale of 10^{-15} of the unit (e.g. for a value of 1.00×10^{25} , the imprecision is of a scale of 10^{10}). This is generally a minor problem for calculations used in palaeomagnetism. However, this can be challenging when trying to identify specific values, e.g. for demagnetisation steps. A demagnetisation step of 0.1 T will be understood in the computer in another way, which should look like this: 0.1000000000000001. This poses a problem when trying to isolate specific steps. To avoid this problem we recommend to round the values to an acceptable level, and to compare them using the all.equal() function, which checks for equality within numerical tolerance (at the opposite of the == comparison relational operator and of the identical() function). This offers a double security to insure that the possible accumulation of computational error will not affect the identification of equal values. The rounding values are equivalent to the amount of digits defined for the writing of the CSV file for the normal numerical values and the scientific numerical values. The following code illustrates the way we advocate to identify specific values in R:

a <- 1 + 1e-15 # this represents a value supposed to be 1, but deviating from it due to computational error

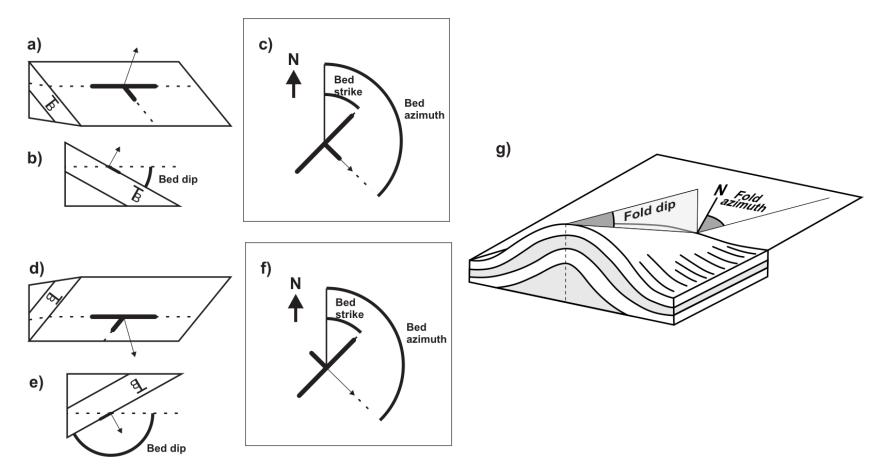


Figure 2: Illustration of the measurement of dip, dip azimuth and strike of a planar surface, generally a bed. Figures a, b & c illustrate normal beds, while figures d, e & f illustrate overturned beds, i.e. stratigraphically upside down (the T_B indicator stands for stratigraphical top and bottom). The horizontal projection of the line perpendicular to the plane oriented in the stratigraphic upward direction (thin arrow in the figures) is used as to define strike and azimuth. Overturned beds have dip values in the]90°,180°] interval. Vertical beds have a dip of 90°. For horizontal beds (dip of 0° or 180°) the dip azimuth and strike can take any value in the [0°, 360°[interval. Figure g illustrates the measurement of the dip and azimuth of folds (illustration modified from https://thehiddenwater.wordpress.com/). In the case of extreme fold plunges overturning the entire axis of the fold, fold dip values are comprised in the [90°, 180°] interval. The fold azimuth (or trend) is the angle from the north of the horizontal projection of the line in the axial plane, perpendicular to the fold axis, and pointing in the stratigraphical upward direction.

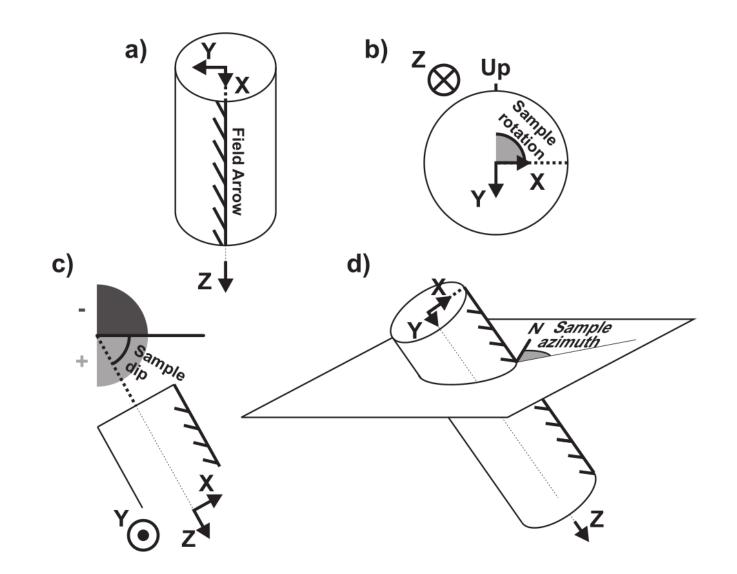
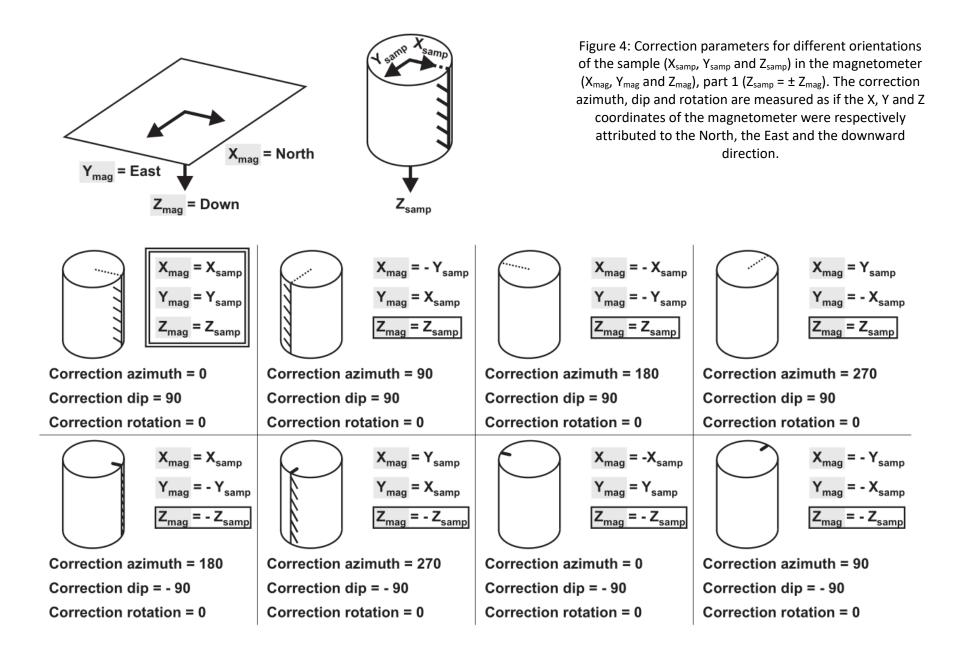
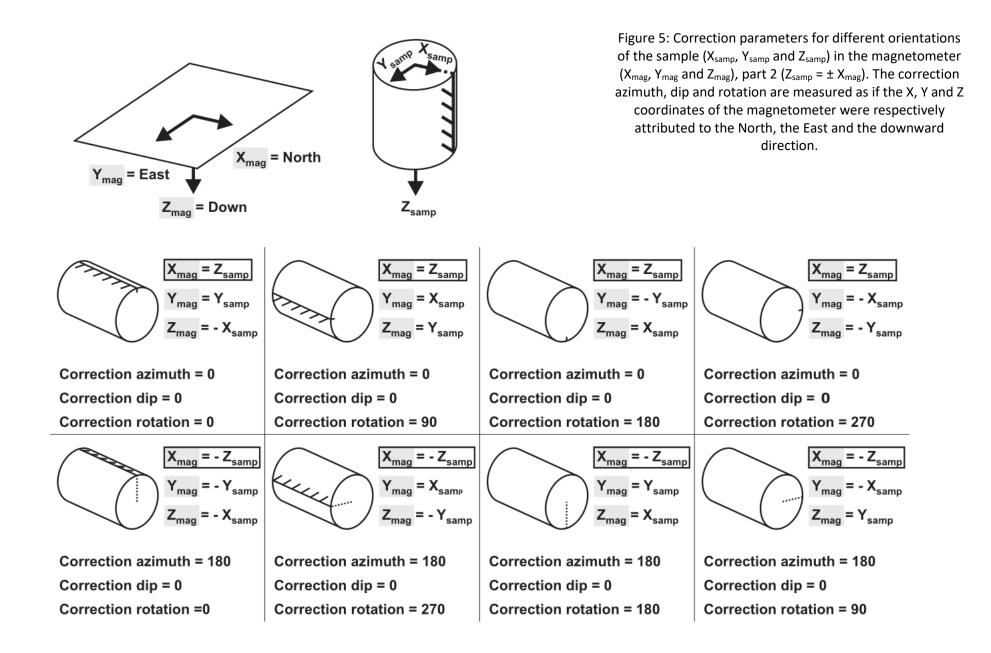
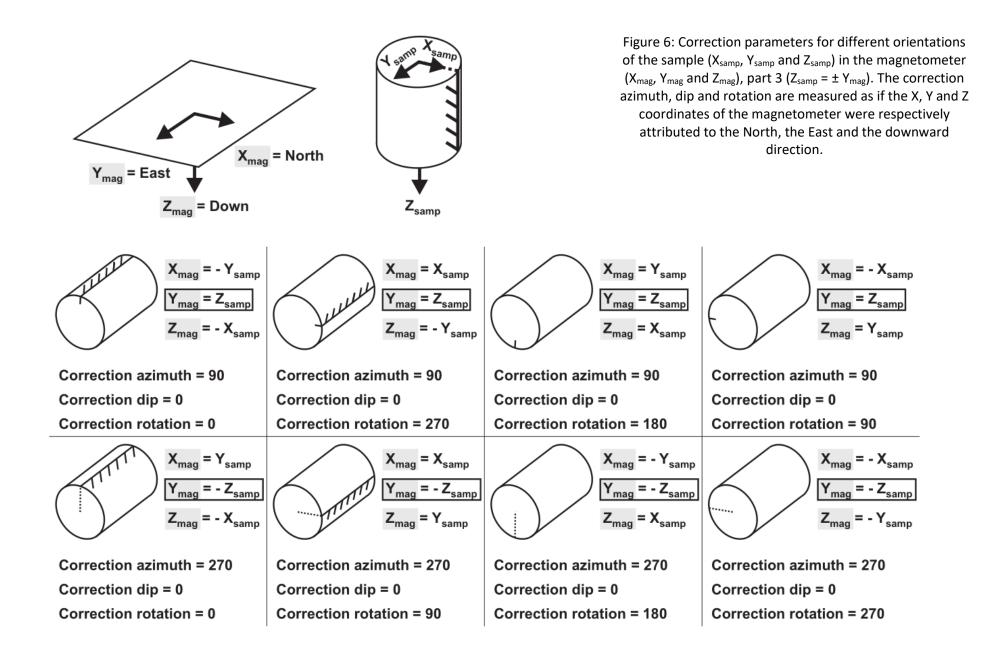


Figure 3: Sample coordinate system. (a) Relation of the sample coordinate system with the field arrow. (b) Measurement of the sample rotation angle. We also refer to X as the 12 o'clock position. (c) Measurement of the sample dip angle. (d) Measurement of the sample azimuth angle.







Header in pmob	Units	Accepted values	Definition
sampleid	-	alphanumeric	Identification of the sample.
specimenid	-	alphanumeric	Identification of the specimen.
slotid	-	alphanumeric	Identification of the tray slot containing the sample for discrete measurements on a multi-sample tray.
measurementid	-	alphanumeric	Identification of the measurement.
depth	m	normal numeric	Sampling depth.
measuresec	second	normal numeric in [0,60[Time of the measurement.
measuremin	minute	integer in [0, 59]	Time of the measurement.
measurehour	hour	integer in [0 ,23]	Time of the measurement.
measureday	day	integer in [1,31]	Time of the measurement.
measuremonth	month	integer in [0,12]	Time of the measurement.
measureyear	year	integer	Time of the measurement.
measurementdevice	-	alphanumeric	Name of the measurement device.
xint	A m ²	scientific numeric	Magnetic moment in the x direction of the measuring device.
yint	A m ²	scientific numeric	Magnetic moment in the y direction of the measuring device.

zint	A m ²	scientific numeric	Magnetic moment in the z direction of the measuring device.
xvol	A m ⁻¹	scientific numeric	Magnetization by volume in the x direction of the measuring device.
yvol	A m ⁻¹	scientific numeric	Magnetization by volume in the y direction of the measuring device.
zvol	A m ⁻¹	scientific numeric	Magnetization by volume in the z direction of the measuring device.
xmass	A m ² kg ⁻¹	scientific numeric	Magnetization by mass in the x direction of the measuring device.
ymass	A m ² kg ⁻¹	scientific numeric	Magnetization by mass in the y direction of the measuring device.
zmass	A m ² kg ⁻¹	scientific numeric	Magnetization by mass in the z direction of the measuring device.
totmagsus	m ⁻³	scientific numeric	Total magnetic susceptibility, which is defined by the magnetic moment m of a sample (expressed in A.m ²) induced by an external field H (expressed in A.m ⁻¹). The total magnetic susceptibility is m/H (expressed in m ⁻³). See also Tauxe, 2010.
volmagsus	SI (dimensionless)	scientific numeric	Magnetic susceptibility by volume.
massmagsus	m ³ kg ⁻¹	scientific numeric	Magnetic susceptibility by mass.
vol	m ³	scientific numeric	Volume of the sample.
mass	kg	scientific numeric	Mass of the sample.
discrete	-	TRUE/FALSE	Whether a single discrete sample is measured (TRUE), or a continuous core (FALSE).
area	m ²	scientific numeric	Cross-sectional area of a long core sample (for continuous cores, applies if the parameter discrete is FALSE).

sampleaz	arc degree	normal numeric in [0,360[Sample azimuth in the field (Fig. 3): it is the angle measured clockwise from the north of the horizontal projection of the field arrow (Tauxe 2010).
sampledip	arc degree	normal numeric in [-90,90]	Sample dip in the field (Fig. 3): it is the angle of the field arrow from the horizontal. It is positive downward, and ranges from +90° for straight down to -90° for straight up (Tauxe, 2010)
samplerot	arc degree	normal numeric in [0,360[Rotation of the sample on its axis, taken in the field (Fig. 3). It is measured clockwise from the 12 o'clock summit (or X sample coordinate, see Fig. 2B), on the sample part opposite of the field arrow. <i>SPECIAL CASE: IN DOWNWARD VERTICAL SAMPLES</i> (dip = 90), the rotation is the angle between the azimuth and the field arrow. <i>SPECIAL CASE: IN UPWARD VERTICAL SAMPLES</i> (dip = -90), the rotation is the angle between the azimuth and the field arrow + 180° (as the upward dip brings the 12 o'clock position (or X sample coordinate, see Fig. 2B) on the sample part opposite of the field arrow, to face the opposite direction of azimuth).
correctionaz	arc degree	normal numeric in [0,360[Azimuth of the sample in the measuring device (Fig. 4, 5 & 6): this is a correction for the difference between the magnetometer coordinates and the sample coordinates. This is equivalent to sample azimuth, considering that the x, y and z coordinates of the magnetometer are attributed to the North, East and downward directions respectively.
correctiondip	arc degree	normal numeric in [-90,90]	Dip of the sample in the measuring device (Fig. 4, 5 & 6): this is a correction for the difference between the magnetometer coordinates and the sample coordinates. This is equivalent to sample dip, considering that the x, y and z coordinates of the magnetometer are attributed to the North, East and downward directions respectively.
correctionrot	arc degree	normal numeric in [0,360[Rotation of the sample in the measuring device (Fig. 4, 5 & 6): this is a correction for the difference between the magnetometer coordinates and the sample coordinates. This is equivalent to sample rotation, considering that the x, y and z coordinates of the

			magnetometer are attributed to the North, East and downward directions respectively.
bedaz	arc degree	normal numeric in [0,360[Bedding azimuth, or dip direction (Fig. 2): it is the azimuth (the angle taken eastward or clockwise from the north) of the line perpendicular to the plane oriented in the stratigraphic upward direction, projected on a horizontal plane. This accounts for stratigraphically overturned beds (Fig. 2d-f).
bedstrike	arc degree	normal numeric in [0,360[Bedding strike (Fig. 1): it is defined as the angle taken eastward (clockwise) from the north of a horizontal line of the plane. It is further defined as the bedding azimuth minus 90° (or plus 270°), to account for stratigraphically overturned beds (Fig. 2d-f).
beddip	arc degree	normal numeric in [0,180]	Bedding dip (Fig. 1): it is the plane's maximum angular deviation from the horizontal. It is positive downward, and ranges from +90° for straight down to 0° for horizontal. Stratigraphically overturned beds are indicated with dip values in the]90°,180°] interval.
foldaz	arc degree	normal numeric in [0,360[Fold dip (Fig. 2):
folddip	arc degree	normal numeric in [0,180]	Fold azimuth (Fig. 2):
magaz	arc degree	numeric in [0,360[Magnetic azimuth of the sample in the field.
usemagaz	-	TRUE/FALSE	If TRUE, the magnetic azimuth (magaz) will be used as the sample azimuth (sampleaz), if FALSE it is the solar azimuth (solaraz) that will be used as the sample azimuth (sampleaz).
solaraz	arc degree	numeric in [0,360[Solar azimuth of the sample in the field.
long	decimal degree	decimal degree in]-180,180]	Longitude.
lat	decimal degree	decimal degree in [-90,90]	Latitude.
samplingmin	minute	Normal numeric in [0,60[Time of sampling.

samplinghour	hour	integer in [0 ,23]	Time of sampling.
samplingday	day	integer in [1,31]	Time of sampling.
samplingmonth	month	integer in [0,12]	Time of sampling.
samplingyear	year	integer	Time of sampling.
samplingtimezonemin	min	Integer in [0,59]	Time zone of the sampling, expressed relative to the UTC (Coordinated Universal Time), e.g. UTC +12:45 for New Zealand. This has to take into account the possible daylight saving time at the moment of the sampling, which changes the effective time zone.
samplingtimezonehour	hour	integer, usually in [-12,14]	Time zone of the sampling, expressed relative to the UTC (Coordinated Universal Time), e.g. UTC +12:45 for New Zealand. This has to take into account the possible daylight saving time at the moment of the sampling, which changes the effective time zone.
magvar	arc degree	numeric in [0,360[Magnetic variation: it is the angle on the horizontal plane between the magnetic north and the geographic north. It is measured as the angle made by the magnetic North eastward (clockwise) from the geographic North.
magazvarcorr	-	TRUE/FALSE	Whether the magnetic azimuth parameter (magaz) has to be corrected for the magnetic variation.
bedazvarcorr	-	TRUE/FALSE	Whether the bedding azimuth parameter (bedaz) has to be corrected for the magnetic variation.
bedstrikevarcorr	-	TRUE/FALSE	Whether the bedding azimuth parameter (bedstrike) has to be
			corrected for the magnetic variation
foldazvarcorr	-	TRUE/FALSE	corrected for the magnetic variation Whether the fold azimuth parameter (foldaz) has to be corrected for the magnetic variation
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	pcacomponent	-	alphanumeric	(e.g. "C1", "C2", "Outlier"), to be used for Principal Component

pcacomponentsingle	- alphanumeric	Which group of measurements to use for Principal Component Analysis (PCA) in files only considering one single group.
circlecomponent	alphanumeric	Identifies groups of measurements considered in one component (e.g. "C1", "C2", "Outlier"), to be used for circle computation.
circlecomponentsingle	- alphanumeric	Which group of measurements to use for circle computation in files only considering one single group.
pmobversion	- alphanumeric	Version of the pmob format.

References

Tauxe, Lisa. 2010. Essentials of Paleomagnetism. First edition. Berkeley: University of California Press.