NAME

mar345_formats - description of image formats for images collected on a mar345 Imaging Plate Detector System.

DESCRIPTION

The 345 mm mar scanners produce the following image file formats:

compressed images ("MAR345"):
Transformed and corrected compressed images. The compression algorithm was kindly provided by Dr. J.P. Abrahams of the LMB in Cambridge, UK.

uncompressed images in old image format ("IMAGE"):
Transformed and corrected uncompressed images that are compatible with the formats of the 180 and 300 mm scanners (see mar_images).

spiral images ("SPIRAL"):
Raw data in spiral coordinates. Before using them in any crystallographic program they have to be transformed into a cartesian coordinate system. During transformation, corrections are applied.

IMAGE SIZES

The mar345 scanner is able to scan the plate using 2 pixel sizes (0.10 mm or 0.15 mm), each at 4 different radii can be chosen, so that in total 8 different image sizes can be produced:

Pixel size	Diameter(mm)	SIZE	Filename extension
0.15	345.0	2300 * 2300	.mar2300 or .pck2300
	300.0	2000 * 2000	.mar2000 or .pck2000
	240.0	1600 * 1600	.mar1600 or .pck1600
	180.0	1200 * 1200	.mar1200 or .pck1200
0.10	345.0	3450 * 3450	.mar3450 or .pck3450
	300.0	3000 * 3000	.mar3000 or .pck3000
	240.0	2400 * 2400	.mar2400 or .pck2400
	180.0	1800 * 1800	.mar1800 or .pck1800

MAR345 FORMAT

One image consists of the following items:

- Header record: 4096 bytes.

- Optional high intensity records: 64 bytes each. Pixels with values > 65535 are stored as pairs of address and actual pixel value. The pixel address is a number corresponding to the linear array starting at pixel 1 and ending at pixel SIZE*SIZE. Both address and value are stored as 32 bit integers. One "high intensity" record thus consists of 8 value pairs (address+intensity). Example: if an image contains 13 values > 65535, there will be 2 high intensity records of 8 value pairs each (8*(4b+4b) = 64 bytes). Pairs 14 to 16 will contain zeroes only. The total number of high intensity has to be taken from the header. The number of high intensity records is calculated as:
  HIGH_RECORDS = (int)(HIGH_PIXELS/8.0 + 0.875)
  where HIGH_PIXELS denotes the total number of high intensity pixels.

- A compressed image data array of variable length. All information is stored in single bytes, so there is no need for byte swapping when moving pck images in between different computer architectures (with exception of the optional high intensity records). There is no loss of information involved in compression. The compressed images take approx. 70% less disk space. After decompression, a linear image data array of SIZE records with SIZE pixels each is obtained. All pixels values are 16-bit unsigned integers with values ranging from 0 to 65535. The first value in the array is in the upper left corner, the fast varying axis is horizontal. This convention differs from the 300 mm mar by a clockwise rotation of 90.0 deg.!

  SIZE denotes the no. of pixels in one dimension, e.g. 1200 or 3450. Each record is 2*SIZE bytes long.

SPIRAL IMAGE FORMAT

A spiral image consists of:

- o Header record: 4096 bytes (as above).

- o An image data array consisting of records. Each record consists of 1024 pixel values (16-bit unsigned integers), i.e 2048 bytes. The header structure is the same as the one for the mar345 images.

MAR345 HEADER

The image header consists of "lines" of 64 bytes each with exception of the first line, that contains 16 4-byte words

(32 bit integers). The very first value always is 1234 for all scanning modes, i.e. it is just a marker for the necessity of byte swapping and does NOT give the size of the image (in contrast to the first value of the old image formats which is 1200 or 2000 or its byte swapped equivalent). Programs of the mar345 suite rely on this value to decide wether the image is in old format or in the new one and/or if byte-swapping is required. The remaining 15 32-bit integers are:

2) Size of image in one dimension

3) Number of high intensity pixels

4) Image format (1=COMPRESSED, 2=SPIRAL)

5) Collection mode (0=DOSE, 1=TIME)

6) Total number of pixels in image

7) Pixel length (in mm * 1.000)

8) Pixel height (in mm * 1.000)

9) Used wavelength (in Ang * 1.000.000)

10) Used distance (in mm * 1.000)

11) Used starting PHI (in deg. * 1.000)

12) Used ending PHI (in deg. * 1.000)

13) Used starting OMEGA (in deg. * 1.000)

14) Used ending OMEGA (in deg. * 1.000)

15) Used CHI (in deg. * 1.000)

16) Used TWOTHETA (in deg. * 1.000)

If the first value is not 1234, the bytes of the following 15 integers must be swapped.

The next 64 character line contains a general identifier string for this type of file: "mar research" (bytes 65 to 76 in the image file). This is for possible use with the "file" command under Unix.

All following lines contain keyworded information. The last keyword should be "END OF HEADER". All keywords are in capital letters and all "lines" are pure ASCII, so they are not affected by the byte order of different computer platforms. Processing of the keywords is not required. For

using the formats correctly, the most important information is contained in the second (bytes 5-8) and third (bytes 9-12) header value: the size of the image and the number of high intensity pixels!

KEYWORDS in MAR345 HEADER

PROGRAM <program name> <version number>
Keyword PROGRAM always is the first in the list of keywords, i.e. at byte 128!

DATE <week day month hh:mm:ss year>
Date and time of production.
Example: DATE Tue Jul 9 13:06:05 1996

SCANNER <serial number>
Serial number of the scanner.
Example: SCANNER 12

FORMAT <size> <type> <no_pixels>
<size> is the number of pixels in one dimension, <type> is "MAR345", "PCK345" or "SPIRAL" and <no_pixels> gives the total number of pixels in the image.
Example: FORMAT 1200 SPIRAL 1111647

HIGH <n_high>
Number of pixels with values > 65535 (16-bit). Depending on this value, programs should try to

read <n_high> high intensity pixel pairs (address in array and 32-bit pixel value) preceding the 16-bit data array.
Example: HIGH 0

PIXEL LENGTH <pix_length> HEIGHT <pix_height>
Size of one pixel in micron units (1000. * mm). In SPIRAL format, length is shorter than height (double sampling).
Example: PIXEL LENGTH 75 HEIGHT 150

OFFSET ROFF <roff> TOFF <toff>
Radial and tangential offset of the scanner in mm (constants).
Example: OFFSET ROFF 0.1 TOFF -0.05

MULTIPLIER <multi>
High intensity multiplier.
Example: MULTIPLIER 1.000

GAIN <gain>
Gain of the detector, i.e. the number of photons required to produce 1 ADC unit.
Example: GAIN 1.000

WAVELENGTH <wave>
Used wavelength in Angstroems.
Example: WAVELENGTH 0.7107

DISTANCE <distance>
Used distance crystal to detector in mm.
Example: DISTANCE 70.0

RESOLUTION <dmax>
Maximum resolution (Ang.) at edge of the plate.
Example: RESOLUTION 2.1

PHI START <phi_start> END <phi_end> OSC <n_osc>
PHI values at start and end of exposure. <n_osc> is the number of PHI oscillations during this exposure.
Example: PHI START 10.000 END 11.000 OSC 1

OMEGA START <omega_start> END <omega_end> OSC <n_osc>
OMEGA values at start and end of exposure. <n_osc> is the number of omega oscillations during this exposure.
Example: OMEGA START 0.000 END 0.000 OSC 0

CHI <chi>
CHI value during this exposure.
Example: CHI 90.0

TWOTHETA <two_theta>
2-theta value during this exposure.
Example: TWOTHETA 0.0

CENTER X <x_cen> Y <y_cen>
Coordinates of direct beam in pixel units.
Example: CENTER X 999.000 Y 1001.100

MODE <dcmode>
Mode of data collection: "TIME" or "DOSE".
Example: MODE TIME

TIME <exp_time>
Exposure time in seconds. In DOSE mode, the time varies depending to X-ray flux.
Example: TIME 60.00

COUNTS START <cnt_beg> END <cnt_end> MIN <cnt_min> MAX <cnt_max> AVE <cnt_ave> SIG <cnt_sig> NMEAS <cnt_n>
X-ray counts as measured by the second ionization chamber: minimum, maximum and average value, values at start and end of exposure and sigma of average reading. <cnt_n> is the number of times the X-ray intensity has actually been read during the exposure.
Example: COUNTS START 12.1 END 11.50 MIN 10.9 MAX 12.4 AVE 11.6 SIG 0.8 NMEAS 120

INTENSITY MIN <int_min> MAX <int_max> AVE <int_ave> SIG <int_sig>
Pixel values in image: minimum, maximum, average value and sigma.
Example: INTENSITY MIN 8 MAX 32987 AVE 432.4 SIG 25.9

HISTOGRAM START <his_beg> END <his_end> MAX <his_max>
Distribution of pixel values in image (used for distributing colours at display). <his_beg> and <his_end> give the limits for the range of intensities to distribute available colours. <his_max> is the most frequent pixel value in the image.
Example: HISTOGRAM START 120 END 640 MAX 216

GENERATOR <type> kV <kiloVolt> mA <milliAmps>

Type of x-ray source ("SEALED TUBE", "ROTATING ANODE" or "SYNCHROTRON") and power settings.
Example: GENERATOR SEALED TUBE kV 40.0 mA 50.0

MONOCHOROMATOR <type> POLAR <polarization>
Type of monochromator ("GRAPHITE", "MIRRORS" or "FILTER") and value of x-ray polarization.
Example: MONOCHROMATOR GRAPHITE POLAR 0.000

COLLIMATOR WIDTH <width> HEIGHT <height>
Aperture of horizontal (<width>) and vertical (<height>) slits in mm. These values are for the second of the two slit systems of the mar research collimation system. They determine the size of the beam.
Example: COLLIMATOR WIDTH 0.3 HEIGHT 0.3

REMARK <text>
Additional remark (one line only)
Example: REMARK Lysozyme crystal 0.5x0.8 mm

SEE ALSO

mar300_formats

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