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2. CONCEPTS AND SPECIFICATIONS

Example 2.3.4.1. (cont.)

```
Example 2.3.4.1. A multiple-block CBF with several images.
###CBF: VERSION 1.0
# CBF file written by cbflib v0.6
# A comment cannot appear before the file identifier,
# but can appear anywhere else, except within the
# binary sections.
# Here the first data block starts
data xxx
### ... various CIF tags and values here
###
        but none that define array data items
# The "data " identifier finishes the first data
# block and starts the second
data yyy
### ... various CIF tags and values here including
###
        ones that define array data items
loop_
array data.array id
_array_data.binary_id
_array_data.data
image_1 1
--CIF-BINARY-FORMAT-SECTION--
Content-Type: application/octet-stream;
     conversions="x-CBF PACKED"
Content-Transfer-Encoding: BINARY
X-Binary-Size: 3745758
X-Binary-ID: 1
X-Binary-Element-Type: "signed 32-bit integer"
Content-MD5: 1zsJjWPfol2GY12V+QSXrw==
START OF BIN
<D5>^P<B8>P^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@ ...
[This is where the raw binary data would be – we can't print them here]
--CIF-BINARY-FORMAT-SECTION----
```

2.3.4. A complex example

In Example 2.3.4.1 only the ARRAY_DATA category CIF identifiers are shown. The other CIF data items are not shown. This shows a possible structuring of a more complicated example. There are two header sections; the first contains two data blocks and defines three binary sections. CIF comment lines, starting with a hash mark '#', are used to clarify the structure.

2.3.5. imgCIF encodings

For an imgCIF, there are several alternative encodings for binary image data as ASCII text. Each binary image may use a different encoding in the same imgCIF data set or even in the same data block. The choice of encoding is specified in the 'Content-Transfer-Encoding' MIME header.

If the Transfer Encoding is x-BASE8, x-BASE10 or x-BASE16, the data are presented as octal, decimal or hexadecimal data, respectively, organized into lines or words. Each word is created by composing octets of data in fixed groups of 2, 3, 4, 6 or 8 octets, either in the order ...4321 ('big-endian') or 1234... ('little-endian'). If there are fewer than the specified number of octets to fill the last word, then the missing octets are presented as '==' for each missing octet. Exactly two equal signs are used for each missing octet even for octal and decimal encoding. The format of lines is

rnd xxxxxx xxxxxx xxxxxx

where r is H, \circ or D for hexadecimal, octal or decimal, n is the number of octets per word, and d is '<' or '>' for the '...4321' and

```
# Following the "end of binary" identifier the file
# is pseudo-ASCII again, so comments are valid
# up to the next "start of binary" identifier.
                                                 Note
# that we have increased the binary ID by one.
image 1 2
--CIF-BINARY-FORMAT-SECTION--
Content-Type: application/octet-stream;
     conversions="x-CBF PACKED"
Content-Transfer-Encoding: BINARY
X-Binary-Size: 3745758
X-Binary-ID: 2
X-Binary-Element-Type: "signed 32-bit integer"
Content-MD5: xR5kxiOetd9T/Nr5vMfAmA==
START OF BIN
<D5>^P<B8>P^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@^@ ...
[This is where the raw binary data would be – we can't print them here]
--CIF-BINARY-FORMAT-SECTION----
;
# Third binary section; note that we have a new
# array ID.
image_2 3
--CIF-BINARY-FORMAT-SECTION--
Content-Type: application/octet-stream;
     conversions="x-CBF PACKED"
Content-Transfer-Encoding: BINARY
X-Binarv-ID: 3
Content-MD5: yS5kxiOetd9T/NrqTLfAmA==
START OF BIN
*****
[This is where the raw binary data would be – we can't print them here]
--CIF-BINARY-FORMAT-SECTION----
;
# Second header section
data zzz
### ... various CIF tags and values here
###
        including ones that define array
###
        data items
# Since we only have one block left, we won't
# use a loop
 array data.array id
                        image
array data.binary_id 1
array data.data
# Note that we can put a comment here
--CIF-BINARY-FORMAT-SECTION--
Content-Type: application/octet-stream;
     conversions="x-CBF_PACKED"
Content-Transfer-Encoding: BINARY
X-Binarv-ID: 1
Content-MD5: fooxiOetd9T/serNufAmA==
START OF BIN
*****
[This is where the raw binary data would be - we can't print them here]
--CIF-BINARY-FORMAT-SECTION----
;
### END OF CBF
```

'1234...' octet orderings, respectively. The '==' padding for the last word should be on the appropriate side to correspond to the missing octets, e.g.

H4< FFFFFFF FFFFFFF 07FFFFFF ====0000

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```
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```

or

H3> FF0700 00====

For these hexadecimal, octal and decimal formats only, comments beginning with '#' are permitted to improve readability.

BASE64 encoding follows MIME conventions. Octets are in groups of three, c1, c2, c3. The resulting 24 bits are reorganized in the following way (where we use the C operators \gg , \ll , & and | to denote, respectively, a right shift, a left shift, bit-wise intersection and bit-wise union). Four six-bit quantities are specified, starting with the high-order six bits ($c1 \gg 2$) of the first octet, then the low-order two bits of the first octet followed by the high-order four bits of the second octet ((c1 & 3) $\ll 4 | (c2 \gg 4)$), then the bottom four bits of the last octet ((c2 & 15) $\ll 2 | (c3 \gg 6)$), then the bottom six bits of the last octet (c3 & 63). Each of these four quantities is translated into an ASCII character using the mapping

```
1 2 3 4
01234567890123456789012345678901234567890123456789
| | | | | |
ABCDEFGHIJKLMNOPQRSTUVWXYZabcdefghijklmnopqrstuvwx
5 6
01234567890123
| | | | | |
yz0123456789+/
```

Short groups of octets are padded on the right with one '=' if c3 is missing, and with '==' if both c2 and c3 are missing.

QUOTED-PRINTABLE encoding also follows MIME conventions, copying octets without translation if their ASCII values are 32...38, 42, 48...57, 59...60, 62, 64...126 and the octet is not a ';' in column 1. All other characters are translated to '=nn', where nn is the hexadecimal encoding of the octet. All lines are 'wrapped' with a terminating '=' (*i.e.* the MIME conventions for an implicit line terminator are never used).

Appendix 2.3.1 Deprecated CBF conventions

There was an earlier, now deprecated, CBF format in which the compression type was given as eight bytes of binary header. In this case, the eight bytes used for the compression type are subtracted from the size, so that the same size will be reported if the compression type is supplied in the MIME header. Use of the MIME header is the recommended way to supply the compression type.

These earlier versions of the specification also included three eight-byte words of information in binary that replicated information now available in the MIME header:

512	Binary section identifier (see <u>array_data.binary_id</u>), 64-bit, little-endian	
1320	The size (<i>n</i>) of the binary section in octets (<i>i.e.</i> the offset from octet 29 to the first byte following the data)	
2128	Compression type:	•
	CBF NONE	0x0040 (64)
	CBF CANONICAL	0x0050 (80)
	CBF PACKED	0x0060 (96)
	–	

The three eight-byte words were followed by binary data. These words are not included when a MIME header is provided.

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References

- Freed, N. & Borenstein, N. (1996a). Multipurpose Internet Mail Extensions (MIME) part five: Conformance criteria and examples. RFC 2049. Network Working Group. http://www.ietf.org/rfc/rfc2049.txt.
- Freed, N. & Borenstein, N. (1996b). Multipurpose Internet Mail Extensions (MIME) part one: Format of Internet message bodies. RFC 2045. Network Working Group. http://www.ietf.org/rfc/rfc2045.txt.
- Freed, N. & Borenstein, N. (1996c). Multipurpose Internet Mail Extensions (MIME) part two: Media types. RFC 2046. Network Working Group. http://www.ietf.org/rfc/rfc2046.txt.
- Freed, N., Klensin, J. & Postel, J. (1996). Multipurpose Internet Mail Extensions (MIME) part four: Registration procedures. RFC 2048. Network Working Group. http://www.ietf.org/rfc/rfc2048.txt.
- Hall, S. R., Allen, F. H. & Brown, I. D. (1991). The Crystallographic Information File (CIF): a new standard archive file for crystallography. Acta Cryst. A47, 655–685.
- IEEE (1985). *IEEE standard for binary floating-point arithmetic.* ANSI/IEEE Std 754–1985. New York: The Institute of Electrical and Electronics Engineers, Inc.
- Moore, K. (1996). *MIME (Multipurpose Internet Mail Extensions) part three: Message header extensions for non-ASCII text.* RFC 2047. Network Working Group. http://www.ietf.org/rfc/rfc2047.txt.
- Rivest, R. (1992). *The MD5 message-digest algorithm*. RFC 1321. Network Working Group. http://www.ietf.org/rfc/rfc1321.txt.