

2.3. SPECIFICATION OF THE CRYSTALLOGRAPHIC BINARY FILE (CBF/imgCIF)

or

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H3> FF0700 00====
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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, c_1 , c_2 , c_3 . 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 ($c_1 \gg 2$) 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 ($(c_1 \& 3) \ll 4 | (c_2 \gg 4)$), then the bottom four bits of the second octet followed by the high-order two bits of the last octet ($(c_2 \& 15) \ll 2 | (c_3 \gg 6)$), then the bottom six bits of the last octet ($c_3 \& 63$). Each of these four quantities is translated into an ASCII character using the mapping

	1	2	3	4	
01234567890123456789012345678901234567890123456789					
ABCDEFGHIJKLMN O PQRSTU VWXYZabcdefghijklmnopqrstu vwx					
5	6				
01234567890123					
yz0123456789+ /					

Short groups of octets are padded on the right with one '=' if c_3 is missing, and with '==' if both c_2 and c_3 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:

5...12	Binary section identifier (see <code>_array_data.binary_id</code>), 64-bit, little-endian
13...20	The size (n) of the binary section in octets (i.e. the offset from octet 29 to the first byte following the data)
21...28	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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