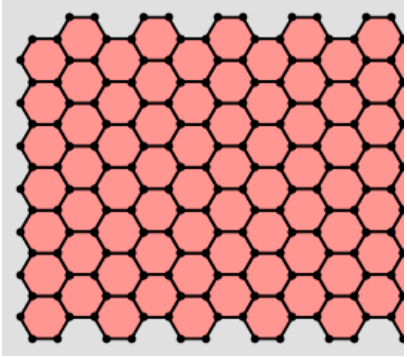
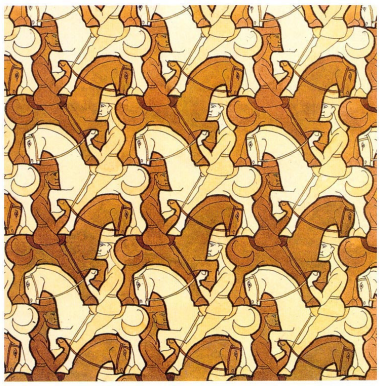


What lattice type is this?

What is the basis?



What lattice type is this?

What is the motif?

CIF for TiO_2 (rutile)

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# This file is available in the Crystallography Open Database (COD),
# http://www.crystallography.net/. The original data for this entry
# were provided the American Mineralogist Crystal Structure Database,
# http://rruff.geo.arizona.edu/AMS/amcsd.php
#
# The file may be used within the scientific community so long as
# proper attribution is given to the journal article from which the
# data were obtained.
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x,y,z
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1/2+x,1/2-y,1/2+z
1/2-x,1/2+y,1/2-z
x,y,-z
-x,-y,z
y,x,z
-y,-x,-z
1/2-y,1/2+x,1/2-z
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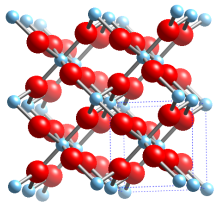
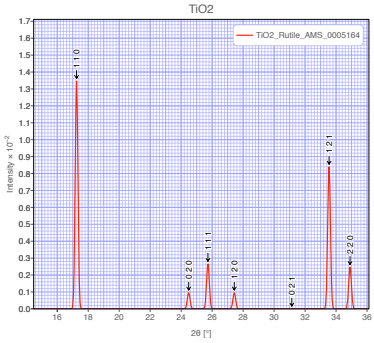
You need to understand what is in the red boxes, especially the first and last, and the concept of the middle one.

TiO_2 (rutile) Structure in real space



TiO_2 (rutile) X-ray diffraction (reciprocal structure; Fourier transform



Other arrangements of the same atoms produce different fingerprints →