## TESSELATION

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Algorithm for filling shells, out $\rightarrow$ in.
6 bits $=1$ byte. Use one byte for set of corresponding positions on 6 edges. Therefore, if $n=$ order of the shell, the descriptive word will have $n$ bytes.

The bytes are in order, ABCDEF, GHIJKL, MNOPQR, STUVWX, YZabcd, and +

1. Partition the shell count among the bytes. (A more efficient algorithm might well extract some symmetries at this point but would complicate the definition of dictionary order. The symmetry involved is reflection, since MNOPQR can interchange with GHIJKL on shell 3 , for example.)

But dictionary order does not directly follow this; viz. ABC < AD. This should not be consequential in producing the canonical forms.
2. Consider first byte.
3. Consider possible arrangements of this byte:

|  | Binary | Octal | Symmet | S left |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| A | 100000 | 40 |  | 1 |  |
| $A B$ | 110000 | 50 |  | /1 | B HNT C C |
| AC | 101000 | 50 |  | $/ 2$ | Y B H N T C I |
| AD | 100100 | 44 | 2 | 1 | SSBHNCIO |
| ABC | 111000 | 70 |  | 12 | M M M B H C I O U |
| ABD | 110100 | 64 | none |  | G G G GBCIOU a |
| ACE | 101010 | 52 | 3 | 1 | AAAAA $A$ D D D D D |
| ABCD | 111100 | 74 |  | 14 | d X R L F E J J J J |
| ABCE | 111010 | 72 |  | /2 | X R L F K E P P P |
| ABDE | 110110 | 66 |  | /1 | R L F Q K EVV |
| ABCDE | 111110 | 76 |  | $/ 4$ | L FWQ K E b |
| ABCDEF | 111111 | 77 | 6 | 1 | FCWQ K E |
| 0 | 000000 | 00 | 6 | 1 |  |

After translation, the figure must be canonicated to compare it with the original. If the latter is later in dictionary order, it is rejected.

To canonicate, set up a look-up table of the function that transforms any 6-bit number to the canonical byte, and execute accordingly for the first byte. The memaining bytes are then tested in sequence under the allowed operations still remaining; the same for the next shell.

For masking one shell on the next: the first byte (ABCDEF) is unique and masks on as many as 3 bytes (1, 2 and last). The last is rotated before being masked.

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Definition of canonical form.
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1. Translate center of coordinates to give the minimum shell-count-vector.
2. (Translate) rotate and reflect to give minimum dictionary value of the list of items, shell by shell.

The outermost shell corresponds to the most significant (leftmost) item of the vector-

$$
\begin{gathered}
D-E F G \\
C C D E K \\
B B B G K I \\
A A+D G J \\
R E F E H X \\
Q K J I G \\
P O N M
\end{gathered}
$$

Notation: list of shells separated by, and with or without terminal + . Empty comma positions are possible at right-hand side of list only.

Examples: ( + ) benzene
(A+) naphthalene
(AB+) phenalene
(ABC+) pyrene
( $A, A D+$ ) napthacene

Possible economies: do not implement now

If more than one alphabetic cycle is needed in a ring,use initial . to set up rank

Commas between non-ascending characters could be dispensed with. Leading $A$ and strings of $A, A, A$ could be more economically coded

Tactical decisions:

1. Partition the count to shell count vector. No interstitial o's allowed. Largest shell allocates entire count to diameter.
2. Build shells from outside inwards. Retain record of symmetry restrictions for calculations on next inner shells.
3. Test for peripheral islandsas each shell is filled.

4- When figure is completed, test (and discard if indicated)
translation to smaller shell count vector discontinuity by masking in and out across shells (breathing)
if translation leaves any ambiguity (shell count vector same) test results of operations (translation, rotation and reflection) for any result with lower value than propesitus.

5 eventually install search for enclaves
6 store list of results on disk!

In process, calculate and store appropriate masks unless the procedure for calculating the mask is quite fast

