Medicinal chemistry
ISSN: 2161-0444
Zhang, Med chem 2016, 6:1
DOI: 10.4172/2161-0444.1000320
Algorithm Open Access

Packing Rectangular-Box Cells Optimally for the Crystal Structure

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Abstract

In crystal structures, if each crystal cell is a special rectangular box (length × width × height=23 × 11.5 × 11.5 angstroms^3), then how to pack these cells onto a enough hard base of a (46 × 46 angstroms^2) square in order to make the crystal reach the stablest/optimal structure as high as the crystal it is? This is a practical problem that we are always thinking in our mind. This short article is to present an algorithm to solve this problem.

Keywords: Crystal cell; Rectangular-box cell; Packing the cells; Optimal crystal structure

We will give an algorithm to solve the problem:

Step 1: Put 2 boxes on one of the four boundaries (denoted as B1) of the base, with their lengths occupying B1.

Step 2: Put 1 box on each of the neighbored boundaries (denoted as B2 and B3) respectively, with each length side occupying each boundary respectively.

Step 3: Put 2 boxes on the remaining boundary (denoted as B4) of the base, with their lengths occupying B4.

Step 4: Now a 23 × 23 angstroms^2 square is inner (or in the center of) the base. Put 2 boxes onto the inner square, with their length sides paralleling to B1 and/or B4. Now we finished the layout of the 1st layer.

Step 5: Determine how many layers that you will lay the boxes, according to your own constraints. Once the number of layers was determined, we will repeat Step 6 to finish the layout onto the inner 23 × 23 angstroms^2 square.

Figure 1: An illumination of the Algorithm.

Step 6: Put 2 boxes in the even number of the layer, with their length sides paralleling to B2 and/or B3; put 2 boxes in the odd number of the layer, with their length sides paralleling to B1 and/or B4.

Step 7: Now we lay boxes onto the outside of the inner 23 × 23 angstroms^2 square: repeating Steps 8 ~ 9 until reaching the maximum number of layers.

Step 8: In the even number of the layer, put 1 box on both sides paralleling to B1 and B4 respectively; in the odd number of the layer, put 1 box on both sides paralleling to B2 and B3 respectively.

Step 9: In the even number of the layer, put 2 boxes on both sides paralleling to B2 and B3 respectively; in the odd number of the layer, put 2 boxes on both sides paralleling to B1 and B4 respectively.

The above algorithm is illuminated in Figure 1 in a workshop. If the maximum number of layers goes to infinity, and each layer produced by the above algorithm is looked as one solution of the algorithm, then the above algorithm is convergent in the strict algorithm convergence theory [1-3].

Acknowledgements

This research was supported by a Victorian Life Sciences Computation Initiative (VLSCI) grant numbered VR0063 on its Peak Computing Facility at the University of Melbourne, an initiative of the Victorian Government, Australia.

References

1. Zhang JP (2011) Derivative-free hybrid methods in global optimization and applications in December 2010. LAP Academic Publishing. ISBN 978-3-8454-3580-0.
2. Zhang JP (2015) Molecular structures and structural dynamics of prion proteins and prions - mechanism underlying the resistance to prion diseases. Springer. ISBN 978-94-017-7317-1.
3. Blow D (2002) Outline of Crystallography for Biologists. Oxford University Press. ISBN 978-0-19-851051-2.

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Received January 14, 2016; **Accepted** January 21, 2016; **Published** January 23, 2016

Citation: Zhang J (2016) Packing Rectangular-Box Cells Optimally for the Crystal Structure. Med chem 6: 039. doi:10.4172/2161-0444.1000320