NATIONAL BUREAU OF STANDARDS REPORT

10 059

Progress Report

on

SIMPLE EXTENSION OF MODEL MAKING TECHNIQUE OF WOOD, GEITH, PAN LIANG AND DOCKRILL



U.S. DEPARTMENT OF COMMERCE

NATIONAL BUREAU OF STANDARDS

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NATIONAL BUREAU OF STANDARDS

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The Bureau comprises the Institute for Basic Standards, the Institute for Materials Research, the Institute for Applied Technology, the Center for Radiation Research, the Center for Computer Sciences and Technology, and the Office for Information Programs.

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Office of Standard Reference Data—Clearinghouse for Federal Scientific and Technical Information [3]—Office of Technical Information and Publications—Library—Office of Public Information—Office of International Relations.

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[1] Headquarters and Laboratories at Gaithersburg, Maryland, unless otherwise noted; mailing address Washington, D.C. 20234.
[2] Located at Boulder, Colorado 80302.
[3] Located at 5285 Port Royal Road, Springfield, Virginia 22151.

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In our structural investigations of ionic compounds, such as the calcium phosphates and hydrated carbonates, we have found it essential to build, routinely, compact (1 Å ≅ 1 cm) and sturdy models (Figure 1) which reveal the packings in the crystal structures. We have adapted a procedure suggested by Wood, Geith, Pan Liang and Dockrill (1961) so that we can use readily available 3/8 inch diameter colored plastic beads and string each bead on its own string without having to tie any knots.

Our method is as follows: A list, conveniently sorted, of all the atoms in a unit cell (translated back into that cell where necessary) is made from the unique set of atoms using a program written for the Univac 1108 computer. The list is used to prepare a template from which two 1/2 inch thick plexiglass plates are drilled with a No. 60 (0.040 inch dia.) drill. The two plates are separated by 1/2 inch diameter plexiglass rods, one at each corner. As pointed out by Wood et al., triclinic cells are easily made by displacing the two plexiglass sheets. One end of a 0.012 inch diameter nylon monofiliament fishing line is passed through a drilled hole

in one of the plates and secured by hammering in a small nail. The appropriately colored beads are threaded on with the fishing line passed through the bead twice to generate enough friction to keep the bead in place, but allow its height to be adjusted readily. The string is then pulled tight and secured in the other plate by another small nail, and the heights of the beads are adjusted. When the model is completed, a grid of the unit cells in the model, with all atoms labelled, is attached to the bottom.

Using this method, we are able to assemble complex models containing several unit cells fairly quickly while avoiding the time-consuming and difficult operations of drilling plastic balls and tying knots in the fishing line.

Reference

Wood, D. L.; Geith, C. R.; Pan Liang, C. Y.; and Dockrill, A. G. Acta Cryst. 14:301 (1961).

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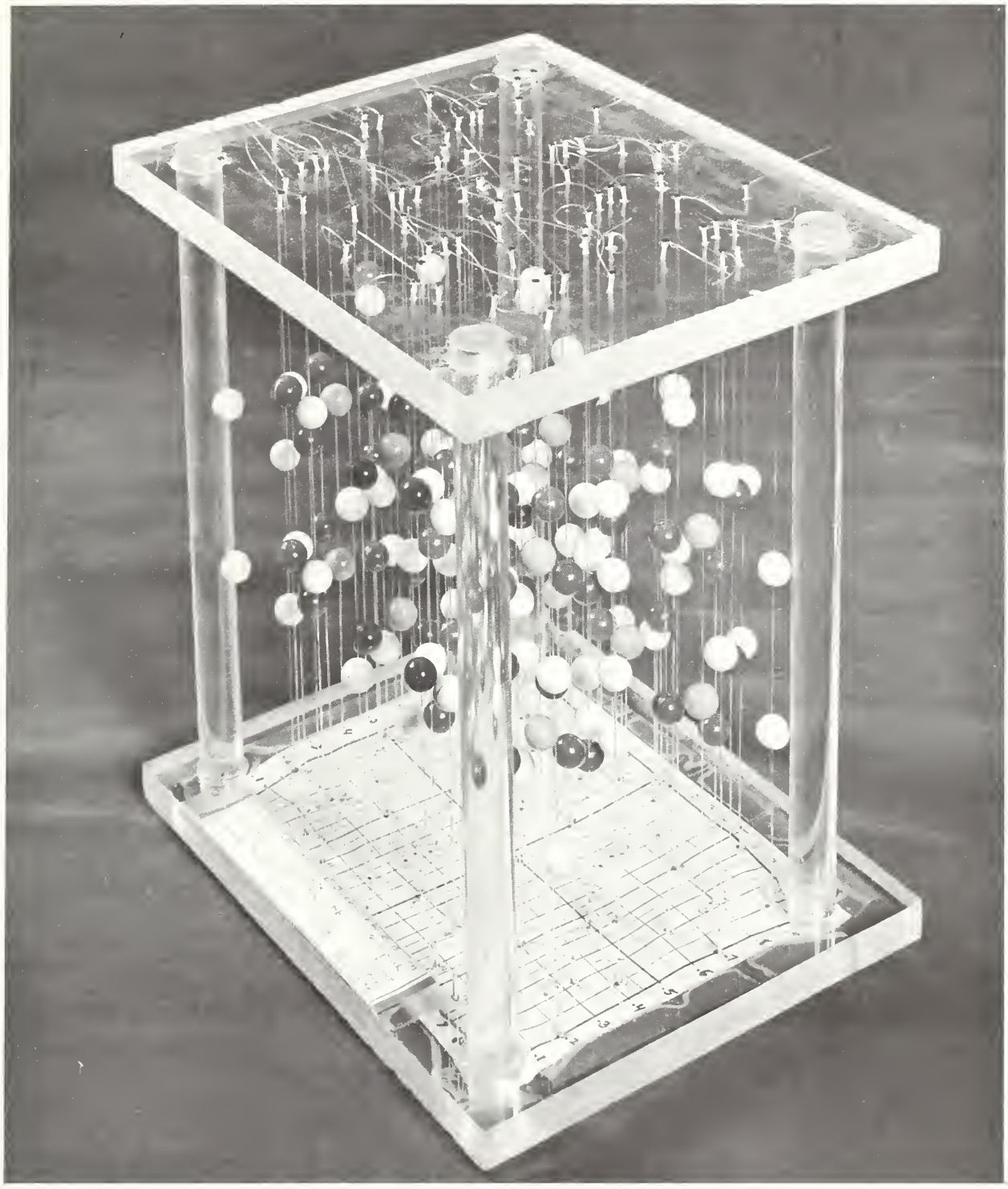


Figure 1

A Model of the Crystal Structure
of $Na_2CO_3 \cdot H_2O$


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