

This article was downloaded by: [Tomsk State University of Control Systems and Radio]

On: 17 February 2013, At: 06:00

Publisher: Taylor & Francis

Informa Ltd Registered in England and Wales Registered Number: 1072954

Registered office: Mortimer House, 37-41 Mortimer Street, London W1T 3JH, UK



## Molecular Crystals

Publication details, including instructions for authors and subscription information:

<http://www.tandfonline.com/loi/gmcl15>

### A Packing Relationship Between 1, 4-Dibenzoyloxybenzene and 4-Benzyloxyphenol

B. Zaslow<sup>a</sup> & Judith L. Dubchansky<sup>a</sup>

<sup>a</sup> Department of Chemistry, Arizona State University, Tempe, Arizona, 85281

Version of record first published: 21 Mar 2007.

To cite this article: B. Zaslow & Judith L. Dubchansky (1967): A Packing Relationship Between 1, 4-Dibenzoyloxybenzene and 4-Benzyloxyphenol, *Molecular Crystals*, 3:2, 297-298

To link to this article: <http://dx.doi.org/10.1080/15421406708083446>

PLEASE SCROLL DOWN FOR ARTICLE

Full terms and conditions of use: <http://www.tandfonline.com/page/terms-and-conditions>

This article may be used for research, teaching, and private study purposes. Any substantial or systematic reproduction, redistribution, reselling, loan, sub-licensing, systematic supply, or distribution in any form to anyone is expressly forbidden.

The publisher does not give any warranty express or implied or make any representation that the contents will be complete or accurate or up to date. The accuracy of any instructions, formulae, and drug doses should be independently verified with primary sources. The publisher shall not be liable for any loss, actions, claims, proceedings, demand, or costs or damages

whatsoever or howsoever caused arising directly or indirectly in connection with or arising out of the use of this material.

## A Packing Relationship Between 1,4-Dibenzyloxybenzene and 4-Benzyloxyphenol

B. ZASLOW and JUDITH L. DUBCHANSKY

Department of Chemistry, Arizona State University, Tempe, Arizona 85281

*Received July 14, 1967*

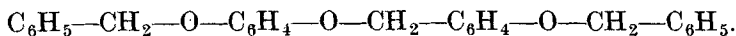
Molecular compounds of a given homologous series often assume closely related modes of packing in the solid state. Kitaigorodskii<sup>1</sup> has called this phenomenon "homologous isomorphism", and it is readily detectable from unit cell parameters. The molecules must be aligned with, or tilted only slightly from, one of the cell directions. Then two cell dimensions of the members of the homologous series are nearly equivalent in size, while the third reflects a change in the length of the molecule; the space groups of the members of the series are often identical. An example of such a series of compounds is biphenyl, terphenyl and quarterphenyl.<sup>2</sup> All crystallize in space group  $P2_1/c$  with both the  $b$  and  $c$  dimensions within  $\pm 0.1$  Å of each other; and  $a$ , the long axis, measured as 9.39 Å, 13.7 Å and 17.8 Å, respectively.

It can be deduced from cell parameters of 1,4-dibenzyloxybenzene and 4-benzyloxyphenol, that the packing similarities described above can exist between molecular compounds which are not members of the same homologous series. The cell dimensions and space group of 1,4-dibenzyloxybenzene and 4-benzyloxyphenol were determined from X-ray diffraction precession photographs. The crystals were fragile, thin plates grown from ethanol solution. Cell parameters for 1,4-dibenzyloxybenzene are  $a = 17.6 \pm 0.1$  Å,  $b = 5.70 \pm 0.05$  Å,  $c = 7.84 \pm 0.05$  Å,  $\beta = 95.5 \pm 1.5^\circ$ ; for 4-benzyloxyphenol, cell parameters are  $a = 23.42 \pm 0.05$  Å,  $b = 5.50 \pm 0.05$  Å,  $c = 7.94 \pm 0.10$  Å,  $\beta = 90.5 \pm 1.0^\circ$ . In both crystals the space groups,  $P2_1/c$ , is established by systematic absences and the plane of the mirror is perpendicular to the plate of the crystal. The number of

molecules per unit cell,  $Z$ , is 2 in 1,4-dibenzyloxybenzene, but 4 in 4-benzyloxyphenol.

With  $Z=2$ , the center of a 1,4-dibenzyloxybenzene molecule is located at  $\bar{1}$  positions, e.g., set  $a$  for the space group as listed in the International Tables;<sup>3</sup> the ends of the molecule are then related through the centers of symmetry, set  $b$ . Molecular models reveal that 1,4-dibenzyloxybenzene can easily assume a planar or near planar conformation. Moreover, the length of 1,4-dibenzyloxybenzene, including terminal van der Waal distances, is roughly 17.5 Å; and, therefore, the molecule must be approximately aligned with the  $a$  axis. The other cell dimensions are also consistent with this alignment. Biphenyl has a similar molecular cross-section, and its cell constants are  $b=5.51$  Å and  $c=8.04$  Å.

The cell dimensions of 4-benzyloxyphenol are those that would be expected for the next member in homologous sequence with 1,4-dibenzyloxybenzene, namely,



This latter molecule has an overall length of about 23.5 Å. The  $a$ -axis length observed for 4-benzyloxyphenol can be accounted for as follows. Dimers, which are extended along the  $a$  axis, pack in the solid. These associate through their phenol groups and are symmetrically located around  $\bar{1}$  positions. The space filling shape of the phenol groups then serves to substitute for the volume occupied by the  $-\text{O}-\text{CH}_2-$  linkage between the middle phenyl rings in the higher homologue. With such a group substitution, an apparent homologous isomorphism exists between 1,4-dibenzyloxybenzene and 4-benzyloxyphenol.

The authors are indebted to Dr. Jay Bishop who supplied the compounds.

#### REFERENCES

1. Kitaigorodskii, A. I., *Organic Chemical Crystallography*, Consultants Bureau, New York, 1961, p. 227.
2. Ibid., pp. 373-5.
3. *International Tables For X-Ray Crystallography*, Vol. I, Edited by Henry, N. F. M. and Lonsdale, K., The Kynoch Press, Birmingham, England, 1952, p. 99.