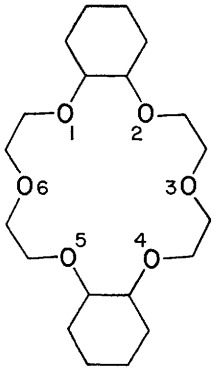
Crystal Structures of Two Isomers of Dicyclohexyl-18-Crown-6

By N. KENT DALLEY,* JUDITH S. SMITH, STEVEN B. LARSON, JAMES J. CHRISTENSEN, and REED M. IZATT
(*Chemistry Department and Center for Thermochemical Studies, Brigham Young University, Provo, Utah* 84602)

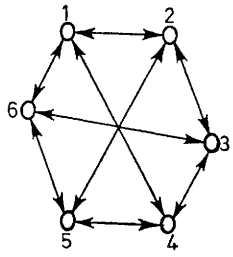
Summary In an *X*-ray diffraction study of the isomers A and B′ of dicyclohexyl-18-crown-6 the oxygen atoms have been found to lie approximately in a plane, with the cavity elliptical in shape and the shorter distance across the ellipse slightly more than 4 Å.

CRYSTAL structure studies of two of the five possible isomers of dicyclohexyl-18-crown-6 (**1**), *viz.* isomer A and the B′ polymorph, are reported to enable comparison of the conformation of the free ligands with that of the complexed form in the Ba^{2+}–isomer A[2] and the Na^{+}–isomer B′[3] complexes.

Crystal data. $C_{20}H_{36}O_6$ Isomer A, space group $P2_12_12_1$, $a = 7{\cdot}907$, $b = 12{\cdot}998$, $c = 20{\cdot}378$ Å, $Z = 4$; 2600 independent reflections collected with Cu–K_α radiation on a diffractometer; current $R = 0{\cdot}108$; isomer B′, space group $P2_1/c$, $a = 8{\cdot}233(2)$, $b = 12{\cdot}379(3)$, $c = 11{\cdot}106(3)$ Å, $\beta = 117{\cdot}09(2)°$, $Z = 2$; 1860 independent reflections collected with Cu–K_α radiation on a diffractometer; current $R = 0{\cdot}081$. The molecule is located about a centre of symmetry.



(1)



(2)

Trial models for both molecules were obtained by symbolic addition and refined by full matrix least-square methods. In both isomers the cavity surrounded by the six oxygen atoms is elliptical in shape (**2**) with the two axial oxygen atoms O(1) and O(4) pointing out of the cavity. The dimensions of the cavities in the two isomers are similar (Table).

TABLE

Oxygen–oxygen contact distances in the ring for isomers A and B′/Å

Oxygen–oxygen	Isomer A	Isomer B′
O(1)–O(2)	2·95	2·95
O(2)–O(3)	3·59	3·58
O(3)–O(4)	2·90	2·87
O(4)–O(5)	2·92	2·95
O(5)–O(6)	3·59	3·58
O(6)–O(1)	2·87	2·87
O(1)–O(4)	>7	>7
O(2)–O(5)	>7	>7
O(3)–O(6)	4·01	4·11

In the complexes previously reported,[2,3] the oxygen atoms all point towards the bound metal atom in the cavity, the distances between opposite oxygen atoms spanning a much smaller range (5·36—5·94 Å) than in the Table. Similar conformational changes for uncomplexed and complexed dibenzo-18-crown-6 were reported by Bright and Truter.[4]

Details of the structures will be published elsewhere.

We thank B. Haymore for crystal preparation, Dr. J. F. Cannon for computer programming assistance, and the U.S. National Institutes of Health for support.

(*Received, 25th September* 1974; *Com.* 1204.)

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