Molecular Rotations of Polyhydroxycyclohexanes in Relation to their Structures. II[1]. *(−)-1, 2, 3, 5/4-Cyclohexanepentol*

By Shukichi YAMANA

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$[M]_D^{20}$(W) of (−)-1, 2, 3, 5/4-cyclohexanepentol ((−)-epi-quercitol[2]) was calculated by using PM-method and Whiffen's method[3], respectively. The orientation of the unit groups, (OH). in the molecule is shown in Table I (Fig. 1).

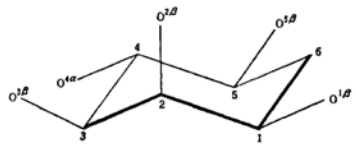

Fig. 1. Perspective drawing of the molecular model of (−)-1,2,3,5/4-cyclohexanepentol.

TABLE I

Name	Orientation of unit group, (OH)	Calcd. $\sum[\mu]_{D\,obs}^{20}$	Calcd. Whiffen
Cyclohexane			
(−)-1,2,3,5/4-pentol	[(1β), (2β), (3β), (4α), (5β)]	−6.8 (−10.9)[5]	0

PM-Method.— $[M]_D^{20}$(W) of (−)-1, 2, 3, 5/4-cyclohexanepentol $\equiv \sum[\mu]_{D\,obs}^{20}$ of (−)-1, 2, 3, 5/4-cyclohexanepentol = (1β) Λ (2β) + (1β) Λ (3β) + (1β) Λ (4α) + (1β) Λ (5β) + (2β) Λ (3β) + (2β) Λ (4α) + (2β) Λ (5β) + (3β) Λ (4α) + (3β) Λ (5β) + (4α) Λ (5β) = $A+0+0+0-A-B+0-A+0+A$[4] $= -B = -6.8$ (-10.9)[5].

1) Part I: S. Yamana, This Bulletin, 33, 1741 (1960).
2) "Advances in Carbohydrate Chemistry", Vol. 14, Academic Press, New York (1959), p. 190.
3) D. H. Whiffen, *Chem. & Ind.*, 1956, 964.
4) Table II in the previous paper[1] is used, here.
5) The values, calculated by supposing that the optical center of (OH) is located at its O atom, are given in parentheses.

Whiffen's Method.

along C^1-C^2
C|C−C|O+O|O−O|H+H|H−H|C
along C^2-C^3
C|H−C|C+O|C−O|O+H|O−H|H
along C^3-C^4
C|C−C|H+O|H−O|O+H|O−H|C
along C^4-C^5
C|H−C|C+O|O−O|H+H|C−H|O
along C^5-C^6
C|C−C|H+O|H−O|H+H|H−H|C
along C^6-C^1
C|H−C|C+H|C−H|O+H|O−H|H

Total=0

As seen above, $[M]_D^{19}$(W) of (−)-1, 2, 3, 5/4-cyclohexanepentol is presumed to be −6.8 (−10.9)[5] (by PM-method) or 0 (by Whiffen's method). The corresponding observed value has not been found in any referential literatures, but $[M]_D$(W) was observed at 27°C as −8.9[6]. This is nearly equal to −6.8 (−10.9)[5], the value calculated by PM-method at 20°C. This fact indicates that in this case also, PM-method is more suitable for estimating $[M]_D^{20}$ (W) than Whiffen's method.

Department of Chemistry
Kyoto Gakugei University
Fushimi-ku, Kyoto

6) B. Magasanik, R. E. Franzl and E. Chargaff, *J. Am. Chem. Soc.*, **74**, 2618 (1952).