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POTENTIAL ENERGY CALCULATIONS OF METHYL α - THIOMALTOSIDE "$C_{13}H_{24}O_{10}S$"

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During the course of present work potential energy calculations are carried out to find the bonded and non bonded interactions in the structure of methyl α - thiomaltoside. The possible allowed conformations of O_6 - O'_6 are found to be in the region of ϕ =O° to 360° and ϕ' = 0° to 230°,ϕ = 40°to 310° and ϕ = 230° to 360° respectively (ϕ and ϕ' are the angles of rotation about the bond C_5 - C_6 and C'_5 - C'_6, respectively). The hydrogen bonds for the pair O_6 - O'_6 are located at the following values of ϕ andϕ'; (I). ϕ=40°, ϕ =260°; (II). ϕ=310°, ϕ'=300°; (III). ϕ'=310°, ϕ'=310°; (IV). ϕ =340°and ϕ'=340°. The distance between the two atoms is 2.70 A° for the above values.

Key words: Methyl α - thiomaltoside.

Introduction

Methyl α-thiomaltoside $C_{13}H_{24}O_{10}$ S belongs to thiodisaccharide system. In the field of polysidascoligosaccharide complexes, 1-thioglyosides have appeared to be good substrate analogues [1-5].

SergePerez and Caroll Vergelati [6] have studied the crystal structure of methyl α - thiomaltoside by X-ray diffraction. Crystal data are as follows; a=14.196 A, b=4.846 A, c=12.410 A, β=110.12° and space group $P2_1$. These workers [7-9] proposed that the hydrogen bonded chains were present between O_2 and O'_3 as found in maltose, methyl β-maltoside and α maltose monohydrate.

The aim of present work is to describe the different possible position of hydrogen bonding and detailed conformational analysis of methyl α-thiomaltoside similar to other drugs [10-14].

Experimental

The perspective view of methyl α - thiomaltoside is shown in Fig. 1. The position of O_6 atom in 1st ring is gauche to C_5 - O_5 and trans to C_4 - C_5 (Fig. 1). In terms of angular variable describing the position with respect to C_5 - C_6 bond we define ϕ (angle of rotation) to be zero in gt position and to increase positively as the plane C_5 - C_6 - O_6 rotates clockwise (Fig. 2). O'_6 atom of the 2nd ring is in gg conformation (Fig. 1). In this C'_6 - O'_6 is gauche to both C'_5 - O'_5 and C'_4 - C'_5 (unprimed and primed atoms represent atom of 1st and 2nd ring, respectively), ϕ' (angle of rotation) is zero in gg position and increases positively as the plane of C'_5 C'_6 - O'_6 rotates clockwise (Fig. 2). The coordinates of the atoms O_6 and O'_6 are evaluated after rotation about the bonds C_5 - C_6(ϕ) and C'_5 - C'_6 (ϕ'), respectively.

The inter molecular distance and potential energy for a pair of atoms i and j separated by a distance rij calculated for the following pairs of 2 methyl α - thiomaltoside residues O_6 - O_5,O_6 - O_4, O_6 - C_4, O'_6 - O_6, O'_6 - O'_5, O'_6 - C'_4.

The detailed mathematical calculations are given elsewhere [12]. Several programmes were written in basic language and Sord M(68) was used throughout this work.

Result and Discussions

The contact distance contours for the pairs O_6 - O'_6 are shown in Fig. 3. The contour maps for the pairs O_6 - O_5, O_6 - O_4, O_6 - C_4, O_6 - O'_6, O'_6 - O'_5 and O'_6 - C'_4 are given in Figs. 4, 5 and 6 respectively.

Figure 7 shows the plot of rij versus ϕ and ϕ' for the pairs mentioned above. Table 1 shows the values of ϕ and ϕ' for intramolecular hydrogen bond formation between the atoms O_6 and O'_6.

In the present work detailed calculations are carried out to study the conformation of side chains in the structure of methyl α - thiomaltoside. Perez and Vergelati [6] reported the occurrence of two intramolecular hydrogen bonds between O_5 - O'_6 and O_6 - O'_6.

In this paper a search is made to find the possible positions of hydrogen bonds for the pair O_6 - O'_6. The criteria used for

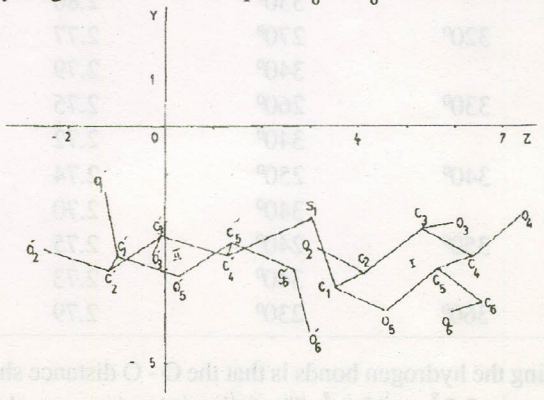

Fig. 1. The 100 projection of methyl - α - Thiomaltoside.

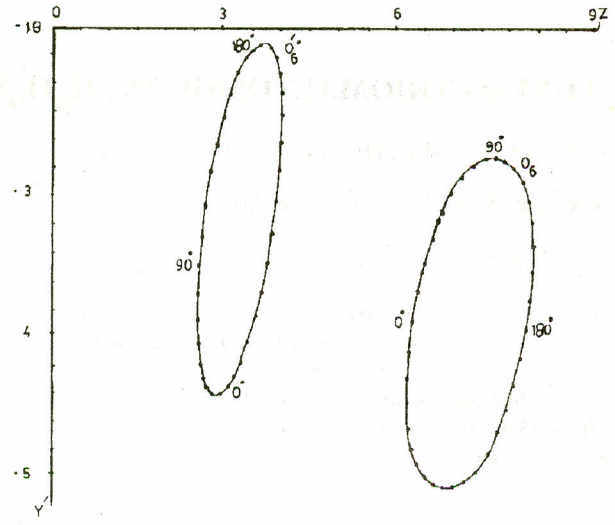

Fig. 2. The 100 projection of coordinates showing clockwise rotation of O_6 and O'_6.

Table 1. VARIOUS REGIONS FOR THE INTRAMOLECULAR HYDROGEN BOND FORMATION BETWEEN THE ATOMS O_6 - O'_6

ϕ	ϕ'	rij
0⁰	230⁰	2.793
10⁰	230⁰	2.741
10⁰	330⁰	2.809
20⁰	330⁰	2.736
30⁰	230⁰	2.776
30⁰	300⁰	2.770
40⁰	240⁰	2.77
	250⁰	2.72
	260⁰	2.70
	270⁰	2.71
	280⁰	2.76
310⁰	290⁰	2.75
	300⁰	2.70
	310⁰	2.70
	320⁰	2.73
	330⁰	2.80
320⁰	270⁰	2.77
	340⁰	2.79
330⁰	260⁰	2.75
	340⁰	2.72
340⁰	250⁰	2.74
	340⁰	2.70
350⁰	240⁰	2.75
	340⁰	2.73
360⁰	230⁰	2.79

deciding the hydrogen bonds is that the O - O distance should lie between 2.7Å and 2.8 Å. The following pairs were selected to study the conformation.

O_6 - O'_6 pair. Contact distance contour for the pair O_6 - O'_6 (Fig. 3) shows that the intramolecular hydrogen bond formation is possible for the following values of ϕ and ϕ′ when the rij is 2.70 Å (Table 1) (i) ϕ =40°, ϕ′=260 (ii) ϕ =310°, ϕ′=300°, (iii) ϕ =310°, ϕ′ =310°, (iv) ϕ =340°, ϕ′ = 340°. Energy calculation for the pair O_6 - O'_6 indicates that the minimum potential energies are found to be 0.379 Kcal/mole when ϕ =350°and ϕ′ =290° (Fig. 4). The allowed conformations are shown outside the zero contour in the regions of ϕ = o to 360° and ϕ′ = 0 ° to 230°, ϕ = 40° to 310° and ϕ ' = 230° to 360°.

O'_6 - C'_4 pair - The maximum potential energy was found to be 0.154 K cal/mole at ϕ = 310°. The rotation of O'_6 from 0° to 280°and 340° to 360°gives allowed conformation, keeping C_4 fixed (Fig. 5).

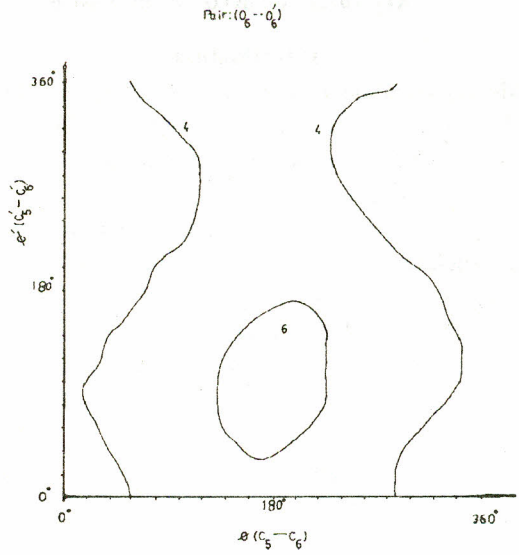

Fig. 3. The contact distance contours for the pair O_6 - O'_6. (Page 518)

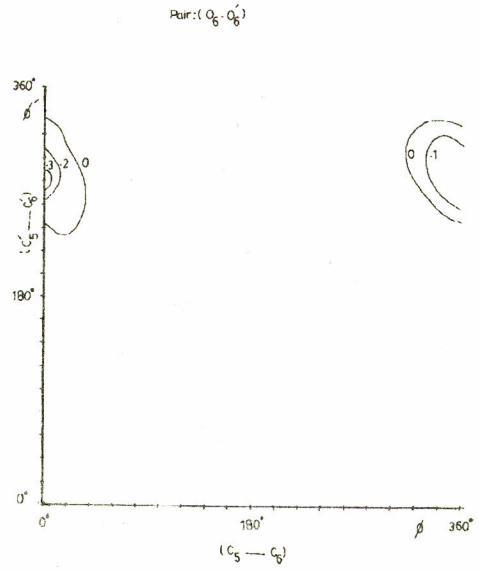

Fig. 4. Energy contours for the pair O_6 - O'_6. The units of energy are K cal/mole.

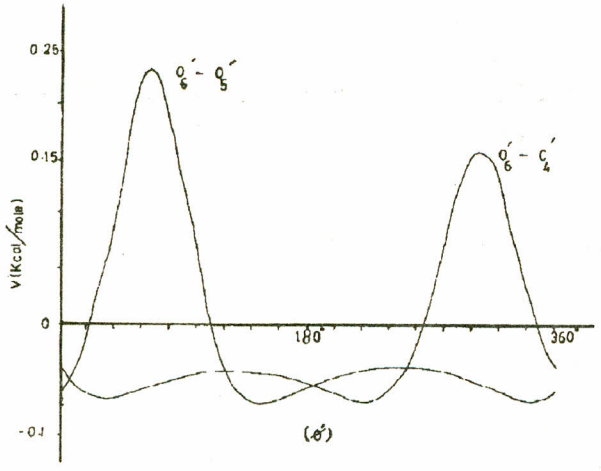

Fig. 5. The plot of potential energy versus, ϕ' for the pairs:- O'_6 - O'_5 and O'_6 - C'_4 (ϕ' represents rolation of O'_6, O_5 and C_4 are kept fixed). The units of energy are K cal/mole.

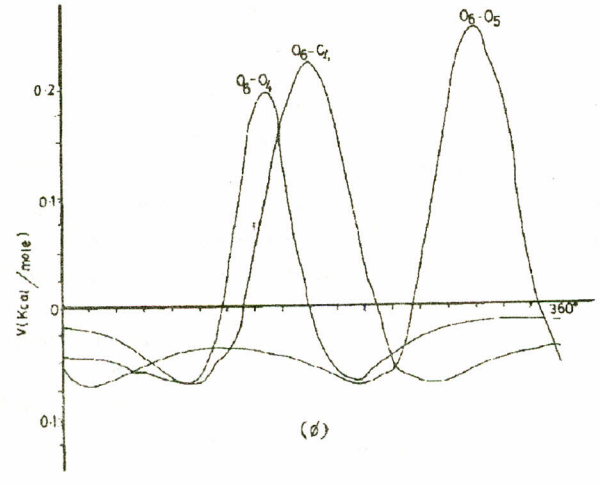

Fig. 6. The plot of potential energy Versus ϕ for the pairs: O_6 - O_4, O_6 - O_4, O_6 - O_5. (ϕ represents rotation of only O_6, O_4, C_4 and O_5 are kept fixed). The units of energy are K cal/mole.

O'_6 - O'_5 pair. The maximum potential energy was found to be 0.230 K cal/mole at ϕ = 70°, O_5 was fixed. The rotation of O_6 from 20° to 110°is not allowed. The allowed conformations are when ϕ'=0° to 20° and 110° to 360° (Fig. 5).

O_6 - C_4 pair. The maximum potential energy was found to be 0.228 K cal/mole at ϕ = 180°, C_4 is fixed. The rotation of O_6 from 140° to 210° indicates unallowed region (Fig. 6).

O_6 - O_4 pair. The maximum potential energy for the pair O_6 - O_4 was found to be 0.192 Kcal/mole at ϕ = 150°, O_4 is fixed. The allowed conformations are observed at ϕ = 0° to 120° and 180° to 360° (Fig. 6).

O_6 - O_5 pair. The maximum potential energy was found to be 0.2503 K cal/mole at ϕ= 300°. The allowed region for this pair is at ϕ = from 0° to 250° (Fig. 6). Figure 7 shows the serious type of short contact for the pairs O_6 - O_5 and O'_6 - O'_5. This is also confirmed from potential energy calculation (Figs. 5 and 6). Present calculations suggest that an intra sheet O_6..H..O_6

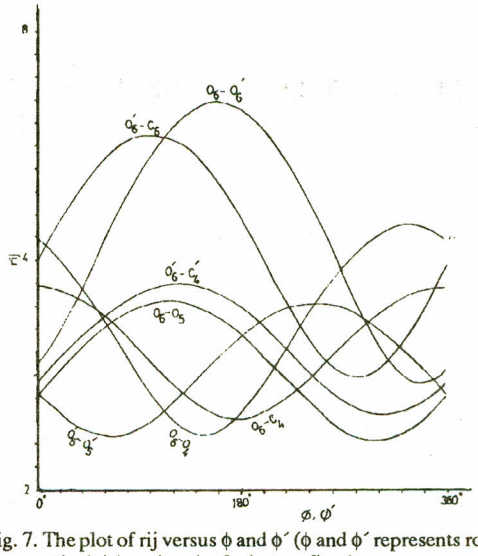

Fig. 7. The plot of rij versus ϕ and ϕ' (ϕ and ϕ' represents rotation of O_6 and O'_6 respectively) keeping the 2nd atom fixed.

hydrogen bond can be formed. Such type of H-bond is necessary to stabilize the structure.

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