RESEARCH PAPER

Crystal Structure Analysis and Conformational Aspects of Oxatricyclo Undeca-Polyene Compound Named Dimethyl 1,8-Diphenyl-11-oxatricyclo-[6.2.1.$0^{2,7}$]undeca-2,4,6,9-tetraene-9,10-dicarboxylate

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ABSTRACT

The title compound $C_{26}H_{20}O_5$, consists of two crystallographically independent molecules (A and B) with similar conformations. Each molecule comprises a fused tricyclic system containing two five-membered rings. In both molecules, the five-membered rings exhibit an envelope conformation and the six-membered ring adopts a boat conformation. The crystal structure is stabilized by C–H···O and C–H···π interactions.

Keywords: Crystal structure; Oxatricyclo undeca-polyene; Dimethyl dicarboxylate; Envelope conformation; Boat conformation; C–H···O interactions; C–H···π interactions; X-ray diffraction

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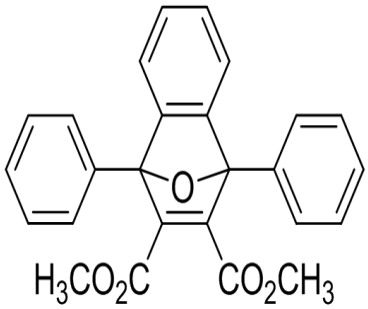


Fig 1 Chemical Diagram

Introduction

Naphthalene derivatives are useful compounds because, they are partial structures of bioactive molecules (Xie &Kozlowski, 2001)and liquid crystals(Svobodaet al., 2003). Recently rhenium complex catalyzed synthesis of naphthalene derivatives is reported by the reactions of aromatic ketimines with benzaldehyde and maleimide. Diels–Alder adducts formed was exposed to acidic conditions, causing dehydrative aromatization.

Anthracene is one of the earliest luminescent materials reported and emits violet both in the solid state and in solution. Derivatives of Anthracene have been used successfully as blue

emitters in commercial OLED products (Shi & Tang, 2002). On the basis of the efficiency reported and stability of anthracene derivatives, recently a new class of blue emitters [7,16 – dihydro - 6,8,15,17 - tetraphenylheptacene , 7,16-dihydro-6,15 - bis(p-tert-butylphenyl)-8,17-diphenylheptacene and 7,16 – dihydro-6,8,15,17-tetrakis(p-tert-butylphenyl)heptacene] has been synthesized and studied (Rajib et al*.,* 2006).They are dihydroheptacene derivatives in which two anthracene moieties are attached to one another via two methylene bridges. These derivatives are prepared by the reaction of in-situ generated furan derivatives with p-benzoquinone which upon dehydration/oxidation yielded heptacene derivatives.

The promise of organic electronics to enable creation of inexpensive, flexible, and multifunctional devices (Anthony, 2008) is presently limited by access to stable high-performance materials. One strategy to develop such materials is to create extended rigid aromatic systems that promote delocalization and minimize energetic disorder in the electronic states. Among the polycyclicaromatic hydrocarbons (PAHs), acenes, defined as linearly annelated arenes with the fewest number of rings containing Clar sextets (Ruiz-Morales, 2002) are considered one of the most important candidates for high-performance organic semiconductors. Recently the synthesis of POAs is achieved (Rebecca & Timothy, 2012) through a series of synthetic transformations using Diels-Alder adduct as the key intermediate.

Tamiflu, a neuraminidase inhibitor, is an antiviral medication used to treat influenza virus in patients who have had symptoms for less than 2 days. The current key starting material for the production of Tamiflu is (-)-shikimic acid(Kim et al., 1997). Besides its industrial uses, (-)-shikimic acid is a pivotal intermediate in the biogenetic synthesis pathway of a variety of aromatic natural products in microorganisms and plants known as the shikimate pathway (Sikorski, 1997). Recently asymmetric synthesis of (-)-shikimic acid from a chiral Diels-Alder adduct between furan and acrylate is reported (Sung et al., 2011).

Macromolecular networks incorporating crosslinks formed by Diels-Alder cycloaddition have been reported in the scientific literature (Rohloff, et al., 1998) the thermally reversible Diels-Alder cycloaddition of a monomer with four furan moieties on each molecule and a monomer with three maleimide moieties on each molecule form a highly-crosslinked network. After casting of a dichloromethane solution of the monomers (with stoichiometric furan-maleimide ratio), the solvent was vacuum evaporated at room temperature and the material was then heated. Cross-linking of furan side chain polymers with bis-maleimide-containing small molecules has also been reported (Sanyal, 2010). Recently novel thermo reversible network of scaffolds are prepared using Diels-Alder oxo adduct as the key intermediates. In view of these significant applications, the crystal structures of the Oxatricyclo undeca-polyene derivatives have been carried out.

Intensity Data Collection

Accurate unit cell parameters and orientation matrix was obtained by least squares fit of several high range reflections in the range $2.3 < \theta < 26.0°$ for this compound, using Mo Kα λ=0.7107Åradiation on Bruker Axs Kappa APEXII CCD diffractometer (Bruker, 2004 ; Bruker, 2008) equipped with a graphite monochromator using ω scan mode. The unit cell parameters were determined from 36 frames measured (0.5°and phi scan) from three different crystallographic zones and using the method of difference vectors. The data reduction and cell refinement were carried out with the help of SAINT (Bruker, 2004) software for this compound. The intensity data were collected with an average four – fold redundancy per reflection and optimum resolution of 0.75Å. A total of 40251 reflections was collected resulting in 8336 independent reflections of which 4142 had $I > 2\sigma$ (1) for this compound and these were considered as observed. The intensity data collection, frames integration, Lorentz and polarization correction and decay correction were done using SAINT (Bruker,2004 ; 2008) software. Empirical absorption correction (multi-scan) is performed using SADABS (Bruker, 2004) program.

Structure Solution And Refinement

The structure of the title compound C 26 H 20 O 5 was solved by direct methods procedure using SIR-92 (Altomare et al., 1993). The normalized structure factors (F) were used for finding the phases. A total of 40251 reflections with $E > 1.2$ were used for phase refinement procedures. A total of 256 phase sets have been refined of which the set with lowest Combined Figure of Merit (CFOM) was taken as the best set. The values of CFOM was 0.0659 . The E – map estimated for the best phase set generated by the program revealed the positions of all the non-hydrogen atoms of this compound. The residual factors (R_E) calculated based on the point atom model was 0.226 for this compound. The trial structure thus obtained were refined by full matrix least – squares technique on F^2 using SHELXL-97 (Sheldrick, 2008) for this compound. In the initial stages of refinement, thermal parameters were assigned a values of 0.05 (U's) for each atom and the refinement was carried out. The scale factor was assigned as 1.0 and isotropic refinement was carried out for all the non-hydrogen atoms until convergence was reached and this was subsequently followed by anisotropic refinement. After a few cycles of anisotropic refinement, the positions of all the hydrogen atoms were taken to be 1.5 Ueq or 1.2 Ueq of the non hydrogen atoms to which they are

attached. The refinement converged to a final R-factor of 0.049 and for this compound. The residual electron density was 0. 0.52 & -0.23 e $Å^{-3}$.

Ressults And Discussioins

Fig 1 shows the chemical diagram of the compound studied. Table1 summarizes the crystal data, intensity data collection and refinement details for this compound. The atomic coordinates of the non – hydrogen atoms with their equivalent temperature factors are presented in Table2. The anisotropic displacement parameters are given in Table3. The corresponding bond lengths and bond angles are given in Table 4 . The torsion angles for non-hydrogen atoms are listed in Table 5. The atomic coordinates and isotropic temperature factors of the hydrogen atoms are listed in Table 6. The least – squares plane calculated using the program PARST (Nardelli, 1983) are tabulated in Table7. The intermolecular and intramolecular hydrogen bonds are listed in Table 8.

Fig 2 shows the ORTEP plot of the molecule drawn at 30% probability displacement ellipsoid with atom numbering scheme. The asymmetric unit of the title compound consists of two crystallographically independent molecules (A and B). Each molecule consists of fused tricyclic systems and two phenyl rings attached to this system. The tricyclic systems consists of two five membered rings and one aromatic ring. In addition, two carboxylate units are attached to the tricyclic systems. Geometrical parameters agree well with reported structures (Bailey et al.,1995 ; Ohwadaet al., 2001).

In molecule A, the five membered rings C1\C2\C7\C8\O1 and C1\C21\C24\C8\O1 rings adopt envelope conformations with atom O1 displaced by 0.773Å and 0.778Å from the mean plane of the other ring atoms. In molecule B, the five membered rings C1A\C2A\C7A\C8A\O1A and C1A\C21A\C24A\C8A\O1A rings also adopt envelope conformations with atom O1A displaced by 0.782Å and 0.776Å from the mean plane of the other ring. The six membered rings C1/C2/C7/C8/C24/C21 and C1A/C2A/C7A/C8A/C24A/C21A adopt boat conformations in molecule (A & B). In both molecules the phenyl rings (C9 - C14) and (C15A-C20A) are disordered over two sets of sites with an occupancy ratios of 0.641(2) : 0.359(2) and 0.775(9) : 0.225(9). The dihedral angles between the two five membered rings (C1\C2\C7\C8\O1) –(C1\C21\C24\C8\O1) in molecule A and (C1A\C2A\C7A\C8A\O1A)-

–(C1A\C21A\C24A\C8A\O1A) in molecule B are 69.6(1)° and 70.1(1)°, respectively. In molecule A and B the phenyl ring system (C15-C20) and (C9A- C14A) make dihedral angles of 80.5(1)° and 78.9(1)° with the mean plane of the tricyclic ring system. In molecule A, the mean plane of the tricyclic ring system make dihedral angles of 33.7(2)° and 39.5(8)° with the major and minor components of the disordered phenyl ring, whereas the corresponding angles are 34.1(3)° and 59.8(1)° in molecule B. In molecule A, the carboxylate ligands at the C21 and C24 carbon atoms are turned out the plane of the five membered ring C21/C1/O1/C8/C24 (the torsion angle being C24—C21— C22—O2= -92.2(4)° and C21—C24— C25—O4 = -28.1(6)°. In molecule B, the carboxylate ligands at the C21A and C24A carbon atoms are turned out the plane of the five membered ring C21A/C1A/O1A/C8A/C24A (the torsion angle being C24A—C21A— C22A—O2A = -28.5(6)° and C21A— C24A— C25A — O4A = 92.4(4)°).

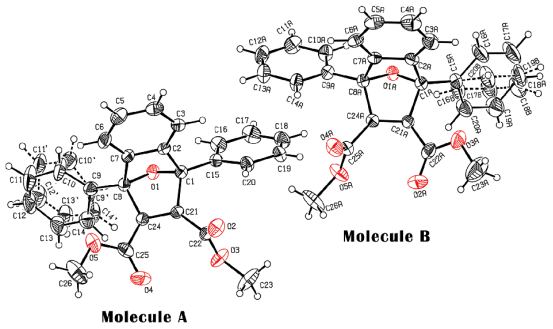


Fig 2: Molecular structure of the title compound, showing 30% probability displacement ellipsoids

Inter And Intra Molecular Features

The pattern of hydrogen bonding and packing in the crystals are shown in Fig 3 and Fig 4. The packing of the molecule is stabilized by intermolecular C--H...O and C--H...π hydrogen bonds. In addition, the intra molecular interactions are observed through C20--H20…O2. Geometric details of hydrogen bondings are listed in Table 8.

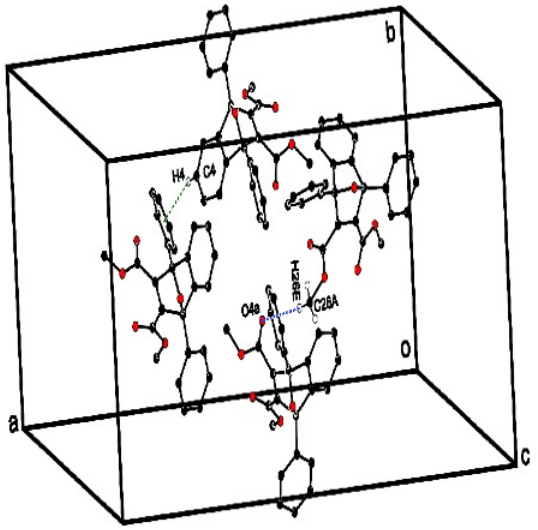


Fig 3 The crystal structure of the Compound with C--H…O hydrogen bonding scheme shown as dashed lines

Ring Puckering Parameters

In molecule A, The total puckering amplitudes (Cremer & Pople, 1975) of the rings (C1\C2\C7\C8\O1), (C1\C1\C21\C24\C8\O1) and (C1/C2/C7/C8/C24/C21) give a quantitative evaluation of puckering and asymmetry parameters (Nardelli, 1983). The five membered rings (C1\C2\C7\C8\O1) and (C1\C21\C24\C8\O1) rings adopt envelope conformations with atom O1 displaced by 0.780Å and 0.785Å from the mean plane of the other ring atoms. In molecule B, the five membered rings (C1A\C2A\C7A\C8A\O1A) and (C1A\C21A\C24A\C8A\O1A) rings also adopt envelope conformations with atom O1A displaced by 0.778Å and 0.773Å from the mean plane of the other ring. The six membered rings (C1/C2/C7/C8/C24/C21) and (C1A/C2A/C7A/C8A/C24A/C21A) adopt boat conformations in molecule (A & B). The total puckering and asymmetry parameters are given the Table9.

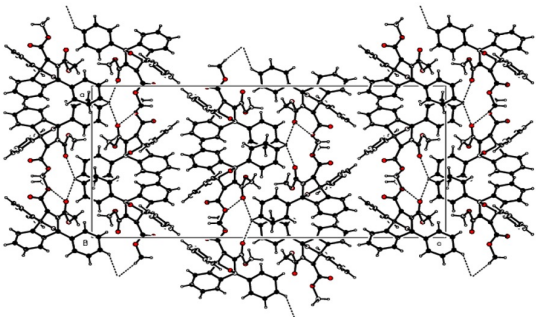


Fig 4 Packing of the Compound viewed down b-axis

Parameters	Compound
Chemical formula	$C_{26}H_{20}O_5$
Formula weight	412.42
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
space group	P $2_12_12_1$
Unit cell dimensions	
a(Å) b(Å) C(Å) α(°) β(°) γ(°)	15.7472(15) 8.3327(8) 11.0961(4) 90 90 90
Volume Å^3	4238.6(7)
Z, Calculated density Mg/m^3	8, 1.293
Absorption coefficient mm^{-1}	0.089
F(000)	1728
Crystal size mm	0.30 x 0.20 x 0.20
θ range	2.29 to 26.00°
Index ranges	-19<=h<=13 -10<=k<=9 -38<=l<=39
Reflections collected / unique	40251 / 8336 [R(int) = 0.0361]
Completeness to theta	99.90%
Refinement method	Full-matrix least-squares on F^2
Diffractometer	Bruker Kappa APEXII CCD diffractometer

Table1: Summary of crystal data, intensity data collection and refinement details for compound Table 2

Atoms	X	Y	Z	U(eq)
C1	6067(2)	4827(4)	1451(1)	37(1)
C2	5429(2)	3721(4)	1671(1)	37(1)
C3	5263(2)	3431(4)	2082(1)	43(1)
C4	4642(2)	2308(5)	2174(1)	58(1)
C5	4226(2)	1502(5)	1866(1)	67(1)
C6	4393(2)	1779(5)	1450(1)	59(1)
C7	5000(2)	2926(4)	1357(1)	43(1)
C8	5403(2)	3548(4)	956(1)	43(1)
C9	4933(11)	3550(30)	559(6)	51(3)
C10	4120(7)	3032(18)	488(4)	83(3)
C11	3788(7)	3030(20)	87(4)	103(3)
C12	4185(10)	3602(18)	-231(5)	89(3)
C13	5042(9)	3977(17)	-193(4)	79(3)
C14	5406(10)	3825(16)	189(5)	67(3)
C9'	5000(20)	3710(50)	518(11)	56(4)
C10'	4091(13)	3860(30)	521(6)	74(4)
C11'	3668(12)	4030(30)	141(6)	87(4)
C12'	4190(20)	4280(30)	-206(9)	90(5)
C13'	4950(17)	4650(30)	-146(7)	81(4)
C14'	5366(17)	4400(30)	225(8)	68(4)
C15	6377(2)	6282(4)	1674(1)	40(1)
C16	6090(2)	7798(4)	1575(1)	56(1)
C17	6405(3)	9122(5)	1787(1)	72(1)
C18	6993(3)	8931(5)	2098(1)	67(1)
C19	7255(2)	7430(5)	2210(1)	60(1)

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for the non-H atoms of Compound with esd's in parentheses

Table 2 Contd…

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for the non-H atoms of Compound with esd's in parentheses.

Atoms	X	Y	Z	U(eq)
C21	6733(2)	3652(4)	1258(1)	38(1)
C22	7583(2)	3314(4)	1438(1)	45(1)
C23	9045(2)	3791(8)	1396(2)	117(2)
C24	6317(2)	2861(4)	964(1)	41(1)
C25	6631(3)	1387(5)	766(1)	57(1)
C26	6318(5)	-1106(7)	486(2)	124(2)
O1	5594(1)	5191(3)	1083(1)	43(1)
O2	7680(2)	2502(3)	1740(1)	64(1)
O3	8194(1)	4057(4)	1234(1)	72(1)
O4	7377(2)	1074(4)	730(1)	93(1)
O5	6020(2)	411(4)	653(1)	80(1)
C1A	2352(2)	-1367(4)	958(1)	42(1)
C2A	2763(2)	-2005(4)	1357(1)	43(1)
C3A	3374(2)	-3106(5)	1449(1)	63(1)
C4A	3548(3)	-3403(6)	1869(2)	75(1)
C5A	3105(2)	-2621(5)	2178(1)	63(1)
C6A	2479(2)	-1530(4)	2082(1)	49(1)
C7A	2325(2)	-1214(4)	1672(1)	40(1)
C8A	1685(2)	-111(4)	1455(1)	38(1)
C9A	1394(2)	1361(4)	1684(1)	43(1)
C10A	1709(2)	2861(4)	1581(1)	54(1)
C11A	1450(3)	4189(5)	1801(1)	68(1)
C12A	895(3)	4054(5)	2126(1)	66(1)
C13A	592(3)	2590(5)	2230(1)	68(1)
C14A	836(2)	1226(5)	2013(1)	57(1)
C15A	2798(2)	-1333(5)	548(1)	52(1)
C16A	3655(4)	-1633(12)	503(2)	93(2)
C17A	4026(5)	-1531(15)	112(3)	112(3)

Table 2 Contd… Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (Å^2 x 10^3) for the non-H atoms of Compound with esd's in parentheses

Atoms	X	Y	Z	U(eq)
C18A	3587(7)	-1140(30)	-222(6)	96(3)
C19A	2699(5)	-856(12)	-186(2)	90(2)
C20A	2332(4)	-979(10)	198(2)	69(2)
C16B	3278(16)	-2470(40)	398(8)	90(5)
C17B	3693(16)	-2410(40)	13(8)	94(5)
C18B	3380(30)	-1190(110)	-260(20)	93(5)
C19B	2988(17)	-80(40)	-125(8)	85(5)
C20B	2622(16)	-140(40)	267(7)	72(4)
C21A	1438(2)	-2061(4)	968(1)	40(1)
C22A	1135(2)	-3549(5)	772(1)	57(1)
C23A	1406(5)	-6014(8)	492(2)	140(3)
C24A	1023(2)	-1274(4)	1262(1)	39(1)
C25A	176(2)	-1634(4)	1438(1)	44(1)
C26A	-1298(2)	-1188(8)	1393(2)	105(2)
O1A	2165(1)	268(3)	1087(1)	42(1)
O2A	386(2)	-3867(4)	739(1)	91(1)
O3A	1739(2)	-4510(4)	659(1)	78(1)
O4A	83(2)	-2453(4)	1739(1)	68(1)
O5A	-438(1)	-920(4)	1235(1)	72(1)

Table 3

Anisotropic displacement parameters ($Å^2x\ 10^3$) for the non-H atoms of Compound

with esd's in parentheses. The anisotropic displacement factor takes the form:

$exp\{-2\pi^2[h^2a^{*2}U_{11} + ... + 2hk\ a^*\ b^*\ U_{12}]\}$

Atoms	U_{11}	U_{22}	U_{33}	U_{23}	U_{12}	U_{13}
C1	37(1)	38(2)	36(2)	3(1)	-1(1)	0(1)
C2	32(1)	34(2)	45(2)	1(1)	5(1)	1(1)
C3	41(2)	44(2)	43(2)	1(2)	5(1)	6(2)
C4	53(2)	59(2)	60(2)	11(2)	19(2)	-3(2)
C5	52(2)	69(3)	81(3)	11(2)	12(2)	-21(2)
C6	46(2)	65(3)	66(2)	-3(2)	-1(2)	-21(2)
C7	34(1)	47(2)	48(2)	-1(2)	-1(1)	0(1)
C8	39(1)	50(2)	40(2)	-3(2)	-4(1)	-4(1)
C9	45(4)	63(6)	45(5)	1(4)	2(3)	0(4)
C10	64(4)	110(7)	74(5)	10(6)	-29(3)	-38(5)
C11	88(5)	131(9)	91(6)	1(7)	-48(4)	-33(6)
C12	95(5)	112(8)	59(4)	-13(6)	-43(4)	1(7)
C13	95(5)	94(8)	49(4)	-4(5)	-12(4)	9(6)
C14	68(4)	80(7)	53(4)	-3(5)	-8(3)	6(5)
C9'	47(7)	80(8)	40(7)	4(7)	-27(7)	-22(6)
C10'	65(6)	103(9)	56(6)	4(8)	-9(5)	-16(8)
C11'	66(6)	123(10)	71(7)	1(8)	-31(5)	-24(8)
C12'	96(7)	112(11)	62(7)	10(9)	-22(6)	-23(9)
C13'	97(8)	96(10)	51(7)	15(8)	-21(6)	-24(9)
C14'	72(7)	87(10)	46(7)	14(8)	-17(6)	-32(8)
C15	41(2)	33(2)	45(2)	0(1)	6(1)	-4(1)
C16	67(2)	40(2)	60(2)	5(2)	1(2)	3(2)
C17	100(3)	30(2)	86(3)	2(2)	15(3)	-3(2)
C18	78(3)	49(3)	75(3)	-20(2)	13(2)	-17(2)
C19	62(2)	61(3)	57(2)	-19(2)	-3(2)	-7(2)
C20	57(2)	44(2)	52(2)	-7(2)	-5(2)	0(2)
C21	35(1)	39(2)	40(2)	5(1)	4(1)	-2(1)
C22	38(2)	46(2)	52(2)	-2(2)	-1(1)	-1(2)
C23	37(2)	128(5)	185(6)	28(5)	-13(3)	-10(3)
C24	39(1)	49(2)	34(2)	-1(2)	3(1)	-4(1)
C25	74(2)	60(2)	37(2)	-1(2)	6(2)	5(2)
C26	185(7)	82(4)	106(4)	-43(4)	4(4)	-3(4)
O1	44(1)	44(1)	41(1)	5(1)	-8(1)	2(1)
O2	59(1)	67(2)	67(2)	20(2)	-12(1)	3(1)
O3	35(1)	92(2)	88(2)	28(2)	-1(1)	-11(1)
O4	71(2)	95(2)	114(2)	-35(2)	25(2)	19(2)
O5	93(2)	67(2)	79(2)	-28(2)	-7(2)	-9(2)
C1A	39(1)	44(2)	44(2)	-1(2)	2(1)	1(1)
C2A	34(1)	42(2)	52(2)	1(2)	-4(1)	0(1)
C3A	53(2)	56(2)	81(3)	4(2)	-4(2)	13(2)
C4A	62(2)	67(3)	97(3)	18(3)	-28(2)	14(2)
C5A	69(2)	58(2)	62(2)	15(2)	-27(2)	-9(2)
C6A	60(2)	40(2)	45(2)	4(2)	-10(2)	-10(2)
C7A	38(1)	37(2)	43(2)	2(2)	-5(1)	-6(1)
C8A	40(1)	36(2)	37(2)	4(1)	3(1)	-1(1)
C9A	49(2)	39(2)	40(2)	2(2)	-2(1)	2(2)
C10A	65(2)	41(2)	56(2)	2(2)	6(2)	1(2)
C11A	88(3)	38(2)	77(3)	1(2)	-6(2)	-2(2)
C12A	82(3)	48(2)	69(3)	-16(2)	-1(2)	15(2)
C13A	77(2)	64(3)	63(2)	-11(2)	19(2)	8(2)
C14A	72(2)	45(2)	53(2)	-3(2)	16(2)	-1(2)
C15A	45(2)	61(2)	49(2)	-3(2)	12(1)	-1(2)
C16A	44(3)	170(7)	66(4)	-1(4)	14(3)	10(4)
C17A	58(4)	190(8)	89(5)	12(5)	34(3)	12(5)

Table 3

Contd…

Anisotropic displacement parameters ($Å^2x\ 10^3$) for the non-H atoms of Compound with esd's in parentheses. The anisotropic displacement factor takes the form:$exp\{-2\pi^2[h^2a^{*2}U_{11} + ... + 2hk\ a^*\ b^*\ U_{12}]\}$

Table 3 Contd…

Anisotropic displacement parameters ($Å^2x\ 10^3$) for the non-H atoms of Compound

with esd's in parentheses. The anisotropic displacement factor takes the form:

$exp\{-2\pi^2[h^2a^{*2}U_{11} + ... + 2hk\ a^*\ b^*\ U_{12}]\}$

Atoms	Distance	Atoms	Distance
C1-O1	1.438(3)	C9'-C14'	1.25(5)
C1-C15	1.491(4)	C9'-C10'	1.43(4)
C1-C2	1.536(4)	C10'-C11'	1.40(2)
C1-C21	1.564(4)	C11'-C12'	1.41(3)
C2-C3	1.376(4)	C12'-C13'	1.24(3)
C2-C7	1.387(4)	C13'-C14'	1.38(3)
C3-C4	1.385(5)	C15-C16	1.379(5)
C4-C5	1.368(5)	C15-C20	1.392(4)
C5-C6	1.388(5)	C16-C17	1.391(6)
C6-C7	1.385(5)	C17-C18	1.375(6)
C7-C8	1.534(4)	C18-C19	1.365(6)
C8-O1	1.460(4)	C19-C20	1.373(5)
C8-C9	1.479(19)	C21-C24	1.328(4)
C8-C24	1.550(4)	C21-C22	1.486(4)
C8-C9'	1.56(3)	C22-O2	1.196(4)
C9-C10	1.37(2)	C22-O3	1.320(4)
C9-C14	1.43(3)	C23-O3	1.457(5)
C10-C11	1.399(14)	C24-C25	1.470(5)
C11-C12	1.295(19)	C25-O4	1.209(4)
C12-C13	1.39(2)	C25-O5	1.311(5)
C13-C14	1.366(18)	C26-O5	1.452(6)

Atoms	U_{11}	U_{22}	U_{33}	U_{23}	U_{12}	U_{13}
C18A	74(7)	151(6)	64(5)	4(5)	35(6)	5(7)
C19A	79(4)	134(6)	57(3)	13(4)	12(3)	-3(4)
C20A	53(3)	101(5)	54(3)	14(3)	11(2)	4(3)
C16B	70(9)	124(11)	77(9)	2(9)	26(8)	19(9)
C17B	65(9)	138(11)	77(9)	-18(9)	34(8)	28(9)
C18B	67(10)	141(10)	72(9)	7(9)	16(9)	20(10)
C19B	77(9)	123(10)	57(8)	14(8)	22(8)	12(9)
C20B	70(9)	94(10)	51(8)	12(8)	21(7)	18(8)
C21A	37(1)	49(2)	34(2)	0(2)	0(1)	0(1)
C22A	75(2)	61(2)	36(2)	-5(2)	1(2)	-9(2)
C23A	192(7)	89(4)	140(5)	-49(4)	-24(5)	7(5)
C24A	38(1)	42(2)	36(2)	6(1)	-1(1)	1(1)
C25A	41(2)	45(2)	46(2)	2(2)	5(1)	1(2)
C26A	40(2)	117(4)	159(5)	36(4)	23(3)	13(3)
O1A	45(1)	42(1)	40(1)	4(1)	7(1)	1(1)
O2A	64(2)	100(3)	111(2)	-31(2)	-16(2)	-25(2)
O3A	90(2)	62(2)	82(2)	-26(2)	9(2)	0(2)
O4A	63(1)	78(2)	62(2)	21(2)	14(1)	-3(2)
O5A	38(1)	88(2)	90(2)	28(2)	6(1)	12(1)

Table 4

Bond lengths (Å) for non-H atoms of Compound with esd's in parentheses

Table 4 Contd…

Bond lengths (Å) for non-H atoms of Compound with esd's in parentheses

Atoms	Distance
C1A-O1A	1.454(4)
C1A-C15A	1.498(4)
C1A-C2A	1.537(4)
C1A-C21A	1.551(4)
C2A-C3A	1.362(5)
C2A-C7A	1.397(4)
C3A-C4A	1.405(6)
C4A-C5A	1.382(6)
C5A-C6A	1.376(5)
C6A-C7A	1.371(4)
C7A-C8A	1.534(4)
C8A-O1A	1.445(3)
C8A-C9A	1.504(5)
C8A-C24A	1.553(4)
C9A-C14A	1.382(5)
C9A-C10A	1.385(5)
C10A-C11A	1.375(5)
C11A-C12A	1.373(6)
C12A-C13A	1.352(6)
C13A-C14A	1.391(5)
C15A-C16B	1.31(2)

Atoms	Distance
C15A-C20B	1.37(2)
C15A-C20A	1.380(7)
C15A-C16A	1.380(6)
C16A-C17A	1.393(9)
C17A-C18A	1.324(19)
C18A-C19A	1.422(15)
C19A-C20A	1.372(9)
C16B-C17B	1.41(3)
C17B-C18B	1.43(8)
C18B-C19B	1.19(8)
C19B-C20B	1.39(3)
C21A-C24A	1.327(4)
C21A-C22A	1.471(5)
C22A-O2A	1.213(4)
C22A-O3A	1.295(5)
C23A-O3A	1.461(7)
C24A-C25A	1.482(4)
C25A-O4A	1.197(4)
C25A-O5A	1.312(4)
C26A-O5A	1.463(4)

Table 4 Contd… Bond angles (°) for non-H atoms of Compound with esd's in parentheses

Table 4 Contd…

Bond angles (°) for non-H atoms of Compound with esd's in parentheses

Atoms	Angle
O1-C1-C15	113.4(3)
O1-C1-C2	99.8(2)
C15-C1-C2	118.6(3)
O1-C1-C21	98.5(2)
C15-C1-C21	118.8(2)
C2-C1-C21	104.3(2)
C3-C2-C7	122.0(3)
C3-C2-C1	132.5(3)
C7-C2-C1	105.5(2)
C2-C3-C4	117.3(3)
C5-C4-C3	121.0(3)
C4-C5-C6	122.1(3)
C7-C6-C5	117.1(3)
C6-C7-C2	120.5(3)
C6-C7-C8	134.6(3)
C2-C7-C8	104.8(3)
O1-C8-C9	110.2(9)
O1-C8-C7	99.5(2)
C9-C8-C7	121.7(8)
O1-C8-C24	98.6(2)
C9-C8-C24	118.7(7)
C7-C8-C24	104.2(2)
O1-C8-C9'	105.0(16)
C9-C8-C9'	7(2)
C7-C8-C9'	128.8(14)
C24-C8-C9'	115.4(14)
C10-C9-C14	113.5(15)
C10-C9-C8	127.7(15)
C14-C9-C8	117.7(13)
C9-C10-C11	120.4(12)
C12-C11-C10	123.7(10)
C11-C12-C13	118.8(11)
C14-C13-C12	117.9(12)

Atoms	Angle
C13-C14-C9	123.5(14)
C14'-C9'-C10'	115(3)
C14'-C9'-C8	122(3)
C10'-C9'-C8	114(3)
C11'-C10'-C9'	118(2)
C10'-C11'-C12'	115.5(18)
C13'-C12'-C11'	118(2)
C12'-C13'-C14'	123(2)
C9'-C14'-C13'	120(2)
C16-C15-C20	118.4(3)
C16-C15-C1	121.8(3)
C20-C15-C1	119.8(3)
C15-C16-C17	119.7(4)
C18-C17-C16	120.6(4)
C19-C18-C17	120.2(4)
C18-C19-C20	119.4(4)
C19-C20-C15	121.6(4)
C24-C21-C22	129.0(3)
C24-C21-C1	105.4(2)
C22-C21-C1	124.5(3)
O2-C22-O3	125.3(3)
O2-C22-C21	122.8(3)
O3-C22-C21	111.8(3)
C21-C24-C25	124.1(3)
C21-C24-C8	106.7(3)
C25-C24-C8	127.8(3)
O4-C25-O5	123.6(4)
O4-C25-C24	123.2(4)
O5-C25-C24	113.1(3)
C1-O1-C8	98.2(2)
C22-O3-C23	114.8(3)
C25-O5-C26	114.0(4)

Table 5

Torsion angles (°) for the non-H atoms of Compound with esd's in parantheses

Atoms	Angle
O1A-C1A-C15A	109.3(3)
O1A-C1A-C2A	99.8(2)
C15A-C1A-C2A	123.2(3)
O1A-C1A-C21A	99.0(2)
C15A-C1A-C21A	117.4(3)
C2A-C1A-C21A	104.2(2)
C3A-C2A-C7A	120.4(3)
C3A-C2A-C1A	135.6(3)
C7A-C2A-C1A	103.9(3)
C2A-C3A-C4A	117.9(4)
C5A-C4A-C3A	121.1(4)
C6A-C5A-C4A	120.6(3)
C7A-C6A-C5A	118.1(4)
C6A-C7A-C2A	121.8(3)
C6A-C7A-C8A	132.3(3)
C2A-C7A-C8A	105.9(2)
O1A-C8A-C9A	112.7(2)
O1A-C8A-C7A	99.4(2)
C9A-C8A-C7A	117.7(3)
O1A-C8A-C24A	99.0(2)
C10A-C9A-C8A	120.6(3)
C11A-C10A-C9A	119.8(3)
C12A-C11A-C10A	121.1(4)
C13A-C12A-C11A	119.3(4)
C12A-C13A-C14A	121.0(4)
C9A-C14A-C13A	119.8(4)
C16B-C15A-C20A	99.1(12)
C20B-C15A-C20A	36.5(11)
C16B-C15A-C16A	42.5(13)
C20B-C15A-C16A	105.0(10)
C20A-C15A-C16A	118.1(4)
C16B-C15A-C1A	125.8(12)

Atoms	Angle
C20B-C15A-C1A	120.2(9)
C20A-C15A-C1A	118.5(3)
C16A-C15A-C1A	123.3(4)
C15A-C16A-C17A	119.7(6)
C18A-C17A-C16A	122.4(8)
C17A-C18A-C19A	119.1(13)
C20A-C19A-C18A	118.5(10)
C19A-C20A-C15A	122.2(5)
C9A-C8A-C24A	120.1(2)
C7A-C8A-C24A	104.6(2)
C14A-C9A-C10A	119.0(3)
C14A-C9A-C8A	120.3(3)
C15A-C16B-C17B	125(3)
C16B-C17B-C18B	114(3)
C19B-C18B-C17B	120(6)
C18B-C19B-C20B	121(5)
C15A-C20B-C19B	123(2)
C24A-C21A-C22A	124.4(3)
C24A-C21A-C1A	106.7(3)
C22A-C21A-C1A	127.3(3)
O2A-C22A-O3A	123.6(4)
O2A-C22A-C21A	122.4(4)
O3A-C22A-C21A	113.9(3)
C21A-C24A-C25A	128.2(3)
C21A-C24A-C8A	105.4(2)
C25A-C24A-C8A	125.2(3)
O4A-C25A-O5A	125.1(3)
O4A-C25A-C24A	122.5(3)
O5A-C25A-C24A	112.3(3)
C8A-O1A-C1A	97.9(2)
C22A-O3A-C23A	111.8(4)
C25A-O5A-C26A	115.9(3)

Atoms	Angle
C8-C9'-C14'-C13'	-174(2)
C12'-C13'-C14'-C9'	3(4)
O1-C1-C15-C16	11.8(4)
C2-C1-C15-C16	-104.8(4)
C21-C1-C15-C16	126.8(3)
O1-C1-C15-C20	-170.5(3)
C2-C1-C15-C20	73.0(4)
C21-C1-C15-C20	-55.4(4)
C20-C15-C16-C17	3.1(5)
C1-C15-C16-C17	-179.1(3)
C15-C16-C17-C18	-0.7(6)
C16-C17-C18-C19	-2.0(7)
C17-C18-C19-C20	2.3(6)
C18-C19-C20-C15	0.2(6)
C16-C15-C20-C19	-2.8(5)
C1-C15-C20-C19	179.3(3)
O1-C1-C21-C24	-34.8(3)
C15-C1-C21-C24	-157.6(3)
C2-C1-C21-C24	67.7(3)
O1-C1-C21-C22	156.4(3)
C15-C1-C21-C22	33.6(4)
C2-C1-C21-C22	-101.2(3)
C24-C21-C22-O2	-92.2(4)
C1-C21-C22-O2	73.9(5)
C24-C21-C22-O3	90.0(4)
C1-C21-C22-O3	-103.9(4)
C22-C21-C24-C25	2.8(5)

Atoms	Angle
C1-C21-C24-C25	-165.4(3)
C22-C21-C24-C8	170.0(3)
C1-C21-C24-C8	1.8(3)
O1-C8-C24-C21	31.2(3)
C9-C8-C24-C21	150.0(10)
C7-C8-C24-C21	-70.9(3)
C9'-C8-C24-C21	142.4(18)
O1-C8-C24-C25	-162.3(3)
C9-C8-C24-C25	-43.5(11)
C7-C8-C24-C25	95.6(4)
C9'-C8-C24-C25	-51.0(18)
C21-C24-C25-O4	-28.1(6)
C8-C24-C25-O4	167.5(4)
C21-C24-C25-O5	148.1(3)
C8-C24-C25-O5	-16.2(5)
C15-C1-O1-C8	-179.8(2)
C2-C1-O1-C8	-52.7(2)
C21-C1-O1-C8	53.5(2)
C9-C8-O1-C1	-177.5(8)
C7-C8-O1-C1	53.5(2)
C24-C8-O1-C1	-52.5(2)
C9'-C8-O1-C1	-171.9(14)
O2-C22-O3-C23	1.7(6)
C21-C22-O3-C23	179.5(4)
O4-C25-O5-C26	0.7(6)
C24-C25-O5-C26	-175.5(4)

Atoms	Angle
O1-C1-C2-C3	-149.2(3)
C15-C1-C2-C3	-25.6(5)
C21-C1-C2-C3	109.3(4)
O1-C1-C2-C7	32.2(3)
C15-C1-C2-C7	155.8(3)
C21-C1-C2-C7	-69.3(3)
C7-C2-C3-C4	-0.3(5)
C1-C2-C3-C4	-178.6(3)
C2-C3-C4-C5	1.3(5)
C3-C4-C5-C6	-0.9(6)
C4-C5-C6-C7	-0.5(6)
C5-C6-C7-C2	1.5(5)
C5-C6-C7-C8	176.8(4)
C3-C2-C7-C6	-1.2(5)
C1-C2-C7-C6	177.6(3)
C3-C2-C7-C8	-177.7(3)
C1-C2-C7-C8	1.1(3)
C6-C7-C8-O1	150.7(4)
C2-C7-C8-O1	-33.5(3)
C6-C7-C8-C9	29.7(11)
C2-C7-C8-C9	-154.4(10)
C6-C7-C8-C24	-107.8(4)
C2-C7-C8-C24	68.0(3)
C6-C7-C8-C9'	33(2)
C2-C7-C8-C9'	-152(2)
O1-C8-C9-C10	-115.9(18)
C7-C8-C9-C10	0(2)

Atoms	Angle
C24-C8-C9-C10	131.6(16)
C9'-C8-C9-C10	-163(19)
O1-C8-C9-C14	77.3(15)
C7-C8-C9-C14	-167.0(10)
C24-C8-C9-C14	-35.3(19)
C9'-C8-C9-C14	30(16)
C14-C9-C10-C11	-9(2)
C8-C9-C10-C11	-176.1(14)
C9-C10-C11-C12	-5(2)
C10-C11-C12-C13	12(2)
C11-C12-C13-C14	-4.7(17)
C12-C13-C14-C9	-10.1(17)
C10-C9-C14-C13	16(2)
C8-C9-C14-C13	-174.9(12)
O1-C8-C9'-C14'	56(4)
C9-C8-C9'-C14'	-169(20)
C7-C8-C9'-C14'	172(2)
C24-C8-C9'-C14'	-51(4)
O1-C8-C9'-C10'	-91(3)
C9-C8-C9'-C10'	44(15)
C7-C8-C9'-C10'	25(4)
C24-C8-C9'-C10'	162(2)
C14'-C9'-C10'-C11'	30(4)
C8-C9'-C10'-C11'	179(2)
C9'-C10'-C11'-C12'	-9(3)
C10'-C11'-C12'-C13'	-14(3)
C11'-C12'-C13'-C14'	19(4)

Table 5 Contd…

Torsion angles (°) for the non-H atoms of Compound with esd's in parantheses

Table 5 Contd…

Torsion angles (°) for the non-H atoms of Compound with esd's in parantheses

Atoms	Angle
O1A-C1A-C2A-C3A	-148.7(4)
C15A-C1A-C2A-C3A	-27.9(6)
C21A-C1A-C2A-C3A	109.3(4)
O1A-C1A-C2A-C7A	34.1(3)
C15A-C1A-C2A-C7A	155.0(3)
C21A-C1A-C2A-C7A	-67.8(3)
C7A-C2A-C3A-C4A	-0.3(5)
C1A-C2A-C3A-C4A	-177.1(4)
C2A-C3A-C4A-C5A	0.9(6)
C3A-C4A-C5A-C6A	0.1(6)
C4A-C5A-C6A-C7A	-1.7(5)
C5A-C6A-C7A-C2A	2.3(5)
C5A-C6A-C7A-C8A	179.1(3)
C3A-C2A-C7A-C6A	-1.3(5)
C1A-C2A-C7A-C6A	176.4(3)
C3A-C2A-C7A-C8A	-178.8(3)
C1A-C2A-C7A-C8A	-1.2(3)
C6A-C7A-C8A-O1A	150.4(3)
C2A-C7A-C8A-O1A	-32.4(3)
C6A-C7A-C8A-C9A	28.5(5)
C2A-C7A-C8A-C9A	-154.3(3)
C6A-C7A-C8A-C24A	-107.6(4)
C2A-C7A-C8A-C24A	69.6(3)
O1A-C8A-C9A-C14A	171.6(3)
C7A-C8A-C9A-C14A	-73.6(4)
C24A-C8A-C9A-C14A	55.6(4)
O1A-C8A-C9A-C10A	-11.3(4)

Atoms	Angle
C24A-C8A-C9A-C10A	-127.3(3)
C14A-C9A-C10A-C11A	-1.3(5)
C8A-C9A-C10A-C11A	-178.5(3)
C9A-C10A-C11A-C12A	1.2(6)
C10A-C11A-C12A-C13A	-0.6(7)
C11A-C12A-C13A-C14A	0.0(7)
C10A-C9A-C14A-C13A	0.8(6)
C8A-C9A-C14A-C13A	177.9(3)
C12A-C13A-C14A-C9A	-0.2(6)
O1A-C1A-C15A-C16B	158.2(18)
C2A-C1A-C15A-C16B	41.8(18)
C21A-C1A-C15A-C16B	-90.3(18)
O1A-C1A-C15A-C20B	-31.8(16)
C2A-C1A-C15A-C20B	-148.2(15)
C21A-C1A-C15A-C20B	79.7(16)
O1A-C1A-C15A-C20A	-73.8(5)
C2A-C1A-C15A-C20A	169.8(5)
C21A-C1A-C15A-C20A	37.7(6)
O1A-C1A-C15A-C16A	106.0(6)
C2A-C1A-C15A-C16A	-10.4(8)
C21A-C1A-C15A-C16A	-142.5(6)
C16B-C15A-C16A-C17A	73.2(18)
C20B-C15A-C16A-C17A	-35.1(16)
C20A-C15A-C16A-C17A	1.7(12)
C1A-C15A-C16A-C17A	-178.1(7)
C15A-C16A-C17A-C18A	0.6(19)
C16A-C17A-C18A-C19A	-2(3)

Table 5 Contd…

Torsion angles (°) for the non-H atoms of Compound with esd's in parantheses

Atoms	Angle
C18A-C19A-C20A-C15A	1.4(16)
C16B-C15A-C20A-C19A	-43.2(16)
C20B-C15A-C20A-C19A	74.0(17)
C16A-C15A-C20A-C19A	-2.7(11)
C1A-C15A-C20A-C19A	177.2(7)
C20B-C15A-C16B-C17B	10(3)
C20A-C15A-C16B-C17B	45(3)
C16A-C15A-C16B-C17B	-77(3)
C1A-C15A-C16B-C17B	-180(2)
C15A-C16B-C17B-C18B	-16(5)
C16B-C17B-C18B-C19B	20(7)
C17B-C18B-C19B-C20B	-18(7)
C16B-C15A-C20B-C19B	-6(3)
C20A-C15A-C20B-C19B	-79(3)
C16A-C15A-C20B-C19B	38(3)
C1A-C15A-C20B-C19B	-177(2)
C18B-C19B-C20B-C15A	11(5)
O1A-C1A-C21A-C24A	-30.9(3)
C15A-C1A-C21A-C24A	-148.1(3)
C2A-C1A-C21A-C24A	71.7(3)
O1A-C1A-C21A-C22A	163.2(3)
C15A-C1A-C21A-C22A	45.9(5)
C2A-C1A-C21A-C22A	-94.2(4)
C24A-C21A-C22A-O2A	28.5(6)
C1A-C21A-C22A-O2A	-167.9(4)
C24A-C21A-C22A-O3A	-148.0(3)

Atoms	Angle
C1A-C21A-C22A-O3A	15.6(5)
C22A-C21A-C24A-C25A	-3.7(5)
C1A-C21A-C24A-C25A	-170.1(3)
C22A-C21A-C24A-C8A	164.2(3)
C1A-C21A-C24A-C8A	-2.2(3)
O1A-C8A-C24A-C21A	34.9(3)
C9A-C8A-C24A-C21A	157.8(3)
C7A-C8A-C24A-C21A	-67.4(3)
O1A-C8A-C24A-C25A	-156.8(3)
C9A-C8A-C24A-C25A	-33.8(4)
C7A-C8A-C24A-C25A	101.0(3)
C21A-C24A-C25A-O4A	92.4(4)
C8A-C24A-C25A-O4A	-73.2(5)
C21A-C24A-C25A-O5A	-89.5(4)
C8A-C24A-C25A-O5A	104.9(4)
C9A-C8A-O1A-C1A	178.6(2)
C7A-C8A-O1A-C1A	53.2(3)
C24A-C8A-O1A-C1A	-53.3(2)
C15A-C1A-O1A-C8A	175.1(2)
C2A-C1A-O1A-C8A	-54.4(2)
C21A-C1A-O1A-C8A	51.8(2)
O2A-C22A-O3A-C23A	-0.4(6)
C21A-C22A-O3A-C23A	176.1(4)
O4A-C25A-O5A-C26A	-0.8(6)
C24A-C25A-O5A-C26A	-178.9(4)

Table 5 Contd…

Torsion angles (°) for the non-H atoms of Compound with esd's in parantheses

Table 6

Atomic coordinates (x 10^4) and their isotropic displacement parameters (Å^2 x 10^3) involving H atoms of Compound

Atoms	X	Y	Z	U(eq)
H3	5555	3967	2291	51
H4	4506	2098	2449	69
H5	3817	744	1937	81
H6	4110	1219	1243	71
H10	3788	2681	708	100
H11	3252	2586	46	124
H12	3903	3762	-481	106
H13	5357	4319	-420	95
H14	5994	3906	209	81
H10'	3791	3845	769	89
H11'	3079	3981	120	104
H12'	3983	4170	-474	108
H13'	5249	5130	-361	97
H14'	5924	4746	257	82
H16	5687	7935	1367	67
H17	6216	10146	1719	86
H18	7213	9826	2232	81
H19	7637	7297	2427	72
H20	7126	5100	2078	61
H23A	9072	4153	1678	175
H23B	9448	4377	1232	175
H23C	9177	2667	1384	175
H26A	6716	-905	267	186
H26B	5844	-1702	379	186
H26C	6589	-1714	701	186
H3A	3668	-3643	1241	76
H4A	3967	-4138	1940	90

Table 6

Atomic coordinates (x 10^4) and their isotropic displacement parameters (Å^2 x 10^3) involving H atoms of Compound

Atoms	X	Y	Z	U(eq)
H5A	3230	-2835	2454	76
H6A	2169	-1022	2289	58
H10A	2094	2969	1365	65
H11A	1655	5196	1727	81
H12A	728	4959	2274	80
H13A	215	2494	2450	82
H14A	624	226	2088	68
H16A	3983	-1902	732	112
H17A	4603	-1747	85	135
H18A	3855	-1050	-478	116
H19A	2375	-594	-417	108
H20A	1750	-818	223	83
H16B	3350	-3389	558	108
H17B	4134	-3097	-59	112
H18B	3483	-1267	-541	112
H19B	2926	840	-285	103
H20B	2240	656	342	86
H23D	805	-6067	541	210
H23E	1679	-6902	627	210
H23F	1514	-6061	200	210
H26D	-1453	-2290	1352	158
H26E	-1689	-508	1248	158
H26F	-1314	-940	1683	158

Table 7 (For Molecule A)

Mean planes through various groups of atoms in the structure of Compound and deviations from the plane. The equation of the plane is of the form: m1x + m2y + m3z - D = 0. where m1, m2, m3 and D are constants. Starred atoms are included in the plane calculations

Plane	m1	m2	m3	D	Atom	Deviation(Å)
1	-0.683	0.729	-0.034	-3.756	C1*	0.003
					C2*	-0.006
					C7*	0.006
					C8*	-0.003
					O1	0.773
2	0.279	0.701	-0.656	2.419	C1*	0.006
					C21*	0.011
					C24*	-0.011
					C8*	0.006
					O1	0.778
3	-0.242	0.871	-0.425	-1.367	C1	0.566
					C2*	-0.294
					C7*	-0.279
					C8	0.572
					C24*	-0.288
					C21*	-0.275
4	0.271	-0.950	-0.148	-0.886	C9*	-0.077
					C10*	0.009
					C11*	0.065
					C12*	-0.067
					C13*	-0.009
					C14*	0.079
5	0.749	0.077	-0.657	4.355	C15*	0.019
					C16*	-0.012
					C17*	-0.005
					C18*	0.015
					C19*	-0.007
					C20*	-0.009

Dihedral angles (º) formed by LSQ-planes with esd's in parantheses

Plane	Plane	Angle
1	2	69.6(1)
3	5	80.5(1)

Table 7 (For Molecule B)

Mean planes through various groups of atoms in the structure of Compound and deviations from the plane. The equation of the plane is of the form: m1x + m2y + m3z - D = 0. where m1, m2, m3 and D are constants. Starred atoms are included in the plane calculations

Plane	m1	m2	m3	D	Atom	Deviation(Å)
1	0.678	0.733	-0.028	1.595	C1A*	-0.004
					C2A*	0.006
					C7A*	-0.006
					C8A*	0.004
					O1A	0.782
2	-0.283	0.702	-0.652	-3.875	C1A*	0.008
					C21A*	-0.013
					C24A*	0.013
					C8A*	-0.007
					O1A	0.776
3	0.239	0.875	-0.418	-1.977	C1A	0.573
					C2A*	-0.278
					C7A*	-0.292
					C8A	0.564
					C24A*	-0.273
					C21A*	-0.293
4	-0.766	0.128	-0.628	-4.961	C9A*	0.005
					C10A*	-0.006
					C11A*	0.003
					C12A*	0.000
					C13A*	-0.000
					C14A	-0.002
5	-0.182	-0.970	-0.154	0.014	C15A*	-0.013
					C16A*	0.000
					C17A*	0.012
					C18A*	-0.011
					C19A*	0.001
					C20A*	0.013

Dihedral angles (º) formed by LSQ-planes with esd's in parantheses

Plane	Plane	Angle
1	2	70.1(1)
3	4	78.9(1)

Table 8

Hydrogen bondings and non - bonded interactions [Å and °] for Compound

D-H…A	D-H	H…A	D…A	D-H…A
C20- H20… O2	0.93	2.58	3.34(4)	139
C12-H12…O4[i]	0.93	2.54	3.39(1)	137
C18A-H18A…O2A[ii]	0.93	2.56	3.29(2)	136
C26A-H26E…O4[iii]	0.96	2.58	3.54(5)	172
C4-H4…Cg [iv]	0.93	2.87	3.68(1)	146

Symmetry codes:

(i) -1/2+x, 1/2-y, -z

(ii) 1/2+x, -1/2-y, -z

(iii) -1+x, y, z

(iv) −x+1, y−1/2, −z+1/2

9(a)

Ring Puckering amplitudes and asymmetry parameters for compound **(Molecule A)**

Ring	Total Puckering amplitudes (Å)	Asymmetry Parameters(°)	Conformation
C1		DS(C1)=0.266 D2(C1)=0.258	
C2		DS(C2)=0.423 D2(C2)=0.094	
C7	q_2 = 0.537(1)	DS(C7)=0.418 D2(C7)=0.106	Envelope
C8		DS(C8)=0.253 D2(C8)=0.265	
O1		DS(O1)=0.008 D2(O1)=0.322	

Table 9(ba)

Ring Puckering amplitudes and asymmetry parameters for compound **(Molecule A)**

Ring	Total Puckering amplitudes (Å)	Asymmetry Parameters (°)	Conformation
C1		DS(C1)=0.249 D2(C1)=0.2699	
C21		DS(C21)=0.419 D2(C21)=0.112	
C24	q_2 = 0.542(1)	DS(C24)=0.428 D2(C24)=0.089	Envelope
C8		DS(C8)=0.275 D2(C8)=0.257	
O1		DS(O1)=0.016 D2(O1)=0.325	

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