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X-ray structure determination of 8-quinoly-l-1,4-butane diether

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Abstract

The title compound 8-quinolyl-1,4-butane diether have been synthesized and prepared crystal. Crystal structure of compound characterized on an four-circle diffractometer. Data of crystallography: a=9.658(1)Å, b=9.810(2)Å, c=11.311(2)Å, α=86.63(1)°, β=68.12(1)°, γ=63.94(1)°. Crystalis triclinic system, space group P-T, V=886.3(2)Å^3, Z=2, Dc=1.30g/cm^3, Mr=344.4, R=0.043. Crystal structure were solved by direct methods (MITHRIL Program).

Keywords

8-quinolyl-1,4-butane diether; Crystal structure.

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INTRODUCTION

A single crystal with dimension 0.28×0.30×0.50nm was sealed in a Lindemann glass capillary. The crystal data were collected at 21±1.5° on an R3M/E four-circle diffractometer with graphite monochromatized M_o-K_α radiation (λ=0.71073 Å), using a ω/2θ scan. Details of the data collection and processing are presented in TABLE 1. The six standard reflections monitored periodically during data collections show the variation of intensities less than 1.5%. Range of Miller indices: h, 0 to 11; h, -11 to 11; and l, -13 to 13.

Crystal stability was monitored by recording two check reflections at intervals of 98. No significant variation in the intensity of these monitoring reflections was observed during data collection. The intensities were corrected for polarization effects but not absorptions.

STRUCTURE ANALYSIS AND REFINEMENT

The positional coordinates of the non-H atoms were refined by the full matric least squares and direct methodÿ first with isotropic and then with anisotropic thermal parameters. All the H atoms were located from successive difference Fourier syntheses. The positions of the H atoms were refined with fixed isotropic thermal parameters. The weight scheme was $\omega=[\acute{a}^2(F)+0.00010F^2]^{-1}\times\{1-\exp[-5(\sin\theta/n)^2]\}$. In a final difference Fourier map the maximum and minimum peaks observed were performed on an Eclipse/s 140 computer with SHELXTL program. Final atomic coordinates are given in TABLE 2.

The torsion angles in the chain of 8-quinolyl-1,4-butane diether are listed in TABLE 3. In the present molecule, the torsion angles of C(9)-O(1)-C(10)-C(11), C(20)-O(2)-C(21)-C(22), O(1)-C(10)-C(11)-C(11a) and O(2)-C(21)-C(22)-C(22a) are close to 180° and ±60°,

which are the stabilization conformation of trans and qauche.

TABLE 1 : Crystallographic data for 8-quinolyl-1,4-butane diether

Chemical formula	$C_{22}H_{20}N_2O_2$	Number of reflections collected	2542
Formula Weight	344.4	Number of reflections for refinement	2527
Crystal system	anorthic	Observed data[I> 1.5σ(I)]	1939
Space group	P-T	Revised parameter	316
a (Å)	9.658(1)	R	0.0431
B (Å)	9.810(2)	R_w	0.0383
c (Å)	11.311(2)	S	1.112
A(°)	86.63(1)	Δe_{max}(e/ Å^3)	0.266
B(°)	68.12(1)	Δe_{min}(e/ Å^3)	-0.248
γ(°)	83.94(1)	Exponential range	
V (Å^3)	886.3(2)	h: 0 —+ 11	
Z	2	h: -11 —+ 11	
M(cm^{-1})	0.90	l: -13 —+ 13	
Dc g/cm^3	1.30		
F(000)	368		

TABLE 2 : Non-hydrogen atomic coordinates (×10^4) and isotropic thermal parameters (Å^2×10^3)

Atom	x	y	z	u
N(1)	7204(2)	3515(2)	9161(2)	50(1)
N(2)	2818(2)	5844(2)	6834(2)	61(1)
O(1)	7330(2)	7811(1)	8945(1)	56(1)
O(2)	1008(2)	7197(2)	6450(1)	75(1)
C(1)	8733(2)	2266(2)	8781(2)	43(1)
C(2)	7162(3)	4867(2)	9234(2)	62(1)
C(3)	8575(4)	5095(3)	8957(2)	69(2)
C(4)	10092(3)	3861(3)	8573(2)	63(1)
C(5)	10237(3)	2386(2)	8466(2)	49(1)
C(6)	11774(3)	1035(3)	8059(2)	64(1)
C(7)	11804(3)	-340(3)	7979(2)	67(1)
C(8)	10330(3)	-478(2)	8270(2)	57(1)
C(9)	8829(2)	79(2)	8666(2)	46(1)
C(10)	7337(3)	-672(2)	8915(2)	55(1)
C(11)	5547(3)	-382(2)	9316(2)	57(1)
C(12)	2931(2)	4953(2)	5893(2)	50(1)
C(13)	3748(3)	5162(3)	7499(3)	71(1)
C(14)	4799(3)	3601(3)	7323(3)	78(2)
C(15)	4899(3)	2719(3)	6408(3)	75(1)
C(16)	3961(3)	3360(2)	5641(2)	60(1)
C(17)	4027(4)	2500(3)	4650(3)	83(2)
C(18)	3123(4)	3210(4)	3943(3)	92(2)
C(19)	2079(4)	4794(4)	4180(3)	79(2)
C(20)	1976(3)	5656(3)	5138(2)	60(1)
C(21)	229(3)	8004(3)	4593(2)	83(1)
C(22)	-598(3)	9674(3)	5049(3)	83(2)

TABLE 3 : The bond distance of compound for 8-quinolyl-1,4-butane diether

Atom 1	Atom 2	Bond Distance(Å)	Atom 1	Atom 2	Bond Distance(Å)
N(1)	C(1)	1.336(2)	N(1)	C(2)	1.315(3)
N(2)	C(12)	1.359(2)	N(2)	C(13)	1.318(4)
O(1)	C(19)	1.367(3)	O(1)	C(10)	1.425(3)
O(2)	C(20)	1.363(2)	O(2)	C(21)	1.437(3)
C(1)	C(5)	1.418(4)	C(1)	C(2)	1.419(3)
C(2)	C(13)	1.398(5)	C(3)	C(4)	1.352(3)
C(4)	C(5)	1.399(4)	C(5)	C(6)	1.416(9)
C(6)	C(7)	1.344(4)	C(7)	C(8)	1.403(2)
C(8)	C(9)	1.359(2)	C(10)	C(11)	1.507(4)
C(11)	C(11a)	1.515(4)	C(12)	C(16)	1.410(3)
C(12)	C(20)	1.419(4)	C(13)	C(14)	1.391(3)
C(14)	C(15)	1.337(5)	C(15)	C(16)	1.411(4)
C(16)	C(13)	1.407(4)	C(13)	C(18)	1.345(6)
C(18)	C(19)	1.405(4)	C(19)	C(20)	1.361(5)
C(21)	C(22)	1.493(4)	C(22)	C(22a)	1.518(7)

TABLE 4 : The bond angles of compound for 8-quinolyl-1,4-butane diether

Atom 1	Atom 2	Atom 3	Angle (°)	Atom 1	Atom 2	Atom 3	Angle (°)
C(1)	N(1)	C(2)	117.4(2)	C(12)	N(2)	C(13)	117.1
C(9)	O(1)	C(10)	117.3(1)	C(20)	O(2)	C(21)	117.5
N(1)	C(1)	C(5)	122.6(2)	N(1)	C(1)	C(9)	118.9
C(5)	C(1)	C(9)	118.6(2)	N(1)	C(2)	C(3)	124.1
C(2)	C(3)	C(4)	118.7(3)	C(3)	C(4)	C(5)	120.5
C(1)	C(5)	C(4)	116.8(2)	C(1)	C(5)	C(6)	119.2
C(4)	C(5)	C(6)	124.2	C(5)	C(6)	C(7)	120.4
C(6)	C(7)	C(8)	121.3(2)	C(7)	C(8)	C(9)	120.1
O(1)	C(9)	C(1)	114.8	O(1)	C(9)	C(8)	124.5
C(1)	C(9)	C(8)	120.7(2)	O(1)	C(10)	C(11)	107.2
C(10)	C(11)	C(11a)	113.5	N(2)	C(12)	C(16)	122.4
N(2)	C(12)	C(20)	118.6	C(16)	C(12)	C(20)	119.0
N(2)	C(13)	C(14)	124.6	C(13)	C(14)	C(15)	118.4
C(14)	C(15)	C(16)	120.6	C(12)	C(16)	C(15)	116.8
C(12)	C(16)	C(13)	119.7	C(15)	C(16)	C(17)	123.5
C(16)	C(17)	C(18)	119.6	C(13)	C(18)	C(19)	121.7
C(18)	C(19)	C(20)	120.1	O(2)	C(20)	C(12)	115.2
O(2)	C(20)	C(19)	124.9	C(12)	C(20)	C(19)	119.8
O(2)	C(21)	C(22)	107.7	C(21)	C(22)	C(22a)	114.5

The torsion angle data was listed in TABLE 5. From the data can be seen, the torsion angle of C-C-C-C and C-O-C-C approach ±60°or ±180°. This belongs to the unstable conformation of the trans-cross type and cross type [3]. The space effect makes repulsion lessen.

TABLE 5 : The torsion angles of compound for 8-quinolyl-1,4-butane diether

C(1)-N(1)-C(2)-C(3)	-0.5(4)
C(12)-N(2)-C(13)-C(14)	-1.4(4)
C(9)-O(1)-C(10)-C(11)	177.3(2)
C(20)-O(2)-C(21)-C(22)	173.8(2)
C(2)-C(3)-C(4)-C(5)	-0.5(4)
C(13)-C(14)-C(15)-C(16)	0.1(4)
C(3)-C(4)-C(5)-C(6)	179.2(2)
C(14)-C(15)-C(164)-C(17)	179.0(3)
C(4)-C(5)-C(6)-C(7)	-179.8(2)
C(15)-C(16)-C(17)-C(18)	-178.3(3)
C(6)-C(7)-C(8)-C(9)	-1.3(4)
C(17)-C(18)-C(19)-C(20)	0.7(5)
C(10)-O(1)-C(9)-C(8)	5.2(3)
C(10)-O(2)-C(20)-C(19)	-9.6(4)
N(1)-C(2)-C(3)-C(4)	0.9(4)
N(2)-C(13)-C(14)-C(15)	0.7(5)
C(5)-C(6)-C(7)-C(8)	1.3(4)
C(16)-C(17)-C(18)-C(19)	-1.2(5)
C(7)-C(8)-C(9)-O(1)	178.5(2)
C(18)-C(19)-C(20)-O(2)	180.0(3)
O(1)-C(10)-C(11)-C(11a)	-63.9(3)
O(2)-C(21)-C(22)-C(22a)	66.0(4)

RESULTS AND DISCUSSION

The molecular structure of 8-quinolyl-1,4-butane diether is shown in Figure 1, the selected parameters in TABLE 3 and TABLE 4, the unitary molecular packing arrangement in the unit cell in Figure 2.

Single 8-quinolyl-1,4-butane diether molecular is symceter ones consisting of two 2-quinolineoxy on the two ends of butane. $[(8\text{-quinolyl-1,4-butane diether})_4]_n$ is one of supermolecular compound. On unitary molecular $(8\text{-quinolyl-1,4-butane diether})_4$, two parallel moleculars 8-quinolyl-1,4-butane diether are

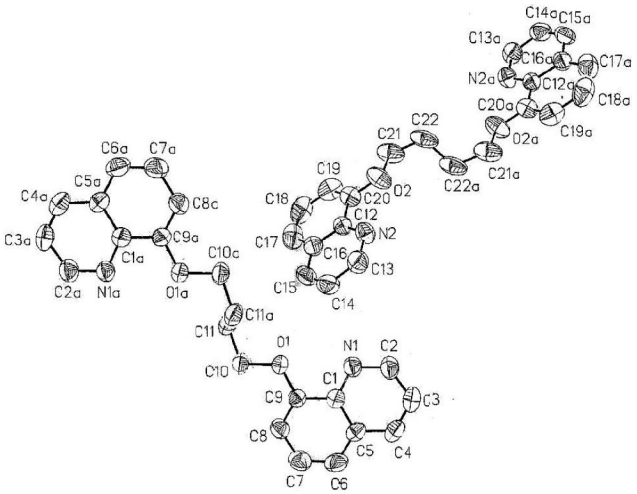

Figure 1 : The complexes perspective of molecular structure

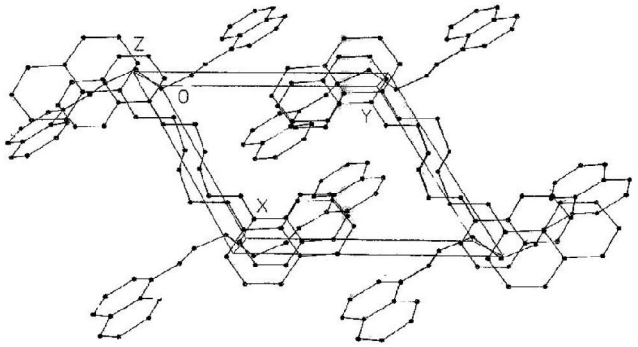

Figure 2 : The molecules accumulation in crystal cell

crisscross bonded together with hydrogen bonds of four equal bonds energy (action pattern is $O_1\cdots\cdots H_{11}—C_{11}$, second atoms generated by transformation 1-x, 0-y, 2-z), in addition to two moleculars 8-quinolyl-1,4-butane diether bonded together with dipole-dipole chemical force (action pattern is $N_2\cdots\cdots H_8—C_8$ and $N_{2a}\cdots\cdots H_{8a}—C_{8a}$, second atoms generated by transformation 1+x, y-1, z), and then N_2 and N_{1a}, N_1 and N_{2a} get together. In a word, weak Vander waals force between unitary molecular $(8\text{-quinolyl-1,4-butane diether})_4$ linked and formed supermolecular compound. $[(8\text{-quinolyl-1,4-butane diether})_4]_n$.

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