Crystal Structure of 2-(2-Pyridyl)-1,3-bis(2-pyridylmethyl)tetrahydropyrimidine

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The ruthenium(VI) complex with *N,N'*-dimethyl-*N,N'*-bis(2-pyridylmethyl)propylenediamine has been investigated electrochemically.¹ The analogous ligand *N,N'*-bis(2-pyridylmethyl)propylenediamine, which was prepared according to a literature method¹, formed complexes with various transition metal ions. In the course of the complex formation researches, a water-insoluble and non-complex forming white product was obtained. Since this product gave colorless prismatic single crystals in an *N,N'*-bis(2-pyridylmethyl)propylenediamine solution, the crystal structure was determined.

The X-ray reflections were collected using a Rigaku AFC7R diffractometer. The single-crystal structure solution was carried out using the program SHELXS86. All non-hydrogen atoms were anisotropically refined, and all hydrogen atoms were isotropically refined. Table 1 summarizes the crystal data. The chemical structure of the title compound is illustrated in Fig. 1. Figures 2 and 3 show the labeling and the packing diagrams of the compound. The atomic coordinates and thermal parameters are presented in Table 2. The bond lengths and angles are presented in Table 3.

The product was a diazacrown ether formed by a

Fig. 1 Chemical structure.

Fig. 2 ORTEP drawing with the atom numbering.

Table 1 Crystal and experimental data

Formula: C ₂₁ H ₂₃ N ₅	
Formula weight=345.45	
Crystal size=0.60×0.20×0.20 mm	
Crystal color: colorless	
Crystal system: triclinic	
Space group: <i>P</i> $\bar{1}$	<i>Z</i> =2
<i>a</i> =10.738(1) Å	α =98.614(10)°
<i>b</i> =14.697(1)	β =103.69(1)
<i>c</i> =6.233(1)	γ =89.813(9)
<i>V</i> =944.5(2) Å ³	
<i>D_x</i> =1.215 g/cm ³	
Radiation: graphite monochromated Cu K α	
μ for Cu K α radiation=5.86 cm ⁻¹	
2 θ range: 0° through 120.1°	
<i>R</i> =0.039	<i>R_w</i> =0.053
No. of reflections measured=2969	
No. of reflections used=2409	
Measurement: Rigaku AFC7R	
Program system: TEXSAN	
Structure determination: direct method	
Refinement: full matrix least-squares	

reaction in which a couple of secondary amines in *N,N'*-bis(2-pyridylmethyl)propylenediamine reacted with the aldehyde group of pyridine-2-aldehyde. This ether was used as the starting material for *N,N'*-bis(2-pyridylmethyl)propylenediamine. The compound 2-(2-pyridyl)-1,3-bis(2-pyridylmethyl)tetrahydropyrimidine has not been reported. The nitrogen atoms of pyridyl and amino groups could not coordinate to metal ions owing to the formation of tetrahydropyrimidine.

We wish to thank Dr. Genta Sakane, Okayama University of Science, for his helpful advice. We also thank Mr. Takaomi Akamatsu and Mr. Kenji Kohara, Okayama University of Science, for their assistance with the X-ray measurements.

Fig. 3 View of the molecular packings.

Table 2 Atomic coordinates and thermal parameters

Atom	x	y	z	$B_{eq}/\text{\AA}^2$
N1	0.8109(1)	0.37748(8)	0.1561(2)	3.74(3)
N2	0.9405(1)	0.24564(7)	0.2216(2)	3.38(3)
N3	1.1369(1)	0.05149(8)	0.2322(2)	4.24(3)
N4	0.6825(1)	0.57497(9)	0.0082(2)	4.87(3)
N5	0.6264(1)	0.17901(8)	-0.0179(2)	4.15(3)
C1	0.8198(1)	0.27766(9)	0.0944(2)	3.28(3)
C2	0.9213(2)	0.4279(1)	0.1253(3)	4.65(4)
C3	1.0439(2)	0.3962(1)	0.2606(4)	4.91(4)
C4	1.0524(2)	0.2947(1)	0.1926(3)	4.37(4)
C5	0.9528(2)	0.14685(10)	0.1545(2)	3.73(3)
C6	1.0564(1)	0.10685(9)	0.3184(2)	3.37(3)
C7	1.0635(2)	0.1235(1)	0.5449(3)	4.27(4)
C8	1.1533(2)	0.0802(1)	0.6876(3)	4.73(4)
C9	1.2344(2)	0.0213(1)	0.6000(3)	4.43(4)
C10	1.2235(2)	0.0096(1)	0.3742(3)	4.60(4)
C11	0.6923(2)	0.4116(1)	0.0263(3)	4.27(4)
C12	0.6708(1)	0.5081(1)	0.1267(3)	3.95(3)
C13	0.6432(2)	0.5267(1)	0.3336(3)	5.00(4)
C14	0.6300(2)	0.6164(1)	0.4249(3)	5.75(5)
C15	0.6441(2)	0.6853(1)	0.3065(4)	5.55(5)
C16	0.6695(2)	0.6615(1)	0.1094(4)	5.56(5)
C17	0.7090(1)	0.23000(9)	0.1495(2)	3.26(3)
C18	0.6964(2)	0.2414(1)	0.3680(3)	4.24(4)
C19	0.5954(2)	0.1993(1)	0.4164(3)	5.32(5)
C20	0.5082(2)	0.1482(1)	0.2458(4)	5.78(5)
C21	0.5273(2)	0.1391(1)	0.0338(4)	5.37(4)

$$B_{eq} = (4/3) \sum_i \sum_j \beta_{ij} (a_i \cdot a_j).$$

Table 3 Bond lengths ($\text{\AA}$) and bond angles ($^\circ$)

N1 - C1	1.469(2)	N1 - C2	1.465(2)
N1 - C11	1.469(2)	N2 - C1	1.467(2)
N2 - C4	1.464(2)	N2 - C5	1.464(2)
N3 - C6	1.335(2)	N3 - C10	1.340(2)
N4 - C12	1.338(2)	N4 - C16	1.340(2)
N5 - C17	1.330(2)	N5 - C21	1.343(2)
C1 - C17	1.515(2)	C2 - C3	1.500(2)
C3 - C4	1.497(2)	C5 - C6	1.505(2)
C6 - C7	1.381(2)	C7 - C8	1.373(2)
C8 - C9	1.372(2)	C9 - C10	1.369(3)
C11 - C12	1.502(2)	C12 - C13	1.379(2)
C13 - C14	1.377(3)	C14 - C15	1.367(3)
C15 - C16	1.361(3)	C17 - C18	1.386(2)
C18 - C19	1.366(2)	C19 - C20	1.366(3)
C20 - C21	1.372(3)		
C1 - N1 - C2	111.6(1)	C1 - N1 - C11	111.4(1)
C2 - N1 - C11	109.3(1)	C1 - N2 - C4	112.1(1)
C1 - N2 - C5	110.8(1)	C4 - N2 - C5	108.7(1)
C6 - N3 - C10	117.3(1)	C12 - N4 - C16	117.0(1)
C17 - N5 - C21	116.6(1)	N1 - C1 - N2	110.4(1)
N1 - C1 - C17	108.5(1)	N2 - C1 - C17	108.8(1)
N1 - C2 - C3	110.5(1)	C2 - C3 - C4	108.8(1)
N2 - C4 - C3	110.4(1)	N2 - C5 - C6	112.2(1)
N3 - C6 - C5	116.5(1)	N3 - C6 - C7	122.0(1)
C5 - C6 - C7	121.4(1)	C6 - C7 - C8	119.7(1)
C7 - C8 - C9	118.7(2)	C8 - C9 - C10	118.4(2)
N3 - C10 - C9	123.8(1)	N1 - C11 - C12	110.2(1)
N4 - C12 - C11	116.9(1)	N4 - C12 - C13	121.8(1)
C11 - C12 - C13	121.2(1)	C12 - C13 - C14	119.7(2)
C13 - C14 - C15	118.8(2)	C14 - C15 - C16	118.2(2)
N4 - C16 - C15	124.5(2)	N5 - C17 - C1	117.6(1)
N5 - C17 - C18	122.7(1)	C1 - C17 - C18	119.7(1)
C17 - C18 - C19	119.5(2)	C18 - C19 - C20	118.6(2)
C19 - C20 - C21	118.2(2)	N5 - C21 - C20	123.8(2)

References

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(Received June 12, 1995)

(Accepted August 3, 1995)