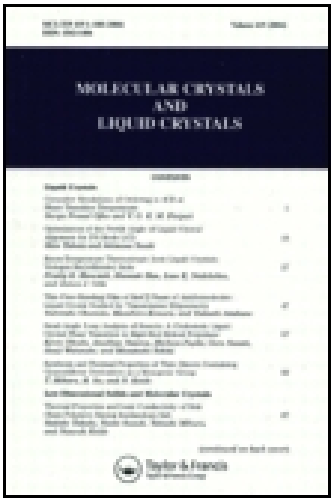

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Crystal and Molecular Structure of Imidazole Derivatives with Different Substituents

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Crystal and Molecular Structure of Imidazole Derivatives with Different Substituents

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The crystal and molecular structures of 1-Methyl-2-Isopropyl-5-Nitroimidazole (A) and 1-Methyl-2(Thiophenyl)-Methyl-5-Nitroimidazole (B) derivatives were determined by X-ray diffraction methods.

The compound A, $C_7H_{11}N_3O_2$, crystallises in the monoclinic space group $P2_1/c$ with $a = 9.9582(2)$ Å, $b = 6.5240(4)$ Å, $c = 13.5560(3)$ Å, $\beta = 99.8930(17)°$, $V = 867.6(5)$ Å^3, $Z = 4$, $D_{calc} = 1.295$ Mg/m^3, $\mu = 0.813$ mm^{-1}, $F_{000} = 360$, Cu$K\alpha = 1.5406$ Å and $R = 0.09$. The five membered ring with two nitrogen atoms is planar. Layering is observed down *a* and *b* axes.

The compound B, $C_{11}H_{11}N_3O_2S$, crystallises in the triclinic space group $P\bar{1}$ with $a = 6.270(10)$ Å, $b = 27.874(12)$ Å, $c = 12.960(3)$ Å, $\alpha = 90°$, $\beta = 89.90°$, $\gamma = 90°$, $V = 2266(35)$ Å^3, $Z = 8$, $D_{calc} = 1.461$ Mg/m^3, $\mu = 2.504$ mm^{-1}, $F_{000} = 1040$, Cu$K\alpha = 1.5406$ Å and $R = 0.11$.

Keywords: Imidazole derivatives; crystal structure

INTRODUCTION

A comprehensive monograph on imidazole and its derivatives by Hofmann [1] was published in 1953. A number of monographs on the chemistry of heterocyclic compounds [2–8] have also dealt with aspects of imidazole chemistry in a necessarily brief manner. A review of imidazole chemistry has been recently published by Grimmett [9]. Takemoto [10] has discussed hydrogen bonding and catalytic activity, while Staab and Rohr [11] have made an extensive coverage of

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the reactive and synthetically important imidazoles. There are not many studies in literature on the crystal structure of imidozole derivatives. Hence we have undertaken crystal structure studies of imidazole derivatives to get a better insight into their chemistry and their use as drugs, as antibacterial agents especially against sporogenes and histolyxicum.

A. 1-METHYL-2-ISOPROPYL-5-NITROIMIDAZOLE

Nitration of 5(4)-methyl-4(5)-nitroimidazole: Nitric acid (16 ml) was added dropwise to 4-methylimidazole (9.6 g) for 15 min whilst cooling in an ice/water bath. Sulfuric acid was added while cooling was maintained. The reaction was then heated at 55°C for 2 hours, poured on to ice (300 ml) and allowed to stand for 18 hours. The mixture was carefully neutralized to pH 8 with potassium carbonate. The aqueous solution was extracted with dichloromethane, the combined organic extracts washed with water, dried over magnesium sulfate, filtered and evaporated to dryness. A 30% yield was obtained.

2-Isopropyl, 5(4)methyl-4(5)-nitroimidazole (595 mg, 3.53 mmol) was methylated wit diazomethane (600 mg) in diethyl ether (100 ml). The solution was stirred for 6 hours. The excess diazomethane was destroyed with acetic acid which was added dropwise (till yellow colour disappeared). The solvent was evaporated to dryness to get a crude solid which was purified using column chromatography with alumina as absorbent and light petroleum: EtOAc (2:1) as eluant. 60% yield M.P. 60–61°C. NMR Result: δ_H 1.35 (6 H, d, Me_2, 2.92–3.33 (1 H,m $CHMe_2$, 3.94 (3 H, s, NMc), 7.81 (1 H, s, 4-H).

Experimental

Single crystals suitable for X-ray diffraction work were obtained by the method of slow evaporation of a mixture of chloroform and ethanol in which material was dissolved. The crystals were stable at room temperature. A crystal of dimension $0.2 \times 0.2 \times 0.3$ mm was selected for data collection. Table I lists the details of data collection, Wilson plot values [12], etc. Data were reduced using teXsan [13] data reduction program. Lorentz and polarisation corrections were applied and a semi-empirical absorption correction based on ψ-scan was applied [14]. The structure was solved by direct methods (SHELXS-97 [15]). All the non-hydrogen atoms were revealed in the first map itself. Least-squares refinement using SHELXL-97 [16] with isotropic temperature factors for all the atoms converged the residual to $R = 0.17$. Refinement of non-hydrogen atoms with ani-

sotropic thermal parameters was started at this stage. After ten cycles of refinement the residuals saturated at $R = 0.09$. The hydrogen atoms were placed at calculated positions and were not refined. The largest peak and hole in the final difference map were 0.311 and –0.237 e.Å^{-3} respectively.

TABLE I Data collections details

	Detail	*A*	*B*
1.	Crystal colour	Colourless	Colourless
2.	Diffractometer	Rigaku AFC7S	Rigaku AFC7S
3.	Wavelengh (Å)	Cu$K\alpha$	Cu$K\alpha$
4.	Monochromator	Graphite	Graphite
5.	Reflections for determining cell parameters	24	16
6.	2θ range for(5)	30° – 50°	32° – 48°
7.	$2\theta_{max}$ for data collection	140°	140°
8.	Scan method	ω-2θ method	ω-2θ method
9.	Unique/Total reflections	966/1161	8339/9193
10.	Reflections with $I \geq 2\sigma(I)$	769	3039
11.	R_{int}	0.0480	0.0255
12.	Wilson plot		
	Temperature factor, B Å^2	6.01	5.27
	Scale factor, K	4.65	2.056

Results and Discussion

The final positional coordinates of all the atoms with equivalent isotropic thermal parameters, bond distances and bond angles for non-hydrogen atoms are given in tables II–IV. The bond distances and bond angles are in good agreement with the standard values. Figure 1 represents the ORTEP [17] of the molecule at 50% probability. There are four molecules in the unit cell. Figure 2 shows packing of the molecules down *a*. Layering of the molecules is observed along both *a* and *b* axes. Intermolecular hydrogen bond of the type CH···N is observed in the structure (see Table V).

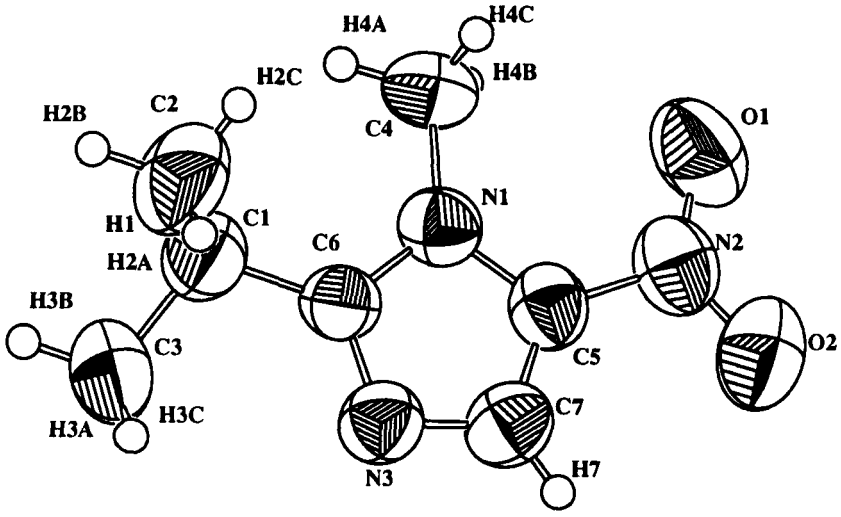

FIGURE 1 ORTEP of the molecule of compound (A)

TABLE II Atomic coordinates and equivalent thermal parameters of the non-hydrogen atoms in Å for compound A

Atom	*x*	*y*	*z*	U_{eq}
O1	0.6322(4)	0.3195(6)	0.5955(3)	0.1198(15)
O2	0.7492(3)	0.0428(6)	0.6347(3)	0.1169(14)
N1	0.3907(3)	0.0989(5)	0.6053(2)	0.0733(11)
N2	0.6397(4)	0.1386(7)	0.6176(3)	0.0892(13)
N3	0.3837(3)	–0.2210(5)	0.6608(2)	0.0787(12)
C1	0.1596(4)	–0.0452(7)	0.6146(3)	0.0875(14)
C2	0.1160(6)	0.0615(9)	0.7032(4)	0.1234(19)
C3	0.0971(5)	–0.2586(6)	0.5987(4)	0.1122(18)
C5	0.5221(3)	0.0237(7)	0.6280(3)	0.0741(13)
C4	0.3438(5)	0.3003(6)	0.5650(4)	0.0950(15)
C6	0.3101(4)	–0.0579(5)	0.6263(3)	0.0701(12)
C7	0.5144(4)	–0.1701(7)	0.6612(3)	0.0797(13)

where $U_{eq} = 1/3\pi^2 \Sigma_i \Sigma_j a_i a_j \mathrm{a}_i^* \cdot \mathrm{a}_j^*$

TABLE III Bond Lengths (Å) for compound A

Atoms	*Length*	*Atoms*	*Length*
O1-N2	1.217(5)	N3-C6	1.330(4)
O2-N2	1.244(4)	N3-C7	1.342(5)
N1-C6	1.360(4)	C1-C6	1.481(5)
N1-C5	1.383(4)	C1-C2	1.515(7)
N1-C4	1.468(5)	C1-C3	1.526(5)
N2-C5	1.417(5)	C5-C7	1.348(6)

TABLE IV Bond Angles (°) for compound A

Atoms	*Angle*	*Atoms*	*Angle*
C6-N1-C5	104.9(3)	C2-C1-C3	111.4(4)
C6-N1-C4	126.1(3)	C7-C5-N1	107.5(3)
C5-N1-C4	129.0(3)	C7-C5-N2	128.7(4)
O1-N2-O2	123.2(4)	N1-C5-N2	123.9(4)
O1-N2-C5	121.4(4)	N3-C6-N1	111.4(3)
O2-N2-C5	115.4(4)	N3-C6-C1	124.6(3)
C6-N3-C7	106.2(3)	N1-C6-C1	123.9(3)
C6-C1-C2	111.3(4)	N3-C7-C5	110.0(4)
C6-C1-C3	110.2(3)		

TABLE V Table of hydrogen bonds

Compound	*Atoms*	*Distance in A*	*Angle in (°)*	*Symmetry Code*
A	C4-H4···N3	3.397	148.38	$x, 1+y, z$
B	C2A-H2A···O2A	3.22(5)	137.01	$x, y, 1+z$
	C2B-H2B···O2B	3.24(5)	138.33	$x, y, 1+z$
	C2C-H2C···O2C	3.24(5)	136.89	$x, y, -1+z$
	C2D-H2D···O2D	3.26(5)	136.55	$x, y, -1+z$
	C9C-H92C···N2C	3.41(6)	160.62	$-1+x, y, z$
	C9D-H92D···N2D	3.43(6)	164.36	$1+x, y, z$
	C9A-H93A···N2A	3.41(6)	162.67	$-1+x, y, z$
	C9B-H93B···N2B	3.43(6)	162.71	$1+x, y, z$

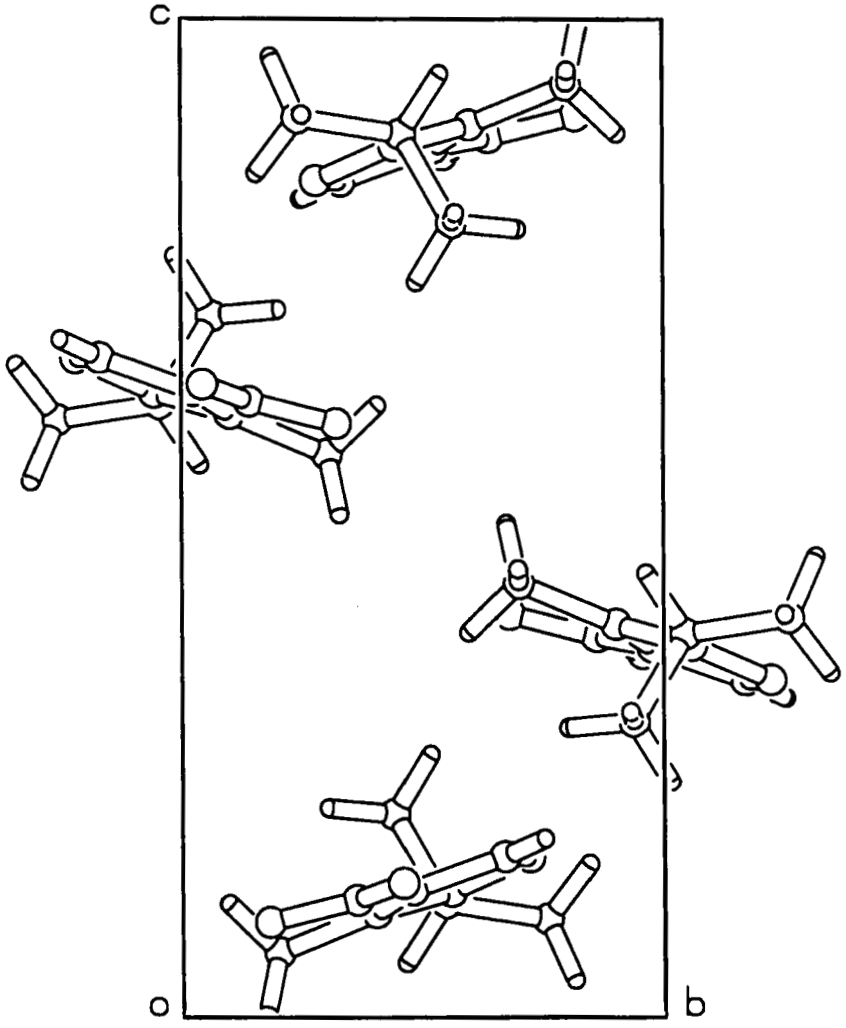

FIGURE 2 Packing of the molecules down *a* of compound (**A**)

B. 1-METHYL-2(THIOPHENYL)-METHYL-5-NITROIMIDAZOLE

5(4)-Methyl-4(5)-nitroimidazole was reacted with thiophenol in the presence of base potassiumcarbonate and refluxed to get the compound B.

Experimental

Single crystals suitable for X-ray diffraction work were obtained by the method of slow evaporation of a mixture of chloroform and ethanol in which material was dissolved. The crystals were stable at room temperature. A crystal of dimension $0.2 \times 0.2 \times 0.3$ mm was selected for data collection. Table I lists the details of data collection, Wilson plot values [12], etc. Data were reduced using teXsan [13] data reduction program. Lorentz and polarisation corrections were applied and a semi-empirical absorption correction based on ψ -scans was applied [14].

During data collection symmetry check failed for the orthorhombic system. Hence the data were collected in triclinic laue group. Solution of the structure was attempted in the orthorhombic space groups unsuccessfuly. The R_{int} values for the data set in orthorhombic, monoclinic and triclinic systems are 0.5313, 0.5287 and 0.0255 respectively. So the structure of the compound was solved in $P\bar{1}$ by direct methods (SHELXS-97 [15]) using 1548 largest E values.

All the non-hydrogen atoms were revealed in the first map itself. Least-squares refinement using SHELXL-97 [16] with isotropic temperature factors for all the atoms converged the residual to $R = 0.18$. Refinement of non-hydrogen atoms with anisotropic thermal parameters was started at this stage. After ten cycles of refinement the residuals saturated at $R = 0.11$. The hydrogen atoms were placed at calculated positions and were not refined. The largest peak and hole in the final difference map were 0.442 and -1.040 e.Å^{-3} respectively.

Results and Discussion

The final positional coordinates of all the atoms with equivalent isotropic thermal parameters, bond distances and bond angles for non-hydrogen atoms are given in tables VI–VIII. The bond distances and bond angles are in good agreement with the standard values. Figure 3 represents the ORTEP [17] of the molecule at 50% probability. Figure 4 shows packing of molecules in the unit cell down $c$axis. Intermolecular hydrogen bonds of the type CH···N and CH···O are observed in the structure (see Table V).

TABLE VI Atomic coordinates and equivalent thermal parameters of the non-hydrogen atoms in Å for compound B

Atom	*x*	*y*	*z*	U_{eq}
S1A	0.2636(4)	0.46007(8)	0.55467(14)	0.0824(7)
O1A	−0.3973(10)	0.3922(2)	0.1706(4)	0.105(2)
O2A	−0.1439(11)	0.4144(2)	0.0703(4)	0.108(2)
N1A	−0.1469(11)	0.4138(2)	0.3447(4)	0.0692(17)

Atom	*x*	*y*	*z*	U_{eq}
N2A	0.1780(12)	0.4453(3)	0.3379(5)	0.088(2)
N3A	–0.2173(12)	0.4078(2)	0.1556(5)	0.083(2)
C1A	0.2369(17)	0.4615(4)	0.9052(6)	0.108(4)
C2A	0.0679(16)	0.4421(3)	0.8515(6)	0.097(3)
C3A	0.0695(14)	0.4401(3)	0.7458(5)	0.082(2)
C4A	0.2376(14)	0.4582(3)	0.6907(5)	0.074(2)
C5A	0.4073(14)	0.4775(3)	0.7459(6)	0.086(3)
C6A	0.4027(15)	0.4793(3)	0.8519(6)	0.099(3)
C7A	0.0306(12)	0.4295(3)	0.5132(5)	0.079(2)
C8A	0.0212(14)	0.4301(3)	0.3971(5)	0.076(2)
C9A	–0.3400(15)	0.3941(4)	0.3884(6)	0.091(3)
C10A	–0.0898(13)	0.4193(3)	0.2417(5)	0.070(2)
C11A	0.1061(13)	0.4394(3)	0.2409(6)	0.085(3)
S1D	0.2361(4)	0.03993(8)	0.44535(14)	0.0830(7)
O1D	0.8983(11)	0.1082(3)	0.8304(4)	0.110(2)
O2D	0.6447(10)	0.0861(2)	0.9278(4)	0.103(2)
N1D	0.6475(11)	0.0862(2)	0.6555(4)	0.0712(18)
N2D	0.3265(11)	0.0542(2)	0.6629(4)	0.080(2)
N3D	0.7225(13)	0.0918(3)	0.8421(5)	0.086(2)
C1D	0.2652(17)	0.0384(3)	0.0958(6)	0.101(3)
C2D	0.4317(16)	0.0583(3)	0.1494(6)	0.098(3)
C3D	0.4281(15)	0.0599(3)	0.2544(5)	0.088(3)
C4D	0.2573(14)	0.0415(3)	0.3098(5)	0.073(2)
C5D	0.0912(15)	0.0221(3)	0.2550(6)	0.095(3)
C6D	0.0957(16)	0.0210(3)	0.1498(7)	0.106(3)
C7D	0.4756(15)	0.0699(3)	0.4860(5)	0.082(3)
C8D	0.4812(13)	0.0703(3)	0.6015(5)	0.070(2)
C9D	0.8410(14)	0.1056(4)	0.6110(6)	0.091(3)
C10D	0.5927(14)	0.0804(3)	0.7577(5)	0.078(2)
C11D	0.3957(14)	0.0610(3)	0.7602(5)	0.086(3)
S1C	0.5144(4)	0.21000(8)	0.94539(14)	0.0830(7)
O1C	–0.1471(10)	0.1419(3)	1.3290(4)	0.108(2)
O2C	0.1078(11)	0.1644(2)	1.4291(4)	0.108(2)
N1C	0.1028(11)	0.1641(2)	1.1552(4)	0.0719(18)
N2C	0.4260(11)	0.1955(3)	1.1625(4)	0.087(2)
N3C	0.0296(13)	0.1577(3)	1.3440(5)	0.087(2)
C1C	0.4849(17)	0.2111(3)	0.5941(6)	0.102(3)
C2C	0.3212(16)	0.1921(3)	0.6487(6)	0.097(3)
C3C	0.3205(14)	0.1899(3)	0.7556(5)	0.081(2)
C4C	0.4946(14)	0.2084(3)	0.8092(5)	0.073(2)
C5C	0.6606(14)	0.2281(3)	0.7542(6)	0.091(3)

Atom	*x*	*y*	*z*	U_{eq}
C6C	0.6546(16)	0.2290(3)	0.6483(6)	0.100(3)
C7C	0.2818(13)	0.1801(3)	0.9866(5)	0.081(2)
C8C	0.2732(14)	0.1803(3)	1.1021(5)	0.074(2)
C9C	−0.0907(15)	0.1448(3)	1.1119(5)	0.092(3)
C10C	0.1591(14)	0.1693(3)	1.2581(5)	0.076(2)
C11C	0.3544(14)	0.1888(3)	1.2595(5)	0.082(3)
S1B	0.9862(4)	0.28990(8)	1.05470(14)	0.0831(7)
O1B	1.6482(10)	0.3586(3)	0.6704(4)	0.111(2)
O2B	1.3931(11)	0.3357(2)	0.5717(4)	0.109(2)
N1B	1.3958(11)	0.3364(2)	0.8443(4)	0.0725(19)
N2B	1.0749(11)	0.3046(2)	0.8384(4)	0.086(2)
N3B	1.4719(12)	0.3422(2)	0.6568(4)	0.081(2)
C1B	1.0135(18)	0.2887(3)	1.4040(6)	0.104(3)
C2B	1.1782(16)	0.3083(3)	1.3526(6)	0.098(3)
C3B	1.1799(14)	0.3100(3)	1.2457(5)	0.085(3)
C4B	1.0084(15)	0.2917(3)	1.1902(5)	0.076(2)
C5B	0.8411(15)	0.2725(3)	1.2445(5)	0.088(3)
C6B	0.8437(17)	0.2706(3)	1.3509(6)	0.109(4)
C7B	1.2207(13)	0.3203(3)	1.0141(5)	0.081(2)
C8B	1.2297(14)	0.3200(3)	0.8978(5)	0.073(2)
C9B	1.5891(13)	0.3563(3)	0.8891(6)	0.093(3)
C10B	1.3377(14)	0.3304(3)	0.7414(5)	0.075(2)
C11B	1.1453(14)	0.3109(3)	0.7409(6)	0.086(3)

where $U_{\text{eq}} = 1/3\pi^2 \Sigma_i \Sigma_j a_i a_j \mathbf{a}_i^* \cdot \mathbf{a}_j^*$

TABLE VII Bond Lengths (Å) for compound B

Atoms	*Length*	*Atoms*	*Length*
S1A-C4A	1.771(8)	S1C-C7C	1.76(2)
S1A-C7A	1.78(2)	S1C-C4C	1.770(7)
O1A-N3A	1.226(18)	O1C-N3C	1.210(18)
O2A-N3A	1.210(9)	O2C-N3C	1.222(9)
N1A-C8A	1.335(16)	N1C-C8C	1.348(17)
N1A-C10A	1.389(9)	N1C-C10C	1.388(9)
N1A-C9A	1.445(19)	N1C-C9C	1.442(18)
N2A-C8A	1.316(16)	N2C-C8C	1.308(15)
N2A-C11A	1.346(10)	N2C-C11C	1.347(10)
N3A-C10A	1.411(12)	N3C-C10C	1.414(14)
C1A-C6A	1.342(18)	C1C-C2C	1.354(17)
C1A-C2A	1.380(18)	C1C-C6C	1.371(18)
C2A-C3A	1.371(9)	C2C-C3C	1.387(10)

Atoms	*Length*	*Atoms*	*Length*
C3A-C4A	1.370(17)	C3C-C4C	1.394(17)
C4A C5A	1.390(17)	C4C-C5C	1.376(17)
C5A-C6A	1.376(10)	C5C-C6C	1.373(10)
C7A-C8A	1.505(9)	C7C-C8C	1.497(9)
C10A-C11A	1.35(2)	C10C-C11C	1.34(2)
S1D-C4D	1.761(8)	S1B-C4B	1.763(8)
S1D-C7D	1.80(2)	S1B-C7B	1.78(2)
O1D-N3D	1.203(18)	O1B-N3B	1.210(18)
O2D-N3D	1.222(9)	O2B-N3B	1.222(9)
N1D-C8D	1.333(16)	N1B-C8B	1.332(17)
N1D-C10D	1.378(9)	N1B-C10B	1.392(9)
N1D-C9D	1.447(18)	N1B-C9B	1.456(18)
N2D-C8D	1.332(15)	N2B-C8B	1.313(15)
N2D-C11D	1.347(10)	N2B-C11B	1.349(10)
N3D-C10D	1.401(13)	N3B-C10B	1.420(14)
C1D-C2D	1.372(17)	C1B-C2B	1.345(18)
C1D-C6D	1.363(18)	C1B-C6B	1.366(19)
C2D-C3D	1.362(10)	C2B-C3B	1.386(10)
C3D-C4D	1.387(17)	C3B-C4B	1.392(17)
C4D-C5D	1.374(17)	C4B-C5B	1.372(17)
C5D-C6D	1.363(11)	C5B-C6B	1.380(10)
C7D-C8D	1.497(8)	C7B-C8B	1.507(9)
C10D-C11D	1.35(2)	C10B-C11B	1.33(2)

TABLE VIII Bond Angles (°) for compound B

Atoms	*Angle*	*Atoms*	*Angle*
C4A-S1A-C7A	102.3(6)	C8D-C7D-S1D	108.4(7)
C8A-N1A-C10A	104.3(9)	N2D-C8D-N1D	111.7(9)
C8A-N1A-C9A	126.3(9)	N2D-C8D-C7D	125.3(8)
C10A-N1A-C9A	129.3(7)	N1D-C8D-C7D	123.0(8)
C8A-N2A-C11A	104.7(10)	C11D-C10D-N1D	107.4(8)
O1A-N3A-O2A	123.2(8)	C11D-C10D-N3D	127.2(9)
O1A-N3A-C10A	118.5(9)	N1D-C10D-N3D	125.4(10)
O2A-N3A-C10A	118.2(10)	C10D-C11D-N2D	109.2(9)
C6A-C1A-C2A	118.8(10)	C7C-S1C-C4C	103.4(6)
C3A-C2A-C1A	121.0(10)	C8C-N1C-C10C	104.6(9)
C2A-C3A-C4A	120.7(9)	C8C-N1C-C9C	126.5(8)
C3A-C4A-C5A	117.7(9)	C10C-N1C-C9C	128.9(8)
C3A-C4A-S1A	126.8(7)	C8C-N2C-C11C	105.6(10)
C5A-C4A-S1A	115.5(8)	O1C-N3C-O2C	124.7(9)
C6A-C5A-C4A	120.8(10)	O1C-N3C-C10C	118.9(9)

Atoms	*Angle*	*Atoms*	*Angle*
C1A-C6A-C5A	121.0(9)	O2C-N3C-C10C	116.4(10)
C8A-C7A-S1A	109.3(7)	C2C-C1C-C6C	117.7(10)
N2A-C8A-N1A	113.8(9)	C1C-C2C-C3C	122.7(9)
N2A-C8A-C7A	123.8(9)	C2C-C3C-C4C	118.7(9)
N1A-C8A-C7A	122.4(9)	C5C-C4C-C3C	118.9(9)
C11A-C10A-N1A	106.7(8)	C5C-C4C-S1C	116.9(8)
C11A-C10A-N3A	127.2(9)	C3C-C4C-S1C	124.2(8)
N1A-C10A-N3A	126.1(9)	C6C-C5C-C4C	120.2(9)
C10A-C11A-N2A	110.4(9)	C5C-C6C-C1C	121.8(10)
C4D-S1D-C7D	102.6(6)	C8C-C7C-S1C	109.3(7)
C8D-N1D-C10D	105.7(9)	N2C-C8C-N1C	112.6(9)
C8D-N1D-C9D	124.9(9)	N2C-C8C-C7C	125.0(9)
C10D-N1D-C9D	129.4(7)	N1C-C8C-C7C	122.4(8)
C8D-N2D-C11D	106.1(9)	C11C-C10C-N1C	106.8(9)
O1D-N3D-O2D	122.0(8)	C11C-C10C-N3C	127.3(8)
O1D-N3D-C10D	121.4(9)	N1C-C10C-N3C	125.9(9)
O2D-N3D-C10D	116.6(10)	C10C-C11C-N2C	110.3(8)
C2D-C1D-C6D	118.6(10)	C4B-S1B-C7B	102.4(6)
C3D-C2D-C1D	120.4(10)	C8B-N1B-C10B	104.6(9)
C2D-C3D-C4D	121.2(9)	C8B-N1B-C9B	125.1(9)
C5D-C4D-C3D	117.6(10)	C10B-N1B-C9B	130.3(8)
C5D-C4D-S1D	116.7(9)	C8B-N2B-C11B	105.4(10)
C3D-C4D-S1D	125.7(7)	O1B-N3B-O2B	124.0(9)
C6D-C5D-C4D	120.8(10)	O1B-N3B-C10B	121.1(9)
C5D-C6D-C1D	121.3(10)	O2B-N3B-C10B	115.0(10)
C2B-C1B-C6B	120.0(10)	C8B-C7B-S1B	108.9(7)
C1B-C2B-C3B	120.9(10)	N2B-C8B-N1B	112.7(9)
C2B-C3B-C4B	119.9(10)	N2B-C8B-C7B	124.1(9)
C5B-C4B-C3B	118.1(9)	N1B-C8B-C7B	123.2(8)
C5B-C4B-S1B	116.0(8)	C11B-C10B-N1B	107.0(8)
C3B-C4B-S1B	126.0(8)	C11B-C10B-N3B	129.1(8)
C6B-C5B-C4B	121.1(9)	N1B-C10B-N3B	123.8(10)
C5B-C6B-C1B	120.0(10)	C10B-C11B-N2B	110.3(8)

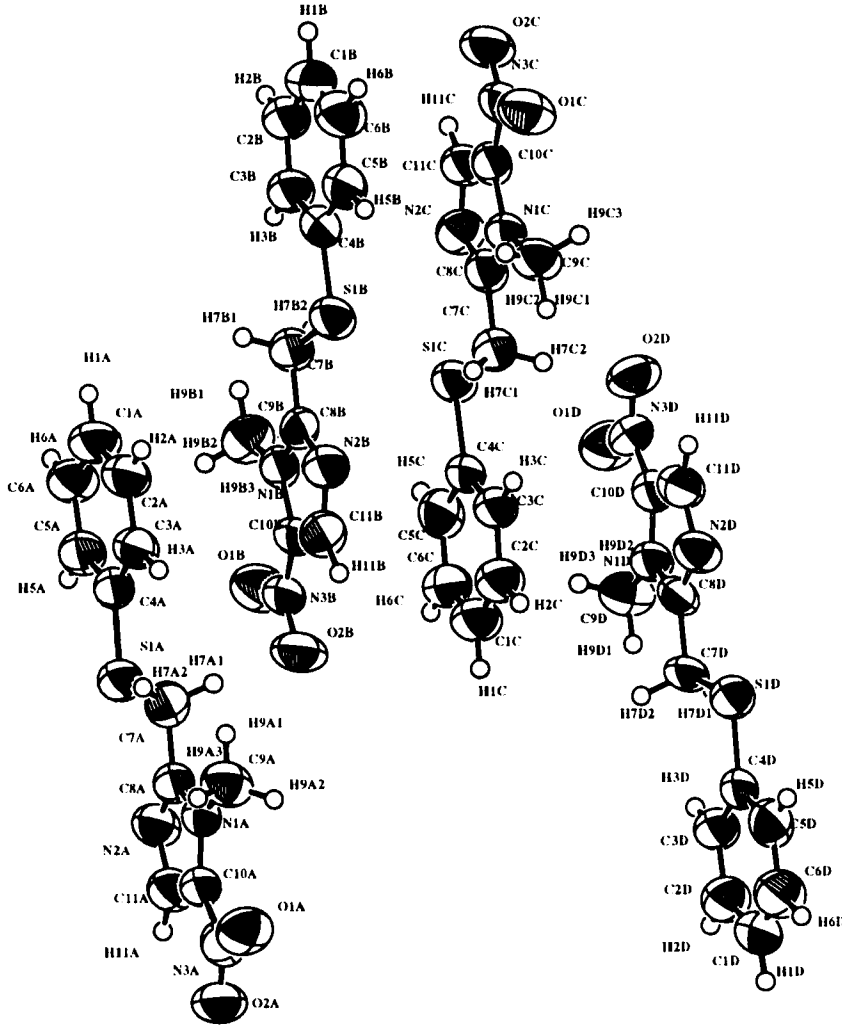

FIGURE 3 ORTEP of the molecule of compound (**B**)

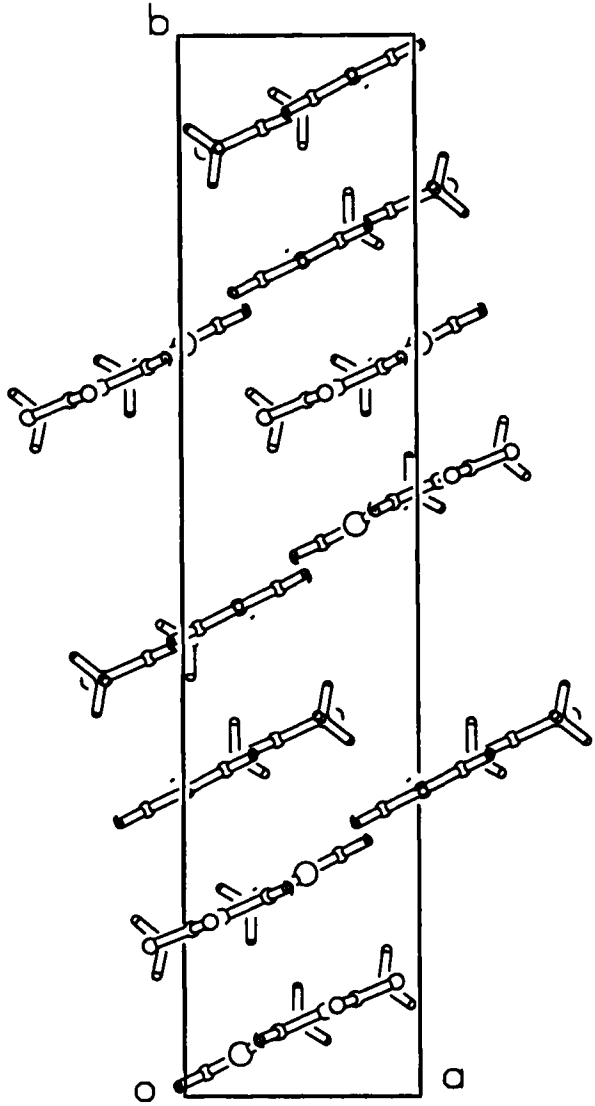

FIGURE 4 Packing of the molecules down *c* of compound (**B**)

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