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Short Communication

Bonding in 1,2,3-Triazoles. V. The Crystal Structure of 2-Phenyl-4-chloro-1,2,3-triazole

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The present structure analysis is part of an investigation of substituted 1,2,3-triazoles.[1–4] The crystals of the title compound, $C_8H_6N_3Cl$, are monoclinic, space group $P2_1/n$, with a=5.742(2), b=10.354(5), c=13.680(4) Å and β=94.17(3)°. M=180.34, Z=4, D_c=1.48 g cm^{-3} and μ(Mo$K\alpha$)=4.1 cm^{-1}.

Three-dimensional data were collected on a four circle diffractometer (CAD-4F) using monochromated Mo$K\alpha$ radiation. Since the crystals are unstable in air, they were sealed in glass capillaries for X-ray work. A total of 1412 reflections with θ<25° were reduced to 806 independent reflections with $I \geq 2\sigma(I)$. The intensities were corrected for Lorentz and polarization effects, but not for absorption. The structure was solved by direct methods.[5] The references to the atomic scattering factors and the refinement technique are those used in Ref. 2. For the

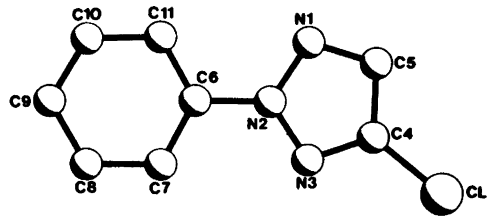

Fig. 1. The structure viewed perpendicular to the plane containing N1, N2 and N3.

Table 1. Atomic coordinates ×10^4. Estimated standard deviations ×10^4 are given in parentheses. The values for hydrogen are multiplied by 10^3.

Atom	x	y	z
Cl	7011(3)	9028(2)	−692(1)
N1	2434(9)	6537(5)	34(4)
N2	4281(7)	6397(4)	684(3)
N3	6062(8)	7183(5)	553(4)
C4	5316(11)	7870(6)	−216(4)
C5	3060(12)	7486(7)	−549(5)
C6	4322(9)	5462(5)	1456(4)
C7	6274(10)	5406(6)	2103(4)
C8	6322(12)	4484(7)	2844(5)
C9	4460(12)	3658(7)	2933(5)
C10	2544(12)	3760(7)	2275(5)
C11	2440(11)	4654(6)	1532(5)
H1	201(13)	776(7)	−111(5)
H2	767(9)	603(5)	208(4)
H3	774(11)	444(6)	335(5)
H4	438(10)	298(6)	349(5)
H5	122(10)	320(6)	231(4)
H6	123(12)	474(7)	105(5)

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Table 2. Bond distances (Å) and bond angles (°) with with estimated standard deviations.

Atoms	Distance	Atoms	Angle
Cl–C4	1.703(6)	Cl–C4–C5	128.1(5)
C4–C5	1.400(8)	Cl–C4–N3	121.7(5)
C5–N1	1.331(9)	N3–C4–C5	110.2(5)
N1–N2	1.342(6)	C4–C5–N1	107.4(5)
N2–N3	1.329(6)	C5–N1–N2	104.0(5)
N3–C4	1.315(8)	N1–N2–N3	115.0(4)
N2–C6	1.432(7)	N2–N3–C4	103.3(4)
C6–C7	1.378(8)	N1–N2–C6	122.1(4)
C7–C8	1.390(9)	N3–N2–C6	122.8(4)
C8–C9	1.382(10)	N2–C6–C11	119.7(5)
C9–C10	1.374(9)	N2–C6–C7	118.1(5)
C10–C11	1.372(10)	C11–C6–C7	122.2(5)
C11–C6	1.376(8)	C6–C7–C8	118.0(5)
C5–H1	0.98(7)	C7–C8–C9	121.0(6)
C7–H2	1.03(5)	C8–C9–C10	118.8(6)
C8–H3	1.03(6)	C9–C10–C11	121.8(7)
C9–H4	1.04(6)	C10–C11–C6	118.2(6)
C10–H5	0.96(6)		
C11–H6	0.92(7)		

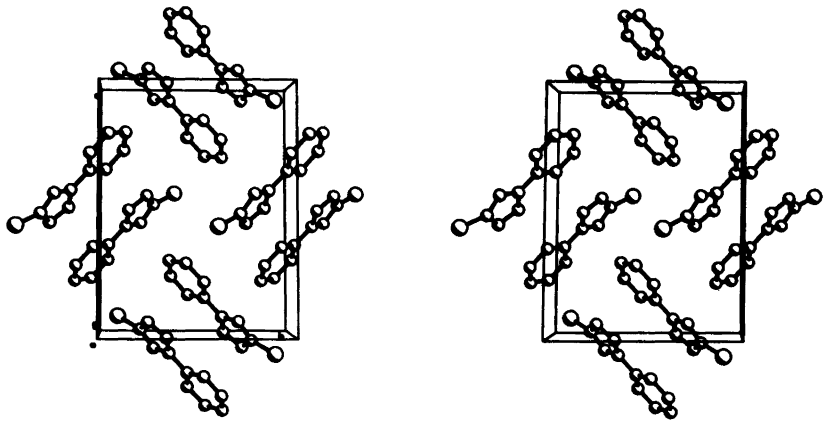

Fig. 2. Stereoview along the a^*-axis of the structure.

illustrations the PLUTO programme[6] was used. The final R-values are $R=0.047$ and $R_w=0.049$. The final positional parameters with their estimated standard deviations are listed in Table 1. The labelling of the atoms is shown in Fig. 1. Lists of thermal parameters as well as lists of observed and calculated structure factors may be obtained from the authors on request.

Description and discussion of the structure. Bond lengths and bond angles with their estimated standard deviations are listed in Table 2. The phenyl and triazole groups are planar, the deviations of the atoms from the least-squares planes through them being less than 0.004 Å. The chlorine atom is 0.022 Å out of the triazole plane. A general discussion of substitution effects on the geometry of the triazole ring is dealt with in subsequent papers.[7,8] The angle between the two planes is 1.6°, and the angle between the normal of the triazole group and the N2–C6–C9 line is 89.7°. The deformations of the endocyclic angles in the phenyl group are symmetric around the

C6–C9 line, with an angle of 122.2° at C6. This indicates a highly electronegative substituent bonded to C6.[9,10]

The packing of the structure is shown in Fig. 2. The shortest non-bonding distances not involving the chlorine atom are found between the triazole ring and the phenyl rings $(1-x, 1-y, -z)$ (a) and $(\frac{3}{2}-x, \frac{1}{2}+y, \frac{1}{2}-z)$ (b). The distances are 3.474 Å [C4–C11(a)], 3.530 Å [N1–C6(a)], 3.502 Å [N3–C8(b)] and 3.530 Å [N3–C9(b)]. The shortest non-bonding distance involving chlorine is the Cl–C9$(\frac{1}{2}+x, \frac{3}{2}-y, z-\frac{1}{2})$ distance of 3.412 Å. The Cl–Cl$(1-x, 2-y, -z)$ distance [3.689 Å] is rather short but of the same order of magnitude as the S–S distance [3.71 Å] in 1-methyl-3-benzyl-4-(1,2,3-triazolio)sulfide.[3]

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