Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å²)*

$$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	U_{eq}
C1	0.9658 (2)	0.8151 (3)	0.21391 (9)	0.0291 (6)
C2	1.0374 (2)	0.9023 (3)	0.24987 (9)	0.0287 (6)
C3	1.1166 (2)	0.7921 (2)	0.24889 (9)	0.0280 (6)
C4	1.0756 (2)	0.6231 (2)	0.24006 (8)	0.0251 (6)
O5	0.97959 (10)	0.6514 (2)	0.22509 (6)	0.0278 (4)
C6	1.0527 (2)	1.0723 (3)	0.23548 (10)	0.0398 (7)
C7	1.0120 (2)	0.8997 (3)	0.29962 (9)	0.0383 (7)
C8	1.0907 (2)	0.5195 (2)	0.28544 (9)	0.0266 (6)
C9	1.0212 (2)	0.4450 (2)	0.30093 (9)	0.0321 (6)
C10	1.0364 (2)	0.3472 (3)	0.34192 (10)	0.0381 (7)
C11	1.1220 (2)	0.3251 (3)	0.36762 (10)	0.0379 (7)
C12	1.1927 (2)	0.3993 (3)	0.35295 (10)	0.0447 (7)
C13	1.1769 (2)	0.4944 (3)	0.31226 (9)	0.0350 (7)
O14	1.14479 (15)	0.2321 (2)	0.40857 (7)	0.0593 (6)
C15	1.0736 (2)	0.1551 (3)	0.42497 (11)	0.0668 (11)
C16	1.1064 (2)	0.5327 (2)	0.19951 (9)	0.0257 (6)
C17	1.1872 (2)	0.5587 (3)	0.18668 (9)	0.0309 (6)
C18	1.2122 (2)	0.4769 (3)	0.14900 (9)	0.0349 (7)
C19	1.1554 (2)	0.3648 (3)	0.12364 (9)	0.0338 (7)
C20	1.0741 (2)	0.3335 (3)	0.13656 (9)	0.0340 (7)
C21	1.0504 (2)	0.4159 (3)	0.17368 (9)	0.0290 (6)
O22	1.17201 (13)	0.2783 (2)	0.08525 (7)	0.0498 (5)
C23	1.2537 (2)	0.3098 (4)	0.07091 (12)	0.0690 (10)
O24	0.97876 (11)	0.8500 (2)	0.16651 (6)	0.0317 (4)
C31	0.9277 (2)	0.7562 (3)	0.12933 (9)	0.0309 (6)
C32	0.9510 (2)	0.8017 (3)	0.08102 (9)	0.0337 (6)
C33	0.8913 (2)	0.9490 (3)	0.06825 (9)	0.0332 (7)
C34	0.8092 (2)	0.9209 (3)	0.09106 (9)	0.0284 (6)
O35	0.83503 (11)	0.7860 (2)	0.12377 (6)	0.0318 (4)
C36	1.0500 (2)	0.8381 (3)	0.08446 (10)	0.0469 (8)
C37	0.9223 (2)	0.6645 (3)	0.04481 (10)	0.0455 (8)
C38	0.7251 (2)	0.8709 (3)	0.05465 (9)	0.0283 (6)
C39	0.6860 (2)	0.7209 (3)	0.05677 (9)	0.0337 (7)
C40	0.6110 (2)	0.6755 (3)	0.02406 (9)	0.0348 (7)
C41	0.5715 (2)	0.7781 (3)	−0.01245 (9)	0.0315 (6)
C42	0.6080 (2)	0.9273 (3)	−0.01514 (9)	0.0338 (7)
C43	0.6843 (2)	0.9716 (3)	0.01813 (9)	0.0322 (7)
O44	0.49594 (12)	0.7214 (2)	−0.04301 (6)	0.0441 (5)
C45	0.4594 (2)	0.8158 (3)	−0.08425 (10)	0.0505 (8)
C46	0.7871 (2)	1.0605 (3)	0.12145 (9)	0.0270 (6)
C47	0.8071 (2)	1.2178 (3)	0.11305 (9)	0.0337 (7)
C48	0.7847 (2)	1.3420 (3)	0.14122 (9)	0.0325 (6)
C49	0.7409 (2)	1.3095 (3)	0.17776 (9)	0.0307 (6)
C50	0.7178 (2)	1.1530 (3)	0.18583 (9)	0.0339 (7)
C51	0.7407 (2)	1.0319 (3)	0.15792 (9)	0.0330 (7)
O52	0.71592 (12)	1.4218 (2)	0.20798 (6)	0.0393 (5)
C53	0.7177 (2)	1.5846 (3)	0.19314 (10)	0.0465 (8)

Table 2. *Selected geometric parameters (Å, °)*

C1—O5	1.415 (3)	O24—C31	1.411 (3)
C1—O24	1.428 (3)	C31—O35	1.415 (3)
C1—C2	1.517 (3)	C31—C32	1.532 (3)
C2—C3	1.529 (3)	C32—C33	1.534 (3)
C3—C4	1.549 (3)	C33—C34	1.545 (3)
C4—O5	1.459 (3)	C34—O35	1.463 (3)
O5—C1—O24	111.4 (2)	O24—C31—O35	111.6 (2)
O5—C1—C2	105.4 (2)	O24—C31—C32	109.4 (2)
O24—C1—C2	108.1 (2)	O35—C31—C32	105.8 (2)
C1—C2—C3	99.1 (2)	C31—C32—C33	99.9 (2)
C2—C3—C4	105.1 (2)	C32—C33—C34	105.9 (2)
O5—C4—C3	104.3 (2)	O35—C34—C33	104.3 (2)
C1—O5—C4	108.4 (2)	C31—O35—C34	109.8 (2)
C31—O24—C1	115.1 (2)		

Conventional diffraction standards were not used. The consistency was checked from successive frames of the area detector and no decay was noted.

Data collection: *MADNES* (Enraf–Nonius, 1990). Cell refinement: *MADNES*. Data reduction: *MADNES*. Program(s)

used to solve structure: *SHELXS*86 (Sheldrick, 1990). Program(s) used to refine structure: *SHELXL*93 (Sheldrick, 1993). Molecular graphics: *PLATON*92 (Spek, 1992*a*) and *PLUTON*92 (Spek, 1992*b*). Software used to prepare material for publication: *SHELXL*93.

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2,10-Dichloro-6-(2,4-dimethylphenoxy)-dibenzo[d,g][1,3,6,2]dioxathiaphosphocine 6-Sulfide

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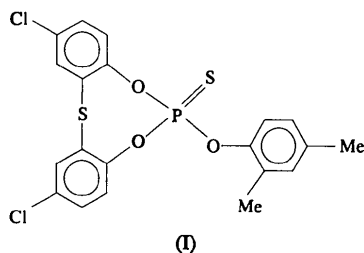
Abstract

In the crystal structure of the title compound, $C_{20}H_{15}Cl_2O_3PS_2$, the dioxathiaphosphocine ring adopts a boat–chair conformation, with the phosphoryl sulfide group axial and the phenoxy group equatorial. The planar chlorobenzene groups fused to the heterocyclic ring form an angle of 67.90 (10)° with one another.

Comment

Considerable interest has been shown in the structural investigation of heterocyclic organophosphorus derivatives because of their potential applications as antioxidants and stabilizers (Spivack, 1982) in polymers and oils. Organophosphorus thionic esters containing the P=S group have proved to be useful nematicides against worms which damage the stems and roots of plants (Emsley & Hall, 1976). These compounds are also useful as insecticides, bactericides, flame retardants and lubricants (Ismail, 1975). The structural data on eight-membered-ring phosphorus heterocycles with sulfur as one of the endo- and exocyclic substituents is limited. The structure determination of the title compound, (I), was undertaken as part of continuous efforts to study the effect of substituents on significant features of the conformation and molecular geometry of the heterocyclic ring.

(I)

In the dioxathiaphosphocine ring system, the corresponding bond lengths and angles (except the endocyclic P—O—C angle) of the P—O—C—C—S fragments are equal within the limits of error. They are also in agreement with values found for related structures (Mani Naidu, Krishnaiah & Sivakumar, 1992; Shanmuga Sundara Raj, Ponnuswamy, Shanmugam, Mani Naidu & Krishnaiah, 1994; Allen et al., 1987). The endocyclic C—S—C angle [102.51 (12)°] is, however, significantly larger than the corresponding one of a related structure [99.5 (1)°; Devendranath Reddy et al., 1996]. This may be due to the bulky dimethylphenoxy group on the P atom.

The dioxathiaphosphocine ring exhibits a boat–chair conformation; deviations are P 0.142 (1), C1 0.359 (2), C6 0.349 (2), C7 0.245 (2) and C12 0.366 (2) Å on one side, and O1 0.411 (1), S2 0.722 (2) and O2 0.329 (2) Å on the other side of the mean plane passing through all the atoms of the heterocyclic ring. This is similar to the situation found in both 2,6-di-tert-butyldibenzo[d,g][1,3,6,2]dioxadiphosphocine 2,6-disulfide (Nietzschmann et al., 1989) and 2,10-dichloro-6-ethoxydibenzo[d,g][1,3,6,2]dioxathiaphosphocine 6-oxide (Devendranath Reddy et al., 1996). These structures differ from the structures of 1,1'-dinaphthoxymethane phenyloxyphosphine sulfide (Shanmuga Sundara Raj et al., 1994) and 8-phenoxy-16H-dinaphtho-[2,1-d;1',2'-g][1,3,2]dioxaphosphocine 8-oxide (Devendranath Reddy et al., 1991). This shows that the influ-
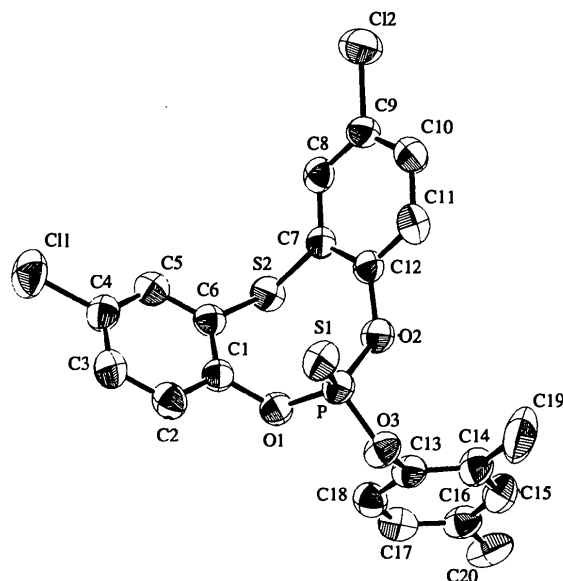
Fig. 1. A perspective view of the title molecule showing the numbering scheme and the boat–chair conformation. Ellipsoids are plotted at the 50% probability level.

ence of the substituents fused to the heterocyclic ring is greater than the influence of those attached to the P atom.

Experimental

The title compound was prepared by the method described by Sankara Reddy, Devendranath Reddy & Mallikarjuna Reddy (1995). The crystals were grown from 2-propanol. The density D_m was measured by flotation in KI solution.

Crystal data

$C_{20}H_{15}Cl_2O_3PS_2$	Mo $K\alpha$ radiation
$M_r = 469.31$	$\lambda = 0.71069$ Å
Monoclinic	Cell parameters from 25
$P2_1/n$	reflections
$a = 13.272$ (2) Å	$\theta = 2-25°$
$b = 9.2251$ (10) Å	$\mu = 0.600$ mm^{-1}
$c = 17.2566$ (10) Å	$T = 293$ (2) K
$\beta = 90.390$ (10)°	Transparent block
$V = 2112.8$ (4) Å^3	0.3 × 0.3 × 0.3 mm
$Z = 4$	Colourless
$D_x = 1.412$ Mg m^{-3}	
$D_m = 1.408$ Mg m^{-3}	

Data collection

Enraf–Nonius CAD-4 diffractometer	$R_{int} = 0.0159$
	$\theta_{max} = 24.98°$
ω–2θ scans	$h = 0 \rightarrow 15$
Absorption correction: none	$k = 0 \rightarrow 10$
	$l = -20 \rightarrow 20$
3153 measured reflections	2 standard reflections
3011 independent reflections	monitored every 100
2874 observed reflections	reflections
[$I > 2\sigma(I)$]	intensity decay: <1%

$C_{20}H_{15}Cl_2O_3PS_2$

Refinement

Refinement on F^2
$R(F) = 0.0359$
$wR(F^2) = 0.0850$
$S = 1.095$
3011 reflections
313 parameters
$w = 1/[\sigma^2(F_o^2) + (0.0408P)^2 + 0.9094P]$
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{max} = 0.184$
$\Delta\rho_{max} = 0.293$ e Å^{-3}
$\Delta\rho_{min} = -0.187$ e Å^{-3}
Extinction correction: none
Atomic scattering factors
from *International Tables
for Crystallography* (1992,
Vol. C, Tables 4.2.6.8 and
6.1.1.4)

Table 1. *Fractional atomic coordinates and equivalent isotropic displacement parameters (Å^2)*

$U_{eq} = (1/3)\Sigma_i\Sigma_j U_{ij}a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j.$

	x	y	z	U_{eq}
P	0.86046 (5)	−0.39638 (8)	0.83335 (4)	0.0471 (2)
S1	0.81174 (6)	−0.54887 (9)	0.89628 (5)	0.0619 (2)
S2	0.78145 (5)	−0.02242 (7)	0.87811 (4)	0.0543 (2)
O1	0.77676 (12)	−0.3054 (2)	0.78794 (9)	0.0512 (4)
O2	0.92998 (12)	−0.2784 (2)	0.87414 (10)	0.0516 (4)
O3	0.93060 (13)	−0.4442 (2)	0.76569 (10)	0.0550 (5)
Cl1	0.38871 (6)	−0.15560 (11)	0.92734 (5)	0.0834 (3)
Cl2	0.90319 (6)	0.01052 (10)	1.17611 (4)	0.0763 (3)
C1	0.6853 (2)	−0.2688 (3)	0.82269 (13)	0.0466 (6)
C2	0.6032 (2)	−0.3556 (3)	0.8086 (2)	0.0571 (7)
C3	0.5116 (2)	−0.3198 (4)	0.8406 (2)	0.0597 (7)
C4	0.5045 (2)	−0.1997 (3)	0.8871 (2)	0.0542 (7)
C5	0.5865 (2)	−0.1125 (3)	0.90132 (15)	0.0507 (6)
C6	0.6786 (2)	−0.1454 (3)	0.86820 (14)	0.0451 (6)
C7	0.8519 (2)	−0.0994 (3)	0.95612 (14)	0.0446 (6)
C8	0.8485 (2)	−0.0314 (3)	1.0279 (2)	0.0497 (6)
C9	0.9066 (2)	−0.0824 (3)	1.08833 (15)	0.0527 (7)
C10	0.9673 (2)	−0.2020 (3)	1.0798 (2)	0.0590 (7)
C11	0.9716 (2)	−0.2690 (3)	1.0083 (2)	0.0553 (7)
C12	0.9150 (2)	−0.2170 (3)	0.94720 (14)	0.0456 (6)
C13	0.9894 (2)	−0.3514 (3)	0.71837 (14)	0.0490 (6)
C14	1.0928 (2)	−0.3596 (3)	0.7258 (2)	0.0597 (7)
C15	1.1491 (2)	−0.2790 (4)	0.6742 (2)	0.0659 (8)
C16	1.1069 (2)	−0.1944 (3)	0.6171 (2)	0.0603 (7)
C17	1.0027 (3)	−0.1888 (4)	0.6132 (2)	0.0625 (8)
C18	0.9433 (2)	−0.2668 (3)	0.6631 (2)	0.0569 (7)
C19	1.1408 (4)	−0.4547 (8)	0.7864 (3)	0.107 (2)
C20	1.1706 (4)	−0.1106 (5)	0.5604 (3)	0.0841 (11)

Table 2. *Selected geometric parameters (Å, °)*

P—O3	1.562 (2)	C5—C6	1.387 (4)
P—O2	1.588 (2)	C7—C12	1.379 (4)
P—O1	1.594 (2)	C7—C8	1.389 (4)
P—S1	1.8937 (14)	C8—C9	1.376 (4)
S2—C7	1.782 (3)	C9—C10	1.375 (4)
S2—C6	1.782 (3)	C10—C11	1.381 (4)
O1—C1	1.399 (3)	C11—C12	1.377 (4)
O2—C12	1.398 (3)	C13—C18	1.373 (4)
O3—C13	1.420 (3)	C13—C14	1.380 (4)
Cl1—C4	1.739 (3)	C14—C15	1.383 (4)
Cl2—C9	1.741 (3)	C14—C19	1.504 (5)
C1—C2	1.371 (4)	C15—C16	1.373 (4)
C1—C6	1.387 (4)	C16—C17	1.385 (4)
C2—C3	1.380 (4)	C16—C20	1.510 (5)
C3—C4	1.372 (4)	C17—C18	1.375 (4)
C4—C5	1.374 (4)		
O3—P—O2	100.22 (10)	C12—C7—S2	123.0 (2)
O3—P—O1	101.42 (10)	C8—C7—S2	118.2 (2)
O2—P—O1	104.95 (10)	C9—C8—C7	120.0 (3)
O3—P—S1	115.25 (9)	C10—C9—C8	121.3 (3)
O2—P—S1	117.04 (8)	C10—C9—Cl2	120.5 (2)
O1—P—S1	115.68 (8)	C8—C9—Cl2	118.3 (2)
C7—S2—C6	102.51 (12)	C9—C10—C11	118.8 (3)
C1—O1—P	121.36 (15)	C12—C11—C10	120.2 (3)
C12—O2—P	126.3 (2)	C11—C12—C7	121.1 (2)
C13—O3—P	126.3 (2)	C11—C12—O2	118.0 (2)
C2—C1—C6	121.8 (2)	C7—C12—O2	120.6 (2)
C2—C1—O1	118.2 (2)	C18—C13—C14	122.3 (3)
C6—C1—O1	120.0 (2)	C18—C13—O3	119.8 (2)
C1—C2—C3	119.4 (3)	C14—C13—O3	117.6 (2)
C4—C3—C2	119.4 (3)	C13—C14—C15	116.8 (3)
C3—C4—C5	121.4 (3)	C13—C14—C19	120.9 (3)
C3—C4—Cl1	119.1 (2)	C15—C14—C19	122.3 (3)
C5—C4—Cl1	119.5 (2)	C16—C15—C14	123.3 (3)
C4—C5—C6	119.8 (3)	C15—C16—C17	117.2 (3)
C1—C6—C5	118.2 (2)	C15—C16—C20	122.0 (3)
C1—C6—S2	121.7 (2)	C17—C16—C20	120.8 (3)
C5—C6—S2	119.9 (2)	C18—C17—C16	121.8 (3)
C12—C7—C8	118.6 (2)	C13—C18—C17	118.5 (3)
O2—P—O1—C1	−91.0 (2)	C7—S2—C6—C1	−86.7 (2)
O1—P—O2—C12	88.1 (2)	C6—S2—C7—C12	78.4 (2)
P—O1—C1—C6	85.4 (3)	S2—C7—C12—O2	2.9 (3)
O1—C1—C6—S2	5.0 (3)	P—O2—C12—C7	−84.7 (3)

Data were corrected for Lorentz and polarization effects, but not for absorption. The structure was solved by direct methods using *SHELXS*86 (Sheldrick, 1990) and refined by full-matrix least squares using *SHELXL*93 (Sheldrick, 1993). All the H atoms were clearly located from difference Fourier syntheses and refined isotropically. All the calculations were carried out on a 486 PC.

Data collection: *MolEN* (Fair, 1990). Cell refinement: *MolEN*. Data reduction: *MolEN*. Molecular graphics: *ORTEP*II (Johnson, 1976). Software used to prepare material for publication: *SHELXL*93.

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4-(5-Methyl-1,3,4-oxadiazol-2-yl)-1,3-phenylene Diacetate

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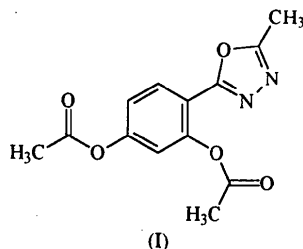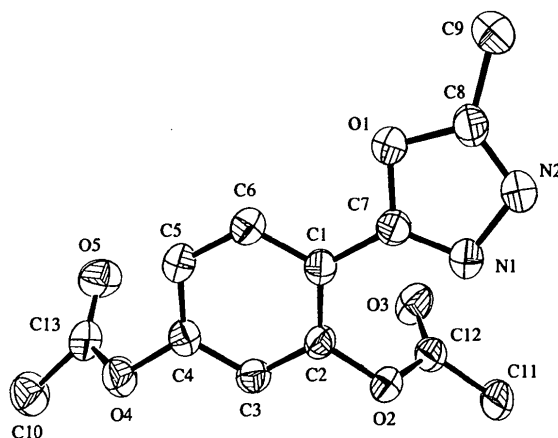
Fig. 1. View of the title compound showing the atomic numbering scheme. Only the positions of the higher occupancy sites of C13, C10 and O5 are shown. Displacement ellipsoids are drawn at the 50% probability level.

Abstract

The title compound, $C_{13}H_{12}N_2O_5$, is a key intermediate in the synthesis of mesogens, which are derivatives of phenyloxadiazole. The oxadiazole and phenyl rings are planar to within 0.003 (2) and 0.010 (7) Å, respectively. The dihedral angle between the least-squares planes through the rings is 10.9 (1)°.

Comment

As part of an ongoing study of the relationship between molecular structure and mesomorphic behaviour, we have been systematically investigating conventional liquid crystals and metallomesogens which include heterocyclic rings (Gallardo & Favarin, 1993; Gallardo, Meyer & Vencato, 1995). The structure of the title compound, (I), was determined in order to obtain further structural information about substituted phenyl-1,3,4-oxadiazoles (Gallardo & Begnini, 1995; Karamysheva, Torgova, Agafonova & Shtikov, 1995).

(I)

The bond lengths and angles of the oxadiazole ring (Table 2) are within the expected ranges (Nygaard, Hansen, Nielsen, Andersen, Sorensen & Steiner, 1972). The phenyl and oxadiazole rings are essentially coplanar with the dihedral angle between their least-squares planes being 10.9 (1)°.

The acetoxy group at the C4 position was found to be disordered. While the introduction of a disorder model improved the structure considerably, the bonds lengths between the disordered atoms are unsatisfactory; C10′—C13′ of 1.55 (2) Å is too long compared with C10—C13 of 1.493 (4) Å.

Experimental

The reaction mixture of 5-(2,4-dihydroxyphenyl)tetrazole and acetic anhydride was heated and refluxed for 2 h, whereupon it was cooled and poured into water. The crude oxadiazole separated as a solid and was recrystallized from ethanol (m.p. 372–373 K). ^1H NMR (200 MHz, CDCl$_3$, 298 K): δ (p.p.m.) 7.91 [1H, d, J_{6-5} = 8.6 Hz, aryl H (C6)], 7.08 [1H, dd, J_{5-3} = 2.2 Hz, J_{5-6} = 8.6 Hz, aryl H (C5)], 6.97 [1H, d, J_{3-5} = 2.2 Hz, aryl H (C3)], 2.49 [3H, s, ArOCOCH$_3$ (C2)], 2.31 [3H, s, ArOCOCH$_3$ (C4)], 2.21 (3H, s, CH$_3$). IR (KBr disk): ν_{max} (cm^{-1}) 3028, 2978, 2930, 2854, 1760, 1616, 1556, 1364, 1216.

Crystal data

$C_{13}H_{12}N_2O_5$	Mo $K\alpha$ radiation
M_r = 276.25	λ = 0.71073 Å
Triclinic	Cell parameters from 25
$P\bar{1}$	reflections
a = 5.6286 (7) Å	θ = 8.72–13.73°
b = 10.257 (1) Å	μ = 0.110 mm^{-1}
c = 12.0111 (5) Å	T = 293 (2) K
α = 100.924 (7)°	Prismatic
β = 100.118 (6)°	0.60 × 0.45 × 0.40 mm
γ = 101.45 (1)°	Colourless
V = 650.7 (1) Å^3	
Z = 2	
D_x = 1.410 Mg m^{-3}	

Data collection

Enraf–Nonius CAD-4 diffractometer	R_{int} = 0.0114
	θ_{max} = 25.02°