| $\mathrm{O}(4)$ | $0.5840(4)$ | $0.0378(1)$ | $-0.107(1)$ | $4.2(2)$ |
| :--- | :--- | :--- | ---: | ---: |
| $\mathrm{O}(5)$ | $0.7566(5)$ | $0.2596(1)$ | $0.308(1)$ | $3.5(2)$ |
| $\mathrm{O}(6)$ | $0.5722(4)$ | $0.2487(1)$ | $0.511(1)$ | $3.5(2)$ |

Table 2. Selected geometric parameters $\left(\AA \AA^{\circ}\right)$

| $\mathrm{C}(1)-\mathrm{C}(2)$ | 1.398 (7) | $\mathrm{C}(10)-\mathrm{O}(2)$ | 1.432 (7) |
| :---: | :---: | :---: | :---: |
| $\mathrm{C}(1)-\mathrm{C}(6)$ | 1.379 (7) | $\mathrm{C}(11)-\mathrm{C}(12)$ | 1.380 (8) |
| $\mathrm{C}(1)-\mathrm{C}(7)$ | 1.471 (7) | $\mathrm{C}(11)-\mathrm{C}(16)$ | 1.389 (7) |
| $\mathrm{C}(2)-\mathrm{C}(3)$ | 1.380 (7) | $\mathrm{C}(12)-\mathrm{C}(13)$ | 1.376 (6) |
| $\mathrm{C}(3)-\mathrm{C}(4)$ | 1.390 (6) | $\mathrm{C}(13)-\mathrm{C}(14)$ | 1.409 (7) |
| $\mathrm{C}(3)-\mathrm{O}(1)$ | 1.377 (6) | $\mathrm{C}(13)-\mathrm{O}(3)$ | 1.360 (7) |
| $\mathrm{C}(4)-\mathrm{C}(5)$ | 1.394 (7) | $\mathrm{C}(14)-\mathrm{C}(15)$ | 1.380 (8) |
| $\mathrm{C}(4)-\mathrm{O}(2)$ | 1.362 (6) | $\mathrm{C}(14)-\mathrm{O}(4)$ | 1.368 (6) |
| $\mathrm{C}(5)-\mathrm{C}(6)$ | 1.385 (7) | $\mathrm{C}(15)-\mathrm{C}(16)$ | 1.384 (7) |
| $\mathrm{C}(7)-\mathrm{C}(8)$ | 1.337 (7) | $\mathrm{C}(17)-\mathrm{O}(3)$ | 1.412 (7) |
| $\mathrm{C}(8)-\mathrm{C}(11)$ | 1.486 (7) | $\mathrm{C}(18)-\mathrm{O}(4)$ | 1.434 (7) |
| $\mathrm{C}(8)-\mathrm{C}(19)$ | 1.505 (8) | $\mathrm{C}(19)-\mathrm{O}(5)$ | 1.209 (6) |
| $\mathrm{C}(9)-\mathrm{O}(1)$ | 1.405 (7) | $\mathrm{C}(19)-\mathrm{O}(6)$ | 1.321 (6) |
| $\mathrm{C}(1)-\mathrm{C}(7)-\mathrm{C}(8)$ | 128.6 (5) | $\mathrm{C}(8)-\mathrm{C}(19)-\mathrm{O}(6)$ | 113.0 (5) |
| $\mathrm{C}(2)-\mathrm{C}(3)-\mathrm{O}(1)$ | 124.7 (4) | $\mathrm{O}(5)-\mathrm{C}(19)-\mathrm{O}(6)$ | 123.2 (5) |
| $\mathrm{C}(5)-\mathrm{C}(4)-\mathrm{O}(2)$ | 125.3 (5) | $\mathrm{C}(3)-\mathrm{O}(1)-\mathrm{C}(9)$ | 116.8 (4) |
| $\mathrm{C}(12)-\mathrm{C}(13)-\mathrm{O}(3)$ | 126.1 (5) | $\mathrm{C}(4)-\mathrm{O}(2)-\mathrm{C}(10)$ | 117.4 (5) |
| $\mathrm{C}(15)-\mathrm{C}(14)-\mathrm{O}(4)$ | 125.8 (5) | $\mathrm{C}(13)-\mathrm{O}(3)-\mathrm{C}(17)$ | 118.3 (4) |
| $\mathrm{C}(8)-\mathrm{C}(19)-\mathrm{O}(5)$ | 123.8 (5) | $\mathrm{C}(14)-\mathrm{O}(4)-\mathrm{C}(18)$ | 116.5 (5) |
| $\mathrm{C}(1)-\mathrm{C}(7)-\mathrm{C}(8)-\mathrm{C}(11)$ |  | -175.9 (5) |  |
| $\mathrm{C}(1)-\mathrm{C}(7)-\mathrm{C}(8)-\mathrm{C}(19)$ |  | 3.6 (9) |  |
| $\mathrm{C}(7)-\mathrm{C}(8)-\mathrm{C}(19)-\mathrm{O}(5)$ |  | -110.5 (6) |  |
| $D-\mathrm{H} \cdots \cdot$ |  | $D \cdots A$ | D-H. . A |
| $\mathrm{O}(6)-\mathrm{H}(\mathrm{O} 6) \cdots \mathrm{O}\left(5^{\mathrm{i}}\right)$ |  | 2.659 (5) 153 |  |
| Symmetry code: (i) $\frac{3}{2}-x, y, \frac{1}{2}+z$. |  |  |  |

The collection of the data was extended to include reflections of the type $h \bar{k} \bar{l}$. A small number of reflections were affected by a minor contribution from a satellite crystal (usually this was not the case for both a reflection of the type $h k l$ and the corresponding reflection of the type $h \bar{k} \bar{l}$ ). The affected reflections were omitted from the data set and average $F$ values were calculated and used in the structure analysis.
Data collection: TEXSAN (Molecular Structure Corporation, 1985). Cell refinement: TEXSAN. Data reduction: TEXSAN. Program(s) used to solve structure: SHELXS86 (Sheldrick, 1985). Program(s) used to refine structure: TEXSAN. Molecular graphics: TEXSAN. Software used to prepare material for publication: TEXSAN.

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## References

Battersby, A. R. \& Greenock, I. A. (1961). J. Chem. Soc. pp. 25922593.

Gadre, S. Y. \& Marathe, K. G. (1988). Synth. Commun. 18, 10151027.

Gierer, J., Lenic, J., Norén, I. \& Szabo-Lin, I. (1974). Acta Chem. Scand. Ser. B, 28, 717-729.
Johnson, C. K. (1976). ORTEPII. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
Li, S. \& Lundquist, K. (1995). Proceedings of the 8th International Symposium on Wood and Pulping Chemistry, June 6-9. Helsinki, Finland, Vol. 1, pp. 163-167, and unpublished data.
Lundquist, K., Stomberg, R. \& von Unge, S. (1987). Acta Chem. Scand. Ser. B, 41, 499-510.

Molecular Structure Corporation (1985). TEXSAN. TEXRAY Structure Analysis Package. MSC, 3200 Research Forest Drive, The Woodlands, TX 77381, USA.
Pandit, S. B. \& Gadre, S. Y. (1988). Synth. Commun. 18, 157-166.
Russell, J. H. \& Hunziker, H. (1969). Tetrahedron Lett. pp. 40354036.

Sheldrick, G. M. (1985). SHELXS86. Program for the Solution of Crustal Structures. Univ. of Göttingen, Germany.
Stomberg, R., Li, S. \& Lundquist, K. (1994). J. Chem. Crystallogr. 24, 407-413.

Acta Cryst. (1995). C51, 2700-2702

## 2-[2-(3,4-Dichlorophenyl)vinyl]benzo[d]thiazole

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#### Abstract

The title compound, $\mathrm{C}_{15} \mathrm{H}_{9} \mathrm{Cl}_{2} \mathrm{NS}$, was synthesized by the condensation of 1-(3,4-dichlorophenyl)-4-methyl-1-penten-3-one and 2 -aminothiophenol. The title compound is essentially planar in the solid state. The $\mathrm{C}=\mathrm{C}$ double bond has the $E$ configuration.


## Comment

The synthesis of the title compound, (III), was unexpected and arose presumably by initial formation of an anil between 1-(3,4-dichlorophenyl)-4-methyl-1-penten-3-one, (I), and 2-aminothiophenol, (II), followed by attack on the carbimino $C$ atom by the $S$ atom leading to the extrusion of the isopropyl group and ring closure forming a benzothiazole. Alternatively, attack by the $S$ atom on the carbonyl $C$ atom of (I) could lead to an intermediate, the amino group of which subsequently forms a bond with this $C$ atom, leading to ring closure and the elimination of the isopropyl group.


(I)

(III)

A review of the literature revealed that while (II) has reacted with certain $\alpha, \beta$-unsaturated ketones and $\alpha, \beta$ unsaturated acids producing benzothiazepines (Lévai, 1979, 1981; Lévai, Toth \& Szollosy, 1982) and benzothiazepiones (Mills \& Whitworth, 1927; Lévai, 1980), respectively, benzothiazoles were not formed. These heterocycles may be obtained by condensation of aldehydes with (II) (Bogert \& Naiman, 1935; Lankelma \& Scharnoff, 1932) and in one instance, reaction of the unsaturated aldehyde cinnamaldehyde with (II) produced a benzothiazole (Lankelma \& Scharnoff, 1932). However, to the best of the authors' knowledge, this is the first report of a benzothiazole being formed from an $\alpha, \beta$ -


Fig. 1. ORTEPII (Johnson, 1976) view of the title compound with non-H-atom displacement ellipsoids at the $50 \%$ probability level. For clarity, the H atoms are drawn as small spheres of arbitrary size.
unsaturated ketone and (II). This observation is important for the following reasons. First, a number of benzothiazoles have pronounced bioactivities (Ince, 1990) and hence the discovery of a novel synthetic route to these heterocycles is noteworthy. Second, the expulsion of the isopropyl group of (I) during the formation of the title compound requires an unusual reaction mechanism, the elucidation of which will require further study.

The X-ray crystallographic data revealed that the molecule is essentially planar. The angles between the benzothiazolyl and halogen-containing aryl rings with the olefinic group were $1.9(4)$ and $2.1(3)^{\circ}$, respectively. The maximum deviation from the least-squares plane of the molecule is 0.121 (4) $\AA$. The C9-S—C10 angle is $89.1(2)^{\circ}$, which suggests that the $S$ atom uses only $p$ orbitals to form bonds with C9 and C10. In order to maintain the planar conformation of the five-membered ring, the other ring bond angles, i.e. $\mathrm{C} 9-\mathrm{N}-\mathrm{C} 11, \mathrm{~S}-$ $\mathrm{C} 10-\mathrm{C} 11, \mathrm{~N}-\mathrm{C} 11-\mathrm{C} 10$ and $\mathrm{N}-\mathrm{C} 9-\mathrm{S}$, are all in the range $109.0-115.4^{\circ}$, less than the ideal $120^{\circ}$ for $s p^{2}$ orbital hybridizations of C and N atoms and greater than the ideal $108^{\circ}$ required for a regular planar pentagon.

The packing of the molecules is shown in Fig. 2. The molecules are arranged in antiparallel pairs attracted by $\pi-\pi$ interactions. There are two intermolecular $\mathrm{N}-\mathrm{H}$ distances $\left[\mathrm{N}-\mathrm{H} 15^{\mathrm{i}}=2.702\right.$ and $\mathrm{N}-\mathrm{H} 5^{\mathrm{ii}}=2.595 \AA$; symmetry codes: (i) $1+x, y, z$; (ii) $1-x,-y, 1-z]$ which are slightly less than the sum of the van der Waals radii ( $2.75 \AA$ ). This may indicate two weak $\mathrm{N} \cdots \mathrm{H}-\mathrm{C}$ interactions. Otherwise, only van der Waals interactions are present.


Fig. 2. PLUTON92 (Spek, 1992) drawing of the molecular packing.

## Experimental

Crystal data
$\mathrm{C}_{15} \mathrm{H}_{9} \mathrm{Cl}_{2} \mathrm{NS}$
$M_{r}=306.21$
Monoclinic
$P 2_{1} / c$
$a=6.2260(16) \AA$
$b=14.3627(15) \AA$
$c=14.5505(22) \AA$
$\beta=92.783$ (17) ${ }^{\circ}$
$V=1299.6(4) \AA^{3}$
$Z=4$
$D_{x}=1.565 \mathrm{Mg} \mathrm{m}^{-3}$

Mo $K \alpha$ radiation
$\lambda=0.7107 \AA$
Cell parameters from 25 reflections
$\theta=8-15^{\circ}$
$\mu=0.66 \mathrm{~mm}^{-1}$
$T=123 \mathrm{~K}$
Rod
$0.40 \times 0.10 \times 0.10 \mathrm{~mm}$ Colorless

Data collection
Enraf-Nonius CAD-4
diffractometer
$\omega / 2 \theta$ scans
Absorption correction: none
2570 measured reflections
2281 independent reflections 1677 observed reflections
$[I>\sigma(I)]$

## Refinement

Refinement on $F$
$R=0.049$
$w R=0.049$
$S=1.26$
1677 reflections
172 parameters $w=1 /\left[\sigma^{2}(F)+0.0005 F^{2}\right]$
$(\Delta / \sigma)_{\max }<0.001$
$R_{\text {int }}=0.021$
$\theta_{\text {max }}=24.92^{\circ}$
$h=-7 \rightarrow 7$
$k=0 \rightarrow 17$
$l=0 \rightarrow 17$
3 standard reflections frequency: 120 min intensity decay: none
$\Delta \rho_{\text {max }}=0.33 \mathrm{e} \AA^{-3}$
$\Delta \rho_{\text {min }}=-0.40 \mathrm{e}^{\AA^{-3}}$
Extinction correction: none Atomic scattering factors from International Tables for X-ray Crystallography (1974, Vol. IV, Table 2.2B)

Table 1. Fractional atomic coordinates and equivalent isotropic displacement parameters $\left(\AA^{2}\right)$
$\mathrm{Cl1}$
Cl
C
S
N
C 1
C 2
C 3
C 4
C 5
C 6
C 7
C 8
C 9
C 10
C 11
C 12
C 13
C 14
C 15

| $U_{\mathrm{eq}}=$ | $(1 / 3) \sum_{i} \sum_{j} U_{i j} a_{i}^{*} a_{j}^{*} \mathbf{a}_{i} \cdot \mathbf{a}_{j}$. |  |  |
| :---: | :---: | :---: | :---: |
| $x$ | $y$ | $z$ | $U_{\mathrm{eq}}$ |
| $0.16566(17)$ | $0.13504(8)$ | $0.06737(7)$ | $0.0353(6)$ |
| $0.62247(16)$ | $0.04523(8)$ | $0.10471(7)$ | $0.0297(5)$ |
| $-0.28655(16)$ | $0.17337(7)$ | $0.57166(7)$ | $0.0248(5)$ |
| $0.0478(5)$ | $0.1134(2)$ | $0.6672(2)$ | $0.023(2)$ |
| $0.1962(6)$ | $0.1037(3)$ | $0.3411(3)$ | $0.022(2)$ |
| $0.1254(6)$ | $0.1243(3)$ | $0.2508(3)$ | $0.023(2)$ |
| $0.2554(6)$ | $0.1056(3)$ | $0.1785(3)$ | $0.023(2)$ |
| $0.4564(6)$ | $0.0666(3)$ | $0.1943(3)$ | $0.022(2)$ |
| $0.5275(6)$ | $0.0448(3)$ | $0.2834(3)$ | $0.022(2)$ |
| $0.3999(6)$ | $0.0632(3)$ | $0.3556(3)$ | $0.023(2)$ |
| $0.0564(6)$ | $0.1244(3)$ | $0.4168(3)$ | $0.023(2)$ |
| $0.1069(6)$ | $0.1099(3)$ | $0.5054(3)$ | $0.026(2)$ |
| $-0.0237(6)$ | $0.1283(3)$ | $0.5833(3)$ | $0.023(2)$ |
| $-0.2991(6)$ | $0.1714(3)$ | $0.6908(3)$ | $0.022(2)$ |
| $-0.1039(6)$ | $0.1374(3)$ | $0.7295(3)$ | $0.020(2)$ |
| $-0.0752(6)$ | $0.1280(3)$ | $0.8252(3)$ | $0.025(2)$ |
| $-0.2421(7)$ | $0.1544(3)$ | $0.8794(3)$ | $0.028(2)$ |
| $-0.4359(6)$ | $0.1875(3)$ | $0.8406(3)$ | $0.025(2)$ |
| $-0.4676(7)$ | $0.1964(3)$ | $0.7460(3)$ | $0.026(2)$ |

Table 2. Selected geometric parameters $\left(\AA^{\circ},^{\circ}\right)$

| $\mathrm{Cl1}-\mathrm{C} 3$ | $1.737(4)$ | $\mathrm{C} 4-\mathrm{C} 5$ | $1.386(5)$ |
| :--- | ---: | :--- | :--- |
| $\mathrm{C} 12-\mathrm{C} 4$ | $1.730(4)$ | $\mathrm{C} 5-\mathrm{C} 6$ | $1.373(6)$ |
| $\mathrm{S}-\mathrm{C} 9$ | $1.760(4)$ | $\mathrm{C} 7-\mathrm{C} 8$ | $1.330(6)$ |
| $\mathrm{S}-\mathrm{C} 10$ | $1.739(4)$ | $\mathrm{C} 8-\mathrm{C} 9$ | $1.450(6)$ |
| $\mathrm{N}-\mathrm{C} 9$ | $1.297(5)$ | $\mathrm{C} 10-\mathrm{C} 11$ | $1.402(5)$ |
| $\mathrm{N}-\mathrm{C} 11$ | $1.384(5)$ | $\mathrm{C} 10-\mathrm{C} 15$ | $1.399(6)$ |
| $\mathrm{C} 1-\mathrm{C} 2$ | $1.397(6)$ | $\mathrm{C} 11-\mathrm{C} 12$ | $1.401(5)$ |
| $\mathrm{C} 1-\mathrm{C} 6$ | $1.402(5)$ | $\mathrm{C} 12-\mathrm{C} 13$ | $1.388(6)$ |
| $\mathrm{C} 1-\mathrm{C} 7$ | $1.466(6)$ | $\mathrm{C} 13-\mathrm{C} 14$ | $1.390(6)$ |
| $\mathrm{C} 2-\mathrm{C} 3$ | $1.385(6)$ | $\mathrm{C} 14-\mathrm{C} 15$ | $1.387(6)$ |
| $\mathrm{C} 3-\mathrm{C} 4$ | $1.380(5)$ |  |  |
| $\mathrm{C} 9-\mathrm{S}-\mathrm{C} 10$ | $89.1(2)$ | $\mathrm{C} 7-\mathrm{C} 8-\mathrm{C} 9$ | $127.9(4)$ |
| $\mathrm{C} 9-\mathrm{N}-\mathrm{C} 11$ | $111.2(3)$ | $\mathrm{S}-\mathrm{C} 9-\mathrm{N}$ | $115.2(3)$ |
| $\mathrm{C} 2-\mathrm{C} 1-\mathrm{C} 6$ | $118.1(4)$ | $\mathrm{S}-\mathrm{C} 9-\mathrm{C} 8$ | $123.1(3)$ |
| $\mathrm{C} 2-\mathrm{C} 1-\mathrm{C} 7$ | $119.4(3)$ | $\mathrm{N}-\mathrm{C} 9-\mathrm{C} 8$ | $121.7(3)$ |
| $\mathrm{C} 6-\mathrm{C} 1-\mathrm{C} 7$ | $122.5(3)$ | $\mathrm{S}-\mathrm{C} 10-\mathrm{Cl1}$ | $109.0(3)$ |
| $\mathrm{C} 1-\mathrm{C} 2-\mathrm{C} 3$ | $120.3(4)$ | $\mathrm{S}-\mathrm{C} 10-\mathrm{C} 15$ | $129.7(3)$ |


| $\mathrm{C} 11-\mathrm{C} 3-\mathrm{C} 2$ | $119.1(3)$ | $\mathrm{C} 11-\mathrm{Cl} 10-\mathrm{C} 15$ | $121.2(4)$ |
| :--- | :--- | :--- | :--- |
| $\mathrm{Cl1}-\mathrm{C} 3-\mathrm{C} 4$ | $120.1(3)$ | $\mathrm{N}-\mathrm{C} 11-\mathrm{C} 10$ | $115.4(3)$ |
| $\mathrm{C} 2-\mathrm{C} 3-\mathrm{C} 4$ | $120.8(4)$ | $\mathrm{N}-\mathrm{C} 11-\mathrm{C} 12$ | $124.7(3)$ |
| $\mathrm{Cl} 2-\mathrm{C} 4-\mathrm{C} 3$ | $121.2(3)$ | $\mathrm{C} 10-\mathrm{C} 11-\mathrm{C} 12$ | $119.9(3)$ |
| $\mathrm{Cl} 2-\mathrm{C} 4-\mathrm{C} 5$ | $119.3(3)$ | $\mathrm{C} 11-\mathrm{C} 12-\mathrm{C} 13$ | $118.4(4)$ |
| $\mathrm{C} 3-\mathrm{C} 4-\mathrm{C} 5$ | $119.5(4)$ | $\mathrm{C} 12-\mathrm{C} 13-\mathrm{C} 14$ | $121.4(4)$ |
| $\mathrm{C} 4-\mathrm{C} 5-\mathrm{C} 6$ | $120.2(4)$ | $\mathrm{C} 13-\mathrm{C} 14-\mathrm{C} 15$ | $120.9(4)$ |
| $\mathrm{C} 1-\mathrm{C}-\mathrm{C} 5$ | $121.2(4)$ | $\mathrm{C} 10-\mathrm{Cl5}-\mathrm{C} 14$ | $118.1(4)$ |
| $\mathrm{C} 1-\mathrm{C} 7-\mathrm{C} 8$ | $125.1(4)$ |  |  |

The $\omega$-scan width was $(0.80+0.35 \tan \theta)^{\circ}$ with a $\theta$-scan rate of $0.37-2.74^{\circ} \mathrm{min}^{-1}$. The scan angle was extended $25 \%$ on each side of each peak for background measurement. All H atoms were placed in calculated positions on the corresponding C atoms ( $\mathrm{C}-\mathrm{H}=1.00 \AA$ ) and were not refined. The $U_{\text {iso }}$ of each H atom was assigned as equal to the $U_{\mathrm{eq}}$ of the attached C atom plus $0.01 \AA^{2}$. Refinement was by full-matrix leastsquares methods.

Data collection: CAD-4 Software (Enraf-Nonius, 1988). Cell refinement: CAD-4 Software. Data reduction: NRCVAX DATRD2 (Gabe, Le Page, Charland, Lee \& White, 1989). Program(s) used to solve structure: $N R C V A X$ SOLVER. Program(s) used to refine structure: NRCVAX LSTSQ. Molecular graphics: NRCVAX, ORTEPII (Johnson, 1976). Software used to prepare material for publication: NRCVAX TABLES and UTILITY.

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Lists of structure factors, anisotropic displacement parameters, $\mathbf{H}$ atom coordinates and complete geometry have been deposited with the IUCT (Reference: PT1025). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square. Chester CH1 2HU, England.

## References

Bogert, M. T. \& Naiman, B. (1935). J. Am. Chem. Soc. 57, 15291533.

Enraf-Nonius (1988). CAD-4 Software. Enraf-Nonius, Delft, The Netherlands.
Gabe, E. J., Le Page, Y., Charland, J.-P., Lee, F. L. \& White, P. S. (1989). J. Appl. Cryst. 22, 384-387.

Ince, F. (1990). Comprehensive Medicinal Chemistry, Vol. 3, edited by J. C. Emmett, p. 309. Oxford: Pergamon.
Johnson, C. K. (1976). ORTEPII. Report ORNL-5138, Oak Ridge National Laboratory, Tennessee, USA.
Lankelma, H. P. \& Scharnoff, P. X. (1932). J. Am. Chem. Soc. 54, 379-381.
Lévai, A. (1979). Pharmazie, 34, 439.
Lévai, A. (1980). Pharmazie, 35, 680-681.
Lévai, A. (1981). Pharmazie, 36, 449-450.
Lévai, A., Toth, G. \& Szollosy, A. (1982). Stud. Org. Chem. (Amsterdam), 11, 41-47; Chem. Abstr. (1983), 98, $34569 f$.
Mills, W. H. \& Whitworth, J. B. (1927). J. Chem. Soc. London, pp. 2738-2753.
Spek, A. L. (1992). PLUTON92. Program for the Display and Analysis of Crystal and Molecular Structures. Univ. of Utrecht, The Netherlands.


[^0]:    Lists of structure factors, anisotropic displacement parameters, H atom coordinates and complete geometry have been deposited with the IUCr (Reference: CR1190). Copies may be obtained through The Managing Editor, International Union of Crystallography, 5 Abbey Square, Chester CHI 2HU, England.

