correspondingly adjusted, *i.e.* diminished from about 125° in TMP to 122–123° in its cation. Another effect of the protonation is to increase the length of the ring bonds adjacent to the N(1) atom from 1·343 (1) Å (the value of both bond lengths in TMP) to 1·355 (4) Å for N(1)—C(2) and to 1·366 (4) Å for N(1)—C(6). The conformation adopted by the TMP cation is described by the torsion angles $\tau_1 = \mathrm{C(4)—C(5)—C(7)—C(1}a)$ of −68·4 (3)° and $\tau_2 = \mathrm{C(5)—C(7)—C(1}a\mathrm{)—C(2}a)$ of 149·1 (2)°. TMP (Koetzle & Williams, 1976) and TMP acetate (Haltiwanger, 1971) adopt similar conformations in the solid state [$\tau_{1(\mathrm{TMP})} = -89·4$ (1); $\tau_{2(\mathrm{TMP})} = 153·3$ (1); $\tau_{1(\mathrm{TMP.Ac})} = -77·9$, $\tau_{2(\mathrm{TMP.Ac})} = 155·1°$], while the conformation of the complex TMP–SMZ is different [$\tau_{1(\mathrm{TSC})} = 173·4$ (4); $\tau_{2(\mathrm{TSC})} = 87·7$ (4)°].

The structural and steric situation of the TMP benzene ring and of the benzoate anion is the same as observed in analogous compounds.

This work was partially supported by a grant from the Ministero Pubblica Istruzione to A. La Manna.

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Acta Cryst. (1984). C**40**, 653–655

1,2,5-Telluradiazole, $C_2H_2N_2Te$

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(*Received* 13 *October* 1983; *accepted* 29 *November* 1983)

Abstract. $M_r = 181·65$, orthorhombic, *Pnma*, $a = 12·308$ (2), $b = 7·840$ (2), $c = 4·136$ (1) Å, $V = 399·1$ (4) Å^3, $Z = 4$, D_m (by flotation) = 3·01, $D_x = 3·022$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0·71069$ Å, $\mu = 72·43$ cm^{-1}, $F(000) = 320$, $T = 293$ K, final conventional R is 0·031 for 339 unique observed reflections. The title compound has been obtained by transformation of the 1,2,5-selenadiazole into the tellurium isologue. The molecule is a heterocycle which contains the bonds N—Te—N, but the tellurium atom forms two other weak bonds with two nitrogen atoms of different molecules. In this way a ribbon polymeric structure is produced which accounts for the exceptionally high melting point and low solubility in common solvents of the compound.

Introduction. When the conversion of 1,2,5-selenadiazoles or 1,2,5-thiadiazoles into the corresponding 1,2,5-telluradiazoles allowed for the first time the synthesis of such derivatives (Bertini, Lucchesini & De Munno, 1982), we were surprised by their unusual physico-chemical properties. The 1,2,5-telluradiazole as well as its methyl and phenyl derivatives melt with decomposition or decompose without melting at a temperature between 458 and 545 K and show very poor solubility in common solvents at room temperature. As a comparison the isologous 1,2,5-selenadiazole melts at 294 K and is soluble in common solvents (Bertini, 1967).

In order to clarify the structural features of 1,2,5-telluradiazole and therefore its rather strange physicochemical behaviour we carried out its X-ray crystal structure determination.

Experimental. Yellow-green parallelepipedal crystals obtained by slow crystallization from peroxide-free tetrahydrofuran in the dark, 0·75 × 0·20 × 0·02 mm, Philips PW 1100 diffractometer, graphite-monochromated Mo *Kα* radiation, 25 reflections having $5{\cdot}2 < \theta < 11{\cdot}2°$ used for measuring lattice parameters, no systematic loss of intensity of the 3 standard reflections 121, 321 and 420, 372 unique measured reflections with $\theta \leq 25°$, 339 with $I \geq 3\sigma(I)$, θ–2θ scan technique, $0 \leq h \leq 14$, $0 \leq k \leq 9$, $0 \leq l \leq 4$, absorption correction with numerical method, transmission factors between 0·24 and 0·85, Lp correction, scattering factors for non-hydrogen atoms (*International Tables for X-ray Crystallography,* 1974, p. 99), and for H atoms (Stewart, Davidson & Simpson, 1965), anomalous-dispersion corrections (*International Tables for X-ray Crystallography,* 1974, p. 149); heavy-atom method, full-matrix refinement, $\sum w(|F_o|-|F_c|)^2$ minimized, anisotropic thermal parameters, max. Δ/σ 0·26, final $R = 0{\cdot}031$, $R_w = 0{\cdot}032$, goodness of fit $S = 2{\cdot}12$, $w = 1/\sigma^2$, max. and min. $\Delta\rho$ excursions 0·88 and −0·99 e Å^{-3}, respectively; SEL 32/70 computer of the ISSECC of Florence, *SHELX76* program (Sheldrick, 1976) and *XRAY* system of programs (Stewart, Kundell & Baldwin, 1970).*

Discussion. Final atomic coordinates are given in Table 1; bond lengths and angles in Table 2.

Table 1. *Fractional atomic coordinates* ($\times 10^4$) *and equivalent isotropic* (*Hamilton,* 1959) *thermal parameters* (Å^2 × 10^4)

	x	*y*	*z*	U_{eq}
Te	−188 (1)	2500	−352 (1)	303 (4)
N	901 (5)	798 (7)	1386 (14)	357 (30)
C	1689 (6)	1594 (10)	2690 (17)	391 (36)
H	2212 (50)	1124 (65)	3559 (72)	648 (77)

Table 2. *Bond distances* (Å) *and angles* (°)

Te—N	2·023 (6)	C—C′	1·421 (11)
Te—N″	2·764 (6)	C—H	0·824 (55)
N—C	1·273 (10)		
N—Te—N′	82·5 (2)	Te′—N—C	140·0 (5)
N—Te—N″	69·4 (2)	N—C—C′	119·4 (7)
N″—Te—N‴	138·6 (2)	N—C—H	124 (4)
Te—N—C	109·4 (5)	C′—C—H	117 (4)
Te—N—Te′	110·6 (2)		

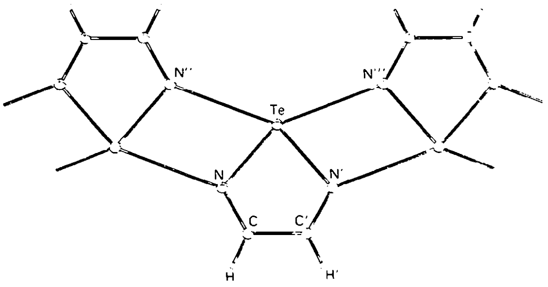

Fig. 1. View of the polymeric array of the structure.

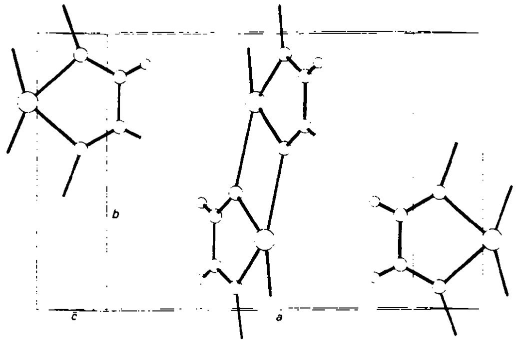

Fig. 2. Packing of the structure.

The 1,2,5-telluradiazole molecules are bonded together through weak bonds between tellurium and nitrogen atoms. The Te—N intermolecular distance [2·764 (6) Å] is much longer than the Te—N distance of the heterocyclic bond [2·023 (6) Å], but also remarkably shorter than the sum of the van der Waals radii of the same atoms (3·70 Å). Each tellurium atom forms two intra- and two intermolecular single bonds with nitrogen atoms, giving rise to a type of ribbon polymeric structure (Fig. 1), which accounts for the observed high melting point and low solubility of the substance. A perspective view of the unit cell is shown in Fig. 2. The spatial orientation of the four mentioned Te—N bonds may be considered planar; in fact the tellurium atom is only 0·023 (1) Å out of the plane, which by construction exactly pertains to the four bonded nitrogens. The heterocycle is close to its least-squares plane, deviations being less than 0·01 Å, and $\sum(\Delta/\sigma)^2$ being 3·70 compared with 5·99 for $\chi^2_{95\%}$. On the other hand, the plane individuated only by carbon and nitrogen atoms displaces the tellurium by 0·023 (1) Å. Such a displacement could assume a

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* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 39072 (4 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

further significance when the physical properties of the heterocycle in solution are examined.

The X-ray structure of 3,4-diphenyl-1,2,5-oxadiazole (Mellini & Merlino, 1976*b*) as well as those of 3,4-diphenyl-1,2,5-thiadiazole and 3,4-diphenyl-1,2,5-selenadiazole (Mellini & Merlino, 1976*a*) show that intermolecular bonds between nitrogen and chalcogen atoms are present only in the selenium derivative. Nevertheless, they are weaker than those observed in the 1,2,5-telluradiazole crystals and do not give rise to a ribbon polymeric structure.

A comparison of the interatomic N—C distances in the four isologous heterocycles shows an increasing localization of the double bond N=C on going from oxygen [1·330 (7) and 1·364 (7) Å] to sulphur [1·327 (5) and 1·342 (6) Å], selenium [1·298 (7) and 1·303 (7) Å] and tellurium [1·273 (10) Å]. The last value agrees well with the expected length (1·275 Å) for a double N=C bond; besides, the observed C—C distance [1·421 (11) Å] is not far from the value of 1·48 Å characteristic of a single C_{sp^2}—C_{sp^2} bond. The aromaticity in the 1,2,5-telluradiazole is therefore almost completely lost.

We wish to thank the ISSECC of Florence for collection of the intensity data and for computer time.

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Acta Cryst. (1984). C**40**, 655–657

Structure of 4-Amino-*N*-(4,6-dimethyl-2-pyrimidinyl)benzenesulphonamide (Sulfadimidine), $C_{12}H_{14}N_4O_2S$

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(*Received* 21 *February* 1983; *accepted* 6 *December* 1983)

Abstract. $M_r = 278·3$, monoclinic, $P2_1/c$, $a = 9·27$ (1), $b = 18·94$ (2), $c = 7·46$ (1) Å, $\beta = 97·3$ (3)°, $V = 1299$ (3) Å^3, $Z = 4$, $D_m = 1·465$ (1), $D_x = 1·423$ (3) Mg m^{-3}, λ(Cu $K\alpha$) = 1·5418 Å, μ(Cu $K\alpha$) = 2·28 mm^{-1}, $F(000) = 584$, room temperature. The structure was determined by direct methods and refined to an R value of 0·065 for 1681 observed reflexions. The mean planes of the benzene and pyrimidine rings are inclined to each other at 78·1 (6)°. The geometry around the S atom is considerably distorted from the ideal tetrahedral geometry. The structure is stabilized by a network of three-dimensional hydrogen bonds and van der Waals forces.

Introduction. Sulphonamides are widely used as antibacterial agents in medical practice. As a part of our programme on the X-ray structure determination of sulphonamides (Joshi, Tiwari, Patel & Singh, 1983), we report here the crystal structure of sulfadimidine.

Experimental. Thin platy crystals of sulfadimidine from the slow evaporation of a solution in acetonitrile at 283 K, crystal used: 0·81 × 0·32 × 0·72 mm. Unit-cell dimensions and space group from oscillation and Weissenberg photographs. Density by flotation in benzene/carbon tetrachloride. 1681 intensity data recorded photographically (h −11–7, k 0–24, l 0–6), 924 unobserved. Corrections for Lorentz and polarization factors and spot-shape distortions. Structure determined by *MULTAN* (Germain, Main & Woolfson, 1971) and by difference Fourier calculations. Refinement by block-diagonal least squares minimizing $\sum w(\Delta F)^2$. H atoms located by ΔF synthesis. Final R for 1681 observed reflexions = 0·065, $R_w = 0·069$, $S = 1·84$; $(\Delta/\sigma)_{\max} = 0·60$, final $\Delta\rho$ excursions −0·12–0·15 e Å^{-3}. The Hughes (1941) weighting function was used in the final cycle of the refinement with $F_{\min} = 8·0$. Atomic scattering factors from Cromer & Waber (1965) for non-hydrogen atoms and Stewart, Davidson & Simpson (1965) for H atoms.

0108-2701/84/040655-03$01.50