Table 1 (cont.)

	x	y	z	U_{11}
N(1)	−1354 (28)	3970 (8)	2642 (10)	29 (4)
N(2)	−3448 (32)	5032 (10)	1655 (12)	44 (5)
C(1)	−1467 (42)	3431 (14)	1880 (15)	46 (6)
C(2)	17 (51)	2689 (15)	2275 (18)	63 (7)
C(3)	−120 (54)	3801 (16)	1178 (19)	75 (9)
C(4)	−3789 (52)	3196 (16)	1516 (18)	68 (8)
C(5)	−4500 (40)	5812 (12)	1532 (14)	39 (5)
C(6)	−4410 (50)	6272 (14)	2382 (18)	62 (7)
C(7)	−6868 (57)	5660 (18)	1125 (20)	77 (9)
C(8)	−3323 (62)	6172 (17)	845 (22)	81 (9)
C(9)	1316 (50)	4041 (15)	5312 (18)	61 (7)
C(10)	2615 (56)	3486 (19)	5064 (19)	77 (8)

Table 2. Bond angles with e.s.d.'s

N(1)–S(1)–N(2)	113 (1)°
S(1)–N(1)–C(1)	125 (1)
S(1)–N(1)–Pt(1)	107 (1)
C(1)–N(1)–Pt(1)	127 (1)
S(1)–N(2)–C(5)	118 (1)
N(1)–C(1)–C(2)	104 (2)
N(1)–C(1)–C(3)	107 (2)
N(1)–C(1)–C(4)	113 (2)
C(2)–C(1)–C(3)	104 (2)
C(2)–C(1)–C(4)	112 (2)
C(3)–C(1)–C(4)	115 (2)
N(2)–C(5)–C(6)	114 (2)
N(2)–C(5)–C(7)	106 (2)
N(2)–C(5)–C(8)	102 (2)
C(6)–C(5)–C(7)	110 (2)
C(6)–C(5)–C(8)	114 (2)
C(7)–C(5)–C(8)	109 (2)

sulphurdiimine group is N-bonded to the metal and situated opposite to the ethylene molecule. The ethylene bond is perpendicular (86)° to the coordination plane of the platinum atom, the sulphurdiimine molecule makes an angle of 71° with this plane.

The sulphurdiimine group provides two independent measure values for the length of the rare double bond between sulphur and nitrogen. This bond was estimated to be 1·54 Å (Goehring, 1956) and up till now only two determinations of 1·53 and 1·54 Å (Webb & Gloss, 1967; Neidle & Rogers, 1970) were known. Our average S–N-length of 1·55 (2) is in agreement with these values. For comparison the single bond S–N has a length of 1·63 (1) Å.

The di-t-butyl-sulphurdiimine molecule is in the cis–trans conformation. C(6) of the t-butyl group C(5)C(6)C(7)C(8) eclipses the double bond S(1)–N(2). In the other t-butyl group C(2) eclipses the ligand bond Pt(1)–N(1).

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SHORT COMMUNICATIONS

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.

The unit cell of a mixed crystal of guanine and 8-azaguanine. By JOHN J. MADDEN,* *Crystallography Department, University of Pittsburgh, Pittsburgh, Pa.* 15213, *U.S.A.*

Guanine ($C_5H_5N_5O$), 8-azaguanine ($C_4H_4N_6O$), and water co-crystallize in the space group $P2_1/c$, with $a = 3·56$ (3), $b = 11·37$ (11), $c = 16·32$ (16) Å, $\beta = 95·33$ (9)°, and $Z = 4$, a form isomorphous with the published structure of 8-azaguanine monohydrate.

A mixed crystal of guanine and 8-azaguanine was prepared by slowly cooling a warm equimolar solution of these compounds in 1M acetic acid. These crystals are isomorphous

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with the published structure of 8-azaguanine (Macintyre, Singh & Werkema, 1965; Sletten, Sletten & Jensen, 1968) as judged by a comparison of the cell parameters for these compounds (Table 1) and the structure factor amplitudes of reflections on two zero-layer precession projectors (a^*b^* and a^*c^*). The intensities for these reflections were visually estimated as absent, weak, medium, and strong and struc-

ture-factor amplitudes calculated. The independent reflections thus calculated yielded $R = 17\%$ when compared with those for 8-azaguanine $(R = \sum ||F_A| - |F_M||/\sum |F_A| \times 100$, where $F_A =$ structure-factor amplitudes for 8-azaguanine [Sletten et al., 1968], and $F_M =$ structure-factor amplitudes for the mixed crystals).

Table 1. *Unit-cell parameters for 8-azaguanine* (*Sletten et al., 1968*), *guanine* (*Thewalt et al., 1971*) *and for the mixed crystal*

	Mixed crystal	8-Azaguanine	Guanine
a	3·57 (3) Å	3·5629 (5) Å	3·645 (5) Å
b	11·37 (11)	11·4404 (9)	11·277 (8)
c	16·32 (16)	16·4685 (16)	16·510 (8)
β	95·33 (9)°	95·13 (1)°	96·8 (1)°
Space group	$P2_1/c$	$P2_1/c$	$P2_1/n$
Z	4	4	4
D_x	~1·68 g cm^{-3}	1·691 g cm^{-3}	1·67 g cm^{-3}
D_m	1·65	1·687 (8)	—

The presence of both guanine and 8-azaguanine in these crystals was confirmed by dissolving exhaustively washed crystals and separating the compounds by column chromatography on Sephadex G-10 (Sweetman & Nyhan, 1968). Optical density measurements on the separated components indicated a two-to-one ratio, azaguanine to guanine, of the compounds in the mixed crystals.

A comparison of the crystal structures of 8-azaguanine monohydrate and of guanine monohydrate (Thewalt, Bugg & Marsh, 1971) has shown that guanine can substitute in

the azaguanine lattice by a single change in the hydrogen-bonding scheme at C(8) [N(8) for 8-azaguanine], as noted by Thewalt et al., 1971. Such a change can occur by adjusting the position of the water molecule in the asymmetric unit, and this is presumably the mechanism for the formation of the mixed crystal. I therefore propose that in the mixed crystal, molecules of guanine and 8-azaguanine occupy isomorphous positions, and that the difference between an asymmetric unit containing guanine and one containing 8-azaguanine lies in the position of the water molecule in the asymmetric unit and in the hydrogen-bonding scheme between position 8 of the base and the water molecule. No further work on the three-dimensional, X-ray analysis of the structure is contemplated.

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The N–S bond lengths in the isomers $S_6(NH)_2$. Refinement of the crystal structure of $S_6(NH)_2$–II.

By H. J. POSTMA, F. VAN BOLHUIS and AAFJE VOS, *Laboratorium voor Structuurchemie, Rijksuniversiteit Groningen, Zernikelaan, Paddepoel, Groningen, The Netherlands*

Refinement of the crystal structure of $S_6(NH)_2$–II has shown that the average length of the N–S bonds in $S_6(NH)_2$–II, 1·680 Å, is approximately equal to the length found in $S_6(NH)_2$–III, 1·672 Å, but smaller than the value observed in $S_6(NH)_2$–I, 1·724 Å. As suggested in an earlier paper the large value observed for the latter compound may be due to disorder.

In a previous paper (Postma, van Bolhuis & Vos, 1971; hereafter referred to as PBV) the average elongation of 0·052 Å of the N–S bonds in $S_6(NH)_2$–I relative to those in $S_6(NH)_2$–III has tentatively been ascribed to disorder in $S_6(NH)_2$–I. The N–S values in $S_6(NH)_2$–II determined by Weiss (1960) were not sufficiently accurate to be compared

Table 1. *Crystallographic data and experimental details*

Data	Method
Space group *Pnma*, $Z = 4$	Weissenberg photographs.
$a = 7\cdot873$ (1) Å	Weissenberg photographs of zero-layer lines;
$b = 12\cdot858$ (2)	$\lambda(Cu\ K\alpha) = 1\cdot5418$, $\lambda(Cu\ K\alpha_1) = 1\cdot54051$,
$c = 7\cdot390$ (1)	$\lambda(Cu\ K\alpha_2) = 1\cdot54433$ Å. Calibration with NaCl reflexion spots. Least-squares adjustment of 17 0*kl* and 22 *hk*0 reflexions.
Crystal size	$0\cdot46 \times 0\cdot44 \times 0\cdot55$ mm.
1682* reliable intensities *hkl*	Computer automated Nonius four-circle diffractometer, Mo-radiation, Zr-filtered, θ–2θ scan, $\sin\theta/\lambda \leq 0\cdot995$ Å^{-1}.
1682 reliable $F(hkl)$ values	Correction for L.P. and for absorption $(\mu = 16\cdot5$ cm$^{-1})$†

* Not including the strong reflexion 020, which was omitted as its intensity was badly influenced by streaks.

† According to the Busing & Levy (1957) scheme.