are stacked along **b** and the Na^+ ion is six-coordinated to oxygen forming triangular prisms. In this case, of course, the NO_2^- groups are oriented with their dipole moments parallel.

$NaClO_2$ is close to orthorhombic since the cell can be transformed to an orthogonal cell by **T**=201/010/001, where, approximately, $a'=11{\cdot}02$, $b'=6{\cdot}42$, $c'=6{\cdot}85$ Å. However, this cannot be considered truly orthorhombic because of the missing mirror symmetry in the intensities.

The sodium chlorite structure may be described in the equivalent space group $C2/c$ by applying the transformation matrix $\mathbf{T}=-101/010/100$; $\mathbf{TA}=\mathbf{B}$ converts the cell parameters **A** in $I2/a$ to those **B** in $C2/c$ and the inverse $\mathbf{XT}^{-1}=\mathbf{Y}$, where $\mathbf{T}^{-1}=00-1/010/10-1$, gives the new atom coordinates **Y** in $C2/c$.

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Note on the Space Group Reported for the Dimeric 6-Mercaptopurine Copper(I) Chloride Complex

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Abstract. The space group is $P\bar{1}$ and not $P1$; the asymmetric unit is $[C_5H_5N_4S.CuCl_2.H_2O]$. The structure has now been refined in $P\bar{1}$ to $R=0{\cdot}046$ for 1584 observed data and yields satisfactory bond lengths and angles.

Introduction. Caira & Nassimbeni (1975) reported the structure of the 6-mercaptopurine copper(I) chloride complex as having the space group $P1$ thus requiring the dimer not only to be the asymmetric unit but also to be chiral. However, if the fractional atomic coordinates as published are summed for each equivalent pair of atoms *A–B*, then it is evident that the sums are identical and that the two halves *A* and *B* are related by a pseudo-centre of inversion at 0·847, −0·153, −0·089. Although R was low (0·051), the standard deviations were high and some chemically equivalent bonds differed in length by over 0·1 Å, *e.g.* C(8)–N(9) *A* 1·39, *B* 1·27 Å; C(4)–C(5) *A* 1·32, *B* 1·41 Å; C(2)–N(3) *A* 1·39, *B* 1·24 Å; N(1)–C(6) *A* 1·44, *B* 1·33 Å (e.s.d. of 0·03 Å in each case, so these differences are as great as 5σ). The planes of the two mercaptopurine units have closely similar direction cosines (0·321, 0·314; 0·884, 0·878; −0·340, −0·360) and thus, within the quoted standard deviations, the planes of these two units are parallel and related by the same pseudo-centre. That a dimeric molecule should apparently retain a centre of inversion yet pack in a non-centrosymmetric space group is most unusual (Kitaigorodskii, 1961).

A statistical analysis of the intensities had originally shown strong indications that the space group was centrosymmetric (av. $|E^2-1|=0{\cdot}965$, av. $|E|=0{\cdot}803$, $|E|>1=31{\cdot}7\%$, $|E|>2=4{\cdot}7\%$, $|E|>3=0{\cdot}1\%$) but repeated attempts to solve the structure in $P\bar{1}$ by both vector and direct methods had failed. The refinement in $P1$ yielded very large correlation coefficients between atomic parameters for each pair of atoms *A–B*; for the Cl and S atoms the mean value of the correlation coefficients for corresponding positional parameters was 0·90.

The structure has been re-examined and successfully refined in $P\bar{1}$ to $R=0{\cdot}046$ and $R_w=0{\cdot}052$ for 1584 reflexions* with $I>2{\cdot}5\sigma I$. The weighting scheme was $w=1/\sigma^2F+gF^2$ with $g=0{\cdot}00196$ chosen to give the

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* A list of structure factors has been deposited with the British Library Lending Division as Supplementary Publication No. SUP 31398 (11 pp., 1 microfiche). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 1. *Final atomic coordinates* ($\times 10^4$) *and thermal parameters* ($\times 10^3$)

(*a*) Heavy atoms

Anisotropic temperature factors refer to the expression

$$T=\exp\,[-2\pi^2(U_{11}h^2a^{*2}+U_{22}k^2b^{*2}+U_{33}l^2c^{*2}+2U_{12}hka^*b^*+2U_{13}hla^*c^*+2U_{23}klb^*c^*)\times 10^3].$$

	x	y	z	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Cu	1530 (1)	1532 (1)	910 (1)	21 (0)	48 (0)	29 (0)	16 (0)	−6 (0)	−17 (0)
Cl(1)	1751 (1)	3029 (1)	4057 (1)	23 (1)	37 (1)	20 (1)	16 (0)	−9 (0)	−18 (0)
Cl(2)	3713 (1)	1298 (1)	877 (1)	16 (1)	32 (1)	19 (1)	5 (0)	2 (0)	−4 (0)
S	−339 (1)	1776 (1)	−1725 (1)	14 (1)	25 (1)	18 (1)	8 (0)	−1 (0)	−9 (0)
N(1)	−1098 (3)	3452 (4)	1155 (5)	14 (2)	21 (2)	17 (2)	4 (1)	−4 (1)	−12 (1)
C(2)	−1938 (4)	4245 (5)	1972 (6)	20 (2)	22 (2)	20 (2)	4 (2)	0 (2)	−9 (2)
N(3)	−3208 (3)	4461 (4)	972 (5)	15 (2)	18 (2)	16 (2)	8 (1)	−1 (1)	−5 (1)
C(4)	−3595 (4)	3771 (4)	−972 (5)	14 (2)	11 (2)	16 (2)	2 (1)	0 (1)	−2 (1)
C(5)	−2800 (4)	2941 (5)	−1895 (5)	14 (2)	13 (2)	12 (2)	3 (1)	−0 (1)	−3 (1)
C(6)	−1440 (4)	2747 (4)	−797 (5)	15 (2)	11 (2)	12 (2)	0 (1)	−2 (1)	−4 (1)
N(7)	−3596 (3)	2417 (4)	−3859 (5)	17 (2)	20 (2)	10 (1)	4 (1)	−3 (1)	−5 (1)
C(8)	−4828 (4)	2915 (5)	−4127 (6)	19 (2)	22 (2)	17 (2)	5 (2)	−2 (2)	−2 (2)
N(9)	−4863 (3)	3750 (4)	−2408 (4)	14 (2)	24 (2)	14 (2)	8 (1)	−2 (1)	−1 (1)
O	2770 (4)	−486 (4)	−3572 (4)	51 (2)	42 (2)	23 (2)	19 (2)	4 (2)	−11 (1)

Table 1 (*cont.*)

(*b*) Hydrogen atoms: theoretical positions ($\times 10^3$)

	x	y	z
H(1)	−7	338	213
H(2)	−154	472	356
H(7)	−328	172	−499
H(8)	−568	269	−553
H(9)	−573	430	−219

Table 2. *Bond lengths* (Å) *and angles* (°) *and their e.s.d.'s*

Cu—Cl(1)	2·365 (2)	N(3)–C(4)	1·350 (5)
Cu—Cl(2)	2·243 (2)	C(4)–C(5)	1·377 (6)
Cu—S	2·252 (2)	C(5)–C(6)	1·405 (5)
Cu—S^{i}	2·733 (2)	C(5)–N(7)	1·374 (4)
C(6)–S	1·691 (5)	N(7)–C(8)	1·329 (6)
C(6)–N(1)	1·362 (5)	C(8)–N(9)	1·344 (5)
N(1)–C(2)	1·355 (6)	N(9)–C(4)	1·378 (4)
C(2)–N(3)	1·315 (5)		

Cl(1)–Cu—Cl(2)	106·2 (1)	N(1)–C(2)–N(3)	124·5 (3)
Cl(1)–Cu—S	117·3 (1)	C(2)–N(3)–C(4)	112·1 (3)
Cl(2)–Cu—S	129·6 (6)	N(3)–C(4)–C(5)	126·5 (3)
Cl(1)–Cu—S^{i}	99·3 (1)	C(4)–C(5)–C(6)	120·2 (3)
Cl(2)–Cu—S^{i}	104·7 (1)	C(6)–C(5)–N(7)	132·2 (4)
S——Cu—S^{i}	92·8 (1)	C(4)–C(5)–N(7)	107·5 (3)
Cu—S——Cu^{i}	87·2 (1)	C(5)–N(7)–C(8)	107·9 (4)
Cu—S——C(6)	108·0 (1)	N(7)–C(8)–N(9)	110·1 (3)
Cu^{i}—S——C(6)	92·6 (1)	C(8)–N(9)–C(4)	107·6 (3)
N(1)–C(6)–S	123·1 (3)	N(9)–C(4)–C(5)	106·9 (3)
S——C(6)–C(5)	125·6 (3)	N(3)–C(4)–N(9)	126·6 (4)
N(1)–C(6)–C(5)	111·2 (4)		
C(6)–N(1)–C(2)	125·5 (3)		

smallest variation of $w\Delta^2$ with $|F|$. All non-hydrogen atoms were treated anisotropically. The H atoms were subjected to constrained refinement 1·08 Å from their parent atoms and were assigned a common isotropic temperature factor which refined to $U=0{\cdot}038$ Å^2. All calculations were done with the SHEL-X program system (Sheldrick, 1976). The revised atomic parameters, bond lengths and angles are listed in Tables 1 and 2. The conclusions about the true symmetry of the structure, based solely upon the published atomic coordinates and simple chemical grounds, are confirmed by this reinvestigation. The present problem is reminiscent of the classic case of dibenzyl disulphide (Donohue, 1974).

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