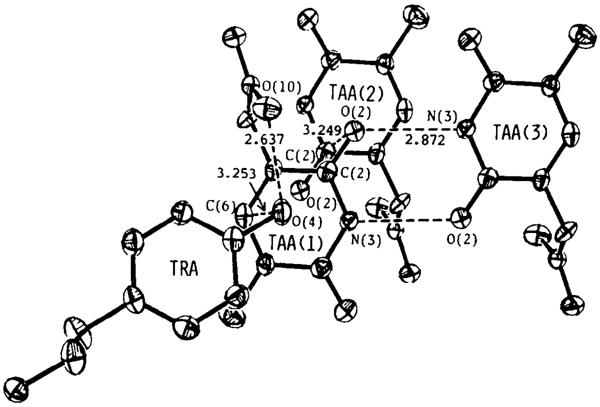

Fig. 3. Partial projection of the molecular packing on to the plane of the TAA(1) pyrimidine ring. The symmetry operations for the TAA(1), TAA(2), TAA(3) and TRA molecules are (x,y,z), $(1-x, -y, 1-z)$, $(1-x, -1-y, 1-z)$ and $(\frac{1}{2}-x, \frac{1}{2}+y, -z)$, respectively.

CNDO/2 method, are −0·23 and +0·15 e Å^{-3}, respectively, so the atoms come close together (3·253 Å) because of an electrostatic interaction.

The structural study of the staphylococcal nuclease–thymidine 3′,5′-diphosphate–Ca^{2+} complex at 1·5 Å resolution (Cotton, Hazen & Legg, 1979) indicates that the thymine ring and the phenol ring of Tyr-113 are almost parallel but are not stacked with each other. On the other hand, as mentioned in the *Introduction*, studies of the interactions between nucleic acids and tyrosine, made by Hélène and co-workers and Cautrecasas *et al.* (1967), suggest the occurrence of stacking and hydrogen-bonding interactions. In the present structural study of the TAA–TRA complex, no hydrogen bond between the thymine ring and the phenolic hydroxyl group was observed, but a hydrogen bond occurs between the carboxyl and hydroxyl groups. It is also interesting to note that the weak interaction between the thymine and phenol rings is probably due to electrostatic or π–π interactions.

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The β Form of Piperidinium 1-Piperidinecarbodithioate

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Abstract

$[C_5H_{12}N]^+$ $[C_6H_{10}NS_2]^-$, monoclinic, $P2_1$, with a = 12·395 (2), b = 15·459 (2), c = 14·320 (2) Å, β = 93·35 (2)°, Z = 8, V = 2739·3 Å^3, D_x = 1·195 Mg m^{-3}. The non-centrosymmetric structure has been refined to $R(F^2)$ = 0·110 for 4991 reflexions and 892 parameters. The structure is built up of two indepen-

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dent dimers with pseudo symmetry $2/m$. Each pseudo-centrosymmetric dimer is composed of two cations and two anions connected by eight N—H···S hydrogen bonds (of which one is weak in one of the dimers). The dimers are packed at van der Waals distances.

Introduction

Systematic structural studies have been performed on $[R_2NH_2]^+[R_2NCS_2]^-$ salts, where R is an alkyl substituent (Wahlberg, 1978*a*,*b*,*c*, 1979, 1980). The present investigation forms part of these studies.

The title compound was synthesized in benzene from piperidine and carbon disulphide (analogous to Wahlberg, 1978*a*), and was recrystallized by evaporation at room temperature from a mixture of benzene and petroleum (b.p. 333–358 K). Two phases, α and β, of transparent pale-yellow crystals were obtained simultaneously. The structure investigation of the α form is in progress (Wahlberg, 1980).

The crystals of the β form appeared as compact parallelepipeds. They sublimed and decomposed on heating. Systematically absent reflexions among $0k0$ for k odd indicated the space groups $P2_1$ or $P2_1/m$. The latter is inconsistent with the final structure. The cell parameters were based on 32 lines from a Guinier–Hägg powder photograph. The internal standard was CoP_3 ($a = 7{\cdot}70778$ Å) and the radiation was Cr $K\alpha_1$ ($\lambda = 2{\cdot}289753$ Å).

A crystal was sealed in a thin-walled glass capillary. Three pairs of surfaces, $(\bar{1}11)$, $(11\bar{1})$ and (101), were all separated by *ca* 0·13 mm. Intensities were collected on a Stoe–Philips four-circle PDP 8/I computer-controlled diffractometer with graphite-monochromatized Mo $K\alpha$ radiation. The count rate was reduced by a factor 2^n, $0 \leq n \leq 5$ (three filters and scan speed). Reflexions within the ranges $-14 \leq h \leq 14$, $0 \leq k \leq 18$ and $0 \leq l \leq 17$ were measured in the ω–2θ mode. The longest scan time was 160 s. The background was measured on each side of a reflexion for 25 s. The intensities of three standard reflexions, 404, $\bar{1}43$ and $\bar{3}\bar{3}3$, measured at intervals of 40 reflexions decreased by *ca* 3%. It was found that the decrease was satisfactorily described by a least-squares line, which was used to scale the data to the mean level. Corrections were applied for background and for Lorentz, polarization and absorption effects [μ(Mo $K\alpha$) = 0·347 mm^{-1}]. The transmission factor varied from 0·95 to 0·97. 6051 reflexions within $0{\cdot}062 < (\sin\theta)/\lambda \leq 0{\cdot}595$ Å^{-1} were reduced to 4991 independent structure factors with $F_m^2 \geq -1{\cdot}70\sigma(F^2)$; 2700 had $F_m^2 < 3{\cdot}0\sigma(F^2)$.

The structure was solved by *MULTAN* (Germain, Main & Woolfson, 1971). The H atom positions were introduced empirically. The scale factor and the non-hydrogen-atom coordinates and isotropic thermal parameters were initially refined by the full-matrix least-squares *UPALS* program (Lundgren, 1976). F_c was kept on an absolute scale. F_m was corrected for non-hydrogen-atom anomalous-dispersion f' terms (*International Tables for X-ray Crystallography*, 1974). The refinement then proceeded by a local version of the block-diagonal least-squares *ORFLS* program (Busing, Martin & Levy, 1962), with scaling on F_c. Eight independent molecular ions formed separate blocks. The thermal parameters of the non-hydrogen atoms were anisotropic. The coordinates and the isotropic thermal parameters of all the H atoms were varied. All structure factors were included in the last cycle, where 892 parameters were varied. The expression minimized was $\sum w\delta^2$, where $\delta = F_m^2 - F_c^2$ and $w^{-1} = \sigma^2(F^2) = \sigma^2_{\text{count}}(F^2) + (0{\cdot}03\ F_m^2)^2$. The refinement converged at $R(F^2) = \sum|\delta|/\sum F_m^2 = 0{\cdot}110$ and $R_w(F^2) = (\sum w\delta^2/\sum wF_m^4)^{1/2} = 0{\cdot}101$. The coordinates are presented in Table 1.* The largest parametric $|\Delta|/\sigma$ was 0·4 for y[1C(1)], U_{33}[1C(2)], y[5S(1)], z[5C(3)], z[6C(5)], x[1H(9)], x[4H(6)], y[6H(3)], U_{iso}[6H(3)] and z[7H(1)]; the average value was 0·100. $|\delta|/\sigma(F^2)$ was $\geq 2{\cdot}0$ for 169 reflexions. A normal δR probability plot (Abrahams & Keve, 1971) had a slope of 1·13 and an intercept of 0·03. A difference synthesis showed some peaks of density $\leq$

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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 35251 (24 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Table 1. *Decimal parts of the fractional coordinates and isotropic thermal parameters B* (Å^2) *defined from* $\exp\{-B[(\sin\theta)/\lambda]^2\}$

For the non-hydrogen atoms the alternative values B_{eq} (Å^2) corresponding to the anisotropic temperature-factor coefficients are given. The atomic labels are preceded by the numbering of the molecular ions.

	x	y	z	B		x	y	z	B
1S(1)	77244 (14)	07320 (12)	49725 (12)	4·65	5S(1)	24267 (15)	03963 (16)	00871 (12)	6·50
1S(2)	54792 (15)	01000	50331 (12)	6·04	5S(2)	00249 (15)	02804 (13)	99302 (13)	4·80
1N	6950 (4)	−0053 (4)	6439 (4)	4·61	5N	1253 (4)	−0120 (4)	1457 (3)	4·50
1C(1)	6722 (5)	0227 (4)	5565 (4)	3·55	5C(1)	1231 (5)	0144 (4)	0572 (4)	3·79
1C(2)	7986 (7)	0116 (7)	6983 (6)	5·96	5C(2)	2231 (7)	−0268 (8)	2037 (6)	6·70
1C(3)	7782 (7)	0629 (7)	7841 (5)	6·05	5C(3)	2277 (7)	0319 (7)	2886 (6)	6·46
1C(4)	6974 (7)	0194 (6)	8461 (6)	5·85	5C(4)	1308 (7)	0190 (7)	3453 (6)	6·30

Table 1 (*cont.*)

	x	*y*	*z*	*B*		*x*	*y*	*z*	*B*
1C(5)	5964 (9)	–0030 (8)	7852 (7)	6·22	5C(5)	0287 (7)	0294 (7)	2821 (6)	6·28
1C(6)	6184 (7)	–0525 (6)	6978 (6)	5·91	5C(6)	0274 (8)	–0292 (7)	1974 (6)	6·22
1H(3)	812 (6)	–052 (5)	716 (6)	7 (3)	5H(3)	220 (5)	–097 (5)	217 (5)	4 (2)
1H(4)	846 (6)	040 (5)	662 (5)	6 (3)	5H(4)	288 (5)	–020 (4)	177 (4)	3 (2)
1H(5)	840 (5)	069 (4)	821 (4)	4 (2)	5H(5)	291 (4)	007 (3)	323 (3)	1 (1)
1H(6)	739 (6)	120 (5)	766 (5)	6 (3)	5H(6)	231 (6)	095 (5)	261 (5)	6 (3)
1H(7)	724 (5)	–045 (5)	863 (5)	5 (2)	5H(7)	140 (5)	–046 (4)	362 (4)	2 (2)
1H(8)	681 (5)	058 (5)	897 (5)	5 (2)	5H(8)	124 (6)	058 (5)	392 (5)	5 (2)
1H(9)	535 (6)	–026 (5)	807 (5)	6 (3)	5H(9)	–032 (4)	006 (3)	308 (3)	1 (1)
1H(10)	568 (6)	042 (4)	775 (5)	2 (2)	5H(10)	031 (6)	099 (5)	266 (5)	6 (3)
1H(11)	656 (5)	–111 (4)	717 (4)	4 (2)	5H(11)	048 (5)	–087 (4)	215 (4)	2 (2)
1H(12)	545 (4)	–051 (3)	660 (3)	1 (1)	5H(12)	–030 (5)	–015 (4)	158 (4)	3 (2)
2S(1)	67207 (15)	28681 (15)	25231 (11)	5·38	6S(1)	20305 (15)	28589 (15)	76591 (12)	5·85
2S(2)	45283 (14)	21087 (13)	26101 (11)	4·35	6S(2)	–01815 (14)	21713 (14)	73740 (11)	5·11
2N	5259 (4)	2834 (4)	1092 (3)	4·42	6N	0837 (5)	2979 (4)	6057 (4)	5·20
2C(1)	5474 (5)	2627 (4)	1990 (4)	4·08	6C(1)	0874 (5)	2694 (4)	6946 (4)	4·12
2C(2)	6010 (7)	3321 (6)	0502 (6)	4·94	6C(2)	1756 (9)	3394 (8)	5621 (8)	7·68
2C(3)	6291 (7)	2763 (6)	–0312 (6)	5·51	6C(3)	2040 (7)	2914 (8)	4771 (7)	7·66
2C(4)	5280 (7)	2465 (6)	–0901 (5)	5·18	6C(4)	1103 (7)	2770 (7)	4095 (5)	6·14
2C(5)	4514 (8)	2037 (8)	–0265 (6)	6·22	6C(5)	0168 (8)	2376 (7)	4580 (6)	7·11
2C(6)	4249 (6)	2597 (6)	0562 (5)	4·98	6C(6)	–0110 (7)	2885 (7)	5414 (6)	6·04
2H(3)	562 (5)	378 (4)	025 (4)	3 (2)	6H(3)	130 (6)	382 (5)	550 (6)	4 (3)
2H(4)	659 (5)	345 (4)	091 (4)	2 (2)	6H(4)	248 (6)	347 (5)	619 (5)	9 (3)
2H(5)	671 (5)	311 (4)	–072 (4)	3 (2)	6H(5)	247 (4)	317 (4)	453 (4)	1 (2)
2H(6)	661 (4)	218 (4)	–020 (3)	1 (1)	6H(6)	238 (4)	224 (4)	498 (4)	2 (1)
2H(7)	489 (5)	293 (4)	–126 (4)	4 (2)	6H(7)	083 (4)	329 (4)	375 (4)	1 (1)
2H(8)	558 (5)	206 (4)	–141 (4)	4 (2)	6H(8)	124 (5)	241 (5)	343 (5)	7 (2)
2H(9)	396 (4)	186 (4)	–062 (4)	1 (1)	6H(9)	–038 (4)	229 (4)	421 (4)	1 (1)
2H(10)	481 (7)	156 (5)	–008 (6)	7 (3)	6H(10)	041 (6)	163 (5)	479 (5)	8 (3)
2H(11)	388 (4)	317 (3)	036 (4)	0 (1)	6H(11)	–042 (6)	345 (5)	525 (5)	5 (2)
2H(12)	364 (5)	229 (4)	109 (4)	5 (2)	6H(12)	–070 (5)	254 (4)	581 (4)	3 (2)
3N	6430 (5)	0558 (4)	2874 (4)	3·96	7N	1774 (4)	0616 (4)	7932 (4)	3·59
3C(2)	5654 (7)	–0122 (5)	2599 (5)	4·32	7C(2)	1073 (7)	–0027 (6)	7474 (6)	5·98
3C(3)	5337 (7)	–0074 (6)	1543 (5)	5·19	7C(3)	1058 (9)	0046 (8)	6412 (7)	7·48
3C(4)	6334 (7)	–0127 (6)	1002 (5)	5·50	7C(4)	2202 (8)	–0016 (7)	6083 (6)	6·08
3C(5)	7120 (7)	0583 (7)	1292 (6)	5·68	7C(5)	2886 (8)	0652 (8)	6551 (6)	6·90
3C(6)	7425 (7)	0497 (7)	2360 (6)	5·41	7C(6)	2902 (6)	0565 (7)	7616 (5)	5·16
3H(1)	657 (4)	055 (4)	353 (4)	2 (1)	7H(1)	187 (6)	051 (5)	871 (5)	8 (2)
3H(2)	604 (4)	113 (4)	280 (4)	2 (2)	7H(2)	143 (4)	110 (3)	775 (3)	–1 (1)
3H(3)	600 (5)	–069 (4)	286 (4)	4 (2)	7H(3)	143 (5)	–059 (4)	767 (4)	2 (2)
3H(4)	498 (5)	–005 (4)	290 (4)	3 (2)	7H(4)	032 (4)	–001 (4)	781 (4)	3 (1)
3H(5)	476 (5)	–053 (4)	143 (4)	2 (2)	7H(5)	066 (6)	–048 (5)	623 (5)	5 (2)
3H(6)	506 (5)	055 (4)	146 (4)	2 (2)	7H(6)	072 (6)	060 (5)	631 (5)	5 (3)
3H(7)	678 (5)	–076 (4)	122 (4)	4 (2)	7H(7)	240 (6)	–057 (5)	620 (5)	4 (2)
3H(8)	609 (5)	–009 (4)	044 (4)	2 (2)	7H(8)	215 (6)	008 (5)	543 (5)	8 (3)
3H(9)	786 (6)	044 (5)	111 (5)	7 (3)	7H(9)	364 (5)	057 (4)	643 (4)	2 (2)
3H(10)	691 (6)	113 (4)	124 (5)	3 (2)	7H(10)	259 (6)	119 (5)	643 (5)	4 (3)
3H(11)	757 (5)	–013 (4)	259 (4)	4 (2)	7H(11)	311 (5)	–004 (4)	781 (4)	2 (2)
3H(12)	779 (4)	087 (4)	255 (4)	0 (2)	7H(12)	314 (5)	107 (5)	792 (5)	4 (2)
4N	5886 (5)	2341 (4)	4690 (4)	3·91	8N	0510 (5)	2371 (4)	9594 (4)	4·65
4C(2)	4876 (8)	2432 (7)	5209 (7)	6·58	8C(2)	–0561 (7)	2699 (7)	9827 (6)	5·69
4C(3)	5073 (7)	2398 (6)	6211 (6)	6·36	8C(3)	–0762 (8)	2566 (8)	0854 (7)	7·14
4C(4)	5932 (7)	3033 (6)	6558 (6)	5·40	8C(4)	0163 (8)	3000 (7)	1440 (6)	6·86
4C(5)	6960 (6)	2879 (7)	6048 (5)	5·26	8C(5)	1221 (8)	2653 (7)	1173 (6)	6·15
4C(6)	6729 (7)	2984 (6)	5026 (6)	5·28	8C(6)	1380 (7)	2778 (7)	0163 (5)	5·60
4H(1)	568 (4)	237 (4)	402 (4)	3 (2)	8H(1)	056 (4)	239 (3)	890 (4)	1 (1)
4H(2)	599 (5)	179 (4)	483 (5)	3 (2)	8H(2)	045 (4)	179 (3)	972 (3)	0 (1)
4H(3)	472 (6)	300 (4)	501 (6)	4 (3)	8H(3)	–049 (6)	327 (5)	970 (5)	4 (2)
4H(4)	439 (5)	198 (4)	497 (4)	3 (2)	8H(4)	–114 (4)	232 (4)	948 (4)	2 (2)
4H(5)	446 (5)	255 (4)	655 (4)	3 (2)	8H(5)	–138 (6)	298 (5)	098 (5)	5 (2)
4H(6)	544 (5)	173 (4)	638 (4)	2 (2)	8H(6)	–069 (6)	194 (4)	098 (5)	4 (2)
4H(7)	572 (4)	364 (4)	650 (4)	1 (2)	8H(7)	004 (6)	370 (5)	125 (5)	7 (3)
4H(8)	607 (5)	299 (5)	721 (4)	3 (2)	8H(8)	004 (5)	298 (5)	206 (5)	4 (2)
4H(9)	749 (6)	332 (5)	630 (5)	6 (3)	8H(9)	178 (6)	298 (5)	148 (5)	5 (2)
4H(10)	724 (5)	229 (5)	624 (4)	4 (2)	8H(10)	129 (5)	202 (4)	137 (4)	3 (2)
4H(11)	639 (5)	356 (4)	477 (5)	4 (2)	8H(11)	132 (5)	342 (4)	998 (4)	3 (2)
4H(12)	722 (5)	289 (4)	468 (4)	2 (2)	8H(12)	200 (5)	247 (4)	991 (5)	5 (2)

0·49 e Å^{-3}. The strongest reflexion, 040, was slightly affected by extinction. Scattering factors were taken from *International Tables for X-ray Crystallography* (1974). No attempt was made to determine the absolute configuration by the introduction of f'' anomalous-dispersion terms (*cf.* Wahlberg, 1979). Lundgren (1976) has described the computer programs. The calculations were performed on the IBM 370/155-158 and IBM 1800 computers in Uppsala.

Discussion

Four formula units, or eight molecular ions, are structurally independent and build up two dimers, (I) and (II), shown in Figs. 1 and 2. These dimers are nearly centrosymmetric and have approximate $2/m$ symmetry. They are almost parallel in the structure and are approximately related by $\frac{1}{2},0,\frac{1}{2}$. Dimer (II) is less regular than dimer (I), which may be seen from the figures. The intra-dimeric N—H···S hydrogen-bond distances are given in Table 2. The occurrence of

Table 2. N—H···S *hydrogen bonds* (Å)

	H···S	N···S
Dimer (I)		
3H(1)···1S(1)	2·46 (5)	3·334 (6)
4H(2)···1S(1)	2·70 (7)	3·382 (7)
3H(1)···1S(2)	2·70 (5)	3·446 (6)
4H(2)···1S(2)	2·71 (7)	3·540 (6)
3H(2)···2S(1)	2·85 (6)	3·627 (7)
4H(1)···2S(1)	2·67 (6)	3·426 (6)
3H(2)···2S(2)	2·41 (6)	3·368 (6)
4H(1)···2S(2)	2·44 (6)	3·354 (6)
Dimer (II)		
7H(1)···5S(1)	2·06 (7)	3·162 (6)
8H(2)···5S(1)*	3·28 (5)	3·907 (7)
7H(1)···5S(2)†	2·97 (7)	3·726 (6)
8H(2)···5S(2)	2·41 (5)	3·327 (7)
7H(2)···6S(1)	2·82 (5)	3·506 (6)
8H(1)···6S(1)	2·72 (5)	3·522 (7)
7H(2)···6S(2)	2·62 (5)	3·474 (6)
8H(1)···6S(2)	2·35 (5)	3·258 (6)

* Very weak bond.

† Weak bond.

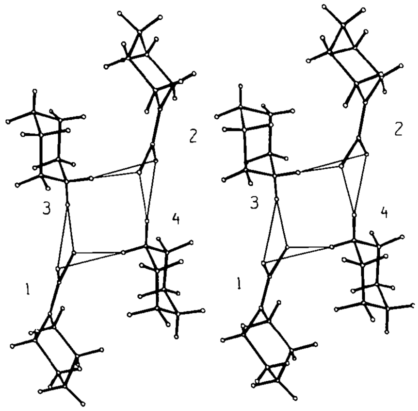

Fig. 1. The pseudo-centrosymmetric dimer (I). The numbering refers to the molecular ions. The vectors 1N → 3N and 1N → 4N are parallel to the corresponding vectors of dimer (II) in Fig. 2.

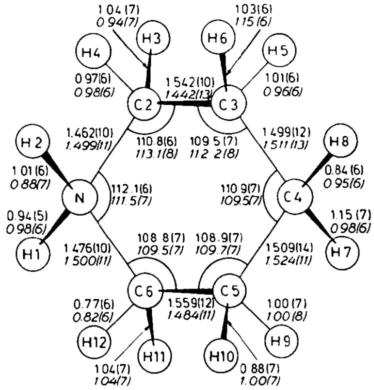

Fig. 3. Distances (Å) and angles (°) in the piperidinium cations in dimer (I). The upper value of a pair refers to molecule (3), the lower value (italic print) to molecule (4).

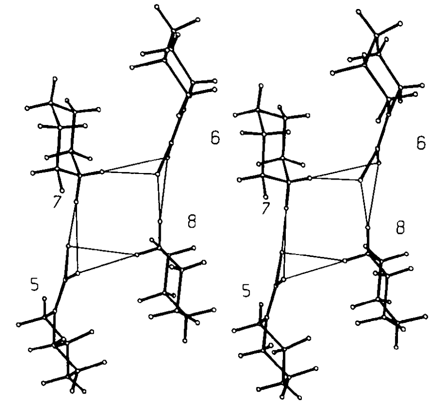

Fig. 2. The pseudo-centrosymmetric dimer (II). The numbering refers to the molecular ions. The vectors 5N → 7N and 5N → 8N are parallel to the corresponding vectors of dimer (I) in Fig. 1.

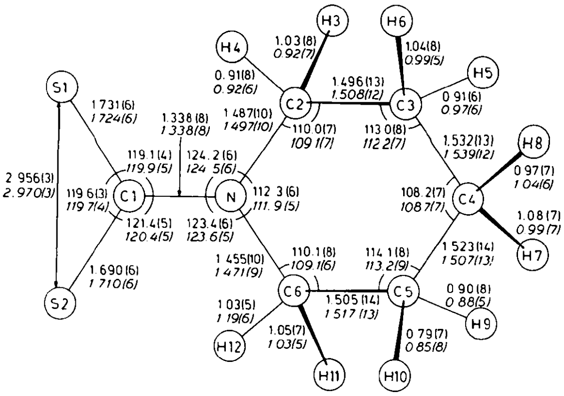

Fig. 4. Distances (Å) and angles (°) in the 1-piperidinecarbodithioate anions in dimer (I). The upper value of a pair refers to molecule (1), the lower value (italic print) to molecule (2).

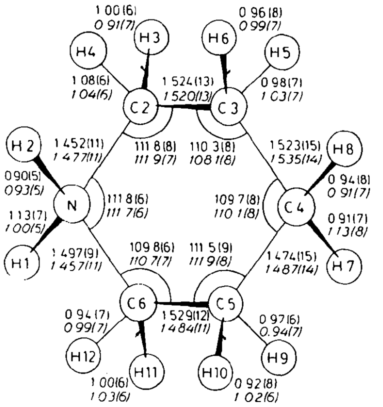

Fig. 5. Distances (Å) and angles (°) in the piperidinium cations in dimer (II). The upper value of a pair refers to molecule (7), the lower value (italic print) to molecule (8).

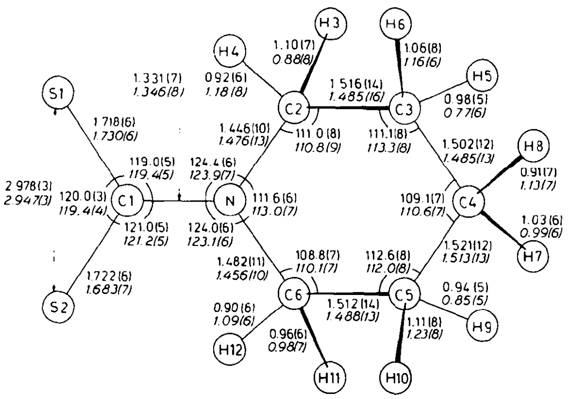

Fig. 6. Distances (Å) and angles (°) in the 1-piperidinecarbodithioate anions in dimer (II). The upper value of a pair refers to molecule (5), the lower value (italic print) to molecule (6).

Table 3. *Deviations* (Å) *from the least-squares plane through the dithiocarbamate-plane atoms* [C(3), C(4) *and* C(5) *are situated on the positive side*]

	Molecule (1)	Molecule (2)	Molecule (5)	Molecule (6)
S(1)	−0·003 (2)	0·004 (2)	0·004 (2)	−0·001 (2)
S(2)	0·001 (1)	−0·003 (2)	−0·001 (2)	0·002 (2)
C(1)	−0·005 (6)	−0·010 (6)	−0·024 (6)	−0·006 (6)
N	−0·008 (5)	−0·005 (6)	−0·005 (5)	−0·004 (6)
C(2)	0·128 (10)	−0·072 (9)	−0·050 (12)	0·072 (12)
C(6)	−0·081 (9)	0·083 (8)	0·079 (11)	−0·037 (10)

centrosymmetric molecules (dimers) in a non-centrosymmetric space group, as in the present case, is unusual (Müller, 1978).

The molecular ions appear in the chair form (Figs. 3–6). Deviations from the least-squares plane through the dithiocarbamate-plane atoms S(1), S(2), C(1), N, C(2) and C(6) are given in Table 3.

The dimers are packed at van der Waals distances (Bondi, 1964). The approximate position of the pseudo centre of symmetry in dimer (I) is at 0·612, 0·143, 0·378 and in dimer (II) at 0·108, 0·144, 0·876. Intramolecular S···S vectors are almost parallel to *a*, and the dithiocarbamate planes are not far from being parallel to *ac*. The dimers form close-packed layers parallel to *ac*. A dimer (II) at *x,y,z* is surrounded by two dimers (II) at *x*, *y*, *z* ± 1, and four dimers (I) [with respect to dimer (II) approximately at $x \pm \frac{1}{2}, y, z \pm \frac{1}{2}$]. The layers parallel to *ac* are stacked along the polar axis *b* by 2_1 screw-axis operations. 1S(2) and 5S(2) lie in the vicinity of these screw axes. In this way, each dimer obtains contacts with four dimers above the layer and four below. The 2_1 screw axes do not coincide with the pseudo centres of symmetry in the dimers. This excludes the space group $P2_1/m$.

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