[0·04 Å], and the Hg atoms lie 0·0894 (6) Å above and below this plane, respectively.

The other trifluoroacetate O atom simultaneously forms secondary O(2)···Hg bonds of 2·844 (11) and 2·878 (13) Å with the pair of Hg atoms in the next molecule. Fig. 2 shows the environment of a molecule, including the Hg···O(2) interactions above and below the molecular plane. The O(2) atoms lie near the approximate mirror plane relating the two metal atoms, at 1·726 (12) Å from the molecular plane, and they define C(11)—Hg(1)—O(2) angles of 99·0 (5) and 96·3 (5)°. This arrangement probably optimizes the coordinative interactions with the Hg—Hg pair, while reducing steric hindrance to a minimum. The extra ligands were similarly positioned in the phenylenedimercury dichloride adducts with DMF or Cl^- (Beauchamp, Olivier, Wuest & Zacharie 1986, 1987) and in the THF complex with the Hg–perfluorosuccinate macrocycle (Wuest & Zacharie, 1987).

ORTEP drawings of the unit cell have been deposited.* Stacking along the *a* axis allows each pair of Hg atoms to interact simultaneously with carboxylate groups in the molecules above and below. Cohesion between these stacks originates from normal van der Waals contacts and complementary pairs of very long Hg···O(1) contacts of 3·057 (13) Å.

We wish to thank M. Simard for collecting the X-ray data.

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* See deposition footnote.

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Structure of Potassium Hydrogen Pimelate

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Abstract. $K^+.C_7H_{11}O_4^-$, $M_r = 198·27$, orthorhombic, *Cmma*, $a = 23·551$ (3), $b = 7·449$ (1), $c = 5·069$ (1) Å, $V = 889·3$ (2) Å^3, $Z = 4$, $D_m = 1·48$, $D_x = 1·48$ g cm^{-3}, λ(Mo $K\alpha$) = 0·71069 Å, $\mu = 5·65$ cm^{-1}, $F(000) = 416$, $T = 293$ K, $R = 0·029$, $wR = 0·041$ for 391 unique observed [$I/\sigma(I) > 2·0$] reflections. Symmetrical hydrogen pimelate anions are linked into infinite chains parallel to **a** by symmetrical hydrogen bonds [OH···O 2·449 (3) Å]. The structure is that of a type A_2 acid salt and in accordance with this the IR spectrum is of Hadzi's type (ii).

Introduction. Acid salts (*MHY*) of dibasic carboxylic acids (H_2Y) with *M* a monovalent cation have been classified (Sime, Speakman & Parthasarathy, 1970) as type A_2 if they contain short and symmetric hydrogen bonds. These structures invariably show anomalous IR spectra. The cell constants of KH pimelate have been reported elsewhere (Speakman, 1972) with the suggestion that the salt was probably of type A_2, and isostructural with KH glutarate (Macdonald & Speakman, 1972). We report here the X-ray analysis of KH pimelate to validate this suggestion.

Experimental. Colourless, platy crystals were obtained by slow evaporation from a solution of pimelic acid in water/ethanol and potassium hydroxide in

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Table 1. *Fractional atomic coordinates and isotropic displacement parameters* (Å^2), *with standard deviations in the least-significant digits in parentheses*

$U_{eq} = (1/3)\sum_i\sum_j U_{ij}a_i^*a_j^*\mathbf{a}_i.\mathbf{a}_j$.

	x	y	z	U/U_{eq}
C(1)	0·16239 (9)	0·25	0·49235 (66)	0·029
C(2)	0·10701 (10)	0·25	0·64195 (62)	0·035
C(3)	0·05408 (10)	0·25	0·47329 (65)	0·033
C(4)	0·0	0·25	0·6381 (9)	0·035
O(1)	0·20710 (7)	0·25	0·63639 (40)	0·037
O(2)	0·16469 (8)	0·25	0·25244 (50)	0·067
K	0·25	0·0	0·0	0·038
H(C2)	0·1077 (8)	0·1462 (31)	0·7564 (54)	0·047 (7)
H(C3)	0·0545 (8)	0·3589 (30)	0·3509 (41)	0·037 (6)
H(C4)	0·0	0·358 (4)	0·758 (7)	0·039 (8)
H(O1)	0·25	0·25	0·5	0·12 (3)

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

C(1)—C(2)	1·509 (4)	C(1)—O(1)	1·281 (4)
C(1)—O(2)	1·217 (5)	C(2)—C(3)	1·512 (4)
C(3)—C(4)	1·523 (4)		
K—O(1^{i})	2·808 (2)	K—O(2^{i})	3·024 (2)
K—O(1^{ii})		K—O(2^{ii})	
K—O(1^{iii})		K—O(2^{iii})	
K—O(1^{iv})		K—O(2^{iv})	
C(2)—C(1)—O(1)	115·1 (3)	C(1)—C(2)—C(3)	115·4 (3)
C(2)—C(1)—O(2)	122·7 (3)	C(2)—C(3)—C(4)	112·3 (3)
O(1)—C(1)—O(2)	122·2 (3)		
O(1^{iii})—K—O(1^{ii})	96·9 (1)	O(2^{ii})—K—O(2^{i})	104·0 (1)
O(1^{iii})—K—O(1^{i})	137·8 (1)	O(2^{ii})—K—O(2^{iv})	96·7 (1)
O(1^{iii})—K—O(1^{iv})	98·0 (1)	O(2^{ii})—K—O(2^{iii})	130·0 (1)

O(1^{iii})—K—O(2^{iii})	68·3 (1)
O(1^{iii})—K—O(2^{iv})	63·4 (1)
O(1^{iii})—K—O(2^{i})	83·8 (1)
O(1_i^{iii})—K—O(2^{ii})	158·0 (1)

Symmetry codes

	O(1)	O(2)
(i)	$x, y, -1+z$	x, y, z
(ii)	$\frac{1}{2}-x, y, 1-z$	$\frac{1}{2}-x, y, -z$
(iii)	$x, -y, 1-z$	$x, -y, -z$
(iv)	$\frac{1}{2}-x, -y, -1+z$	$\frac{1}{2}-x, -y, z$

water (1:1 mol ratio). The density was measured by flotation in heptane/1,2-dibromoethane. A crystal of dimensions 0·5 × 0·2 × 0·07 mm was used for the measurement of 537 unique X-ray intensities by ω–2θ scan on a Nonius CAD-4 diffractometer, these comprising all possible reflections with $(\sin\theta)/\lambda <$ 0·64 Å^{-1} in the index ranges $0 < h < 30$, $0 < k < 9$, $0 < l < 6$. Two standard reflections showed no appreciable intensity variation. 391 reflections having $I > 2\sigma(I)$ were considered observed. Intensities were not corrected for absorption. Lattice parameters were determined from setting angles for 25 reflections with $12 < \theta < 15°$. The structure was solved by the heavy-atom method, with K placed in the position found for potassium hydrogen glutarate. Anisotropic least-squares refinement gave a final R value (on F) of 0·029, with $wR = 0·041$, $S = 3·8$, $w = 1/\sigma^2(F_o)$. The H atoms were located in difference maps and refined isotropically. Total number of refined parameters = 44. After the final refinement cycle $(\Delta/\sigma)_{max} = 0·3$, $\Delta\rho_{max} = 0·4$, $\Delta\rho_{min} = -0·4$ e Å^{-3}. Computations were carried out with the *GX* crystallographic package (Mallinson & Muir, 1985). Atomic scattering factors were taken from *International Tables for X-ray Crystallography* (1974). Atomic coordinates, bond lengths and angles are in Tables 1 and 2.* The atom labels are shown on Fig. 1.

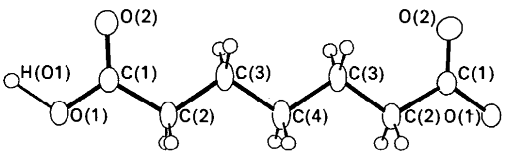

Fig. 1. The pimelate anion showing the atom labels.

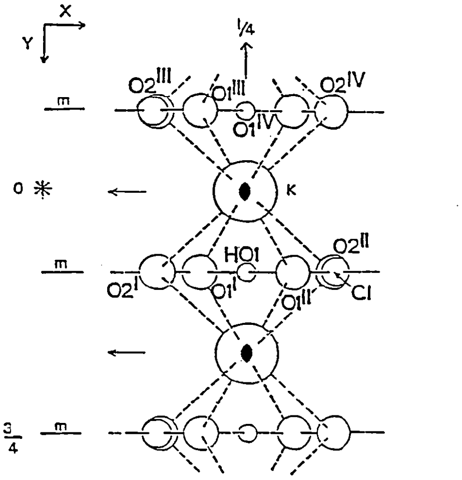

Fig. 2. The environment of the potassium ion.

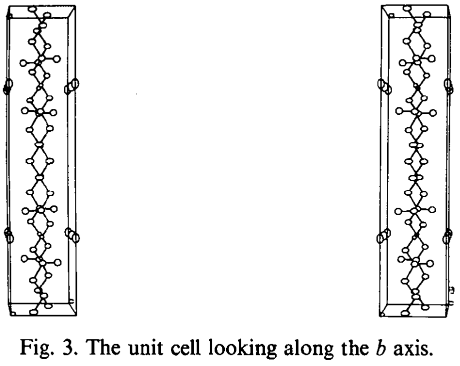

Fig. 3. The unit cell looking along the b axis.

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* Lists of structure factors and anisotropic displacement parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 52194 (6 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Discussion. Fig. 2 shows the environment of the K^+ ion and Fig. 3 the contents of the unit cell. The pimelate residue has *mm* symmetry and the K^+ cation is at a site of symmetry 222. The acidic H atom H(O1) occupies a site of $2/m$ symmetry. The pimelate anions are linked into infinite chains by very short, symmetric hydrogen bonds [O—H(O1)···O 2·449 (3) Å]. There are two such chains lying in mirror planes at $y = \frac{1}{4}$ and $y = \frac{3}{4}$, related by a glide plane. Layers of pimelate residues are interspersed by layers of K^+ ions at $y = 0$ and $y = \frac{1}{2}$, such that each K^+ is eight-coordinate. The K^+ ion makes contact with two sets of four equivalent O atoms. Because of the crystal symmetry there are only two independent K^+ contacts: $K^+\cdots O(1)$ 2·808 (2) and $K^+\cdots O(2)$ 3·024 (2) Å. The structure is that of a typical A_2 salt, as predicted by Speakman (1972) and the IR spectrum (Hadzi, 1965), and is isostructural with potassium hydrogen glutarate. A comparison of the unit-cell parameters for KH glutarate and KH pimelate is given in Table 3. Two cell dimensions, *b* and *c*, are nearly the same, but the *a* dimension in KH pimelate is increased to accommodate the extra methylene groups.

Table 3. *Comparison of crystal data of potassium hydrogen glutarate and potassium hydrogen pimelate*

	KH glutarate	KH pimelate
a (Å)	18·476 (4)	23·551 (3)
b (Å)	7·282 (3)	7·449 (1)
c (Å)	5·133 (1)	5·069 (1)
Z	4	4
Space group	*Cmma*	*Cmma*
OH···O (Å)	2·445 (3)	2·449 (3)

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Structure of Chlorobis(*N*,*N*-dimethyldithiocarbamato)(3-methoxy-3-oxopropyl)tin(IV)

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Abstract. $[SnCl(C_3H_6NS_2)_2(C_4H_7O_2)]$, $M_r = 469{\cdot}57$, monoclinic, $P2_1/n$, $a = 9{\cdot}656\,(2)$, $b = 18{\cdot}478\,(2)$, $c = 10{\cdot}519\,(3)$ Å, $\beta = 101{\cdot}04\,(2)^\circ$, $V = 1842\,(7)$ Å^3, $Z = 4$, $D_x = 1{\cdot}693$ g cm^{-3}, Mo $K\alpha$, $\lambda = 0{\cdot}71073$ Å, $\mu = 18{\cdot}34$ cm^{-1}, $F(000) = 964{\cdot}00$, $T = 293$ K, final $R = 0{\cdot}0488$ for 2518 unique observed reflections. Intramolecular carbonyl oxygen-to-tin coordination is not allowed in order to accommodate the two bidentate dithiocarbamate ligands, and thus the coordination geometry around the Sn^{IV} atom is a distorted octahedral arrangement with the ester group and Cl atom occupying mutually *cis* positions.

Introduction. Details of intramolecular carbonyl-to-tin coordination and the Lewis acidity of β-alkoxycarbonylethyltin(IV) chlorides (so-called 'estertins') have been published by Howie, Paterson, Wardell & Burley (1983, 1986). In a continuing effort to understand the coordination geometry of such complexes we have studied the estertin complexes with the dithiocarbamate (dtc) ligand, R_2NCS_2—, which is potentially bidentate (Jung, Jeong & Sohn, 1989*a*,*b*) and here report the crystal structure of $[CH_3OOCCH_2CH_2Sn(S_2CNMe_2)_2Cl]$. From ^{119}Sn NMR spectroscopy the authors (Jung *et al.*, 1989*a*) suggested that in this complex the Sn center is six-coordinate.

Experimental. The title compound was prepared by the authors' procedure (Jung *et al.*, 1989*a*). Analysis: calculated for $C_{10}H_{19}ClN_2O_2S_4Sn$: C 25·58; H 4·09; N 5·97; found: C 25·34; H 4·01; N 5·86%. A colorless crystal, 0·33 × 0·52 × 0·68 mm, was sealed in a glass capillary and mounted on an Enraf–Nonius CAD-4 diffractometer with graphite-monochromated molybdenum radiation. The unti-cell parameters were determined by least-squares refinement of 25 intense reflections ($11 \leq \theta \leq 15^\circ$). Data were collected at ambient temperature [296 (2) K] in $\omega/2\theta$ scan mode using variable rates, $\theta_{\max} = 25^\circ$ for the range $0 \leq h \leq 11$, $0 \leq k \leq 22$, $-12 \leq l \leq 12$ and two standard reflections measured after every hour did not reveal any systematic variations in intensity. Max. $\sin\theta/\lambda$ reached in intensity measurement was

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