puted the 'difference' Patterson function, with coefficients $(F_D^2-F_H^2)$, where $|F_D|$ and $|F_H|$ are the respective neutron structure amplitudes, each on an absolute scale. The outcome is represented on the left-hand side of Fig. 1.

As these acid salts are almost identically isomorphous, as the single hydrogen atom lies at a centre of symmetry ($I2/a$, $Z=4$), and as the neutron-scattering lengths of D and H are $+6{\cdot}5$ and $-3{\cdot}8$ fermi, the map shows a complete image of the structure. The nine peaks shown are the nine highest, and only significant, independent peaks of the Patterson function. (The peak representing the hydrogen atom has a poor profile in the y direction, but this (origin) peak is sensitive to slight errors in the data.)

This exercise is a logical, and obvious, extension of a method of absolute structure determination developed in the 1930's (Beevers & Lipson, 1934; Robertson, 1936; Robertson & Woodward, 1940). Whether we refer to the heavy-atom method or to that of isomorphous replacement may be debated. We prefer to regard the 'difference atom', (D–H), as 'heavy', with a scattering power of $+10{\cdot}3$ fermi.

A crystal belonging to the space group $I2/a$ yields a vector pattern in $I2/m$; hence any image of the true structure is doubled by a mirror-plane. Fortunately all the atoms are free from overlap except for the one oxygen atom which, consequently, has a peak of nearly double height. So we easily recognize an acceptable molecule in a correct position in the cell. The mirror ambiguity would equally have compromised the absolute structure determination of platinum phthalocyanine ($P2_1/a \rightarrow P2/m$) had it been possible, at the time, to apply the method three-dimensionally.

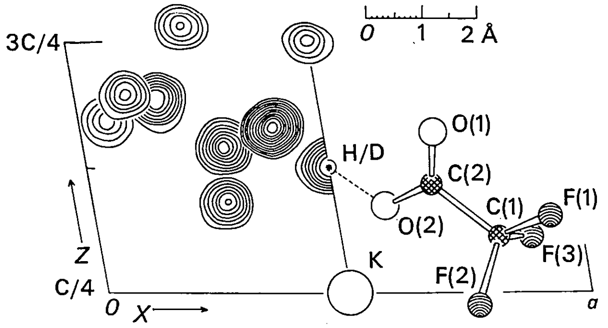

Fig. 1. On the left-hand side are sections from the three-dimensional 'difference' Patterson function, with positive contours at 4,6,8 ... in arbitrary units. On the right is the crystal structure established and refined by normal X-ray and neutron diffraction analysis. (The asterisk symbolizes a centre of inversion at $\frac{1}{2},\frac{1}{2},\frac{1}{2}$.)

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The crystal structure of $K_7Th_6F_{31}$.*

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The complex fluoride $K_7Th_6F_{31}$ is isostructural with $Na_7Zr_6F_{31}$. It is trigonal, $R\bar{3}$, with hexagonal axes $a_0=15{\cdot}293$ (2) and $c_0=10{\cdot}449$ (2) Å, $Z=3$ and $\varrho_{cal}=5{\cdot}307$ g.cm^{-3}. The eight Th–F distances range from 2·24 (1) to 2·41 (1) Å. The K–F distances range from 2·63 (2) to 3·36 (2) Å.

The structure of $K_7Th_6F_{31}$ is identical to that of $Na_7Zr_6F_{31}$ (Burns, Ellison & Levy, 1968) and was determined to confirm the supposition that all 7AF.6MF$_4$ complexes are probably isostructural, (A = Na, K, Rb and NH$_4$, and M = most of the tetravalent lanthanides and actinides) (Thoma, 1962).

The reflection data were collected from an ellipsoidal

Table 1. *Lattice and atomic parameters for* $K_7Th_6F_{31}$

Space group $R\bar{3}$, $a_0=15{\cdot}293$ (2), $c_0=10{\cdot}449$ (2) Å, $Z=3$, $\varrho_{cal}=5{\cdot}307$ g.cm^{-3}.

Standard errors in parentheses, corresponding to the last significant digit, are given by the variance–covariance matrix.

	x	y	z	$^*\beta_{11}\times 10^4$	$\beta_{22}\times 10^4$	$\beta_{33}\times 10^4$	$\beta_{12}=10^4$	$\beta_{13}\times 10^4$	$\beta_{23}\times 10^4$
K(1)	0·0824 (4)	0·3088 (4)	0·4948 (5)	30 (3)	37 (3)	53 (4)	20 (2)	−4 (3)	1 (3)
K(2)	0	0	$\frac{1}{2}$	26 (4)	β_{11}	37 (8)	$(\frac{1}{2}\beta_{11})$	0	0
Th	0·18917 (4)	0·05122 (4)	0·17732 (6)	16 (1)	14 (1)	24 (1)	7 (1)	1 (1)	1 (1)
F(1)	0·3548 (7)	0·1126 (7)	0·0938 (9)	1·4 (2)†					
F(2)	0·1834 (8)	0·0551 (8)	0·392 (1)	1·8 (2)					
F(3)	0·2747 (8)	0·3717 (8)	0·425 (1)	1·7 (2)					
F(4)	0·2103 (9)	0·1602 (9)	0·004 (2)	2·8 (3)					
F(5)	0·2442 (9)	0·544 (1)	0·446 (2)	2·9 (3)					
F(6)	0	0	0·03 (2)	10 (6)					

* Coefficients in the temperature factor: $\exp[-(\beta_{11}h^2+\beta_{22}k^2+\beta_{33}l^2+2\beta_{12}hk+2\beta_{13}hl+2\beta_{23}kl)]$.

† Isotropic B.

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Table 2. *Interatomic distances for* $K_7Th_6F_{31}$

Atom labels correspond to those of Burns *et al.* (1968).

Th—F(3)	2·24 (1) Å	Th—F(2)	2·24 (2) Å	Th—F(5)	2·32 (2) Å
Th—F(5)	2·33 (2)	Th—F(4)	2·34 (2)	Th—F(4)	2·37 (2)
Th—F(1)	2·38 (1)	Th—F(1)	2·41 (1)	K(1)—F(2)	2·63 (2)
K(1)—F(3)	2·66 (2)	K(1)—F(3)	2·67 (2)	K(1)—F(3)	2·70 (2)
K(1)—F(2)	2·72 (2)	2[K(1)-F(1)]	2·78 (2)	K(1)—F(5)	3·23 (2)
K(1)—F(4)	3·28 (2)	K(1)—F(4)	3·31 (2)	6[K(2)-F(2)]	2·74 (2)
6[K(2)-F(5)]	3·36 (2)	F(1)—F(1)	2·56 (2)	F(1)—F(3)	2·79 (2)
F(1)—F(2)	2·80 (2)	2[F(1)-F(4)]	2·81 (2)	F(1)—F(4)	2·95 (2)
F(1)—F(5)	2·96 (2)	F(1)—F(3)	3·28 (2)	F(2)—F(3)	2·75 (2)
F(2)—F(5)	2·80 (2)	F(2)—F(1)	2·80 (2)	F(2)—F(5)	2·87 (2)
F(2)—F(3)	3·24 (2)	2[F(2)-F(2)]	3·37 (2)	F(3)—F(4)	2·84 (2)
F(3)—F(5)	2·90 (2)	F(4)—F(5)	2·80 (2)	F(4)—F(5)	2·91 (2)
2[F(4)-F(4)]	2·91 (2)	F(4)—F(6)	2·93 (3)	F(4)—F(6)	2·94 (4)
F(5)—F(6)	2·6 (2)	2[F(5)-F(5)]	2·91 (3)		

Table 3. *Observed and calculated structure factors and extinction correction for* $K_7Th_6F_{31}$

ECOR $= 10^3 \times$ extinction correction.

crystal 0·26 × 0·241 × 0·26 mm using unfiltered Ag $K\alpha$ radiation. The experimental and processing details are identical to those previously described by Brunton (1971). Because of the identity of the $K_7Th_6F_{31}$ and $Na_7Zr_6F_{31}$ structures, the description of the structure by Burns *et al.* (1968) need not be repeated here. The lattice and atomic parameters are listed in Table 1, interatomic distances in Table 2, and the 1853 observed and calculated structure factors in Table 3. An isotropic extinction correction was applied to F_o, and the reflections with an extinction correction different from 1·0 are also listed in Table 3 (Coppens & Hamilton, 1970). Tables 1, 2 & 3.

The Th–F distances range from 2·24 (1) to 2·41 (1) Å and the K–F distances range from 2·63 (2) to 3·36 (2) Å. The Th–F and K–F distances average respectively 0·21 and 0·30 Å longer than corresponding Zr–F and Na–F distances, and the corresponding F–F distances average 0·30 Å longer for $K_7Th_6F_{31}$. The discrepancy indices $R(F_o)$ and weighted $R(F_o)$ are 0·0660 and 0·1188 respectively for all reflections less than $\sigma(F_o^2)$.

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Bond lengths and angles in the molecule of palladium n-propyl mercaptide.

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Revised values are given which supersede those in *Acta Cryst.* (1968) **B24**, 1623.

The structure of palladium n-propyl mercaptide was solved by Kunchur (1968) and the values for the various bond lengths and angles within the molecule were reported. Owing to a fault in the program which was used in these calculations on a computer, errors were introduced in the values of bond lengths and angles reported. The author wishes to thank Dr R. O. Gould of the University of Edinburgh for pointing out this error. In Table 1 the corrected values of bond lengths and angles are given. The labelling scheme is the same as reported in the earlier work. However, a correction should be made in the labelling of two carbon atoms. The carbon atoms C(17) and C(18) in Table 1 of the previous work (Kunchur, 1968) should be read as C(18′) and C(17′) respectively.

Table 1. *Dimensions of the molecule; corrected values*

Bond lengths (Å)		Angles (°)	
Pd(1)–S(2)	2·311	S(5)—Pd(1)–S(4)	82·2
Pd(1)–S(3)	2·332	S(5)—Pd(1)–S(3)	98·2
Pd(1)–S(4)	2·334	S(5)—Pd(1)–S(2)	177·8
Pd(1)–S(5)	2·336	S(4)—Pd(1)–S(3)	176·6
Pd(2)–S(1)	2·332	S(4)—Pd(1)–S(2)	97·6
Pd(2)–S(4)	2·338	S(3)—Pd(1)–S(2)	81·9
Pd(2)–S(5)	2·332	S(6)—Pd(2)–S(5)	97·1
Pd(2)–S(6)	2·318	S(6)—Pd(2)–S(4)	174·6
Pd(3)–S(1)	2·320	S(6)—Pd(2)–S(1)	81·8
Pd(3)–S(2)	2·326	S(5)—Pd(2)–S(4)	82·2
Pd(3)–S(3)	2·338	S(5)—Pd(2)–S(1)	177·7
Pd(3)–S(6)	2·327	S(4)—Pd(2)–S(1)	98·7
S(1)—C(1)	1·83	S(6)—Pd(3)–S(3)	174·3
C(1)—C(2)	1·52	S(6)—Pd(3)–S(2)	97·5
C(2)—C(3)	1·48	S(6)—Pd(3)–S(1)	81·9
S(2)—C(4)	1·84	S(3)—Pd(3)–S(2)	81·9
C(4)—C(5)	1·62	S(2)—Pd(3)–S(1)	177·6
C(5)—C(6)	1·47	S(3)—Pd(3)–S(1)	98·5
S(3)—C(7)	1·82	C(1)—S(1)—Pd(3)	109·2
C(7)—C(8)	1·50	C(1)—S(1)—Pd(2)	111·1
C(8)—C(9)	1·54	C(4)—S(2)—Pd(1)	107·5
S(4)—C(10)	1·87	C(4)—S(2)—Pd(3)	109·4
C(10)–C(11)	1·52	C(7)—S(3)—Pd(3)	103·8
C(11)–C(12)	1·47	C(7)—S(3)—Pd(1)	104·5
S(5)—C(13)	1·85	Pd(3)–S(1)—Pd(2)	85·1
C(13)–C(14)	1·45	Pd(3)–S(2)—Pd(1)	83·8
C(14)–C(15)	1·51	Pd(3)–S(3)—Pd(1)	83·5
S(6)—C(16)	1·86		
C(16)–C(17)	1·44		
C(17)–C(18)	1·55		
Pd(1)–Pd(3)	3·111		
Pd(1)–Pd(2)	3·088		
Pd(2)–Pd(3)	3·147		

The estimated standard deviations in the values of bond lengths and angles are not given here since they are not affected and are the same as reported previously.

Reference

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