to Dr M. A. Quader for helpful discussions. One of the authors (S.P.S.G.) is thankful to the C.S.I.R. (New Delhi) for financial assistance.

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The Crystal Structure of Protactinium Pentachloride

By Richard P. Dodge,* Gordon S. Smith, Quintin Johnson and Robert E. Elson
University of California, Lawrence Radiation Laboratory, Livermore, California, U.S.A.

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$PaCl_5$ forms monoclinic crystals with lattice constants $a=7{\cdot}97$, $b=11{\cdot}35$, $c=8{\cdot}36$ Å; $\beta=106{\cdot}4°$. The probable space group is $C2/c$, and the unit cell contains four $PaCl_5$ units. The structure consists of infinite chains of non-regular pentagonal bipyramidal $PaCl_7$ groups which share pentagon edges. $PaCl_5$ therefore provides an example of the comparatively rare coordination number of seven, and illustrates a new way of achieving an overall stoichiometry of 1:5. Pa-Cl bond distances fall into two classes: (*a*) 2·43 (twice) and 2·46 Å to non-bridging Cl, and (*b*) 2·70 (twice) and 2·76 Å (twice) to bridging Cl. The Cl–Pa–Cl bond angle along the axis of the pentagon is $176\pm1°$.

Introduction

Chlorine compounds of protactinium (element 91) were first prepared by Grosse (1934), who reported a transparent, nearly colorless pentachloride melting at 301 °C and sublimable below its melting point. Only microgram amounts being available, no chemical analysis was carried out, and the formulation as a pentachloride was predicated by an expected analogy with the pentachlorides of Nb^{V} and Ta^{V}. The present crystal-structure analysis was undertaken to confirm the stoichiometry as well as to provide structural data on the volatile chloride. Of especial interest was whether the molecular structure would prove to be similar to that found for the pentachlorides of niobium and tantalum (Zalkin & Sands, 1958).

Experimental

Our sample of protactinium, in the form of $PaO_{2{\cdot}25}$ was received from Oak Ridge National Laboratory. This sample, originally part of a gram-scale lot recovered by investigators at the Atomic Energy Research Establishment, Harwell, England, is now known to contain about 4% Nb [for further details see Stein (1964)]. The pentachloride was prepared as previously reported (Elson, 1954), namely, by the action of carbon tetrachloride on the oxide at about 200°C, followed by a fractional sublimation to separate out a less volatile component (possibly $PaOCl_3$). These compounds are highly sensitive to atmospheric moisture and are radioactive as well (the most stable isotope, ^{231}Pa, is an α emitter). Manipulations during the preparative stages were performed in a (glass) vacuum system. Samples for X-ray diffraction photography were then sealed off in thin-walled glass capillaries.

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* Permanent address: Chemistry Department, University of the Pacific, Stockton, California, U.S.A.

Because $PaCl_5$ turns out not to be isostructural with $NbCl_5$ and because fractional sublimation techniques were used in the preparation, the Nb content in these samples is believed to be considerably less than the original 4%.

An examination of these sample-tubes showed a goodly number of well-formed crystals which were pale yellow for thicker specimens and nearly colorless for the thin ones. Oscillation, Weissenberg, and precession photographs indicated monoclinic symmetry; the systematic extinctions (hkl, $h+k=2n+1$; $h0l$, $l=2n+1$) are characteristic of the space groups $C2/c$ and Cc. Unit cell data are as follows: $a=7{\cdot}97$, $b=11{\cdot}35$, $c=8{\cdot}36$ Å; $\beta=105{\cdot}4°$ (with an accuracy of about 0·3%); $D_x=3{\cdot}74$ g.cm^{-3} for four $PaCl_5$ units per unit cell. These lattice constants differ from those reported for $PaCl_5$ by Brown & Maddock (1963). Dr Brown in a personal communication writes that further work has led to revised values. These agree satisfactorily with ours reported above.

Two different crystals were used to collect intensity data. One, a blade-like specimen, was used for a set of equi-inclination Weissenberg photographs with Cu $K\alpha$ radiation. Another, a prism along the c axis measuring approximately 0·45 mm in length and 0·30 × 0·26 mm in cross section, was used on a General Electric XRD-5 diffractometer equipped with a goniostat. Although somewhat larger than desired, this crystal was an exception among the samples examined in that it was positionable at the center of arcs of a eucentric goniometer head.* The stationary-crystal stationary-counter technique (Furnas, 1957) was employed; the radiation was Zr-filtered Mo $K\alpha$. In all, 344 reflections were recorded up to a 2θ-cutoff of 40°. Both sets of intensities were reduced to relative $|F|$'s through the application of Lorentz–polarization factors. The $|F|$'s used in the refinement (and reported in this paper) were those collected with the counter.

Determination of the structure

With four molecules of $PaCl_5$ per unit cell being indicated, the Pa atoms could be placed in general positions of Cc or in one of several fourfold sets of $C2/c$ (*International Tables for X-ray Crystallography*, 1952). Of these latter, only the 4(e) set [$\pm(0,y,\frac{1}{4})$ plus C-centering] was also consistent with the observed intensities. The symmetry operations in Cc do not select any fixed origin for the x and z parameters. Hence the x and z parameters for Pa could be specified as 0 and $\frac{1}{4}$ respectively, so that the positions of Pa are the same in the two space groups. The space group assignment therefore depends on the Cl positions.

A three-dimensional Patterson prepared from the film data gave the y parameter of Pa. With phases determined by Pa, electron density maps were synthesized which gave peaks identifiable as Cl in pentagonal bipyramidal coordination about Pa. These Cl atoms were placed in a 4(e) set and in two eightfold positions of $C2/c$. This structure model, however, would not refine below an R value of 30%. The linear absorption coefficient for Cu $K\alpha$ is high ($\sim$1,000 cm^{-1}), and we judged absorption to be the principal cause of the rather large R value.

At this time the diffractometer data obtained with Mo $K\alpha$ radiation became available. A repeat of the preceding calculations confirmed the model deduced from the film data. Four cycles of full-matrix least-squares refinement (based on $|F_o|$) with individual isotropic temperature parameters gave an overall R value of 8·5%. Final shifts in the 13 variable parameters were in all cases $<0{\cdot}001$ times the e.s.d.'s. The program used was that of Gantzel, Sparks & Trueblood (ACA Program No. 319, unpublished) with the weighting scheme (Smith, Johnson & Nordine, 1965) as follows: $w=F_o^{1/4}$ for $F_o<A$; $w=A^{5/4}F_o^{-1}$ for $F_o>A$. On the scale of the data of Table 1, A is 125. The atomic scattering factors were those listed in *International Tables for X-ray Crystallography* (1962) for the neutral atoms.

Attempts to improve the agreement by inclusion of absorption corrections were not successful. A φ-dependent absorption curve experimentally measured at $\chi=90°$ and applied to all structure amplitudes yielded a refinement with an R of 9·6%. (Maximum deviation in these intensities at $\chi=90°$ from the mean was about 30%). Absorption factors calculated by the method of Wehe, Busing & Levy (1962) led to an R of 10·1%. (Maximum deviation in the corrections from the mean was about 50%). The absorption coefficient used in this calculation was derived from Roof's (1959) mass absorption data for Th and U; the value for Pa (268 cm^{-1}; Mo $K\alpha$ radiation) was obtained by linear interpolation. Fairly drastic approximations were used to describe the crystal shape: one end of the crystal could not be clearly seen, and the other end followed the curved contour of the capillary wall rather than displaying faces.

A comparison (Table 2) of atomic parameters from the three separate refinements showed the coordinates differed but little, despite the dissimilar ways of handling absorption. The largest difference is about $\frac{3}{2}\sigma$; temperature parameters understandably show more variation. Completely valid absorption corrections would undoubtedly lead to better definition of the coordinates. Whether or not the changes in these values would prove to be significant in a statistical sense is problematical. Because absorption effects were present, we decided not to generalize the model to allow for the effects of anisotropic thermal motion or anomalous dispersion effects in the scattering factors. Increased flexibility of the model could be also achieved by considering all Cl atoms in fourfold positions of Cc. There

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* In response to a referee's query, we point out that the goniometer heads used allow only limited adjustments with which to center a crystal in the X-ray beam. Thus, while a crystal might be sufficiently separated from neighboring specimens in the capillary, the crystal still might not be positionable in the beam because of its location from the ends of the capillary.

is nothing, however, to suggest that the centrosymmetric arrangement in $C2/c$ is unsatisfactory.

Results for the data without absorption corrections were accepted as final. Table 1 lists observed and calculated structure factors; atomic parameters are given in Table 2.

As a final check of our results, a difference map was prepared in which the Pa atoms were subtracted out. This synthesis gave circular contours for Cl with little evidence for any pronounced anisotropy. Saddle-shaped contours at the Pa sites undoubtedly reflect errors caused by sample absorption, although some amount of anisotropy in the thermal motion is not ruled out. The R value of 24% for this calculation, compared with the final R of 8·5%, illustrates the overall contribution made by the Cl atoms to the structure factors.

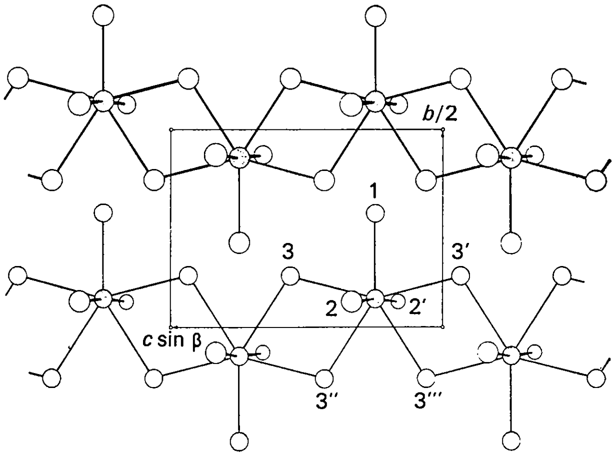

Fig. 1. Portion of infinite chains in $PaCl_5$. Coordination of Cl around each Pa is pentagonal bipyramidal.

Table 1. *Observed and calculated structure factors*

```
H,K= 0, 0
L FOB FCA
2 205-179
4 155 133
6 145-115

H,K= 0, 2
L FOB FCA
0 137 119
1 137-131
2  88 -93
3 141 142
4  56  52
5  42 -40
6  46 -38
7  78  65

H,K= 0, 4
L FOB FCA
0  88 -71
1 200-206
2  18  -9
3 126 139
4  18 -18
5  94 -99
6  32  31
7  81  79

H,K= 0, 6
L FOB FCA
0 148-139
1  75 -69
2 135 128
3  12   7
4  88 -90
5  47 -40
6  70  68

H,K= 0, 8
L FOB FCA
0 114-100
1  47  39
2 139 127
3  30 -29
4  83 -78
5  32  32

H,K= 0,10
L FOB FCA
0  48 -27
1 134 115

 2  13  12
 3  71 -71

H,K= 1, 1
 L FOB FCA
-7  69 -56
-6 132-113
-5  63  56
-4 158 149
-3 145-137
-2 114-144
-1 108  90
 0 145 169
 1  81 -68
 2  68 -61
 3 114  96
 4 111  97
 5  50  44
 6 124-108
 7  66  60

H,K= 1, 3
 L FOB FCA
-7  87 -82
-6  18 -19
-5  93 103
-4  52  52
-3 168-181
-2  98 -84
-1 124 125
 0  14   3
 1  77 -82
 2  60 -56
 3 102 110
 4  34  31
 5  83 -80
 6  21 -20
 7  95  93

H,K= 1, 5
 L FOB FCA
-7  60 -61
-6  93  83
-5 117 120
-4  98 -97
-3 106-105
-2 102  95
-1 138 131
 0 133-125
 1 102 -96
 2  69  69

 3  55  55
 4  82 -78
 5 106 -99
 6  78  78

H,K= 1, 7
 L FOB FCA
-6  62  68
-5  18  16
-4 109-109
-3  10   7
-2 136 131
-1  17   9
 0  66 -68
 1  10   1
 2  97  92
 3  18 -19
 4  80 -76
 5  15 -11

H,K= 1, 9
 L FOB FCA
-4  80 -76
-3  71  70
-2  96  87
-1 106 -95
 0  56 -51
 1  92  84
 2  68  60
 3  55 -55

H,K= 2, 0
 L FOB FCA
-8  87  89
-6 176-159
-4 152 141
-2  95 -97
 0 217 212
 2 167-149
 4 175 164
 6 139-127

H,K= 2, 2
 L FOB FCA
-7  89 -88
-6  64 -65
-5  56  65
-4  48  60
-3 125-121
-2  49 -42
-1  49  52

 0  46  48
 1  83 -86
 2  87 -80
 3 149 142
 4  86  77
 5  73 -66
 6  59 -54

H,K= 2, 4
 L FOB FCA
-7  95-111
-6  37  34
-5 118 120
-4  13 -17
-3 120-115
-2  17  -7
-1 119 119
 0  65  61
 1 139-144
 2  12  -6
 3 147 148
 4  19 -20
 5 117-124
 6  29  27

H,K= 2, 6
 L FOB FCA
-6  84  90
-5  61  55
-4  97 -96
-3  17   5
-2  97  94
-1  34  32
 0  95 -95
 1  43 -42
 2 118 115
 3  23  21
 4 112-104
 5  60 -56

H,K= 2, 8
 L FOB FCA
-5  32 -33
-4  92 -85
-3  28  28
-2 101  93
-1  37 -36
 0  60 -60
 1  39  36
 2 121 116
 3  29 -28

 4 102 -94

H,K= 2,10
 L FOB FCA
-2  13  -3
-1  98 -91
 0  11  -9
 1  98  95

H,K= 3, 1
 L FOB FCA
-7  58 -53
-6  96 -87
-5  36  37
-4  68  86
-3 105-102
-2  94-113
-1  81  83
 0 173 195
 1  96 -87
 2 129-115
 3  97  89
 4  93  90
 5  37 -32
 6  76 -70

H,K= 3, 3
 L FOB FCA
-7  67 -70
-6  11  -9
-5  55  61
-4  33  32
-3 125-126
-2  63 -64
-1 113 132
 0  31  26
 1 136-139
 2  61 -64
 3 121 122
 4  28  27
 5  62 -57

H,K= 3, 5
 L FOB FCA
-7  51 -57
-6  74  73
-5  86  83
-4  75 -74
-3  65 -66
-2  86  82
-1 129 131

 0 116-124
 1 137-129
 2  86  78
 3  79  73
 4  73 -70
 5  74 -75

H,K= 3, 7
 L FOB FCA
-5   8   5
-4  77 -74
-3  24  16
-2 111 111
-1  16  13
 0  93 -93
 1  12 -11
 2 128 115
 3  12  -9
 4  78 -70

H,K= 3, 9
 L FOB FCA
-4  54 -50
-3  61  57
-2  75  74
-1  94 -93
 0  70 -68
 1  90  88
 2  82  78

H,K= 4, 0
 L FOB FCA
-6 135-134
-4 136 157
-2 149-157
 0 167 180
 2  87 -84
 4 102  99

H,K= 4, 2
 L FOB FCA
-7  59 -65
-6  37 -51
-5  59  65
-4  78  77
-3 129-143
-2  80 -84
-1  79  85
 0  58  59
 1  64 -68
 2  42 -43

 3  79  84
 4  45  40
 5  50 -41

H,K= 4, 4
 L FOB FCA
-7  67 -83
-6  36  33
-5 118 123
-4  42 -14
-3 138-148
-2  15   1
-1 139 143
 0  46 -48
 1 103-108
 2   7  -4
 3  82  86
 4  39 -17

H,K= 4, 6
 L FOB FCA
-6  75  77
-5  52  53
-4 102-104
-3  21 -22
-2 107 114
-1  51  52
 0  94 -92
 1  31 -29
 2  80  79
 3  13  -1

H,K= 4, 8
 L FOB FCA
-4  95 -98
-3  25  27
-2 108 114
-1  34 -34
 0  65 -63
 1  36  30
 2  88  81

H,K= 5, 1
 L FOB FCA
-7  40 -57
-6  81-110
-5  42  46
-4  79  93
-3  62 -83
-2  62 -69
-1  39  44

 0  85 100
 1  51 -53
 2  86 -78
 3  66  70
 4  97  91

H,K= 5, 3
 L FOB FCA
-6  16 -19
-5  82  85
-4  32  35
-3  87-104
-2  32 -38
-1  63  67
 0   8   6
 1  76 -81
 2  37 -45
 3 100 103

H,K= 5, 5
 L FOB FCA
-6  72  78
-5  92  97
-4  61 -70
-3  49 -56
-2  55  61
-1  72  76
 0  78 -83
 1  76 -76
 2  64  58
 3  73  65

H,K= 5, 7
 L FOB FCA
-4  74 -80
-3  16  14
-2  69  77
-1   2   1
 0  57 -50
 1   3  -0

H,K= 6, 0
 L FOB FCA
-6  87-103
-4  73  87
-2  95-102
 0 139 154
 2 106 -99

H,K= 6, 2
 L FOB FCA

-6  35 -36
-5  34  38
-4  34  39
-3  72 -89
-2  46 -52
-1  70  67
 0  65  61
 1  79 -78
 2  61 -57

H,K= 6, 4
 L FOB FCA
-5  68  80
-4  11 -10
-3  84 -89
-2  15   3
-1 110 112
 0  31 -37
 1 111-113
 2   9  -2

H,K= 6, 6
 L FOB FCA
-4  56 -68
-3   6  -1
-2  84  82
-1  41  43
 0  94 -85

H,K= 7, 1
 L FOB FCA
-5  29  37
-4  74  85
-3  54 -71
-2  84 -87
-1  44  45
 0  75  92
 1  31 -42

H,K= 7, 3
 L FOB FCA
-4  25  33
-3  97-105
-2  33 -39
-1  79  79
 0  14  12
```

Discussion of the structure

Each protactinium atom (Fig. 1) is coordinated to seven chlorine atoms at the vertices of a non-regular pentagonal bipyramid. These $PaCl_7$ units, each of which has a crystallographic twofold axis as a symmetry element, share pentagon edges to form infinite (zigzag) chains in the c-axis direction. It is to be noted that this configuration differs fundamentally from the octahedrally coordinated, dimeric M_2Cl_{10} units found in $NbCl_5$ and $TaCl_5$ (Zalkin & Sands, 1958). As far as is known, the present arrangement, in fact, constitutes a new way of achieving an overall stoichiometry of 1:5.

Bond data for an isolated $PaCl_7$ group are given in Table 3 and pictorially in Fig. 2. The Pa–Cl bond distances fall into two classes: (*a*) 2·43 (twice), 2·46 Å to terminal (or non-bridging) Cl, and (*b*) 2·70 (twice), 2·76 Å (twice) to bridging Cl. The Cl atoms in (*a*) are two 'axial' atoms and one within the pentagonal girdle; those of (*b*) are the remaining four in the equatorial pentagon. Similar variations between bridging and terminal Cl have, of course, been reported in a number of complexes including, for example, $NbCl_5$. This distinction eliminates the possibility of a molecular fivefold axis along the line Cl(2)–Pa–Cl(2′). (It will still be convenient to speak of equatorial and axial Cl; for the latter we adopt the designation 'axial'.) Cl···Cl distances within the pentagonal bipyramid likewise separate into two groups. One set, from 'axial' to equatorial chlorine atoms, has distances (3·52–3·68 Å) not appreciably different from those corresponding to normal van der Waals contacts. Distances between equatorial chlorine atoms are, however, significantly smaller (3·11–3·19 Å). From a purely steric point of view, a five-coordinate, trigonal bipyramidal arrangement of Cl [as found in $SbCl_5$ (Ohlberg, 1959)] would be preferable. Apparently the free energy associated with two additional Pa–Cl bonds in the pentagonal bipyramidal configuration more than offsets the steric disadvantages of five equatorial chlorine atoms.

Examination of the bond data indicates also a slight shifting (by ~0·05 Å) of Pa away from the center of the equatorial section and toward Cl(1), *i.e.* along the

Table 2. *Atomic parameters resulting from different methods of treating absorption (standard deviations in parentheses)*

	I. No corrections $R=8{\cdot}5\%$				II. φ-dependent corrections $R=9{\cdot}6\%$				III. Corrections by the method of Wehe, Busing & Levy $R=10{\cdot}1\%$			
	10^4x	10^4y	10^4z	B	10^4x	10^4y	10^4z	B	10^4x	10^4y	10^4z	B
Pa	0	717 (2)	2500	1·2 ± 0·1 Å²	0	715	2500	1·1 Å²	0	715	2500	1·8 Å²
Cl(1)	0	2885 (18)	2500	1·8 ± 0·4	0	2887	2500	2·7	0	2905	2500	3·7
Cl(2)	3181 (21)	637 (16)	3365 (19)	3·1 ± 0·5	3179	647	3350	3·3	3168	650	3373	3·9
Cl(3)	−56 (18)	1290 (13)	5624 (17)	1·9 ± 0·3	−55	1291	5631	2·0	−68	1270	5632	2·6

twofold axis. This shifting, which occurs in opposite directions in adjacent bipyramids, serves to increase the mutual separation of these Pa atoms, and is also effective in reducing the Pa–Cl(1) bond distance. As mentioned above, Cl(1) is the only terminal Cl within the equatorial girdle. The effect of such a displacement on the geometry of a bipyramid of D_{5h} symmetry is illustrated in Fig. 3. In quantitative terms, a shift in the Pa position by 0·050 Å produces a splitting in the four Pa–Cl(3) bond distances into two sets which differ by 0·056 Å. The angles Cl(1)–Pa–Cl(2) and Cl(2)–Pa–Cl(2′) become 91·2° and 177·6° respectively, and within the equatorial section the pattern of bond angle deviations from the pentagon angle of 72° is in directions as observed. Deviations in the bond angles are, in fact, slightly in excess of the values produced by the displacement of Pa alone. The most notable example is an increase of the Cl(1)–Pa–Cl(3) angle to 76·1° (from a calculated value of 73·7°). This and attendant adjustments in other bond angles within the equatorial section are apparently a consequence of the perturbing effect of one short Pa–Cl(1) bond.

The six atoms comprising the equatorial section are slightly ruffled from coplanarity. (Exact coplanarity would result if the x coordinate of Cl(3) were zero. Table 2 shows this coordinate differs from zero by about 3σ.) Deviations from a least-squares plane are indicated in Fig. 3. The atoms Pa, Cl(1), Cl(2), and Cl(2′) are coplanar within 10^{-4} Å. These two least-squares planes are perpendicular to one another within 0·1°.

The infinite chains are packed side by side to give a quasi-hexagonal arrangement when viewed along the chain direction. The axial ratio of the cross section, $a \sin \beta : b$, is 0·674 as compared with 0·577 ($=1/\sqrt{3}$) for

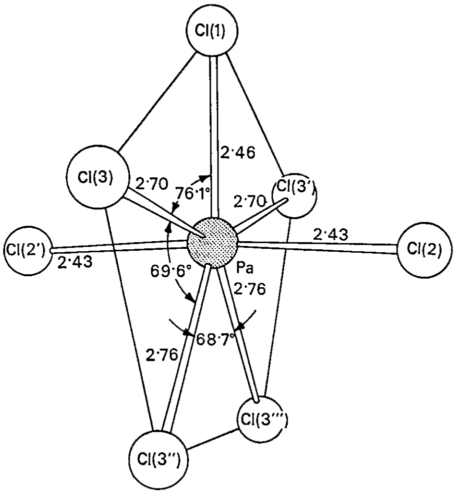

Fig. 2. Bond distances (Å) and angles within an isolated $PaCl_7$ group. The four Cl(3) atoms are bridging; the other three Cl are nonbridging atoms.

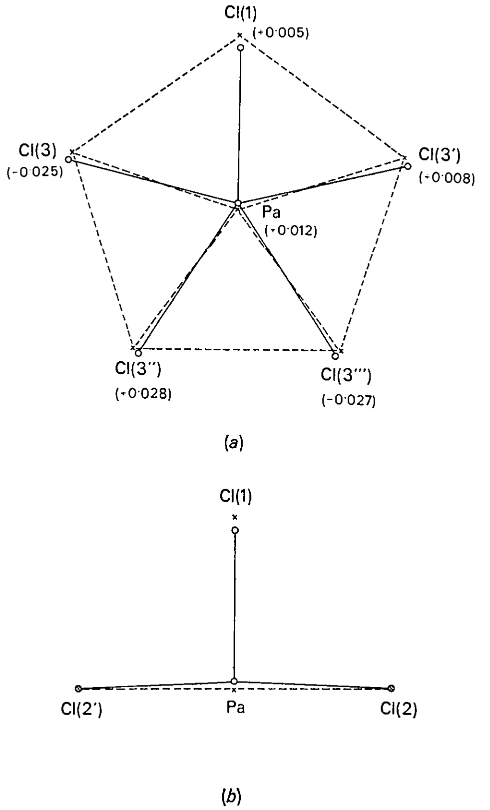

Fig. 3. Illustration of distortion in (a) the equatorial section; (b) the plane through Pa, Cl(1), Cl(2) and Cl(2′). ×'s correspond to positions of D_{5h} symmetry. Open circles mark observed positions. Values in parentheses in (a) are deviations in Å from a least-squares plane through the six atoms.

Table 3. *Distances and angles in* $PaCl_5$*

Pa–Cl(1)	2·461 ± 0·020 Å	Cl(3″)···Cl(3‴)	3·11 ± 0·03 Å
Pa–Cl(2)	2·434 ± 0·016	Cl(2)····Cl(1)	3·52 ± 0·02
Pa–Cl(3)	2·704 ± 0·014	Cl(2)····Cl(3″)	3·59 ± 0·02
Pa–Cl(3″)	2·759 ± 0·014	Cl(2)····Cl(3′)	3·63 ± 0·02
Cl(1)···Cl(3)	3·19 ± 0·02	Cl(2)····Cl(3‴)	3·65 ± 0·02
Cl(3)···Cl(3″)	3·12 ± 0·03	Cl(2)····Cl(3)	3·68 ± 0·02
Cl(1)–Pa–Cl(2)	92·1 ± 0·4°	Cl(2)—Pa—Cl(3‴)	89·2 ± 0·5°
Cl(1)–Pa–Cl(3)	76·1 ± 0·3	Cl(3)—Pa—Cl(3″)	69·6 ± 0·5
Cl(2)–Pa–Cl(3)	91·2 ± 0·5	Cl(3″)–Pa—Cl(3‴)	68·7 ± 0·6
Cl(2)–Pa–Cl(3′)	89·8 ± 0·5	Cl(2)—Pa—Cl(2′)	175·8 ± 0·9
Cl(2)–Pa–Cl(3″)	87·3 ± 0·5	Pa——Cl(3)–Pa′	110·4 ± 0·5

* Numbering of atoms follows that of Fig. 2. E.S.D.'s include only uncertainties in the positional parameters.

the analogous orthohexagonal cell. Interchain contacts, almost exclusively between terminal chlorines, range from 3·59–3·79 Å (Table 4); all are seen to correspond to normal van der Waals distances.

Table 4. *Interatomic* Cl···Cl *distances less than* 4·0 Å

Atom (*i*)	Atom (*j*)	Symmetry (*j*)*	Distance
Cl(1)	Cl(2)	*M*1	3·60 ± 0·02 Å
	Cl(2)	*M*2	3·60 ± 0·02
	Cl(2)	*M*3	3·75 ± 0·02
	Cl(2)	*M*4	3·75 ± 0·02
Cl(2)	Cl(2)	*M*5	3·59 ± 0·03
	Cl(2)	*M*6	3·67 ± 0·03
	Cl(3)	*M*4	3·79 ± 0·02

* Coordinates of atom (*j*) are related to those in Table 2 by the following operations:

$M1 = \frac{1}{2}-x,\ \frac{1}{2}+y,\ \frac{1}{2}-z$ $M4 = \frac{1}{2}-x,\ \frac{1}{2}-y,\ 1-z$
$M2 = x-\frac{1}{2},\ \frac{1}{2}+y,\ z$ $M5 = 1-x,\ y,\ \frac{1}{2}-z$
$M3 = x-\frac{1}{2},\ \frac{1}{2}-y,\ -\frac{1}{2}+z$ $M6 = 1-x,\ -y,\ 1-z$

No other Pa–Cl distances are available in the literature for comparison with the present results. However, using the unit-cell data for $PaCl_4$ (Zachariasen, 1954*a*) and the atomic coordinates in isostructural UCl_4 (Mooney, 1949), one obtains Pa–Cl distances of 2·43 and 3·09 Å for Pa in eight-coordination.

Only a few examples of pentagonal bipyramidal coordination are known to occur in crystals. These include $UO_2F_5^{3-}$ in $K_3UO_2F_5^{3-}$ (Zachariasen, 1954*b*) and UF_7^{3-} in K_3UF_7 (Zachariasen, 1954*c*). The coordination polyhedron in β-UF_5 (Zachariasen, 1949) resembles the present one. (A detailed comparison of configurations, however, is not warranted since the fluorine positions were deduced from spatial considerations alone.) Interestingly enough, the 1:5 composition in β-UF_5 is achieved by the sharing of *vertices* at four positions in the pentagonal section.

One other actinide element is reported to form a pentachloride, that being uranium. Zachariasen (1948) mentioned that UCl_5 is monoclinic, but no unit cell data were given. In view of the pronounced similarity in crystal chemistry among the actinide elements, there is a strong possibility that UCl_5 is isostructural with $PaCl_5$.

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