of the I.B.M. Research Center, Poughkeepsie, N.Y. This program refines both the structure parameters and the temperature factors for each set of atoms. Refinement of the structure was done with the 8(*b*) positions 0%, 25%, 50%, 75%, and 100% occupied. Fig. 1 shows a plot of the reliability factor, $R = \Sigma||F_o|-|F_c||\div\Sigma|F_o|$, obtained from the calculations. The most intense reflection, (880), was omitted when computing R to avoid scaling errors. The magnitudes of F_o and F_c are shown in Table 1; the tabulated F_c is based on the structure with 8(*b*) sites 50% occupied. There is excellent agreement between the three structure parameters obtained by the least-squares refinement and those obtained by Brown:

Position		Brown	These data (8(*b*), 50% occupied)
96(*g*)	(x, x, z)	$x = 0{\cdot}0654$	$x = 0{\cdot}0644$
		$z = 0{\cdot}3009$	$z = 0{\cdot}3009$
48(*f*)	$(x, 0, 0)$	$x = 0{\cdot}1407$	$x = 0{\cdot}1408$

A lattice parameter of 14·516 Å was obtained from data taken on a back-reflection Weissenberg camera; Brown obtained 14·492 Å. The difference in the two values is in the direction which might be expected from the indicated difference in aluminum content.

The temperature factors are related to the vibrational amplitudes and hence to the strength of the bonds. The temperature-factor values are consistent with the bond strengths indicated by interatomic distances given by Brown. The values (Table 2) show that the vanadium atoms are most localized owing to their greater mass and strong bonding. Similarly, the aluminum atoms in the 96(*g*) and 48(*f*) sets, which are coordinated to vanadium, are more localized than the aluminum atoms in the 16(*d*) and 8(*b*) sets, which are not bonded directly to vanadium. Finally, the aluminum atoms in 8(*b*) with no bonds shorter than 3·1 Å have the most vibrational freedom and hence the lowest bond energy, and these are the atoms which do not seem necessary for stability of the structure.

Table 2. *Temperature factors*

Set	Temperature factor
16(*c*) (V)	0·12 Å
96(*g*) (Al)	0·52
48(*f*) (Al)	0·39
16(*d*) (Al)	1·35
8(*b*) (Al, 50%)	1·53

Since the crystals used in this investigation and those used by Brown were all grown on the aluminum-rich side of the compound, the difference in composition quite probably indicates a slope in the phase boundary as a function of temperature.

Reference

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Kristalldaten von Thorium-tetrakis-(dibenzoylmethan) und den isomorphen Komplexen des vierwertigen Cers und Urans.

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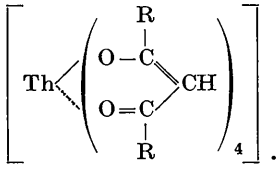
Angeregt durch präparative Arbeiten auf dem Gebiet der inneren Komplexe des Thoriums mit β-Diketonen (Wolf & Jahn, 1955) interessierten wir uns für den räumlichen Bau der Verbindungen des Typs



Mit Dibenzoylmethan als Ligand gelang uns nach anfänglichen Schwierigkeiten die Röntgenstrukturanalyse bis zur Raumgruppe. Für die weitere Strukturaufklärung ist die Isomorphie des Thoriumkomplexes mit Cer-tetrakis-(dibenzoylmethan) — dargestellt von Sacconi & Ercoli (1949) — wertvoll. Das bisher in reiner Form lediglich von Albers, Deutsch, Krastinat & Osten (1952) erhaltene Urantetrakis-(dibenzoylmethan) ist ebenfalls dem Thoriumkomplex isomorph.

Zu Röntgenuntersuchungen geeignete Einkristalle der drei genannten Verbindungen wurden durch langsames Abkühlen von in der Hitze mässig konzentrierten Xylol-Lösungen erhalten. Die langen, tafeligen Kristalle gehören dem äusseren Habitus nach zur rhombisch-bipyramidalen Kristallklasse (D_{2h}–*mmm*) mit den Begrenzungsflächen {010}, {110}, {012}. Nach Gitterkonstantenbestimmungen aus Drehkristallaufnahmen und der rechnerischen Indizierung von Schwenkaufnahmen wurden genaue Gitterkonstanten nach Straumanis aus Äquatorinterferenzen hoher Beugungswinkel auf Schwenkaufnahmen — symmetrisch zu den drei rhombischen Achsen — ermittelt (Tabelle 1).

Tabelle 1. *Gitterkonstanten*

	Cer-tetrakis-(dibenzoyl-methan)	Thorium-tetrakis-(dibenzoyl-methan)	Uran-tetrakis-(dibenzoyl-methan)
a (Å)	10,320±0,002	10,398±0,002	10,303±0·002
b (Å)	20,109±0,003	20,298±0,003	20,136±0,003
c (Å)	23,514±0,005	23,334±0,005	23,613±0,005

Die Statistik der vorhandenen Interferenzen (*hkl* alle Ordnungen, *hk*0 mit $h+k = 2n$, *h*0*l* mit $l = 2n$, 0*kl* mit $l = 2n$) führt zu der wahrscheinlichen Raumgruppe D_{2h}^{10}–*Pccn*.

Bei Annahme von 4 Molekülen in der Elementarzelle beträgt die Röntgendichte 1,52 g.cm.$^{-3}$ in Übereinstimmung mit der pyknometrisch ermittelten Dichte 1,50 g.cm.$^{-3}$.

Da der Beitrag leichter Atome zum Strukturfaktor infolge ungleich stärkeren Abfalls des Atomformfaktors mit steigendem sin θ/λ neben dem der schweren Atome vernachlässigt werden kann, liess sich aus dem visuell geschätzten Gang der Intensitäten bei hohen Beugungswinkeln die Punktlage der schweren Atome (Ce, Th, U) angenähert bestimmen.

Vierzählige spezielle Punktlage (*c*) in der Raumgruppe *Pccn*:

$$\tfrac{1}{4}, \tfrac{1}{4}, \tfrac{1}{8}\pm\varDelta z; \quad \tfrac{3}{4}, \tfrac{3}{4}, -\tfrac{1}{8}\pm\varDelta z; \quad \tfrac{1}{4}, \tfrac{1}{4}, \tfrac{5}{8}\pm\varDelta z; \quad \tfrac{3}{4}, \tfrac{3}{4}, \tfrac{3}{8}\pm\varDelta z ,$$

mit $\varDelta z = 0{,}015\pm0{,}002$ für Thorium und $\varDelta z = 0{,}018\pm0{,}002$ für Cer und Uran.

Um die weitere Aufklärung der Struktur sind wir bemüht.

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Structure factor algebra. II.

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The simple rules for finding symmetry relations between structure factors and for the linearization of structure factors stated in the paper entitled 'Algèbre des facteurs de structure' (Bertaut, 1956, henceforth referred to as I) do not always apply without modification.

Symmetry relations

Consider two equivalent vectors $\mathbf{r}$ and $\mathbf{r}'$, related by the symmetry operation C: $\mathbf{r}' = C\mathbf{r}$. The operation C contains in general a translational component $\mathbf{t}$ and a dyadic part A (proper or improper rotation):

$$\mathbf{r}' = C\mathbf{r} = A\mathbf{r}+\mathbf{t}\,.$$

Now, as was stated by Waser (1955), the relationship between $\mathbf{r}$ and $\mathbf{r}'$ in direct space engenders the relationship

$$F(\mathbf{h}) = F(\mathbf{h}') \exp\,(2\pi i\mathbf{h}.\mathbf{t}) \tag{1}$$

between structure factors $F(\mathbf{h}')$, and $F(\mathbf{h})$, where $\mathbf{h}' = \mathbf{h}A = A^{-1}\mathbf{h}$.

In general A^{-1} is not identical with A, as was implied by the simple rule of paper I. However, $A^{-1} = A$ whenever A is of order $2 (m, \bar{1}, 2)$, and then the rule given in I is correct.

The index triple (h', k', l') symbolized by $\mathbf{h}' = A^{-1}\mathbf{h} = \mathbf{h}A$ may be obtained by post-multiplication of the row matrix (h, k, l) with the 3×3 matrix representing A (cf. MacGillavry, 1950), or by the following method of inspection.

Consider, for example, the equivalent points $\mathbf{r} = x, y, z$, and $\mathbf{r}' = C\mathbf{r} = \frac{1}{2}-y, x, z$ (space group *Pn*3*n*, cf. Waser, 1955). The latter contributes to the structure factor the term $(-1)^h \exp 2\pi i(-hy+kx+lz)$. Rearrange so as to bring the parameters x, y, z into their usual sequence again. This regrouping of the parenthesis casts $\mathbf{h}.\mathbf{r}'$ into the equivalent form $(\mathbf{h}A)\mathbf{r}+\mathbf{h}.\mathbf{t}$ and here results in $(-1)^h \exp 2\pi i(kx+\bar{h}y+lz)$. From this the symmetry relation

$$F(hkl) = (-1)^h F(k\bar{h}l)$$

may be read off directly.

Linearization

The correct linearization relation for a structure-factor product (cf. Bertaut, 1955, equation III–12) is shown below to be

$$\xi(\mathbf{h}_1)\xi(\mathbf{h}_2) = \sum_{s=1}^{n} \exp\,(2\pi i\mathbf{h}_2\mathbf{t}_s)\xi(\mathbf{H}_s)\,, \tag{2}$$

where

$$\xi(\mathbf{h}) \sum_{s=1}^{n} = \exp 2\pi i\mathbf{h}C_s\mathbf{r} \tag{3}$$

is the trigonometric part of the structure factor, and where

$$\mathbf{H}_s = \mathbf{h}_1+\mathbf{h}_2A_s\,.$$

This follows from the expansion

$$\begin{aligned}\xi(\mathbf{h}_1)\xi(\mathbf{h}_2) &= \sum_p \sum_q \exp\,(2\pi i\mathbf{h}_1C_p\mathbf{r}) \exp 2\pi i\mathbf{h}_2C_q\mathbf{r})\\ &= \sum_p \sum_s \exp 2\pi i(\mathbf{h}_1+\mathbf{h}_2C_s)C_p\mathbf{r} \end{aligned} \tag{5}$$

with $C_s = C_qC_p^{-1}$. As q runs from 1 to n with p fixed, s varies from 1 to n also, only in different order. Furthermore, $\mathbf{h}_2C_s(C_p\mathbf{r}) = \mathbf{h}_2A_s(C_p\mathbf{r})+\mathbf{h}_2\mathbf{t}_s$. Thus rearrangement of the last double sum in (3) yields

$$\sum_s \left(\sum_p \exp 2\pi i(\mathbf{h}_1+\mathbf{h}_2A_s)C_p\mathbf{r}\right) \exp 2\pi i\mathbf{h}_2\mathbf{t}\,,$$

which can be rewritten in the form (2).

The rule for linearization may also be stated as follows: Find all symmetry relations (1) for the structure factor $F(\mathbf{h}_2)$ and list all the reciprocal vectors $\mathbf{h}_2A_s$ as well as the phase factors $\exp 2\pi i\mathbf{h}_2\mathbf{t}_s$, $s = 1, \ldots, n$. Add $\mathbf{h}_1$ to all $\mathbf{h}_2A_s$ to give $\mathbf{H}_s$. Multiply each $\xi(\mathbf{H}_s)$ with the corresponding phase factor and sum.

The simpler rule given in I applies to all space groups containing symmetry elements of order 2 only. It also applies to space groups in which those symmetry operations that interrelate coordinate axes have no translational components. Fortunately, the correct rules were used in the derivation of the *Tables de Linéarisation des Produits et Puissances des Facteurs de Structure* (Bertaut