

trépiéd en *endo* est plus difficile puisque les proportions des deux diastéréoisomères obtenus sont de 82% *exo* et 18% *endo*.

Nous remercions vivement MM Faure et Loiseleur de l'Université de Lyon I pour les conseils et l'aide qu'ils nous ont apportés.

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## The Structure of Chlorotris[1–3- $\eta$ -(1,4,7-trimethylindenyl)]thorium

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#### Abstract

$[\text{Th}(\text{C}_{12}\text{H}_{13})_3\text{Cl}]$  crystallizes in space group  $P2_1/c$  with  $a = 9.781$  (2),  $b = 16.565$  (2),  $c = 18.913$  (2) Å,  $\beta = 100.96$  (1)° and  $D_c = 1.632$  Mg m<sup>-3</sup> for  $Z = 4$ . The crystal structure was solved by direct methods. Full-matrix least-squares refinement with all atoms except H treated anisotropically gave an  $R$  value of 0.022 for 3759 reflections. Coordination about the Th atom is a slightly distorted tetrahedron. The Th atom is bonded to the Cl atom with a Th–Cl bond length of 2.664 (1) Å. The distances from the Th atom to the C atoms of each five-membered ring of the three indenyl moieties range from 2.721 (3) to 2.962 (3) Å. The orientation of the trimethylindenyl rings and the shorter bonds observed between the Th atom and the three isolated C atoms of the five-membered ring of each indenyl moiety suggest a trihapto character of the metal–carbon bonding.

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#### Introduction

Since the initial report of the preparation and characterization of uranocene (Streitwieser & Muller-Westerhoff, 1968; Zalkin & Raymond, 1969; Avdeef, Raymond, Hodgson & Zalkin, 1972), considerable interest has been generated about the nature of the metal–carbon bond in organoactinide complexes.

While structural data have been reported for a number of  $\pi$ -sandwich organouranium compounds (Hodgson, Dempf & Raymond, 1971; Hodgson & Raymond, 1973; Wong, Yen & Lee, 1965; Burns & Laubereau, 1971; Burns, 1974; Leong, Hodgson & Raymond, 1973; Fischer, Klahne & Kopf, 1978; Perego, Cesari, Farina & Lugli, 1975, 1976; Atwood, Hains, Tsutsui & Gebala, 1973), thorium complexes have not been extensively investigated to date. Structural data exist only for bis(cyclooctatetraene)thorium (Avdeef *et al.*, 1972), bis(cyclopentadienyl)dithorium (Baker, Raymond, Marks & Wachter, 1974) and bis(2-butene-2,3-diolato)bis(pentamethylcyclopenta-

dienyl)thorium (Manriquez, Fagan, Marks, Day & Day, 1978). In these compounds, the carbocyclic species  $C_nH_n$ ,  $\pi$ -bonded to the thorium, are restricted to the cases with  $n = 5$  and  $n = 8$ .

We report, in the present paper, the structure of a new complex, chlorotris(1,4,7-trimethylindenyl)-thorium  $[Th(C_{12}H_{13})_3Cl]$ , to clarify the role of the Th atom in an environment of five- and six-membered conjugated ring systems.

The closest analogous organoactinide compound whose structure has been reported in the literature is chlorotris(indenyl)uranium,  $[U(C_9H_7)_3Cl]$  (Burns & Laubereau, 1971), in which indenyl rings are  $\pi$ -linked to the U atom through the C atoms of the five-membered ring portion. Substantial differences were found in the U—C bond lengths. The three C atoms of the indenyl anion which are in the five-membered ring but not in the six-membered ring were found to have shorter U—C bond lengths than the remaining two C atoms of the five-membered ring, while in the cyclopentadienyl complexes, either of uranium or thorium, the actinide atom appears to be symmetrically bonded to the C atoms. This result would apparently impose a trihapto character on the bonding in the structure of  $[U(C_9H_7)_3Cl]$  but the authors do not rule out the possibility of a pentahapto bonding. The lengthening of bonds to the C atoms common to the five- and six-membered ring portions could result from steric interference between the Cl atom and the six-membered rings.

The determination of the structure of the title compound was undertaken to provide accurate details on the Th—C bonds.

### Experimental

The space group was unequivocally established by precession photographs. The cell dimensions were determined by the least-squares method from angle data recorded at  $293 \pm 1$  K for 25 reflections.

Intensities of 5857 observed independent reflections were collected, in the  $\theta$ - $2\theta$  scan mode, with an Enraf-Nonius CAD-4 X-ray diffractometer using monochromatic Mo  $K\alpha$  radiation ( $\lambda = 0.71073$  Å).

As a check on the stability of the diffractometer and of the crystal, two reflections were measured at 30 min intervals during data collection.

The intensities were then corrected for Lorentz, polarization and absorption effects ( $\mu = 48.694$  cm $^{-1}$ ). The calculated transmission factors range from 23.85 to 31.35%.

The structure was solved by direct methods. Full-matrix least-squares refinement was carried out on 3759 independent reflections for which  $F^2 \geq 3\sigma(F^2)$ . The calculation included both  $f'$  and  $f''$  for anomalous-dispersion effects of the Th and Cl atoms.

Table 1. Atomic positional and equivalent isotropic thermal parameters with standard deviations

	$B_{eq} = \frac{1}{3} \text{trace } \bar{B}$			$B_{eq}$ (Å $^2$ )
	x	y	z	
Th	0.25985 (1)	0.21574 (1)	0.93712 (1)	2.605 (5)
Cl	0.0078 (1)	0.16041 (7)	0.94558 (6)	4.583 (4)
C(1)	0.2116 (4)	0.2715 (3)	1.0734 (2)	4.0 (2)
C(1')	0.0691 (5)	0.2739 (3)	1.0916 (3)	5.9 (2)
C(2)	0.2682 (4)	0.3348 (2)	1.0382 (2)	3.8 (2)
C(3)	0.4067 (5)	0.3201 (2)	1.0359 (2)	3.9 (2)
C(4)	0.5784 (4)	0.2113 (2)	1.1009 (2)	4.2 (2)
C(4')	0.7030 (5)	0.2478 (4)	1.0820 (3)	6.1 (2)
C(5)	0.5834 (4)	0.1476 (2)	1.1421 (2)	4.5 (2)
C(6)	0.4631 (5)	0.1115 (2)	1.1600 (2)	4.9 (2)
C(7)	0.3318 (5)	0.1423 (2)	1.1372 (2)	4.2 (2)
C(7')	0.2052 (6)	0.1025 (3)	1.1549 (3)	6.3 (2)
C(8)	0.3238 (4)	0.2155 (2)	1.0966 (2)	3.4 (1)
C(9)	0.4452 (4)	0.2479 (2)	1.0760 (2)	3.3 (1)
C(10)	0.2923 (4)	0.0469 (2)	0.9348 (2)	3.8 (2)
C(10')	0.1969 (6)	-0.0099 (3)	0.9658 (3)	6.2 (2)
C(11)	0.4149 (4)	0.0808 (2)	0.9753 (2)	4.0 (2)
C(12)	0.4890 (4)	0.1227 (2)	0.9303 (2)	4.1 (2)
C(13)	0.4589 (4)	0.1272 (2)	0.7916 (2)	4.7 (2)
C(13')	0.5983 (6)	0.1682 (4)	0.7910 (3)	8.2 (3)
C(14)	0.3704 (5)	0.1025 (3)	0.7305 (2)	5.5 (2)
C(15)	0.2440 (5)	0.0618 (2)	0.7323 (2)	4.8 (2)
C(16)	0.2011 (4)	0.0450 (2)	0.7944 (2)	4.1 (2)
C(16')	0.0660 (5)	0.0024 (3)	0.7940 (3)	5.7 (2)
C(17)	0.2928 (4)	0.0656 (2)	0.8616 (2)	3.3 (1)
C(18)	0.4172 (4)	0.1095 (2)	0.8578 (2)	3.5 (2)
C(19)	0.0782 (5)	0.2798 (2)	0.8136 (2)	4.0 (2)
C(19')	-0.0632 (5)	0.2457 (4)	0.7847 (3)	6.6 (2)
C(20)	0.2029 (5)	0.2577 (2)	0.7948 (2)	4.0 (2)
C(21)	0.3118 (4)	0.3101 (3)	0.8262 (2)	4.2 (2)
C(22)	0.3064 (6)	0.4457 (3)	0.8923 (2)	6.0 (2)
C(22')	0.4573 (7)	0.4644 (4)	0.8891 (3)	9.2 (3)
C(23)	0.2161 (8)	0.4942 (3)	0.9183 (3)	7.7 (3)
C(24)	0.0773 (6)	0.4756 (3)	0.9173 (2)	7.3 (3)
C(25)	0.0189 (5)	0.4052 (3)	0.8887 (2)	6.1 (2)
C(25')	-0.1272 (6)	0.3855 (4)	0.8903 (3)	9.0 (3)
C(26)	0.1060 (4)	0.3516 (2)	0.8570 (2)	3.9 (1)
C(27)	0.2493 (5)	0.3703 (2)	0.8622 (2)	3.9 (2)

All atoms were treated anisotropically, except H atoms which were all given the same isotropic temperature factor  $B = 4.0$  Å $^2$ . The H-atom positions were calculated by assuming the appropriate geometry and C—H bond lengths of 1.087 Å. The final agreement factors  $R_1 = \sum [|F_o| - |F_c|] / \sum |F_o|$  and  $R_2 = [\sum w(|F_o| - |F_c|)^2 / \sum wF_o^2]^{1/2}$  (weighted  $R$  factor) are 0.022 and 0.034 respectively.\*

The positional parameters from the final least-squares cycle and their associated standard deviations are listed in Table 1.

\* Lists of structure factors, anisotropic thermal parameters, hydrogen coordinates, bond angles for the indenyl groups and equations for least-squares planes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 36873 (22 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

### Description of the structure and discussion

The structure is illustrated in Fig. 1, which represents one molecule, and in Fig. 2, which shows the packing in the unit cell.

The thermal motions of the Th, Cl and C atoms are depicted as 50% probability ellipsoids. To clarify the drawings we did not include H atoms.

The motion of the Th atom is almost isotropic but the C atoms exhibit relatively large anisotropic thermal motion and show a preferential oscillation about their respective pseudo-fivefold and sixfold axes. For the ring

C atoms, the r.m.s. amplitudes of vibration along the major axes of the ellipsoids range from 0.161 to 0.442 Å.

The intramolecular bond lengths and angles with standard deviations are listed in Table 2.

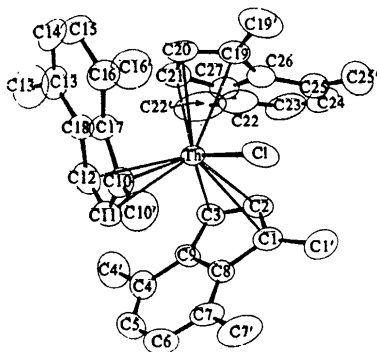


Fig. 1. The molecule of  $[\text{Th}(\text{C}_{12}\text{H}_{13})_3\text{Cl}]$ .

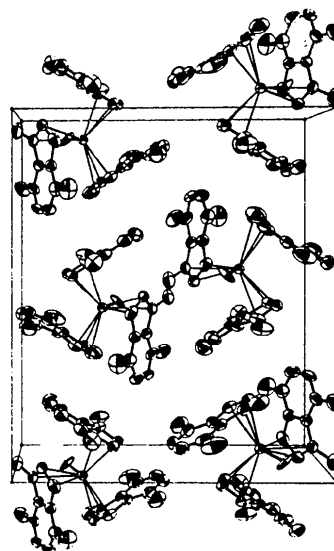


Fig. 2. Packing in the crystal. Viewing direction is along *a*; *b* is horizontal from left to right.

Table 2. Intramolecular bond lengths (Å) and angles ( $^{\circ}$ ) with standard deviations in parentheses

#### (a) Bond lengths

Th—Cl 2.664 (1)

#### Indenyl group I

Th—C(2) 2.738 (4)  
Th—C(3) 2.742 (4)  
Th—C(1) 2.862 (4)  
Th—C(9) 2.942 (3)  
Th—C(8) 2.962 (3)  
Th—C(7) 3.909 (3)  
Th—C(4) 3.955 (4)  
Th—C(6) 4.639 (4)  
Th—C(5) 4.653 (3)  
Th—I 2.554 (1)

#### Indenyl group II

—C(11) 2.721 (3)  
—C(12) 2.744 (4)  
—C(10) 2.816 (4)  
—C(18) 2.932 (4)  
—C(17) 2.917 (3)  
—C(16) 3.877 (3)  
—C(13) 3.943 (4)  
—C(15) 4.616 (4)  
—C(14) 4.644 (4)  
Th—II 2.530 (1)

#### Indenyl group III

—C(20) 2.733 (4)  
—C(21) 2.740 (4)  
—C(19) 2.856 (3)  
—C(27) 2.918 (3)  
—C(26) 2.960 (3)  
—C(25) 3.927 (4)  
—C(22) 3.948 (4)  
—C(24) 4.648 (5)  
—C(23) 4.640 (5)  
Th—III 2.549 (1)

C(1)—C(2) 1.411 (6)  
C(1)—C(8) 1.441 (5)  
C(2)—C(3) 1.386 (6)  
C(3)—C(9) 1.427 (5)  
C(4)—C(5) 1.307 (5)  
C(4)—C(9) 1.433 (5)  
C(5)—C(6) 1.418 (6)  
C(6)—C(7) 1.372 (6)  
C(7)—C(8) 1.428 (5)  
C(8)—C(9) 1.424 (6)  
C(1)—C(1') 1.498 (6)  
C(4)—C(4') 1.464 (7)  
C(7)—C(7') 1.496 (6)

C(10)—C(11) 1.411 (5)  
C(10)—C(17) 1.419 (5)  
C(11)—C(12) 1.401 (6)  
C(12)—C(18) 1.434 (5)  
C(13)—C(14) 1.369 (6)  
C(13)—C(18) 1.418 (6)  
C(14)—C(15) 1.414 (6)  
C(15)—C(16) 1.349 (6)  
C(16)—C(17) 1.451 (4)  
C(17)—C(18) 1.431 (5)  
C(10)—C(10') 1.519 (6)  
C(13)—C(13') 1.525 (6)  
C(16)—C(16') 1.496 (6)

C(19)—C(20) 1.383 (6)  
C(19)—C(26) 1.441 (5)  
C(20)—C(21) 1.414 (6)  
C(21)—C(27) 1.411 (6)  
C(22)—C(23) 1.354 (8)  
C(22)—C(27) 1.442 (6)  
C(23)—C(24) 1.389 (9)  
C(24)—C(25) 1.365 (8)  
C(25)—C(26) 1.438 (6)  
C(26)—C(27) 1.420 (6)  
C(19)—C(19') 1.498 (6)  
C(22)—C(22') 1.520 (8)  
C(25)—C(25') 1.471 (8)

#### (b) Selected bond angles

Cl—Th—I 98.5  
Cl—Th—II 99.8

Cl—Th—III 99.0  
I—Th—II 118.4

I—Th—III 117.6  
II—Th—III 116.8

Table 3. *Intramolecular non-bonded distances (Å) with standard deviations in parentheses*

(1) Cl...C							
Indenyl group I		Indenyl group II		Indenyl group III			
Cl...C(1)	3.373 (4)	Cl...C(10)	3.397 (4)	Cl...C(19)	3.357 (4)		
Cl...C(2)	4.027 (4)	Cl...C(11)	4.131 (4)	Cl...C(20)	4.055 (4)		
Cl...C(3)	4.755 (4)	Cl...C(12)	4.811 (4)	Cl...C(21)	4.758 (4)		
Cl...C(8)	3.898 (3)	Cl...C(17)	3.801 (4)	Cl...C(26)	3.792 (4)		
Cl...C(9)	4.741 (3)	Cl...C(18)	4.694 (4)	Cl...C(27)	4.644 (4)		
(2) Cl...C' (<4.0 Å)							
Cl...C(1')	3.300 (5)	Cl...C(10')	3.355 (5)	Cl...C(19')	3.306 (5)		
(3) C...C (<3.6 Å)							
C(2)...C(22)	3.395 (6)	C(3)...C(22)	3.413 (5)	C(7)...C(11)	3.468 (6)	C(14)...C(20)	3.395 (6)
C(2)...C(23)	3.455 (6)	C(3)...C(27)	3.453 (5)	C(8)...C(11)	3.438 (5)	C(15)...C(20)	3.503 (5)
C(2)...C(24)	3.540 (6)	C(4)...C(11)	3.382 (5)	C(9)...C(11)	3.342 (5)	C(16)...C(20)	3.524 (5)
C(2)...C(25)	3.562 (5)	C(4)...C(12)	3.501 (5)	C(9)...C(12)	3.539 (6)	C(17)...C(20)	3.475 (5)
C(2)...C(26)	3.505 (5)	C(5)...C(11)	3.453 (5)	C(13)...C(20)	3.317 (6)	C(18)...C(20)	3.300 (5)
C(2)...C(27)	3.351 (5)	C(6)...C(11)	3.474 (5)	C(13)...C(21)	3.468 (6)	C(18)...C(21)	3.496 (6)

The shortest intramolecular non-bonded distances and the shortest intermolecular distances are reported in Tables 3 and 4 respectively.

The crystal structure consists of four discrete molecules of  $[\text{Th}(\text{C}_{12}\text{H}_{13})_3\text{Cl}]$  per unit cell. In the molecule, the chlorine and the five-membered rings of the three indenyl moieties are arranged in an approximate tetrahedron about the Th atom. The extent of deviation of the structure from a regular tetrahedron is shown by the angles between normals from the Th atom to the planes of the three indenyl groups (designated as I, II and III) and the Th—Cl bond direction (Table 2*b*). The average Cl—Th—indenyl angle of  $99.1^\circ$  and the average indenyl—Th—indenyl angle of  $117.6^\circ$  agree well with the corresponding angles found in similar pseudotetrahedral 'bent sandwich' uranium complexes (Wong *et al.*, 1965; Burns & Laubereau, 1971; Leong *et al.*, 1973; Perego *et al.*, 1976; Atwood *et al.*, 1973). The distances from the Th atom to the planes of the rings I, II, and III are reported in Table 2(*a*).

The results of least-squares-plane calculations are shown in Table 5. The five- and six-membered portions of the indenyl rings are almost planar although each indenyl ring as a whole exhibits significant deviations from planarity. A bending of about  $7.5^\circ$  occurs

between the five- and the six-membered ring portions as shown by the dihedral angles reported in Table 5. This bending would result from steric hindrance between the three trimethylindenyl groups around the Th atom. Indeed there appear to be several non-bonded intramolecular contacts (Table 3) between C atoms of the indenyls equal to or slightly shorter than the normal van der Waals contact of  $3.4 \text{ \AA}$  between aromatic molecules (Pauling, 1960).

Table 5. *Deviations (Å) from the least-squares planes*

Plane A		Plane D		Plane G	
C(1)	0.020 (4)	C(10)	-0.004 (4)	C(19)	-0.006 (4)
C(2)	-0.020 (4)	C(11)	0.021 (4)	C(20)	0.018 (4)
C(3)	0.030 (4)	C(12)	-0.030 (4)	C(21)	-0.023 (4)
C(8)	0.016 (4)	C(17)	-0.015 (4)	C(26)	-0.008 (4)
C(9)	-0.028 (4)	C(18)	0.027 (4)	C(27)	0.019 (4)
C(1')	-0.188 (5)	C(10')	0.192 (5)	C(19')	0.181 (5)
Plane B		Plane E		Plane H	
C(4)	0.014 (4)	C(13)	0.003 (4)	C(22)	0.003 (4)
C(5)	-0.023 (4)	C(14)	-0.010 (5)	C(23)	0.012 (5)
C(6)	0.002 (4)	C(15)	-0.005 (4)	C(24)	-0.004 (4)
C(7)	0.027 (4)	C(16)	0.025 (4)	C(25)	-0.018 (4)
C(8)	-0.035 (4)	C(17)	-0.031 (4)	C(26)	0.032 (4)
C(9)	0.016 (4)	C(18)	0.018 (4)	C(27)	-0.025 (4)
C(4')	0.001 (6)	C(13')	-0.060 (6)	C(22')	0.078 (6)
C(7')	0.089 (5)	C(16')	0.042 (5)	C(25')	-0.078 (6)
Plane C		Plane F		Plane I	
C(1)	-0.064 (4)	C(10)	0.056 (4)	C(19)	0.055 (4)
C(2)	-0.085 (4)	C(11)	0.084 (4)	C(20)	0.085 (4)
C(3)	0.065 (4)	C(12)	-0.062 (4)	C(21)	-0.055 (4)
C(4)	-0.007 (4)	C(13)	0.016 (4)	C(22)	0.020 (4)
C(5)	-0.085 (4)	C(14)	0.067 (5)	C(23)	0.070 (5)
C(6)	-0.028 (4)	C(15)	0.032 (4)	C(24)	0.028 (4)
C(7)	0.073 (4)	C(16)	-0.067 (4)	C(25)	-0.059 (4)
C(8)	0.057 (4)	C(17)	-0.056 (4)	C(26)	-0.058 (4)
C(9)	0.074 (4)	C(18)	-0.072 (4)	C(27)	-0.086 (4)
C(1')	-0.349 (5)	C(10')	0.340 (5)	C(19')	0.328 (5)
C(4')	-0.053 (6)	C(13')	0.111 (6)	C(22')	0.121 (6)
C(7')	0.168 (5)	C(16')	-0.114 (5)	C(25')	-0.146 (6)

Table 4. *Intermolecular distances (Å) with standard deviations in parentheses*

Symmetry code	
(i) $-x, -\frac{1}{2} + y, \frac{1}{2} - z$ ;	(iv) $-1 + x, y, z$
(ii) $x, \frac{1}{2} - y, -\frac{1}{2} + z$ ;	(v) $1 + x, y, z$
(iii) $-x, \frac{1}{2} + y, \frac{1}{2} - z$ ;	
(1) C...C' (<3.8 Å)	
C(15)...C(25 <sup>(i)</sup> )	3.767 (9)
C(20)...C(7 <sup>(ii)</sup> )	3.535 (8)
C(21)...C(7 <sup>(iii)</sup> )	3.528 (8)
C(25)...C(16 <sup>(iii)</sup> )	3.762 (8)
(2) C'...C' (<4.0 Å)	
C(1')...C(4 <sup>(iv)</sup> )	3.556 (8)
C(13')...C(19 <sup>(v)</sup> )	3.604 (10)

Dihedral angles ( $^\circ$ )

C/F	118.2 (1)	A/B	172.4 (1)
C/I	117.6 (1)	D/E	172.8 (1)
F/I	116.8 (1)	G/H	172.4 (1)

Bond lengths and angles within the trimethylindenyl rings (Table 2) are all normal and within the range expected for five- and six-membered conjugated ring systems (Atwood *et al.*, 1973; Burns & Laubereau, 1971; Webb & Marsh, 1967). Corresponding dimensions in the three trimethylindenyl groups are equal within experimental error.

The Th—Cl bond length of 2.664 (1) Å corresponds to the value expected for a single covalent bond (2.64 Å). A similar value (2.69 Å) has recently been reported for the Th—Cl bonds in [Th(C<sub>8</sub>H<sub>8</sub>)(C<sub>4</sub>H<sub>8</sub>O)<sub>2</sub>Cl<sub>2</sub>] (Zalkin, Templeton & Levanda, 1979).

The Th—C distances reported in Table 2 show that the Th atom is bonded to the C atoms of each five-membered ring of the three indenyl moieties with distances ranging from 2.721 (3) to 2.962 (3) Å. As in [U(C<sub>9</sub>H<sub>7</sub>)<sub>3</sub>Cl] (Burns & Laubereau, 1971) the closest Th—C approaches are, in each case, to the three non-bridging atoms (1, 2 and 3 ring positions) of the five-membered rings. The Th—C(2)\* and Th—C(3)\* distances, 2.731 (4) and 2.742 (4) Å respectively (averaged values for the three indenyl rings), are comparable while the average Th—C(1)\* distance, 2.845 (4) Å, is slightly longer. As for the other two (bridging) C atoms, they are respectively at distances of 2.931 (3) and 2.946 (3) Å (averaged values) apart from the Th atom. These last distances are 0.1 Å greater than the values reported for the pentahapto Th—C bond lengths in [Th(C<sub>5</sub>H<sub>4</sub>)(C<sub>5</sub>H<sub>5</sub>)<sub>2</sub>]<sub>2</sub> (Baker *et al.*, 1974) and [Th{C<sub>5</sub>(CH<sub>3</sub>)<sub>5</sub>]<sub>2</sub>{C<sub>2</sub>(CH<sub>3</sub>)<sub>2</sub>O<sub>2</sub>}]<sub>2</sub> (Manriquez *et al.*, 1978). The lengthening of Th—C(8)\* and Th—C(9)\* bond distances, in comparison with Th—C(2)\* and Th—C(3)\* bond lengths, cannot be ascribed to steric interference since there are no short intra- or intermolecular non-bonded contacts involving the C atoms in the 8 and 9 positions (Tables 3 and 4). On the other hand, there appear to be some rather short intramolecular non-bonded distances between the Cl atom and the C atoms in the 1 ring position and also between the Cl and the methyl group attached to the C(1) atoms of the three trimethylindenyl groups. [The normal van der Waals distance between a Cl atom and an aromatic ring is about 3.5 Å while the corresponding distance between a Cl atom and a methyl group is about 3.8 Å (Pauling, 1960).] Therefore the lengthening of the Th—C(1) distance in comparison with Th—C(2) and Th—C(3) may be interpreted as resulting from steric interactions between the bulky Cl atom and methyl groups in the 1 ring position. Based on these observations, the three shorter bonds between the Th atom and the C atoms in the 1, 2, 3 ring positions of the indenyl groups lend support to a model involving 1, 2, 3 trihapto-indenyl coordination. There

would be only very weak interactions between the metal and the bridging C atoms of the indenyls. This is not surprising since molecular-orbital calculations indicate that the negative charge of an indenyl anion primarily resides on the three isolated C atoms.

In conclusion, while there is no doubt concerning the pentahapto character of the metal—carbon bond in cyclopentadienyl organoactinide complexes, in indenyl compounds, the actinide atom seems to be more properly described as  $\eta^3$  covalently bonded. It is evident that in addition to electronic factors, the size of the ligands bonded to the metal is also a determining factor in the character of the metal—carbon bond.

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\* The numbers used here as indices to identify the C atoms correspond to their ring positions in the indenyl ring I, II or III (Table 2).