



Cite this: *Chem. Commun.*, 2024, 60, 10414

DOI: 10.1039/d4cc90297a

rsc.li/chemcomm

Correction: Thorium amidates function as single-source molecular precursors for thorium dioxide

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Correction for 'Thorium amidates function as single-source molecular precursors for thorium dioxide' by Mark D. Straub et al., *Chem. Commun.*, 2021, 57, 4954–4957, <https://doi.org/10.1039/D1CC00867F>.

The single crystal X-ray crystallographic data for Th(ITA)₄ (ITA = *N*-*tert*-butylisobutyramidate) has been reanalysed using a $P2_1/n$ unit cell. The structure of Th(ITA)₄ displayed full-molecule disorder when solved in the space group $C2/m$, as originally reported. However, revisiting the same single crystal X-ray crystallographic data showed a weaker $P2_1/n$ supercell containing an ordered arrangement of the ligands. The supercell was overlooked previously due to the strength of the heavy atoms in the crystal. The revised X-ray crystal structure of Th(ITA)₄ is shown in Fig. 1, with associated bond metrics and crystallographic data given in Tables 1 and 2. This change to the model of the X-ray structural data does not impact any other aspects of the data or conclusions reported previously.

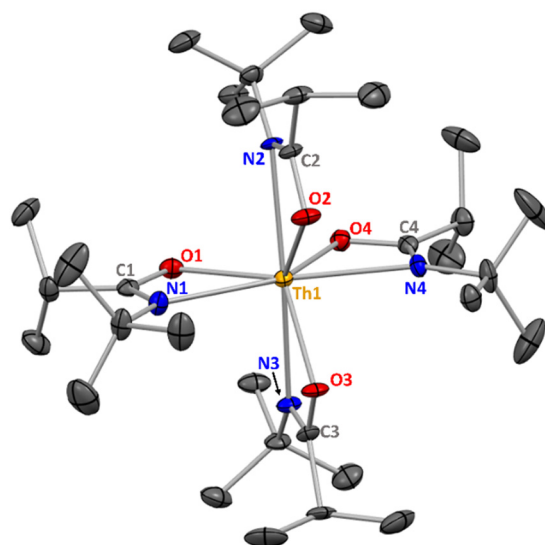


Fig. 1 X-ray crystal structure of **1** with 50% probability ellipsoids. Hydrogen atoms and structural disorder are omitted for clarity.

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Table 1 Selected atomic distances (Å) and angles (°) for Th(ITA)₄

Th1–O1	2.361(3)	C3–O3	1.305(6)
Th1–O2	2.416(3)	C4–O4	1.308(5)
Th1–O3	2.424(3)	C1–N1	1.299(5)
Th1–O4	2.356(3)	C2–N2	1.309(7)
Th1–N1	2.565(4)	C3–N3	1.310(7)
Th1–N2	2.557(5)	C4–N4	1.312(6)
Th1–N3	2.557(5)	O1–C1–N1	115.9(4)
Th1–N4	2.536(4)	O2–C2–N2	116.0(5)
C1–O1	1.312(5)	O3–C3–N3	116.7(5)
C2–O2	1.306(6)	O4–C4–N4	115.6(4)

Table 2 Crystallographic details and refinement metrics for Th(ITA)₄

Chemical formula	C ₃₂ H ₆₄ N ₄ O ₄ Th
Formula weight	800.91
Color, habit	Colorless, block
Crystal system	Monoclinic
Space group	<i>P</i> ₂ ₁ / <i>n</i>
<i>a</i> (Å)	8.8073(4)
<i>b</i> (Å)	24.7927(11)
<i>c</i> (Å)	17.2472(7)
α (°)	90
β (°)	94.9595(16)
γ (°)	90
<i>V</i> (Å ³)	3751.9(3)
<i>Z</i>	4
Density (g cm ⁻³)	1.418
<i>F</i> (000)	1624.0
Radiation type	Synchrotron
Radiation wavelength	(λ = 0.7288 Å)
μ (mm ⁻¹)	4.275
Crystal size (mm)	0.18 × 0.10 × 0.09
Meas. refl.	11 511
Indep. refl.	6998
Obsvd. [<i>I</i> > 2 σ (<i>I</i>)] refl.	6998
<i>R</i> _{int}	0.0422
Final [<i>I</i> ≥ 2 σ (<i>I</i>)] <i>R</i> indices	<i>R</i> ₁ = 0.0313 <i>wR</i> ₂ = 0.0660
Goodness-of-fit	1.047
CCDC	2377153

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

