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CORRECTION

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# 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.

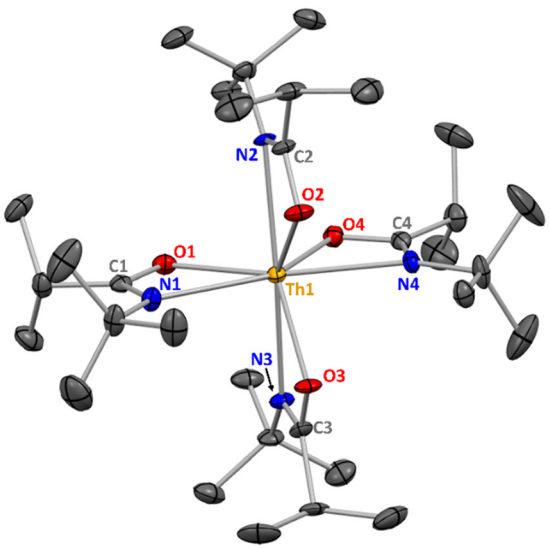


Fig. 1 X-ray crystal structure of **1** with 50% probability ellipsoids. Hydrogen atoms and structural disorder are omitted for clarity.

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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 | $C_{32}H_{64}N_4O_4Th$ |
| Formula weight | 800.91 |
| Color, habit | Colorless, block |
| Crystal system | Monoclinic |
| Space group | $P2_1/n$ |
| $a$ (Å) | 8.8073(4) |
| $b$ (Å) | 24.7927(11) |
| $c$ (Å) | 17.2472(7) |
| $\alpha$ (°) | 90 |
| $\beta$ (°) | 94.9595(16) |
| $\gamma$ (°) | 90 |
| $V$ (Å$^3$) | 3751.9(3) |
| $Z$ | 4 |
| Density (g cm$^{-3}$) | 1.418 |
| $F(000)$ | 1624.0 |
| Radiation type | Synchrotron |
| Radiation wavelength | ($\lambda$ = 0.7288 Å) |
| $\mu$ (mm$^{-1}$) | 4.275 |
| Crystal size (mm) | 0.18 × 0.10 × 0.09 |
| Meas. refl. | 11 511 |
| Indep. refl. | 6998 |
| Obsvd. [$I > 2\sigma(I)$] refl. | 6998 |
| $R_{int}$ | 0.0422 |
| Final [$I \geq 2\sigma(I)$] $R$ indices | $R_1$ = 0.0313 |
| | w$R_2$ = 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.