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The crystal structure of tris(µ₂-1,3-bis(4,4,4-trifluoro-3-oxido-1-(oxo)but-2-en-1-yl)phenyl-κ⁴O,O’:O’’,O’’’)-bis(1,2-dimethoxyethane-κ²O,O’)dicerium(III), C₅₀H₃₈F₁₈O₁₆Ce₂

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Abstract
C₅₀H₃₈F₁₈O₁₆Ce₂, monoclinic, C2/c (no. 15), a = 15.589(3) Å, b = 13.118(2) Å, c = 29.118(5) Å, β = 92.285(2)°, V = 5949.8(18) Å³, Z = 4, Rgt(F) = 0.0452, wRref(F²) = 0.1321, T = 273 K.

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Table 1: Data collection and handling.

| Crystal: | Crimson blocks |
| Wavelength: | Mo Kα radiation (0.71073 Å) |
| μ: | 16.3 cm⁻¹ |
| Diffractometer, scan mode: | Bruker APEX-II, ϕ and ω |
| 2θmax, completeness: | 56.8°, >98% |
| N(hkl)measured, N(hkl)unique, Rint: | 23328, 7330, 0.022 |
| Criterion for Iobs, N(hkl)gt: | Iobs > 2 σ(Iobs), 6502 |
| N(param)refined: | 391 |
| Programs: | SHELX [6], Bruker programs [7] |

The title crystal structure is shown in the figure. Tables 1 and 2 contain details of the measurement method and a list of the atoms including atomic coordinates and displacement parameters.

Source of material
Tris(µ₂-1,3-bis(4,4,4-trifluoro-3-oxido-1-(oxo)but-2-en-1-yl)phenyl-κ⁴O,O’:O’’,O’’’)-bis(1,2-dimethoxyethane-κ²O,O’)dicerium(III) was synthesised following a literature method [1, 2]. In a typical reaction, to a solution of 1,3-bis(4,4,4-trifluoro-1,3-dioxobutyl)phenyl (1 g, 2.8 mmol) in 10 mL methanol, NaOH (0.2 g, 5.6 mmol) was added, and the mixture was allowed to stir for 5 min. Then CeCl₃·7H₂O (0.693 g, 1.86 mmol) in 5 mL water was added dropwise, and the mixture was allowed...
to stir for 24 h at room temperature. Then 20 mL water was added to this mixture. The formed precipitate was filtered, washed with water, and dried in air. The block-shaped crystals of the title complex were obtained in about ten days by recrystallization from a mixture of dimethylether and hexane.

**Experimental details**

All H atoms on C atoms were placed in idealized positions [C–H = 0.97 Å (methylene) and 0.93 Å (aromatic)] and included in the refinement in the riding-model approximation, with $U_{iso}$(H) = 1.2$U_{eq}$(methylene and aromatic C).

**Discussion**

$\beta$-Diketonate ligands have been widely used to construct different lanthanide complexes for their luminescence properties or they are used as precursors of metalorganic chemical vapor deposition for single and multi-component oxide thin films [3–5]. Herein, we report the crystal structure of a dinuclear Ce(III) complex with 1,3-bis(4,4,4-trifluoro-1,3-dioxobutyl)phenyl. The structural analysis reveals that the complex is a triple-bridged dinuclear complex by the coordination of three bis-$\beta$-diketonate ligands to two crystallographically equivalent Ce(III) metal centers. The crystallographically distinct Ce(III) is ligated to six oxygen atoms from the three bis-diketonate and two oxygen atoms from dimethylether, resulting in the distorted square antiprism geometry. The Ce–O distances are in the range of 2.413(3)–2.607(4) Å. There is no classical hydrogen bond in the complex; interactions of CH···F(2.723(6)–2.750(7) Å) and CH···O(2.722(6)–2.758(4) Å) play a subordinate role in the stabilization of the structures.

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**References**


2. Hou, Y. J.; Shi, J.; Chu, W. Y.; Sun, Z. Z.: Synthesis, crystal structure, and near-IR luminescent properties of lanthanide...


