

Tetrakis(μ -2,4-difluorobenzoato)bis[(2,4-difluorobenzoato)(1,10-phenanthroline)-gadolinium(III)]

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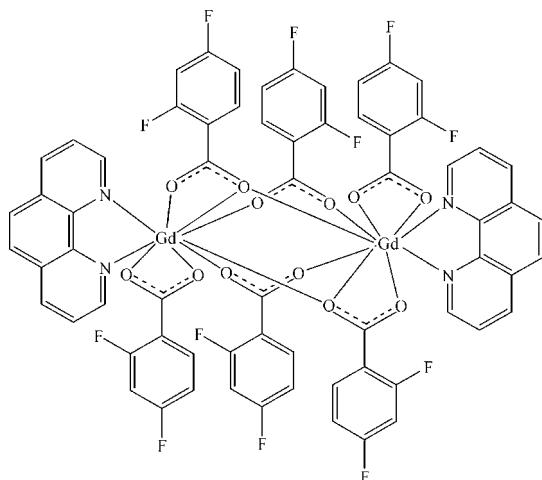
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.008$ Å; R factor = 0.032; wR factor = 0.095; data-to-parameter ratio = 12.8.

In the title compound, $[\text{Gd}_2(\text{C}_7\text{H}_3\text{F}_2\text{O}_2)_6(\text{C}_{12}\text{H}_8\text{N}_2)_2]$, the asymmetric unit comprises one Gd^{3+} cation chelated by two 2,4-difluorobenzoate and one 1,10-phenanthroline ligands. Two cations are linked into a centrosymmetric dimer via three bridging carboxylate groups of 2,4-difluorobenzoate ligands. Each Gd^{3+} ion is nine-coordinated by seven O atoms and two N atoms.

Related literature

For related literature, see: Church & Halvorson (1959); Chung *et al.* (1971); Okabe & Oya (2000); Serre *et al.* (2005); Pocker & Fong (1980); Scapin *et al.* (1997).



Experimental

Crystal data

$[\text{Gd}_2(\text{C}_7\text{H}_3\text{F}_2\text{O}_2)_6(\text{C}_{12}\text{H}_8\text{N}_2)_2]$
 $M_r = 1617.47$
Monoclinic, $P2_1/n$
 $a = 15.132$ (3) Å
 $b = 13.663$ (3) Å
 $c = 15.286$ (3) Å
 $\beta = 109.364$ (2)°

$V = 2981.6$ (9) Å³
 $Z = 2$
Mo $K\alpha$ radiation
 $\mu = 2.31$ mm⁻¹
 $T = 295$ (2) K
 $0.33 \times 0.14 \times 0.08$ mm

Data collection

Bruker APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2001)
 $T_{\min} = 0.516$, $T_{\max} = 0.837$
15634 measured reflections
5535 independent reflections
4598 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.037$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.032$
 $wR(F^2) = 0.095$
 $S = 1.00$
5535 reflections

433 parameters
H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 1.69$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.64$ e Å⁻³

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT-Plus (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CF2184).

References

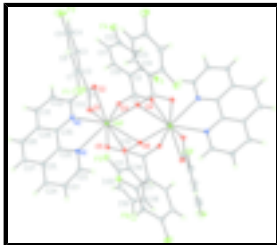
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