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μ-Acetato-diacetato{μ-6,6′-dimethoxy-2,2′-[*o*-phenylenebis(nitrilomethanylylidene)]diphenolato}gadolinium(III)zinc

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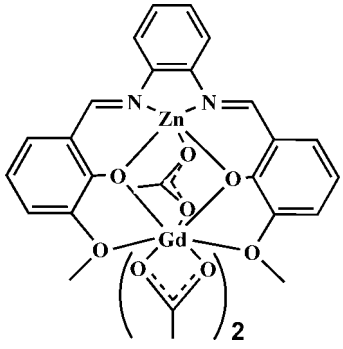
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.008 Å; R factor = 0.041; wR factor = 0.078; data-to-parameter ratio = 16.9.

In the heterodinuclear title complex, $[GdZn(C_{22}H_{18}N_2O_4)(CH_3COO)_3]$, the Zn^{II} ion is five-coordinated in a square-pyramidal environment defined by two O atoms and two N atoms from the ligand, forming the square plane, and one acetate O atom serving as the apex, while the Gd^{III} ion is nine-coordinated in an approximate mono-capped tetragonal–antiprismatic environment defined by four O atoms from the ligand and five acetate O atoms.

Related literature

For the synthesis of the ligand, see: Costes *et al.* (2000). For similar 3*d*–4*f* complexes of similar ligands, see: Bao *et al.* (2010); Liao *et al.* (2010); Xu *et al.* (2011).



Experimental

Crystal data

$[GdZn(C_{22}H_{18}N_2O_4)(C_2H_3O_2)_3]$
M_r = 774.16
Monoclinic, $P2_1/c$
a = 14.012 (3) Å
b = 13.581 (3) Å
c = 15.426 (3) Å
β = 103.65 (3)°
V = 2852.6 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 3.21 mm^{-1}
T = 293 K
0.15 × 0.14 × 0.13 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.645, T_{max} = 0.681
26483 measured reflections
6488 independent reflections
4513 reflections with $I > 2\sigma(I)$
R_{int} = 0.073

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.078
S = 1.01
6488 reflections
384 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

Data collection: *RAPID-AUTO* (Rigaku, 1998); cell refinement: *RAPID-AUTO*; data reduction: *CrystalClear* (Rigaku/MSC, 2002); 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: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG5198).

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