Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Poly[di-μ_4-benzene-1,4-dicarboxylato-μ_6-succinato-diholmium(III)]

Qin He* and Bao-Jun Huang

Department of Chemistry, Xuchang University, Xuchang 461000, People's Republic of China
Correspondence e-mail: qhe.xcu@163.com

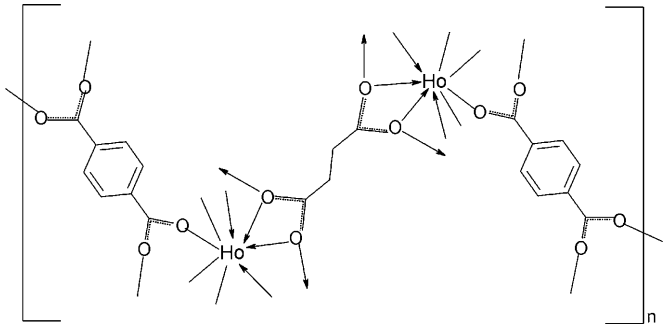
Received 25 October 2007; accepted 14 December 2007

Key indicators: single-crystal X-ray study; T = 291 K; mean σ(C–C) = 0.004 Å; R factor = 0.015; wR factor = 0.042; data-to-parameter ratio = 15.6.

The title compound, $[Ho_2(C_4H_4O_4)(C_8H_4O_4)_2]_n$, was synthesized hydrothermally. The Ho atom is coordinated by four O atoms from four benzene-1,4-dicarboxylate (BDC) anions and four O atoms from three succinate anions, in a distorted square-antiprismatic coordination geometry. The antiprisms are bridged by the benzene-1,4-dicarboxylate and succinate anions, into a three-dimensional coordination network. The succinate anions are located on centres of inversion.

Related literature

For related literature, see: Li & Wang (2005); Li *et al.* (2006); Wang & Li (2005); He *et al.* (2006).



Experimental

Crystal data

$[Ho_2(C_4H_4O_4)(C_8H_4O_4)_2]$
M_r = 387.08
Orthorhombic, *Pbca*
a = 13.8147 (3) Å
b = 6.7850 (2) Å
c = 21.7103 (5) Å
V = 2034.97 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 7.79 mm^{-1}
T = 291 (2) K
0.18 × 0.15 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.245, T_{max} = 0.682
11598 measured reflections
2411 independent reflections
2140 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.015
$wR(F^2)$ = 0.042
S = 1.06
2411 reflections
155 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.94 e Å^{-3}
$\Delta\rho_{min}$ = −0.60 e Å^{-3}

Table 1
Selected bond lengths (Å).

Ho—O1	2.2899 (17)	Ho—O5	2.4753 (16)
Ho—O2^{i}	2.2320 (17)	Ho—O5^{iv}	2.4015 (18)
Ho—O3^{ii}	2.3208 (16)	Ho—O6^{v}	2.4633 (17)
Ho—O4^{iii}	2.3013 (16)	Ho—O6	2.5230 (16)

Symmetry codes: (i) $-x+2, -y+2, -z+1$; (ii) $x, -y+\frac{3}{2}, z+\frac{1}{2}$; (iii) $-x+\frac{3}{2}, -y+2, z+\frac{1}{2}$; (iv) $-x+\frac{3}{2}, y+\frac{1}{2}, z$; (v) $-x+\frac{3}{2}, y-\frac{1}{2}, z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1998); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2068).

References

Bruker (1998). *SMART* (Version 5.16), *SAINT* (Version 6.01) and *SHELXTL* (Version 6.14). Bruker AXS Inc., Madison, Wisconsin, USA.
He, Q., Zi, J.-F. & Zhang, F.-J. (2006). *Acta Cryst.* E**62**, m997–m998.
Li, Z.-F. & Wang, C.-X. (2005). *Acta Cryst.* E**61**, m2689–m2690.
Li, Z.-F., Wang, C.-X., Li, Y., Cai, D.-J. & Xiao, Y.-J. (2006). *Acta Cryst.* E**62**, m251–m252.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Wang, C.-X. & Li, Z.-F. (2005). *Acta Cryst.* E**61**, m2212–m2213.

 doi:10.1107/S1600536807066950

supporting information

Acta Cryst. (2008). E**64**, m237 [https://doi.org/10.1107/S1600536807066950]

Poly[di-μ_4-benzene-1,4-dicarboxylato-μ_6-succinato-diholmium(III)]

Qin He and Bao-Jun Huang

S1. Comment

The title compound, (I), is isostructural with its $[M_2(C_8H_4O_4)_2(C_4H_4O_4)]_n$ [*M* = Gd (Wang & Li, 2005), Dy ((Li & Wang, 2005), Nd (Li *et al.*, 2006) and Er (He *et al.*, 2006)] analogues. The Ho^{3+} ion is located at the center of a distorted square antiprism and is coordinated by four oxygen atoms from four benzene-1,4-dicarboxylate anions and four oxygen atoms from three succinate anions (Fig. 1). The Ho—O bond distances ranging from 2.2851 (2) to 2.5764 (16) Å.

The succinate anions are located on centres of inversion and acts as a bis-chelating ligands for each two symmetry related Ho atoms. Each of the four oxygen atom are additionally connected by Ho atoms into layers which are parallel to the (001) plane. These layers are connected *via* the benzene-1,4-dicarboxylate anions into a three-dimensional coordination network.

S2. Experimental

A mixture of $HoCl_3.6H_2O$ (2.00 mmol, 0.74 g), benzene-1,4-dicarboxylic acid (1.0 mmol, 0.16 g), succinic acid (1.0 mmol, 0.10 g), NaOH (6.0 ml, 1 mol/*L*) and H_2O (20.0 ml) was heated in a 35 ml stainless steel reactor with a Teflon liner at 453 K for 48 h. The column-like crystals were filtered and washed with ethanol. Yield: 30% based on Ho.

S3. Refinement

H atoms were included at calculated positions and treated as riding atoms, with C—H distances of 0.93–0.97 Å and $U_{iso}(H) = 1.2U_{eq}(C)$].

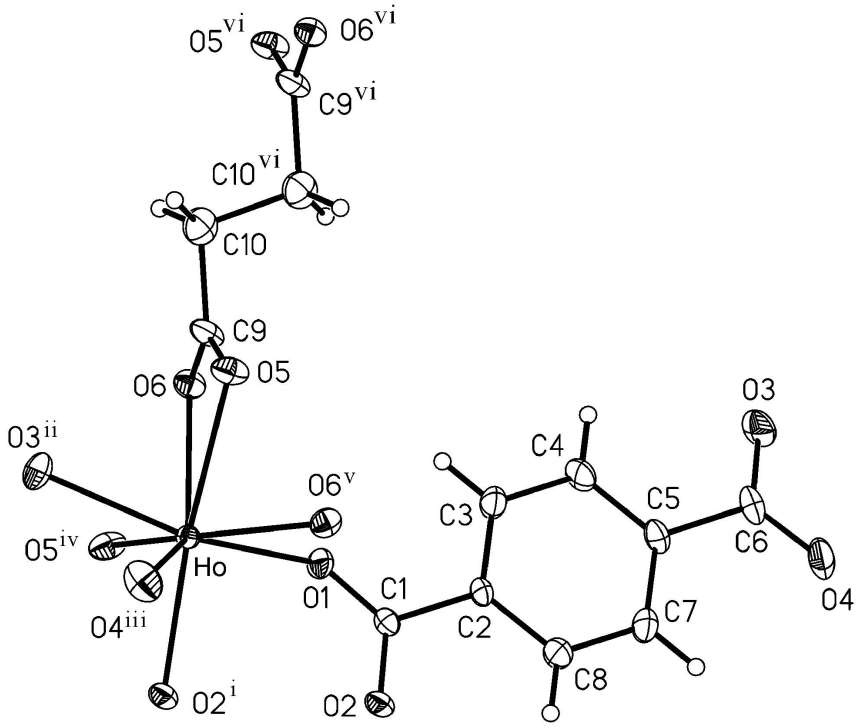


Figure 1

The coordination environment of the Ho atom, with the atom-numbering scheme, showing displacement ellipsoids drawn at the 50% probability level. Symmetry codes: (i) 2 - *x*, 2 - *y*, 1 - *z*; (ii) *x*, 3/2 - *y*, *z* + 1/2; (iii) 3/2 - *x*, 2 - *y*, *z* + 1/2; (iv) 3/2 - *x*, *y* + 1/2, *z*; (v) 3/2 - *x*, *y* - 1/2, *z*; (vi) 1 - *x*, 2 - *y*, 1 - *z*.

Poly[di-μ_4-benzene-1,4-dicarboxylato-μ_6-succinato-diholmium(III)]

Crystal data

$[Ho_2(C_4H_4O_4)(C_8H_4O_4)_2]$
M_r = 387.08
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
a = 13.8147 (3) Å
b = 6.7850 (2) Å
c = 21.7103 (5) Å
V = 2034.97 (9) Å^3
Z = 8
F(000) = 1448
D_x = 2.527 Mg m^{-3}
Mo *Kα* radiation, λ = 0.71073 Å
Cell parameters from 254 reflections
θ = 2.1–27.1°
μ = 7.79 mm^{-1}
T = 291 K
Column, orange
0.18 × 0.15 × 0.05 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.245, T_{max} = 0.682
11598 measured reflections
2411 independent reflections
2140 reflections with $I > 2\sigma(I)$
R_{int} = 0.019
θ_{max} = 28.0°, θ_{min} = 1.9°
h = −17→16
k = −7→8
l = −28→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.015$
$wR(F^2) = 0.042$
$S = 1.06$
2411 reflections
155 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0238P)^2 + 0.923P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.002$
$\Delta\rho_{max} = 0.94$ e Å^{-3}
$\Delta\rho_{min} = -0.60$ e Å^{-3}
Extinction correction: *SHELXTL* (Bruker, 1998), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.00060 (5)

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Ho	0.830676 (8)	1.016049 (15)	0.554834 (5)	0.01275 (6)
O1	0.86282 (15)	1.0368 (2)	0.45156 (8)	0.0198 (4)
O2	1.01131 (12)	0.9282 (3)	0.43269 (7)	0.0206 (3)
C1	0.92600 (17)	0.9674 (3)	0.41630 (11)	0.0148 (4)
C2	0.89870 (17)	0.9259 (3)	0.35070 (10)	0.0177 (5)
C3	0.96527 (18)	0.8440 (4)	0.31009 (11)	0.0257 (5)
H3A	1.0274	0.8143	0.3237	0.031*
C4	0.93977 (19)	0.8064 (4)	0.24966 (11)	0.0276 (6)
H4A	0.9846	0.7510	0.2228	0.033*
C5	0.84715 (17)	0.8514 (3)	0.22885 (11)	0.0208 (5)
C6	0.81879 (18)	0.8035 (3)	0.16377 (11)	0.0213 (5)
C7	0.78017 (19)	0.9332 (4)	0.26926 (11)	0.0259 (5)
H7A	0.7181	0.9634	0.2555	0.031*
C8	0.8056 (2)	0.9698 (4)	0.32984 (13)	0.0244 (5)
H8A	0.7605	1.0240	0.3568	0.029*
O3	0.87624 (13)	0.6998 (3)	0.13253 (8)	0.0284 (4)
O4	0.73920 (13)	0.8685 (3)	0.14403 (7)	0.0265 (4)
O5	0.66712 (11)	0.8691 (3)	0.54719 (8)	0.0229 (4)
O6	0.67647 (11)	1.1742 (2)	0.51694 (8)	0.0205 (4)
C9	0.6257 (2)	1.0274 (3)	0.53160 (14)	0.0240 (6)
C10	0.5157 (2)	1.0403 (4)	0.53093 (15)	0.0313 (6)
H10A	0.4883	0.9627	0.5641	0.038*
H10B	0.4948	1.1760	0.5356	0.038*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Ho	0.01198 (8)	0.01651 (7)	0.00977 (8)	−0.00044 (3)	0.00010 (4)	0.00131 (3)
O1	0.0203 (10)	0.0274 (9)	0.0118 (9)	0.0012 (7)	0.0002 (7)	−0.0009 (6)
O2	0.0158 (9)	0.0311 (8)	0.0149 (8)	−0.0020 (7)	−0.0033 (7)	−0.0017 (7)
C1	0.0166 (12)	0.0170 (10)	0.0108 (11)	−0.0019 (8)	0.0003 (9)	0.0010 (8)
C2	0.0190 (12)	0.0229 (11)	0.0112 (11)	0.0006 (9)	−0.0022 (9)	−0.0021 (8)
C3	0.0203 (13)	0.0393 (14)	0.0175 (13)	0.0050 (10)	−0.0054 (10)	−0.0067 (10)
C4	0.0250 (14)	0.0385 (14)	0.0193 (13)	0.0056 (11)	−0.0008 (10)	−0.0087 (11)
C5	0.0278 (13)	0.0224 (11)	0.0123 (12)	0.0005 (9)	−0.0051 (10)	−0.0036 (9)
C6	0.0302 (14)	0.0206 (11)	0.0131 (12)	−0.0036 (9)	−0.0049 (10)	−0.0017 (9)
C7	0.0228 (13)	0.0364 (13)	0.0186 (13)	0.0066 (11)	−0.0097 (11)	−0.0037 (11)
C8	0.0210 (13)	0.0356 (13)	0.0167 (13)	0.0063 (10)	−0.0022 (11)	−0.0065 (10)
O3	0.0338 (10)	0.0312 (9)	0.0203 (10)	0.0021 (8)	−0.0054 (8)	−0.0088 (7)
O4	0.0264 (10)	0.0378 (10)	0.0154 (8)	0.0011 (8)	−0.0072 (7)	0.0012 (7)
O5	0.0173 (9)	0.0174 (8)	0.0341 (11)	0.0002 (6)	−0.0071 (7)	0.0010 (7)
O6	0.0189 (9)	0.0188 (8)	0.0238 (10)	−0.0010 (6)	−0.0022 (7)	0.0019 (7)
C9	0.0197 (14)	0.0212 (12)	0.0310 (16)	−0.0020 (9)	−0.0089 (12)	0.0025 (10)
C10	0.0376 (18)	0.0236 (12)	0.0326 (17)	0.0037 (11)	−0.0005 (14)	−0.0019 (11)

Geometric parameters (Å, º)

Ho—O1	2.2899 (17)	C4—C5	1.391 (3)
Ho—O2^{i}	2.2320 (17)	C4—H4A	0.9300
Ho—O3^{ii}	2.3208 (16)	C5—C7	1.391 (3)
Ho—O4^{iii}	2.3013 (16)	C5—C6	1.502 (3)
Ho—O5	2.4753 (16)	C6—O3	1.259 (3)
Ho—O5^{iv}	2.4015 (18)	C6—O4	1.260 (3)
Ho—O6^{v}	2.4633 (17)	C7—C8	1.384 (4)
Ho—O6	2.5230 (16)	C7—H7A	0.9300
O1—C1	1.253 (3)	C8—H8A	0.9300
O2—C1	1.259 (3)	O5—C9	1.263 (3)
C1—C2	1.500 (3)	O6—C9	1.259 (3)
C2—C3	1.390 (3)	C9—C10	1.523 (4)
C2—C8	1.395 (4)	C10—C10^{vi}	1.514 (6)
C3—C4	1.382 (3)	C10—H10A	0.9700
C3—H3A	0.9300	C10—H10B	0.9700
O2^{i}—Ho—O1	85.34 (7)	C3—C2—C8	119.3 (2)
O2^{i}—Ho—O4^{iii}	104.50 (6)	C3—C2—C1	120.7 (2)
O1—Ho—O4^{iii}	152.17 (6)	C8—C2—C1	120.0 (2)
O2^{i}—Ho—O3^{ii}	75.73 (6)	C4—C3—C2	120.5 (2)
O1—Ho—O3^{ii}	134.25 (7)	C4—C3—H3A	119.8
O4^{iii}—Ho—O3^{ii}	73.56 (7)	C2—C3—H3A	119.8
O2^{i}—Ho—O5^{iv}	80.03 (6)	C3—C4—C5	120.2 (2)
O1—Ho—O5^{iv}	82.44 (6)	C3—C4—H4A	119.9
O4^{iii}—Ho—O5^{iv}	73.97 (6)	C5—C4—H4A	119.9

O3^{ii}—Ho—O5^{iv}	132.55 (6)	C7—C5—C4	119.7 (2)
O2^{i}—Ho—O6^{v}	103.85 (6)	C7—C5—C6	120.4 (2)
O1—Ho—O6^{v}	74.86 (6)	C4—C5—C6	119.9 (2)
O4^{iii}—Ho—O6^{v}	125.79 (6)	O3—C6—O4	124.2 (2)
O3^{ii}—Ho—O6^{v}	70.08 (6)	O3—C6—C5	117.6 (2)
O5^{iv}—Ho—O6^{v}	156.47 (6)	O4—C6—C5	118.2 (2)
O2^{i}—Ho—O5	165.74 (6)	C8—C7—C5	120.1 (2)
O1—Ho—O5	97.82 (7)	C8—C7—H7A	119.9
O4^{iii}—Ho—O5	79.09 (6)	C5—C7—H7A	119.9
O3^{ii}—Ho—O5	92.42 (6)	C7—C8—C2	120.3 (2)
O5^{iv}—Ho—O5	114.12 (5)	C7—C8—H8A	119.9
O6^{v}—Ho—O5	64.00 (6)	C2—C8—H8A	119.9
O2^{i}—Ho—O6	142.50 (6)	C6—O3—Ho^{vii}	124.97 (15)
O1—Ho—O6	79.54 (6)	C6—O4—Ho^{viii}	140.49 (16)
O4^{iii}—Ho—O6	77.02 (6)	C9—O5—Ho^{v}	150.76 (16)
O3^{ii}—Ho—O6	137.25 (6)	C9—O5—Ho	95.09 (15)
O5^{iv}—Ho—O6	64.15 (5)	Ho^{v}—O5—Ho	112.68 (6)
O6^{v}—Ho—O6	104.93 (5)	C9—O6—Ho^{iv}	129.67 (17)
O5—Ho—O6	51.58 (6)	C9—O6—Ho	92.94 (15)
O2^{i}—Ho—C9	168.32 (6)	Ho^{iv}—O6—Ho	108.99 (6)
O1—Ho—C9	91.01 (8)	O6—C9—O5	119.2 (2)
O4^{iii}—Ho—C9	74.08 (8)	O6—C9—C10	120.5 (2)
O3^{ii}—Ho—C9	114.28 (7)	O5—C9—C10	120.2 (2)
O5^{iv}—Ho—C9	88.50 (6)	O6—C9—Ho	61.15 (13)
O6^{v}—Ho—C9	85.82 (6)	O5—C9—Ho	58.99 (13)
O5—Ho—C9	25.92 (6)	C10—C9—Ho	170.3 (2)
O6—Ho—C9	25.91 (6)	C10^{vi}—C10—C9	105.9 (3)
C1—O1—Ho	135.25 (16)	C10^{vi}—C10—H10A	110.6
C1—O2—Ho^{i}	156.02 (15)	C9—C10—H10A	110.6
O1—C1—O2	124.0 (2)	C10^{vi}—C10—H10B	110.6
O1—C1—C2	118.4 (2)	C9—C10—H10B	110.6
O2—C1—C2	117.6 (2)	H10A—C10—H10B	108.7

Symmetry codes: (i) $-x+2, -y+2, -z+1$; (ii) $x, -y+3/2, z+1/2$; (iii) $-x+3/2, -y+2, z+1/2$; (iv) $-x+3/2, y+1/2, z$; (v) $-x+3/2, y-1/2, z$; (vi) $-x+1, -y+2, -z+1$; (vii) $x, -y+3/2, z-1/2$; (viii) $-x+3/2, -y+2, z-1/2$.