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catena-Poly[(diaquastrontium)-bis{μ-5-[4-(1*H*-imidazol-1-yl)phenyl]-tetrazolido}]

Shao-Wei Tong,[a] Shi-Jie Li,[b] Wen-Dong Song,[c]* Dong-Liang Miao[a] and Qi Deng[a]

[a]College of Food Science and Technology, Guangdong Ocean University, Zhanjiang 524088, People's Republic of China, [b]School of Environment Science and Engineering, Donghua University, Shanghai 200051, People's Republic of China, and [c]College of Science, Guangdong Ocean University, Zhanjiang 524088, People's Republic of China
Correspondence e-mail: songwd60@163.com

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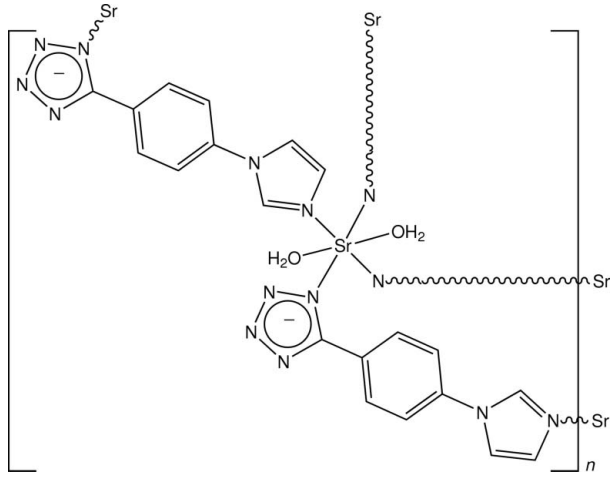
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; R factor = 0.036; wR factor = 0.118; data-to-parameter ratio = 11.1.

In the title complex polymer, $[Sr(C_{10}H_7N_6)_2(H_2O)_2]_n$, the Sr^{II} atom lies on an inversion centre and is coordinated by four N atoms from two bidentate bridging *trans*-related 5-[4-(1*H*-imidazol-1-yl)phenyl]tetrazolide ligands [Sr—N = 2.387 (4) Å for the tetrazolide moiety and Sr—N = 2.273 (5) Å for the imidazole moiety], and by two O atoms from water molecules [Sr—O = 2.464 (4) Å], giving a distorted octahedral coordination. Pairs of ligand bridges link the complex units, forming chains which extend along [111] and are inter-associated through O_{water}—H···N hydrogen bonds, giving a two-dimensional network structure parallel to (001). Weak π–π stacking interactions between the benzene and imidazole rings are also present [minimum ring centroid separation = 3.691 (4) Å].

Related literature

For our previous work on imidazole derivatives as ligands, see: Tong *et al.* (2011); Li *et al.* (2010). Wang *et al.* (2010). For related structures, see: Huang *et al.* (2009); Cheng (2011).



Experimental

Crystal data

$[Sr(C_{10}H_7N_6)_2(H_2O)_2]$
M_r = 546.08
Triclinic, $P\overline{1}$
a = 7.6210 (6) Å
b = 8.0589 (7) Å
c = 9.1641 (9) Å
α = 102.783 (1)°
β = 97.544 (1)°
γ = 106.036 (2)°
V = 516.29 (8) Å^3
Z = 1
Mo $K\alpha$ radiation
μ = 2.66 mm^{-1}
T = 298 K
0.37 × 0.30 × 0.21 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2007)
T_{min} = 0.439, T_{max} = 0.605
2616 measured reflections
1789 independent reflections
1756 reflections with $I > 2\sigma(I)$
R_{int} = 0.013

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.118
S = 1.17
1789 reflections
161 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1C···N1^{i}	0.85	2.07	2.915 (7)	171
O1—H1D···N2^{ii}	0.85	2.10	2.948 (6)	171

Symmetry codes: (i) $x, y+1, z+1$; (ii) $-x, -y-1, -z$.

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; 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: ZS2191).

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supplementary materials

Acta Cryst. (2012). E**68**, m523–m524 [doi:10.1107/S1600536812013347]

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Shao-Wei Tong, Shi-Jie Li, Wen-Dong Song, Dong-Liang Miao and Qi Deng

Comment

Recently, our research group has shown great interest in the solid-state coordination chemistry of *N*-heterocyclic carboxylic acids, such as 2-propyl-1*H*-imidazole-4,5-dicarboxylic acid and 1*H*-benzimidazole-5,6-dicarboxylic acid. We have synthesized a number of metal complexes using the monoanionic 5-[(4-imidazol-1-yl)phenyl]tetrazolide ligand with a series of metals, e.g. Mn, Cd and Sr (Tong *et al.*, 2011; Li *et al.*, 2010; Wang *et al.*, 2010). In this paper, we report the structure of a new strontium complex with this ligand, obtained under hydrothermal conditions, the title complex polymer, $[Sr(C_{10}H_7N_6)_2(H_2O)_2]_n$. The centrosymmetric complex molecule (Fig. 1) comprises a Sr^{II} ion coordinated by four N atoms from the two bidentate bridging *trans*- related 5-[(4-imidazol-1-yl)phenyl]tetrazolido ligands (two tetrazole and two imidazole) and two O atoms from the water molecules, giving a distorted octahedral stereochemistry [Sr—N = 2.273 (4), 2.387 (5) Å and Sr—O = 2.464 (4) Å]. Duplex bridging ligand molecules link the complex molecules forming polymer chains which extend along [111] and are inter-associated through water O—H···N hydrogen bonds (Table 1) giving a two-dimensional network structure. Weak π–π stacking interactions are also present between the phenyl and the imidazole rings [minimum ring centroid separation, 3.691 (4) Å]. The structures of similar complexes are also known (Huang *et al.*, 2009; Cheng, 2011).

Experimental

A mixture of strontium chloride (0.1 mmol, 0.027 g) and 5-[4-imidazol-1-yl)phenyl]tetrazole (0.2 mmol, 0.043 g) in 12 ml of water was sealed in an autoclave equipped with a Teflon liner (25 ml) and then heated at 413 K for 3 days. Crystals of the title compound were obtained by slow evaporation of the solvent at room temperature.

Refinement

H atoms of the water molecule were located in a difference-Fourier map and refined as riding with an O—H distance restraint of 0.85 Å, with U_{iso}(H) = 1.2 U_{eq}(O). The imidazolyl and phenyl H atoms were located in a difference-Fourier but were refined as riding with C—H = 0.93 Å also with U_{iso}(H) = 1.2U_{eq}(C).

Computing details

Data collection: *SMART* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT* (Bruker, 2007); 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* (Sheldrick, 2008).

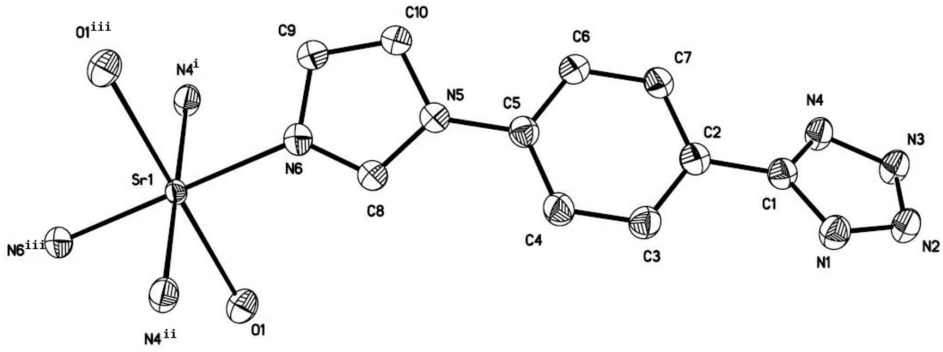

Figure 1

Molecular configuration and atom numbering scheme for the title complex showing 30% probability ellipsoids. For symmetry codes: (i) *x* + 1, *y* + 1, *z* + 1; (ii) -*x*, -*y*, -*z*; (iii) -*x* + 1, -*y* + 1, -*z* + 1.

catena-Poly[(diaquastrontium)-bis{μ-5-[4-(1*H*-imidazol- 1-yl)phenyl]tetrazolido}]

Crystal data

$[Sr(C_{10}H_7N_6)_2(H_2O)_2]$
M_r = 546.08
Triclinic, $P\overline{1}$
Hall symbol: -P 1
a = 7.6210 (6) Å
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c = 9.1641 (9) Å
α = 102.783 (1)°
β = 97.544 (1)°
γ = 106.036 (2)°
V = 516.29 (8) Å^3
Z = 1
$F(000)$ = 276
D_x = 1.756 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2869 reflections
θ = 2.8–28.3°
μ = 2.66 mm^{-1}
T = 298 K
Block, colourless
0.37 × 0.30 × 0.21 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*; Bruker, 2007)
T_{min} = 0.439, T_{max} = 0.605
2616 measured reflections
1789 independent reflections
1756 reflections with $I > 2\sigma(I)$
R_{int} = 0.013
θ_{max} = 25.0°, θ_{min} = 2.7°
h = −9→9
k = −9→7
l = −10→9

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.036
$wR(F^2)$ = 0.118
S = 1.17
1789 reflections
161 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
$w = 1/[\sigma^2(F_o^2) + (0.0473P)^2 + 1.6581P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.43 e Å^{-3}
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.260 (15)

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Sr1	0.50000	0.50000	0.50000	0.0271 (2)
O1	0.3110 (6)	0.2631 (5)	0.5968 (5)	0.0511 (12)
N1	−0.0566 (7)	−0.7449 (6)	−0.3419 (5)	0.0468 (16)
N2	−0.2033 (7)	−0.8777 (6)	−0.4402 (6)	0.0478 (16)
N3	−0.3273 (6)	−0.8089 (6)	−0.4930 (6)	0.0480 (16)
N4	−0.2656 (6)	−0.6290 (6)	−0.4306 (5)	0.0451 (14)
N5	0.3031 (6)	0.1033 (6)	0.0479 (5)	0.0411 (12)
N6	0.4352 (6)	0.3262 (6)	0.2555 (5)	0.0435 (14)
C1	−0.0992 (7)	−0.5942 (7)	−0.3381 (6)	0.0402 (17)
C2	0.0161 (7)	−0.4150 (7)	−0.2417 (6)	0.0418 (17)
C3	0.1352 (8)	−0.3925 (8)	−0.1057 (7)	0.0477 (17)
C4	0.2324 (8)	−0.2232 (7)	−0.0114 (7)	0.0481 (17)
C5	0.2105 (7)	−0.0735 (7)	−0.0516 (6)	0.0403 (17)
C6	0.0955 (8)	−0.0935 (7)	−0.1875 (6)	0.0473 (17)
C7	−0.0003 (8)	−0.2634 (7)	−0.2825 (6)	0.0454 (17)
C8	0.3753 (8)	0.1501 (7)	0.1989 (6)	0.0433 (17)
C9	0.4015 (8)	0.3956 (7)	0.1358 (6)	0.0460 (17)
C10	0.3208 (8)	0.2604 (7)	0.0071 (6)	0.0475 (17)
H1C	0.20900	0.27310	0.61930	0.0610*
H1D	0.29230	0.15410	0.55030	0.0610*
H3	0.14980	−0.49270	−0.07760	0.0580*
H4	0.31260	−0.21000	0.07910	0.0570*
H6	0.08210	0.00710	−0.21560	0.0570*
H7	−0.07670	−0.27600	−0.37480	0.0540*
H8	0.38200	0.06900	0.25590	0.0520*
H9	0.42970	0.51710	0.14180	0.0550*
H10	0.28420	0.27160	−0.09020	0.0570*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Sr1	0.0303 (4)	0.0239 (4)	0.0238 (4)	0.0093 (2)	0.0006 (2)	0.0018 (2)
O1	0.049 (2)	0.043 (2)	0.061 (2)	0.0155 (17)	0.0138 (19)	0.0107 (18)
N1	0.046 (3)	0.043 (2)	0.050 (3)	0.016 (2)	0.007 (2)	0.009 (2)
N2	0.049 (3)	0.036 (2)	0.054 (3)	0.013 (2)	0.007 (2)	0.006 (2)
N3	0.044 (3)	0.038 (2)	0.057 (3)	0.012 (2)	0.004 (2)	0.008 (2)
N4	0.044 (2)	0.036 (2)	0.049 (3)	0.0105 (19)	0.004 (2)	0.0048 (19)
N5	0.045 (2)	0.040 (2)	0.037 (2)	0.0126 (19)	0.0065 (19)	0.0099 (18)

N6	0.048 (3)	0.039 (2)	0.039 (2)	0.012 (2)	0.0053 (19)	0.0061 (19)
C1	0.039 (3)	0.041 (3)	0.041 (3)	0.015 (2)	0.008 (2)	0.009 (2)
C2	0.039 (3)	0.044 (3)	0.042 (3)	0.014 (2)	0.010 (2)	0.009 (2)
C3	0.049 (3)	0.042 (3)	0.051 (3)	0.018 (2)	0.001 (3)	0.011 (2)
C4	0.049 (3)	0.046 (3)	0.045 (3)	0.017 (2)	−0.002 (2)	0.008 (2)
C5	0.040 (3)	0.042 (3)	0.038 (3)	0.012 (2)	0.010 (2)	0.009 (2)
C6	0.055 (3)	0.039 (3)	0.044 (3)	0.010 (2)	0.004 (2)	0.013 (2)
C7	0.048 (3)	0.044 (3)	0.038 (3)	0.009 (2)	0.003 (2)	0.009 (2)
C8	0.051 (3)	0.039 (3)	0.039 (3)	0.015 (2)	0.005 (2)	0.010 (2)
C9	0.056 (3)	0.039 (3)	0.042 (3)	0.013 (2)	0.008 (2)	0.013 (2)
C10	0.061 (3)	0.041 (3)	0.038 (3)	0.013 (3)	0.006 (2)	0.012 (2)

Geometric parameters (Å, º)

Sr1—O1	2.464 (4)	N6—C9	1.363 (7)
Sr1—N6	2.273 (4)	C1—C2	1.473 (8)
Sr1—N4^{i}	2.387 (5)	C2—C7	1.387 (8)
Sr1—N4^{ii}	2.387 (5)	C2—C3	1.386 (8)
Sr1—O1^{iii}	2.464 (4)	C3—C4	1.382 (9)
Sr1—N6^{iii}	2.273 (4)	C4—C5	1.382 (8)
O1—H1C	0.8500	C5—C6	1.375 (8)
O1—H1D	0.8500	C6—C7	1.385 (8)
N1—N2	1.362 (7)	C9—C10	1.352 (8)
N1—C1	1.336 (8)	C3—H3	0.9300
N2—N3	1.313 (7)	C4—H4	0.9300
N3—N4	1.355 (7)	C6—H6	0.9300
N4—C1	1.350 (7)	C7—H7	0.9300
N5—C8	1.347 (7)	C8—H8	0.9300
N5—C10	1.375 (7)	C9—H9	0.9300
N5—C5	1.435 (7)	C10—H10	0.9300
N6—C8	1.321 (7)		

O1—Sr1—N6	94.69 (16)	N1—C1—N4	110.9 (5)
O1—Sr1—N4^{i}	81.30 (16)	N4—C1—C2	124.4 (5)
O1—Sr1—N4^{ii}	98.70 (16)	N1—C1—C2	124.7 (5)
O1—Sr1—O1^{iii}	180.00	C3—C2—C7	118.4 (5)
O1—Sr1—N6^{iii}	85.31 (16)	C1—C2—C7	119.8 (5)
N4^{i}—Sr1—N6	90.56 (16)	C1—C2—C3	121.7 (5)
N4^{ii}—Sr1—N6	89.44 (16)	C2—C3—C4	120.9 (6)
O1^{iii}—Sr1—N6	85.31 (16)	C3—C4—C5	120.0 (6)
N6—Sr1—N6^{iii}	180.00	N5—C5—C4	121.0 (5)
N4^{i}—Sr1—N4^{ii}	180.00	N5—C5—C6	119.2 (5)
O1^{iii}—Sr1—N4^{i}	98.70 (16)	C4—C5—C6	119.8 (5)
N4^{i}—Sr1—N6^{iii}	89.44 (16)	C5—C6—C7	120.0 (5)
O1^{iii}—Sr1—N4^{ii}	81.30 (16)	C2—C7—C6	120.9 (5)
N4^{ii}—Sr1—N6^{iii}	90.56 (16)	N5—C8—N6	111.2 (5)
O1^{iii}—Sr1—N6^{iii}	94.69 (16)	N6—C9—C10	109.4 (5)
H1C—O1—H1D	108.00	N5—C10—C9	106.7 (5)
Sr1—O1—H1D	119.00	C2—C3—H3	120.00
Sr1—O1—H1C	118.00	C4—C3—H3	120.00

N2—N1—C1	105.0 (5)	C3—C4—H4	120.00
N1—N2—N3	109.8 (5)	C5—C4—H4	120.00
N2—N3—N4	108.9 (5)	C5—C6—H6	120.00
N3—N4—C1	105.5 (5)	C7—C6—H6	120.00
Sr1^{iv}—N4—N3	110.5 (3)	C2—C7—H7	120.00
Sr1^{iv}—N4—C1	143.5 (4)	C6—C7—H7	120.00
C8—N5—C10	106.5 (5)	N5—C8—H8	124.00
C5—N5—C8	128.0 (5)	N6—C8—H8	124.00
C5—N5—C10	125.3 (4)	N6—C9—H9	125.00
Sr1—N6—C8	131.1 (4)	C10—C9—H9	125.00
Sr1—N6—C9	120.4 (4)	N5—C10—H10	127.00
C8—N6—C9	106.2 (4)	C9—C10—H10	127.00
O1—Sr1—N6—C8	−20.5 (5)	C10—N5—C8—N6	0.7 (7)
O1—Sr1—N6—C9	139.5 (4)	C5—N5—C10—C9	174.7 (5)
N4^{i}—Sr1—N6—C8	60.8 (5)	C8—N5—C10—C9	−0.6 (7)
N4^{i}—Sr1—N6—C9	−139.2 (4)	Sr1—N6—C8—N5	161.7 (4)
N4^{ii}—Sr1—N6—C8	−119.2 (5)	C9—N6—C8—N5	−0.5 (7)
N4^{ii}—Sr1—N6—C9	40.8 (4)	Sr1—N6—C9—C10	−164.3 (4)
O1^{iii}—Sr1—N6—C8	159.5 (5)	C8—N6—C9—C10	0.1 (7)
O1^{iii}—Sr1—N6—C9	−40.5 (4)	N1—C1—C2—C3	−26.5 (9)
C1—N1—N2—N3	0.3 (6)	N1—C1—C2—C7	156.8 (6)
N2—N1—C1—N4	−0.3 (6)	N4—C1—C2—C3	151.0 (6)
N2—N1—C1—C2	177.6 (5)	N4—C1—C2—C7	−25.6 (8)
N1—N2—N3—N4	−0.1 (6)	C1—C2—C3—C4	−175.4 (6)
N2—N3—N4—C1	−0.1 (6)	C7—C2—C3—C4	1.3 (9)
N2—N3—N4—Sr1^{iv}	−173.6 (4)	C1—C2—C7—C6	174.8 (5)
N3—N4—C1—N1	0.2 (6)	C3—C2—C7—C6	−2.0 (9)
N3—N4—C1—C2	−177.6 (5)	C2—C3—C4—C5	0.5 (9)
Sr1^{iv}—N4—C1—N1	170.0 (4)	C3—C4—C5—N5	177.0 (5)
Sr1^{iv}—N4—C1—C2	−7.8 (10)	C3—C4—C5—C6	−1.7 (9)
C8—N5—C5—C4	−19.4 (9)	N5—C5—C6—C7	−177.7 (5)
C8—N5—C5—C6	159.3 (6)	C4—C5—C6—C7	1.0 (9)
C10—N5—C5—C4	166.4 (6)	C5—C6—C7—C2	0.8 (9)
C10—N5—C5—C6	−14.9 (8)	N6—C9—C10—N5	0.3 (7)
C5—N5—C8—N6	−174.4 (5)		

Symmetry codes: (i) *x*+1, *y*+1, *z*+1; (ii) −*x*, −*y*, −*z*; (iii) −*x*+1, −*y*+1, −*z*+1; (iv) *x*−1, *y*−1, *z*−1.

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1*C*···N1^{v}	0.85	2.07	2.915 (7)	171
O1—H1*D*···N2^{vi}	0.85	2.10	2.948 (6)	171

Symmetry codes: (v) *x*, *y*+1, *z*+1; (vi) −*x*, −*y*−1, −*z*.