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catena-Poly[[bis(thiocyanato-κ*N*)-zinc(II)]-μ-1,4-bis(1,2,4-triazol-1-yl)-butane]

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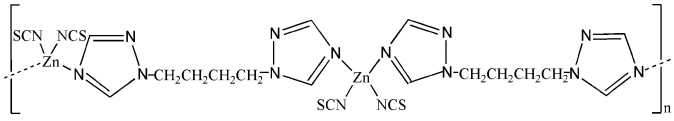
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.004 Å; R factor = 0.034; wR factor = 0.132; data-to-parameter ratio = 19.4.

The structure of the title complex, $[Zn(NCS)_2(C_8H_{12}N_6)]_n$, exhibits a one-dimensional zigzag chain through a 1,4-bis(1,2,4-triazol-1-yl)butane bridge, in which the Zn^{II} atom, lying on a twofold rotation axis, is in a distorted tetrahedral environment formed by two N atoms of the triazoles and two N atoms from two thiocyanate ligands.

Related literature

For related literature, see: Gromova *et al.* (2000); Li *et al.* (2006); Liu *et al.* (2006).



Experimental

Crystal data

$[Zn(NCS)_2(C_8H_{12}N_6)]$
M_r = 373.76
Monoclinic, $C2/c$
a = 15.1950 (9) Å
b = 5.8261 (2) Å
c = 18.8040 (7) Å
β = 100.893 (2)°
V = 1634.68 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 1.76 mm^{-1}
T = 298 (1) K
0.38 × 0.28 × 0.11 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*ABSCOR*; Higashi, 1995)
T_{min} = 0.515, T_{max} = 0.824
7229 measured reflections
1867 independent reflections
1473 reflections with $F^2 > 2\sigma(F^2)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.132
S = 1.00
1867 reflections
96 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—N1	2.017 (2)	Zn1—N4	1.934 (3)
N1—Zn1—N1^{i}	102.75 (8)	N1—Zn1—N4^{i}	109.46 (10)
N1—Zn1—N4	108.35 (10)	N4—Zn1—N4^{i}	117.45 (13)

Symmetry code: (i) $-x+1, y, -z+\frac{3}{2}$.

Data collection: *PROCESS-AUTO* (Rigaku, 1998); cell refinement: *PROCESS-AUTO*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SIR97* (Altomare *et al.*, 1999); program(s) used to refine structure: *CRYSTALS* (Betteridge *et al.*, 2003); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *CrystalStructure*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2425).

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supplementary materials

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catena-Poly[[bis(thiocyanato-κN)zinc(II)]-μ-1,4-bis(1,2,4-triazol-1-yl)butane]

L. Shen

Comment

Recently a new class of flexible ligands, [bis(1,2,4-triazol-1-yl)-alkanes], have been found to be very effective in the formation of various interesting extended structures. As bridging ligands, these 1,2,4-triazole derivatives show a great coordination diversity. Among these ligands, 1,4-bis(1,2,4-triazol-1-yl)butane(btb), with a appropriate length between two hetercyclic donors, is expected to play an important role in the construction of transition-metal supramolecular structures. To our knowledge, there are a few reports on the crystal structures of manganese(II) and cadmium(II) complexes with bridging 1,4-bis(1,2,4-triazol-1-yl)butane ligand [Li *et al.*, 2006; Liu *et al.*, 2006]. As part of our investigations of the coordination mode of the ligand in metal complexes incorporating 1,2,4-triazole derivatives, we here report the synthesis and crystal structure of a new polymeric Zn(II) with btb bridges.

The molecular structure of the title complex, with the atom-numbering scheme, is shown in Fig. 1. The Zn(II) atoms are surrounded by two triazoles and two NCS– ions, forming a distorted tetrahedral geometry. The Zn—N bond distances of btb [2.017 (2) Å] are slightly longer than the Zn—N from NCS [1.934 (3) Å]. The N—Zn—N angles around Zn centers range from 102.75 (8)^o to 117.45 (13)^o. The Zn—N—C angles are 176.8 (3)^o, which deviating from 180º expected for *sp* hybrid orbital of the N atom. The NCS group is almost linear with a N(4)—C(5)—S(1) angle of 177.0 (3)^o. The C—N distances [1.143 (4) Å] and C—S distances [1.610 (3) Å] in the SCN moiety show the normal structure of the thiocyanate in the complex.

As shown in Fig. 2, the Zn(II) ions are linked by btb ligands, building up coordination polymers to one-dimensional zigzag chain. The btb ligand adopts an anti-*gauche* conformation in this complex.

Experimental

1,4-Bis(1,2,4-triazol-1-yl)butane (btb) was prepared according to literature method (Gromova *et al.*, 2000). A 15 mL me thanol of $ZnCl_2$(0.136 g, 1 mmol) was added to a 15 ml me thanol of KSCN (0.348 g, 2 mmol). The resulting precipitate of KCl was filtered off. A 15 ml aqueous solution of btb (0.192 g, 1 mmol) was added to the above filtrate. The reaction mixture was stirred at reflux temperature for 2 h. The colourless single crystals of the title complex were obtained by evaporating the reaction solution at room temperature for one week.

Refinement

The H atoms were placed in a calculated positions, with C—H = 0.93 or 0.97 Å. All H atoms were included in the final cycle of refinement in riding mode, with U_{iso}(H) = 1.2U_{eq}(C,*N*,*O*).

Figures

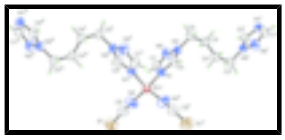

Fig. 1. Molecular structure showing 50% probability displacement ellipsoids.

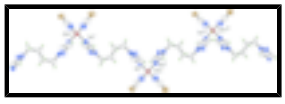

Fig. 2. The extended structure of the title complex.

catena-Poly[[bis(thiocyanato-κ*N*)zinc(II)]-μ-1,4-bis(1,2,4-triazol-1- yl)butane]

Crystal data

$[Zn(NCS)_2(C_8H_{12}N_6)]$	F_{000} = 760.00
M_r = 373.76	D_x = 1.519 Mg m^{-3}
Monoclinic, *C*2/*c*	Mo *K*α radiation λ = 0.71069 Å
Hall symbol: -C 2yc	Cell parameters from 5666 reflections
a = 15.1950 (9) Å	θ = 4.0–27.4º
b = 5.8261 (2) Å	μ = 1.76 mm^{-1}
c = 18.8040 (7) Å	*T* = 298 (1) K
β = 100.893 (2)º	Platelet, colourless
V = 1634.68 (13) Å^3	0.38 × 0.28 × 0.11 mm
Z = 4	

Data collection

Rigaku R-AXIS RAPID diffractometer	1473 reflections with $F^2 > 2\sigma(F^2)$
Detector resolution: 10.00 pixels mm^{-1}	R_{int} = 0.049
ω scans	θ_{max} = 27.5º
Absorption correction: multi-scan (ABSCOR; Higashi, 1995)	*h* = −19→19
T_{min} = 0.515, T_{max} = 0.824	*k* = −7→7
7229 measured reflections	*l* = −24→23
1867 independent reflections	

Refinement

Refinement on F^2	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.034	$w = 1/[0.002F_o^2 + \sigma(F_o^2)]/(4F_o^2)$
$wR(F^2)$ = 0.132	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max}$ = 0.50 e Å^{-3}
1867 reflections	$\Delta\rho_{min}$ = −0.46 e Å^{-3}
96 parameters	Extinction correction: none

Special details

Refinement. Refinement using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (*S*) are based on F^2. *R*-factor (gt) are based on *F*. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating *R*-factor (gt).

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Zn1	0.5000	0.23651 (6)	0.7500	0.04427 (14)
S1	0.38748 (10)	−0.21390 (18)	0.91869 (6)	0.0815 (3)
N1	0.40464 (14)	0.4526 (3)	0.69942 (11)	0.0434 (5)
N2	0.29337 (19)	0.7082 (5)	0.68471 (14)	0.0552 (7)
N3	0.34510 (17)	0.7371 (3)	0.63403 (12)	0.0423 (5)
N4	0.45101 (19)	0.0641 (5)	0.82138 (17)	0.0697 (9)
C1	0.33192 (19)	0.5365 (5)	0.72290 (14)	0.0514 (8)
C2	0.41033 (18)	0.5847 (4)	0.64281 (14)	0.0452 (7)
C3	0.3238 (2)	0.9165 (4)	0.57881 (14)	0.0525 (7)
C4	0.24236 (19)	0.8540 (4)	0.52201 (14)	0.0468 (7)
C5	0.4231 (2)	−0.0470 (5)	0.86203 (17)	0.0560 (8)
H1	0.3114	0.4770	0.7627	0.063*
H2	0.4535	0.5716	0.6140	0.055*
H32	0.3118	1.0586	0.6021	0.061*
H31	0.3748	0.9375	0.5553	0.061*
H42	0.1926	0.8225	0.5462	0.055*
H41	0.2275	0.9833	0.4895	0.055*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0450 (2)	0.0382 (2)	0.0481 (3)	0.0000	0.0050 (2)	0.0000
S1	0.0995 (8)	0.0692 (6)	0.0903 (7)	−0.0024 (5)	0.0551 (6)	0.0129 (5)
N1	0.0409 (11)	0.0462 (11)	0.0422 (11)	−0.0023 (9)	0.0056 (9)	0.0020 (9)
N2	0.0512 (14)	0.0688 (16)	0.0481 (13)	0.0132 (11)	0.0162 (11)	0.0018 (11)
N3	0.0425 (12)	0.0445 (12)	0.0383 (11)	−0.0014 (9)	0.0033 (9)	0.0008 (9)
N4	0.0612 (17)	0.0663 (17)	0.0835 (19)	−0.0009 (13)	0.0181 (14)	0.0246 (15)
C1	0.0490 (16)	0.0660 (18)	0.0422 (13)	0.0042 (13)	0.0160 (11)	0.0065 (13)
C2	0.0405 (13)	0.0523 (15)	0.0442 (13)	0.0006 (11)	0.0115 (10)	0.0024 (11)
C3	0.0634 (18)	0.0432 (14)	0.0468 (14)	−0.0039 (13)	0.0001 (12)	0.0039 (12)
C4	0.0507 (15)	0.0426 (14)	0.0440 (12)	0.0090 (11)	0.0012 (11)	−0.0004 (12)
C5	0.0516 (17)	0.0522 (16)	0.0664 (18)	0.0015 (13)	0.0167 (13)	0.0038 (15)

Geometric parameters (Å, °)

Zn1—N1	2.017 (2)	N3—C3	1.466 (3)
Zn1—N1^{i}	2.017 (2)	N4—C5	1.143 (4)
Zn1—N4	1.934 (3)	C3—C4	1.518 (3)
Zn1—N4^{i}	1.934 (3)	C4—C4^{ii}	1.510 (4)

S1—C5	1.610 (3)	C1—H1	0.930
N1—C1	1.356 (3)	C2—H2	0.930
N1—C2	1.330 (3)	C3—H32	0.970
N2—N3	1.356 (4)	C3—H31	0.970
N2—C1	1.304 (4)	C4—H42	0.970
N3—C2	1.318 (3)	C4—H41	0.970
N1—Zn1—N1^{i}	102.75 (8)	C3—C4—C4^{ii}	112.9 (2)
N1—Zn1—N4	108.35 (10)	S1—C5—N4	177.0 (3)
N1—Zn1—N4^{i}	109.46 (10)	N1—C1—H1	123.0
N1^{i}—Zn1—N4	109.46 (10)	N2—C1—H1	123.0
N1^{i}—Zn1—N4^{i}	108.35 (10)	N1—C2—H2	125.4
N4—Zn1—N4^{i}	117.45 (13)	N3—C2—H2	125.4
Zn1—N1—C1	128.93 (18)	N3—C3—H32	108.9
Zn1—N1—C2	126.10 (19)	N3—C3—H31	108.9
C1—N1—C2	103.4 (2)	C4—C3—H32	108.9
N3—N2—C1	102.9 (2)	C4—C3—H31	108.9
N2—N3—C2	110.5 (2)	H32—C3—H31	109.5
N2—N3—C3	120.5 (2)	C3—C4—H42	108.6
C2—N3—C3	129.0 (2)	C3—C4—H41	108.6
Zn1—N4—C5	176.8 (3)	C4^{ii}—C4—H42	108.6
N1—C1—N2	114.0 (2)	C4^{ii}—C4—H41	108.6
N1—C2—N3	109.2 (2)	H42—C4—H41	109.5
N3—C3—C4	111.6 (2)		
N1—Zn1—N1^{i}—C1^{i}	−93.0 (2)	Zn1—N1—C1—N2	166.49 (19)
N1—Zn1—N1^{i}—C2^{i}	70.5 (2)	Zn1—N1—C2—N3	−166.57 (17)
N1^{i}—Zn1—N1—C1	−93.0 (2)	C1—N1—C2—N3	0.3 (2)
N1^{i}—Zn1—N1—C2	70.5 (2)	C2—N1—C1—N2	0.2 (3)
N4—Zn1—N1—C1	22.8 (2)	N3—N2—C1—N1	−0.5 (3)
N4—Zn1—N1—C2	−173.7 (2)	C1—N2—N3—C2	0.7 (3)
N4^{i}—Zn1—N1—C1	152.0 (2)	C1—N2—N3—C3	179.6 (2)
N4^{i}—Zn1—N1—C2	−44.5 (2)	N2—N3—C2—N1	−0.6 (3)
N4—Zn1—N1^{i}—C1^{i}	152.0 (2)	N2—N3—C3—C4	−73.6 (3)
N4—Zn1—N1^{i}—C2^{i}	−44.5 (2)	C2—N3—C3—C4	105.1 (3)
N4^{i}—Zn1—N1^{i}—C1^{i}	22.8 (2)	C3—N3—C2—N1	−179.4 (2)
N4^{i}—Zn1—N1^{i}—C2^{i}	−173.7 (2)	N3—C3—C4—C4^{ii}	−64.9 (3)

Symmetry codes: (i) −*x*+1, *y*, −*z*+3/2; (ii) −*x*+1/2, −*y*+3/2, −*z*+1.

Fig. 1

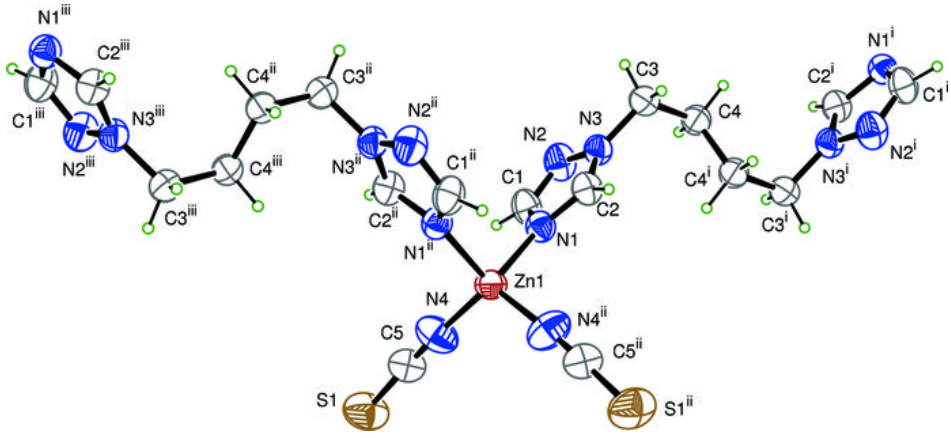
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Fig. 2