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Bis(tetra-*n*-butylammonium) tetrabromidozincate(II)

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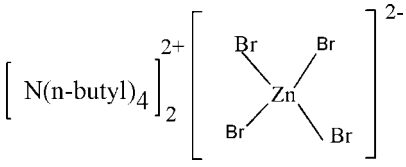
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.013 Å; disorder in main residue; R factor = 0.050; wR factor = 0.161; data-to-parameter ratio = 23.6.

In the title complex, $[(C_4H_9)_4N]_2[ZnBr_4]$, the Zn^{II} ion is coordinated by four Br atoms, forming a slightly distorted tetrahedral geometry. The Zn—Br bonds range from 2.3986 (11) to 2.4162 (11) Å and the Br—Zn—Br angles range from 106.59 (4) to 112.84 (4)°. One of the cations is disordered essentially equally over two orientations.

Related literature

Some research related to zinc(II) compounds has already been published (Wang, Zhuang *et al.*, 2007; Yu *et al.*, 2007; Zhang *et al.*, 2007; Liu *et al.*, 2007; Tian *et al.*, 2007; Wang, Moorefield *et al.*, 2007).



Experimental

Crystal data

$[(C_4H_9)_4N]_2[ZnBr_4]$
M_r = 869.93
Monoclinic, $P2_1/n$
a = 16.530 (2) Å
b = 15.4906 (18) Å
c = 18.657 (2) Å
β = 116.133 (2)°
V = 4289.0 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 4.32 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.16 mm

Data collection

Bruker APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.399, T_{max} = 0.500
24548 measured reflections
8766 independent reflections
3455 reflections with $I > 2\sigma(I)$
R_{int} = 0.079

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.050
$wR(F^2)$ = 0.161
S = 0.96
8766 reflections
371 parameters
106 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.50 e Å^{-3}
$\Delta\rho_{min}$ = −0.65 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Zn1—Br1	2.3986 (11)	Zn1—Br3	2.4082 (11)
Zn1—Br2	2.4014 (11)	Zn1—Br4	2.4162 (11)
Br1—Zn1—Br2	111.42 (4)	Br1—Zn1—Br4	112.84 (4)
Br1—Zn1—Br3	106.59 (4)	Br2—Zn1—Br4	107.59 (4)
Br2—Zn1—Br3	110.10 (4)	Br3—Zn1—Br4	108.26 (4)

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2361).

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supplementary materials

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Bis(tetra-*n*-butylammonium) tetrabromidozincate(II)

F.-X. Gao, W. Gu, Y.-S. Yang, J. Qian and S.-P. Yan

Comment

In recent years, the crystal engineering of materials containing Zn(II) has become an intensively active field due to not only their structural diversity, but also their promising applications in the fields of catalysis, (Wang, Zhuang *et al.*, 2007) medicine, magnetism, photochemistry, fluorescence (Yu *et al.*, 2007; Zhang *et al.*, 2007) and electrical chemistry (Liu *et al.*, 2007; Tian *et al.*, 2007; Wang, Moorefield *et al.*, 2007). With this in mind , we have synthesized the title complex and its crystal structure is determined herein. The Zn^{II} ion is coordinated by four Br atoms in a slightly distorted tetrhedral geometry. The asymmetric unit of (I) is shown in Fig. 1.

Experimental

A solution of $ZnBr_2$ 0.0207 g (0.1 mmol) in CH_3CN (5 ml) was added to a solution of tacntp (0.1 mmol) (tacntp = 1,4,7-triazacyclononane-1,4,7-tripropionate) in CH_3CN (15 ml). The reaction mixture was stirred at room temperature for 30 min. Then $(C_4H_9)_4N$ (0.1 mmol) was added to the solution. The reaction mixture was continuously stirred for 2 h at room temperature. Several months later, crystals suitable for X-ray diffraction were obtained by slow evaporation of the filtrate. Calculated for $[(C_4H_9)_4N]_2[ZnBr_4]$: C 44.14, H 8.28, N 3.22, Br 32.65%; found: C 44.15, H 8.27, N3.24, Br 32.67%.

Refinement

H atoms were placed in calculated positions with C—H = 0.96–0.97 Å and were included in the riding-motion approximation with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}(C)$ for methyl H atoms. In one of the cation molecules three C atoms are disordered over two sites with refined occupancies of 0.500 (16). The C—C bonds distances of the disorder components were restained to 1.54 (1) Å.

Figures

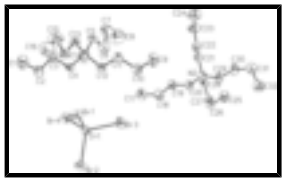


Fig. 1. The asymmtric unit of (I) shown with 30% displacement ellipsoids. The disorder is not showm.

Bis(tetra-n-butylammonium) tetrabromozincate(II)

Crystal data

$[(C_4H_9)_4N]_2[ZnBr_4]$ $F_{000} = 1792$

M_r = 869.93	D_x = 1.347 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3229 reflections
a = 16.530 (2) Å	θ = 1.4–26.4º
b = 15.4906 (18) Å	μ = 4.32 mm^{-1}
c = 18.657 (2) Å	T = 294 (2) K
β = 116.133 (2)º	Block, colourless
V = 4289.0 (9) Å^3	0.22 × 0.20 × 0.16 mm
Z = 4	

Data collection

Bruker APEXII diffractometer	8766 independent reflections
Radiation source: fine-focus sealed tube	3455 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.079
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.4º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −20→20
T_{min} = 0.399, T_{max} = 0.500	k = −14→19
24548 measured reflections	l = −19→23

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.050	$w = 1/[\sigma^2(F_o^2) + (0.0697P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.161	$(\Delta/\sigma)_{max}$ = 0.001
S = 0.96	$\Delta\rho_{max}$ = 0.50 e Å^{-3}
8766 reflections	$\Delta\rho_{min}$ = −0.65 e Å^{-3}
371 parameters	Extinction correction: none
106 restraints	
Primary atom site location: structure-invariant direct methods	
Secondary atom site location: difference Fourier map	

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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}	Occ. (<1)
Zn1	0.49076 (5)	0.13616 (5)	0.72626 (5)	0.0547 (2)	
Br1	0.57269 (6)	0.25277 (5)	0.70430 (5)	0.0833 (3)	
Br2	0.57414 (5)	0.07205 (6)	0.85543 (5)	0.0858 (3)	
Br3	0.35194 (6)	0.19646 (5)	0.71636 (6)	0.0862 (3)	
Br4	0.45436 (5)	0.02280 (5)	0.62795 (5)	0.0744 (3)	
N1	0.3318 (3)	0.2229 (3)	0.4325 (3)	0.0540 (14)	
N2	0.2736 (4)	0.9413 (3)	0.7667 (4)	0.0663 (17)	
C1	0.6498 (6)	0.2236 (6)	0.4602 (6)	0.128 (4)	
H1A	0.7102	0.2102	0.4985	0.192*	
H1B	0.6460	0.2837	0.4463	0.192*	
H1C	0.6341	0.1891	0.4132	0.192*	
C2	0.5864 (5)	0.2049 (6)	0.4955 (5)	0.093 (3)	
H2A	0.5910	0.1442	0.5094	0.111*	
H2B	0.6049	0.2379	0.5444	0.111*	
C3	0.4911 (5)	0.2254 (5)	0.4419 (5)	0.080 (2)	
H3A	0.4704	0.1892	0.3946	0.096*	
H3B	0.4863	0.2851	0.4250	0.096*	
C4	0.4325 (4)	0.2106 (4)	0.4837 (4)	0.0573 (18)	
H4A	0.4518	0.2498	0.5288	0.069*	
H4B	0.4426	0.1523	0.5047	0.069*	
C5	0.3112 (5)	0.3131 (5)	0.3960 (4)	0.067 (2)	
H5A	0.3422	0.3201	0.3627	0.081*	
H5B	0.2471	0.3166	0.3614	0.081*	
C6	0.3363 (5)	0.3872 (5)	0.4531 (5)	0.094 (3)	
H6A	0.3981	0.3808	0.4933	0.113*	
H6B	0.2975	0.3885	0.4797	0.113*	
C7	0.3262 (7)	0.4708 (6)	0.4068 (6)	0.118 (3)	
H7A	0.3636	0.4671	0.3789	0.142*	
H7B	0.2641	0.4757	0.3669	0.142*	
C8	0.3496 (10)	0.5466 (8)	0.4538 (8)	0.210 (7)	
H8A	0.3421	0.5958	0.4202	0.316*	
H8B	0.4113	0.5430	0.4931	0.316*	
H8C	0.3113	0.5525	0.4800	0.316*	
C9	0.0428 (6)	0.2096 (6)	0.4610 (6)	0.126 (4)	
H9A	0.0193	0.2193	0.4991	0.189*	
H9B	0.0286	0.1518	0.4405	0.189*	
H9C	0.0163	0.2500	0.4179	0.189*	
C10	0.1426 (5)	0.2213 (5)	0.5007 (5)	0.085 (2)	
H10A	0.1565	0.2793	0.5221	0.103*	
H10B	0.1688	0.1812	0.5450	0.103*	

C11	0.1841 (4)	0.2070 (5)	0.4452 (4)	0.068 (2)
H11A	0.1623	0.2509	0.4039	0.081*
H11B	0.1648	0.1513	0.4195	0.081*
C12	0.2862 (4)	0.2096 (4)	0.4861 (4)	0.0585 (19)
H12A	0.3049	0.2556	0.5253	0.070*
H12B	0.3078	0.1557	0.5148	0.070*
C13	0.2967 (5)	0.1583 (5)	0.3646 (4)	0.071 (2)
H13A	0.2328	0.1691	0.3332	0.085*
H13B	0.3258	0.1703	0.3305	0.085*
C14	0.3083 (5)	0.0645 (5)	0.3845 (4)	0.076 (2)
H14A	0.3719	0.0504	0.4115	0.092*
H14B	0.2813	0.0505	0.4199	0.092*
C15	0.2641 (7)	0.0134 (6)	0.3095 (5)	0.120 (4)
H15A	0.2028	0.0340	0.2794	0.144*
H15B	0.2960	0.0232	0.2773	0.144*
C16	0.2618 (7)	−0.0797 (7)	0.3230 (6)	0.148 (5)
H16A	0.2315	−0.1087	0.2726	0.223*
H16B	0.2301	−0.0901	0.3546	0.223*
H16C	0.3222	−0.1012	0.3505	0.223*
C17	0.5576 (8)	0.7840 (8)	0.8043 (7)	0.176 (6)
H17A	0.5868	0.7288	0.8185	0.263*
H17B	0.5938	0.8265	0.8424	0.263*
H17C	0.5504	0.8000	0.7521	0.263*
C18	0.4636 (8)	0.7787 (7)	0.8040 (7)	0.141 (4)
H18A	0.4276	0.7353	0.7658	0.170*
H18B	0.4712	0.7606	0.8564	0.170*
C19	0.4140 (6)	0.8633 (5)	0.7832 (5)	0.089 (3)
H19A	0.4505	0.9072	0.8206	0.107*
H19B	0.4046	0.8807	0.7302	0.107*
C20	0.3271 (5)	0.8575 (4)	0.7856 (5)	0.078 (2)
H20A	0.3372	0.8384	0.8384	0.094*
H20B	0.2911	0.8139	0.7477	0.094*
C21	0.2545 (5)	0.9748 (4)	0.6845 (5)	0.071 (2)
H21A	0.2243	1.0301	0.6770	0.085*
H21B	0.3116	0.9850	0.6830	0.085*
C22	0.1991 (5)	0.9184 (5)	0.6164 (5)	0.086 (2)
H22A	0.1431	0.9040	0.6186	0.104*
H22B	0.2312	0.8652	0.6190	0.104*
C23	0.1789 (7)	0.9655 (6)	0.5384 (6)	0.115 (3)
H23A	0.1562	1.0224	0.5416	0.138*
H23B	0.2356	0.9737	0.5355	0.138*
C24	0.1164 (8)	0.9265 (8)	0.4647 (7)	0.166 (5)
H24A	0.1099	0.9628	0.4207	0.249*
H24B	0.0589	0.9198	0.4652	0.249*
H24C	0.1387	0.8710	0.4590	0.249*
C25	0.3386 (7)	1.1502 (6)	0.9471 (6)	0.127 (4)
H25A	0.3734	1.1972	0.9797	0.191*
H25B	0.2897	1.1374	0.9599	0.191*
H25C	0.3151	1.1660	0.8918	0.191*

C26	0.3968 (6)	1.0731 (6)	0.9623 (5)	0.096 (3)	
H26A	0.4200	1.0575	1.0182	0.115*	
H26B	0.4478	1.0876	0.9520	0.115*	
C27	0.3496 (6)	0.9970 (5)	0.9126 (5)	0.088 (3)	
H27A	0.2946	0.9863	0.9177	0.106*	
H27B	0.3877	0.9464	0.9321	0.106*	
C28	0.3269 (5)	1.0111 (4)	0.8248 (5)	0.067 (2)	
H28A	0.2933	1.0646	0.8078	0.081*	
H28B	0.3829	1.0189	0.8208	0.081*	
C29	0.1874 (5)	0.9230 (5)	0.7726 (5)	0.083 (3)	
H29A	0.1562	0.8769	0.7356	0.099*	
H29B	0.2027	0.9019	0.8260	0.099*	
C30	0.1237 (6)	0.9969 (6)	0.7561 (7)	0.114 (3)	0.500 (16)
H30A	0.1183	1.0251	0.7077	0.137*	0.500 (16)
H30B	0.1511	1.0382	0.7992	0.137*	0.500 (16)
C31	0.0270 (9)	0.9777 (17)	0.7460 (11)	0.127 (8)	0.500 (16)
H31A	−0.0148	1.0234	0.7172	0.152*	0.500 (16)
H31B	0.0044	0.9231	0.7191	0.152*	0.500 (16)
C32	0.0444 (17)	0.9742 (15)	0.8335 (11)	0.136 (9)	0.500 (16)
H32A	−0.0102	0.9585	0.8366	0.205*	0.500 (16)
H32B	0.0641	1.0298	0.8575	0.205*	0.500 (16)
H32C	0.0902	0.9321	0.8613	0.205*	0.500 (16)
C30'	0.1237 (6)	0.9969 (6)	0.7561 (7)	0.114 (3)	0.500 (16)
H30C	0.0942	1.0101	0.6994	0.137*	0.500 (16)
H30D	0.1550	1.0481	0.7850	0.137*	0.500 (16)
C32'	−0.0040 (13)	1.0404 (12)	0.7878 (14)	0.128 (9)	0.500 (16)
H32D	−0.0465	1.0203	0.8063	0.192*	0.500 (16)
H32E	−0.0358	1.0641	0.7352	0.192*	0.500 (16)
H32F	0.0336	1.0841	0.8234	0.192*	0.500 (16)
C31'	0.0545 (15)	0.9649 (13)	0.7856 (18)	0.118 (7)	0.500 (16)
H31C	0.0167	0.9204	0.7501	0.141*	0.500 (16)
H31D	0.0861	0.9402	0.8386	0.141*	0.500 (16)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0535 (5)	0.0543 (5)	0.0499 (5)	−0.0035 (4)	0.0170 (4)	−0.0008 (4)
Br1	0.0844 (6)	0.0921 (6)	0.0646 (6)	−0.0296 (5)	0.0249 (4)	−0.0038 (4)
Br2	0.0744 (6)	0.0979 (7)	0.0682 (6)	−0.0048 (5)	0.0159 (4)	0.0198 (5)
Br3	0.0811 (6)	0.0670 (5)	0.1121 (8)	0.0109 (4)	0.0442 (5)	0.0056 (5)
Br4	0.0878 (6)	0.0639 (5)	0.0726 (6)	−0.0061 (4)	0.0362 (5)	−0.0105 (4)
N1	0.047 (3)	0.073 (4)	0.038 (3)	0.001 (3)	0.015 (3)	0.007 (3)
N2	0.067 (4)	0.045 (4)	0.090 (5)	−0.010 (3)	0.037 (4)	0.005 (3)
C1	0.084 (7)	0.153 (10)	0.156 (10)	−0.011 (6)	0.061 (7)	−0.017 (8)
C2	0.062 (5)	0.119 (7)	0.100 (7)	0.003 (5)	0.038 (5)	0.004 (5)
C3	0.058 (5)	0.106 (6)	0.077 (6)	−0.003 (4)	0.028 (5)	0.003 (5)
C4	0.043 (4)	0.067 (5)	0.049 (4)	−0.003 (3)	0.008 (3)	0.007 (3)
C5	0.058 (5)	0.078 (6)	0.048 (5)	0.000 (4)	0.008 (4)	0.014 (4)

C6	0.083 (6)	0.076 (6)	0.102 (7)	−0.008 (5)	0.022 (5)	0.004 (6)
C7	0.133 (9)	0.069 (7)	0.139 (10)	−0.003 (6)	0.047 (7)	0.019 (7)
C8	0.32 (2)	0.099 (10)	0.189 (15)	−0.028 (11)	0.089 (14)	−0.005 (9)
C9	0.075 (6)	0.169 (10)	0.161 (11)	0.020 (6)	0.077 (7)	0.033 (8)
C10	0.083 (6)	0.089 (6)	0.094 (7)	0.009 (5)	0.048 (5)	0.008 (5)
C11	0.057 (5)	0.087 (6)	0.063 (5)	0.010 (4)	0.029 (4)	0.006 (4)
C12	0.054 (4)	0.066 (5)	0.051 (5)	0.000 (4)	0.019 (4)	0.003 (4)
C13	0.057 (5)	0.108 (7)	0.041 (4)	−0.006 (4)	0.015 (4)	−0.007 (4)
C14	0.082 (6)	0.077 (6)	0.061 (5)	0.006 (4)	0.024 (4)	−0.003 (4)
C15	0.149 (9)	0.104 (8)	0.073 (7)	0.001 (7)	0.018 (6)	−0.018 (6)
C16	0.183 (11)	0.107 (9)	0.114 (9)	0.023 (8)	0.027 (8)	−0.026 (7)
C17	0.177 (13)	0.215 (14)	0.141 (11)	0.101 (11)	0.075 (10)	0.013 (9)
C18	0.162 (11)	0.134 (9)	0.145 (11)	0.064 (8)	0.082 (9)	0.038 (7)
C19	0.093 (7)	0.074 (6)	0.100 (7)	0.017 (5)	0.043 (5)	0.006 (5)
C20	0.088 (6)	0.053 (5)	0.104 (7)	0.008 (4)	0.052 (5)	0.015 (4)
C21	0.066 (5)	0.059 (5)	0.081 (6)	−0.014 (4)	0.027 (4)	0.000 (4)
C22	0.072 (6)	0.090 (6)	0.101 (7)	−0.016 (5)	0.041 (5)	−0.008 (6)
C23	0.113 (8)	0.131 (9)	0.078 (7)	−0.041 (6)	0.021 (6)	−0.011 (6)
C24	0.158 (11)	0.196 (13)	0.118 (10)	−0.036 (10)	0.038 (9)	−0.005 (9)
C25	0.132 (9)	0.119 (9)	0.140 (10)	0.000 (7)	0.069 (8)	−0.035 (7)
C26	0.099 (7)	0.111 (8)	0.080 (7)	0.005 (6)	0.042 (5)	0.001 (6)
C27	0.106 (7)	0.079 (6)	0.093 (7)	0.002 (5)	0.056 (6)	0.003 (5)
C28	0.082 (5)	0.052 (5)	0.076 (6)	−0.001 (4)	0.042 (5)	0.008 (4)
C29	0.078 (6)	0.065 (5)	0.131 (8)	−0.013 (4)	0.070 (6)	0.002 (5)
C30	0.091 (5)	0.122 (5)	0.147 (6)	−0.005 (4)	0.068 (4)	−0.003 (5)
C31	0.123 (10)	0.134 (10)	0.125 (11)	0.006 (8)	0.055 (8)	0.008 (8)
C32	0.134 (12)	0.143 (12)	0.136 (12)	−0.002 (8)	0.063 (9)	0.000 (8)
C30'	0.091 (5)	0.122 (5)	0.147 (6)	−0.005 (4)	0.068 (4)	−0.003 (5)
C32'	0.119 (11)	0.150 (12)	0.131 (12)	0.001 (8)	0.070 (8)	0.007 (8)
C31'	0.109 (9)	0.134 (10)	0.126 (10)	0.004 (8)	0.067 (8)	0.001 (8)

Geometric parameters (Å, °)

Zn1—Br1	2.3986 (11)	C16—H16A	0.9600
Zn1—Br2	2.4014 (11)	C16—H16B	0.9600
Zn1—Br3	2.4082 (11)	C16—H16C	0.9600
Zn1—Br4	2.4162 (11)	C17—C18	1.555 (13)
N1—C12	1.507 (8)	C17—H17A	0.9600
N1—C13	1.516 (8)	C17—H17B	0.9600
N1—C4	1.524 (7)	C17—H17C	0.9600
N1—C5	1.526 (8)	C18—C19	1.503 (11)
N2—C29	1.502 (8)	C18—H18A	0.9700
N2—C28	1.509 (8)	C18—H18B	0.9700
N2—C21	1.515 (9)	C19—C20	1.459 (10)
N2—C20	1.522 (8)	C19—H19A	0.9700
C1—C2	1.490 (11)	C19—H19B	0.9700
C1—H1A	0.9600	C20—H20A	0.9700
C1—H1B	0.9600	C20—H20B	0.9700
C1—H1C	0.9600	C21—C22	1.481 (9)

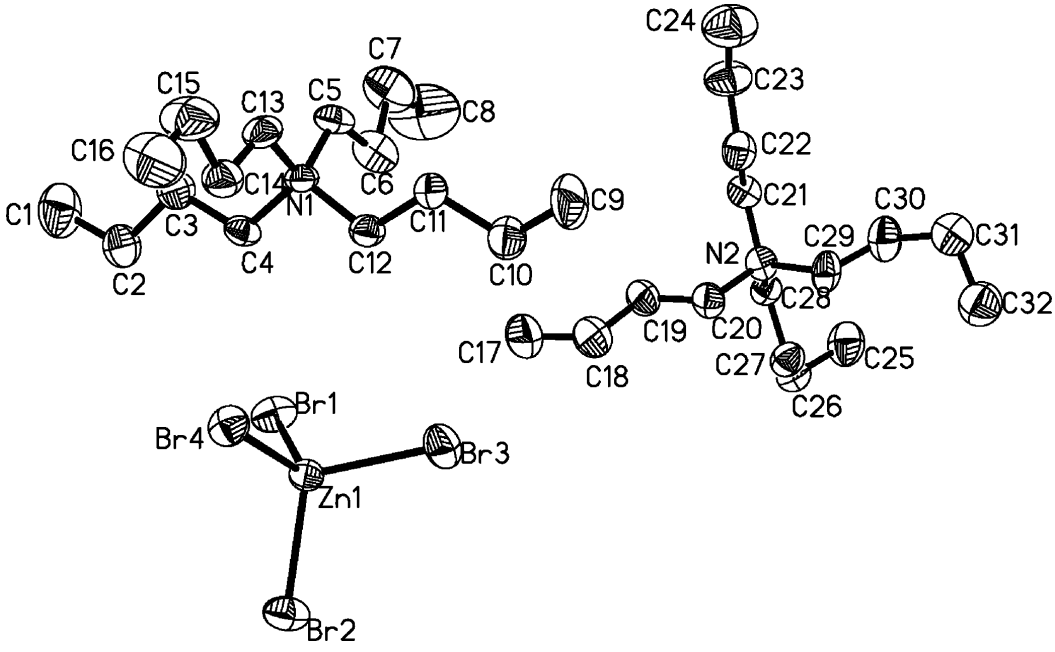
C2—C3	1.483 (9)	C21—H21A	0.9700
C2—H2A	0.9700	C21—H21B	0.9700
C2—H2B	0.9700	C22—C23	1.526 (11)
C3—C4	1.503 (9)	C22—H22A	0.9700
C3—H3A	0.9700	C22—H22B	0.9700
C3—H3B	0.9700	C23—C24	1.440 (12)
C4—H4A	0.9700	C23—H23A	0.9700
C4—H4B	0.9700	C23—H23B	0.9700
C5—C6	1.495 (10)	C24—H24A	0.9600
C5—H5A	0.9700	C24—H24B	0.9600
C5—H5B	0.9700	C24—H24C	0.9600
C6—C7	1.523 (11)	C25—C26	1.480 (11)
C6—H6A	0.9700	C25—H25A	0.9600
C6—H6B	0.9700	C25—H25B	0.9600
C7—C8	1.414 (13)	C25—H25C	0.9600
C7—H7A	0.9700	C26—C27	1.489 (10)
C7—H7B	0.9700	C26—H26A	0.9700
C8—H8A	0.9600	C26—H26B	0.9700
C8—H8B	0.9600	C27—C28	1.527 (10)
C8—H8C	0.9600	C27—H27A	0.9700
C9—C10	1.492 (10)	C27—H27B	0.9700
C9—H9A	0.9600	C28—H28A	0.9700
C9—H9B	0.9600	C28—H28B	0.9700
C9—H9C	0.9600	C29—C30	1.493 (10)
C10—C11	1.489 (9)	C29—H29A	0.9700
C10—H10A	0.9700	C29—H29B	0.9700
C10—H10B	0.9700	C30—C31	1.555 (9)
C11—C12	1.515 (8)	C30—H30A	0.9700
C11—H11A	0.9700	C30—H30B	0.9700
C11—H11B	0.9700	C31—C32	1.528 (10)
C12—H12A	0.9700	C31—H31A	0.9700
C12—H12B	0.9700	C31—H31B	0.9700
C13—C14	1.492 (9)	C32—H32A	0.9600
C13—H13A	0.9700	C32—H32B	0.9600
C13—H13B	0.9700	C32—H32C	0.9600
C14—C15	1.490 (10)	C32'—C31'	1.529 (10)
C14—H14A	0.9700	C32'—H32D	0.9600
C14—H14B	0.9700	C32'—H32E	0.9600
C15—C16	1.467 (11)	C32'—H32F	0.9600
C15—H15A	0.9700	C31'—H31C	0.9700
C15—H15B	0.9700	C31'—H31D	0.9700
Br1—Zn1—Br2	111.42 (4)	H16A—C16—H16B	109.5
Br1—Zn1—Br3	106.59 (4)	C15—C16—H16C	109.5
Br2—Zn1—Br3	110.10 (4)	H16A—C16—H16C	109.5
Br1—Zn1—Br4	112.84 (4)	H16B—C16—H16C	109.5
Br2—Zn1—Br4	107.59 (4)	C18—C17—H17A	109.5
Br3—Zn1—Br4	108.26 (4)	C18—C17—H17B	109.5
C12—N1—C13	110.2 (5)	H17A—C17—H17B	109.5
C12—N1—C4	107.2 (5)	C18—C17—H17C	109.5

C13—N1—C4	110.6 (5)	H17A—C17—H17C	109.5
C12—N1—C5	110.1 (5)	H17B—C17—H17C	109.5
C13—N1—C5	107.7 (5)	C19—C18—C17	112.7 (9)
C4—N1—C5	111.2 (5)	C19—C18—H18A	109.1
C29—N2—C28	110.8 (6)	C17—C18—H18A	109.1
C29—N2—C21	110.9 (6)	C19—C18—H18B	109.1
C28—N2—C21	106.1 (5)	C17—C18—H18B	109.1
C29—N2—C20	107.2 (5)	H18A—C18—H18B	107.8
C28—N2—C20	110.4 (6)	C20—C19—C18	111.7 (8)
C21—N2—C20	111.5 (6)	C20—C19—H19A	109.3
C2—C1—H1A	109.5	C18—C19—H19A	109.3
C2—C1—H1B	109.5	C20—C19—H19B	109.3
H1A—C1—H1B	109.5	C18—C19—H19B	109.3
C2—C1—H1C	109.5	H19A—C19—H19B	107.9
H1A—C1—H1C	109.5	C19—C20—N2	114.9 (6)
H1B—C1—H1C	109.5	C19—C20—H20A	108.6
C3—C2—C1	114.0 (8)	N2—C20—H20A	108.6
C3—C2—H2A	108.8	C19—C20—H20B	108.6
C1—C2—H2A	108.8	N2—C20—H20B	108.6
C3—C2—H2B	108.8	H20A—C20—H20B	107.5
C1—C2—H2B	108.8	C22—C21—N2	116.2 (6)
H2A—C2—H2B	107.7	C22—C21—H21A	108.2
C2—C3—C4	110.7 (7)	N2—C21—H21A	108.2
C2—C3—H3A	109.5	C22—C21—H21B	108.2
C4—C3—H3A	109.5	N2—C21—H21B	108.2
C2—C3—H3B	109.5	H21A—C21—H21B	107.4
C4—C3—H3B	109.5	C21—C22—C23	109.2 (7)
H3A—C3—H3B	108.1	C21—C22—H22A	109.8
C3—C4—N1	115.6 (5)	C23—C22—H22A	109.8
C3—C4—H4A	108.4	C21—C22—H22B	109.8
N1—C4—H4A	108.4	C23—C22—H22B	109.8
C3—C4—H4B	108.4	H22A—C22—H22B	108.3
N1—C4—H4B	108.4	C24—C23—C22	118.2 (9)
H4A—C4—H4B	107.4	C24—C23—H23A	107.8
C6—C5—N1	116.6 (6)	C22—C23—H23A	107.8
C6—C5—H5A	108.1	C24—C23—H23B	107.8
N1—C5—H5A	108.1	C22—C23—H23B	107.8
C6—C5—H5B	108.1	H23A—C23—H23B	107.1
N1—C5—H5B	108.1	C23—C24—H24A	109.5
H5A—C5—H5B	107.3	C23—C24—H24B	109.5
C5—C6—C7	108.8 (8)	H24A—C24—H24B	109.5
C5—C6—H6A	109.9	C23—C24—H24C	109.5
C7—C6—H6A	109.9	H24A—C24—H24C	109.5
C5—C6—H6B	109.9	H24B—C24—H24C	109.5
C7—C6—H6B	109.9	C26—C25—H25A	109.5
H6A—C6—H6B	108.3	C26—C25—H25B	109.5
C8—C7—C6	115.0 (10)	H25A—C25—H25B	109.5
C8—C7—H7A	108.5	C26—C25—H25C	109.5
C6—C7—H7A	108.5	H25A—C25—H25C	109.5

C8—C7—H7B	108.5	H25B—C25—H25C	109.5
C6—C7—H7B	108.5	C25—C26—C27	113.7 (8)
H7A—C7—H7B	107.5	C25—C26—H26A	108.8
C7—C8—H8A	109.5	C27—C26—H26A	108.8
C7—C8—H8B	109.5	C25—C26—H26B	108.8
H8A—C8—H8B	109.5	C27—C26—H26B	108.8
C7—C8—H8C	109.5	H26A—C26—H26B	107.7
H8A—C8—H8C	109.5	C26—C27—C28	111.6 (7)
H8B—C8—H8C	109.5	C26—C27—H27A	109.3
C10—C9—H9A	109.5	C28—C27—H27A	109.3
C10—C9—H9B	109.5	C26—C27—H27B	109.3
H9A—C9—H9B	109.5	C28—C27—H27B	109.3
C10—C9—H9C	109.5	H27A—C27—H27B	108.0
H9A—C9—H9C	109.5	N2—C28—C27	117.3 (6)
H9B—C9—H9C	109.5	N2—C28—H28A	108.0
C11—C10—C9	112.6 (7)	C27—C28—H28A	108.0
C11—C10—H10A	109.1	N2—C28—H28B	108.0
C9—C10—H10A	109.1	C27—C28—H28B	108.0
C11—C10—H10B	109.1	H28A—C28—H28B	107.2
C9—C10—H10B	109.1	C30—C29—N2	116.4 (6)
H10A—C10—H10B	107.8	C30—C29—H29A	108.2
C10—C11—C12	113.5 (6)	N2—C29—H29A	108.2
C10—C11—H11A	108.9	C30—C29—H29B	108.2
C12—C11—H11A	108.9	N2—C29—H29B	108.2
C10—C11—H11B	108.9	H29A—C29—H29B	107.3
C12—C11—H11B	108.9	C29—C30—C31	118.2 (12)
H11A—C11—H11B	107.7	C29—C30—H30A	107.8
N1—C12—C11	116.2 (5)	C31—C30—H30A	107.8
N1—C12—H12A	108.2	C29—C30—H30B	107.8
C11—C12—H12A	108.2	C31—C30—H30B	107.8
N1—C12—H12B	108.2	H30A—C30—H30B	107.1
C11—C12—H12B	108.2	C32—C31—C30	100.3 (14)
H12A—C12—H12B	107.4	C32—C31—H31A	111.7
C14—C13—N1	118.4 (6)	C30—C31—H31A	111.7
C14—C13—H13A	107.7	C32—C31—H31B	111.7
N1—C13—H13A	107.7	C30—C31—H31B	111.7
C14—C13—H13B	107.7	H31A—C31—H31B	109.5
N1—C13—H13B	107.7	C31—C32—H32A	109.5
H13A—C13—H13B	107.1	C31—C32—H32B	109.5
C15—C14—C13	109.1 (7)	H32A—C32—H32B	109.5
C15—C14—H14A	109.9	C31—C32—H32C	109.5
C13—C14—H14A	109.9	H32A—C32—H32C	109.5
C15—C14—H14B	109.9	H32B—C32—H32C	109.5
C13—C14—H14B	109.9	C31'—C32'—H32D	109.5
H14A—C14—H14B	108.3	C31'—C32'—H32E	109.5
C16—C15—C14	113.6 (8)	H32D—C32'—H32E	109.5
C16—C15—H15A	108.9	C31'—C32'—H32F	109.5
C14—C15—H15A	108.9	H32D—C32'—H32F	109.5
C16—C15—H15B	108.9	H32E—C32'—H32F	109.5

C14—C15—H15B	108.9	C32'—C31'—H31C	109.7
H15A—C15—H15B	107.7	C32'—C31'—H31D	109.7
C15—C16—H16A	109.5	H31C—C31'—H31D	108.2
C15—C16—H16B	109.5		
C1—C2—C3—C4	−176.0 (7)	C17—C18—C19—C20	−178.4 (8)
C2—C3—C4—N1	−175.5 (6)	C18—C19—C20—N2	178.9 (7)
C12—N1—C4—C3	−177.3 (6)	C29—N2—C20—C19	−179.6 (7)
C13—N1—C4—C3	62.6 (7)	C28—N2—C20—C19	−58.8 (9)
C5—N1—C4—C3	−56.9 (8)	C21—N2—C20—C19	58.9 (9)
C12—N1—C5—C6	57.0 (7)	C29—N2—C21—C22	−57.2 (8)
C13—N1—C5—C6	177.1 (6)	C28—N2—C21—C22	−177.6 (6)
C4—N1—C5—C6	−61.6 (8)	C20—N2—C21—C22	62.2 (8)
N1—C5—C6—C7	170.2 (7)	N2—C21—C22—C23	174.6 (7)
C5—C6—C7—C8	−178.8 (10)	C21—C22—C23—C24	−172.3 (9)
C9—C10—C11—C12	−174.1 (7)	C25—C26—C27—C28	69.3 (10)
C13—N1—C12—C11	−51.8 (7)	C29—N2—C28—C27	55.2 (8)
C4—N1—C12—C11	−172.1 (6)	C21—N2—C28—C27	175.6 (7)
C5—N1—C12—C11	66.8 (7)	C20—N2—C28—C27	−63.4 (8)
C10—C11—C12—N1	−162.0 (6)	C26—C27—C28—N2	−176.2 (6)
C12—N1—C13—C14	−59.8 (8)	C28—N2—C29—C30	59.6 (9)
C4—N1—C13—C14	58.6 (8)	C21—N2—C29—C30	−57.9 (9)
C5—N1—C13—C14	−179.8 (6)	C20—N2—C29—C30	−179.9 (8)
N1—C13—C14—C15	176.5 (7)	N2—C29—C30—C31	169.0 (10)
C13—C14—C15—C16	−172.9 (8)	C29—C30—C31—C32	82 (2)

Fig. 1


C24
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C17
C18
C27
C25
C26
Br1
Br4
Br3
Zn1
Br2