catena-Poly[[diaquadinitratozinc(II)]bis(μ-1,4-di-3-pyridyl-2,3-diaza-1,3-butadiene)Poly[[diaquadinitratozinc(II)]bis(μ-1,4-di-3-pyridyl-2,3-diaza-1,3-butadiene)]

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catena-Poly[[diaquadinitratozinc(II)]bis(μ-1,4-di-3-pyridyl-2,3-diaza-1,3-butadiene)]

Shakoya Paulin, Pierre Kelly, Kenneth B. Williams, Andrea M. Goforth, Mark D. Smith, LeRoy Peterson Jr and Hans-Conrad zur Loye
catena-Poly[[diaquadinitratozinc(II)]]-bis(μ-1,4-di-3-pyridyl-2,3-diaza-1,3-butadiene)]

The polymeric title complex, [Zn(NO$_3$)$_2$(C$_{24}$H$_{20}$N$_8$)(H$_2$O)$_2$]$_n$, features distorted ZnN$_2$O$_4$ octahedra with each Zn$^{II}$ atom being located on an inversion center. Adjacent Zn ions are doubly bridged by two equivalent 1,4-di-3-pyridyl-2,3-diaza-1,3-butadiene ligands to form linear chains.

Comment
There has been much effort directed at the construction of new coordination polymers due to their potentially interesting and useful properties (Chin et al., 1993; Kitagawa et al., 2004; Janiak, 2003). In this context, we have been highly successful in utilizing N,N$^0$-bipyridyl-type ligands to link metal centers to form such polymeric materials (Perkins et al., 2005; Khalil et al., 2005; Davis et al., 2004; Dong et al., 2000a,b). As a continuation of this work, we report the details of the crystal structure of the title complex, (I), in which 1,4-di-3-pyridyl-2,3-diaza-1,3-butadiene (L$_2$) is used to link Zn$^{II}$ centers into one-dimensional chains.
involved in an intramolecular O4—H4•••O2 hydrogen bond (Table 2) to a coordinated water molecule located on the same ZnII center. It is noteworthy that only one of the two pyridyl N atoms of L2 directly coordinates a ZnII ion. The other pyridyl N atom interacts indirectly with an adjacent ZnII ion by forming an outer-sphere O4—H4•••N4 hydrogen bond (Table 2) with a coordinated water molecule located on the adjacent ZnII center. This interaction, along with the inner-sphere ZnII—N2 coordination bond noted previously, generates a double chain structure (Fig. 2) involving two equivalent L2 ligands. The chains run along the [111] direction with a non-bonded ZnII•••ZnII distance of 15.578 (1) Å.

To our knowledge, the generation of such a double chain structure involving both inner- and outer-sphere coordination by L2 is the first of its kind for this ligand.

**Experimental**

All chemicals and solvents were purchased from commercial sources and used without further purification. The L2 ligand (Dong et al., 2000) was prepared as previously described. Complex (I) was obtained by slow diffusion of an ethanol solution containing zinc nitrate hexahydrate (0.50 mmol) into a dichloromethane solution (8 ml) containing a mixture of L2 (1.0 mmol) and of 4,4'-bipyridine (1.0 mmol). A mixture of yellow, irregularly shaped crystals of (I) and colorless bar-shaped crystals of formula [ZnII(4,4'-bipyridine)2•••(NO3)2•••CH2Cl2]n were obtained at the interface of the two solutions after several weeks.

**Crystal data**

[Zn(NO3)2(C24H20N8)(H2O)2]  
Mr = 645.90  
Triclinic, P1  
a = 7.8267 (11) Å  
b = 8.5320 (11) Å  
c = 11.7409 (16) Å  
α = 81.113 (2)°  
β = 73.696 (2)°  
γ = 66.468 (2)°  
V = 691.12 (16) Å³  
Z = 1  
Dx = 1.556 Mg m⁻³  
Mo Kα radiation  
T = 150 (1) K  
Irregular fragment, yellow  
0.40 × 0.26 × 0.14 mm

**Data collection**

Bruker SMART APEX CCD diffractometer  
ω scans  
Absorption correction: multi-scan (SADABS; Bruker, 2001)  
 Tmin = 0.670, T max = 0.870  
6421 measured reflections  
2831 independent reflections  
2720 reflections with I > 2σ(I)  
R int = 0.027  
θ max = 26.4°

**Refinement**

Refinement on F²  
R[F² > 2σ(F²)] = 0.029  
wR(F²) = 0.082  
S = 1.07  
2831 reflections  
205 parameters  
H atoms treated by a mixture of independent and constrained refinement

Extinction correction: SHELXL97  
Extinction coefficient: 0.026 (4)

**Table 1**

Selected geometric parameters (Å, °).

<table>
<thead>
<tr>
<th>Bond/Angle</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Zn1—O1</td>
<td>2.1839 (12)</td>
</tr>
<tr>
<td>Zn1—O4</td>
<td>2.0795 (12)</td>
</tr>
<tr>
<td>Zn1—N1</td>
<td>2.1487 (13)</td>
</tr>
<tr>
<td>O1—Zn1—O1'</td>
<td>180</td>
</tr>
<tr>
<td>O4—Zn1—O1</td>
<td>95.05 (5)</td>
</tr>
<tr>
<td>O4—Zn1—O4'</td>
<td>84.95 (5)</td>
</tr>
</tbody>
</table>

Symmetry code: (i) −x + 1, −y + 1, −z.
Table 2
Hydrogen-bond geometry (Å, °).

<table>
<thead>
<tr>
<th>D—H—A</th>
<th>D—H</th>
<th>H—A</th>
<th>D—A</th>
<th>D—H—A</th>
</tr>
</thead>
<tbody>
<tr>
<td>O4—H4A···N4ii</td>
<td>0.79 (3)</td>
<td>1.97 (3)</td>
<td>2.750 (2)</td>
<td>170 (2)</td>
</tr>
<tr>
<td>O4—H4B···O2</td>
<td>0.78 (3)</td>
<td>2.29 (3)</td>
<td>2.856 (2)</td>
<td>130 (2)</td>
</tr>
</tbody>
</table>

Symmetry code: (ii) x + 1, y + 1, z — 1.

The water-bound H atoms were refined without constraint; see Table 2. The remaining H atoms were included in the riding-model approximation, with C—H = 0.95 Å and Uiso(H) = 1.2Ueq(C).

Data collection: SMART (Bruker, 2001); cell refinement: SAINT (Bruker, 2001); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: SHELXTL (Sheldrick, 2000) and DIAMOND (Brandenburg, 2005); software used to prepare material for publication: SHELXTL.

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References