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# Hexaaquamagnesium dibromide 5-(pyridinium-3-yl)tetrazol-1-ide

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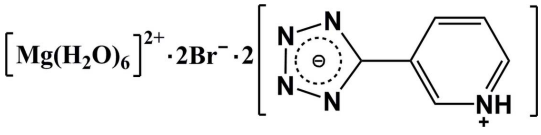
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.040; $wR$ factor = 0.097; data-to-parameter ratio = 18.5.

In the title compound, $[Mg(H_2O)_6]Br_2\cdot 2C_6H_5N_5$, the $Mg^{II}$ atom, lying on an inversion center, is coordinated by six water molecules in a distorted octahedral geometry. The pyridine and tetrazole rings in the 5-(pyridinium-3-yl)tetrazol-1-ide zwitterion are nearly coplanar, twisted from each other by a dihedral angle of 5.70 (1)°. The zwitterions, Br anions and complex cations are connected by O—H···Br, O—H···N and N—H···Br hydrogen bonds, leading to the formation of a three-dimensional network.

## Related literature

For tetrazole derivatives, see: Fu *et al.* (2008); Zhao *et al.* (2008). For the crystal structures and properties of related compounds, see: Fu *et al.* (2007, 2009); Fu & Xiong (2008).



## Experimental

### Crystal data

$[Mg(H_2O)_6]Br_2\cdot 2C_6H_5N_5$
$M_r$ = 586.53
Triclinic, $P\overline{1}$
$a$ = 7.3439 (15) Å
$b$ = 8.7786 (18) Å
$c$ = 9.5863 (19) Å
$\alpha$ = 94.04 (3)°
$\beta$ = 90.94 (3)°
$\gamma$ = 111.75 (3)°
$V$ = 572.0 (2) Å$^3$
$Z$ = 1
Mo $K\alpha$ radiation
$\mu$ = 3.62 mm$^{-1}$
$T$ = 298 K
0.40 × 0.05 × 0.05 mm

### Data collection

Rigaku SCXmini CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005)
$T_{min}$ = 0.89, $T_{max}$ = 0.95
5933 measured reflections
2627 independent reflections
2172 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.040

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.097
$S$ = 1.09
2627 reflections
142 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.52 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$A$···Br1$^{i}$ | 0.86 | 2.41 | 3.240 (3) | 161 |
| O1$W$—H1$WA$···N5 | 0.81 | 1.98 | 2.780 (3) | 171 |
| O1$W$—H1$WB$···Br1$^{ii}$ | 0.89 | 2.66 | 3.382 (3) | 138 |
| O2$W$—H2$WA$···N4 | 0.86 | 1.89 | 2.738 (3) | 167 |
| O2$W$—H2$WB$···Br1$^{iii}$ | 0.76 | 2.53 | 3.296 (2) | 178 |
| O3$W$—H3$WA$···Br1$^{iv}$ | 0.91 | 2.48 | 3.328 (2) | 156 |
| O3$W$—H3$WB$···N2$^{v}$ | 0.96 | 1.78 | 2.730 (3) | 174 |

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

Data collection: *CrystalClear* (Rigaku, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL* and *DIAMOND* (Brandenburg, 1999); 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: HY2389).

## References

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# supplementary materials

*Acta Cryst.* (2011). E**67**, m113 [ **doi:10.1107/S1600536810052992** ]

# Hexaaquamagnesium dibromide 5-(pyridinium-3-yl)tetrazol-1-ide

**J. Dai and X.-Y. Chen**

## Comment

Tetrazole compounds have attracted more attention as phase transition dielectric materials for its applications in micro-electronics, memory storage. With the purpose of obtaining phase transition crystals of 3-(1*H*-tetrazol-5-yl)pyridine compounds, its interaction with various metal ions has been studied and a series of new materials have been elaborated with this organic molecule (Fu *et al.*, 2007, 2008; Fu & Xiong 2008; Zhao *et al.*, 2008). In this paper, we describe the crystal structure of the title compound.

The asymmetric unit of the title compound (Fig. 1) is composed of one zwitterionic organic molecule, half $[Mg(H_2O)_6]^{2+}$ cation and one Br anion. In the zwitterionic organic molecule, the pyridine N atom is protonated. The pyridine and tetrazole rings are nearly coplanar and only twisted from each other by a dihedral angle of 5.70 (1)°. The geometric parameters of the tetrazole ring are comparable to those in related molecules (Fu *et al.*, 2009; Zhao *et al.*, 2008).

In the crystal structure, the intermolecular hydrogen bonds are formed by all H atoms of the water molecules and pyridine N atoms with the tetrazole N atoms or Br anions. The complex cations $[Mg(H_2O)_6]^{2+}$ and Br anions are linked in the crystal through O—H···Br hydrogen bonds into an infinite cation–anion sheet parallel to (0 0 1). The two-dimensional sheets are linked by organic molecules through O—H···N and N—H···Br hydrogen bonds into a three-dimensional network (Table 1 and Fig. 2).

## Experimental

$MgBr_2.6H_2O$ (2 mmol) and 3-(1*H*-tetrazol-5-yl)pyridine (0.528 g, 2 mmol) were dissolved in 70% methanol aqueous solution, and then 2 ml HBr was added. Single crystals suitable for X-ray diffraction analysis were obtained by slow evaporation of the solution at room temperature after two weeks. The crystals were colourless, block, and of average size 0.2×0.3×0.4 mm.

The permittivity measurement shows that there is no phase transition within temperature range from 100 to 400 K, and the permittivity is 9.1 at 1 MHz at room temperature.

## Refinement

H atoms attached to C and N atoms were positioned geometrically and treated as riding, with C—H = 0.93 and N—H = 0.86 Å and with $U_{iso}(H) = 1.2U_{eq}(C, N)$. H atoms of water molecules were located in a difference Fourier map and refined using a riding model, with $U_{iso}(H) = 1.5U_{eq}(O)$.

## Figures

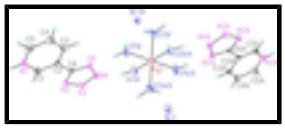

Fig. 1. Molecular structure of the title compound. Displacement ellipsoids are drawn at the 30% probability level. [Symmetry code: (A) 1 - *x*, 1 - *y*, 2 - *z*.]

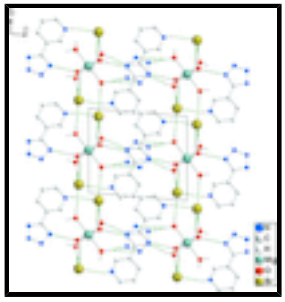

Fig. 2. The crystal packing of the title compound. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

## Hexaaquamagnesium dibromide 5-(pyridinium-3-yl)tetrazol-1-ide

*Crystal data*

| | |
|---|---|
| $[Mg(H_2O)_6]Br_2·2C_6H_5N_5$ | $Z = 1$ |
| $M_r = 586.53$ | $F(000) = 294$ |
| Triclinic, $P\overline{1}$ | $D_x = 1.703$ Mg m$^{-3}$ |
| Hall symbol: -P 1 | Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å |
| $a = 7.3439$ (15) Å | Cell parameters from 2627 reflections |
| $b = 8.7786$ (18) Å | $\theta = 3.1$–$24.5°$ |
| $c = 9.5863$ (19) Å | $\mu = 3.62$ mm$^{-1}$ |
| $\alpha = 94.04$ (3)° | $T = 298$ K |
| $\beta = 90.94$ (3)° | Block, colourless |
| $\gamma = 111.75$ (3)° | 0.40 × 0.05 × 0.05 mm |
| $V = 572.0$ (2) Å$^3$ | |

*Data collection*

| | |
|---|---|
| Rigaku SCXmini CCD diffractometer | 2627 independent reflections |
| Radiation source: fine-focus sealed tube | 2172 reflections with $I > 2\sigma(I)$ |
| graphite | $R_{int} = 0.040$ |
| Detector resolution: 13.6612 pixels mm$^{-1}$ | $\theta_{max} = 27.5°$, $\theta_{min} = 3.1°$ |
| ω scans | $h = -9 \rightarrow 9$ |
| Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2005) | $k = -11 \rightarrow 11$ |
| $T_{min} = 0.89$, $T_{max} = 0.95$ | $l = -12 \rightarrow 12$ |
| 5933 measured reflections | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Primary atom site location: structure-invariant direct methods |
| Least-squares matrix: full | Secondary atom site location: difference Fourier map |
| $R[F^2 > 2\sigma(F^2)] = 0.040$ | Hydrogen site location: inferred from neighbouring sites |
| $wR(F^2) = 0.097$ | H-atom parameters constrained |
| $S = 1.09$ | $w = 1/[\sigma^2(F_o^2) + (0.0426P)^2 + 0.1011P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| 2627 reflections | $(\Delta/\sigma)_{max} = 0.001$ |
| 142 parameters | $\Delta\rho_{max} = 0.32$ e Å$^{-3}$ |
| 0 restraints | $\Delta\rho_{min} = -0.52$ e Å$^{-3}$ |

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N4 | 0.3716 (3) | 0.6009 (3) | 0.6076 (3) | 0.0347 (6) |
| N2 | 0.2637 (3) | 0.5318 (3) | 0.3932 (2) | 0.0315 (5) |
| C6 | 0.1639 (4) | 0.4135 (3) | 0.4740 (3) | 0.0263 (6) |
| N5 | 0.2266 (3) | 0.4528 (3) | 0.6073 (2) | 0.0328 (5) |
| C2 | 0.0038 (4) | 0.2612 (3) | 0.4229 (3) | 0.0272 (6) |
| C3 | −0.1073 (4) | 0.1506 (4) | 0.5142 (3) | 0.0319 (6) |
| H3 | −0.0792 | 0.1730 | 0.6101 | 0.038* |
| N1 | −0.1923 (4) | 0.0847 (4) | 0.2374 (3) | 0.0481 (7) |
| H1A | −0.2202 | 0.0642 | 0.1489 | 0.058* |
| N3 | 0.3947 (3) | 0.6479 (3) | 0.4800 (3) | 0.0360 (6) |
| C1 | −0.0427 (5) | 0.2234 (4) | 0.2822 (3) | 0.0398 (7) |
| H1 | 0.0296 | 0.2941 | 0.2180 | 0.048* |
| C5 | −0.3000 (5) | −0.0234 (4) | 0.3232 (4) | 0.0464 (8) |
| H5 | −0.4017 | −0.1188 | 0.2873 | 0.056* |
| C4 | −0.2598 (4) | 0.0073 (4) | 0.4639 (4) | 0.0408 (7) |
| H4 | −0.3335 | −0.0668 | 0.5253 | 0.049* |
| Mg1 | 0.5000 | 0.5000 | 1.0000 | 0.0303 (3) |
| O1W | 0.2634 (3) | 0.3471 (3) | 0.8692 (2) | 0.0497 (6) |
| H1WA | 0.2453 | 0.3674 | 0.7906 | 0.075* |
| H1WB | 0.1806 | 0.2467 | 0.8849 | 0.075* |
| O2W | 0.5507 (3) | 0.6851 (2) | 0.8697 (2) | 0.0465 (6) |
| H2WA | 0.5117 | 0.6602 | 0.7829 | 0.070* |
| H2WB | 0.6098 | 0.7777 | 0.8780 | 0.070* |
| O3W | 0.3123 (4) | 0.5786 (3) | 1.1155 (2) | 0.0532 (6) |
| H3WA | 0.2760 | 0.6585 | 1.0834 | 0.080* |
| H3WB | 0.3030 | 0.5606 | 1.2130 | 0.080* |
| Br1 | 0.79518 (5) | 0.08632 (4) | 0.89951 (3) | 0.04481 (14) |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N4 | 0.0315 (12) | 0.0309 (13) | 0.0353 (14) | 0.0055 (11) | −0.0054 (10) | −0.0025 (11) |
| N2 | 0.0307 (12) | 0.0285 (12) | 0.0293 (13) | 0.0041 (10) | 0.0010 (10) | 0.0027 (10) |
| C6 | 0.0242 (13) | 0.0277 (14) | 0.0257 (14) | 0.0080 (11) | 0.0012 (10) | 0.0028 (11) |
| N5 | 0.0325 (12) | 0.0336 (13) | 0.0262 (13) | 0.0053 (11) | −0.0038 (10) | 0.0027 (10) |
| C2 | 0.0270 (13) | 0.0270 (14) | 0.0269 (14) | 0.0097 (11) | 0.0010 (11) | 0.0009 (11) |
| C3 | 0.0309 (14) | 0.0311 (15) | 0.0313 (15) | 0.0083 (12) | 0.0010 (11) | 0.0051 (12) |
| N1 | 0.0513 (16) | 0.0464 (17) | 0.0333 (15) | 0.0059 (14) | −0.0096 (12) | −0.0124 (13) |
| N3 | 0.0332 (13) | 0.0292 (13) | 0.0411 (15) | 0.0063 (11) | 0.0026 (11) | 0.0039 (11) |
| C1 | 0.0410 (16) | 0.0376 (17) | 0.0297 (16) | 0.0025 (14) | 0.0027 (13) | −0.0010 (13) |
| C5 | 0.0369 (17) | 0.0301 (17) | 0.061 (2) | 0.0016 (14) | −0.0041 (16) | −0.0084 (16) |
| C4 | 0.0344 (16) | 0.0307 (16) | 0.052 (2) | 0.0049 (13) | 0.0049 (14) | 0.0061 (15) |
| Mg1 | 0.0387 (7) | 0.0245 (7) | 0.0216 (7) | 0.0047 (6) | 0.0004 (5) | 0.0022 (5) |
| O1W | 0.0520 (13) | 0.0454 (14) | 0.0302 (12) | −0.0069 (11) | −0.0088 (10) | 0.0073 (10) |
| O2W | 0.0710 (15) | 0.0213 (10) | 0.0310 (12) | −0.0015 (10) | −0.0103 (10) | 0.0041 (9) |
| O3W | 0.0792 (17) | 0.0629 (17) | 0.0342 (13) | 0.0432 (15) | 0.0173 (12) | 0.0161 (12) |
| Br1 | 0.0546 (2) | 0.03047 (19) | 0.0402 (2) | 0.00473 (15) | 0.00206 (14) | 0.00592 (14) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| N4—N3 | 1.312 (4) | C5—H5 | 0.9300 |
| N4—N5 | 1.341 (3) | C4—H4 | 0.9300 |
| N2—N3 | 1.336 (3) | Mg1—O2W$^{i}$ | 2.048 (2) |
| N2—C6 | 1.336 (3) | Mg1—O2W | 2.048 (2) |
| C6—N5 | 1.329 (3) | Mg1—O3W$^{i}$ | 2.061 (2) |
| C6—C2 | 1.460 (4) | Mg1—O3W | 2.061 (2) |
| C2—C1 | 1.373 (4) | Mg1—O1W | 2.087 (2) |
| C2—C3 | 1.390 (4) | Mg1—O1W$^{i}$ | 2.087 (2) |
| C3—C4 | 1.386 (4) | O1W—H1WA | 0.8068 |
| C3—H3 | 0.9300 | O1W—H1WB | 0.8907 |
| N1—C5 | 1.333 (4) | O2W—H2WA | 0.8615 |
| N1—C1 | 1.339 (4) | O2W—H2WB | 0.7636 |
| N1—H1A | 0.8600 | O3W—H3WA | 0.9085 |
| C1—H1 | 0.9300 | O3W—H3WB | 0.9576 |
| C5—C4 | 1.363 (5) | | |
| N3—N4—N5 | 110.0 (2) | O2W$^{i}$—Mg1—O2W | 180.000 (1) |
| N3—N2—C6 | 105.2 (2) | O2W$^{i}$—Mg1—O3W$^{i}$ | 91.93 (10) |
| N5—C6—N2 | 111.4 (2) | O2W—Mg1—O3W$^{i}$ | 88.07 (10) |
| N5—C6—C2 | 124.2 (2) | O2W$^{i}$—Mg1—O3W | 88.07 (10) |
| N2—C6—C2 | 124.4 (2) | O2W—Mg1—O3W | 91.93 (10) |
| C6—N5—N4 | 104.5 (2) | O3W$^{i}$—Mg1—O3W | 180.000 (1) |
| C1—C2—C3 | 117.8 (3) | O2W$^{i}$—Mg1—O1W | 89.55 (9) |
| C1—C2—C6 | 120.7 (3) | O2W—Mg1—O1W | 90.45 (9) |
| C3—C2—C6 | 121.5 (3) | O3W$^{i}$—Mg1—O1W | 90.10 (11) |

| | | | |
|---|---|---|---|
| C4—C3—C2 | 120.7 (3) | O3W—Mg1—O1W | 89.90 (11) |
| C4—C3—H3 | 119.6 | $O2W^{i}$—Mg1—$O1W^{i}$ | 90.45 (9) |
| C2—C3—H3 | 119.6 | O2W—Mg1—$O1W^{i}$ | 89.55 (9) |
| C5—N1—C1 | 123.3 (3) | $O3W^{i}$—Mg1—$O1W^{i}$ | 89.90 (11) |
| C5—N1—H1A | 118.3 | O3W—Mg1—$O1W^{i}$ | 90.10 (11) |
| C1—N1—H1A | 118.3 | O1W—Mg1—$O1W^{i}$ | 180.000 (1) |
| N4—N3—N2 | 108.8 (2) | Mg1—O1W—H1WA | 122.5 |
| N1—C1—C2 | 119.9 (3) | Mg1—O1W—H1WB | 126.6 |
| N1—C1—H1 | 120.1 | H1WA—O1W—H1WB | 110.2 |
| C2—C1—H1 | 120.1 | Mg1—O2W—H2WA | 119.0 |
| N1—C5—C4 | 119.4 (3) | Mg1—O2W—H2WB | 133.7 |
| N1—C5—H5 | 120.3 | H2WA—O2W—H2WB | 107.0 |
| C4—C5—H5 | 120.3 | Mg1—O3W—H3WA | 118.6 |
| C5—C4—C3 | 119.0 (3) | Mg1—O3W—H3WB | 118.7 |
| C5—C4—H4 | 120.5 | H3WA—O3W—H3WB | 119.2 |
| C3—C4—H4 | 120.5 | | |

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

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1A···$Br1^{ii}$ | 0.86 | 2.41 | 3.240 (3) | 161 |
| O1W—H1WA···N5 | 0.81 | 1.98 | 2.780 (3) | 171 |
| O1W—H1WB···$Br1^{iii}$ | 0.89 | 2.66 | 3.382 (3) | 138 |
| O2W—H2WA···N4 | 0.86 | 1.89 | 2.738 (3) | 167 |
| O2W—H2WB···$Br1^{iv}$ | 0.76 | 2.53 | 3.296 (2) | 178 |
| O3W—H3WA···$Br1^{i}$ | 0.91 | 2.48 | 3.328 (2) | 156 |
| O3W—H3WB···$N2^{v}$ | 0.96 | 1.78 | 2.730 (3) | 174 |

Symmetry codes: (ii) *x*−1, *y*, *z*−1; (iii) *x*−1, *y*, *z*; (iv) *x*, *y*+1, *z*; (i) −*x*+1, −*y*+1, −*z*+2; (v) *x*, *y*, *z*+1.

**Fig. 1**

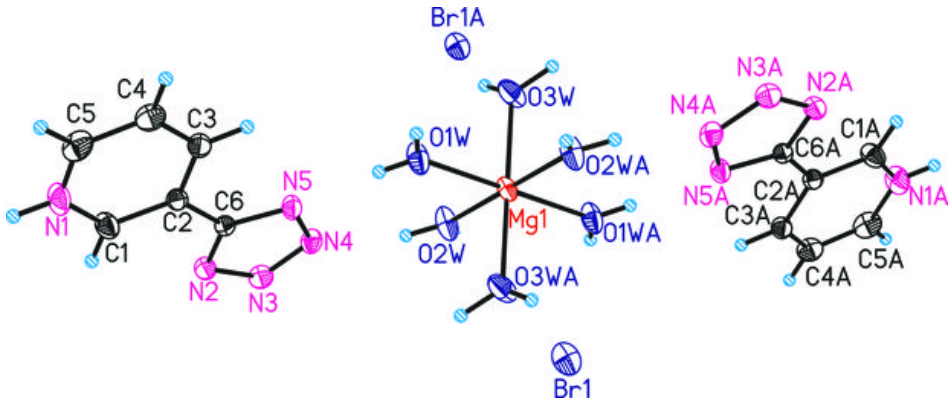
Br1A
O3W
O1W
O2WA
Mg1
O1WA
O2W
O3WA
Br1
C4
C5
C3
N5
C6
N1
C2
N4
C1
N2
N3
N3A
N2A
N4A
C1A
C6A
N5A
C2A
N1A
C3A
C5A
C4A

**Fig. 2**