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trans,trans,trans-Diaquabis(nicotinamide-κ*N*)bis(2-nitrobenzoato-κ*O*)cadmium(II) dihydrate

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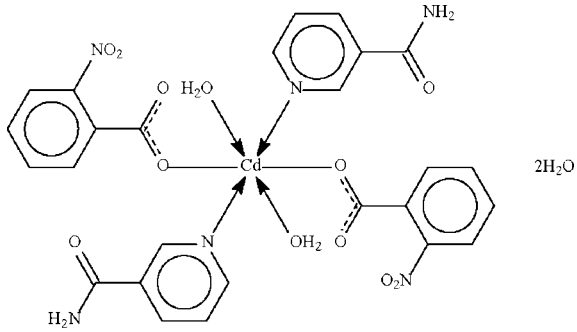
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.034; wR factor = 0.093; data-to-parameter ratio = 10.8.

The cadmium atom in the title compound, $[Cd(C_7H_4NO_4)_2(C_6H_6N_2O)_2(H_2O)_2]\cdot 2H_2O$, lies on a center of inversion in an all-*trans* octahedral environment. In the crystal, the complex interacts with the uncoordinated water molecules through O—H···O and N—H···O hydrogen bonds, forming a layered network.

Related literature

There are several examples of diaquadi(arylcarboxylato)di(nicotinamide)metal(II) compounds. For recent examples, see: Hökelek & Necefoğlu (2007*a*,*b*); Hökelek *et al.* (2007); Koksharova *et al.* (2006); Şahin *et al.* (2007*a*,*b*); Stachova *et al.* (2006); Çaylak *et al.* (2007).



Experimental

Crystal data

$[Cd(C_7H_4NO_4)_2(C_6H_6N_2O)_2(H_2O)_2]\cdot 2H_2O$
M_r = 760.94
Monoclinic, $P2_1/n$
a = 7.9365 (8) Å
b = 19.589 (2) Å
c = 10.059 (1) Å
β = 103.178 (2)°
V = 1522.6 (3) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.80 mm^{-1}
T = 293 K
0.50 × 0.18 × 0.18 mm

Data collection

Bruker SMART area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.619, T_{max} = 0.866
4427 measured reflections
2651 independent reflections
2396 reflections with $I > 2\sigma(I)$
R_{int} = 0.016

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.093
S = 1.13
2651 reflections
246 parameters
9 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −1.04 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1w—H11···O2w	0.85 (4)	1.92 (4)	2.764 (4)	174 (4)
O1w—H12···O2^{i}	0.85 (4)	1.95 (5)	2.718 (4)	150 (4)
O2w—H21···O5^{i}	0.85 (3)	2.08 (3)	2.910 (4)	166 (4)
O2w—H22···O1^{ii}	0.85 (3)	2.00 (1)	2.846 (3)	177 (5)
N3—H31···O2^{iii}	0.85 (3)	2.22 (2)	3.038 (4)	165 (4)
N3—H32···O5^{iv}	0.85 (3)	2.05 (3)	2.873 (4)	164 (4)

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2136).

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supporting information

Acta Cryst. (2009). E**65**, m292 [doi:10.1107/S1600536809005479]

trans,trans,trans-Diaquabis(nicotinamide-κN)bis(2-nitrobenzoato-κO)cadmium(II) dihydrate

Kou-Lin Zhang, Bo Yang, Jian-Guo Lin and Seik Weng Ng

S1. Experimental

A water/methanol (1:1 *v*/*v*) solution (3 ml) of cadmium nitrate trihydrate (0.082 g, 0.3 mmol) was added to a water/methanol (1:1 *v*/*v*) solution (3 ml) of 2-nitrobenzoic acid (0.100 g, 0.6 mmol), sodium hydroxide (0.024 g, 0.6 mmol) and nicotinamide (0.073 g, 0.6 mmol). A white powder was obtained after several days; this was recrystallized from DMF/methanol (3:1 *v*/*v*) to give colorless crystals in 50% yield. CH&N elemental analysis. Calculated for $C_{26}H_{28}CdN_6O_{14}$: C 41.04 H 3.68 N 11.04%; found: C 40.08, H 3.87, N 10.93%.

S2. Refinement

Carbon-bound H atoms were placed in calculated positions and were allowed to ride on the parent atoms. N and O-bound H atoms were located in a difference Fourier map, and were refined with distance restraints N–H = O–H = 0.85±0.01 Å; for the water molecules, an additional H···H 1.39±0.01 Å restraint was used. Their temperature factors were freely refined.

The measurements are 100% at the 2θ limit of 50 °.

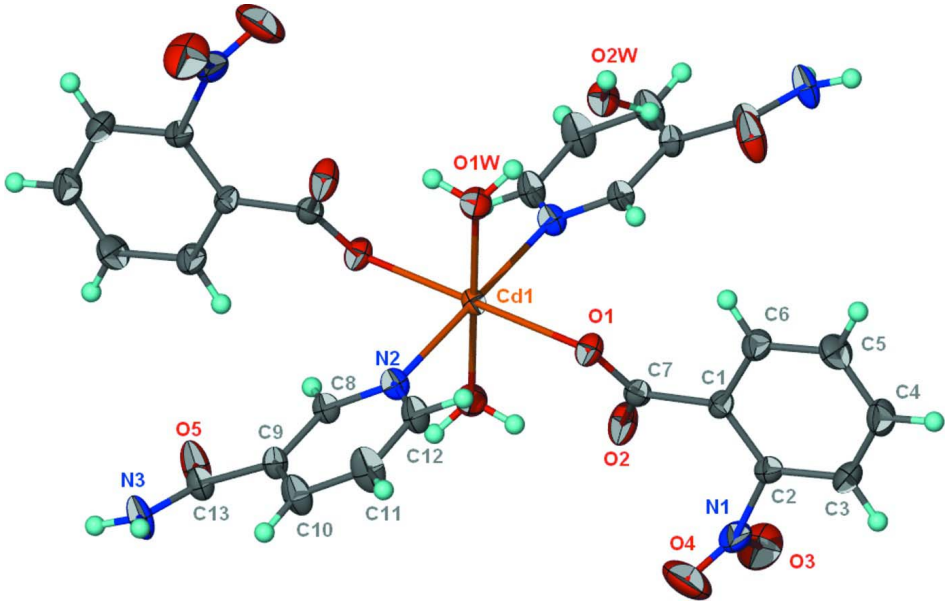

Figure 1

Thermal ellipsoid plot of $Cd(H_2O)_2(C_7H_4NO_4)_2(C_6H_6N_2O)_2.2H_2O$; displacement ellipsoids are drawn at the 50% probabability level, and H atoms as spheres of arbitrary radii.

trans,trans,trans-Diaquabis(nicotinamide-κN)bis(2- nitrobenzoato-κO)cadmium(II) dihydrate

Crystal data

$[Cd(C_7H_4NO_4)_2(C_6H_6N_2O)_2(H_2O)_2]\cdot 2H_2O$
$M_r = 760.94$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 7.9365\ (8)$ Å
$b = 19.589\ (2)$ Å
$c = 10.059\ (1)$ Å
$\beta = 103.178\ (2)°$
$V = 1522.6\ (3)$ Å^3
$Z = 2$
$F(000) = 772$
$D_x = 1.660$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3417 reflections
$\theta = 2.1–25.1°$
$\mu = 0.80$ mm^{-1}
$T = 293$ K
Rod, colorless
0.50 × 0.18 × 0.18 mm

Data collection

Bruker SMART area-detector diffractometer
Radiation source: medium-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.619$, $T_{max} = 0.866$
4427 measured reflections
2651 independent reflections
2396 reflections with $I > 2\sigma(I)$
$R_{int} = 0.016$
$\theta_{max} = 25.1°$, $\theta_{min} = 2.1°$
$h = -9\rightarrow3$
$k = -20\rightarrow23$
$l = -11\rightarrow11$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.093$
$S = 1.13$
2651 reflections
246 parameters
9 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0433P)^2 + 2.3534P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.42$ e Å^{-3}
$\Delta\rho_{min} = -1.04$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cd1	0.5000	0.5000	0.5000	0.02349 (13)
O1	0.6570 (3)	0.40982 (12)	0.4385 (2)	0.0312 (5)
O2	0.4256 (3)	0.36571 (14)	0.2970 (3)	0.0428 (7)
O3	0.3595 (4)	0.23243 (19)	0.1217 (4)	0.0693 (10)
O4	0.4552 (5)	0.2124 (2)	0.3355 (4)	0.0835 (12)
O5	0.0789 (4)	0.48477 (17)	0.8538 (3)	0.0505 (8)
O1W	0.7685 (3)	0.55083 (13)	0.5819 (3)	0.0362 (6)
H11	0.842 (5)	0.561 (2)	0.536 (4)	0.055 (14)*
H12	0.737 (6)	0.5868 (14)	0.616 (5)	0.082 (19)*
O2W	0.9923 (3)	0.57871 (14)	0.4149 (3)	0.0375 (6)
H21	0.987 (5)	0.556 (2)	0.342 (3)	0.079 (18)*
H22	1.097 (2)	0.581 (2)	0.460 (3)	0.050 (13)*

N1	0.4713 (4)	0.23414 (16)	0.2260 (4)	0.0438 (8)
N2	0.5129 (3)	0.44979 (15)	0.7119 (3)	0.0291 (6)
N3	0.1940 (4)	0.44256 (19)	1.0627 (3)	0.0405 (8)
H31	0.274 (4)	0.424 (2)	1.122 (3)	0.055 (13)*
H32	0.114 (4)	0.457 (2)	1.098 (3)	0.049 (12)*
C1	0.6994 (4)	0.32348 (16)	0.2832 (3)	0.0237 (6)
C2	0.6421 (4)	0.26190 (17)	0.2198 (3)	0.0282 (7)
C3	0.7386 (5)	0.22316 (19)	0.1503 (4)	0.0386 (9)
H3	0.6942	0.1829	0.1070	0.047 (12)*
C4	0.9033 (5)	0.2454 (2)	0.1459 (4)	0.0407 (9)
H4	0.9714	0.2196	0.1008	0.047 (12)*
C5	0.9655 (5)	0.3057 (2)	0.2087 (4)	0.0430 (9)
H5	1.0761	0.3205	0.2063	0.057 (13)*
C6	0.8643 (4)	0.34455 (19)	0.2755 (4)	0.0337 (8)
H6	0.9075	0.3855	0.3161	0.046 (12)*
C7	0.5842 (4)	0.36885 (16)	0.3458 (3)	0.0262 (7)
C8	0.3792 (4)	0.46351 (17)	0.7674 (3)	0.0256 (7)
H8	0.2975	0.4951	0.7238	0.044 (12)*
C9	0.3553 (4)	0.43356 (17)	0.8857 (3)	0.0273 (7)
C10	0.4767 (5)	0.3864 (2)	0.9499 (4)	0.0399 (9)
H10	0.4645	0.3648	1.0295	0.044 (11)*
C11	0.6165 (5)	0.3721 (2)	0.8941 (4)	0.0461 (10)
H11A	0.7004	0.3410	0.9362	0.055 (13)*
C12	0.6301 (5)	0.40434 (19)	0.7751 (4)	0.0352 (8)
H12A	0.7239	0.3942	0.7375	0.052 (12)*
C13	0.1972 (4)	0.45472 (18)	0.9337 (3)	0.0312 (7)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cd1	0.02157 (19)	0.0277 (2)	0.0224 (2)	−0.00033 (12)	0.00743 (13)	0.00046 (12)
O1	0.0292 (12)	0.0324 (13)	0.0303 (12)	0.0020 (10)	0.0034 (10)	−0.0075 (10)
O2	0.0268 (13)	0.0550 (17)	0.0443 (15)	0.0049 (12)	0.0033 (11)	−0.0207 (13)
O3	0.0398 (17)	0.078 (2)	0.085 (3)	−0.0141 (16)	0.0042 (17)	−0.027 (2)
O4	0.087 (3)	0.098 (3)	0.078 (3)	−0.041 (2)	0.044 (2)	0.003 (2)
O5	0.0388 (16)	0.084 (2)	0.0318 (15)	0.0297 (15)	0.0135 (12)	0.0122 (14)
O1W	0.0273 (13)	0.0406 (14)	0.0416 (15)	−0.0066 (11)	0.0094 (11)	−0.0085 (12)
O2W	0.0276 (13)	0.0452 (15)	0.0390 (15)	0.0019 (11)	0.0061 (11)	−0.0039 (12)
N1	0.0417 (19)	0.0363 (18)	0.057 (2)	−0.0114 (14)	0.0190 (17)	−0.0155 (16)
N2	0.0251 (14)	0.0348 (15)	0.0274 (15)	0.0037 (12)	0.0059 (11)	0.0027 (12)
N3	0.0366 (17)	0.066 (2)	0.0223 (15)	0.0158 (16)	0.0128 (13)	0.0093 (15)
C1	0.0281 (16)	0.0240 (16)	0.0173 (14)	0.0011 (13)	0.0015 (12)	−0.0017 (12)
C2	0.0282 (17)	0.0258 (17)	0.0313 (17)	−0.0024 (13)	0.0083 (14)	−0.0016 (14)
C3	0.051 (2)	0.0263 (18)	0.041 (2)	−0.0017 (16)	0.0154 (17)	−0.0088 (16)
C4	0.042 (2)	0.040 (2)	0.045 (2)	0.0102 (17)	0.0185 (17)	−0.0024 (17)
C5	0.0305 (19)	0.047 (2)	0.056 (3)	−0.0013 (17)	0.0203 (18)	−0.0033 (19)
C6	0.0303 (18)	0.0349 (19)	0.0359 (19)	−0.0044 (15)	0.0075 (15)	−0.0083 (15)
C7	0.0254 (16)	0.0243 (16)	0.0297 (17)	0.0019 (13)	0.0078 (13)	0.0013 (13)

C8	0.0246 (16)	0.0309 (18)	0.0201 (15)	0.0033 (13)	0.0025 (12)	0.0029 (13)
C9	0.0282 (17)	0.0336 (18)	0.0199 (15)	0.0028 (14)	0.0051 (13)	−0.0012 (13)
C10	0.042 (2)	0.053 (2)	0.0267 (18)	0.0173 (18)	0.0117 (15)	0.0150 (17)
C11	0.041 (2)	0.062 (3)	0.035 (2)	0.027 (2)	0.0095 (17)	0.0190 (19)
C12	0.0303 (18)	0.046 (2)	0.0317 (19)	0.0088 (16)	0.0117 (15)	0.0022 (16)
C13	0.0304 (18)	0.0375 (19)	0.0274 (17)	0.0051 (15)	0.0098 (14)	0.0027 (14)

Geometric parameters (Å, º)

Cd1—O1^{i}	2.325 (2)	C1—C2	1.391 (4)
Cd1—O1	2.325 (2)	C1—C6	1.391 (5)
Cd1—O1W^{i}	2.326 (2)	C1—C7	1.512 (4)
Cd1—O1W	2.326 (2)	C2—C3	1.377 (5)
Cd1—N2	2.329 (3)	C3—C4	1.388 (5)
Cd1—N2^{i}	2.329 (3)	C3—H3	0.9300
O1—C7	1.266 (4)	C4—C5	1.378 (6)
O2—C7	1.244 (4)	C4—H4	0.9300
O3—N1	1.211 (5)	C5—C6	1.386 (5)
O4—N1	1.214 (5)	C5—H5	0.9300
O5—C13	1.237 (4)	C6—H6	0.9300
O1W—H11	0.85 (4)	C8—C9	1.378 (5)
O1W—H12	0.85 (4)	C8—H8	0.9300
O2W—H21	0.85 (3)	C9—C10	1.383 (5)
O2W—H22	0.85 (3)	C9—C13	1.502 (5)
N1—C2	1.476 (4)	C10—C11	1.382 (5)
N2—C8	1.334 (4)	C10—H10	0.9300
N2—C12	1.339 (4)	C11—C12	1.379 (5)
N3—C13	1.325 (4)	C11—H11A	0.9300
N3—H31	0.84 (3)	C12—H12A	0.9300
N3—H32	0.85 (3)		
O1^{i}—Cd1—O1	180.000 (1)	C1—C2—N1	120.5 (3)
O1^{i}—Cd1—O1W^{i}	85.20 (9)	C2—C3—C4	118.7 (3)
O1—Cd1—O1W^{i}	94.80 (9)	C2—C3—H3	120.7
O1^{i}—Cd1—O1W	94.80 (9)	C4—C3—H3	120.7
O1—Cd1—O1W	85.20 (9)	C5—C4—C3	119.8 (3)
O1W^{i}—Cd1—O1W	180.00 (12)	C5—C4—H4	120.1
O1^{i}—Cd1—N2	89.52 (9)	C3—C4—H4	120.1
O1—Cd1—N2	90.48 (9)	C4—C5—C6	120.4 (3)
O1W^{i}—Cd1—N2	89.36 (10)	C4—C5—H5	119.8
O1W—Cd1—N2	90.64 (10)	C6—C5—H5	119.8
O1^{i}—Cd1—N2^{i}	90.48 (9)	C5—C6—C1	121.4 (3)
O1—Cd1—N2^{i}	89.52 (9)	C5—C6—H6	119.3
O1W^{i}—Cd1—N2^{i}	90.64 (10)	C1—C6—H6	119.3
O1W—Cd1—N2^{i}	89.36 (10)	O2—C7—O1	125.0 (3)
N2—Cd1—N2^{i}	180.0	O2—C7—C1	117.4 (3)
C7—O1—Cd1	119.7 (2)	O1—C7—C1	117.5 (3)
Cd1—O1W—H11	126 (3)	N2—C8—C9	123.7 (3)

Cd1—O1W—H12	100 (3)	N2—C8—H8	118.2
H11—O1W—H12	109 (4)	C9—C8—H8	118.2
H21—O2W—H22	109.4 (17)	C8—C9—C10	118.0 (3)
O3—N1—O4	124.7 (4)	C8—C9—C13	116.7 (3)
O3—N1—C2	118.2 (4)	C10—C9—C13	125.3 (3)
O4—N1—C2	117.1 (4)	C11—C10—C9	118.9 (3)
C8—N2—C12	117.9 (3)	C11—C10—H10	120.5
C8—N2—Cd1	115.1 (2)	C9—C10—H10	120.5
C12—N2—Cd1	126.6 (2)	C12—C11—C10	119.3 (3)
C13—N3—H31	126 (3)	C12—C11—H11A	120.4
C13—N3—H32	122 (2)	C10—C11—H11A	120.4
H31—N3—H32	111.4 (18)	N2—C12—C11	122.2 (3)
C2—C1—C6	116.4 (3)	N2—C12—H12A	118.9
C2—C1—C7	122.4 (3)	C11—C12—H12A	118.9
C6—C1—C7	121.0 (3)	O5—C13—N3	122.8 (3)
C3—C2—C1	123.3 (3)	O5—C13—C9	119.2 (3)
C3—C2—N1	116.2 (3)	N3—C13—C9	118.0 (3)
O1W^{i}—Cd1—O1—C7	22.2 (2)	C4—C5—C6—C1	1.0 (6)
O1W—Cd1—O1—C7	−157.8 (2)	C2—C1—C6—C5	−0.3 (5)
N2—Cd1—O1—C7	111.6 (2)	C7—C1—C6—C5	−174.8 (3)
N2^{i}—Cd1—O1—C7	−68.4 (2)	Cd1—O1—C7—O2	−11.8 (5)
O1^{i}—Cd1—N2—C8	29.7 (2)	Cd1—O1—C7—C1	163.9 (2)
O1—Cd1—N2—C8	−150.3 (2)	C2—C1—C7—O2	−27.5 (5)
O1W^{i}—Cd1—N2—C8	−55.5 (2)	C6—C1—C7—O2	146.7 (3)
O1W—Cd1—N2—C8	124.5 (2)	C2—C1—C7—O1	156.4 (3)
O1^{i}—Cd1—N2—C12	−157.2 (3)	C6—C1—C7—O1	−29.4 (4)
O1—Cd1—N2—C12	22.8 (3)	C12—N2—C8—C9	0.0 (5)
O1W^{i}—Cd1—N2—C12	117.6 (3)	Cd1—N2—C8—C9	173.7 (3)
O1W—Cd1—N2—C12	−62.4 (3)	N2—C8—C9—C10	−0.3 (5)
C6—C1—C2—C3	−1.2 (5)	N2—C8—C9—C13	−179.8 (3)
C7—C1—C2—C3	173.2 (3)	C8—C9—C10—C11	0.7 (6)
C6—C1—C2—N1	178.0 (3)	C13—C9—C10—C11	−179.9 (4)
C7—C1—C2—N1	−7.5 (5)	C9—C10—C11—C12	−0.8 (7)
O3—N1—C2—C3	−69.1 (5)	C8—N2—C12—C11	−0.1 (6)
O4—N1—C2—C3	108.4 (4)	Cd1—N2—C12—C11	−173.0 (3)
O3—N1—C2—C1	111.6 (4)	C10—C11—C12—N2	0.6 (7)
O4—N1—C2—C1	−70.9 (5)	C8—C9—C13—O5	15.8 (5)
C1—C2—C3—C4	1.9 (6)	C10—C9—C13—O5	−163.7 (4)
N1—C2—C3—C4	−177.4 (3)	C8—C9—C13—N3	−161.5 (3)
C2—C3—C4—C5	−1.1 (6)	C10—C9—C13—N3	19.0 (6)
C3—C4—C5—C6	−0.3 (6)		

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1w—H11···O2w	0.85 (4)	1.92 (4)	2.764 (4)	174 (4)

O1w—H12···O2^{i}	0.85 (4)	1.95 (5)	2.718 (4)	150 (4)
O2w—H21···O5^{i}	0.85 (3)	2.08 (3)	2.910 (4)	166 (4)
O2w—H22···O1^{ii}	0.85 (3)	2.00 (1)	2.846 (3)	177 (5)
N3—H31···O2^{iii}	0.85 (3)	2.22 (2)	3.038 (4)	165 (4)
N3—H32···O5^{iv}	0.85 (3)	2.05 (3)	2.873 (4)	164 (4)

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