Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Bis[5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine-κ^2N,N']bis(nitrato-κO)cadmium(II)

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Received 9 November 2006
Accepted 9 November 2006

In the centrosymmetric title compound, $[Cd(NO_3)_2(C_{20}H_{14}N_4)_2]$, the dihedral angle between the phenyl rings attached to one heterocycle is 54.13 (5)°. The crystal structure is stabilized by O···C, C—H···O, C—H···π and π–π interactions.

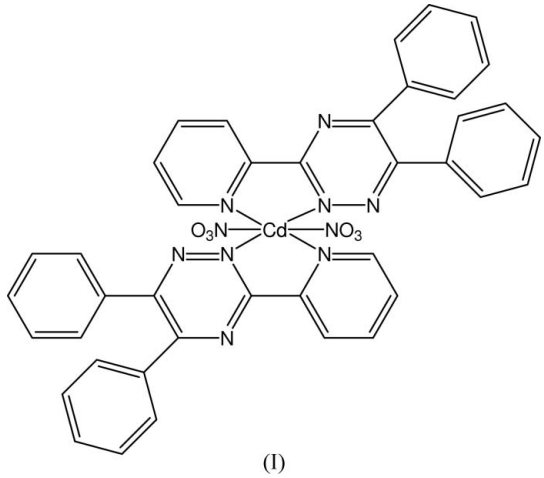
Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.001 Å
R factor = 0.028
wR factor = 0.082
Data-to-parameter ratio = 43.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Comment

1,2,4-Triazine compounds are well known natural products and show interesting biological, pharmacological and medicinal properties. The 3,5,6-trisubstituted 1,2,4-triazines are a principal class of N-donor heterocyclic ligands. Some can be active as blood platelet aggregation inhibitors and others exhibit antiviral inhibitory activity, significant activity towards leukemia and ovarian cancer, and anti-HIV activity (Soudi *et al.*, 2005; Mashaly *et al.*, 1999). Also 1,2,4-triazine has been used in analytical chemistry to determine the concentration of some trace metal ions (Almog *et al.*, 1996; Croot & Hunter, 2000). Recently we have reported the crystal structure of the Mn^{II} complex with 5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine (Eltayeb *et al.*, 2006). Now we report the crystal of the Cd^{II} complex with the same ligand.



(I)

The bond lengths and angles in (I) have normal values (Allen *et al.*, 1987), comparable to a related structure (Eltayeb *et al.*, 2006). The chelate ring (Cd1/N1/C5/C6/N2) is planar, with a maximum deviation of 0.070 (1) Å for atom C6. The dihedral angle between the two phenyl rings is 54.13 (5)°.

The relatively short distance [2.940 (1) Å] between atoms O3 and C7($\frac{3}{2}-x, \frac{1}{2}-y, -z$) indicates the presence of intermolecular O···C interactions, which contribute to the stabilization of the crystal structure, along with C—H···O and C—H···π interactions, the latter involving the C8–C13 phenyl

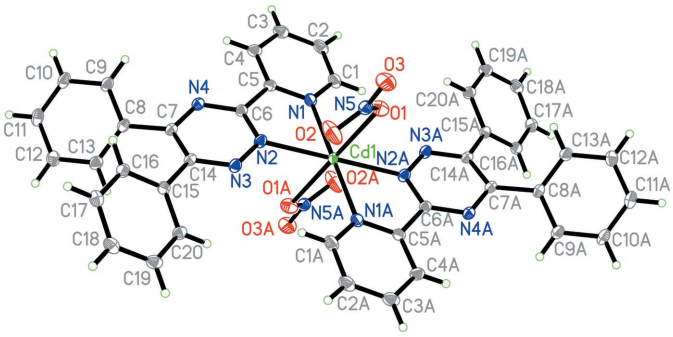


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids and the atomic numbering. The suffix A indicates the symmetry code ($\frac{3}{2} - x, \frac{3}{2} - y, -z$).

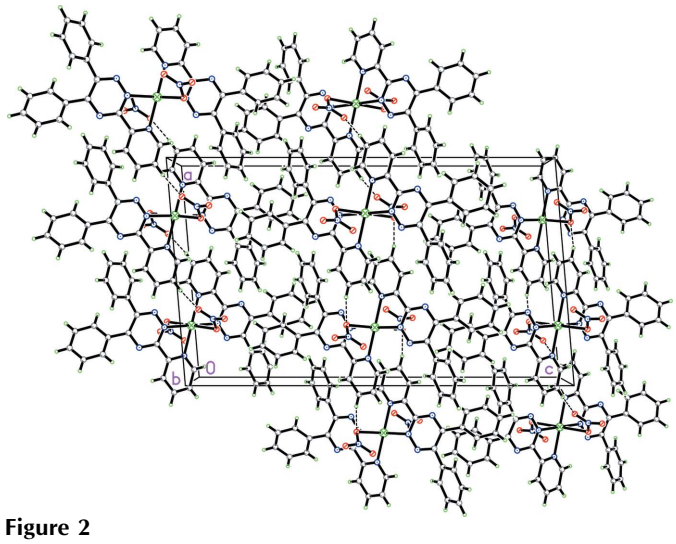


Figure 2
The crystal packing of (I), viewed down the *b* axis. Dashed lines indicate hydrogen bonds.

ring (Table 1). *Cg* is the C8–C13 ring centroid. The crystal structure is further stabilized by π–π interactions, in which the centroid–centroid distance between the N1/C1–C5 rings at (x, y, z) and ($2 - x$, $1 - y$, $-z$) is 3.606 (1) Å, and that between the N1/C1–C5 ring at (x, y, z) and the C15–C20 ring at ($\frac{1}{2} + x$, $\frac{1}{2} + y$, z) is 3.727 (1) Å.

Experimental

To a solution of 5,6-diphenyl-3-(2-pyridyl)-1,2,4-triazine (0.31 g, 1 mmol) in ethanol (20 ml) was added cadmium nitrate tetrahydrate (0.154 g, 0.5 mmol). The mixture was refluxed for 1 h. The resulting pale-yellow solution was filtered and left to evaporate slowly at room temperature. Yellow crystals suitable for X-ray diffraction were obtained after two weeks (m.p. 559–561 K). IR (KBr, cm^{-1}): ν(C—H) 3070, 3040, ν(C═N) 1618, ν(C═C) 1599, 1574, 1509, ν_{asym}(N—O) 1482, ν_{sym}(N—O) 1384, ν(C—N) 1255.

Crystal data

$[Cd(NO_3)_2(C_{20}H_{14}N_4)_2]$
M_r = 857.12
Monoclinic, $C2/c$
a = 15.8191 (2) Å
b = 8.4756 (1) Å
c = 26.8765 (4) Å
β = 94.809 (1)°
V = 3590.82 (8) Å^3
Z = 4
D_x = 1.585 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.67 mm^{-1}
T = 100.0 (1) K
Slab, yellow
0.31 × 0.26 × 0.12 mm

Data collection

Bruker SMART APEX-2 CCD diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*;, Bruker, 2005)
T_{min} = 0.817, T_{max} = 0.923
81732 measured reflections
11133 independent reflections
9320 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 40.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.028
$wR(F^2)$ = 0.082
S = 1.13
11133 reflections
259 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0397P)^2 + 1.338P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.64 e Å^{-3}
$\Delta\rho_{min}$ = −0.42 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···O2^{i}	0.93	2.41	3.309 (2)	162
C3—H3A···O1^{ii}	0.93	2.47	3.337 (1)	155
C13—H13A···Cg^{iii}	0.93	3.06	3.672 (1)	125
C17—H17A···Cg^{iv}	0.93	3.16	3.852 (1)	132

Symmetry codes: (i) $x + \frac{1}{2}, y + \frac{1}{2}, z$; (ii) $-x + 2, -y + 1, -z$; (iii) $-x + \frac{3}{2}, y + \frac{1}{2}, -z + \frac{1}{2}$; (iv) $-x + \frac{3}{2}, y - \frac{1}{2}, -z + \frac{1}{2}$.

H atoms were positioned geometrically and treated as riding, with C—H = 0.93 Å, and U_{iso}(H) = 1.2U_{eq}(C).

Data collection: *APEX2* (Bruker, 2005); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2005); program(s) used to solve structure: *SHELXTL* (Sheldrick, 1998); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2003).

The authors thank the Malaysian Government, Academy of Sciences Malaysia and Universiti Sains Malaysia for research grants and facilities. The International University of Africa (Sudan) is acknowledged for providing study leave to NEE.

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