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Bis[1,3-dimethyl-3,4,5,6-tetrahydropyrimidin-2(1*H*)-one-κ*O*]diiodocadmium(II)

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Key indicators

Single-crystal X-ray study
T = 100 K
Mean σ(C–C) = 0.012 Å
R factor = 0.043
wR factor = 0.107
Data-to-parameter ratio = 29.3

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

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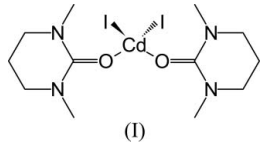
The title compound, $[CdI_2(C_6H_{12}N_2O)_2]$, displays distorted tetrahedral coordination at the CdO_2I_2 centre. Intramolecular C—H···O interactions appear to be present.

Comment

The space-demanding, oxygen electron-pair donating ligand 1,3-dimethyl-3,4,5,6-tetrahydropyrimidin-2(1*H*)-one (also known as *N*,*N*′-dimethylpropyleneurea, dmpu), forms a four-coordinate complex, (I) (Fig. 1), with cadmium(II) iodide. The resulting CdO_2I_2 grouping forms a distorted tetrahedron (Table 1).



(I)

The six-membered rings of the dmpu ligands in (I) adopt envelope conformations [displacement of atom C14 from the C1/N11/N12/C13/C15 mean plane = 0.65 (1) Å; displacement of atom C24 from the C2/N21/N22/C23/C25 plane = 0.60 (1) Å]. These two mean planes are inclined at 84.4 (3)° to each other.

Two non-classical C—H···O intramolecular hydrogen bonds could be identified (Table 2), one in each dmpu ligand, between one of the methyl H atoms and the O atom. The molecules of (I) pack with close contacts between the dmpu ligands, along the *a*-axis direction, as shown in Fig. 2.

This is only the second molecular CdI_2O_2 complex reported to date. No geometrical comparisons with the previously reported complex, bis(urea)diiodocadmium(II) (Durski *et al.*, 1975) could be made as no coordinates are available in the Cambridge Structural Database (Version of November 2005; Allen, 2002) for the urea complex.

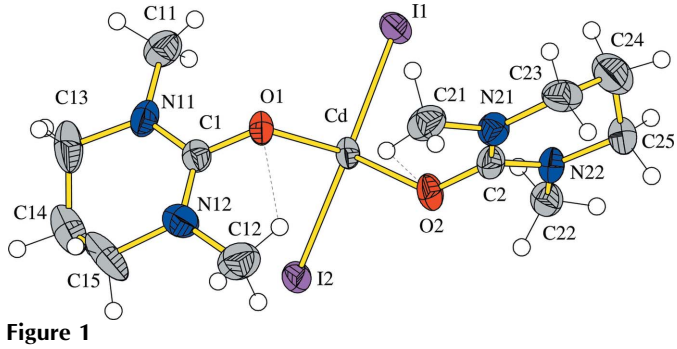


Figure 1
The molecular structure of (I), showing 50% probability displacement ellipsoids (arbitrary spheres for the H atoms).

Experimental

Anhydrous cadmium iodide (Aldrich) was dried in an evacuated desiccator using P_2O_5 as a drying agent. Compound (I) was synthesized by dissolving anhydrous cadmium(II) iodide (200 mg) in freshly distilled DPMU (2 ml). The solution was heated gently (*ca* 323 K) in an oil bath and then allowed to cool, whereupon crystal formation took place almost immediately. These crystals were used for data collection.

Crystal data

$[CdI_2(C_6H_{12}N_2O)_2]$
M_r = 622.56
Monoclinic, $P2_1/c$
a = 14.4849 (3) Å
b = 15.8909 (1) Å
c = 8.4871 (2) Å
β = 90.522 (2)°
V = 1953.46 (6) Å^3
Z = 4
D_x = 2.117 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1623 reflections
θ = 4.2–30.0°
μ = 4.29 mm^{-1}
T = 100 (2) K
Plate, colourless
0.25 × 0.20 × 0.05 mm

Data collection

Oxford Xcalibur-3 κ diffractometer with Sapphire-III CCD
ω scans at different φ
Absorption correction: numerical (*X-RED*; Stoe & Cie, 1997)
T_{min} = 0.33, T_{max} = 0.80
28468 measured reflections
5680 independent reflections
4982 reflections with $I > 2\sigma(I)$
R_{int} = 0.040
θ_{max} = 30.0°
$h = -20 \rightarrow 20$
$k = -22 \rightarrow 22$
$l = -11 \rightarrow 11$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.107
S = 1.20
5680 reflections
194 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0212P)^2 + 15.0583P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.59 e Å^{-3}
$\Delta\rho_{min}$ = −1.24 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd—O2	2.200 (4)	Cd—I1	2.6889 (6)
Cd—O1	2.215 (4)	Cd—I2	2.7184 (5)
O2—Cd—O1	94.78 (16)	O2—Cd—I2	105.90 (12)
O2—Cd—I1	110.21 (11)	O1—Cd—I2	103.91 (10)
O1—Cd—I1	110.84 (11)	I1—Cd—I2	126.47 (2)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12A···O1	0.98	2.30	2.711 (9)	104
C21—H21B···O2	0.98	2.23	2.691 (9)	107

The H atoms were positioned geometrically (C—H = 0.98–0.99 Å) and refined as riding, with U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(methyl C).

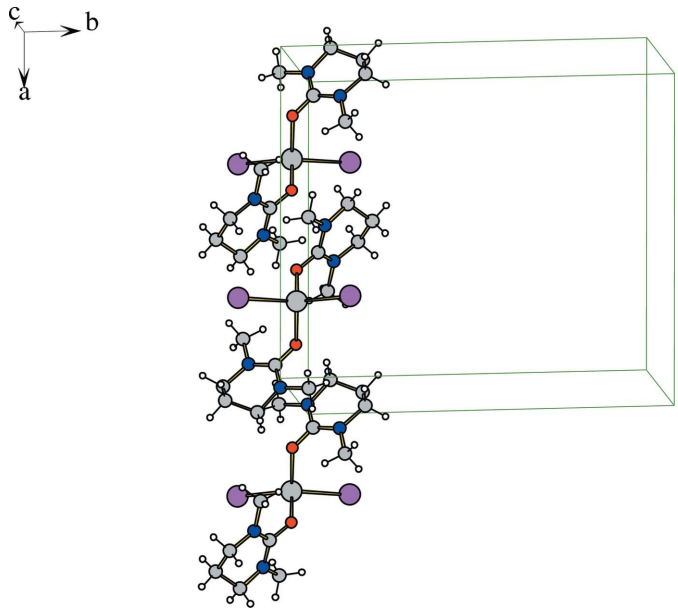


Figure 2
View of the packing of three molecules of (I), showing close intermolecular contacts between dmpu ligands along the *a*-axis direction. From top to bottom, the symmetry relations are (1 − x, −y, 1 − z), (x, y, z) and (2 − x, −y, 1 − z).

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2003); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2003); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *DIAMOND* (Bergerhoff, 1996); software used to prepare material for publication: *SHELXL97*.

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References

Allen, F. H. (2002). *Acta Cryst.* B**58**, 380–388.
Bergerhoff, G. (1996). *DIAMOND*. Gerhard-Domagk-Strasse 1, 53121 Bonn, Germany.
Durski, Z., Boniuk, H. & Majorowski, S. (1975). *Rocz. Chem.* **49**, 2101–2105.
Oxford Diffraction. (2003). *CrysAlis CCD* and *CrysAlis RED*. Oxford Diffraction Ltd, Abingdon, Oxfordshire, England.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Stoe & Cie (1997). *X-RED*. Version 1.09. Stoe & Cie GmbH, Hilpertstrasse 10, D-64295 Darmstadt, Germany.