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Tris(1,3-dimethylurea)diiodidocadmium(II)

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(N–C) = 0.013 Å
R factor = 0.047
wR factor = 0.124
Data-to-parameter ratio = 19.2

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

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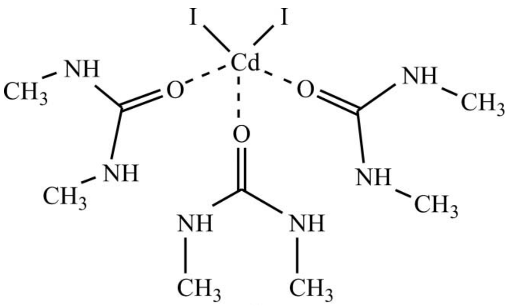
In the title compound, $[CdI_2(C_3H_8N_2O)_3]$, the Cd atom is five-coordinated by O atoms of three monodentate dimethylurea ligands and two iodide ligands. The coordination polyhedron is a distorted trigonal bipyramid of molecular symmetry C_2. Two dimethylurea ligands are involved in intermolecular N—H$\cdots$O hydrogen bonds, whereas the third participates in N—H$\cdots$I contacts.

Comment

The present work is a part of the systematic study of transition metal iodido complexes with amides (Kuz'mina *et al.*, 2000, 2001, 2005; Savinkina *et al.*, 2005). In the crystal structure of $[Cd(C_6H_5CONH_2)I_2]$, the I atoms are in the axial positions, whereas the O atoms of the benzamide ligand are in equatorial positions (Kuz'mina *et al.*, 2005). 1,3-Dimethylurea (DMU) forms various complexes with transition metals. The crystal structures of $[M(\mathrm{DMU})_6][M\mathrm{Cl}_6]$ complexes (M is Nd or Y) contain octahedral cations and anions, while the crystal structures of $[M(\mathrm{DMU})_3(\mathrm{NO}_3)_3]$ (M is Nd or Y) contain complexes where the central atoms are coordinated by monodentate DMU molecules and bidentate nitrate ions (Diamantopoulou *et al.*, 2003; Boudalis *et al.*, 2005). In $[\mathrm{Mn}(\mathrm{DMU})_3\mathrm{I}_2]$, the Mn atom is coordinated by three O atoms of the DMU molecules and two iodido ligands (Delaunay & Hugel, 1986). Nickel complexes with DMU are octahedral (except for a thiocyanate-containing complex) (Bailey *et al.*, 1969).



(I)

In the title DMU complex with Cd, (I), the Cd atom and one C=O group are located on a crystallographic twofold rotation axis, and thus the molecular symmetry is C_2 (Fig. 1). The uncommon coordination of five for Cd involves three monodentate DMU ligands bound *via* their O atoms and two I atoms (Table 1, Fig. 1). The Cd1—O1 distance to the axial DMU molecules (2.427 Å) is noticeably longer than the Cd1—O7 distance to the equatorial DMU molecule (2.172 Å). The

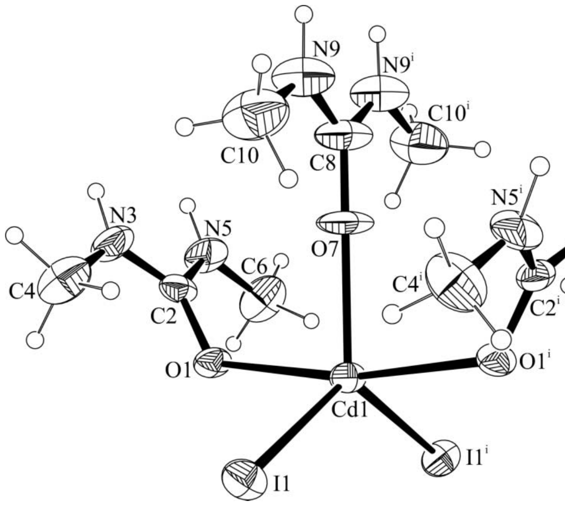


Figure 1
The molecular structure of compound (I) with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code (i) as given in Table 1.]

coordination polyhedron is a distorted trigonal bipyramid, with two I atoms and an O atom in the equatorial plane.

The NH H atoms of the two axial DMU molecules participate in two N—H···O hydrogen bonds (Table 2, Fig. 2). The equatorial DMU molecule acts as a donor to I atoms.

Experimental

Cadmium iodide (1 g, 2.73 mmol) and DMU (0.55 g, 5.39 mmol) were dissolved in water (9 ml). The reaction mixture was allowed to stand at room temperature for 4 d. The resulting colourless solid was recrystallized from water (yield 50%).

Crystal data

$[\mathrm{CdI_2(C_3H_8N_2O)_3I_2}]$
$M_r = 630.54$
Monoclinic, $C2/c$
$a = 13.712$ (9) Å
$b = 8.807$ (5) Å
$c = 17.265$ (9) Å
$\beta = 108.74$ (5)°
$V = 1974$ (2) Å^3
$Z = 4$
Mo $K\alpha$ radiation
$\mu = 4.25$ mm^{-1}
$T = 293$ (2) K
0.10 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
1939 measured reflections
1919 independent reflections
1596 reflections with $I > 2\sigma(I)$
$R_{\mathrm{int}} = 0.059$
1 standard reflections
frequency: 60 min
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.124$
$S = 1.08$
1919 reflections
100 parameters
H-atom parameters constrained
$\Delta\rho_{\mathrm{max}} = 0.99$ e Å^{-3}
$\Delta\rho_{\mathrm{min}} = -0.74$ e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

Cd1—O7	2.170 (8)	N3—C4	1.432 (13)
Cd1—O1	2.428 (5)	N5—C6	1.433 (13)
Cd1—I1	2.7319 (14)	O7—C8	1.230 (16)
O1—C2	1.275 (9)	C8—N9	1.333 (12)
C2—N3	1.331 (11)	N9—C10	1.432 (16)
C2—N5	1.346 (11)		
O7—Cd1—O1	84.61 (12)	O1—C2—N5	120.1 (8)
O1—Cd1—O1^{i}	169.2 (2)	N3—C2—N5	118.4 (7)
O1—Cd1—I1^{i}	92.05 (14)	C2—N3—C4	122.6 (8)
O7—Cd1—I1	117.68 (3)	C2—N5—C6	123.6 (8)
O1—Cd1—I1	92.95 (14)	C8—O7—Cd1	180
I1^{i}—Cd1—I1	124.64 (5)	O7—C8—N9	121.5 (6)
C2—O1—Cd1	125.4 (5)	N9^{i}—C8—N9	116.9 (13)
O1—C2—N3	121.5 (8)	C8—N9—C10	122.7 (10)

Symmetry code: (i) $-x, y, -z + \frac{1}{2}$.

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1^{ii}	0.86	2.20	3.019 (9)	160
N5—H5···O1^{ii}	0.86	2.47	3.228 (9)	148
N9—H9···I1^{iii}	0.86	2.91	3.677 (9)	150

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

All H atoms were included in calculated positions and refined as riding atoms, with N—H = 0.86 Å and C—H = 0.96 Å, and with $U_{\mathrm{iso}}(\mathrm{H}) = 1.2U_{\mathrm{eq}}(\mathrm{N})$ and $1.5U_{\mathrm{eq}}(\mathrm{C})$.

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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