

Acta Crystallographica Section E

## Structure Reports

Online

ISSN 1600-5368

(2-Carbamoylethyl- $\kappa^2C^1,O$ )triiodido-tin(IV)Geraldo M. de Lima,<sup>a</sup> Edward R. T. Tiekink,<sup>b\*</sup> James L. Wardell<sup>a,c,‡</sup> and Solange M. S. V. Wardell<sup>d</sup>

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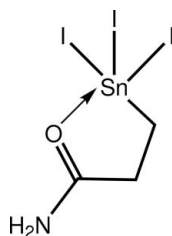
Received 6 October 2011; accepted 10 October 2011

Key indicators: single-crystal X-ray study;  $T = 120$  K; mean  $\sigma(C-C) = 0.008$  Å;  $R$  factor = 0.027;  $wR$  factor = 0.079; data-to-parameter ratio = 27.1.

Two independent but virtually identical molecules comprise the asymmetric unit of the title compound,  $[Sn(C_3H_6NO)I_3]$ . The  $Cl_3O$  coordination geometry around the  $Sn^{IV}$  atom is defined by a chelating carbamoylethyl ligand ( $C^1,O$ -bidentate) and three I atoms, and is based on a distorted trigonal bipyramid with the carbonyl O atom occupying a position *trans* to one of the I atoms which forms the longer of the Sn—I bonds. The independent molecules are linked *via* N—H...O hydrogen bonds, which leads to the formation on an eight-membered amide  $\{\cdots HNCO\}_2$  synthon. N—H...I hydrogen-bonding interactions are also present between neighbouring molecules.

## Related literature

For background to and for related  $Sn[OCH(NH_2)CH_2CH_2]Cl_3L$  structures ( $L =$  amide), see: Howie *et al.* (2011*a,b*); Wardell *et al.* (2010); Tiekink *et al.* (2006). For additional geometric analysis, see: Addison *et al.* (1984); Spek (2009).



## Experimental

## Crystal data

 $[Sn(C_3H_6NO)I_3]$  $M_r = 571.48$ Triclinic,  $P\bar{1}$  $a = 7.8530$  (1) Å $b = 10.6264$  (1) Å $c = 14.1250$  (2) Å $\alpha = 98.801$  (1)° $\beta = 105.523$  (1)° $\gamma = 102.383$  (1)° $V = 1081.22$  (2) Å<sup>3</sup> $Z = 4$ Mo  $K\alpha$  radiation $\mu = 10.87$  mm<sup>-1</sup> $T = 120$  K

0.20 × 0.20 × 0.02 mm

## Data collection

Bruker–Nonius APEXII CCD diffractometer

Absorption correction: multi-scan (SADABS; Sheldrick, 2007)

 $T_{\min} = 0.379$ ,  $T_{\max} = 1.000$ 

14061 measured reflections

4414 independent reflections

4342 reflections with  $I > 2\sigma(I)$  $R_{\text{int}} = 0.039$ 

## Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.027$  $wR(F^2) = 0.079$  $S = 1.12$ 

4414 reflections

163 parameters

H-atom parameters constrained

 $\Delta\rho_{\text{max}} = 1.37$  e Å<sup>-3</sup> $\Delta\rho_{\text{min}} = -1.46$  e Å<sup>-3</sup>

Table 1

Selected bond lengths (Å).

Sn1—C1	2.146 (5)	Sn2—C4	2.147 (5)
Sn1—O1	2.347 (3)	Sn2—O2	2.330 (3)
Sn1—I1	2.6953 (4)	Sn2—I4	2.6987 (4)
Sn1—I2	2.7796 (4)	Sn2—I5	2.6880 (4)
Sn1—I3	2.6904 (4)	Sn2—I6	2.8060 (4)

Table 2

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1n...O2	0.88	2.29	3.085 (7)	150
N2—H3n...O1	0.88	2.26	3.018 (7)	145
N2—H4n...I1	0.88	3.06	3.784 (6)	141

Data collection: COLLECT (Hooft, 1998); cell refinement: DENZO (Otwinowski & Minor, 1997) and COLLECT; data reduction: DENZO and COLLECT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997) and DIAMOND (Brandenburg, 2006); software used to prepare material for publication: pubCIF (Westrip, 2010).

The use of the EPSRC X-ray crystallographic service at the University of Southampton, England, and the valuable assistance of the staff there is gratefully acknowledged. JLW acknowledges support from CAPES (Brazil).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WM2541).

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## supporting information

*Acta Cryst.* (2011). E67, m1536–m1537 [doi:10.1107/S1600536811041778]

**(2-Carbamoylethyl- $\kappa^2C^1,O$ )triiodidotin(IV)**

Geraldo M. de Lima, Edward R. T. Tiekink, James L. Wardell and Solange M. S. V. Wardell

**S1. Comment**

The title compound, (I), was studied as a continuation of structural investigations of 2-amidoethyl compounds of stannanes(IV) (Tiekink *et al.*, 2006; Wardell *et al.*, 2010; Howie *et al.*, 2011*a,b*, and references therein).

Two independent molecules comprise the asymmetric unit of (I), (Fig. 1). The two molecules are virtually identical with the r.m.s. deviations for distances and angles being 0.0132 Å and 3.291°, respectively (Spek, 2009). The greatest difference in equivalent bond lengths is found in the Sn1—I2 and Sn2—I6 bonds (Table 1). The Sn<sup>IV</sup> atom in each molecule is chelated by the amidoethyl ligand and additionally coordinated by three I atoms. Each of the five-membered chelate rings is twisted, with the twist occurring about the CH<sub>2</sub>—CH<sub>2</sub> bond in each case. The resulting Cl<sub>3</sub>O donor set defines a coordination geometry intermediate between square-pyramidal and trigonal-bipyramidal, with a leaning towards the latter description. This is quantified by the value of  $\tau = 0.80$  [Sn1] which compares to the  $\tau$  values of 0.0 and 1.0 for ideal square-pyramidal and trigonal-bipyramidal geometries, respectively (Addison *et al.*, 1984). The  $\tau$  value for the Sn2 atom is 0.72. The disparity in the Sn—I bond lengths (Table 1), shows that the I atoms in the axial positions, each of which is *trans* to an O atom, form longer bonds than the I atoms occupying equatorial positions.

It is of interest that while (H<sub>2</sub>NCOCH<sub>2</sub>CH<sub>2</sub>-C,O)SnCl<sub>3</sub> readily forms six-coordinate complexes, [(H<sub>2</sub>NCOCH<sub>2</sub>CH<sub>2</sub>-C,O)SnCl<sub>3</sub>.L] with oxygen ligands, L, *e.g.* L = amide, as illustrated by the isolation of [(H<sub>2</sub>NCOCH<sub>2</sub>CH<sub>2</sub>-C,O)(EtCONH<sub>2</sub>-O)SnCl<sub>3</sub>] from reaction mixtures containing SnCl<sub>2</sub>, HCl and H<sub>2</sub>C=CHCONH<sub>2</sub> in Et<sub>2</sub>O (Howie *et al.*, 2011*b*), the triiodido analogue is reluctant to form similar complexes. This is a consequence of the reduced Lewis acidity of the tin atom in iodidostannanes compared to chloridostannanes.

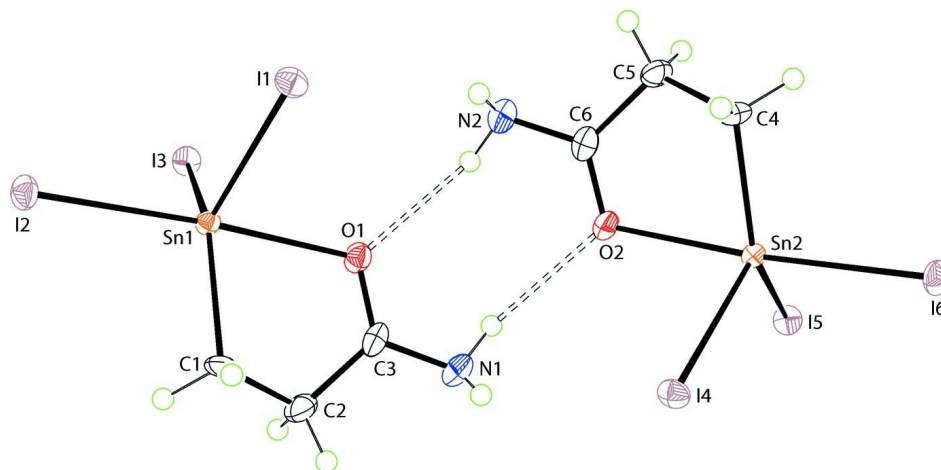
The two molecules comprising the asymmetric unit are linked *via* N—H···O hydrogen bonds, leading to the formation of an eight-membered {···HNCO}<sub>2</sub> synthon (Fig. 1, Table 2). The other H atom on each N forms an interaction with an I atom of the other molecule, in the case of the N1—H2n atom, this distance is long at 3.14 Å.

**S2. Experimental**

A solution of the complex, (H<sub>2</sub>NCOCH<sub>2</sub>CH<sub>2</sub>-C,O)(EtCONH<sub>2</sub>-O)SnCl<sub>3</sub> (0.74 g, 2 mmol), isolated from a reaction mixture containing SnCl<sub>2</sub>, HCl and H<sub>2</sub>C=CHCONH<sub>2</sub> in Et<sub>2</sub>O (Howie *et al.*, 2011*b*), and sodium iodide (10 mmol) in acetone (30 ml) was refluxed for 3 h, filtered to remove sodium chloride and rotary evaporated. The residue was extracted into chloroform (30 ml), the organic solution was rotary evaporated and the resulting residue was recrystallized from ethanol to give the title compound, melting point 461–463 K. IR:  $\nu(C=O)$  1660, 1581 cm<sup>-1</sup>.

**S3. Refinement**

The C-bound H atoms were geometrically placed (N—H = 0.88 Å and C—H = 0.99 Å) and refined as riding with  $U_{iso}(H) = 1.2U_{eq}(N, C)$ . The maximum and minimum residual electron density peaks of 1.37 and 1.46 e<sup>-</sup> Å<sup>-3</sup>, respectively, are located 1.34 Å and 0.85 Å from the I5 and I3 atoms, respectively.

**Figure 1**

The molecular structure of the two independent molecules comprising the asymmetric unit in (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level. The N—H...O hydrogen bonds are shown as dashed lines.

### (2-Carbamoylethyl- $\kappa^2C^1,O$ )triiodidotin(IV)

#### Crystal data

[Sn(C<sub>3</sub>H<sub>6</sub>NO)I<sub>3</sub>]

$M_r = 571.48$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 7.8530$  (1) Å

$b = 10.6264$  (1) Å

$c = 14.1250$  (2) Å

$\alpha = 98.801$  (1)°

$\beta = 105.523$  (1)°

$\gamma = 102.383$  (1)°

$V = 1081.22$  (2) Å<sup>3</sup>

$Z = 4$

$F(000) = 992$

$D_x = 3.511$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 4411 reflections

$\theta = 2.9$ – $27.5$ °

$\mu = 10.87$  mm<sup>-1</sup>

$T = 120$  K

Plate, yellow

$0.20 \times 0.20 \times 0.02$  mm

#### Data collection

Bruker–Nonius APEXII CCD  
diffractometer

Radiation source: Bruker–Nonius FR591  
rotating anode

10cm confocal mirrors monochromator

Detector resolution: 9.091 pixels mm<sup>-1</sup>

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan  
(SADABS; Sheldrick, 2007)

$T_{\min} = 0.379$ ,  $T_{\max} = 1.000$

14061 measured reflections

4414 independent reflections

4342 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 26.5$ °,  $\theta_{\min} = 3.0$ °

$h = -9 \rightarrow 9$

$k = -13 \rightarrow 13$

$l = -17 \rightarrow 17$

#### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.027$

$wR(F^2) = 0.079$

$S = 1.12$

4414 reflections

163 parameters

0 restraints

Primary atom site location: structure-invariant  
direct methods

Secondary atom site location: difference Fourier  
map

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0384P)^2 + 3.8857P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} = 0.001$   
 $\Delta\rho_{\max} = 1.37 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -1.46 \text{ e } \text{\AA}^{-3}$

#### Special details

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

**Refinement.** Refinement of  $F^2$  against ALL reflections. The weighted  $R$ -factor  $wR$  and goodness of fit  $S$  are based on  $F^2$ , conventional  $R$ -factors  $R$  are based on  $F$ , with  $F$  set to zero for negative  $F^2$ . The threshold expression of  $F^2 > 2\sigma(F^2)$  is used only for calculating  $R$ -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement.  $R$ -factors based on  $F^2$  are statistically about twice as large as those based on  $F$ , and  $R$ -factors based on ALL data will be even larger.

#### Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Sn1	0.84744 (4)	0.81052 (3)	0.07941 (2)	0.01343 (9)
I1	0.79233 (5)	0.56511 (3)	0.11465 (2)	0.02019 (10)
I2	1.13298 (5)	0.80096 (3)	-0.00043 (3)	0.02164 (10)
I3	0.58439 (4)	0.79311 (3)	-0.09302 (2)	0.01808 (9)
O1	0.6302 (5)	0.8274 (4)	0.1636 (3)	0.0196 (7)
N1	0.5852 (8)	0.9523 (5)	0.2928 (4)	0.0324 (12)
H1N	0.4849	0.8870	0.2762	0.039*
H2N	0.6529	0.9568	0.3546	0.039*
C1	0.9830 (7)	0.9848 (5)	0.1974 (4)	0.0190 (10)
H1A	1.0707	0.9634	0.2533	0.023*
H1B	1.0533	1.0528	0.1714	0.023*
C2	0.8454 (9)	1.0397 (5)	0.2370 (4)	0.0266 (12)
H2A	0.9052	1.0874	0.3083	0.032*
H2B	0.8057	1.1037	0.1978	0.032*
C3	0.6791 (7)	0.9313 (5)	0.2296 (4)	0.0198 (10)
Sn2	0.27996 (4)	0.67003 (3)	0.46025 (2)	0.01266 (9)
I4	0.61233 (4)	0.84602 (3)	0.54333 (3)	0.01904 (10)
I5	0.02318 (4)	0.80393 (3)	0.43118 (2)	0.01823 (9)
I6	0.25104 (5)	0.60910 (3)	0.64270 (2)	0.02072 (10)
O2	0.3235 (5)	0.6994 (4)	0.3074 (3)	0.0208 (8)
N2	0.3498 (7)	0.5858 (5)	0.1668 (4)	0.0286 (11)
H3N	0.3856	0.6666	0.1585	0.034*
H4N	0.4401	0.5480	0.1716	0.034*
C4	0.2650 (7)	0.4737 (5)	0.3869 (4)	0.0171 (9)
H4A	0.3835	0.4533	0.4140	0.021*
H4B	0.1684	0.4090	0.4005	0.021*
C5	0.2215 (7)	0.4620 (5)	0.2734 (4)	0.0213 (11)
H5A	0.2708	0.3921	0.2449	0.026*
H5B	0.0868	0.4358	0.2414	0.026*
C6	0.3029 (7)	0.5905 (5)	0.2496 (4)	0.0188 (10)

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
Sn1	0.01254 (17)	0.01471 (17)	0.01161 (16)	0.00316 (13)	0.00254 (13)	0.00162 (12)
I1	0.02194 (19)	0.01739 (17)	0.02113 (18)	0.00547 (14)	0.00490 (14)	0.00694 (13)
I2	0.01880 (18)	0.02449 (18)	0.02683 (19)	0.00877 (14)	0.01201 (14)	0.00795 (14)
I3	0.01449 (17)	0.02295 (18)	0.01437 (17)	0.00462 (13)	0.00081 (13)	0.00423 (13)
O1	0.0162 (18)	0.0241 (18)	0.0176 (17)	0.0048 (14)	0.0059 (14)	0.0023 (14)
N1	0.044 (3)	0.027 (2)	0.032 (3)	0.009 (2)	0.025 (2)	-0.001 (2)
C1	0.021 (3)	0.013 (2)	0.016 (2)	-0.0025 (19)	0.001 (2)	-0.0023 (18)
C2	0.045 (4)	0.016 (2)	0.024 (3)	0.010 (2)	0.018 (3)	0.003 (2)
C3	0.025 (3)	0.026 (3)	0.016 (2)	0.014 (2)	0.011 (2)	0.008 (2)
Sn2	0.01234 (17)	0.01365 (16)	0.01193 (16)	0.00425 (12)	0.00339 (13)	0.00231 (12)
I4	0.01251 (17)	0.01815 (17)	0.02403 (18)	0.00266 (13)	0.00420 (13)	0.00230 (13)
I5	0.01529 (18)	0.02042 (17)	0.02122 (18)	0.00887 (13)	0.00530 (13)	0.00606 (13)
I6	0.01956 (18)	0.02811 (19)	0.01277 (16)	0.00340 (14)	0.00347 (13)	0.00657 (13)
O2	0.028 (2)	0.0208 (18)	0.0155 (17)	0.0060 (15)	0.0108 (15)	0.0032 (14)
N2	0.035 (3)	0.030 (3)	0.022 (2)	0.005 (2)	0.015 (2)	0.003 (2)
C4	0.022 (3)	0.013 (2)	0.013 (2)	0.0072 (19)	0.0009 (19)	0.0001 (17)
C5	0.022 (3)	0.021 (2)	0.016 (2)	0.002 (2)	0.004 (2)	-0.0031 (19)
C6	0.014 (2)	0.029 (3)	0.016 (2)	0.009 (2)	0.0047 (19)	0.006 (2)

*Geometric parameters (Å, °)*

Sn1—C1	2.146 (5)	Sn2—C4	2.147 (5)
Sn1—O1	2.347 (3)	Sn2—O2	2.330 (3)
Sn1—I1	2.6953 (4)	Sn2—I4	2.6987 (4)
Sn1—I2	2.7796 (4)	Sn2—I5	2.6880 (4)
Sn1—I3	2.6904 (4)	Sn2—I6	2.8060 (4)
O1—C3	1.244 (6)	O2—C6	1.262 (6)
N1—C3	1.324 (7)	N2—C6	1.313 (6)
N1—H1N	0.8800	N2—H3N	0.8800
N1—H2N	0.8800	N2—H4N	0.8800
C1—C2	1.521 (7)	C4—C5	1.526 (7)
C1—H1A	0.9900	C4—H4A	0.9900
C1—H1B	0.9900	C4—H4B	0.9900
C2—C3	1.512 (8)	C5—C6	1.506 (7)
C2—H2A	0.9900	C5—H5A	0.9900
C2—H2B	0.9900	C5—H5B	0.9900
C1—Sn1—O1	76.52 (16)	C4—Sn2—O2	77.38 (16)
C1—Sn1—I3	125.92 (14)	C4—Sn2—I5	129.25 (14)
O1—Sn1—I3	87.71 (9)	O2—Sn2—I5	89.69 (9)
C1—Sn1—I1	122.64 (14)	C4—Sn2—I4	118.64 (14)
O1—Sn1—I1	83.18 (9)	O2—Sn2—I4	84.58 (9)
I3—Sn1—I1	105.788 (15)	I5—Sn2—I4	108.400 (14)
C1—Sn1—I2	98.50 (14)	C4—Sn2—I6	96.42 (13)
O1—Sn1—I2	173.92 (9)	O2—Sn2—I6	172.63 (9)

I3—Sn1—I2	98.106 (14)	I5—Sn2—I6	97.373 (13)
I1—Sn1—I2	96.853 (14)	I4—Sn2—I6	95.120 (13)
C3—O1—Sn1	112.5 (3)	C6—O2—Sn2	111.5 (3)
C3—N1—H1N	109.5	C6—N2—H3N	109.5
C3—N1—H2N	109.5	C6—N2—H4N	109.5
H1N—N1—H2N	109.5	H3N—N2—H4N	109.5
C2—C1—Sn1	111.0 (4)	C5—C4—Sn2	110.1 (3)
C2—C1—H1A	109.4	C5—C4—H4A	109.6
Sn1—C1—H1A	109.4	Sn2—C4—H4A	109.6
C2—C1—H1B	109.4	C5—C4—H4B	109.6
Sn1—C1—H1B	109.4	Sn2—C4—H4B	109.6
H1A—C1—H1B	108.0	H4A—C4—H4B	108.1
C3—C2—C1	111.7 (4)	C6—C5—C4	111.5 (4)
C3—C2—H2A	109.3	C6—C5—H5A	109.3
C1—C2—H2A	109.3	C4—C5—H5A	109.3
C3—C2—H2B	109.3	C6—C5—H5B	109.3
C1—C2—H2B	109.3	C4—C5—H5B	109.3
H2A—C2—H2B	107.9	H5A—C5—H5B	108.0
O1—C3—N1	121.5 (5)	O2—C6—N2	121.2 (5)
O1—C3—C2	120.3 (4)	O2—C6—C5	120.6 (4)
N1—C3—C2	118.2 (5)	N2—C6—C5	118.2 (5)
C1—Sn1—O1—C3	6.4 (4)	C4—Sn2—O2—C6	5.8 (3)
I3—Sn1—O1—C3	-121.4 (3)	I5—Sn2—O2—C6	-124.7 (3)
I1—Sn1—O1—C3	132.4 (3)	I4—Sn2—O2—C6	126.8 (3)
O1—Sn1—C1—C2	-19.9 (3)	O2—Sn2—C4—C5	-20.4 (3)
I3—Sn1—C1—C2	57.1 (4)	I5—Sn2—C4—C5	58.6 (4)
I1—Sn1—C1—C2	-92.5 (4)	I4—Sn2—C4—C5	-97.0 (3)
I2—Sn1—C1—C2	163.6 (3)	I6—Sn2—C4—C5	163.6 (3)
Sn1—C1—C2—C3	31.0 (6)	Sn2—C4—C5—C6	32.4 (5)
Sn1—O1—C3—N1	-172.4 (4)	Sn2—O2—C6—N2	-169.0 (4)
Sn1—O1—C3—C2	9.8 (6)	Sn2—O2—C6—C5	11.7 (6)
C1—C2—C3—O1	-27.7 (7)	C4—C5—C6—O2	-30.2 (7)
C1—C2—C3—N1	154.4 (5)	C4—C5—C6—N2	150.5 (5)

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1n $\cdots$ O2	0.88	2.29	3.085 (7)	150
N2—H3n $\cdots$ O1	0.88	2.26	3.018 (7)	145
N2—H4n $\cdots$ I1	0.88	3.06	3.784 (6)	141