Supporting information

Diorganotin(IV) 2-pyridyl selenolates: Synthesis, structures and their utility as molecular precursors for the preparation of tin selenide nanocrystals and thin films

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Figure Captions

Fig. S1 $^{77}Se\{^{1}H\}$NMR spectrum of $[Me_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)Cl]$ (**7**).

Fig. S2 $^{119}Sn\{^{1}H\}$NMR spectrum of $[Me_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)Cl]$ (**7**).

Fig. S3 $^{77}Se\{^{1}H\}$NMR spectrum of $[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**).

Fig. S4 $^{119}Sn\{^{1}H\}$NMR spectrum of $[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**).

Fig. S5 TG curves of a) $[Me_2Sn(Se\text{-}C_5H_4N)_2]$ (**1**), b) $[Me_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)_2]$ (**2**) and c) $[Me_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)Cl]$ (**7**).

Fig. S6 TG curves of a) $[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**) and b) $[Et_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)_2]$ (**4**).

Fig. S7 TG curves of a) $[^tBu_2Sn(Se\text{-}C_5H_4N)_2]$ (**5**) and b) $[^tBu_2Sn(Se\text{-}C_5H_4N)Cl]$ (**8**).

Fig. S8 a) XRD pattern, b) EDX spectrum and c) SEM image of SnSe obtained by thermolysis of $[Me_2Sn(Se\text{-}C_5H_4N)_2]$ (**1**) in 3 ml of oleylamine at 215 ^oC for 15 min.

Fig. S9 a) XRD pattern, b) EDX spectrum and c) SEM image of $SnSe_2$ obtained by thermolysis of $[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**) in 3 ml of oleylamine at 215 ^oC for 25 min.

Fig. S10 a) XRD pattern, b) EDX spectrum and c) SEM image of SnSe obtained by thermolysis of $[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**) in 6 ml of oleylamine at 215 ^oC for 25 min.

Fig. S11 a) XRD pattern and b) EDX spectrum of SnSe obtained by thermolysis of $[Et_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)_2]$ (**4**) in 3 ml of oleylamine at 215 ^oC for 25 min.

Fig. S12 a) XRD pattern and b) EDX spectrum of $SnSe_2$ obtained by thermolysis of $[Et_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)_2]$ (**4**) in 6 ml of oleylamine at 215 ^oC for 25 min.

Fig. S13 a) XRD pattern, b) EDX spectrum and c) SEM image of SnSe obtained by thermolysis of $[^tBu_2Sn(Se\text{-}C_5H_4N)_2]$ (**5**) in 3 ml of oleylamine at 215 ^oC for 25 min.

Fig. S14 a) XRD pattern, b) EDX spectrum and c) SEM image of SnSe obtained by thermolysis of $[^tBu_2Sn(Se\text{-}C_5H_4N)_2]$ (**5**) in 6 ml of oleylamine at 215 ^oC for 25 min.

Fig. S15 a) XRD pattern and b) EDX spectrum of SnSe obtained by the AACVD of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) at 490 ^{o}C for 3 h on glass substrate.

Fig. S16 a) XRD pattern, b) EDX spectrum and c) SEM of SnSe deposited by the AACVD of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) at 490 ^{o}C for 3 h on silicon substrate.

.**Fig. S17** a) EDX spectrum and b) SEM of SnSe obtained by the AACVD of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) at 530 ^{o}C for 3 h on glass substrate.

Fig. S18 a) XRD pattern, b) EDX spectrum and c) SEM of SnSe obtained by AACVD of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) at 530 ^{o}C for 3 h on silicon substrate.

Fig. S19 a) TEM image and b) SAED pattern of SnSe obtained by thermolysis of [$Me_2Sn(Se\text{-}C_5H_4N)_2$] (**1**) in 3 ml oleylamine at 215 ^{o}C for 25 min.

Fig. S20 a) TEM image and b) SAED pattern of $SnSe_2$ obtained by thermolysis of [$Et_2Sn(Se\text{-}C_5H_4N)_2$] (**3**) in 3 ml oleylamine at 215 ^{o}C for 25 min.

Fig. S21 a) TEM image and b) SAED pattern of SnSe obtained by thermolysis of [$Et_2Sn(Se\text{-}C_5H_4N)_2$] (**3**) in 6 ml oleylamine at 215 ^{o}C for 25 min.

Fig. S22 a), c) TEM image and b), d) SAED pattern of SnSe obtained by thermolysis of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) in 3 ml oleylamine at 215 ^{o}C for 25 min.

Fig. S23 a) TEM image and b) SAED pattern of $SnSe_2$ obtained by thermolysis of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) in 6 ml oleylamine at 215 ^{o}C for 25 min.

Table S1. Experimental details and results of tin selenide nanostructures obtained from the complexes, **1** and **3-5.**

Table S2. Lattice parameters of tin selenide nanostructures calculated by using eq 1.

Table S3. Experimental details and results of tin selenide thin films deposited by AACVD of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**).

Crystal Information File of [$Me_2Sn(Se\text{-}C_5H_4N)_2$] (**1**)
Crystal Information File of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**)
Crystal Information File of [$Me_2Sn(Se\text{-}C_5H_4N)Cl$] (**7**)

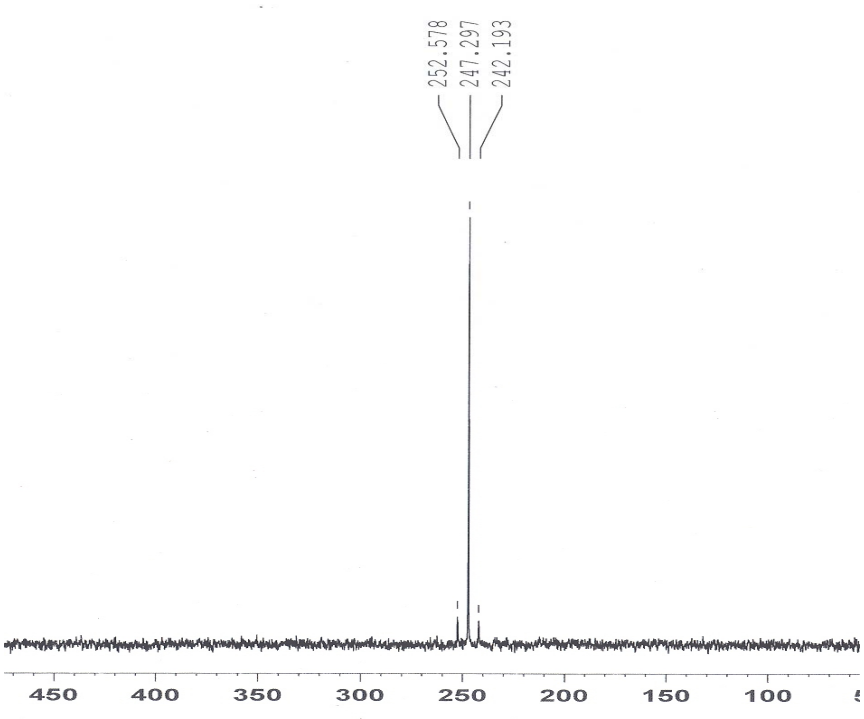


Fig. S1 $^{77}Se\{^{1}H\}$NMR spectrum of [$Me_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)Cl$] (**7**)

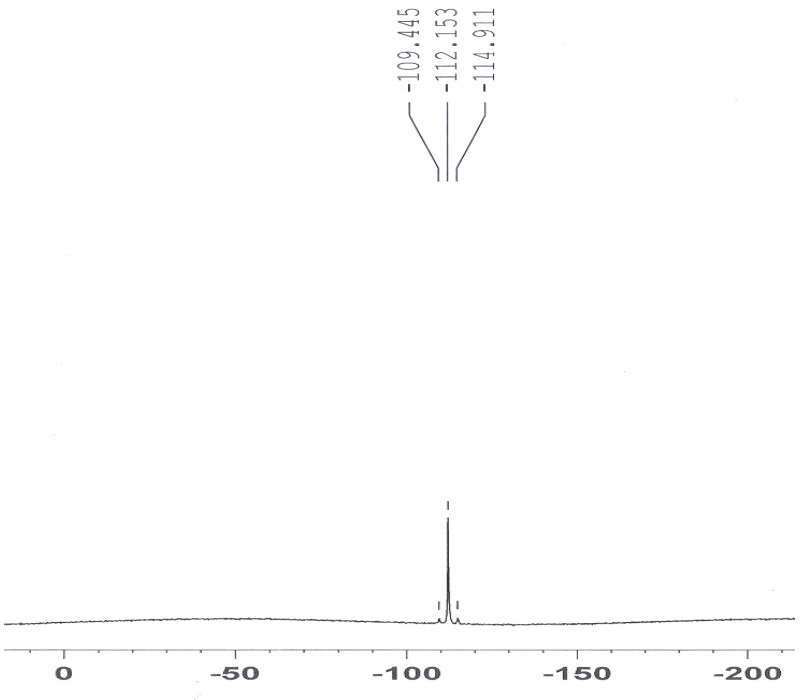


Fig. S2 $^{119}Sn\{^{1}H\}$NMR spectrum of [$Me_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)Cl$] (**7**)

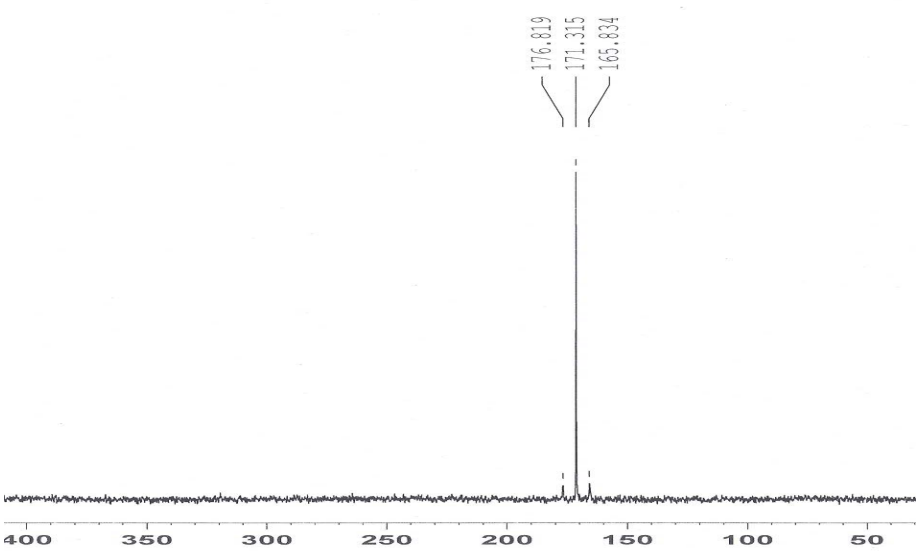


Fig. S3 $^{77}Se\{^{1}H\}$NMR spectrum of $[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**)

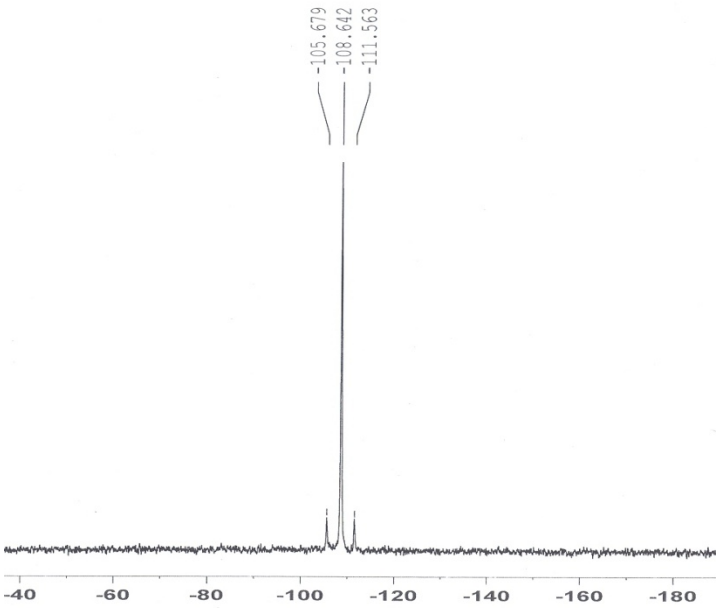


Fig. S4 $^{119}Sn\{^{1}H\}$NMR spectrum of $[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**)

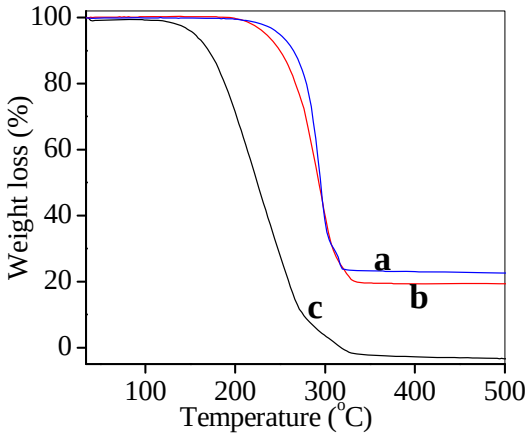


Fig. S5 TG curves of a) $[Me_2Sn(Se\text{-}C_5H_4N)_2]$ (**1**), b) $[Me_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)_2]$ (**2**) and c) $[Me_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)Cl]$ (**7**).

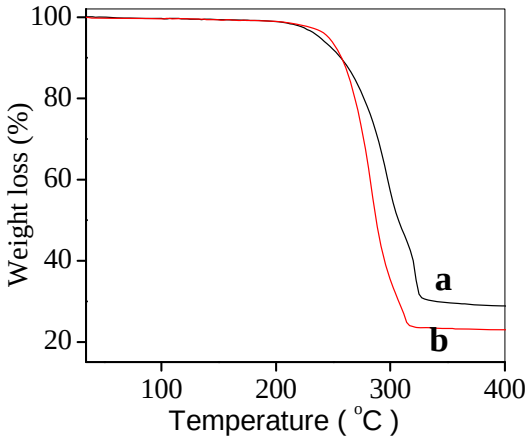


Fig. S6 TG curves of a) $[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**) and b) $[Et_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)_2]$ (**4**).

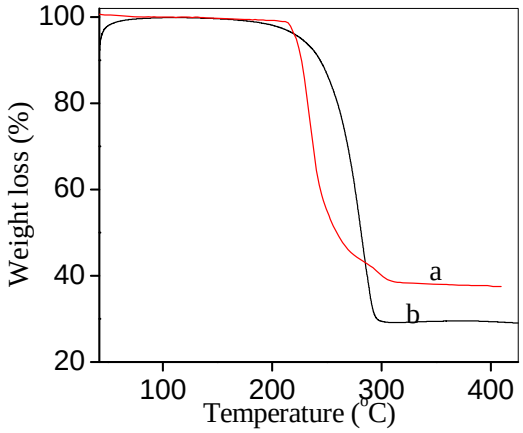
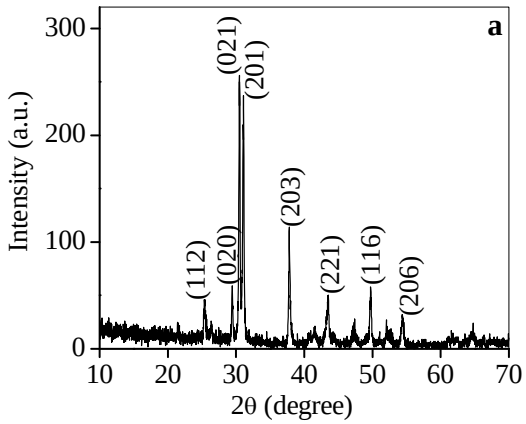
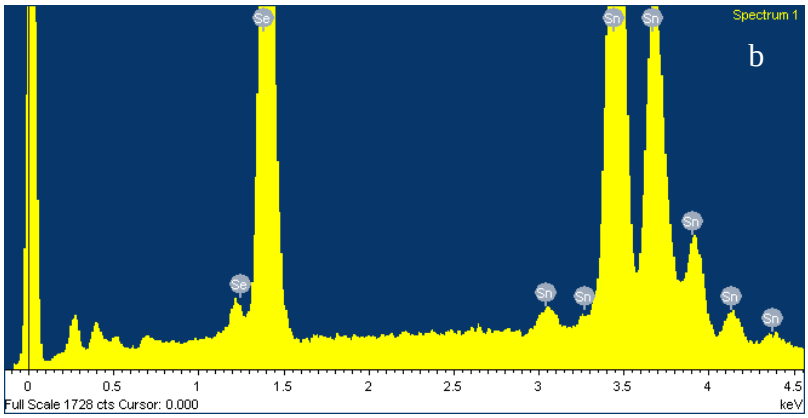


Fig. S7 TG curves of a) $[^tBu_2Sn(Se\text{-}C_5H_4N)_2]$ (**5**) and b) $[^tBu_2Sn(Se\text{-}C_5H_4N)Cl]$ (**8**).





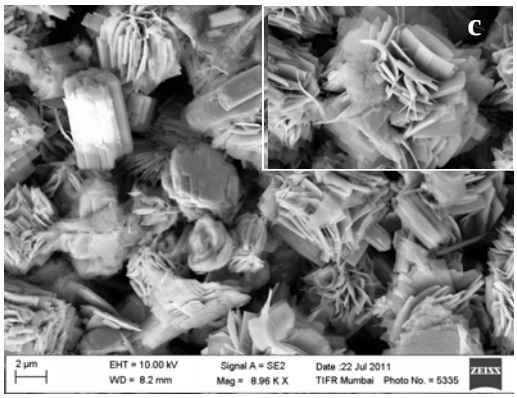
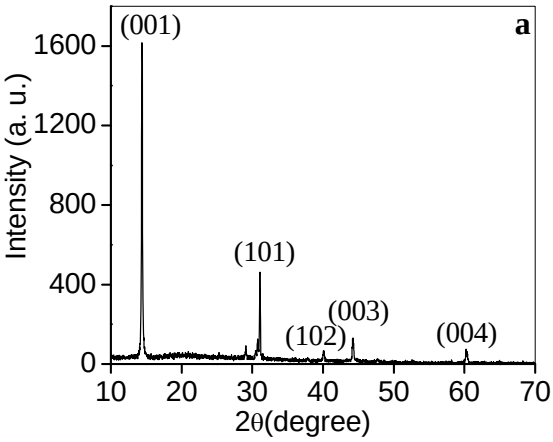
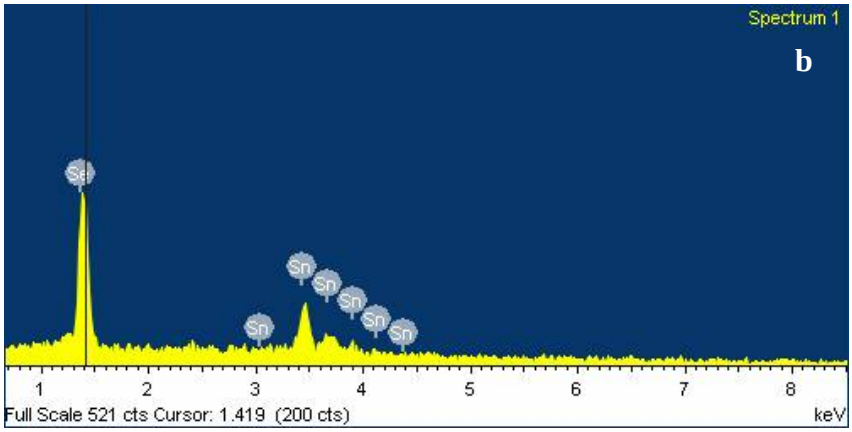


Fig. S8 a) XRD pattern, b) EDX spectrum and c) SEM image of SnSe obtained by the thermolysis of $[Me_2Sn(Se\text{-}C_5H_4N)_2]$ (**1**) in 3 ml of oleylamine at 215 ^oC for 15 min.





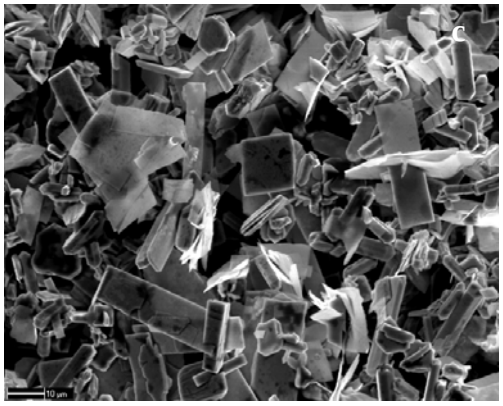
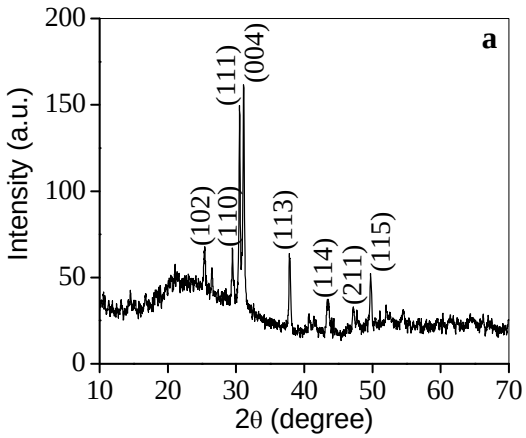
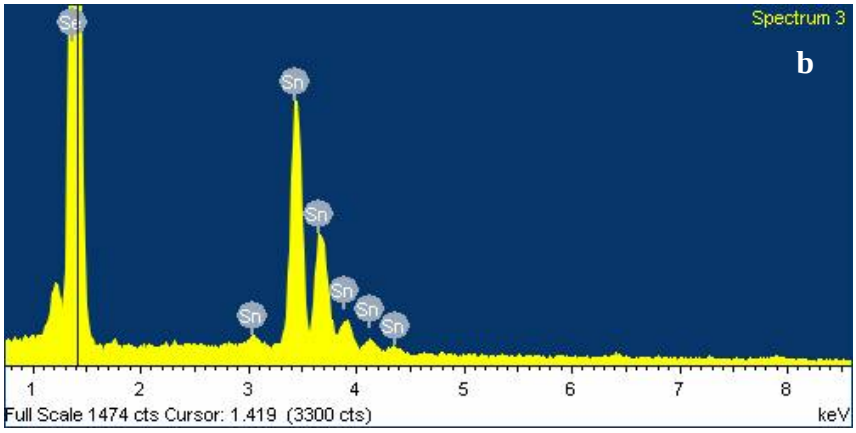


Fig. S9 a) XRD pattern, b) EDX spectrum and c) SEM image of $SnSe_2$ obtained by thermolysis of $[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**) in 3 ml of oleylamine at 215 ^oC for 25 min.





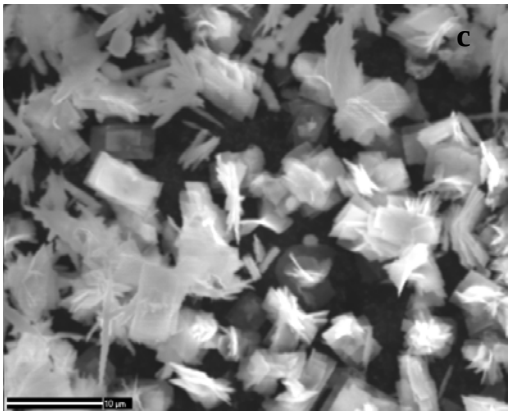


Fig. S10 a) XRD pattern, b) EDX spectrum and c) SEM image of SnSe obtained by thermolysis of $[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**) in 6 ml of oleylamine at 215 ^oC for 25 min.

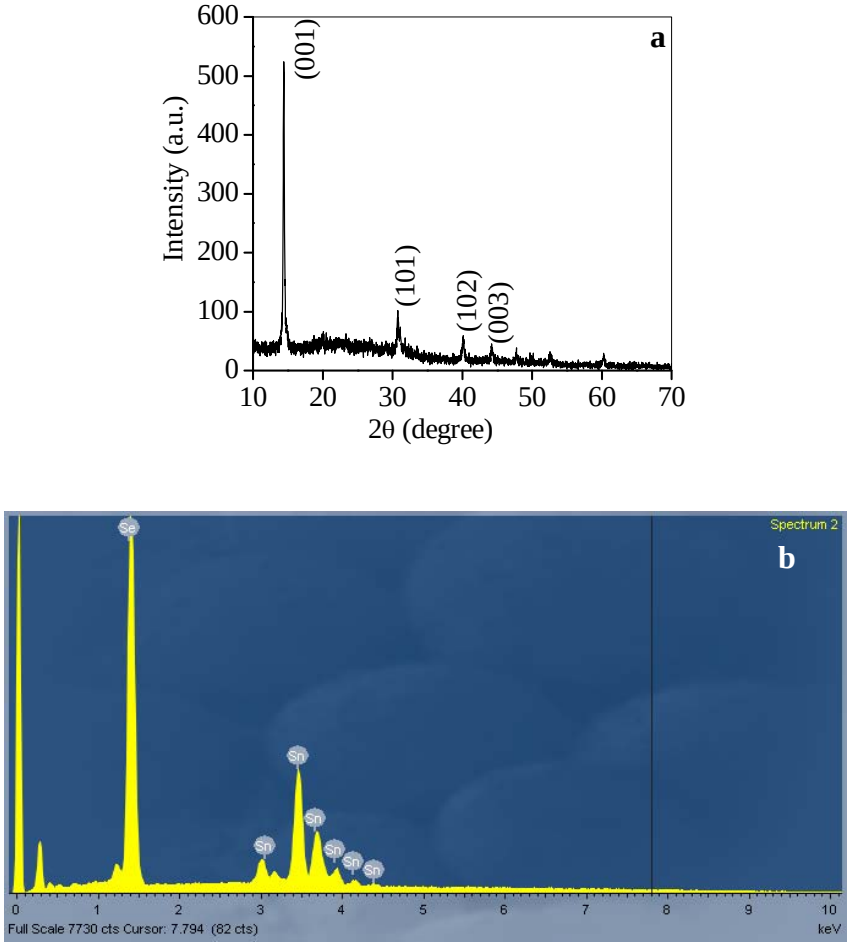


Fig. S11 a) XRD pattern and b) EDX of $SnSe_2$ obtained by thermolysis of [$Et_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)_2$] (**4**) in 3 ml of oleylamine at 215 ^oC for 25 min.

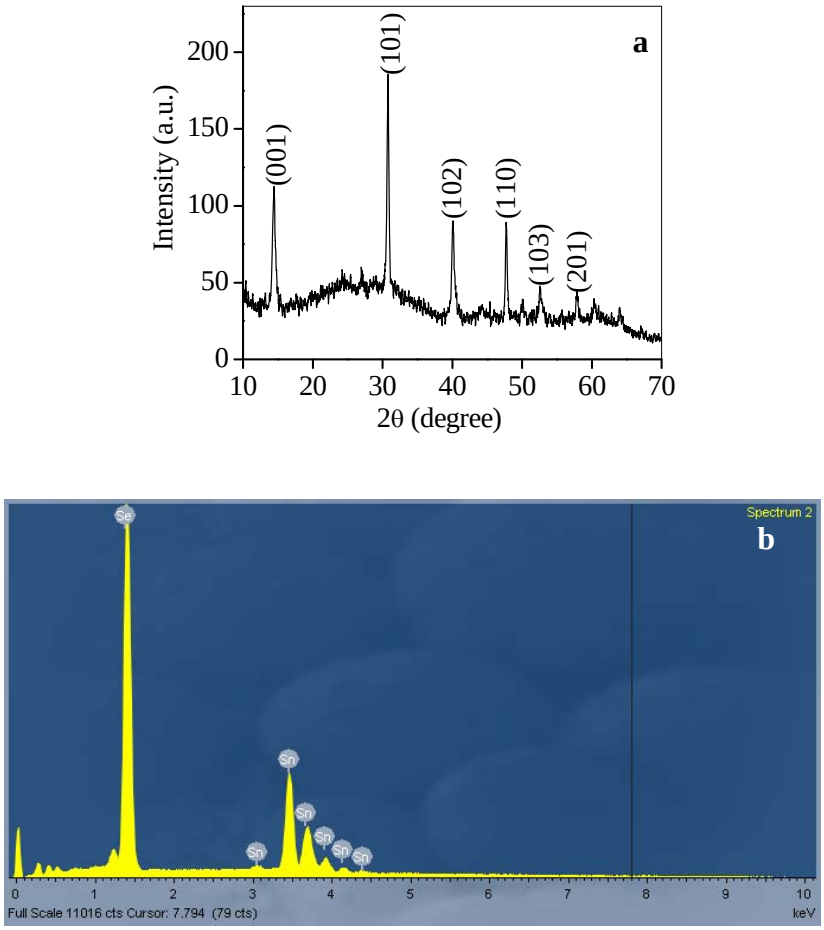


Fig. S12 a) XRD pattern and b) EDX spectrum of $SnSe_2$ obtained by thermolysis of $[Et_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)_2]$ (**4**) in 6 ml of oleylamine at 215 ^oC for 25 min.

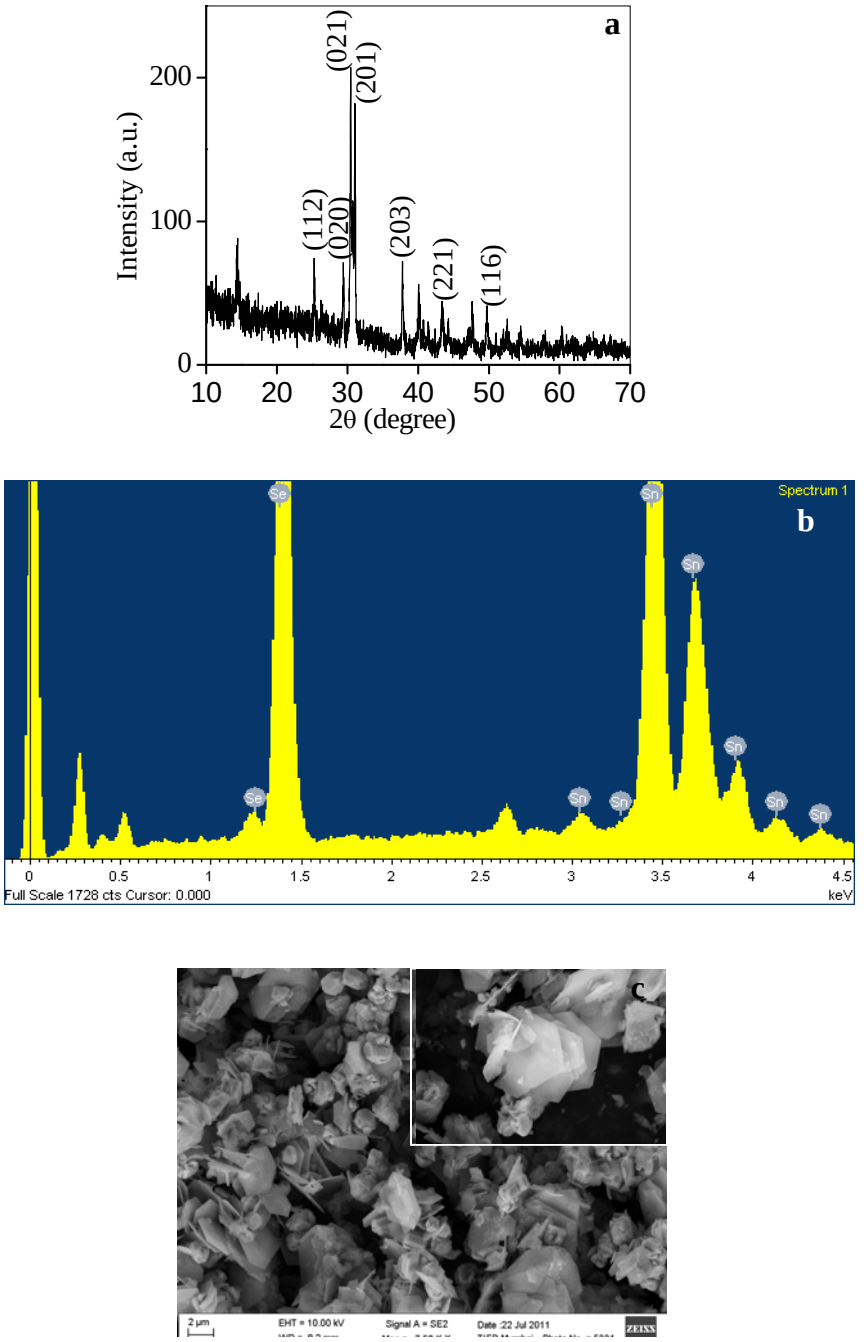


Fig. S13 a) XRD pattern, b) EDX spectrum and c) SEM image of SnSe obtained by thermolysis of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) in 3 ml of oleylamine at 215 ^{o}C for 25 min.

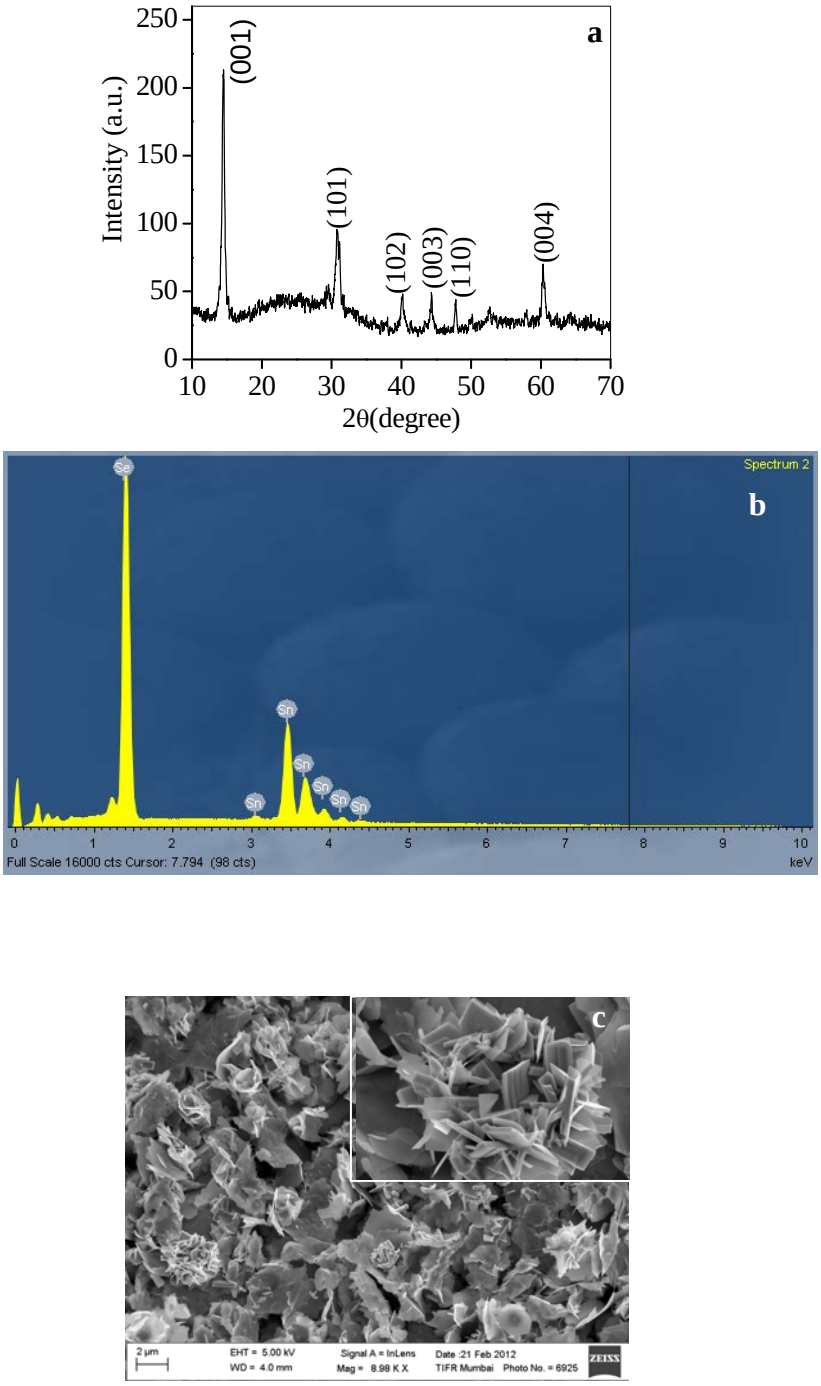


Fig. S14 a) XRD pattern, b) EDX spectrum and c) SEM image of SnSe obtained by thermolysis of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) in 6 ml of oleylamine at 215 ^{o}C for 25 min.

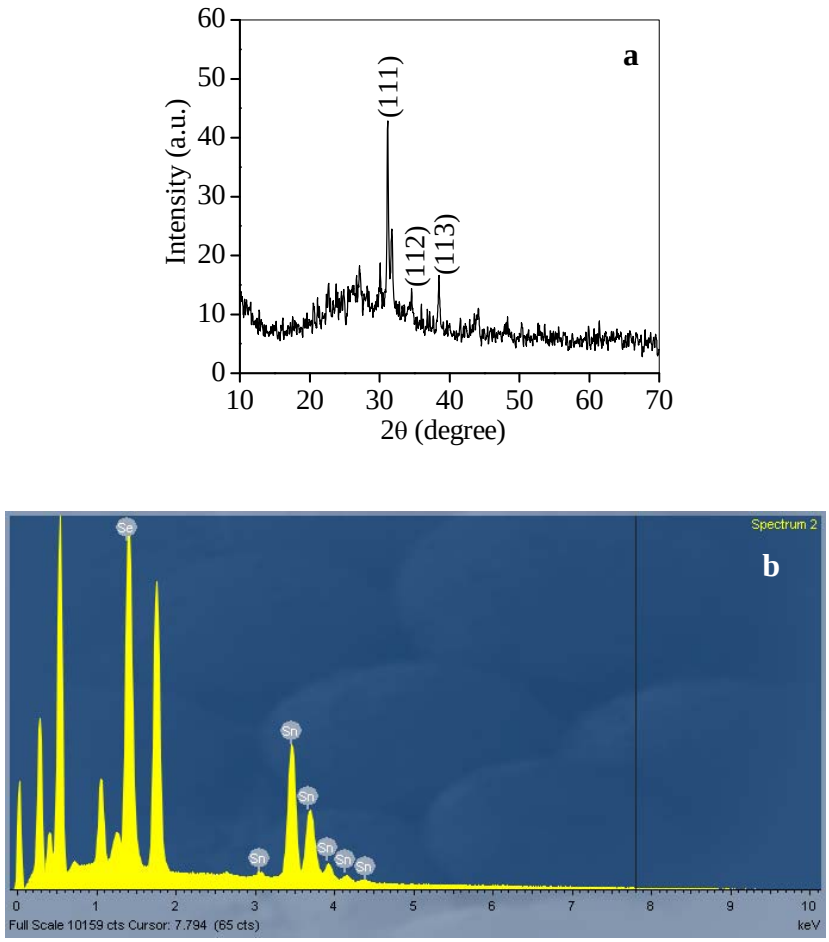


Fig. S15 a) XRD pattern and b) EDX spectrum of SnSe deposited by AACVD of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) at 490 ^{o}C for 3 h on glass substrate.

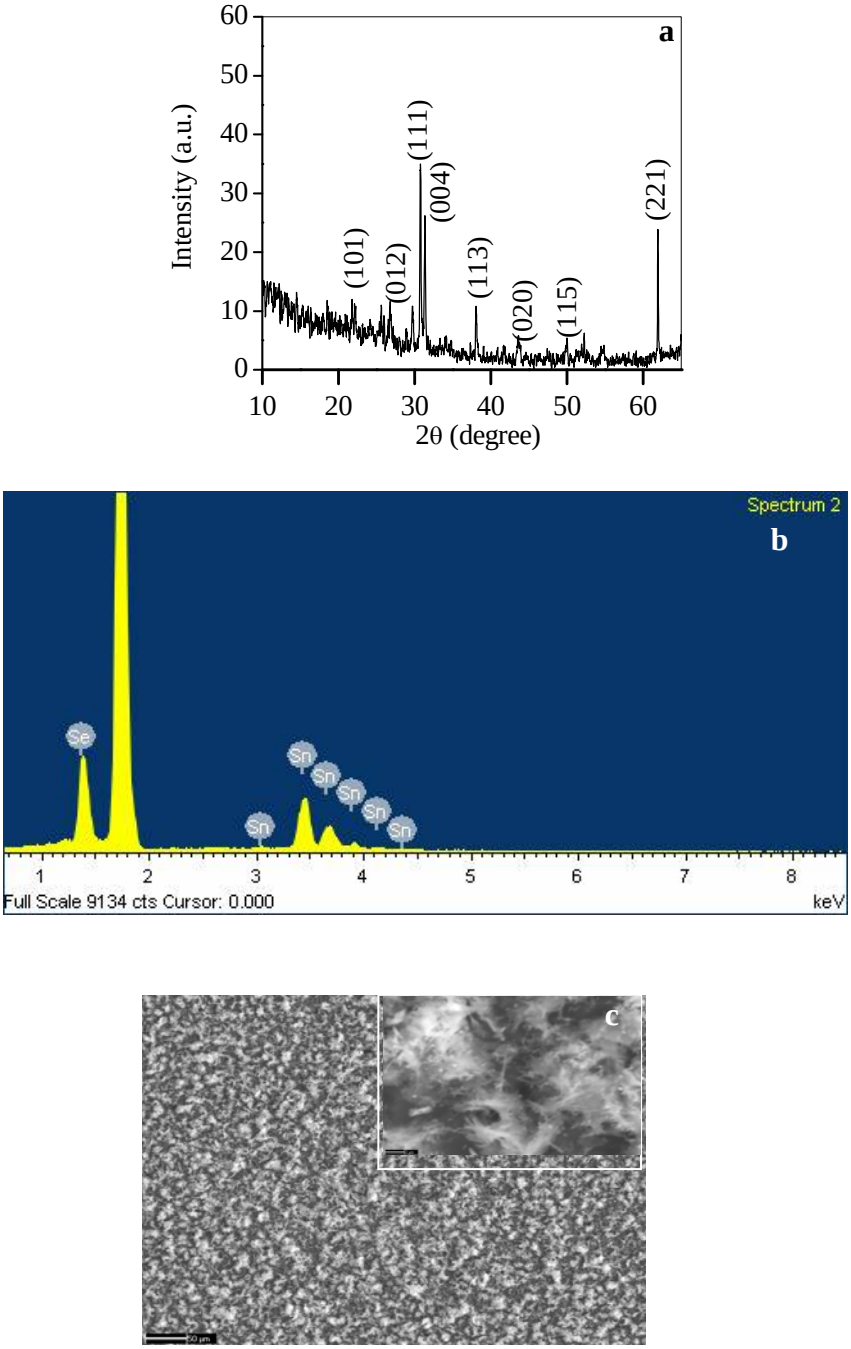
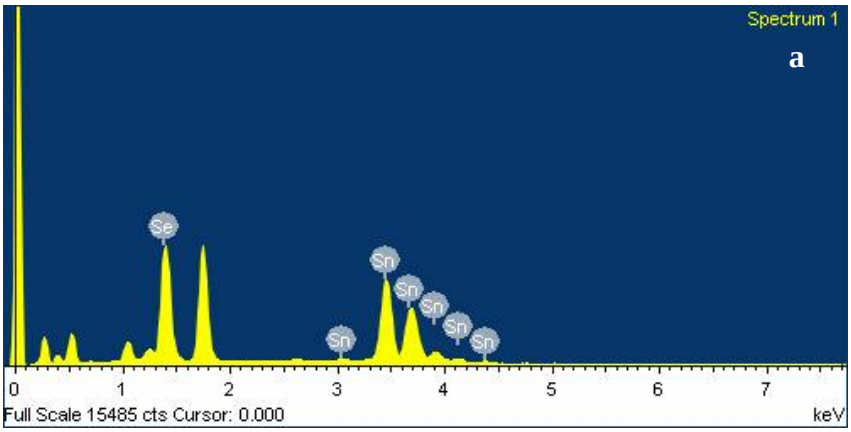


Fig. S16 a) XRD pattern, b) EDX spectrum and c) SEM of SnSe deposited by the AACVD of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) at 490 ^{o}C for 3 h on silicon substrate.



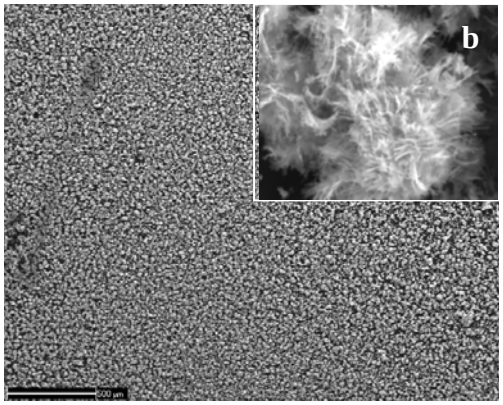


Fig. S17 a) EDX spectrum and b) SEM of SnSe deposited by AACVD of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) at 530^{o}C for 3 h on glass substrate.

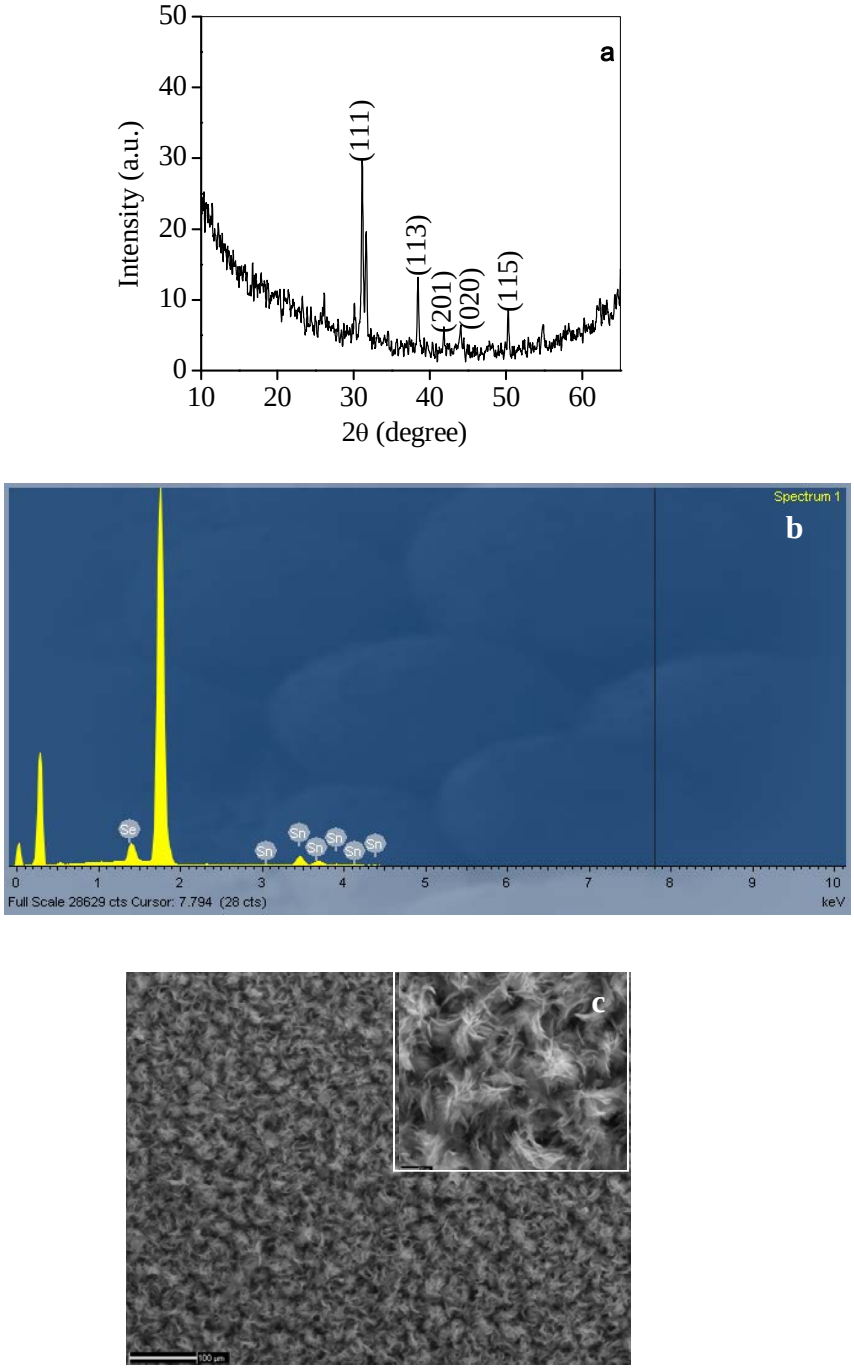


Fig. S18 a) XRD pattern, b) EDX spectrum and c) SEM of SnSe obtained by AACVD of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) at 530 ^{o}C for 3 h on silicon substrate.

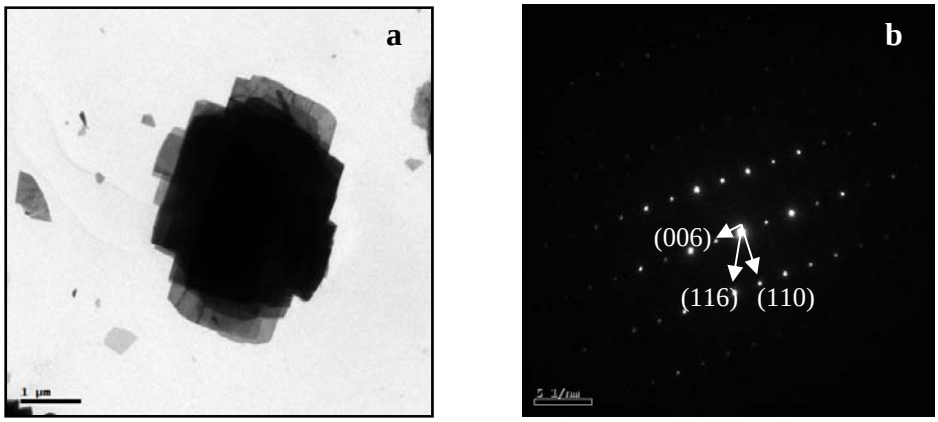


Fig. S19 a) TEM image and b) SAED pattern of SnSe obtained by thermolysis of $[Me_2Sn(Se\text{-}C_5H_4N)_2]$ (**1**) in 3 ml oleylamine at 215 ^oC for 25 min.

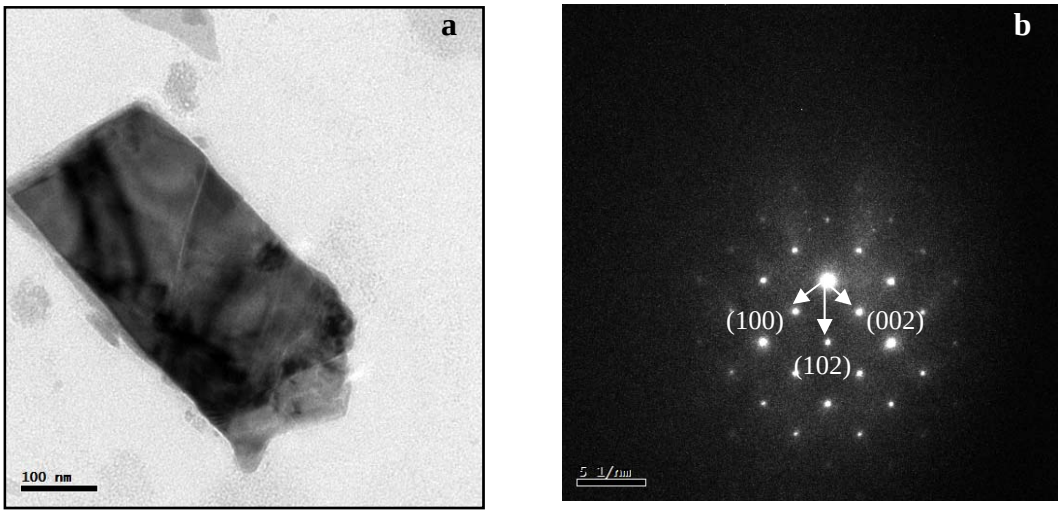


Fig. S20 a) TEM image and b) SAED pattern of $SnSe_2$ obtained by thermolysis of $[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**) in 3 ml oleylamine at 215 ^oC for 25 min.

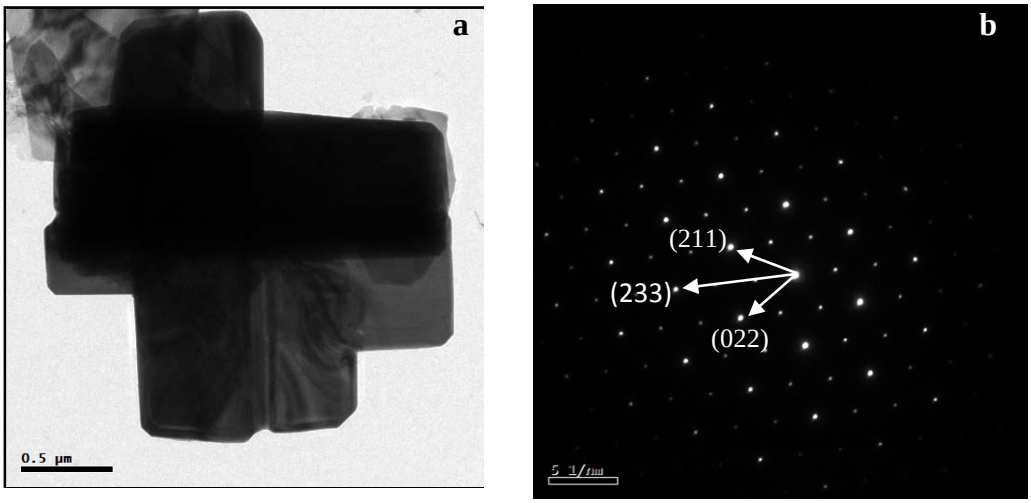


Fig. S21 a) TEM image and b) SAED pattern of SnSe obtained by thermolysis of $[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**) in 6 ml oleylamine at 215 ^oC for 25 min.

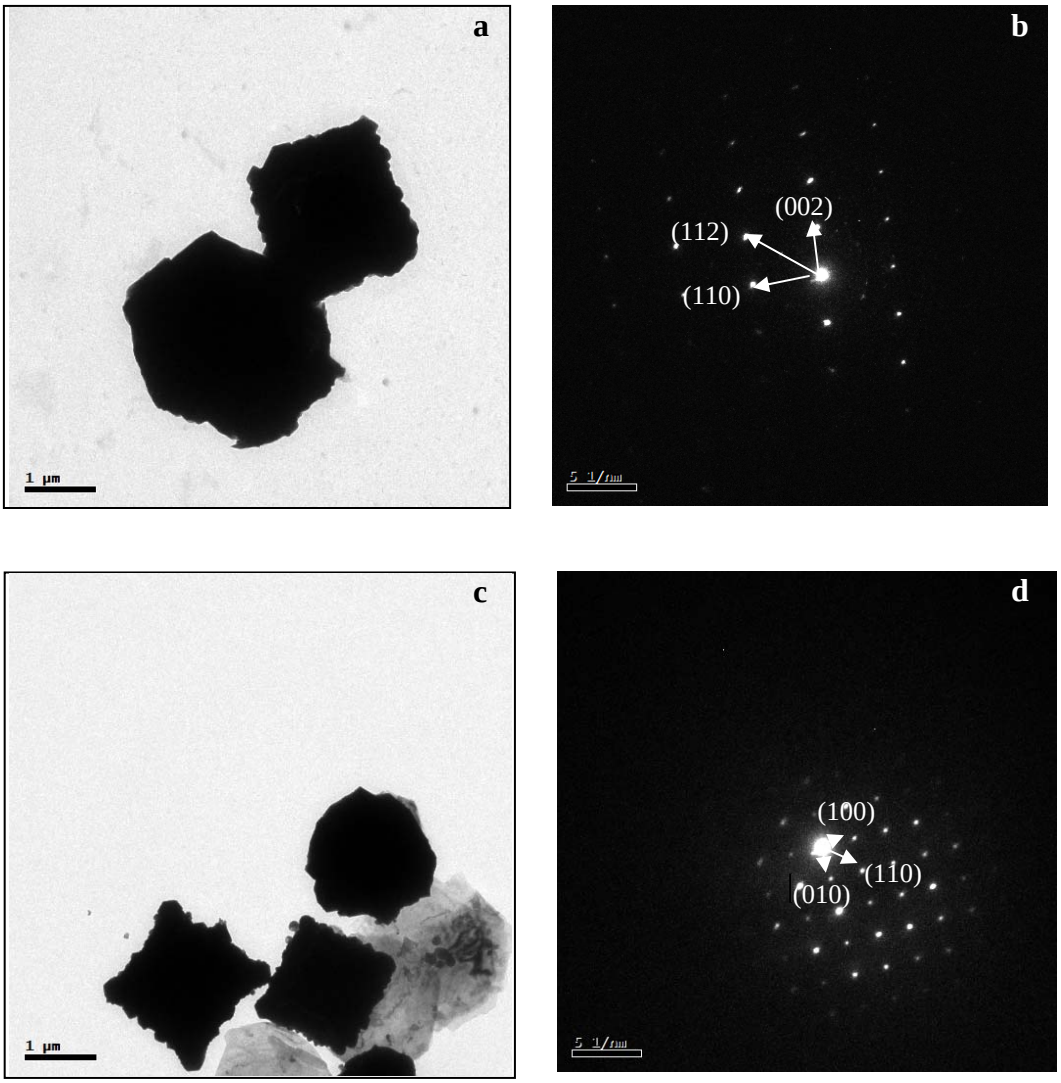


Fig. S22 a), c) TEM images and SAED patterns of b) hexagonal and d) square like SnSe obtained by thermolysis of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) in 3 ml oleylamine at 215 ^{o}C for 25 min.

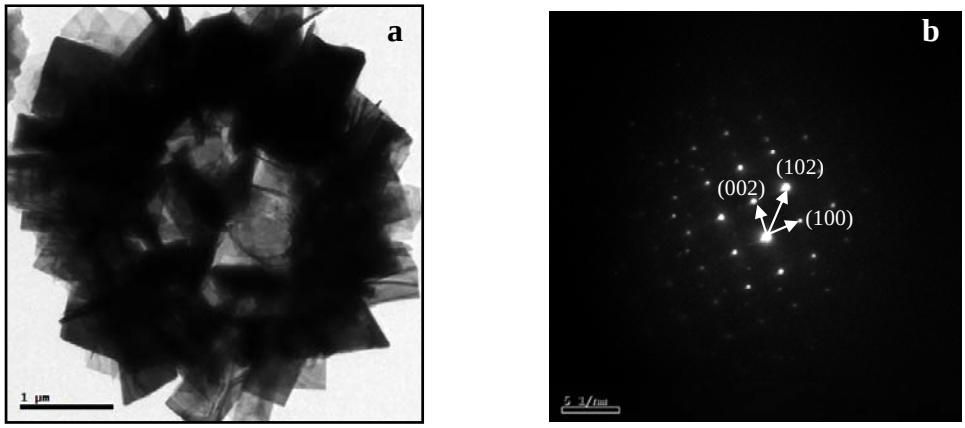


Fig. S23 a) TEM image and b) SAED pattern of $SnSe_2$ obtained by thermolysis of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**) in 6 ml oleylamine at 215 ^{o}C for 25 min.

Table S1. Experimental details and results of tin selenide nanostructures obtained from the complexes, **1** and **3-5**.

Exp. No.	Precursor	Amount of OA taken in the flask (ml)	Amount of OA/CH_2Cl_2 taken with the precursor (ml)		Reaction duration (minutes)	EDX Se/Sn ratio	Phase/composition/JCPDS No.	Morphology as revealed by SEM
			OA	CH_2Cl_2				
1	$[Me_2Sn(Se\text{-}C_5H_4N)_2]$ (**1**)	3	_	2	15	0.87	Ortho/SnSe/81-0013	Bundles of rectangular sheets
3	$[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**)	3	_	2	25	2.10	Hex/$SnSe_2$/23-0602	Rectangular bars
4	$[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**)	3	3	_	25	0.99	Ortho/SnSe/72-1460	Regular bars
5	$[Et_2Sn\{Se\text{-}C_5H_3(3\text{-}Me\}N)_2]$ (**4**)	3	_	2	25	1.52	Hex/$SnSe_2$/23-0602	Irregular hexagonal sheets
6	$[Et_2Sn\{Se\text{-}C_5H_3(3\text{-}Me\}N)_2]$ (**4**)	3	3	_	25	1.74	Hex/$SnSe_2$/23-0602	Regular hexagons
5	$[^tBu_2Sn(Se\text{-}C_5H_4N)_2]$ (**5**)	3	_	2	25	0.96	Mixture of Ortho/SnSe/81-0013 and Hex/$SnSe_2$/23-0602	Hexagon sheets and square like structures
6	$[^tBu_2Sn(Se\text{-}C_5H_4N)_2]$ (**5**)	3	3	_	25	1.50	Hex/$SnSe_2$/23-0602	Rectangular sheets

Table S2. Lattice parameters of tin selenide nanostructures calculated by using eq 1.

Exp. No.	Precursor	Amount of OA taken in the flask (ml)	Amount of OA/CH_2Cl_2 taken with the precursor (ml)		Reaction duration (minutes)	JCPDS No.	Lattice parameter Calculated by eq. 1 Reported in JCPDS)		
			OA	CH_2Cl_2			a	b	c
1	$[Me_2Sn(Se\text{-}C_5H_4N)_2]$ (**1**)	3	_	2	15	81-0013	5.905(8) (5.928)	6.020(6) (5.970)	12.406(9) (12.28)
2	$[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**)	3	_	2	25	23-0602	3.810 (3.810)	3.810 (3.810)	6.133(1) (6.140)
3	$[Et_2Sn(Se\text{-}C_5H_4N)_2]$ (**3**)	3	3	_	25	72-1460	4.424(10) (4.460)	4.149(8) (4.190)	11.491(11) (11.570)
4	$[Et_2Sn\{Se\text{-}C_5H_3(3\text{-}Me\}N)_2]$ (**4**)	3	_	2	25	23-0602	3.810 (3.810)	3.810 (3.810)	6.137(4) (6.140)
5	$[Et_2Sn\{Se\text{-}C_5H_3(3\text{-}Me\}N)_2]$ (**4**)	3	3	_	25	23-0602	3.810 (3.810)	3.810 (3.810)	6.141(7) (6.140)
6	$[^tBu_2Sn(Se\text{-}C_5H_4N)_2]$ (**5**)	3	3	_	25	23-0602	3.810 (3.810)	3.810 (3.810)	6.131(9) (6.140)

Table S3. Experimental details and results of tin selenide thin films deposited by AACVD of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (**5**).

Exp. No.	Substrate on which thin film was deposited by AACVD	Substrate temperature (^{o}C)	Reaction duration (in hour)	JCPDS No.	Lattice parameter calculated by eq 1. (Reported in JCPDS File)		
					a	b	c
1	Si	490	3	72-1460	4.445(10) (4.460)	4.218(3) (4.190)	11.584(6) (11.570)
2	Glass	490	3	72-1460	4.528(8) (4.460)	4.173(5) (4.190)	11.483(5) (11.570)
3	Si	530	3	72-1460	4.513(25) (4.460)	4.194(13) (4.190)	11.509(19) (11.570)
4	glass	530	3	72-1460	4.520(7) (4.460)	4.177(10) (4.190)	11.523(8) (11.570)

Crystal Information File of $[Me_2Sn(Se\text{-}C_5H_4N)_2]$ (1)

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 'H'  'H'   0.0000   0.0000
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 'N'  'N'   0.0061   0.0033
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
 'Se'  'Se'  -0.0929   2.2259
 'International Tables Vol C Tables 4.2.6.8 and 6.1.1.4'
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 F^2^ > 2sigma(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
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 factors based on ALL data will be even larger.
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H2 H 0.3629 1.9121 1.2700 0.068 Uiso 1 1 calc R . .
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H3 H 0.3768 2.0692 1.4375 0.089 Uiso 1 1 calc R . .
C4 C 0.4198(8) 1.946(3) 1.519(3) 0.083(8) Uani 1 1 d . . .
H4 H 0.4291 2.0106 1.5769 0.099 Uiso 1 1 calc R . .
C5 C 0.4368(6) 1.812(2) 1.523(2) 0.061(6) Uani 1 1 d . . .
H5 H 0.4552 1.7866 1.5882 0.074 Uiso 1 1 calc R . .
N1 N 0.4282(6) 1.7159(18) 1.4368(15) 0.057(5) Uani 1 1 d . . .
C6 C 0.4896(7) 1.157(2) 1.3130(16) 0.044(5) Uani 1 1 d . . .
C7 C 0.5033(8) 1.030(2) 1.2936(18) 0.051(5) Uani 1 1 d . . .
H7 H 0.4916 0.9790 1.2285 0.061 Uiso 1 1 calc R . .
C8 C 0.5356(7) 0.971(2) 1.371(3) 0.086(7) Uani 1 1 d . . .
H8 H 0.5471 0.8817 1.3583 0.103 Uiso 1 1 calc R . .
C9 C 0.5502(7) 1.054(3) 1.471(2) 0.075(7) Uani 1 1 d . . .
H9 H 0.5727 1.0228 1.5251 0.090 Uiso 1 1 calc R . .
C10 C 0.5296(7) 1.181(3) 1.485(2) 0.073(7) Uani 1 1 d . . .
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N2 N 0.4998(6) 1.2318(18) 1.4077(17) 0.063(5) Uani 1 1 d . . .
C11 C 0.4108(6) 1.400(2) 1.5185(17) 0.066(6) Uani 1 1 d . . .
H11A H 0.4071 1.3011 1.5193 0.099 Uiso 1 1 calc R . .
H11B H 0.3811 1.4437 1.5193 0.099 Uiso 1 1 calc R . .
H11C H 0.4279 1.4285 1.5889 0.099 Uiso 1 1 calc R . .
C12 C 0.5126(6) 1.556(2) 1.336(3) 0.091(8) Uani 1 1 d . . .
H12A H 0.5238 1.5861 1.4139 0.137 Uiso 1 1 calc R . .
H12B H 0.5098 1.6349 1.2830 0.137 Uiso 1 1 calc R . .
H12C H 0.5338 1.4906 1.3015 0.137 Uiso 1 1 calc R . .
C13 C 0.2736(7) 0.882(2) 1.946(2) 0.076(3) Uani 1 1 d . . .
C14 C 0.2597(7) 0.748(2) 1.974(2) 0.076(3) Uani 1 1 d . . .
H14 H 0.2723 0.7018 2.0400 0.091 Uiso 1 1 calc R . .
C15 C 0.2272(6) 0.684(2) 1.903(2) 0.076(3) Uani 1 1 d . . .
H15 H 0.2186 0.5933 1.9206 0.091 Uiso 1 1 calc R . .
C16 C 0.2076(7) 0.747(3) 1.809(2) 0.076(3) Uani 1 1 d . . .
H16 H 0.1843 0.7032 1.7659 0.091 Uiso 1 1 calc R . .
C17 C 0.2216(9) 0.875(3) 1.778(2) 0.090(8) Uani 1 1 d . . .
H17 H 0.2094 0.9163 1.7085 0.109 Uiso 1 1 calc R . .
N3 N 0.2529(6) 0.9444(17) 1.8440(19) 0.072(5) Uani 1 1 d . . .
C18 C 0.3497(7) 1.487(2) 1.865(3) 0.076(3) Uani 1 1 d . . .
C19 C 0.3721(7) 1.616(2) 1.869(2) 0.073(6) Uani 1 1 d . . .
H19 H 0.3921 1.6367 1.9326 0.087 Uiso 1 1 calc R . .
C20 C 0.3639(8) 1.713(2) 1.776(2) 0.070(7) Uani 1 1 d . . .
H20 H 0.3780 1.7998 1.7770 0.084 Uiso 1 1 calc R . .
C21 C 0.3333(8) 1.675(3) 1.682(2) 0.079(8) Uani 1 1 d . . .
H21 H 0.3272 1.7365 1.6186 0.095 Uiso 1 1 calc R . .
C22 C 0.3141(7) 1.555(3) 1.6842(19) 0.071(8) Uani 1 1 d . . .
H22 H 0.2937 1.5329 1.6219 0.085 Uiso 1 1 calc R . .
N4 N 0.3215(5) 1.4594(18) 1.7710(15) 0.054(4) Uani 1 1 d . . .
C23 C 0.2342(6) 1.268(2) 1.884(2) 0.078(8) Uani 1 1 d . . .
H23A H 0.2275 1.3256 1.8153 0.118 Uiso 1 1 calc R . .
H23B H 0.2315 1.3220 1.9574 0.118 Uiso 1 1 calc R . .
H23C H 0.2129 1.1921 1.8870 0.118 Uiso 1 1 calc R . .
C24 C 0.3363(7) 1.130(2) 1.705(2) 0.093(8) Uani 1 1 d . . .
H24A H 0.3149 1.0822 1.6538 0.140 Uiso 1 1 calc R . .
H24B H 0.3617 1.0695 1.7236 0.140 Uiso 1 1 calc R . .
H24C H 0.3475 1.2113 1.6646 0.140 Uiso 1 1 calc R . .
Se1 Se 0.38945(7) 1.6087(2) 1.2296(2) 0.0661(7) Uani 1 1 d . . .
```

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Se2 Se 0.44429(7) 1.2472(2) 1.21052(19) 0.0664(7) Uani 1 1 d . . .
Se3 Se 0.31632(8) 0.9919(3) 2.0269(2) 0.0736(8) Uani 1 1 d . . .
Se4 Se 0.35976(8) 1.3498(3) 1.9829(2) 0.0760(8) Uani 1 1 d . . .
Sn1 Sn 0.44709(4) 1.46049(14) 1.35786(13) 0.0560(4) Uani 1 1 d . . .
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C3 0.089(19) 0.024(13) 0.108(19) -0.011(13) 0.008(16) 0.008(13)
C4 0.072(18) 0.08(2) 0.10(2) 0.007(17) -0.006(16) 0.040(15)
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N1 0.063(11) 0.057(13) 0.052(11) -0.014(9) -0.008(10) 0.018(10)
C6 0.068(15) 0.032(12) 0.031(11) -0.005(10) -0.009(10) -0.013(12)
C7 0.059(14) 0.049(15) 0.043(12) -0.006(11) 0.003(11) -0.002(13)
C8 0.054(14) 0.071(16) 0.13(2) -0.01(2) 0.00(2) 0.001(13)
C9 0.042(14) 0.11(2) 0.077(17) 0.028(17) 0.001(14) 0.004(16)
C10 0.053(14) 0.09(2) 0.080(17) -0.021(17) 0.005(14) -0.006(15)
N2 0.058(11) 0.057(13) 0.075(13) 0.008(11) -0.032(11) 0.012(10)
C11 0.061(13) 0.081(17) 0.056(13) 0.011(12) 0.014(12) 0.003(12)
C12 0.065(14) 0.069(16) 0.14(2) 0.005(17) 0.012(17) 0.010(13)
C13 0.063(7) 0.061(8) 0.104(8) -0.016 -0.043 -0.002
C14 0.063(7) 0.061(8) 0.104(8) -0.016 -0.043 -0.002
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C16 0.063(7) 0.061(8) 0.104(8) -0.016 -0.043 -0.002
C17 0.13(2) 0.077(19) 0.063(16) -0.006(15) -0.040(16) 0.017(18)
N3 0.063(11) 0.074(13) 0.081(14) -0.039(12) -0.002(12) 0.002(10)
C18 0.063(7) 0.061(8) 0.104(8) -0.016 -0.043 -0.002
C19 0.067(14) 0.092(18) 0.059(14) -0.004(17) 0.018(14) -0.007(13)
C20 0.075(17) 0.061(17) 0.074(16) 0.007(14) 0.011(14) -0.009(14)
C21 0.085(18) 0.067(18) 0.085(19) 0.015(15) -0.055(16) -0.012(16)
C22 0.069(16) 0.11(2) 0.037(13) 0.041(14) -0.023(11) -0.027(16)
N4 0.038(10) 0.060(12) 0.063(11) -0.011(10) -0.010(9) -0.007(9)
C23 0.055(13) 0.076(17) 0.10(2) 0.015(16) 0.030(15) 0.006(11)
C24 0.086(16) 0.10(2) 0.10(2) -0.011(17) 0.023(16) 0.032(16)
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Se2 0.0740(15) 0.0677(16) 0.0573(14) -0.0043(13) -0.0094(14) 0.0135(13)
Se3 0.0730(16) 0.0781(19) 0.0697(16) 0.0110(14) -0.0109(14) -0.0028(14)
Se4 0.0806(17) 0.0809(18) 0.0666(16) 0.0121(13) -0.0236(14) -0.0150(14)
Sn1 0.0542(8) 0.0595(9) 0.0545(8) 0.0000(9) 0.0034(10) -0.0019(7)
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 and torsion angles; correlations between esds in cell parameters are only
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 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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C5 H5 0.9300 . ?
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C6 C7 1.31(3) . ?
C6 Se2 1.94(2) . ?
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C7 H7 0.9300 . ?
C8 C9 1.43(3) . ?
C8 H8 0.9300 . ?
C9 C10 1.37(3) . ?
C9 H9 0.9300 . ?
C10 N2 1.31(2) . ?
C10 H10 0.9300 . ?
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C11 H11B 0.9600 . ?
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C12 H12C 0.9600 . ?
C13 C14 1.39(3) . ?
C13 N3 1.41(3) . ?
C13 Se3 1.86(2) . ?
C14 C15 1.37(2) . ?
C14 H14 0.9300 . ?
C15 C16 1.32(3) . ?
C15 H15 0.9300 . ?
C16 C17 1.34(3) . ?
C16 H16 0.9300 . ?
C17 N3 1.34(3) . ?
C17 H17 0.9300 . ?
C18 N4 1.35(3) . ?
C18 C19 1.41(2) . ?
C18 Se4 1.87(3) . ?
C19 C20 1.41(3) . ?
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C20 H20 0.9300 . ?
C21 C22 1.28(3) . ?
C21 H21 0.9300 . ?
C22 N4 1.34(2) . ?
C22 H22 0.9300 . ?
C23 Sn2 2.149(16) . ?
C23 H23A 0.9600 . ?
C23 H23B 0.9600 . ?
C23 H23C 0.9600 . ?
C24 Sn2 2.13(2) . ?
C24 H24A 0.9600 . ?
C24 H24B 0.9600 . ?
C24 H24C 0.9600 . ?
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Se2 Sn1 2.618(3) . ?
Se3 Sn2 2.595(3) . ?
Se4 Sn2 2.585(3) . ?

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C3 C2 H2 121.5 . . ?
C4 C3 C2 119(2) . . ?
C4 C3 H3 120.4 . . ?
C2 C3 H3 120.4 . . ?
C3 C4 C5 120(3) . . ?
C3 C4 H4 119.9 . . ?
C5 C4 H4 119.9 . . ?
N1 C5 C4 124(2) . . ?
N1 C5 H5 118.2 . . ?
C4 C5 H5 118.2 . . ?
C1 N1 C5 118.1(18) . . ?
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N2 C6 Se2 111.8(16) . . ?
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H11A C11 H11C 109.5 . . ?
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Sn1 C12 H12B 109.5 . . ?
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H24B C24 H24C 109.5 . . ?
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C18 Se4 Sn2 89.3(7) . . ?
C12 Sn1 C11 130.7(9) . . ?
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Crystal Information File of [$^{t}Bu_2Sn(Se\text{-}C_5H_4N)_2$] (5)

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 'Se'  'Se'  -0.0929   2.2259
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 'x+1/2, y+1/2, z'
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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 on F, with F set to zero for negative F^2^. The threshold expression of
 F^2^ > 2sigma(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-
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N1 N 0.6795(7) 0.1900(15) 0.2318(11) 0.047(3) Uani 1 1 d . . .
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C1 C 0.7074(8) 0.016(2) 0.2723(14) 0.044(3) Uani 1 1 d . . .
C2 C 0.7966(8) -0.024(2) 0.3876(13) 0.056(3) Uani 1 1 d . . .
H2 H 0.8147 -0.1447 0.4162 0.067 Uiso 1 1 calc R . .
C7 C 0.5047(9) 0.165(2) -0.2927(11) 0.070(4) Uani 1 1 d . . .
H7A H 0.5363 0.2094 -0.3476 0.105 Uiso 1 1 calc R . .
H7B H 0.4419 0.2208 -0.3281 0.105 Uiso 1 1 calc R . .
H7C H 0.4976 0.0348 -0.3027 0.105 Uiso 1 1 calc R . .
C4 C 0.8315(10) 0.296(2) 0.4199(15) 0.073(5) Uani 1 1 d . . .
H4 H 0.8726 0.3923 0.4689 0.088 Uiso 1 1 calc R . .
C3 C 0.8571(9) 0.118(3) 0.4579(14) 0.072(5) Uani 1 1 d . . .
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H9B H 0.6624 0.0081 -0.0894 0.104 Uiso 1 1 calc R . .
H9C H 0.7060 0.1787 0.0110 0.104 Uiso 1 1 calc R . .
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N1 0.050(6) 0.040(6) 0.046(6) -0.012(5) 0.017(5) -0.001(5)
C1 0.033(6) 0.057(8) 0.039(7) -0.003(6) 0.014(5) 0.010(5)
C2 0.045(6) 0.068(9) 0.048(8) 0.015(7) 0.016(6) 0.008(7)
C7 0.084(9) 0.092(11) 0.045(7) -0.012(7) 0.040(7) -0.029(8)
C4 0.079(10) 0.078(12) 0.058(9) -0.023(9) 0.028(8) -0.029(9)
C3 0.046(6) 0.093(14) 0.066(8) -0.024(11) 0.016(6) -0.011(9)
C6 0.029(5) 0.057(7) 0.037(6) 0.001(5) 0.015(4) -0.008(5)
C9 0.051(6) 0.091(13) 0.089(9) 0.007(8) 0.051(7) 0.008(7)
C5 0.082(8) 0.053(7) 0.064(8) -0.011(8) 0.038(7) -0.019(8)
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N1 C1 1.344(14) . ?
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C9 C6 Sn1 109.5(8) . . ?
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H9B C9 H9C 109.5 . . ?
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C5 N1 C1 C2 1(2) . . . . ?
C5 N1 C1 Se1 -179.7(8) . . . . ?
Sn1 Se1 C1 N1 2.0(12) . . . . ?
Sn1 Se1 C1 C2 -178.9(11) . . . . ?
N1 C1 C2 C3 -1(2) . . . . ?
Se1 C1 C2 C3 179.5(10) . . . . ?
C1 C2 C3 C4 1(2) . . . . ?
```

```
C5 C4 C3 C2 -1(2) . . . . ?
C6 Sn1 C6 C9 125.5(9) 2_655 . . . ?
Se1 Sn1 C6 C9 -101.1(8) 2_655 . . . ?
Se1 Sn1 C6 C9 -6.8(9) . . . . ?
C6 Sn1 C6 C8 6.0(8) 2_655 . . . ?
Se1 Sn1 C6 C8 139.4(9) 2_655 . . . ?
Se1 Sn1 C6 C8 -126.3(9) . . . . ?
C6 Sn1 C6 C7 -115.9(9) 2_655 . . . ?
Se1 Sn1 C6 C7 17.5(9) 2_655 . . . ?
Se1 Sn1 C6 C7 111.8(9) . . . . ?
C1 N1 C5 C4 -1(2) . . . . ?
C3 C4 C5 N1 1(2) . . . . ?

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Crystal Information File of [$Me_2Sn(Se\text{-}C_5H_3(Me\text{-}3)N)Cl$] (7)

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 'Sn'  'Sn'  -0.6537   1.4246
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_symmetry_Int_Tables_number          14

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 '-x, -y, -z'
 'x, -y-1/2, z-1/2'

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 Refinement of F^2^ against ALL reflections.  The weighted R-factor wR and
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 F^2^ > 2sigma(F^2^) is used only for calculating R-factors(gt) etc. and is
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 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.
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Se1 Se 0.40581(11) 0.14351(12) 1.03607(9) 0.0639(4) Uani 1 1 d . . .
Cl1 Cl 0.1570(3) -0.0925(3) 0.8331(3) 0.1002(12) Uani 1 1 d . . .
N1 N 0.2475(9) 0.3680(9) 0.9567(7) 0.058(2) Uani 1 1 d . . .
C1 C 0.3696(11) 0.3327(11) 1.0409(9) 0.055(3) Uani 1 1 d . . .
C7 C -0.0208(10) 0.1644(11) 0.9051(8) 0.076(4) Uani 1 1 d . . .
H7A H -0.0833 0.2316 0.8584 0.114 Uiso 1 1 calc R . .
H7B H 0.0047 0.1888 0.9814 0.114 Uiso 1 1 calc R . .
H7C H -0.0686 0.0787 0.8914 0.114 Uiso 1 1 calc R . .
C5 C 0.2082(14) 0.4967(14) 0.9504(11) 0.085(4) Uani 1 1 d . . .
H5 H 0.1228 0.5218 0.8941 0.101 Uiso 1 1 calc R . .
C3 C 0.4137(14) 0.5557(13) 1.1090(10) 0.078(4) Uani 1 1 d . . .
H3 H 0.4681 0.6199 1.1594 0.094 Uiso 1 1 calc R . .
C2 C 0.4584(12) 0.4229(11) 1.1202(10) 0.061(3) Uani 1 1 d . . .
C4 C 0.2866(16) 0.5946(13) 1.0223(13) 0.091(4) Uani 1 1 d . . .
H4 H 0.2566 0.6840 1.0140 0.109 Uiso 1 1 calc R . .
C8 C 0.1828(10) 0.2155(13) 0.7207(8) 0.084(4) Uani 1 1 d . . .
H8A H 0.1686 0.1399 0.6717 0.126 Uiso 1 1 calc R . .
H8B H 0.2758 0.2531 0.7369 0.126 Uiso 1 1 calc R . .
H8C H 0.1115 0.2827 0.6860 0.126 Uiso 1 1 calc R . .
C6 C 0.5886(11) 0.3765(11) 1.2128(8) 0.075(4) Uani 1 1 d . . .
H6A H 0.6548 0.4500 1.2383 0.113 Uiso 1 1 calc R . .
H6B H 0.6318 0.3044 1.1878 0.113 Uiso 1 1 calc R . .
H6C H 0.5635 0.3451 1.2725 0.113 Uiso 1 1 calc R . .

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Se1 0.0587(7) 0.0508(7) 0.0681(8) -0.0012(7) 0.0086(6) 0.0088(7)
Cl1 0.097(3) 0.071(2) 0.116(3) -0.025(2) 0.022(2) -0.005(2)
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N1 0.068(6) 0.045(6) 0.059(6) 0.004(5) 0.024(5) 0.014(5)
C1 0.062(7) 0.054(8) 0.056(7) 0.010(6) 0.032(6) 0.008(6)
C7 0.056(7) 0.112(10) 0.067(7) 0.000(8) 0.032(6) -0.011(7)
C5 0.114(12) 0.072(10) 0.079(10) 0.009(9) 0.050(9) 0.023(9)
C3 0.102(10) 0.062(10) 0.077(9) -0.006(8) 0.042(8) 0.000(8)
C2 0.069(8) 0.037(7) 0.080(8) -0.016(7) 0.031(7) -0.007(6)
C4 0.121(13) 0.039(8) 0.121(12) -0.001(9) 0.056(10) 0.018(8)
C8 0.073(8) 0.132(12) 0.058(7) -0.004(8) 0.037(6) -0.004(8)
C6 0.069(8) 0.078(9) 0.067(8) -0.006(7) 0.013(6) -0.019(7)

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 All esds (except the esd in the dihedral angle between two l.s. planes)
 are estimated using the full covariance matrix.  The cell esds are taken
 into account individually in the estimation of esds in distances, angles
 and torsion angles; correlations between esds in cell parameters are only
 used when they are defined by crystal symmetry.  An approximate (isotropic)
 treatment of cell esds is used for estimating esds involving l.s. planes.
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Sn1 C7 2.120(9) . ?
Sn1 N1 2.425(9) . ?
Sn1 Cl1 2.457(3) . ?
Sn1 Se1 2.5667(14) . ?
Se1 C1 1.917(11) . ?
N1 C5 1.330(13) . ?
N1 C1 1.350(12) . ?
C1 C2 1.404(13) . ?
C7 H7A 0.9600 . ?
C7 H7B 0.9600 . ?
C7 H7C 0.9600 . ?
C5 C4 1.374(15) . ?
C5 H5 0.9300 . ?
C3 C2 1.382(14) . ?
C3 C4 1.405(15) . ?
C3 H3 0.9300 . ?
C2 C6 1.482(13) . ?
C4 H4 0.9300 . ?
C8 H8A 0.9600 . ?
C8 H8B 0.9600 . ?
C8 H8C 0.9600 . ?
C6 H6A 0.9600 . ?
C6 H6B 0.9600 . ?
C6 H6C 0.9600 . ?

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C8 Sn1 N1 91.7(4) . . ?
C7 Sn1 N1 90.9(4) . . ?
C8 Sn1 Cl1 97.3(4) . . ?
C7 Sn1 Cl1 97.7(3) . . ?
N1 Sn1 Cl1 160.7(2) . . ?
C8 Sn1 Se1 113.8(3) . . ?
C7 Sn1 Se1 117.0(3) . . ?
N1 Sn1 Se1 65.6(2) . . ?
Cl1 Sn1 Se1 95.12(9) . . ?
C1 Se1 Sn1 82.4(3) . . ?
C5 N1 C1 117.3(11) . . ?
C5 N1 Sn1 141.4(9) . . ?
C1 N1 Sn1 101.1(7) . . ?
N1 C1 C2 124.4(10) . . ?
N1 C1 Se1 110.8(8) . . ?
C2 C1 Se1 124.8(8) . . ?
Sn1 C7 H7A 109.5 . . ?
Sn1 C7 H7B 109.5 . . ?
H7A C7 H7B 109.5 . . ?
Sn1 C7 H7C 109.5 . . ?
H7A C7 H7C 109.5 . . ?
H7B C7 H7C 109.5 . . ?
N1 C5 C4 123.7(12) . . ?
N1 C5 H5 118.2 . . ?
C4 C5 H5 118.2 . . ?
C2 C3 C4 120.6(12) . . ?
C2 C3 H3 119.7 . . ?
C4 C3 H3 119.7 . . ?
C3 C2 C1 115.9(11) . . ?
C3 C2 C6 122.4(11) . . ?
C1 C2 C6 121.6(10) . . ?
C5 C4 C3 118.0(12) . . ?
C5 C4 H4 121.0 . . ?
C3 C4 H4 121.0 . . ?
Sn1 C8 H8A 109.5 . . ?
Sn1 C8 H8B 109.5 . . ?
H8A C8 H8B 109.5 . . ?
Sn1 C8 H8C 109.5 . . ?
H8A C8 H8C 109.5 . . ?
H8B C8 H8C 109.5 . . ?
C2 C6 H6A 109.5 . . ?
C2 C6 H6B 109.5 . . ?
H6A C6 H6B 109.5 . . ?
C2 C6 H6C 109.5 . . ?
H6A C6 H6C 109.5 . . ?
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C7 Sn1 Se1 C1 -76.5(4) . . . . ?
N1 Sn1 Se1 C1 1.3(3) . . . . ?
Cl1 Sn1 Se1 C1 -177.8(3) . . . . ?
C8 Sn1 N1 C5 67.1(12) . . . . ?
C7 Sn1 N1 C5 -57.9(12) . . . . ?
Cl1 Sn1 N1 C5 -174.8(9) . . . . ?
Se1 Sn1 N1 C5 -177.4(12) . . . . ?
C8 Sn1 N1 C1 -117.3(6) . . . . ?
C7 Sn1 N1 C1 117.6(6) . . . . ?
Cl1 Sn1 N1 C1 0.8(10) . . . . ?
Se1 Sn1 N1 C1 -1.9(5) . . . . ?
C5 N1 C1 C2 -1.4(15) . . . . ?
Sn1 N1 C1 C2 -178.2(8) . . . . ?
C5 N1 C1 Se1 179.3(8) . . . . ?
Sn1 N1 C1 Se1 2.5(6) . . . . ?
Sn1 Se1 C1 N1 -2.3(6) . . . . ?
Sn1 Se1 C1 C2 178.4(9) . . . . ?
C1 N1 C5 C4 1.9(17) . . . . ?
Sn1 N1 C5 C4 177.0(9) . . . . ?
C4 C3 C2 C1 -0.2(17) . . . . ?
C4 C3 C2 C6 -177.5(10) . . . . ?
N1 C1 C2 C3 0.6(16) . . . . ?
Se1 C1 C2 C3 179.8(8) . . . . ?
N1 C1 C2 C6 177.9(9) . . . . ?
Se1 C1 C2 C6 -2.9(14) . . . . ?
N1 C5 C4 C3 -1.7(19) . . . . ?
C2 C3 C4 C5 0.8(18) . . . . ?

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_diffrn_measured_fraction_theta_full   0.998
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_refine_diff_density_rms    0.148
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