Electronic Supplementary Information for *Dalton Transactions*

Supplementary material

2-Pyridyl selenolates of antimony and bismuth: Synthesis, characterization, structures and their use as single source molecular precursor for the preparation of metal selenide nanostructures and thin films

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Figure Captions

Fig. S1 a) XRD pattern and b) EDAX spectrum of Sb_2Se_3 obtained by pyrolysis of [Sb{Se-C_5H_3(Me-3)N}$_3$] at 400 ^oC for 1 h.

Fig. S2 a) XRD pattern and b) EDAX spectrum of BiSe obtained by pyrolysis of [Bi{Se-C_5H_3(Me-3)N}$_3$] at 450 ^oC for 1 h.

Fig. S3 Absorption spectra of a) Sb_2Se_3 and b) Bi_2Se_3 nanoparticles obtained by the pyrolysis of [M{Se-C_5H_3(Me-3)N}$_3$] (M = Sb or Bi) in HDA at 200 and 230 ^oC, respectively for 25 min.

Fig. S4 XRD patterns of Sb_2Se_3 obtained by AACVD of [Sb{Se-C_5H_3(Me-3)N}$_3$] at a) 425,c) 450, d) 475, f) 500 ^oC for a deposition time of 1 h and b) 425, e) 475 for a deposition time of 2h.

Fig. S5 EDX spectra of Sb_2Se_3 films obtained by AACVD of [Sb{Se-C_5H_3(Me-3)N}$_3$] at a)425, b) 450 and c) 475 ^oC for 1 h.

Fig. S6 EDX spectra of Sb_2Se_3 films obtained by AACVD of [Sb{Se-C_5H_3(Me-3)N}$_3$] at a) 425 and b) 475 ^oC for 2 h.

Fig. S7 SEM images of Sb_2Se_3 films obtained by AACVD of [Sb{Se-C_5H_3(Me-3)N}$_3$] at a) 425, b) 450, c) 475 and d) 500 ^oC for 1 h.

Fig. S8 SEM images of Sb_2Se_3 films obtained by AACVD of [Sb{Se-C_5H_3(Me-3)N}$_3$] at a) 425 and b) 475 ^oC for 2 h.

Fig. S9 XRD patterns of bismuth selenide films obtained by AACVD of [Bi{Se-C_5H_3(Me-3)N}$_3$] at a) 350, b) 375, c) 400, d) 425 and e) 475 ^oC for 1 h.

Fig. S10 XRD patterns of bismuth selenide films obtained by AACVD of [Bi{Se-C_5H_3(Me-3)N}$_3$] at a) 375, b) 400 and c) 425 ^oC for 2 h.

Fig. S11 EDX spectra of bismuth selenide films obtained by AACVD of [Bi{SeC_5H_3(Me-3)N}$_3$] at a) 350, b) 375, c) 400, d) 425 and e) 475 ^oC for 1 h.

Fig. S12 SEM images of bismuth selenide films obtained by AACVD of [Bi{Se-C_5H_3(Me-3)N}$_3$] at a) 350, b) 375, c) 400, d) 425 and e) 475 ^oC for 1 h.

Fig. S13 a) SEM images of uniformly coated bismuth selenide films obtained by AACVD of [Bi{Se-C_5H_3(Me-3)N}$_3$] at 375 and b) 400 ^oC, respectively for 1 h.

Fig. S14 Packing diagram of [Sb{Se-C_5H_3(Me-3)N}$_3$].1.5H_2O (**2**).1.5H_2O.

Fig. S15 Packing diagram of [Bi{Se-C_5H_3(Me-3)N}$_3$].0.5H_2O (**4**).0.5H_2O.

Table S1**.** Experimental data of antimony selenide thin films.

Table S2**.** Experimental data of bismuth selenide thin films.

CIF for [Sb{Se-C_5H_3(Me-3)N}$_3$].1.5H_2O

CIF for [Bi{Se-C_5H_3(Me-3)N}$_3$].0.5H_2O

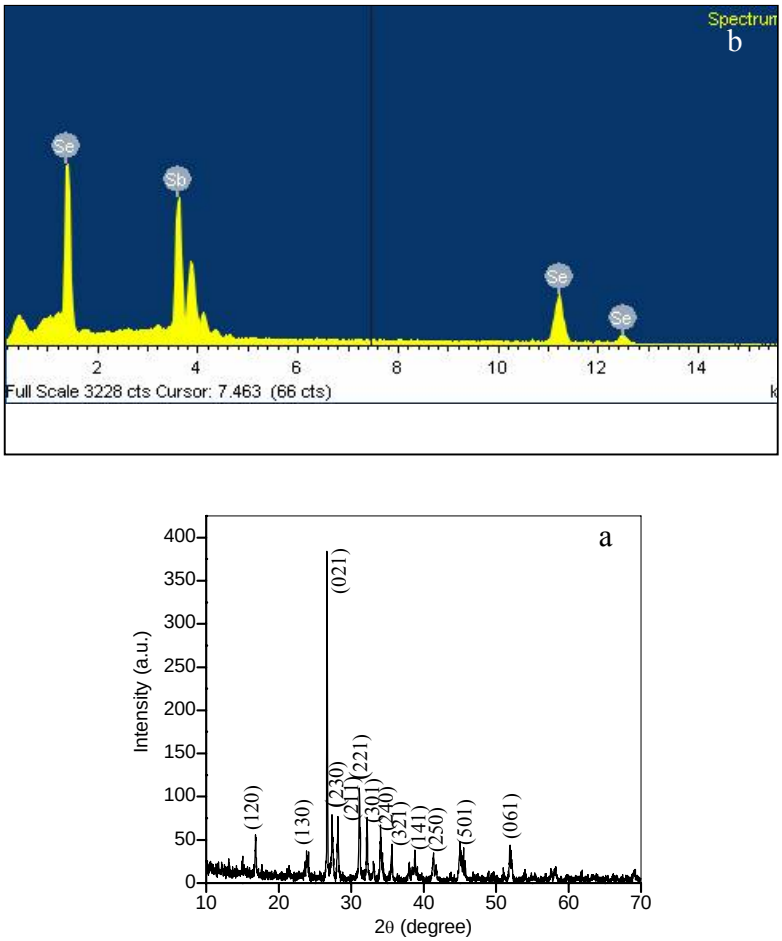


Fig. S1 a) XRD pattern and b) EDAX spectrum of Sb_2Se_3 obtained by pyrolysis of $[Sb\{Se\text{-}C_5H_3(Me\text{-}3)N\}_3]$ at 400 ^oC for 1 h.

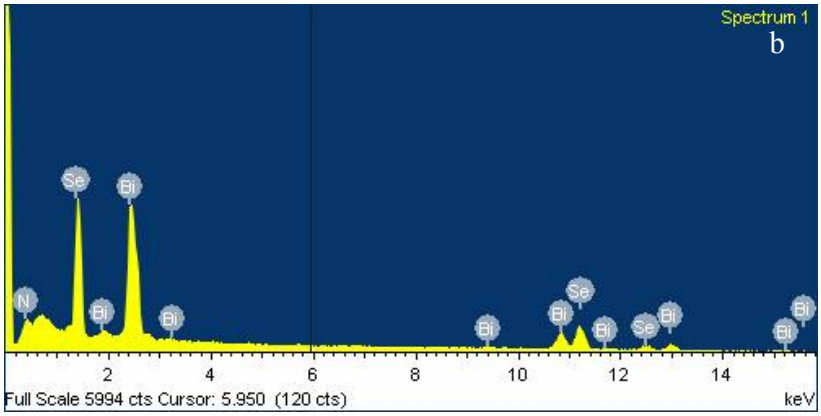
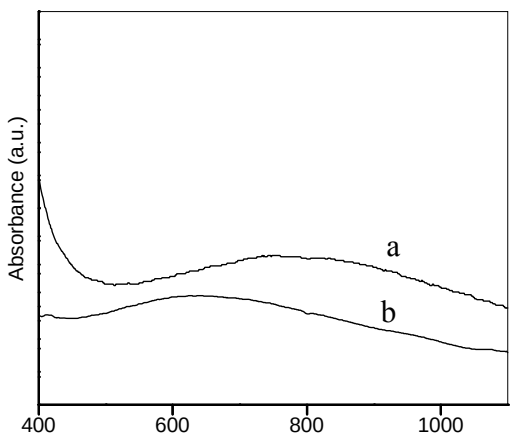
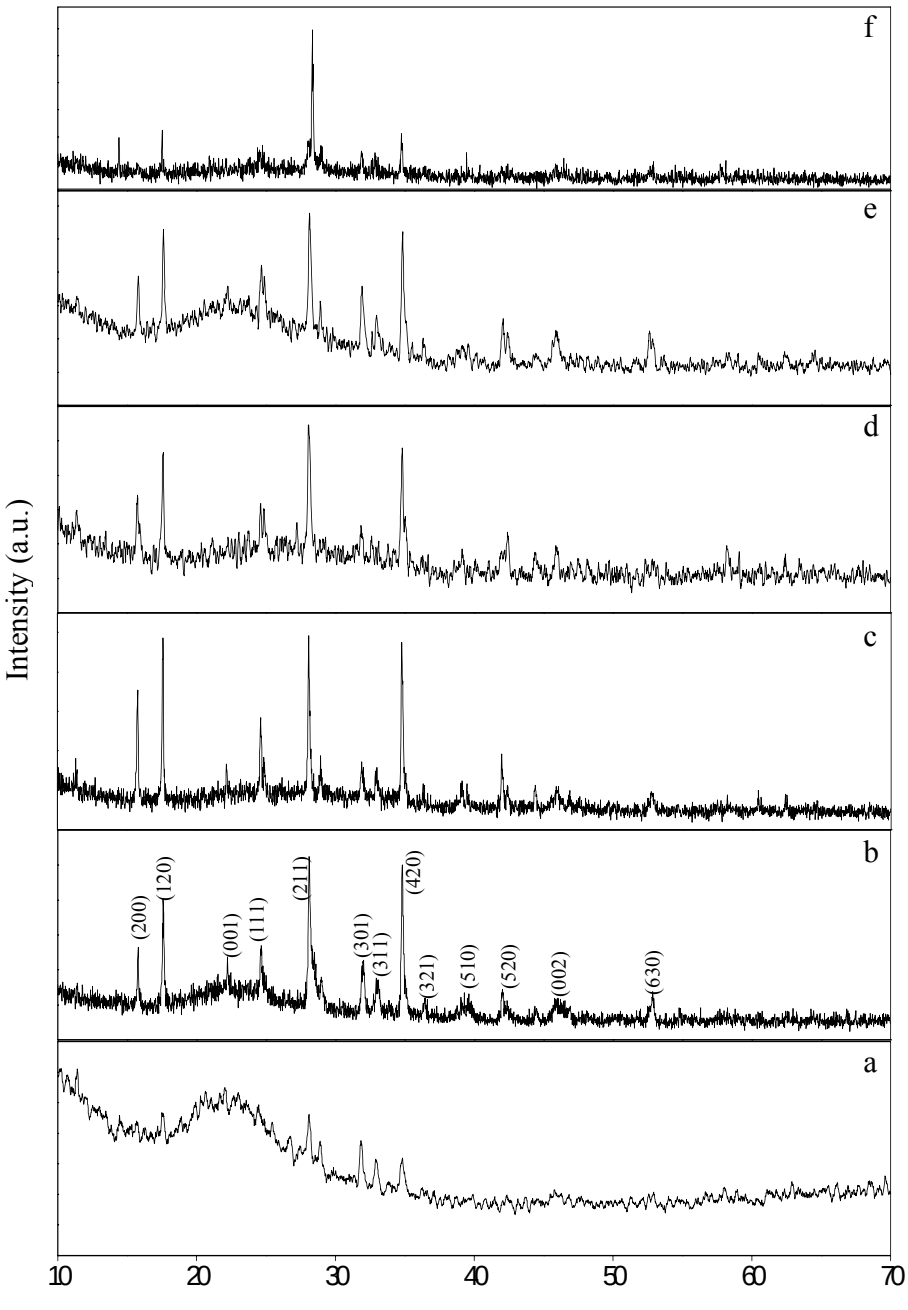


Fig. S2 a) XRD pattern and b) EDAX spectrum of BiSe obtained by pyrolysis of [Bi{Se-C_5H_3(Me-3)N}$_3$] at 450 ^oC for 1 h.





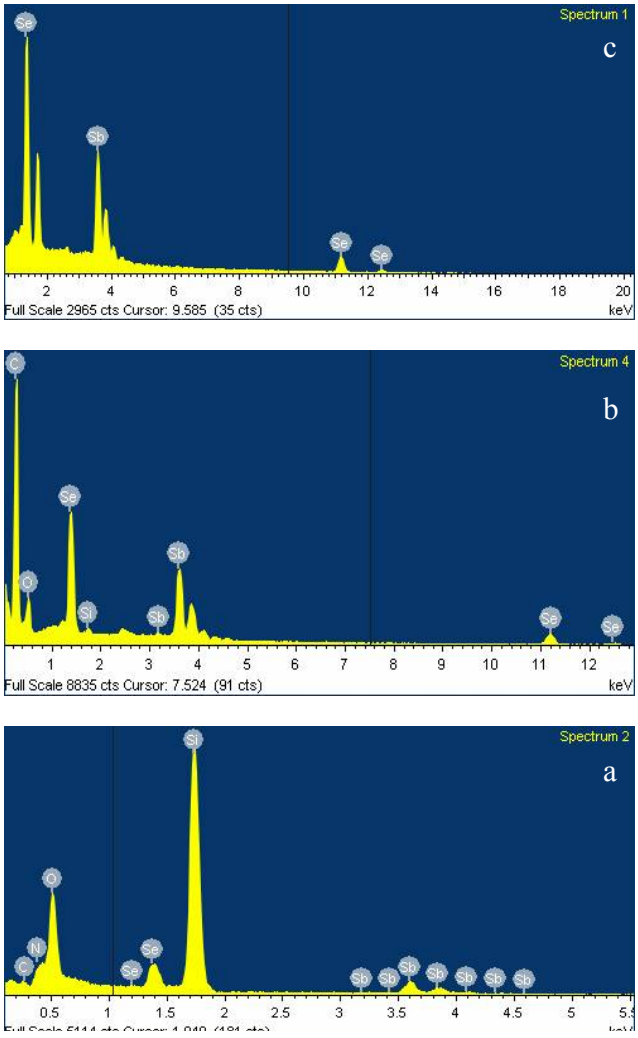


Fig. S5 EDAX spectra of Sb_2Se_3 films obtained by AACVD of $[Sb\{Se\text{-}C_5H_3(Me\text{-}3)N\}_3]$ at a) 425, b) 450 and c) 475 ^oC for 1 h.

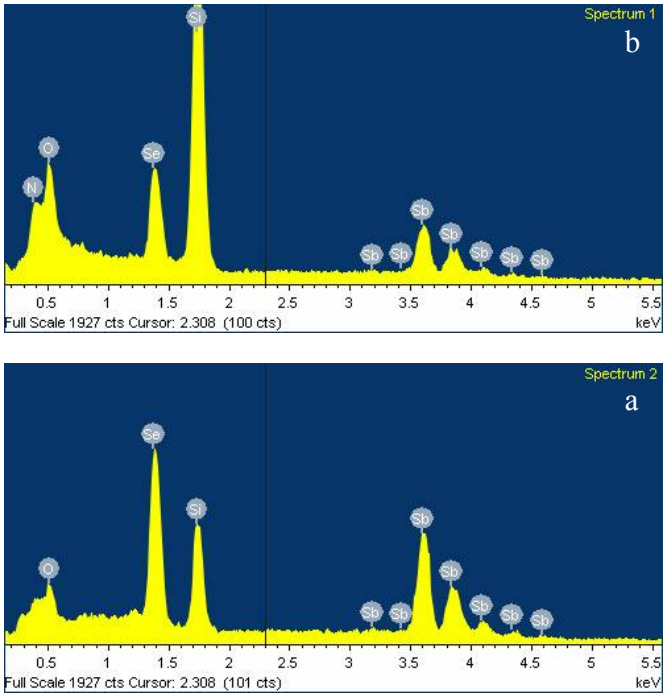


Fig. S6 EDAX spectra of Sb_2Se_3 films obtained by AACVD of $[Sb\{Se\text{-}C_5H_3(Me\text{-}3)N\}_3]$ at a) 425 and b) 475 ^oC for 2 h.

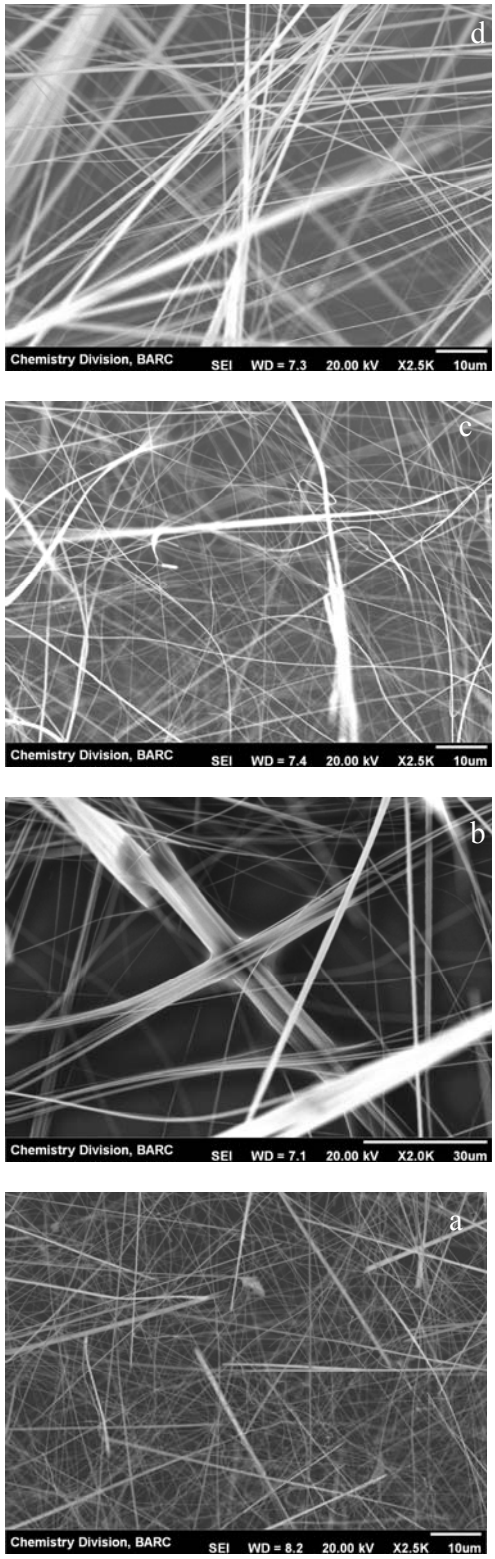


Fig. S7 SEM images of Sb_2Se_3 films obtained by AACVD of [Sb{Se-C_5H_3(Me-3)N}$_3$] at a) 425, b) 450, c) 475 and d) 500 ^oC for 1 h.

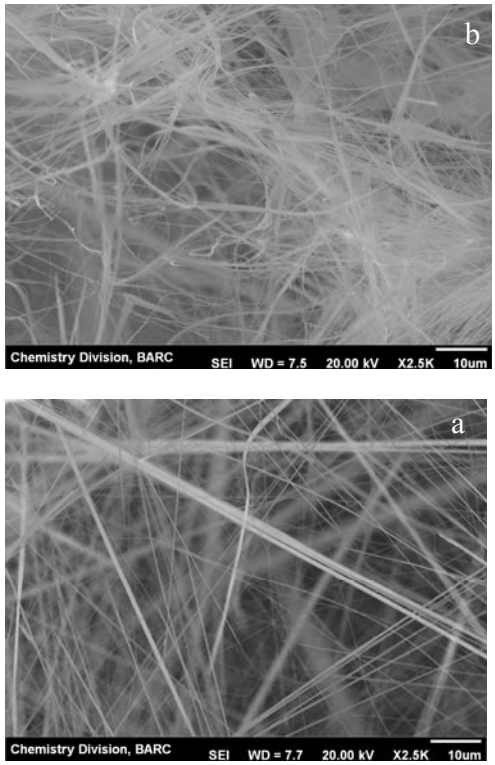


Fig. S8 SEM images of Sb_2Se_3 films obtained by AACVD of [Sb{Se-C_5H_3(Me-3)N}$_3$] at a) 425 and b) 475 ^oC for 2 h.

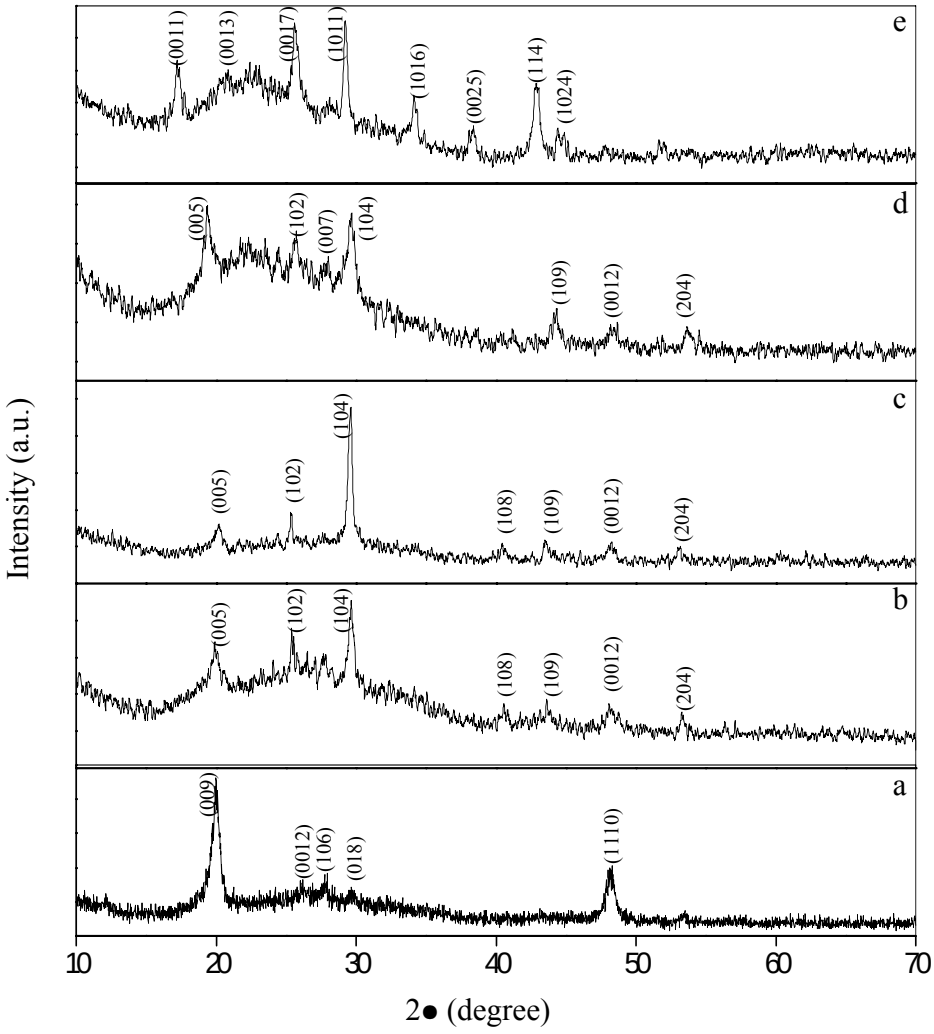


Fig. S9 XRD patterns of bismuth selenide films obtained by AACVD of [Bi{Se-C_5H_3(Me-3)N}$_3$] at a) 350, b) 375, c) 400, d) 425 and e) 475 ^oC for 1 h.

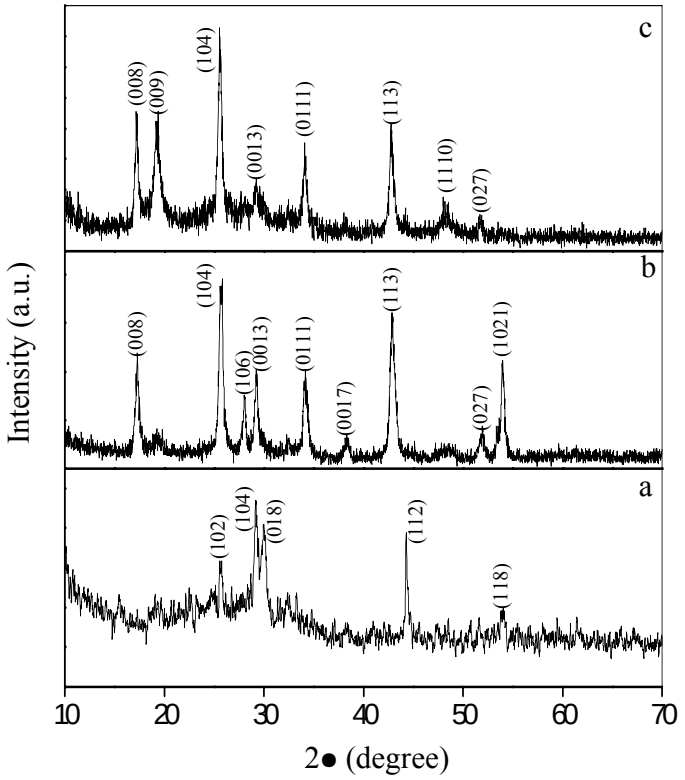


Fig. S10 XRD patterns of bismuth selenide films obtained by AACVD of [Bi{Se-C_5H_3(Me-3)N}$_3$] at a) 375, b) 400 and c) 425 ^oC for 2 h.

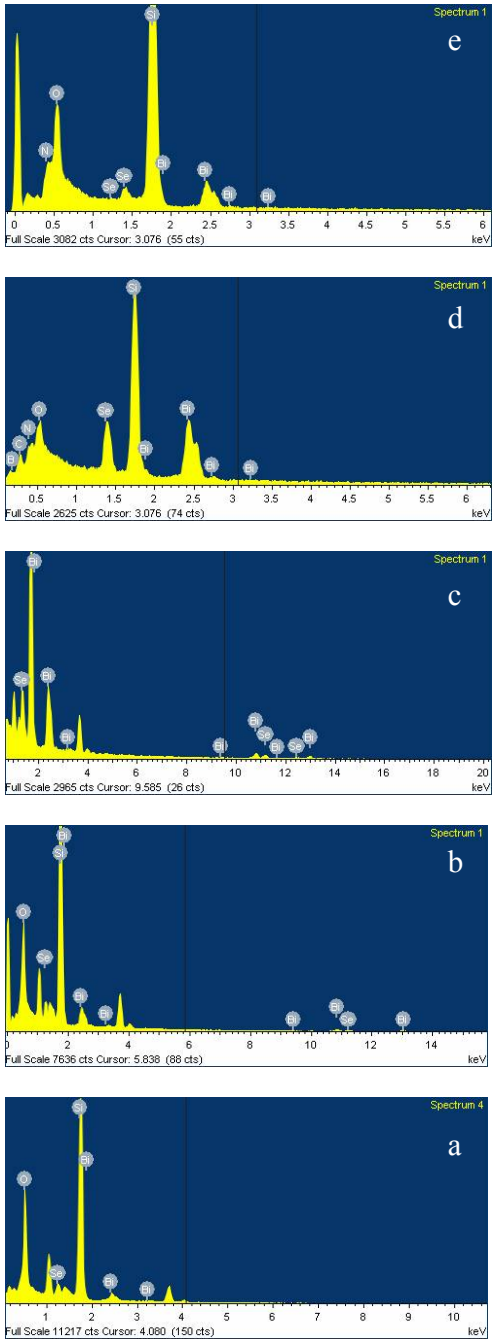


Fig. S11 EDAX spectra of bismuth selenide films obtained by AACVD of [Bi{Se-C_5H_3(Me-3)N}$_3$] at a) 350, b) 375, c) 400, d) 425 and e) 475 ^{o}C for 1 h.

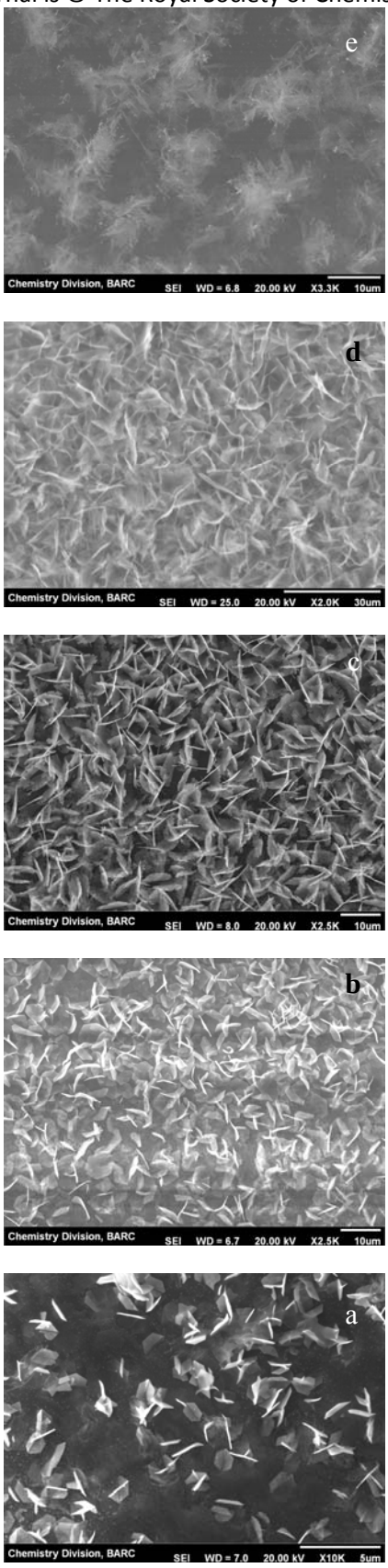


Fig. S12 SEM images of bismuth selenide films obtained by AACVD of [Bi{Se-C_5H_3(Me-3)N}$_3$] at a) 350, b) 375, c) 400, d) 425 and e) 475 ^oC for 1 h.

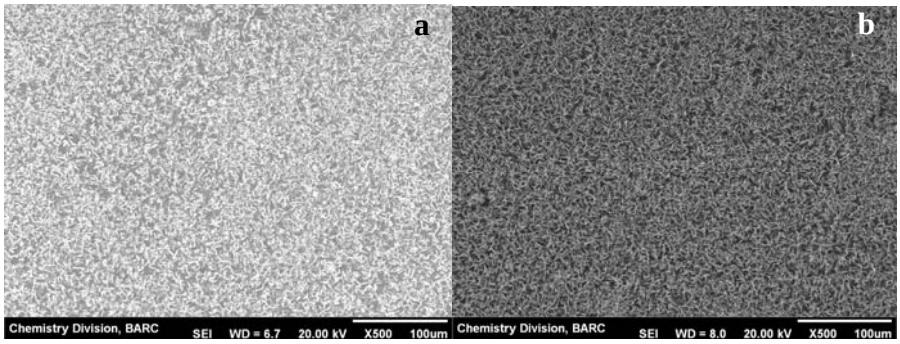


Fig. 13 a) SEM images of uniformly coated bismuth selenide films obtained by AACVD of [Bi{Se-C_5H_3(Me-3)N}$_3$] at 375 and b) 400 ^oC, respectively for 1 h.

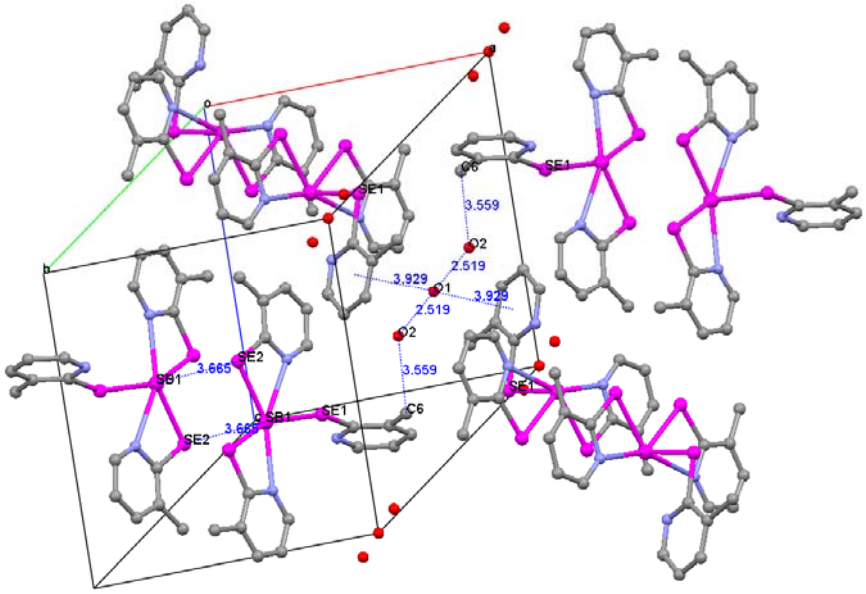


Fig. S14 Packing diagram of [Sb{Se-C_5H_3(Me-3)N}$_3$].1.5H_2O (**2**).1.5H_2O.

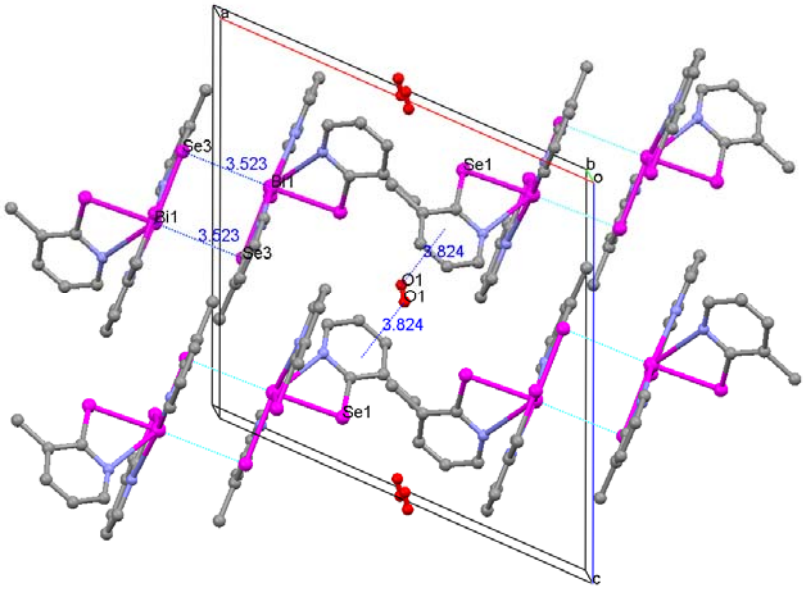


Fig. S15 Packing diagram of [Bi{Se-C_5H_3(Me-3)N}$_3$].0.5H_2O (**4**).0.5H_2O.

Discussion of crystal packing

The water molecules are trapped almost halfway between the planar pyridine rings attached to Se1 of different molecules in the cell. On careful examination of the packing diagrams, it is observed that O1 atom in **2** lies at distances of 3.930 Å and 3.942 Å on the axis joining centers of two parallel pyridine rings attached to Se1 of neighboring molecules. O2 is situated at a distance of 3.559 from C6 of neighboring molecule due to which the methyl group on C6 seems to be slightly disordered. Similarly, water molecule in **4** is also highly disordered; hence the packing diagram shows two sites with 0.5 occupancy. Each of O1 atoms with 0.5 occupancy lies at a distance of 3.824 Å, which is approximately half the inter-planar distance (7.832 Å) of the two pyridine rings attached to Se1 of neighboring parent molecules in the cell. Thus the high disorders in the water molecules in **2** and **4** may be attributed to the interactions between the delocalized π orbitals of the pyridine rings and the water molecules.

Table S1**.** Experimental data of antimony selenide thin films.

Substrate temperature (^{o}C)	Deposition time (hours)	XRD Orientation of film and phase	EDX Se/Sb Atom ratio
425	1	(211) orthorhombic	1.52
425	2	(211) orthorhombic	1.48
450	1	(211) orthorhombic	1.3
475	1	(211) orthorhombic	1.45
475	2	(211) orthorhombic	1.34
500	1	(211) orthorhombic	

Table S2**.** Experimental data of bismuth selenide thin films.

Substrate temperature (^{o}C)	Deposition time (hours)	XRD Orientation of film and phase	EDX Se/Bi Atom ratio
350	1	(009) rhombohedral Bi_3Se_4	1.2
375	1	(104) hexagonal BiSe	0.96
375	2	(104) hexagonal BiSe	1.00
400	1	(104) hexagonal BiSe	0.89
400	2	(104) rhombohedral Bi_4Se_3	0.81
425	1	(104) hexagonal BiSe	1.08
425	2	(104) rhombohedral Bi_4Se_3	0.87
475	1	(1011) hexagonal Bi_3Se_2	0.63

Electronic Supplementary Information for *Dalton Transactions*

Crystal Information File of $[Sb\{Se\text{-}C_5H_3(Me\text{-}3)N\}_3] .1.5H_2O$

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C11 C 0.3689(8) 0.3553(8) 0.4704(8) 0.058(2) Uani 1 1 d . . .
H11 H 0.3456 0.3820 0.4044 0.070 Uiso 1 1 calc R . .
C2 C 0.0481(8) 0.2269(10) 0.2284(10) 0.076(3) Uani 1 1 d . . .
C16 C 0.2203(8) -0.1907(10) 0.0801(9) 0.070(3) Uani 1 1 d . . .
H16 H 0.1967 -0.1860 0.0102 0.084 Uiso 1 1 calc R . .
C15 C 0.2344(8) -0.2979(9) 0.1261(8) 0.065(3) Uani 1 1 d . . .
H15 H 0.2189 -0.3643 0.0868 0.079 Uiso 1 1 calc R . .
C3 C 0.0362(10) 0.3122(12) 0.1537(12) 0.096(4) Uani 1 1 d . . .
H3' H -0.0206 0.3568 0.1278 0.115 Uiso 1 1 calc R . .
O1 O 0.0000 0.0000 0.0000 0.093 Uani 1 2 d S . .
O2 O 0.1054(6) 0.0618(7) -0.0906(7) 0.093 Uani 1 1 d . . .
C6 C -0.0321(12) 0.1999(16) 0.2675(16) 0.147(8) Uani 1 1 d . . .
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H6A H -0.0348 0.1183 0.2769 0.221 Uiso 1 1 calc R . .
H6B H -0.0947 0.2262 0.2194 0.221 Uiso 1 1 calc R . .
H6C H -0.0168 0.2385 0.3307 0.221 Uiso 1 1 calc R . .

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Se3 0.0702(7) 0.0385(5) 0.0537(5) 0.0031(4) 0.0289(5) -0.0021(4)
Se2 0.0593(6) 0.0394(4) 0.0479(5) 0.0047(4) 0.0180(4) -0.0004(4)
Se1 0.0476(6) 0.0715(7) 0.0725(7) 0.0112(5) 0.0306(5) 0.0002(5)
N2 0.065(5) 0.043(4) 0.042(4) 0.004(3) 0.019(4) 0.009(4)
C8 0.041(5) 0.045(5) 0.051(5) 0.001(4) 0.016(4) 0.001(4)
N3 0.056(5) 0.050(4) 0.037(4) 0.007(3) 0.016(4) 0.000(3)
N1 0.052(5) 0.066(5) 0.058(5) 0.010(4) 0.026(4) 0.002(4)
C18 0.078(8) 0.036(4) 0.081(8) -0.002(5) 0.035(6) 0.005(5)
C9 0.051(6) 0.052(5) 0.064(7) -0.019(5) 0.016(5) 0.001(4)
C10 0.090(9) 0.036(5) 0.084(8) -0.002(5) 0.041(7) 0.003(5)
C14 0.045(5) 0.046(5) 0.072(7) -0.008(4) 0.033(5) -0.003(4)
C7 0.041(5) 0.053(5) 0.044(5) 0.006(4) 0.023(4) 0.004(4)
C13 0.041(5) 0.049(5) 0.057(6) -0.006(4) 0.022(4) -0.005(4)
C1 0.037(5) 0.055(5) 0.064(6) -0.005(5) 0.017(4) -0.003(4)
C17 0.054(6) 0.059(6) 0.076(8) 0.016(5) 0.030(6) 0.019(5)
C12 0.057(6) 0.069(6) 0.055(6) -0.005(5) 0.016(5) -0.005(5)
C5 0.073(8) 0.082(8) 0.095(9) 0.009(7) 0.049(7) -0.003(7)
C4 0.071(8) 0.072(7) 0.082(8) 0.027(6) 0.033(7) 0.024(6)
C11 0.069(7) 0.044(5) 0.065(6) 0.010(4) 0.030(5) 0.011(4)
C2 0.051(7) 0.083(8) 0.102(10) 0.025(7) 0.038(6) 0.018(6)
C16 0.063(7) 0.085(8) 0.060(6) 0.007(6) 0.022(5) 0.016(6)
C15 0.072(7) 0.067(7) 0.058(6) -0.011(5) 0.027(6) 0.006(5)
C3 0.070(9) 0.099(9) 0.120(12) 0.015(9) 0.039(8) 0.036(7)
O1 0.060 0.087 0.117 0.030 0.019 0.038
O2 0.060 0.087 0.117 0.030 0.019 0.038
C6 0.078(10) 0.174(16) 0.23(2) 0.068(15) 0.102(14) 0.044(10)

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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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Sb1 Se3 2.6466(11) . ?
Sb1 Se2 2.6643(12) . ?
Se3 C13 1.891(9) . ?
Se2 C7 1.906(9) . ?
Se1 C1 1.915(10) . ?
N2 C7 1.333(11) . ?
N2 C11 1.357(12) . ?
C8 C9 1.374(12) . ?
C8 C7 1.397(12) . ?
C8 C12 1.512(13) . ?
N3 C17 1.323(13) . ?
N3 C13 1.363(11) . ?
N1 C1 1.323(12) . ?
N1 C5 1.330(14) . ?
C18 C14 1.488(13) . ?
C18 H18A 0.9600 . ?
C18 H18B 0.9600 . ?
C18 H18C 0.9600 . ?
C9 C10 1.351(15) . ?
C9 H9 0.9300 . ?
C10 C11 1.379(14) . ?
C10 H10 0.9300 . ?
C14 C15 1.355(14) . ?
C14 C13 1.407(12) . ?
C1 C2 1.391(14) . ?
C17 C16 1.339(15) . ?
C17 H17 0.9300 . ?
C12 H12A 0.9600 . ?
C12 H12B 0.9600 . ?
C12 H12C 0.9600 . ?
C5 C4 1.368(15) . ?
C5 H5 0.9300 . ?
C4 C3 1.348(17) . ?
C4 H4 0.9300 . ?
C11 H11 0.9300 . ?
C2 C3 1.425(17) . ?
C2 C6 1.544(17) . ?
C16 C15 1.387(15) . ?
C16 H16 0.9300 . ?
C15 H15 0.9300 . ?
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Se1 Sb1 Se2 91.94(4) . . ?
Se3 Sb1 Se2 82.73(3) . . ?
C13 Se3 Sb1 85.1(3) . . ?
C7 Se2 Sb1 86.5(3) . . ?
C1 Se1 Sb1 92.6(3) . . ?
C7 N2 C11 118.9(8) . . ?
C9 C8 C7 116.0(8) . . ?
C9 C8 C12 121.8(9) . . ?
C7 C8 C12 122.2(8) . . ?
C17 N3 C13 119.9(8) . . ?
C1 N1 C5 117.0(9) . . ?
C14 C18 H18A 109.5 . . ?
C14 C18 H18B 109.5 . . ?
H18A C18 H18B 109.5 . . ?
C14 C18 H18C 109.5 . . ?
H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
C10 C9 C8 122.4(9) . . ?
C10 C9 H9 118.8 . . ?
C8 C9 H9 118.8 . . ?
C9 C10 C11 118.7(9) . . ?
C9 C10 H10 120.7 . . ?
C11 C10 H10 120.7 . . ?
C15 C14 C13 116.4(9) . . ?
C15 C14 C18 123.1(9) . . ?
C13 C14 C18 120.5(9) . . ?
N2 C7 C8 123.0(8) . . ?
N2 C7 Se2 113.9(6) . . ?
C8 C7 Se2 123.2(6) . . ?
N3 C13 C14 121.7(9) . . ?
N3 C13 Se3 113.8(6) . . ?
C14 C13 Se3 124.5(7) . . ?
N1 C1 C2 123.4(10) . . ?
N1 C1 Se1 115.4(7) . . ?
C2 C1 Se1 121.1(7) . . ?
N3 C17 C16 120.6(10) . . ?
N3 C17 H17 119.7 . . ?
C16 C17 H17 119.7 . . ?
C8 C12 H12A 109.5 . . ?
C8 C12 H12B 109.5 . . ?
H12A C12 H12B 109.5 . . ?
C8 C12 H12C 109.5 . . ?
H12A C12 H12C 109.5 . . ?
H12B C12 H12C 109.5 . . ?
N1 C5 C4 124.7(10) . . ?
N1 C5 H5 117.7 . . ?
C4 C5 H5 117.7 . . ?
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C3 C4 C5 118.8(11) . . ?
C3 C4 H4 120.6 . . ?
C5 C4 H4 120.6 . . ?
N2 C11 C10 121.0(9) . . ?
N2 C11 H11 119.5 . . ?
C10 C11 H11 119.5 . . ?
C1 C2 C3 117.1(10) . . ?
C1 C2 C6 120.1(11) . . ?
C3 C2 C6 122.8(11) . . ?
C17 C16 C15 120.9(11) . . ?
C17 C16 H16 119.5 . . ?
C15 C16 H16 119.5 . . ?
C14 C15 C16 120.5(10) . . ?
C14 C15 H15 119.8 . . ?
C16 C15 H15 119.8 . . ?
C4 C3 C2 118.8(11) . . ?
C4 C3 H3' 120.6 . . ?
C2 C3 H3' 120.6 . . ?
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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Crystal Information File of $[Bi\{Se\text{-}C_5H_3(Me\text{-}3)N\}_3].0.5H_2O$

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 'H'  'H'   0.0000   0.0000
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 'N'  'N'   0.0061   0.0033
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 'Bi'  'Bi'  -4.1077  10.2566
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 'O'  'O'   0.0106   0.0060
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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
 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.
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Se3 Se 0.08047(12) 0.46504(13) -0.09930(11) 0.0459(4) Uani 1 1 d . . .
Se2 Se 0.15846(13) 0.70560(13) 0.07935(12) 0.0508(4) Uani 1 1 d . . .
Se1 Se 0.34021(14) 0.44538(16) 0.12352(14) 0.0624(5) Uani 1 1 d . . .
N3 N 0.1253(10) 0.2682(11) 0.0098(10) 0.053(3) Uani 1 1 d . . .
N2 N 0.2224(10) 0.6078(10) 0.2650(9) 0.051(4) Uani 1 1 d . . .
N1 N 0.2908(11) 0.3207(11) 0.2578(11) 0.057(4) Uani 1 1 d . . .
C8 C 0.2320(13) 0.8168(12) 0.2751(13) 0.055(4) Uani 1 1 d . . .
C6 C 0.5349(17) 0.295(2) 0.2351(18) 0.129(4) Uani 1 1 d . . .
H6A H 0.5210 0.2522 0.1745 0.194 Uiso 1 1 calc R . .
H6B H 0.5961 0.2686 0.2857 0.194 Uiso 1 1 calc R . .
H6C H 0.5396 0.3752 0.2228 0.194 Uiso 1 1 calc R . .
C15 C 0.0656(12) 0.1089(14) -0.1428(12) 0.055(4) Uani 1 1 d . . .
H15 H 0.0464 0.0555 -0.1947 0.066 Uiso 1 1 calc R . .
C16 C 0.1039(14) 0.0714(15) -0.0431(14) 0.066(5) Uani 1 1 d . . .
H16 H 0.1112 -0.0069 -0.0283 0.079 Uiso 1 1 calc R . .
C17 C 0.1302(14) 0.1504(15) 0.0315(12) 0.063(5) Uani 1 1 d . . .
H17 H 0.1518 0.1261 0.0976 0.075 Uiso 1 1 calc R . .
C14 C 0.0563(10) 0.2267(14) -0.1640(12) 0.045(4) Uani 1 1 d . . .
C11 C 0.2608(12) 0.6023(15) 0.3679(13) 0.058(5) Uani 1 1 d . . .
H11 H 0.2692 0.5303 0.3982 0.069 Uiso 1 1 calc R . .
C5 C 0.3038(16) 0.2497(17) 0.3322(16) 0.077(6) Uani 1 1 d . . .
H5 H 0.2557 0.2455 0.3577 0.092 Uiso 1 1 calc R . .
C1 C 0.3627(11) 0.3339(13) 0.2265(12) 0.047(4) Uani 1 1 d . . .
C2 C 0.4524(14) 0.2755(19) 0.2707(15) 0.082(6) Uani 1 1 d . . .
C18 C 0.0143(14) 0.2684(13) -0.2735(12) 0.063(5) Uani 1 1 d . . .
H18A H -0.0399 0.3197 -0.2847 0.094 Uiso 1 1 calc R . .
H18B H -0.0081 0.2034 -0.3176 0.094 Uiso 1 1 calc R . .
H18C H 0.0645 0.3083 -0.2865 0.094 Uiso 1 1 calc R . .
C12 C 0.2115(16) 0.9298(13) 0.2197(14) 0.077(6) Uani 1 1 d . . .
H12A H 0.2456 0.9906 0.2650 0.115 Uiso 1 1 calc R . .
H12B H 0.1421 0.9449 0.1922 0.115 Uiso 1 1 calc R . .
H12C H 0.2338 0.9260 0.1664 0.115 Uiso 1 1 calc R . .
C7 C 0.2100(12) 0.7110(12) 0.2230(11) 0.044(4) Uani 1 1 d . . .
C3 C 0.4599(18) 0.1891(16) 0.3476(17) 0.096(7) Uani 1 1 d . . .
H3 H 0.5154 0.1427 0.3754 0.115 Uiso 1 1 calc R . .
C10 C 0.2877(15) 0.6997(16) 0.4286(13) 0.067(5) Uani 1 1 d . . .
H10 H 0.3160 0.6943 0.4981 0.080 Uiso 1 1 calc R . .
C13 C 0.0854(10) 0.3029(11) -0.0862(10) 0.033(3) Uani 1 1 d . . .
C9 C 0.2696(13) 0.8069(17) 0.3790(13) 0.064(5) Uani 1 1 d . . .
H9 H 0.2834 0.8738 0.4172 0.077 Uiso 1 1 calc R . .
C4 C 0.3890(16) 0.1789(17) 0.3754(15) 0.076(6) Uani 1 1 d . . .
H4 H 0.3930 0.1250 0.4240 0.091 Uiso 1 1 calc R . .
O1 O 0.504(3) 0.508(3) 0.480(3) 0.093 Uani 0.50 1 d P . .
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Se3 0.0557(10) 0.0368(8) 0.0435(8) 0.0046(7) 0.0181(8) -0.0007(8)
Se2 0.0667(12) 0.0379(8) 0.0513(10) 0.0040(7) 0.0272(9) -0.0022(8)
Se1 0.0509(11) 0.0713(13) 0.0737(12) 0.0137(9) 0.0341(10) 0.0013(9)
N3 0.045(9) 0.049(8) 0.063(9) -0.016(7) 0.019(7) -0.003(7)
N2 0.073(11) 0.041(8) 0.045(8) 0.001(6) 0.032(8) -0.013(7)
N1 0.065(11) 0.050(8) 0.069(10) 0.008(7) 0.039(9) 0.007(7)
C8 0.061(12) 0.026(8) 0.083(13) 0.003(8) 0.033(11) 0.001(7)
C6 0.071(17) 0.183 0.160 0.060(18) 0.074(14) 0.043(16)
C15 0.055(12) 0.052(11) 0.056(11) -0.022(9) 0.019(9) -0.015(9)
C16 0.081(15) 0.043(10) 0.071(13) 0.002(9) 0.029(11) 0.014(9)
C17 0.087(15) 0.061(12) 0.045(10) 0.017(9) 0.032(11) 0.026(10)
C14 0.023(8) 0.062(11) 0.061(10) -0.010(8) 0.028(8) -0.011(7)
C11 0.043(11) 0.065(12) 0.069(13) 0.015(9) 0.026(10) 0.012(9)
C5 0.076(16) 0.084(14) 0.088(15) -0.014(12) 0.051(14) 0.006(12)
C1 0.021(9) 0.055(9) 0.062(10) 0.001(8) 0.012(8) 0.004(7)
C2 0.043(13) 0.120(18) 0.080(14) -0.014(13) 0.022(11) 0.014(12)
C18 0.094(16) 0.045(10) 0.063(11) -0.009(8) 0.046(11) -0.001(10)
C12 0.123(19) 0.036(9) 0.106(16) -0.008(9) 0.083(15) 0.005(10)
C7 0.044(10) 0.037(8) 0.063(10) 0.001(7) 0.033(9) -0.005(7)
C3 0.10(2) 0.056(13) 0.119(19) 0.042(12) 0.030(16) 0.030(13)
C10 0.081(15) 0.065(13) 0.052(11) -0.019(10) 0.024(11) -0.002(10)
C13 0.020(8) 0.035(8) 0.045(9) 0.001(7) 0.015(7) 0.000(6)
C9 0.061(13) 0.078(14) 0.060(12) -0.031(10) 0.031(11) -0.006(10)
C4 0.069(15) 0.078(14) 0.085(15) -0.011(11) 0.035(13) -0.032(13)
O1 0.050 0.088 0.129 0.006 0.022 0.020

_geom_special_details
;
 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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C8 C12 1.51(2) . ?
C6 C2 1.53(3) . ?
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C6 H6C 0.9600 . ?
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H6A C6 H6B 109.5 . . ?
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H6A C6 H6C 109.5 . . ?
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H18A C18 H18C 109.5 . . ?
H18B C18 H18C 109.5 . . ?
C8 C12 H12A 109.5 . . ?
C8 C12 H12B 109.5 . . ?
H12A C12 H12B 109.5 . . ?
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H12A C12 H12C 109.5 . . ?
H12B C12 H12C 109.5 . . ?
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N2 C7 Se2 113.3(11) . . ?
C8 C7 Se2 121.3(11) . . ?
C4 C3 C2 119(2) . . ?
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C11 C10 C9 116.3(16) . . ?
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N3 C13 C14 122.1(13) . . ?
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