

Supporting Information for

The Tungsten Allylimido Complexes  $\text{Cl}_4(\text{RCN})\text{W}(\text{NC}_3\text{H}_5)$  as Single-source CVD Precursors for  $\text{WN}_x\text{C}_y$  Thin Films. Correlation of Precursor Fragmentation to Film Properties

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**Table S1.** Atomic coordinates ( $\times 10^4$ ) and equivalent isotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **3a**.  $U(\text{eq})$  is defined as one third of the trace of the orthogonalized  $U^{\text{ij}}$  tensor.

	x	y	z	U(eq)
W	3673(1)	8599(10)	2535(1)	49(1)
N1	5066(15)	8370(40)	1429(7)	70(6)
N2	1708(12)	8700(50)	4039(6)	44(2)
Cl1	5703(14)	10782(10)	3533(7)	76(3)
Cl2	1187(11)	6445(7)	1876(6)	59(2)
Cl3	5635(13)	6364(9)	3495(7)	68(3)
Cl4	1046(15)	10783(8)	1997(7)	79(3)
C1	6430(20)	8580(40)	484(10)	93(5)
C2	5470(60)	9880(60)	-410(30)	66(9)
C3	3800(60)	8730(120)	-1180(30)	80(10)
C2'	5130(30)	8860(50)	-592(16)	65(7)
C3'	3020(30)	8270(30)	-748(16)	53(5)
C4	665(13)	8640(50)	4747(7)	44(3)
C5	-633(17)	8530(50)	5692(8)	52(3)

**Table S2.** Bond lengths [Å] and angles [°] for **3a**.

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W-N1	1.687(9)
W-N2	2.308(8)
W-C12	2.317(8)
W-C13	2.324(9)
W-C11	2.339(10)
W-C14	2.351(9)
N1-C1	1.508(17)
N2-C4	1.130(12)
C1-C2'	1.51(2)
C1-C2	1.55(4)
C2-C3	1.59(6)
C2'-C3'	1.36(3)
C4-C5	1.476(14)
N1-W-N2	175.8(15)
N1-W-C12	90.6(8)
N2-W-C12	86.0(7)
N1-W-C13	93.6(7)
N2-W-C13	84.0(6)
C12-W-C13	88.7(4)
N1-W-C11	102.4(8)
N2-W-C11	81.1(7)
C12-W-C11	167.0(3)
C13-W-C11	90.18(13)
N1-W-C14	103.1(7)
N2-W-C14	79.1(6)
C12-W-C14	88.14(11)
C13-W-C14	163.0(3)
C11-W-C14	89.2(4)
C1-N1-W	167(2)
C4-N2-W	175(3)
C2'-C1-N1	114.2(12)
C2'-C1-C2	30.9(16)
N1-C1-C2	114.8(17)

C1-C2-C3	106(4)
C3'-C2'-C1	120(2)
N2-C4-C5	178(2)

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Symmetry transformations used to generate equivalent atoms:

**Table S3.** Anisotropic displacement parameters ( $\text{\AA}^2 \times 10^3$ ) for **3a**. The anisotropic displacement factor exponent takes the form:  $-2\pi^2 [ h^2 a^{*2} U^{11} + \dots + 2 h k a^* b^* U^{12} ]$

	U <sup>11</sup>	U <sup>22</sup>	U <sup>33</sup>	U <sup>23</sup>	U <sup>13</sup>	U <sup>12</sup>
W	31(1)	79(1)	38(1)	-1(1)	2(1)	-1(1)
N1	53(5)	115(16)	41(4)	1(8)	1(4)	51(11)
N2	35(3)	51(7)	47(4)	13(12)	3(3)	8(10)
Cl1	58(5)	101(7)	65(5)	18(5)	-10(4)	-30(5)
Cl2	40(3)	86(5)	51(3)	-8(3)	9(2)	-14(3)
Cl3	52(4)	94(7)	58(5)	2(5)	-4(3)	22(4)
Cl4	87(5)	69(5)	73(4)	7(3)	-30(4)	0(4)
C1	69(8)	146(13)	67(7)	-6(16)	17(7)	75(13)
C4	35(4)	53(6)	45(5)	-21(12)	1(4)	14(12)
C5	52(5)	58(7)	48(5)	-8(15)	13(4)	19(14)

**Table S4.** Hydrogen coordinates ( $\times 10^4$ ) and isotropic displacement parameters ( $\text{\AA}^2 \times 10^{-3}$ ) for **3a**.

	x	y	z	U(eq)
H1B	6628	7394	154	112
H1A	7896	9024	761	112
H1B'	7403	9632	623	112
H1A'	7373	7516	438	112
H2	5816	11109	-492	80
H3B	3577	7498	-1024	96
H3A	3011	9267	-1789	96
H2'	5774	9445	-1165	78
H3B'	2371	7687	-177	63
H3A'	2207	8450	-1429	63
H5A	-750	7281	5915	78
H5B	-2097	9017	5497	78
H5C	85	9229	6294	78