

Electronic Supplementary Information

**The Deposition of Cadmium Selenide and Cadmium Phosphide Thin Films from Cadmium Thioselenoimidodiphosphate by AACVD and the Formation of Aromatic Species**

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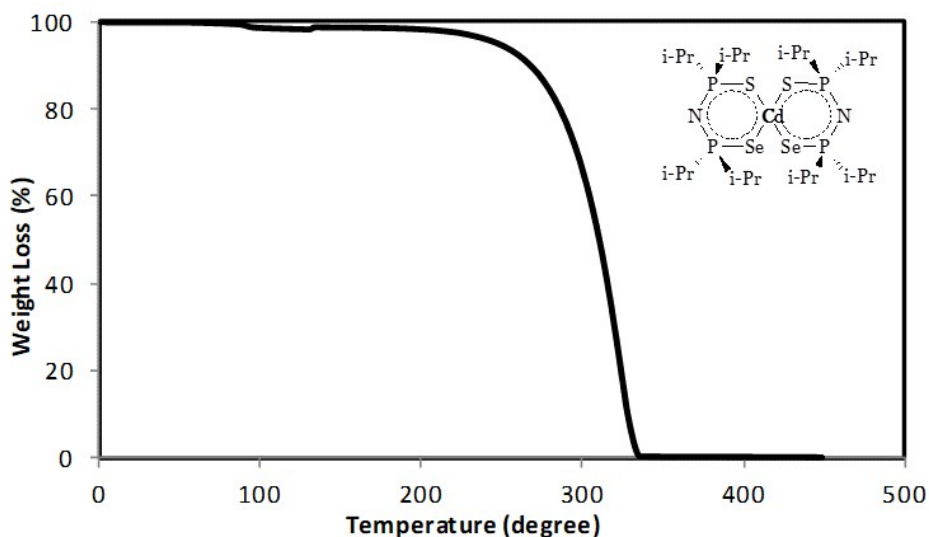
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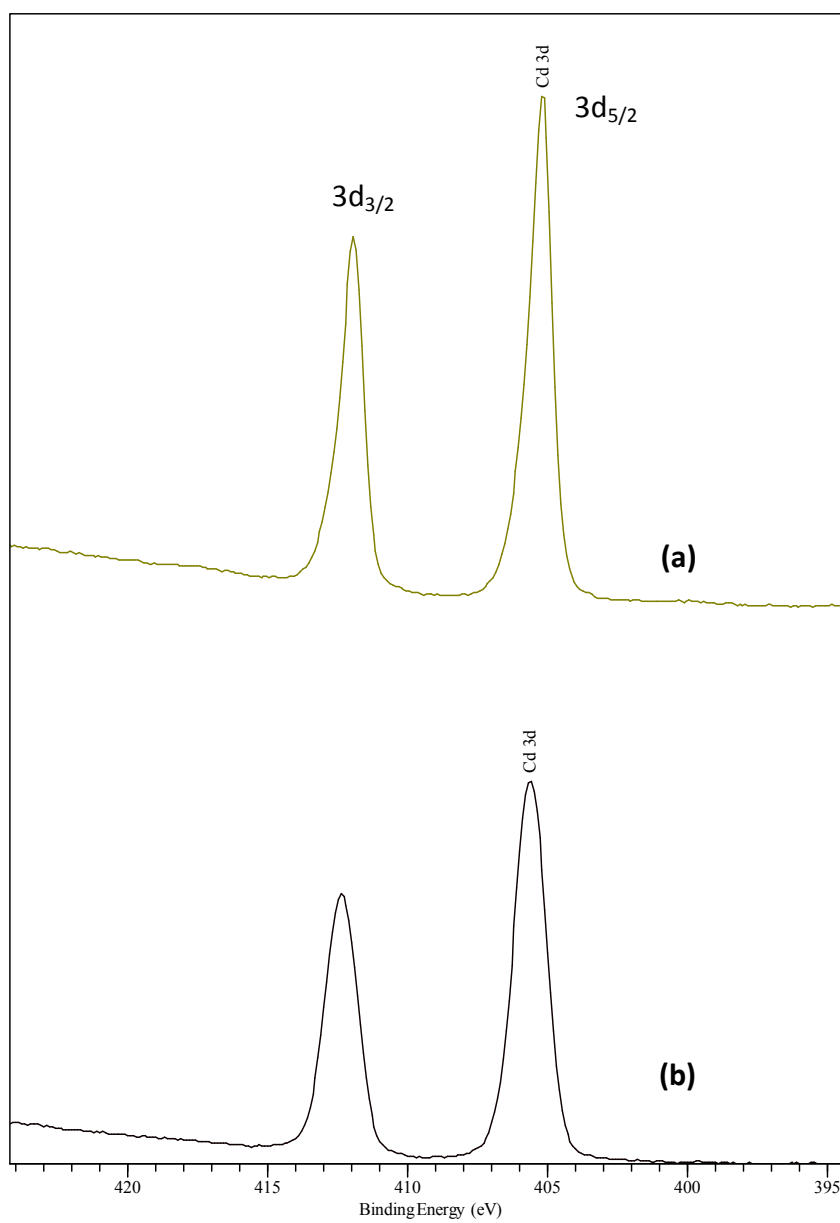
**Figure S1.** Thermogravimetry analysis of  $\text{Cd}[(\text{SP}^i\text{Pr}_2)(\text{SeP}^i\text{Pr}_2)_2\text{N}]_2$ . Inset shows the structure of precursor.

Compound	Dep. Temp (°C)	Flow Rate (sccm)	Phase	Lattice Constant (Å)	
				Experimental	Literature <sup>1,2</sup>
CdSe	525/500	240	Hexagonal	$a = 4.290(3)$ $c = 7.013(3)$	$a = 4.299$ $c = 7.010$
CdSe/Cd <sub>2</sub> P <sub>3</sub>	500/475	160	Monoclinic	$a = 18.035(1)$ $b = 4.610(3)$ $c = 17.854(2)$	$a = 18.030$ $b = 4.610$ $c = 17.850$

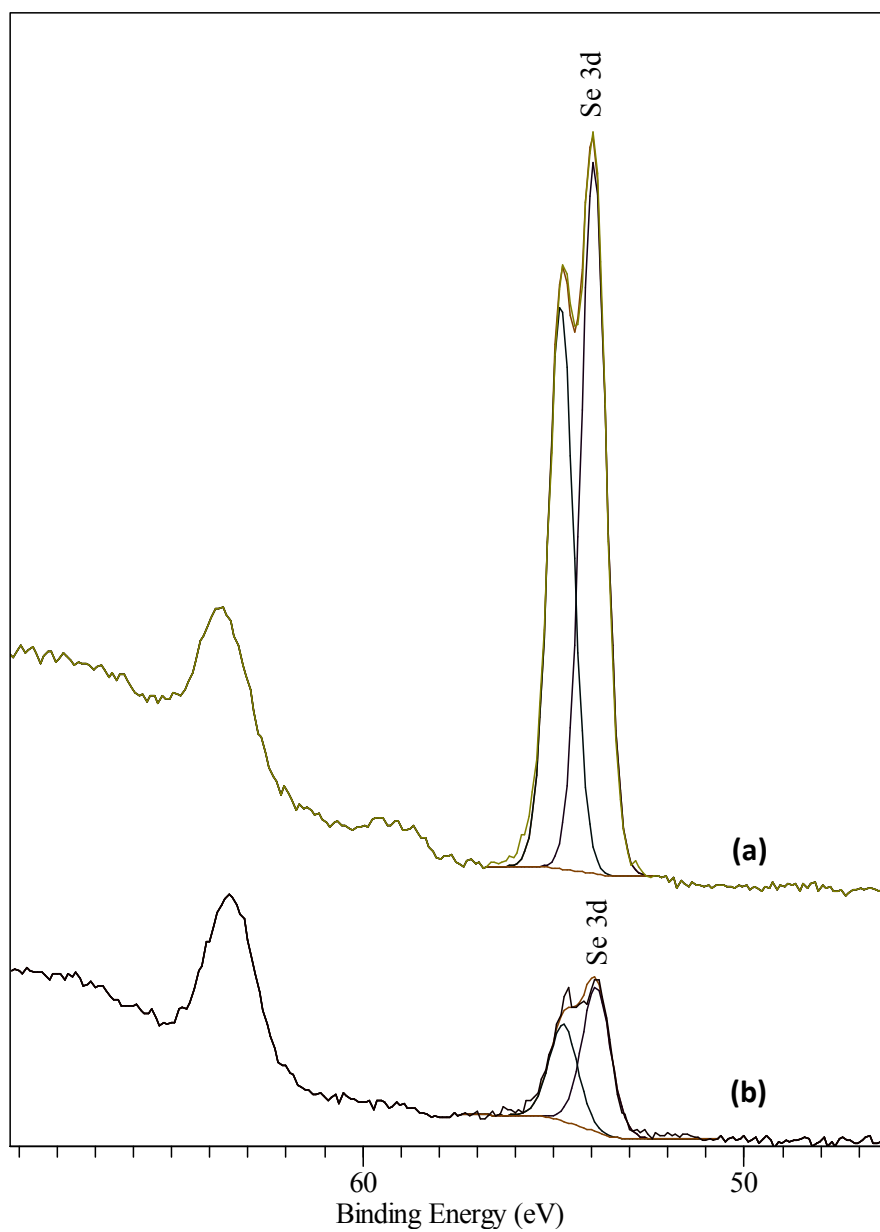
**Table S1.** Lattice parameters of the deposited thin films .

Compound	Dep. Temp (°C)	Flow Rate (sccm)	Cd (%)	Se (%)	P (%)
CdSe	525	240	39.3	30.6	29.8
	500	240	42.4	34.2	22.7
CdSe/Cd <sub>2</sub> P <sub>3</sub>	500	160	43.4	33.9	22.5
	475	160	37.2	34.9	27.1

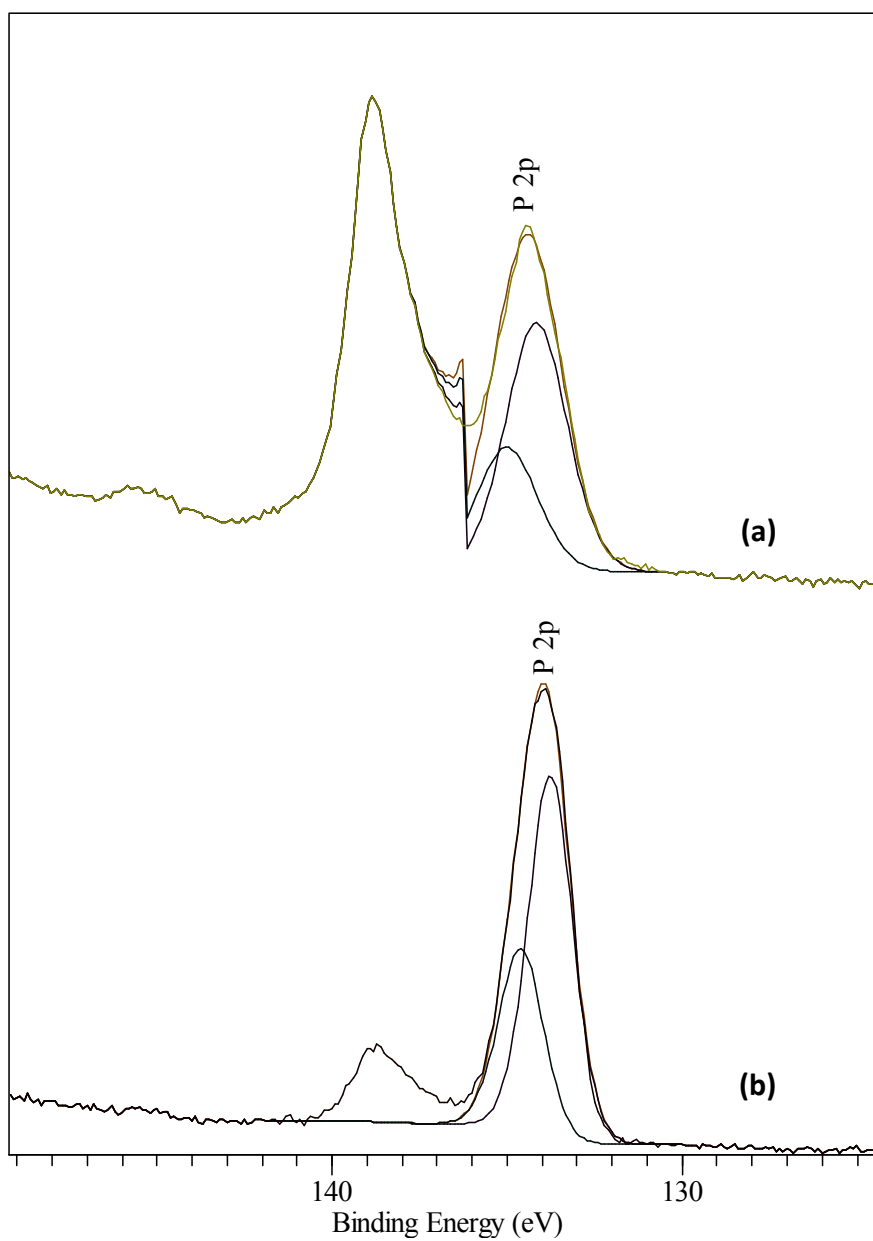
**Table S2.** Compositional analysis of films determined by EDAX.



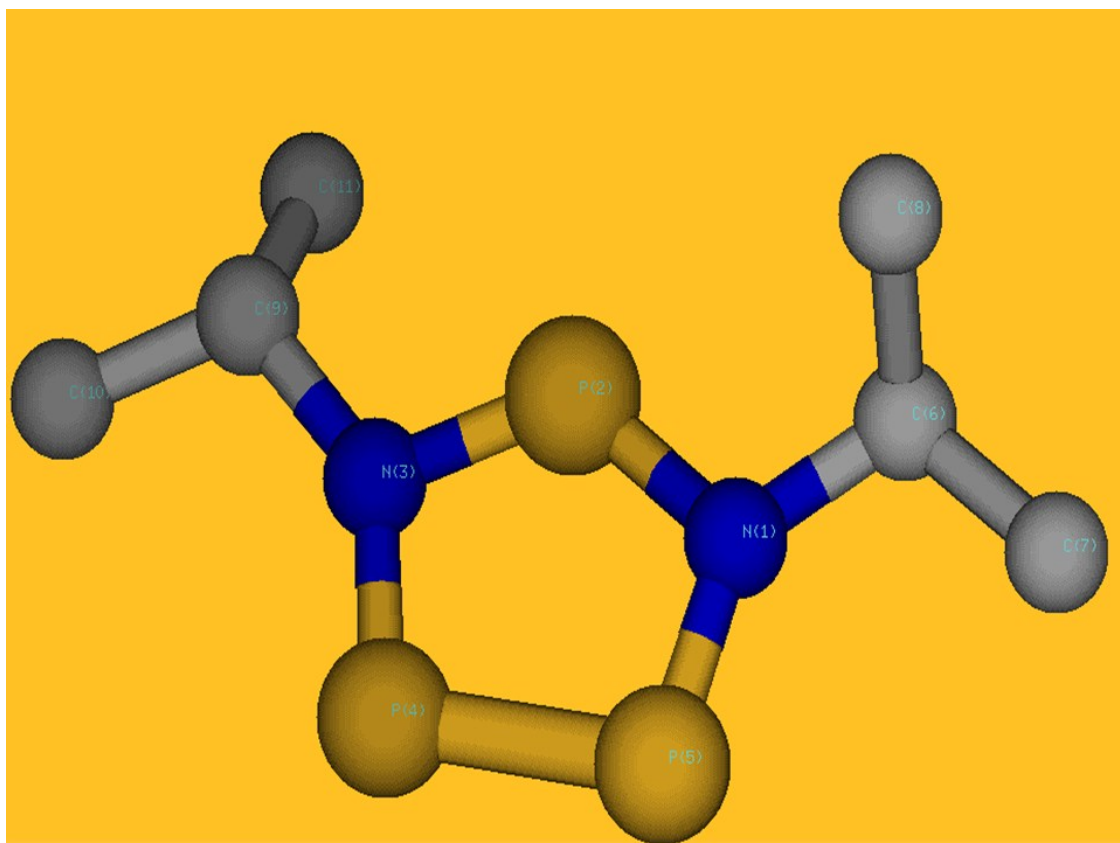
**Figure S2.** XPS of Cd 3d peaks of (a)  $\text{Cd}[(\text{SP}^i\text{Pr}_2)(\text{SeP}^i\text{Pr}_2)_2\text{N}]_2$  and (b)  $\text{Cd}[(\text{SeP}^i\text{Pr}_2)_2\text{N}]_2^3$ .



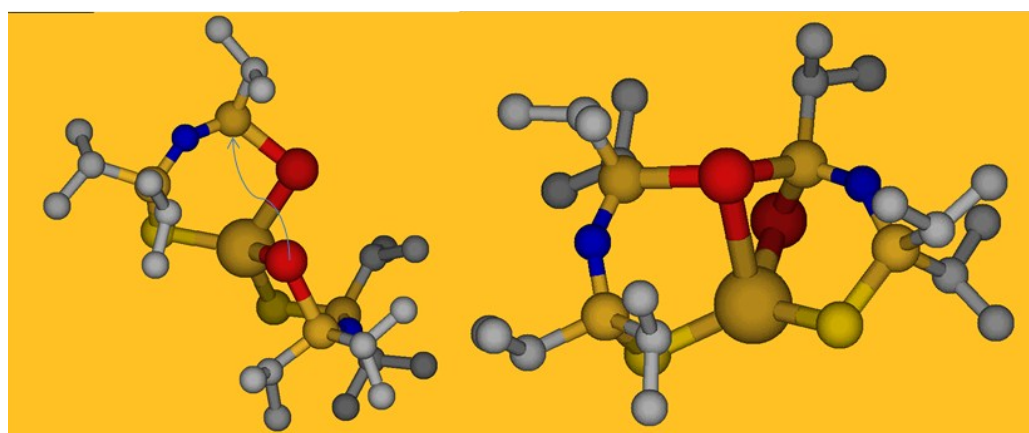
**Figure S3.** XPS of Se 3d peaks of (a)  $\text{Cd}[(\text{SP}^i\text{Pr}_2)(\text{SeP}^i\text{Pr}_2)_2\text{N}]_2$  and (b)  $\text{Cd}[(\text{SeP}^i\text{Pr}_2)_2\text{N}]_2^3$ .



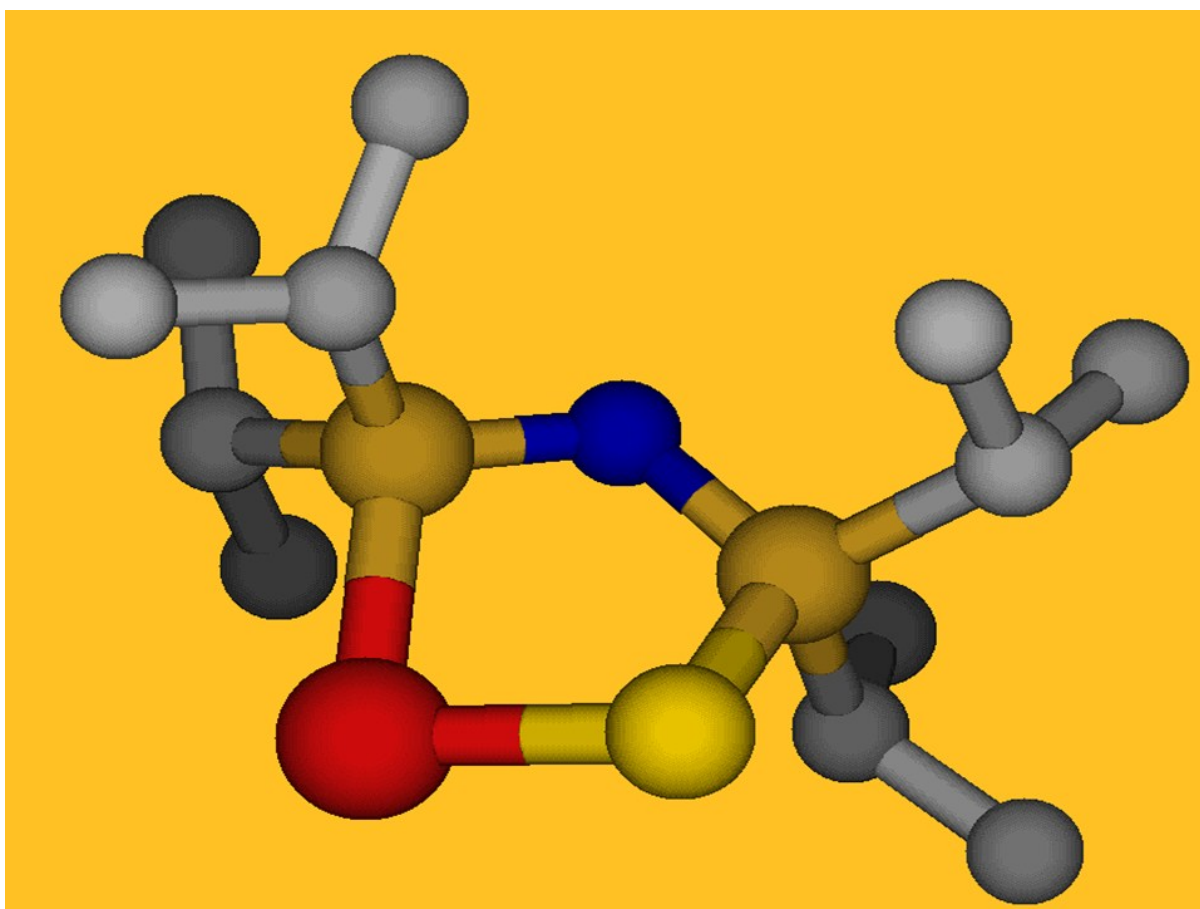
**Figure S4.** XPS of P 2p peaks of (a)  $\text{Cd}[(\text{SP}^i\text{Pr}_2)(\text{SeP}^i\text{Pr}_2)_2\text{N}]_2$  and (b)  $\text{Cd}[(\text{SeP}^i\text{Pr}_2)_2\text{N}]_2^3$ .



**Figure. S5.** The aromatic ion found in our previous study, at a charge to mass ratio of 207 in the MS. We assigned it this structure due to its stability. For clarity the hydrogens are omitted<sup>4</sup>.



**Figure. S6.** The  $\text{Cd}[(\text{SP}^i\text{Pr}_2)(\text{SeP}^i\text{Pr})\text{N}][(\text{SP}^i\text{Pr}_2)(\text{SeP}^i\text{Pr}_2)\text{N}]^+$  ion, which is the parent ion with the loss of an *iso*-propyl group from P bound to Se (shown in Red). The Se from the other complete ligand attacks the trivalent P as indicated by the arrow in the left image, to yield the structure shown on the right. For clarity the hydrogens have been omitted<sup>4</sup>.



**Figure S7.** The stable ion  $(SPiPr_2)(SePiPr_2)_2N^+$  formed by the loss of an entire ligand from the ionized complex  $Cd[(SPiPr_2)(SePiPr_2)_2N]_2^+$  (formed during MS analysis). Once this ligand has been lost from the complex, it spontaneously cyclized as this results in each element being in a stable valence state. Thus with the positive charge on N, this forms two double bonds to each P and these in turn form two bonds to the *iso*-propyl groups and one bond to either S or Se, giving two five valent P atoms. The Se and S form a bond to each other to complete the cyclization of the ion and to give them two single bonds each. For clarity the hydrogens have been omitted<sup>4</sup>.

**References:**

1. (a) T. Logu, K. Sankarasubramanian, P. Soundarrajan and K. Sethuraman, *Elect. Mater. Lett.*, 2015, **Vol 11, No 2**, 206-212. (b) H. Chauhan, Y. Kumar and S. Deka, *Nanoscale.*, 2014, **6**, 10347-10354.
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4. G. Schaftenaar, E. Vlieg and G. Vriend, "Molden 2.0: quantum chemistry meets proteins", *J Comput Aided Mol. Des.*, **2017**, 31, 789. G.Schaftenaar and J.H. Noordik, "Molden: a pre- and post-processing program for molecular and electronic structures", *J. Comput.-Aided Mol. Design*, 2000, **14**, 123-134.