

## Supporting Information

# Development of molecular precursors for deposition of indium sulphide thin film electrodes for photoelectrochemical applications

### CHN Analysis

Precursor  $[\text{In}(\text{S}_2\text{CNCy}_2)_3] \cdot 2\text{Py}$  (1)

Run Details				Results			Simplest Empirical Formula		
Run	Run #	Created On	Weight	Carbon	Hydrogen	Nitrogen	Carbon	Hydrogen	Nitrogen
DD4	90	2012-8-27 4:39 PM	1.495	56.73	7.831	6.329	10.453	17.194	1

Precursor  $[\text{In}(\text{S}_2\text{CN}(\text{iPr})_2)_3] \cdot 1.5\text{Py}$  (2)

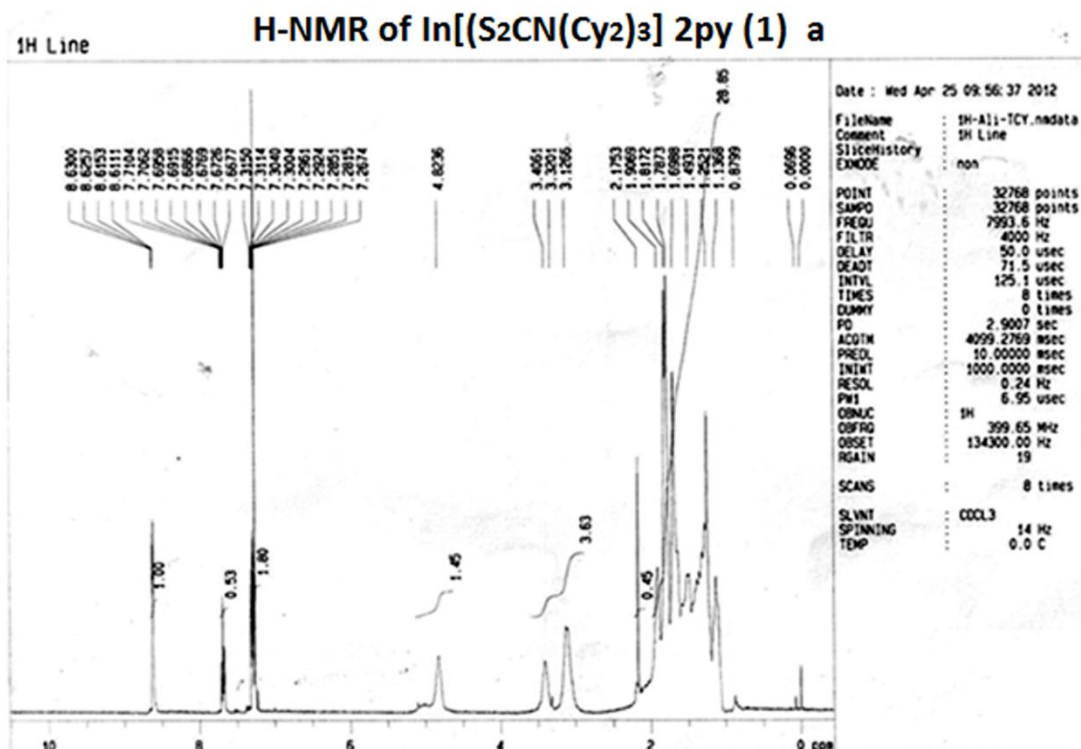
Run Details				Results			Simplest Empirical Formula		
Run	Run #	Created On	Weight	Carbon	Hydrogen	Nitrogen	Carbon	Hydrogen	Nitrogen
AA2	8	2012-10-16 11:40 AM	1.57	43.722	6.688	7.941	6.421	11.703	1

Precursor  $[\text{In}(\text{S}_2\text{CPip})_3] \cdot 0.5\text{Py}$  (3)

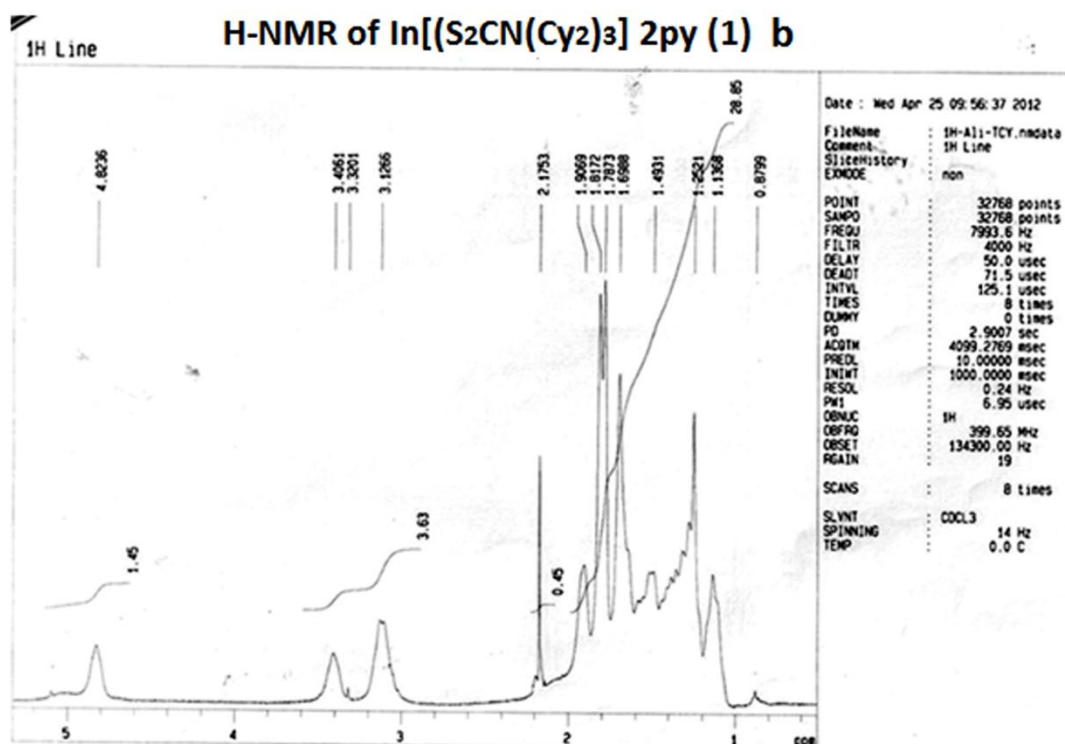
Run Details				Results			Simplest Empirical Formula		
Run	Run #	Created On	Weight	Carbon	Hydrogen	Nitrogen	Carbon	Hydrogen	Nitrogen
E10	74	2012-10-3 11:24 AM	1.585	37.708	5.057	7.407	5.937	9.487	1

Precursor  $[\text{In}(\text{S}_2\text{CNBzMe})_3]$  (4)

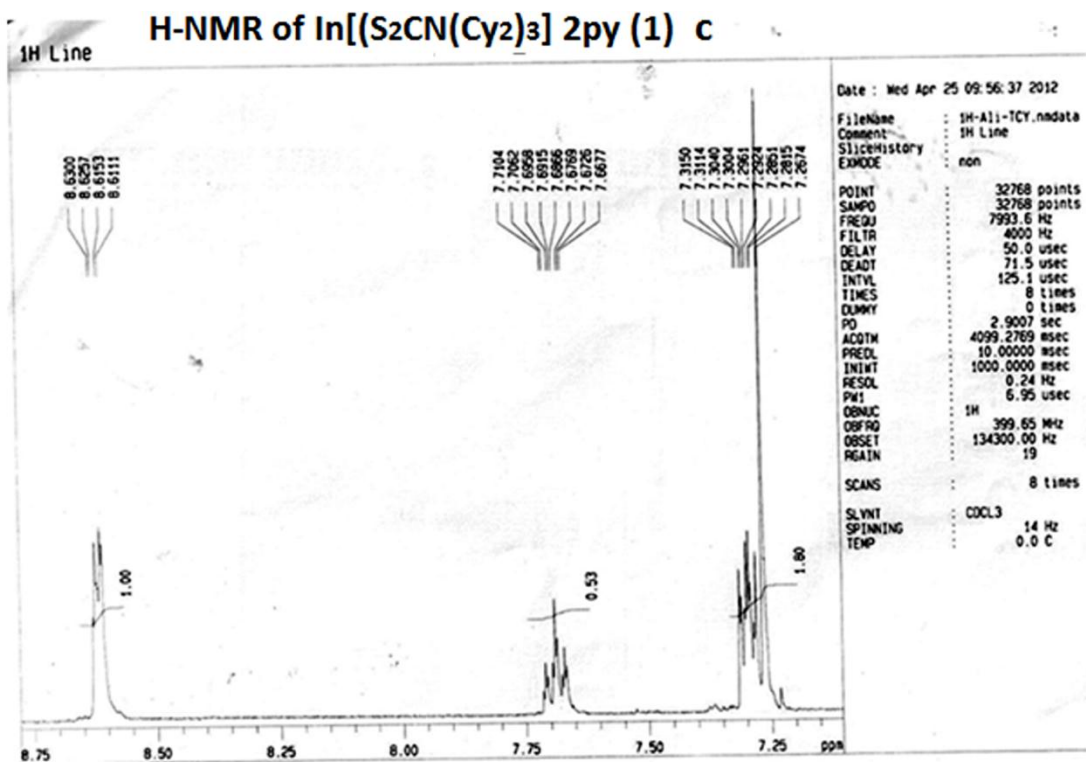
Run Details				Results			Simplest Empirical Formula		
Run	Run #	Created On	Weight	Carbon	Hydrogen	Nitrogen	Carbon	Hydrogen	Nitrogen
DB2	87	2012-7-10 12:29 PM	2.071	45.696	4.334	6.057	8.893	9.983	1



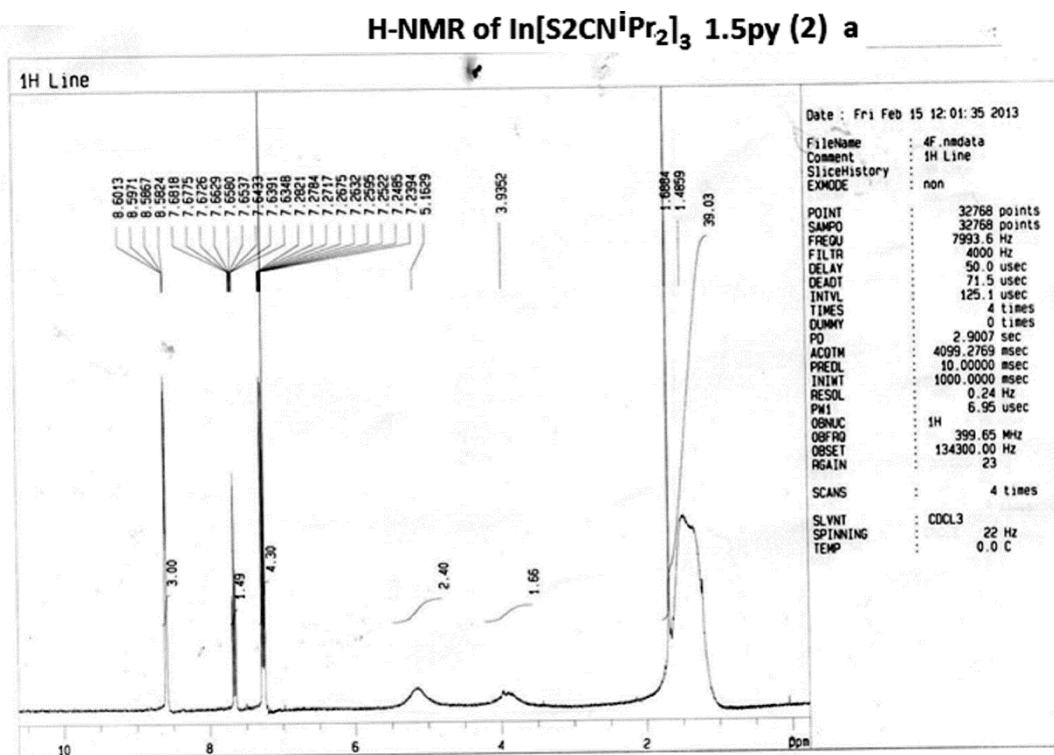
S.Fig. 1a: H-NMR of Precursor  $[\text{In}(\text{S}_2\text{CNCy}_2)_3] \cdot 2\text{Py}(\mathbf{1})$



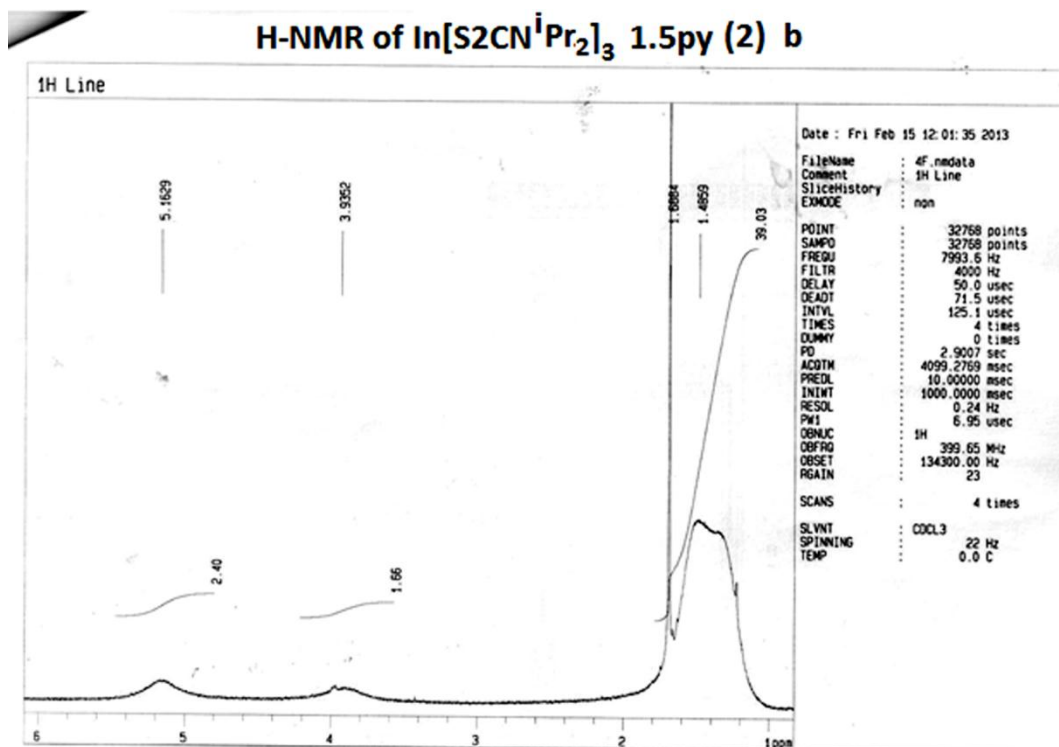
S.Fig. 1b: H-NMR of Precursor  $[\text{In}(\text{S}_2\text{CNCy}_2)_3] \cdot 2\text{Py}(\mathbf{1})$



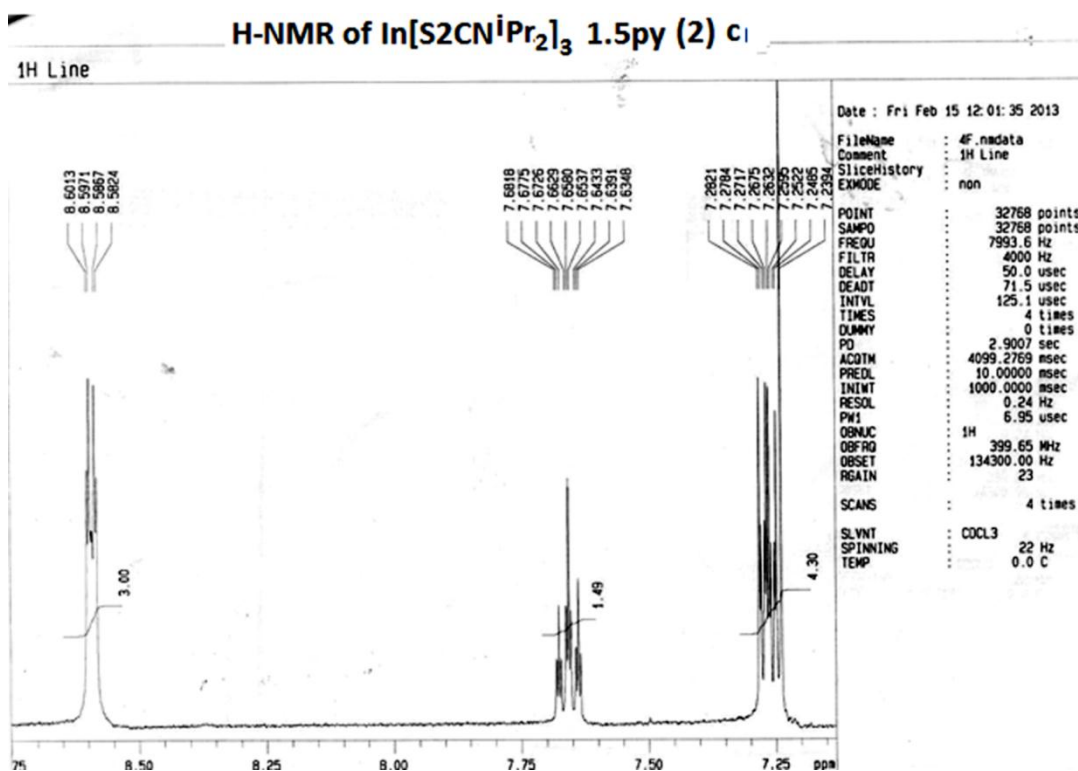
**S.Fig. 1c:** H-NMR of Precursor  $[\text{In}(\text{S}_2\text{CNCy}_2)_3] \cdot 2\text{Py}(1)$



**S.Fig. 2a:** H-NMR of Precursor  $[\text{In}(\text{S}_2\text{CN}^i\text{Pr}_2)_3] \cdot 1.5\text{py} (2)$

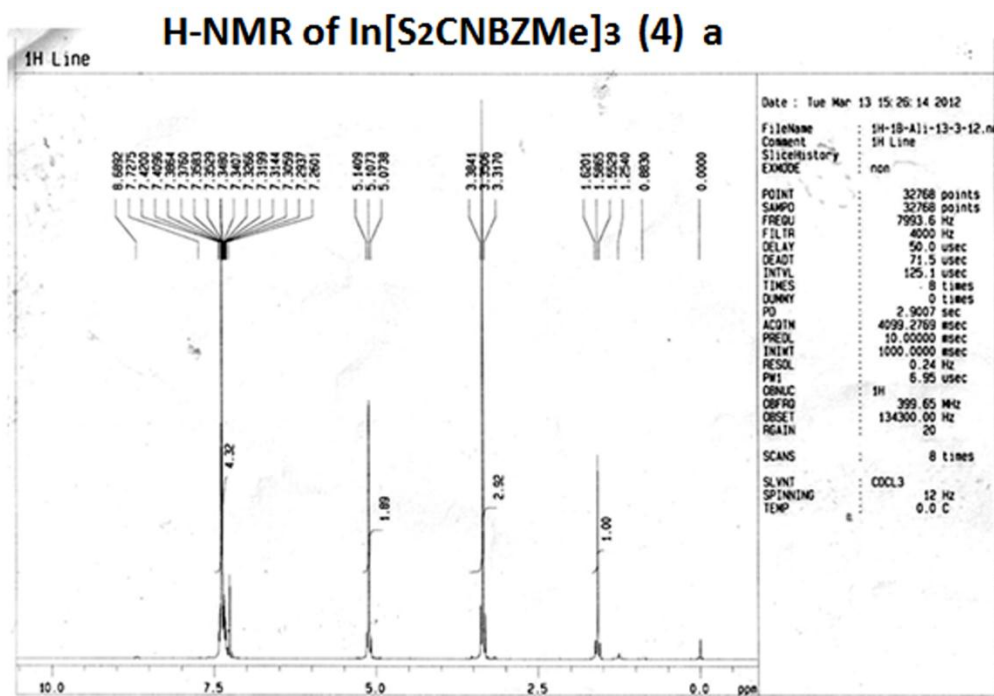


**S.Fig. 2b:** H-NMR of Precursor  $[\text{In}(\text{S}_2\text{CN}^i\text{Pr})_2]_3 \cdot 1.5\text{py}$  (2)

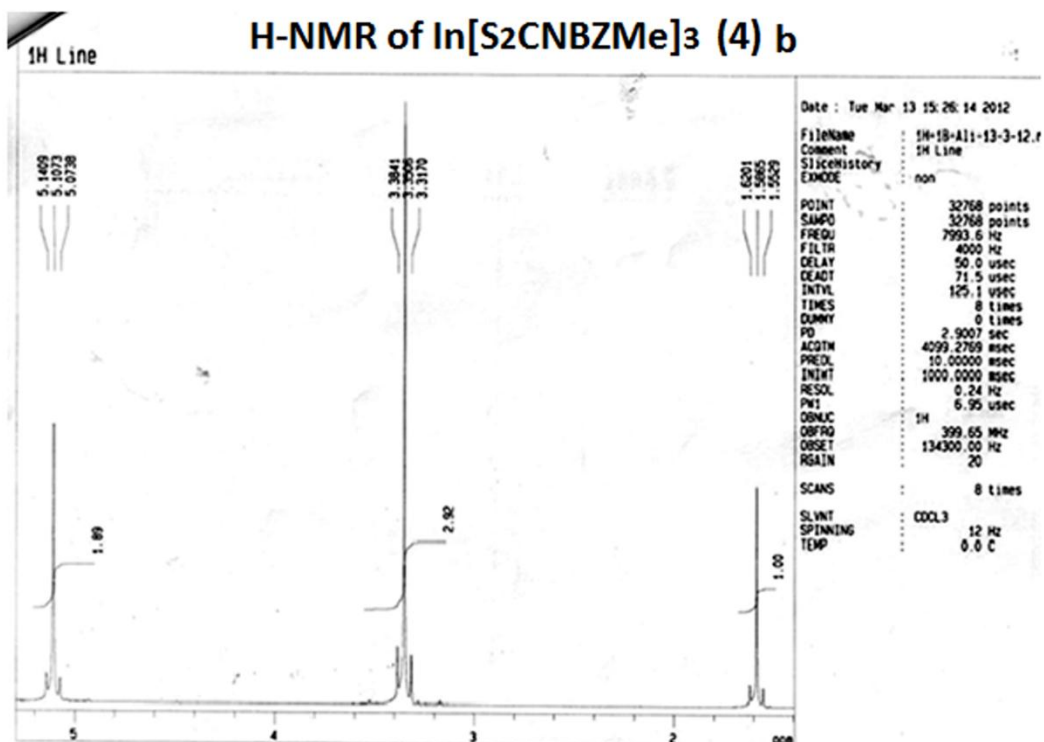


**S.Fig. 2c:** H-NMR of Precursor  $[\text{In}(\text{S}_2\text{CN}^i\text{Pr})_2]_3 \cdot 1.5\text{py}$  (2)

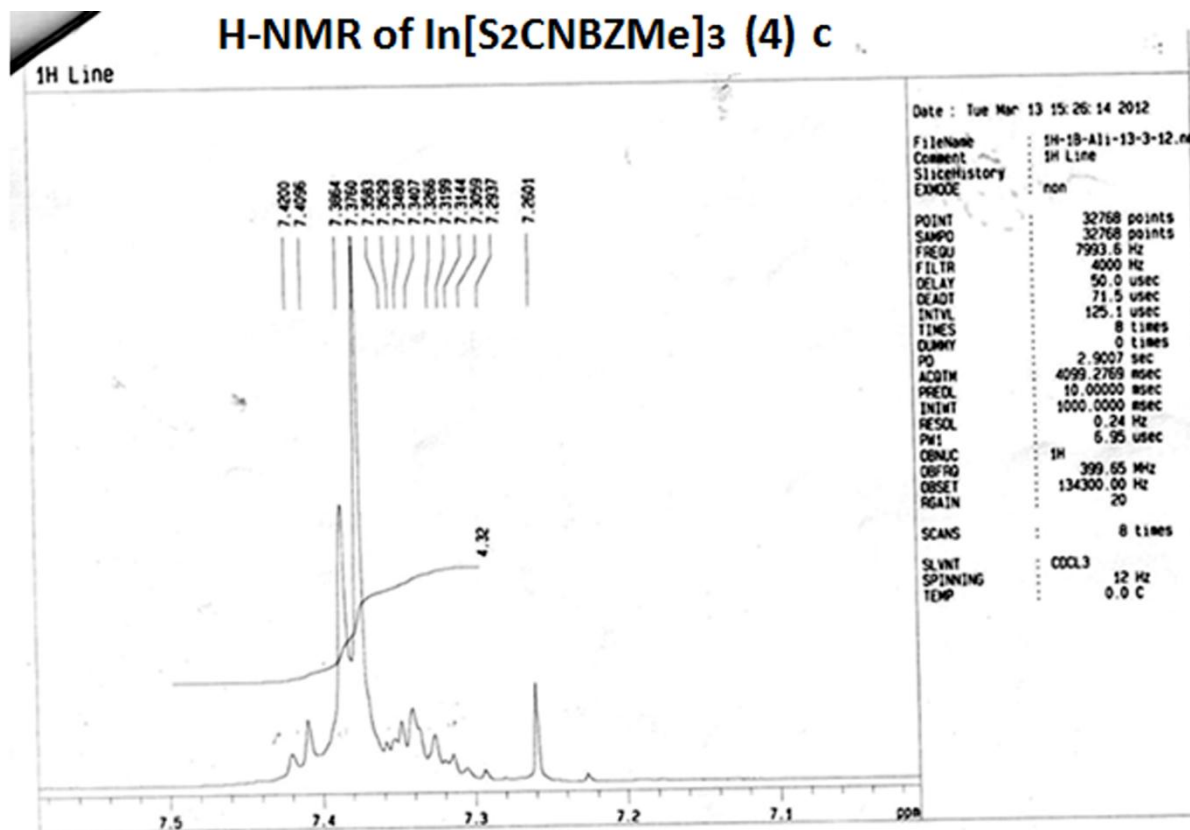




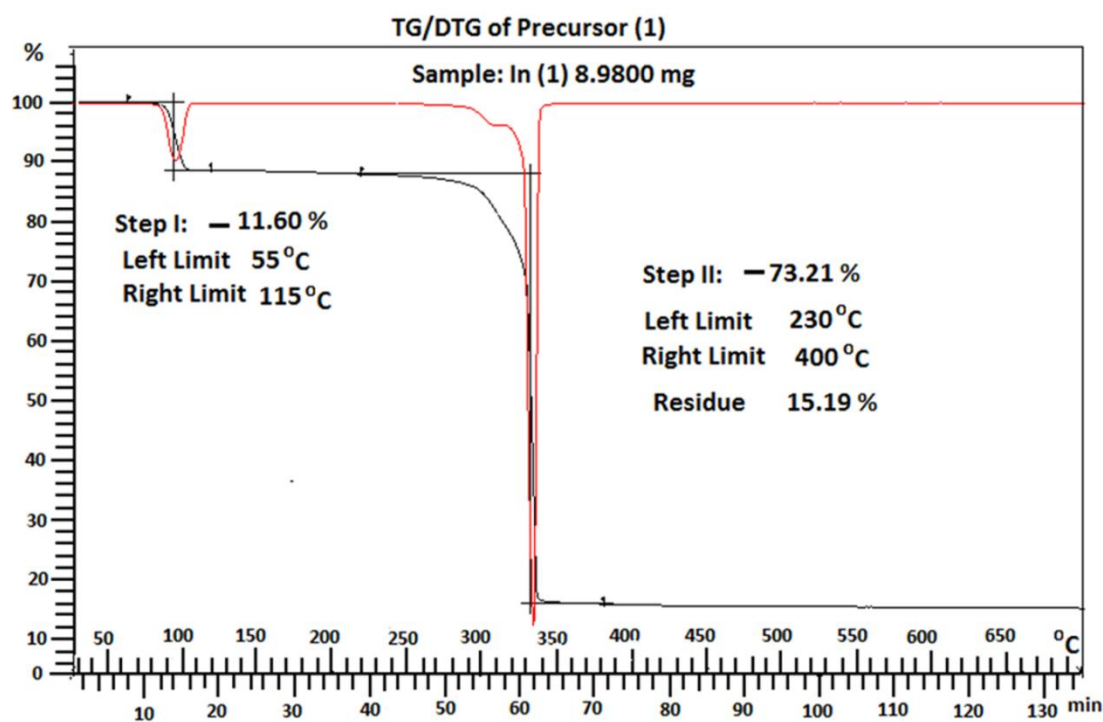
S.Fig. 4a: H-NMR of Precursor [In(S<sub>2</sub>CNBzMe)<sub>3</sub>] (4)



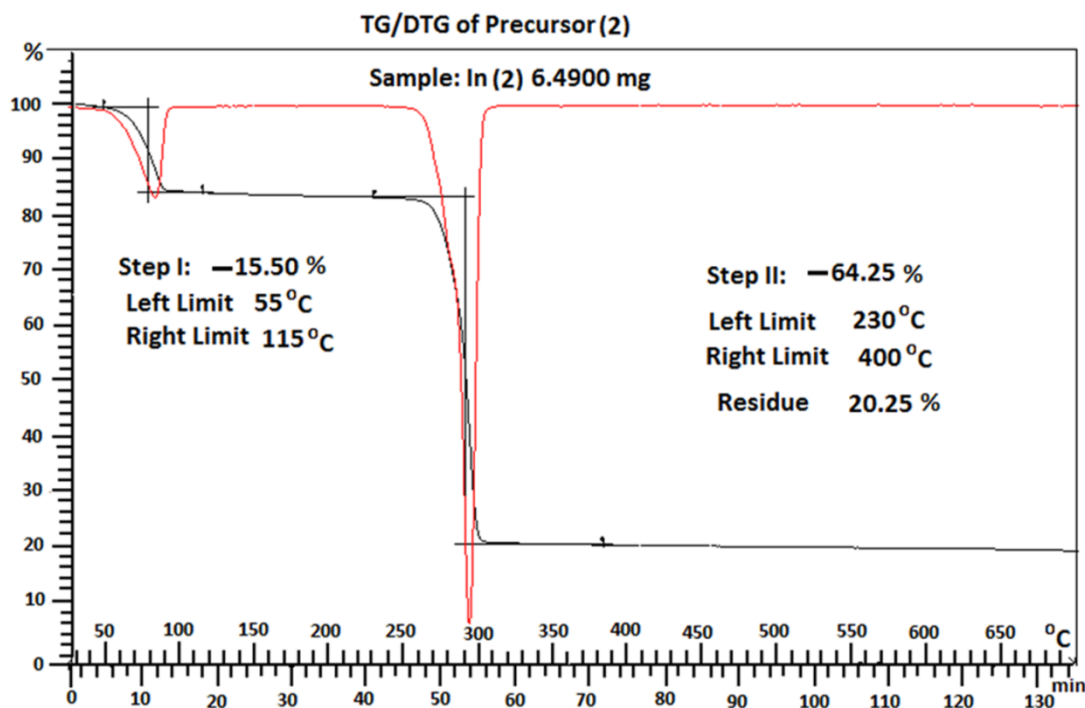
S.Fig. 4b: H-NMR of Precursor [In(S<sub>2</sub>CNBzMe)<sub>3</sub>] (4)



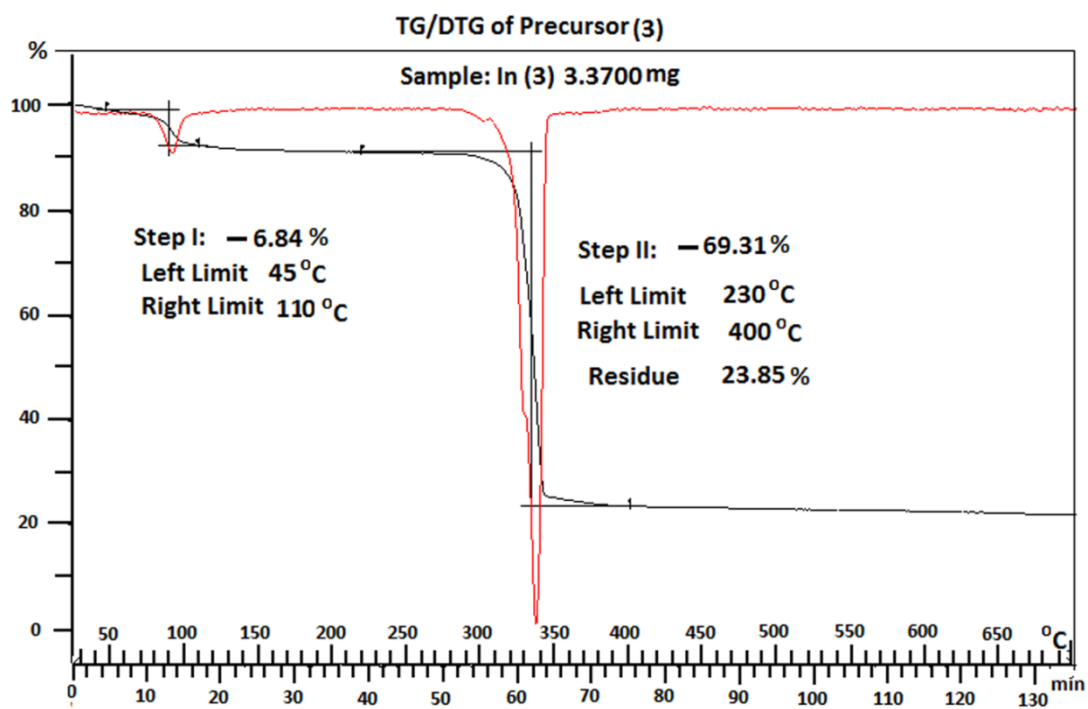
**S. Fig. 4c:** H-NMR of Precursor  $[\text{In}(\text{S}_2\text{CNBzMe})_3]$  (4)



**S. Fig. 5a:** TG/DTG curves presenting losses in weight against temperature for precursor  $[\text{In}(\text{S}_2\text{CNCy}_2)_3] \cdot 2\text{py}$  (1)

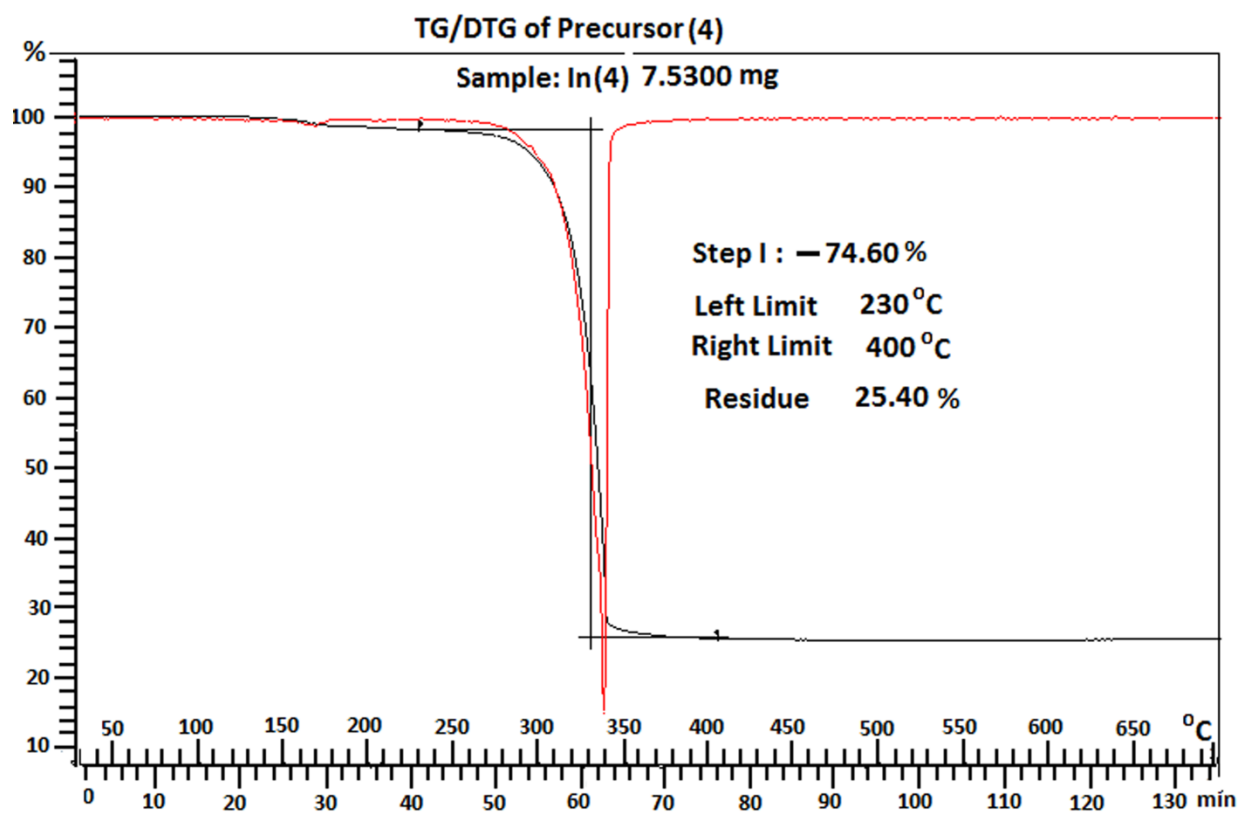


**S. Fig. 5b:** TG/DTG curves presenting losses in weight against temperature for precursor  $[\text{In}(\text{S}_2\text{CN}(\text{Pr})_2)_3] \cdot 1.5\text{py}$  (2)

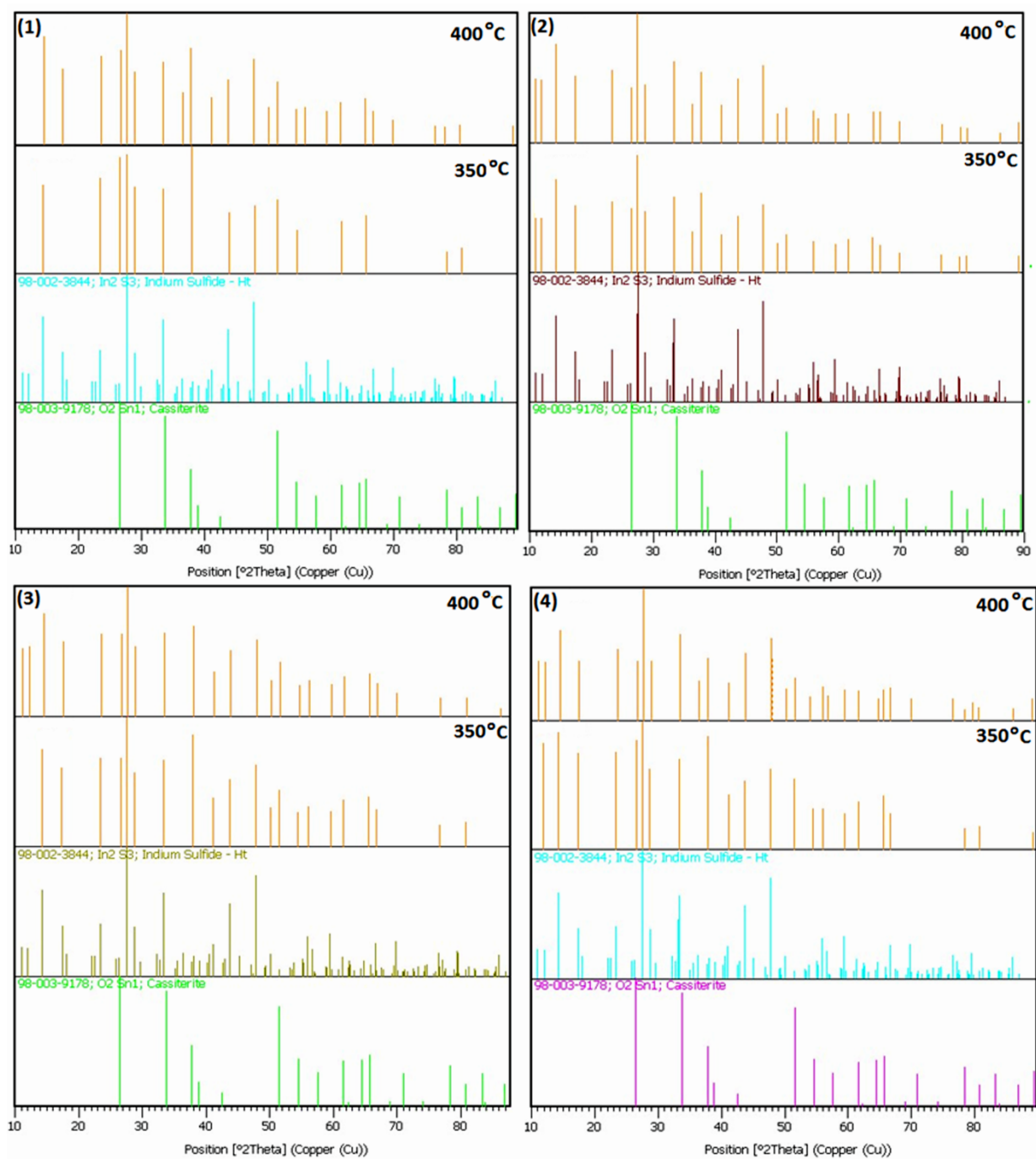


**S. Fig. 5c:** TG/DTG curves presenting losses in weight against temperature for precursor  $[\text{In}(\text{S}_2\text{CPip})_3] \cdot 0.5\text{Py}$  (3)

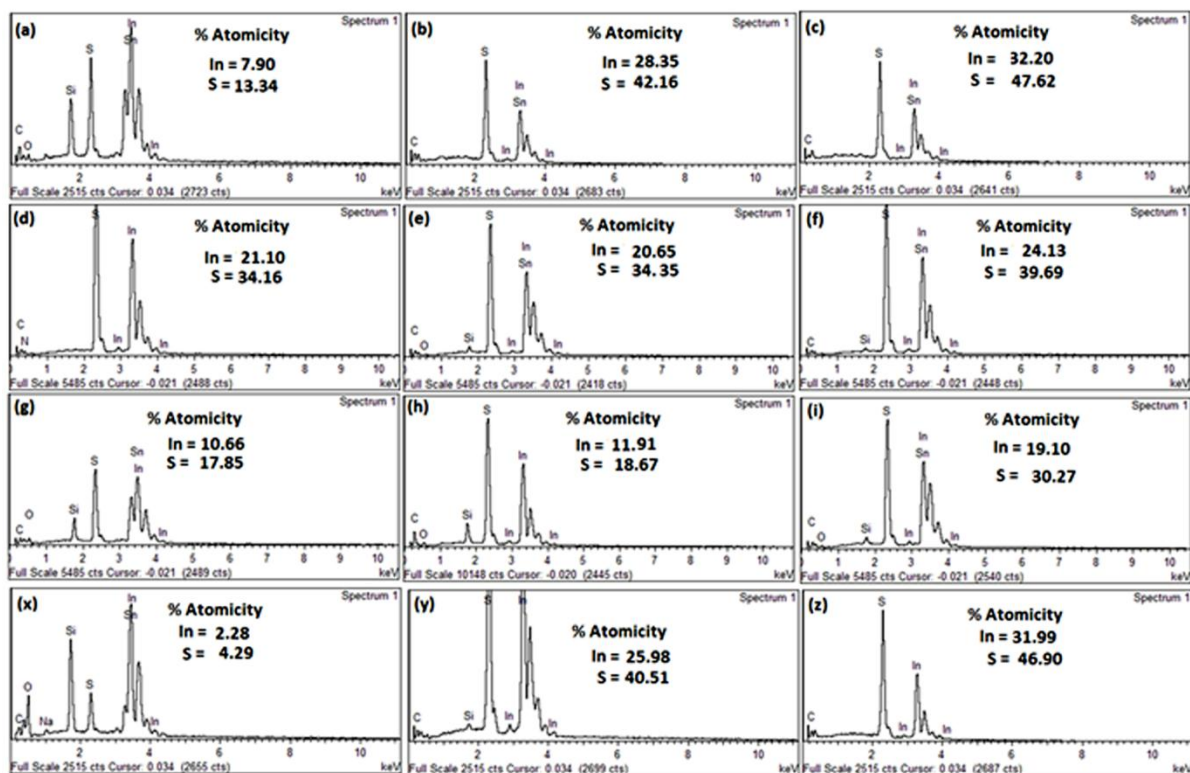




**S. Fig. 5d:** TG/DTG curves presenting losses in weight against temperature for precursor  $[\text{In}(\text{S}_2\text{CNBzMe})_3]$  (4)



**S. Fig. 6:** Comparisons of PXRD patterns of  $\beta$ - $\text{In}_2\text{S}_3$  thin films deposited from precursor  $[\text{In}(\text{S}_2\text{CNCy}_2)_3] \cdot 2\text{py}$  (1),  $[\text{In}(\text{S}_2\text{CN}(\text{iPr})_2)_3] \cdot 1.5\text{py}$  (2),  $[\text{In}(\text{S}_2\text{CPip})_3] \cdot 0.5\text{py}$  (3) and  $[\text{In}(\text{S}_2\text{CNBzMe})_3]$  (4) at 350 and 400°C with the standard ICSD= [98-002-3844] file.



**S. Fig. 7** : EDX spectra of  $\beta$ -In<sub>2</sub>S<sub>3</sub> thin films deposited using precursors [In(S<sub>2</sub>CNCy<sub>2</sub>)<sub>3</sub>]•2py (**1**) at **(a)** 300 °C **(b)** 350 °C **(c)** 400 °C [In(S<sub>2</sub>CN(Pr)<sub>2</sub>)<sub>3</sub>]•1.5py (**2**) at **(d)** 300 °C **(e)** 350 °C and **(f)** 400 °C; [In(S<sub>2</sub>CPip)<sub>3</sub>]•0.5py (**3**) at **(g)** 300 °C **(h)** 350 °C **(i)** 400 °C and [In(S<sub>2</sub>CNBzMe)<sub>3</sub>] (**4**) at **(x)** 300 °C **(y)** 350 °C and **(z)** 400 °C.