Synthesis and Theoretical Study of a Mixed-Ligand Indium(III) Complex for Fabrication of ß-In₂S₃ Thin Films via Chemical Vapor Deposition

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Figure S1: ¹H NMR spectrum of N-Methyldiethanethiolamine ligand in CDCl₃.



Figure S2: ¹H NMR spectrum of ß-heteroarylalkenol ligand in CDCl₃.



Figure S3: ¹⁹F NMR spectrum of ß-heteroarylalkenol ligand in CDCl₃.



Figure S4: ¹H NMR spectrum of [1] recorded in DMSO-d6 (Bruker-600 MHz)



Figure S5: ¹³C (¹H)DEPTQ-135 spectrum of [1] recorded in DMSO-d6 (Bruker-600 MHz)



Figure S6: ¹³C (¹H)DEPTQ-135 NMR spectrum of [2] recorded in CDCl₃.



Figure S7: ${}^{1}H-{}^{13}C$ Heteronuclear multiple quantum coherence (HMQC) spectrum of [2] at room temperature in CDCl₃.



Figure S8: ${}^{1}H-{}^{13}C$ heteronuclear multiple bond correlation (HMBC) spectrum of [2] at room temperature recorded in CDCl₃



Figure S9: ¹⁹F NMR spectrum of [2] recorded in CDCl₃.

Bond lengths	Length/Å
In1-Cl1	2.4147(10)
In1-S1	2.4039(10)
In1-S2	2.4848(11)
In1_a -S2	2.6759(11)
In1-N1	2.394(4)
Bond Angle	Angle/°
Cl1-In1-S1	114.63(4)
Cl1-In1-S2	113.10(4)
Cl1-In1-S2_b	87.18(4)
S1-In1-S2_b	101.49(4)
S1-In1-S2	131.39(4)
S2-In1-S2_b	89.35(6)
N1-In1-Cl1	95.16(9)
N1-In1-S1	84.82(9)
N1-In1-S2_b	171.66(9)
N1-In1-S2	82.36(9)
In1-S2_b-In1_b	111.10(4)

 Table S1: Selected bond lengths and angles of compound [1]



Figure S10: A) Packing of **[2]** along the crystallographic b axis, and B) Packing of **[1]** along the c axis.



Figure S11: Absorption spectrum of complex [2] in CH₃CN as solvent at room temperature.



re S12: EI mass spectrum (70eV) of heteroleptic complex [1].

Figure S13: EI mass spectrum (70eV) of heteroleptic complex [2]

Electron Image 1



Figure S14. Electron image of the obtained In_2S_3 CVD film from compound **[2]**.



Figure S15. Map data of the obtained In_2S_3 CVD film from compound [2].



Figure S16. EDS mapping of the obtained In_2S_3 CVD film from compound **[2]** (The (stoichiometric ratio of In:S = 2:3.35).



Figure S17. Map sum spectrum of the obtained In_2S_3 CVD film from compound [2] (stoichiometric ratio of In:S = 2:3.31)



Figure S18. High-resolution X-ray photoelectron spectra A) O 1s region B) C Is region of CVD

film from compound [2].

 Table S2. XPS elemental quantification of CVD films obtained from compound [2]

Peak	At%
O 1s	10.51
C 1s	50.98
N 1s	2.12
In 3d _{5/2}	13.32
S 2p	22.05
F 1s	1.03

Coordinates (Å) Atom Х Υ Ζ -0.42251 0.008914 1 In -0.59875 2 S -1.38951 -1.02343 2.23854 3 S -1.43449 -1.36759 -2.07935 4 F 1.817605 3.460741 0.978623 5 F 3.629507 2.957203 -0.11797 6 0 0.547052 1.247734 -0.12113 7 F 1.796592 3.429363 -1.19416 8 Ν 1.345433 -1.61805 0.022604 9 Ν -2.56689 0.954945 -0.08248 10 С 1.209859 -2.96148 0.04356 н 11 0.188637 -3.33161 0.02462 12 С 2.592508 -1.063 0.028524 13 С 2.282923 -3.83466 0.078901 14 н -4.905122.114816 0.094662 С 15 -3.14553 0.800556 -1.44508 н 16 -2.55075 1.424835 -2.1177 17 Н -4.17698 1.188749 -1.44993 2.793262 С 18 0.36617 -0.00718 19 н 3.824756 0.691532 0.014054 С 20 1.845038 1.344809 -0.07685 21 С -3.48261 0.417898 0.959962 22 н -3.8857 -0.53093 0.598553 23 н -4.32659 1.114351 1.091245 С 3.723369 -1.91249 0.065328 24 25 Н 4.710247 -1.46249 0.070161 С 26 -2.79873 0.173226 2.306925 27 н -3.54165 -0.24951 2.988547 28 н -2.45262 1.110829 2.750539 С 29 -3.12747 -0.63651 -1.97043 30 Н -3.5341 -0.62616 -2.98524 31 Н -3.77243 -1.28978-1.37553 32 С 3.571849 -3.28663 0.09142 33 н 4.445373 -3.93146 0.118951 34 С -2.25752 2.380936 0.172619 35 Н -1.8278 2.498641 1.168019 36 Н 0.099788 -3.16597 2.996247 37 н -1.51668 2.72695 -0.5482 38 С 2.288167 2.80585 -0.10382

Table S3. The XYZ coordinates of the optimised ground state for [2] (B3lyp/6-31G(d,p)/LanL2DZ level of theory).

Table S4. DFT-calculated compositions (%) of frontier MOs in the S_0 ground state for [2] (B3lyp/6-31G(d, p)/LanL2DZ level of theory).

МО	energy (eV)	component %					
		In	Pyridine	Carbony I: C2, 3, O	S1 and S2	CF ₃	L' = N1, C9, 10,12,13
LUMO+4	1.127	14	23	29	19	5	10
LUMO+3	0.995	15	10	1	21	1	52
LUMO+2	0.381	51	10	6	22	1	10
LUMO+1	-1.042	1	87	7	2	2	1
LUMO	-1.696	0	74	20	1	4	1
номо	-5.748	1	3	6	81	0	9
HOMO-1	-5.931	1	24	53	18	2	2
HOMO-2	-5.960	3	1	2	83	1	10

HOMO-3	-6.891	8	4	2	75	0	11
HOMO-4	-7.089	5	12	1	41	0	41

LUMO: Lowest unoccupied molecular orbital, and HOMO: Highest occupied molecular orbital.



Figure S19. FT-IR spectra of [2] showing the experimental (black) and calculated (red).