Electronic Supplementary Information

Preparation of Seven-Coordinated Hypervalent Tin(IV)-Fused Azobenzene and Applications for Stimuli-Responsive π-Conjugated Polymer Films

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General

^{1}H, $^{13}C\{^{1}H\}$ and ^{119}Sn NMR spectra were recorded on JEOL ECZ400, ECZ400S and ECZ500R instruments at 400, 100 and 186 MHz, respectively. Samples were analyzed in $CDCl_3$ and benzene-d_6, and the chemical shift values were expressed relative to benzene or Me_4Si as an internal standard in $CDCl_3$ for ^{1}H, $^{13}C\{^{1}H\}$ NMR. ^{119}Sn NMR spectra were measured using double NMR tube. The benzene, PA, EDA or DMSO solution of **TAz** were placed in external tube and benzene-d_6 in inner tube. The chemical shift values were expressed relative to Me_4Sn as an external capillary standard. Gel permeation chromatography (GPC) was carried out on a Shimadzu Prominence system equipped with three consecutive polystyrene gel columns (TOSOH TSKgel: $G4000H_{XL}$, $G3000H_{XL}$, $G2500H_{XL}$) using chloroform as an eluent after calibration with standard polystyrene samples. High-resolution mass spectrometry (HRMS) was performed at the Technical Support Office (Department of Synthetic Chemistry and Biological Chemistry, Graduate School of Engineering, Kyoto University), and the HRMS spectra were obtained on a Thermo Fisher Scientific EXACTIVE spectrometer for electrospray ionization (ESI) and a Bruker Daltonics ultrafleXtreme for matrix assisted laser desorption ionization (MALDI) (negative, matrix: *trans*-2-[3-(4-*tert*-butylphenyl)-2-methyl-2-propenylidene]malononitrile (DCTB)). UV–vis spectra were recorded on a SHIMADZU UV-3600i Plus spectrophotometer, and samples were analyzed at room temperature or valuable temperature (VT) with an Oxford Optistat DN2 under N_2. HORIBA JOBIN YVON Fluorolog-3 was used for PL spectra at room temperature under air or VT with an Oxford Optistat DN2 under N_2. Absolute photoluminescence quantum efficiency (Φ_{PL}) was recorded on a Hamamatsu Photonics Quantaurus-QY Plus C13534-01. IKA C-MAG HS 7 digital was used as a hot stirrer. X-ray crystallographic analysis was carried out by Rigaku Saturn 724+ with MicroMax-007HF CCD diffractometer with Varimax Mo optics using graphite-monochromated MoKα radiation. A symmetry-related absorption correction was carried out by using the program ABSCOR.[1] The analysis was carried out with Yadokari-XG.[2] The program ORTEP3[3] and Mercury-4.2.0 were used to generate the X-ray structural diagram. Thermogravimetric analysis (TGA) was recorded on a Hitachi High-Tech Science Corporation STA7200RV. Differential scanning calorimetry (DSC) was recorded on a Hitachi High-Tech Science Corporation DSC7020.

Materials.

Commercially available compounds used without purification:

$Pd_2(dba)_3$ (dba = dibenzylideneacetone) (Tokyo Chemical Industry Co, Ltd.)

2-Dicyclohexylphosphino-2′,4′,6′-triisopropylbiphenyl (XPhos) (Strem Chemicals, Inc.)

Propylamine (PA) (FUJIFILM Wako Pure Chemical Corporation)

Ethylenediamine (EDA) (FUJIFILM Wako Pure Chemical Corporation)

N,*N*,*N*′,*N*′-Tetramethylethylenediamine (TMEDA) (FUJIFILM Wako Pure Chemical Corporation)

N,*N*′-Dimethylethylenediamine (DMEDA) (Tokyo Chemical Industry Co, Ltd.)

1,3-Propanediamine (PDA) (Tokyo Chemical Industry Co, Ltd.)

1,10-Phenanthroline (phen) (FUJIFILM Wako Pure Chemical Corporation)

Commercially available solvents used without purification:

Toluene (deoxidized grade, FUJIFILM Wako Pure Chemical Corporation)

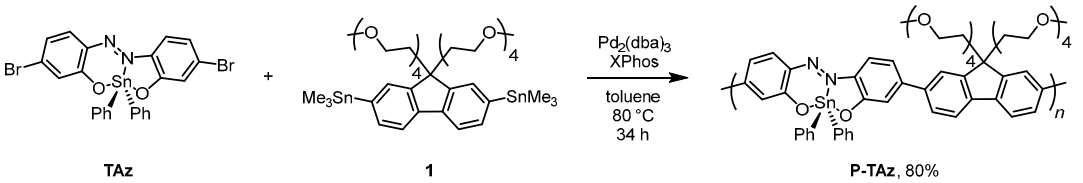
Compounds prepared as described in the literatures:

TAz[4]

(9,9-Di(2,5,8,11-tetraoxatridecan-13-yl)-9*H*-fluorene-2,7-diyl)bis(trimethylstannane) (**1**)[4]

Synthetic procedures and characterization

Synthesis of P-TAz



TAz **1** **P-TAz**, 80%

A mixture of **TAz** (0.0643 g, 0.10 mmol, 1 equiv.), **1** (0.0872 g, 0.10 mmol, 1 equiv.), $Pd_2(dba)_3$ (0.0027 g, 0.0030 mmol, 0.03 equiv.), XPhos (0.0029 g, 0.006 mmol, 0.06 equiv.) in toluene (2.0 mL) was stirred at 80 °C for 34 h under N_2 atmosphere. After cooling to room temperature, the solution was poured into a large amount of hexane to collect the polymer by filtration to afford **P-TAz** (0.0826 g, 80%) as a black solid.

M_n = 18,800, M_w = 80,400, M_w/M_n = 4.3. ^{1}H NMR ($CDCl_3$, 400 MHz) δ 8.10 (br), 7.91 (br), 7.84 (br), 7.80 (br), 7.75 (br), 7.47 (br), 7.29 (br) 7.16 (br), 3.55 (br), 3.42 (br), 3.34 (br), 3.34 (br), 3.32 (br), 3.27 (br), 2.90 (br), 2.57 (br) ppm; $^{13}C\{^1H\}$ NMR ($CDCl_3$, 100 MHz) δ 161.8, 150.3, 139.3, 136.4, 135.9, 130.6, 128.9, 121.9, 121.6, 121.0, 118.0, 117.8, 117.6, 117.5, 71.9, 10.5, 70.4, 70.1, 67.1, 59.0, 51.7, 39.9 ppm. The other $^{13}C\{^1H\}$ signals were not detected due to broadening peaks in a polymer even at high temperature (50 °C). ^{119}Sn NMR ($CDCl_3$, 186 MHz) δ −363.1 (br). The peaks are picked with reference to our previous work including the original NMR spectra of **TAz** and **1**.[4]

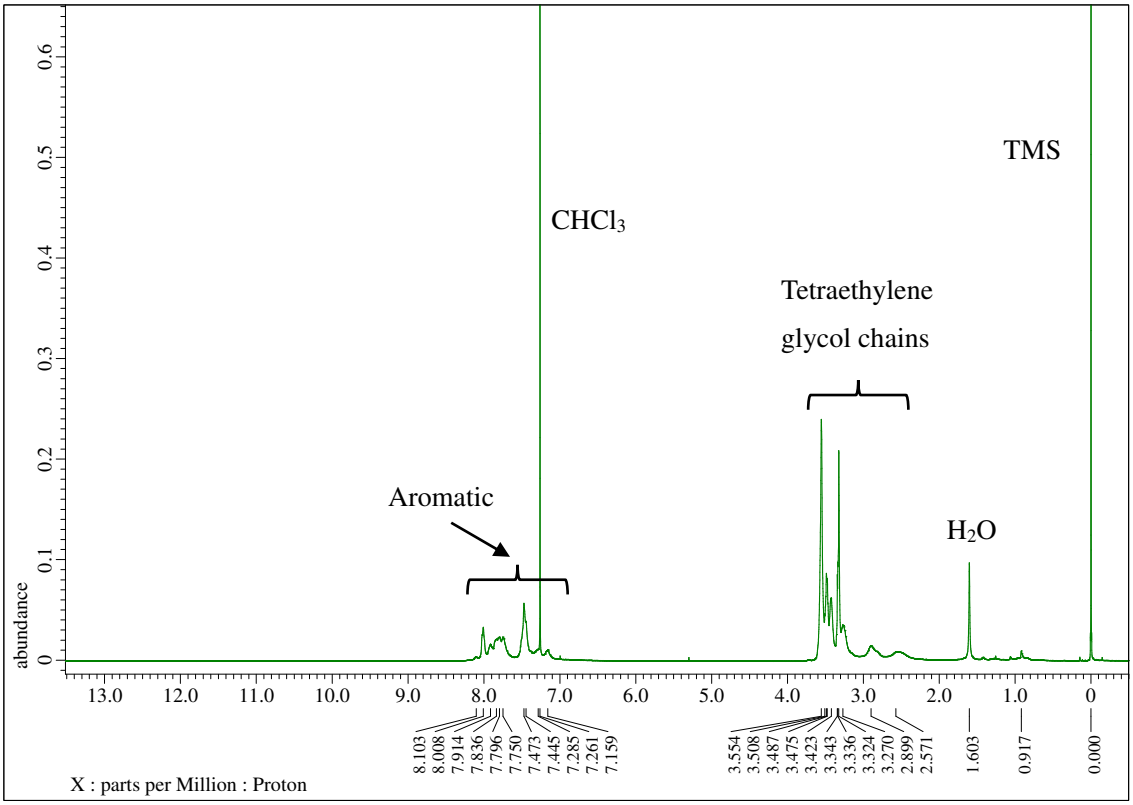


Chart S1. ^{1}H NMR spectrum of **P-TAz** in $CDCl_3$ at 400 MHz.

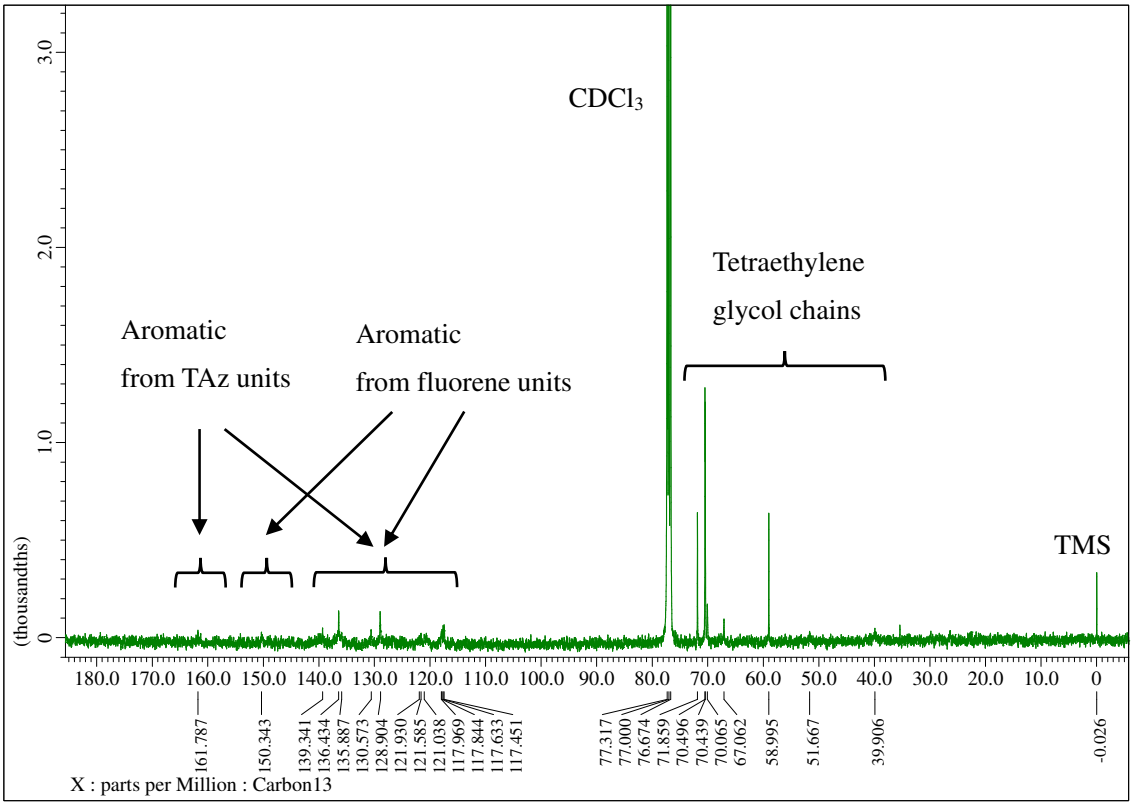


Chart S2. ^{13}C{^{1}H} NMR spectrum of **P-TAz** in $CDCl_3$ at 100 MHz.

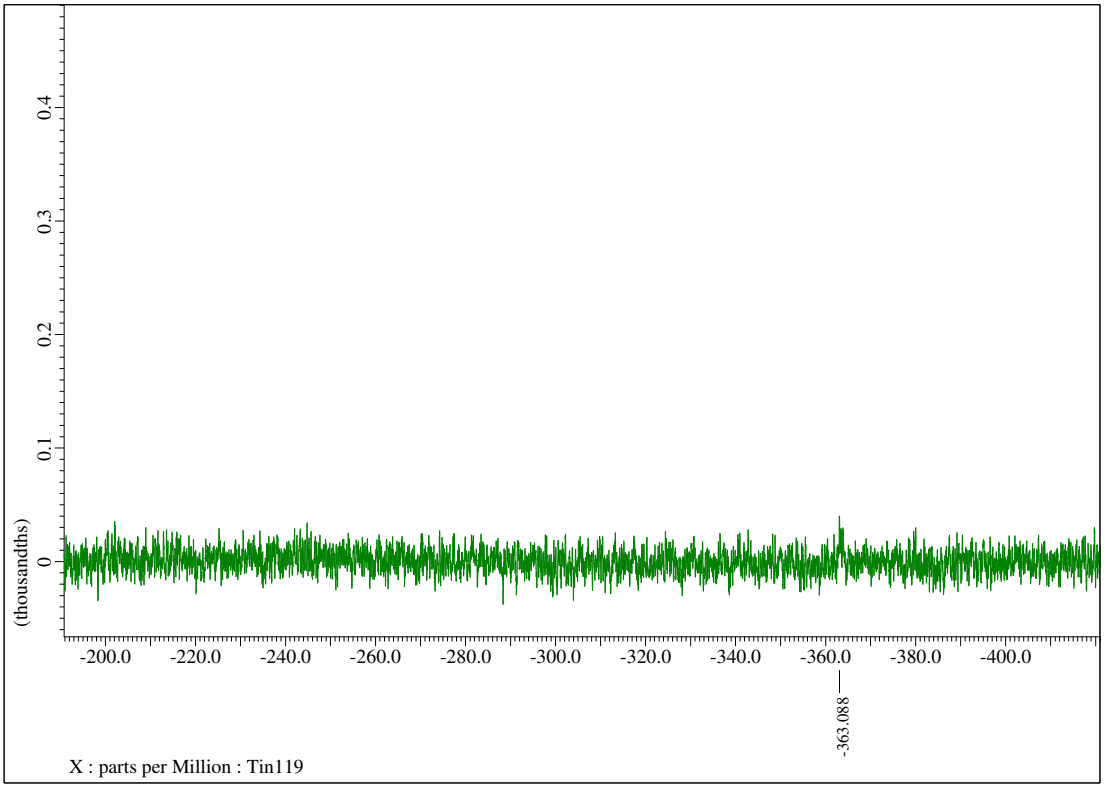


Chart S3. ^{119}Sn NMR spectrum of **P-TAz** in $CDCl_3$ at 186 MHz at 50 °C.

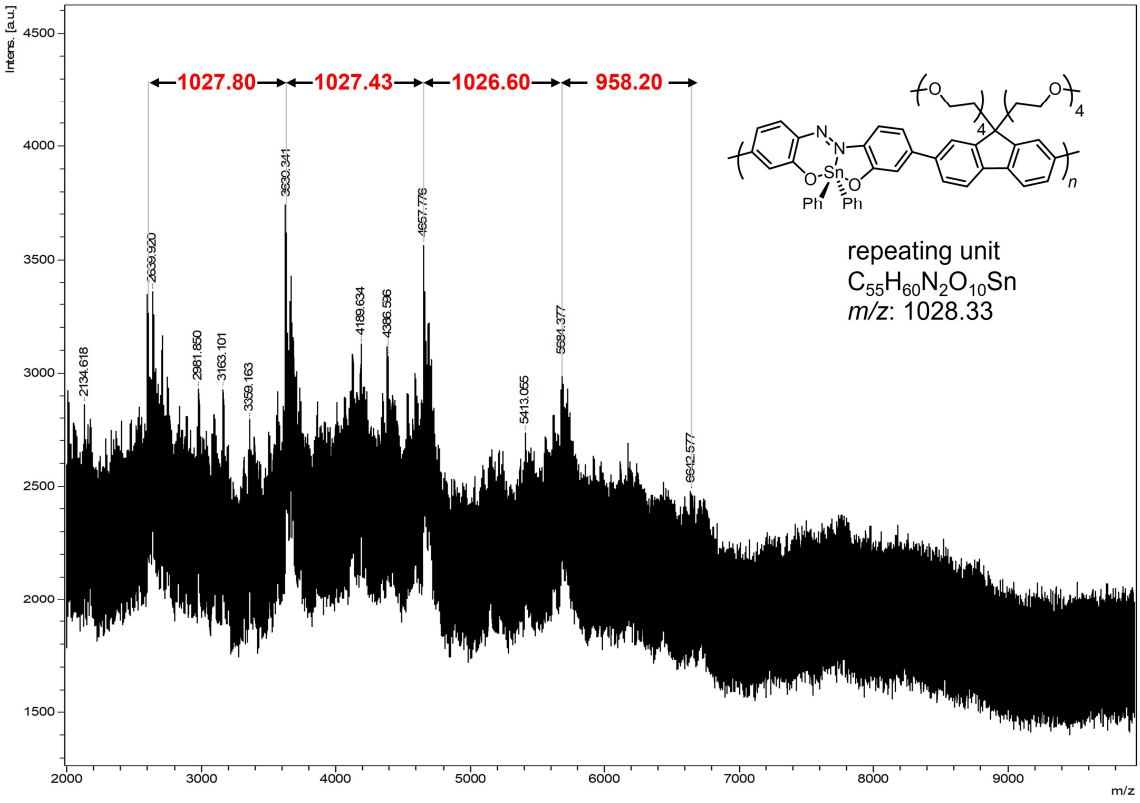


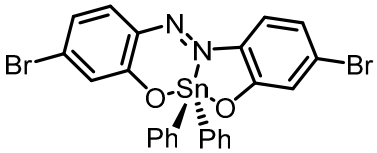
Chart S4. MADLI-TOF MS spectrum of **P-TAz**.

Single crystal X-ray structure analysis of TAz

Intensity data were collected on a Rigaku Saturn 724+ with MicroMax-007HF CCD diffractometer with Varimax Mo optics using graphite-monochromated Mo Kα radiation. The structures were solved and refined by full-matrix least-squares procedures based on F^2 (SHELXL-2018/3).[5]

Table S1. Crystallographic data of **TAz**

Empirical formula	$C_{24}H_{16}Br_2N_2O_2Sn$
Formula weight	642.90
Temperature (K)	143(2)
Wavelength (Å)	0.71075
Crystal system, space group	Monoclinic, $P2_1/c$
Unit cell dimensions (Å)	a = 17.877(7)
	b = 17.298(6)
	c = 7.251(2)
Unit cell dimensions (º)	α = 90
	β = 90.373(5)
	γ = 90
Volume (Å^3)	2242.2(13)
Z, calculated density (g cm^{-3})	4, 1.904
Absorption coefficient	4.727
F(000)	1240
Crystal size (mm)	0.16 × 0.07 × 0.02
θ range for data collection (°)	3.046–27.493
Limiting indices	$-9 \le h \le 8$, $-22 \le k \le 22$, $-22 \le l \le 23$
Reflections collected (unique)	17923/5091 [R(int) = 0.0503]
Completeness to theta	0.989
Max. and min. transmission	1.000, 0.792
Goodness-of-fit on F^2	1.085
Final R indices [$I > 2\sigma(I)$] [a]	R_1 = 0.0391, wR_2 = 0.0673
R indices (all data)	R_1 = 0.0543, wR_2 = 0.0727



TAz

CCDC 2349665

[a] $R_1 = \Sigma(||F_0|-|F_c||)/\Sigma|F_0|$. w$R_2 = [\Sigma w(F^2_0-F^2_c)^2/\Sigma w(F^2_0)^2]^{1/2}$. w $= 1/[\sigma^2(F^2_0)+[(ap)^2+bp]]$, where $p = [\max(F^2_0,0)+2F^2_c]/3$.

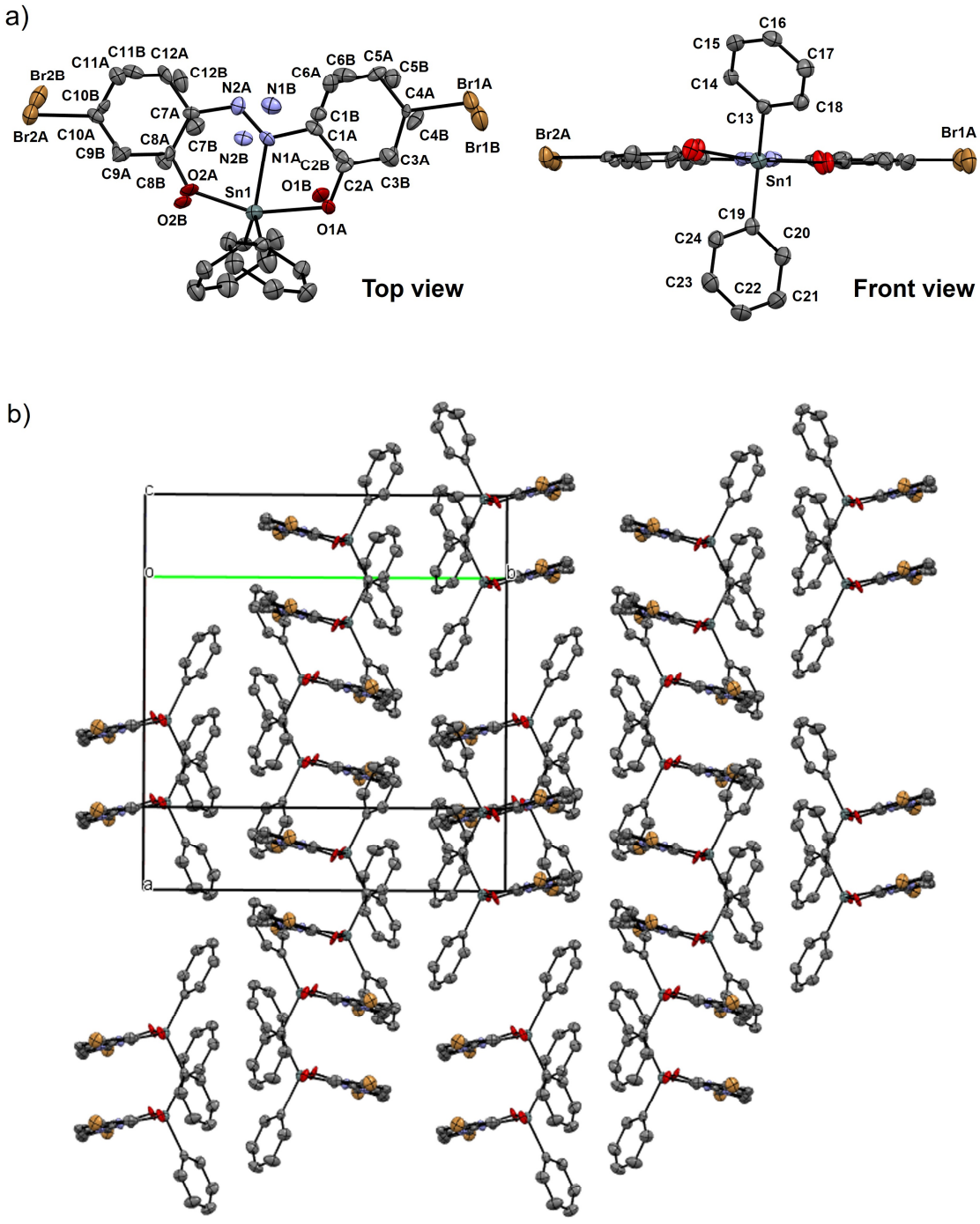


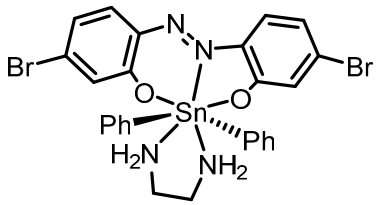
Figure S1. a) ORTEP drawings (occupancy of major conformation A: 51%, occupancy of minor conformation B: 49%) and b) packing diagrams of **TAz**. Thermal ellipsoids are scaled to the 50% probability level. Hydrogen atoms are omitted for the clarity.

Single crystal X-ray structure analysis of TAz-EDA

Intensity data were collected on a Rigaku Saturn 724+ with MicroMax-007HF CCD diffractometer with Varimax Mo optics using graphite-monochromated Mo Kα radiation. The structures were solved and refined by full-matrix least-squares procedures based on F^2 (SHELXL-2018/3).[6] Heavily disordered solvent molecules from EDA were removed by using SQUEEZE procedure.[7]

Table S2. Crystallographic data of **TAz-EDA**

Empirical formula	$C_{26}H_{24}Br_2N_4O_2Sn$
Formula weight	703.00
Temperature (K)	143(2)
Wavelength (Å)	0.71075
Crystal system, space group	Orthorhombic, $P-1$
Unit cell dimensions (Å)	a = 8.454(4)
	b = 12.256(7)
	c = 14.860(8)
Unit cell dimensions (º)	α = 107.396(8)
	β = 95.828(4)
	γ = 103.868(6)
Volume (Å^3)	1401.3(13)
Z, calculated density (g cm^{-3})	2, 1.666
Absorption coefficient	3.792
F(000)	688
Crystal size (mm)	0.20 × 0.12 × 0.06
θ range for data collection (°)	3.100–27.484
Limiting indices	$-10 \le h \le 10$, $-15 \le k \le 14$, $-16 \le l \le 19$
Reflections collected (unique)	11269/6096 [R(int) = 0.0489]
Completeness to theta	0.953
Max. and min. transmission	1.000, 0.544
Goodness-of-fit on F^2	0.988
Final R indices [$I > 2\sigma(I)$] [a]	R_1 = 0.0516, wR_2 = 0.0918
R indices (all data)	R_1 = 0.0691, wR_2 = 0.1018



TAz-EDA

CCDC 2349666

[a] $R_1 = \Sigma(||F_0|-|F_c||)/\Sigma|F_0|$. w$R_2 = [\Sigma w(F^2_0-F^2_c)^2/\Sigma w(F^2_0)^2]^{1/2}$. w $= 1/[\sigma^2(F^2_0)+[(ap)^2+bp]]$, where $p = [\max(F^2_0,0)+2F^2_c]/3$.

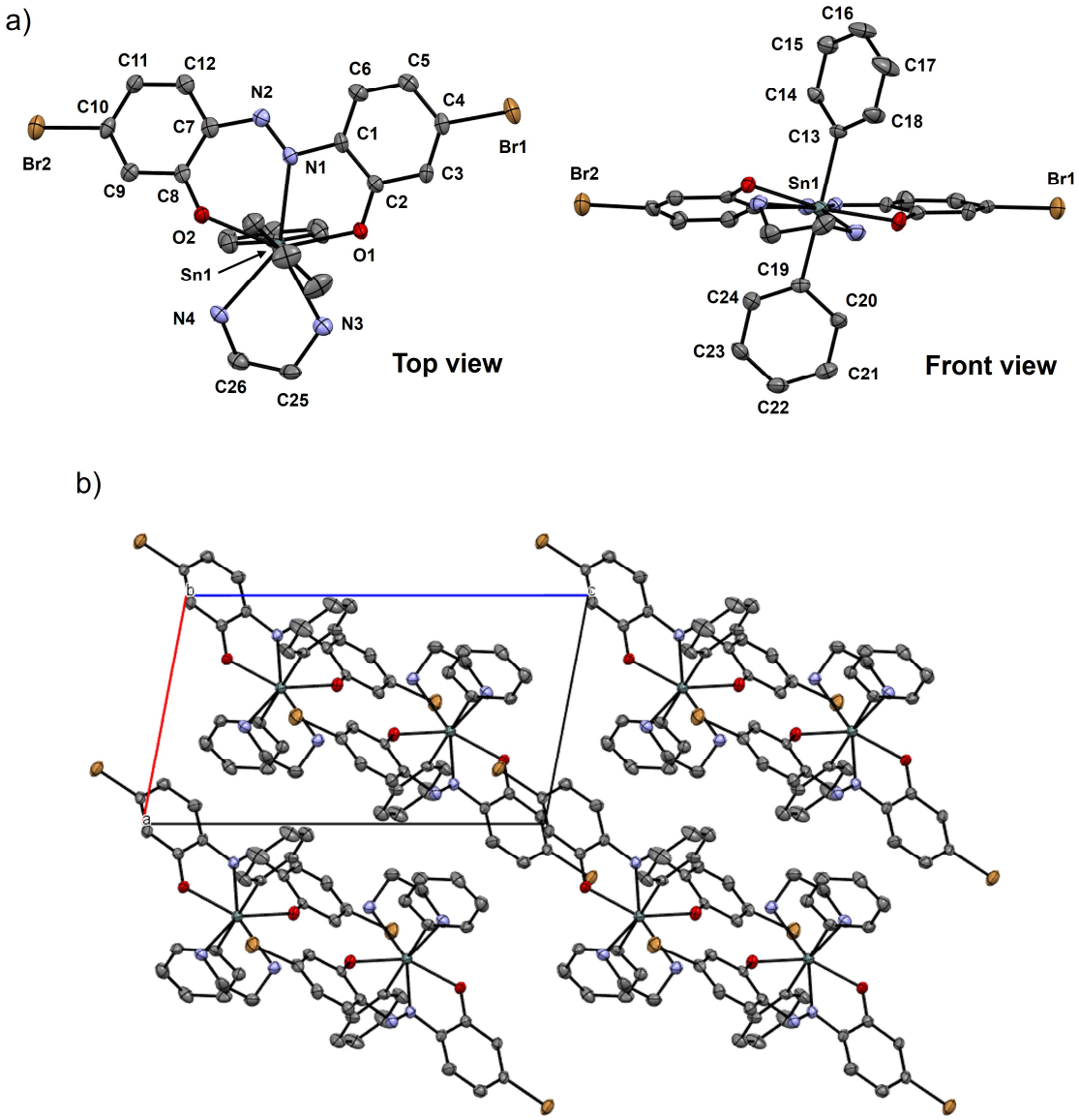


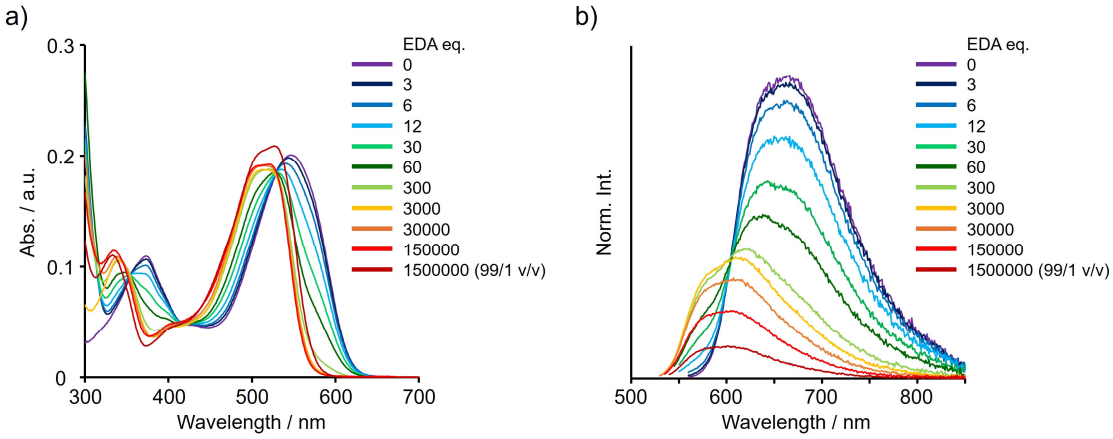
Figure S2. a) ORTEP drawings and b) packing diagrams of **TAz-EDA**. Thermal ellipsoids are scaled to the 50% probability level. Hydrogen atoms are omitted for the clarity.

Selected bond lengths, angles and torsion angles

Table S3. Selected bond lengths, angles, τ_5, and torsion angles from single crystals.

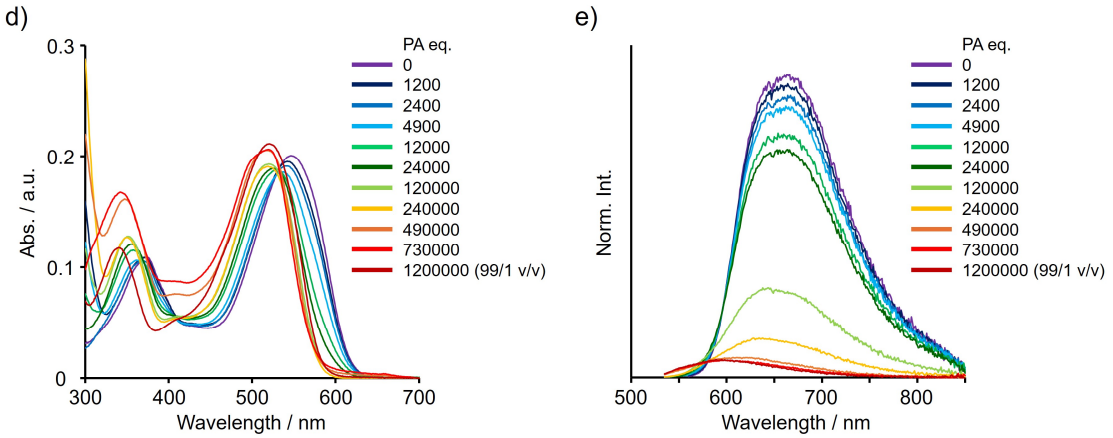
	TAz (major conformation)	**TAz-EDA**
Bond / Å		
Sn(1)–C(13)	2.116(3)	2.140(5)
Sn(1)–C(19)	2.109(3)	2.150(5)
Sn(1)–O(1)	2.16(2)	2.179(3)
Sn(1)–O(2)	2.02(2)	2.230(3)
Sn(1)–N(1)	2.231(7)	2.440(5)
N(1)–N(2)	1.27(1)	1.276(7)
N(1)–C(1)	1.41(2)	1.414(5)
N(2)–C(7)	1.38(2)	1.407(5)
O(1)–C(2)	1.35(2)	1.326(6)
O(2)–C(8)	1.24(3)	1.315(7)
C(1)–C(2)	1.41(3)	1.410(7)
C(7)–C(8)	1.40(3)	1.416(7)
Sn(1)–N(3)	–	2.392(6)
Sn(1)–N(4)	–	2.374(4)
Angle / °		
C(13)–Sn(1)–C(19)	127.9(1)	178.0(2)
N(1)–Sn(1)–C(13)	125.1(2)	91.5(2)
N(1)–Sn(1)–C(19)	106.5(2)	86.9(2)
O(1)–Sn(1)–O(2)	156.6(7)	144.8(1)
N(1)–Sn(1)–O(1)	75.3(4)	71.5(1)
N(1)–Sn(1)–O(2)	82.6(6)	73.9(1)
O(1)–Sn(1)–N(3)	–	73.4(2)
O(2)–Sn(1)–N(4)	–	71.4(1)
N(3)–Sn(1)–N(4)	–	70.5(2)
C(13)–Sn(1)–N(3)	–	87.2(2)
O(13)–Sn(1)–N(4)	–	88.8(2)
Torsion Angle / °		
C(1)–N(1)–N(2)–C(7)	179(1)	179.8(4)
C(1)–C(2)–O(1)–Sn(1)	4(2)	−12.7(6)
C(7)–C(8)–O(2)–Sn(1)	−12(4)	−34.4(7)
C(6)–C(1)–N(1)–N(2)	4(2)	8.3(7)
N(1)–N(2)–C(7)–C(8)	8(2)	12.6(8)

UV–vis absorption and PL titration spectra



c)

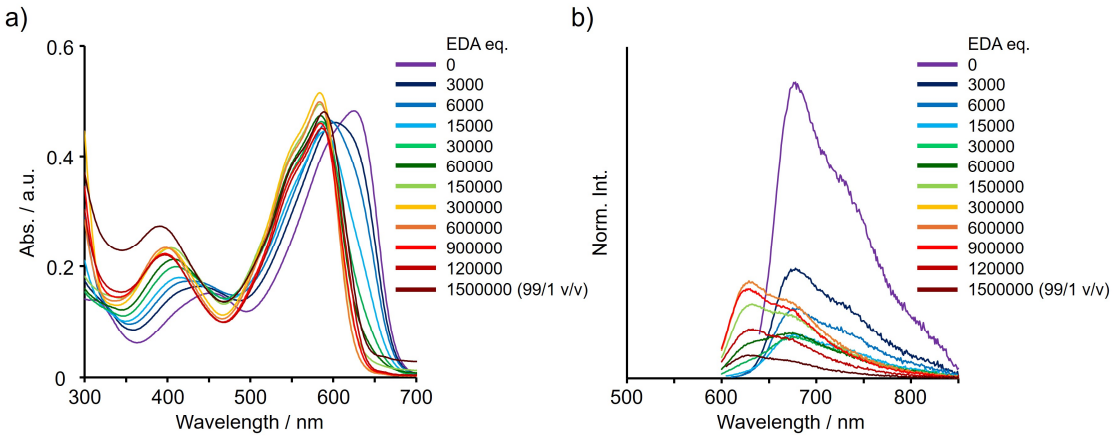
EDA eq.	0	3	6	12	30	60	300	3000	30000	150000	1500000
λ_{abs} / nm	547	544	542	535	531	528	520	513	514	519	527
λ_{PL} / nm	666	666	660	650	643	638	624	609	607	600	601
Φ_{PL} / %	15.6	15.5	15.2	14.1	11.9	9.1	6.2	5.5	4.3	2.8	1.2



f)

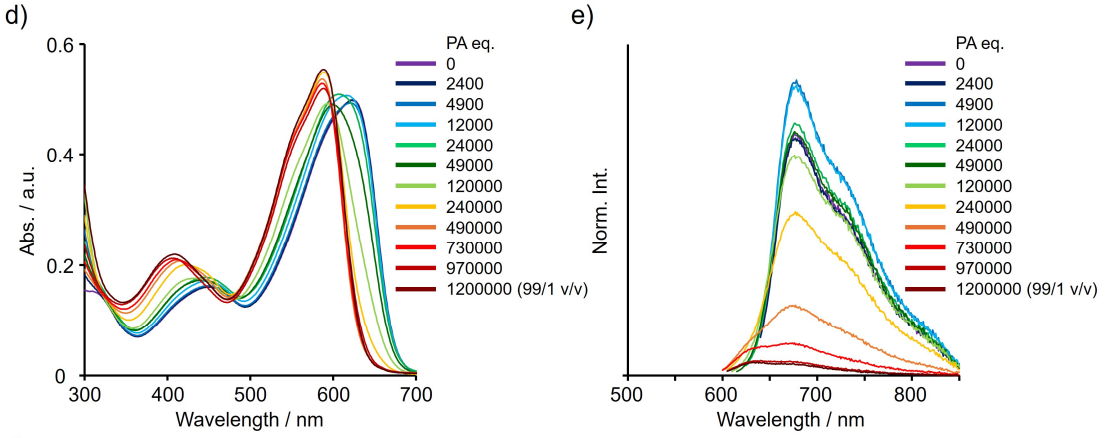
PA eq.	0	1200	2400	4800	12000	24000	120000	240000	480000	730000	1200000
λ_{abs} / nm	547	543	542	537	530	525	520	519	517	519	521
λ_{PL} / nm	666	664	667	662	654	664	638	634	614	598	589
Φ_{PL} / %	15.6	15.4	15.1	14.6	13.4	12.1	4.3	1.9	1.1	1.1	1.0

Figure S3. a) UV–vis absorption, b) PL titration spectra, and c) spectroscopic data of **TAz** (1.0×10^{-5} M) to EDA in toluene, excited at λ_{abs}. d) UV–vis absorption, e) PL titration spectra, and f) spectroscopic data of **TAz** (1.0×10^{-5} M) to PA in toluene, excited at λ_{abs}.



c)

EDA eq.	0	3000	6000	15000	30000	60000	150000	300000	600000	900000	120000	1500000
λ_{abs} / nm	625	602	596	589	586	584	584	584	584	585	586	589
λ_{PL} / nm	676	678	683	678	675	675	632	629	630	628	633	629
Φ_{PL} / %	23.5	9.3	6.7	4.4	3.9	4.6	8.4	7.4	6.3	4.0	3.2	1.4



f)

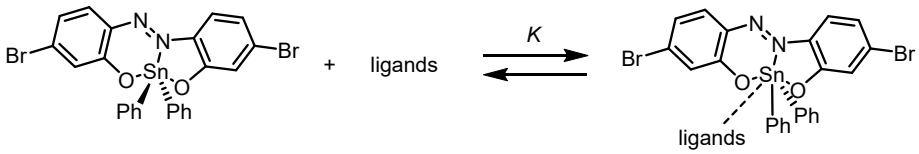
PA eq.	0	2400	4900	12000	24000	49000	120000	240000	490000	730000	970000	1200000
λ_{abs} / nm	625	623	621	616	607	600	593	589	587	586	589	589
λ_{PL} / nm	676	677	678	678	676	676	676	677	677	677	640	637
Φ_{PL} / %	23.5	25.1	29.1	29.1	28.9	28.5	25.7	18.7	8.1	3.6	1.6	1.0

Figure S4. a) UV–vis absorption, b) PL titration spectra, and c) spectroscopic data of **P-TAz** (1.0×10^{-5} M per repeating unit) to EDA in $CHCl_3$, excited at λ_{abs}. d) UV–vis absorption, e) PL titration spectra, and f) spectroscopic data of **P-TAz** (1.0×10^{-5} M per repeating unit) to PA in $CHCl_3$, excited at λ_{abs}.

Determination of binding constant

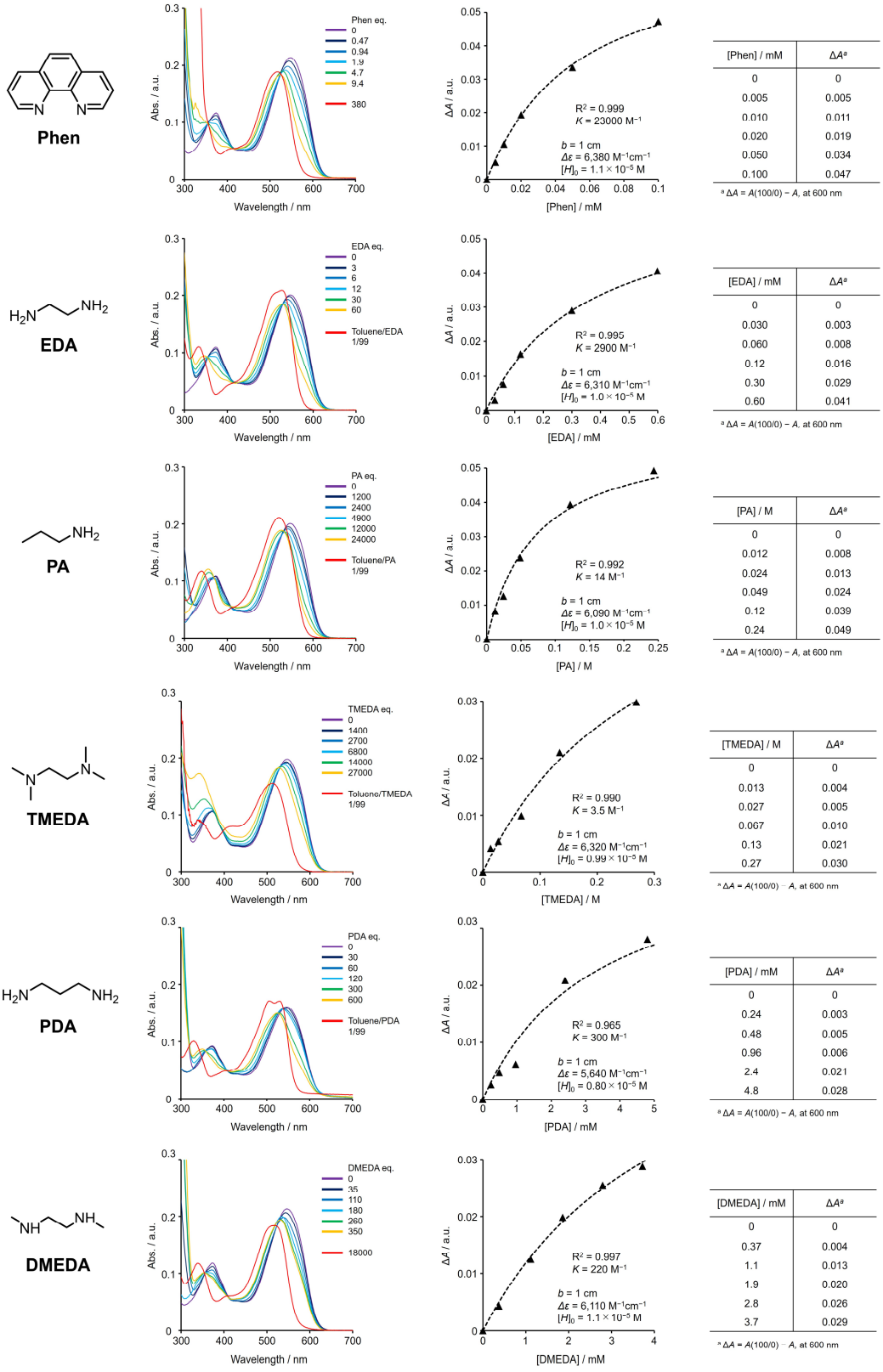
Determination of binding constants for **TAz** was carried out by means of an absorption titration technique in toluene at room temperature (25 °C) (Figure S5) according to our previous research.[6] We assumed equilibrium 1:1 binding of **TAz** and ligands (Scheme S1). The concentration of **TAz**, $[H]_0$ was kept constant and the concentration of guest (ligands), $[G]$ was varied in non-coordinating solvent, toluene. The mixed solutions of **TAz** and guests were prepared, and UV–vis absorption spectra were recorded. The host-guest complexation immediately reach equilibrium after preparation of the mixed solutions. The binding constants were determined by a non-linear curve fitting analysis of hypsochromic shifts and reduction of absorption spectra by increasing guest concentration. The *y*-axis is ΔA and the *x*-axis is $[G]$. The binding constants K_{guest} were calculated from eq(1) using non-linear curve fitting (A: absorbance, b: optical path length, ε: molar extinction coefficient, $\Delta\varepsilon = \varepsilon(100/0) - \varepsilon(1/99)$). A(x/y) or ε(x/y) means a value of an absorbance or a molar extinction coefficient of a sample in toluene/ligands = x/y v/v, respectively. Since isosbestic points were observed with most bidentate ligands, especially for pairs with large binding constants, K was calculated assuming that the binding of the amine to the tin center is the rate-determining step in the reaction.

$$\Delta A = (b\Delta\varepsilon/2K_{guest})[1 + K_{a,guest}[G] + K_{guest}[H_0] - \{(1 + K_{guest}[H_0] + K_{guest}[G])^2 - 4K_{guest}^2[G][H_0]\}^{1/2}] \quad (1)$$



Host **Guest** **1:1 Complex**

Scheme S1. Equilibrium reaction between host **TAz** and guest ligands.



[Phen] / mM	ΔA^a
0	0
0.005	0.005
0.010	0.011
0.020	0.019
0.050	0.034
0.100	0.047

[a] $\Delta A = A(100/0) - A$, at 600 nm

[EDA] / mM	ΔA^a
0	0
0.030	0.003
0.060	0.008
0.12	0.016
0.30	0.029
0.60	0.041

[a] $\Delta A = A(100/0) - A$, at 600 nm

[PA] / M	ΔA^a
0	0
0.012	0.008
0.024	0.013
0.049	0.024
0.12	0.039
0.24	0.049

[a] $\Delta A = A(100/0) - A$, at 600 nm

[TMEDA] / M	ΔA^a
0	0
0.013	0.004
0.027	0.005
0.067	0.010
0.13	0.021
0.27	0.030

[a] $\Delta A = A(100/0) - A$, at 600 nm

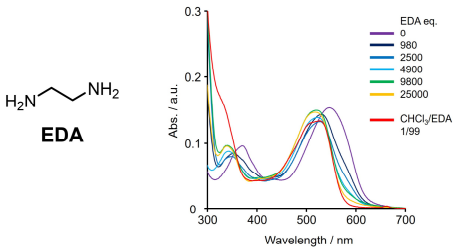
[PDA] / mM	ΔA^a
0	0
0.24	0.003
0.48	0.005
0.96	0.006
2.4	0.021
4.8	0.028

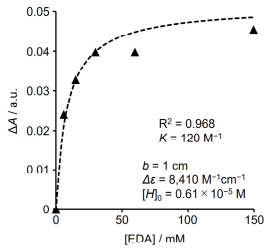
[a] $\Delta A = A(100/0) - A$, at 600 nm

[DMEDA] / mM	ΔA^a
0	0
0.37	0.004
1.1	0.013
1.9	0.020
2.8	0.026
3.7	0.029

[a] $\Delta A = A(100/0) - A$, at 600 nm

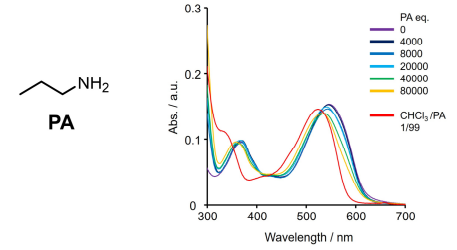
Figure S5. UV–vis absorption titration spectra, non-linear curve fitting graphs, and parameters of **TAz** with ligands in toluene at room temperature.

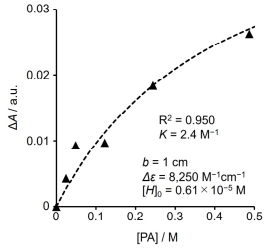




[EDA] / mM	ΔA^a
0	0
6.0	0.024
15	0.033
30	0.040
60	0.040
150	0.046

[a] $\Delta A = A(100/0) - A$, at 600 nm





[PA] / M	ΔA^a
0	0
0.024	0.004
0.049	0.009
0.12	0.010
0.24	0.018
0.49	0.026

[a] $\Delta A = A(100/0) - A$, at 600 nm

Figure S6. UV–vis absorption titration spectra, non-linear curve fitting graphs, and parameters of **TAz** with ligands in $CHCl_3$ at room temperature.

Computational details for theoretical calculation

The Gaussian 16 program package[8] was used for computation of single molecules. We optimized the structures of **TAz**, **TAz-PA**, **TAz-EDA**, **TAz-Phen**, **M-TAz**, **M-TAz-PA**, **M-TAz-EDA**, **M-TAz-Phen** in the ground state (S_0) and calculated their molecular orbitals. The density functional theory (DFT) was applied for the optimization in the S_0 at an LanL2DZ level for Sn and an B3LYP/6-311G(d,p) level for the other elements. We calculated energy of the $S_0 \rightarrow S_1$ and $S_0 \rightarrow S_2$ transition with optimized geometries in the S_0 states by time-dependent (TD-) DFT at an B3LYP/6-311G(d,p) level. Natural bond orbital (NBO) calculation was carried out by DFT at an B3LYP/6-311G(d,p).

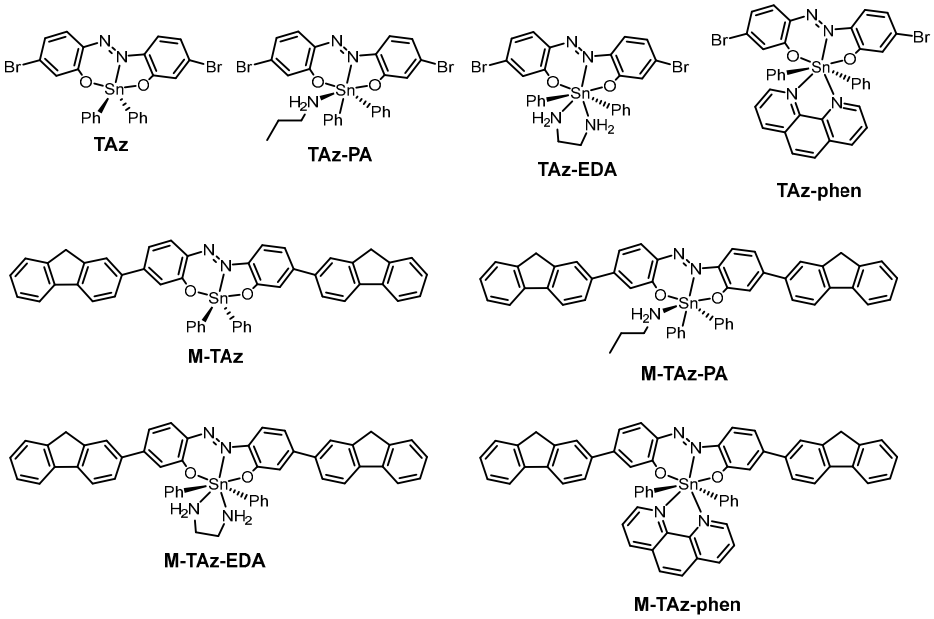


Table S4. Results of the $S_0 \rightarrow S_1$ transition of TAz compounds from TD-DFT calculations

	Transition	Energy gap / eV	Wavelength / nm	Oscillator Strength	Assignment (Weight)
TAz	$S_0 \rightarrow S_1$	2.4739	501.17	0.4048	HOMO → LUMO (0.69160)
					HOMO–2 → LUMO (0.13029)
TAz-PA	$S_0 \rightarrow S_1$	2.6004	476.79	0.3946	HOMO → LUMO (0.69268)
TAz-EDA	$S_0 \rightarrow S_1$	2.6044	476.06	0.4088	HOMO → LUMO (0.69694)
					HOMO–2 → LUMO (0.11487)
TAz-Phen	$S_0 \rightarrow S_1$	2.5309	489.89	0.0073	HOMO → LUMO (0.36133)
					HOMO → LUMO+1 (0.60413)
	$S_0 \rightarrow S_2$	2.6016	476.57	0.3075	HOMO → LUMO (0.56881)
					HOMO → LUMO+1 (–0.35845)
					HOMO → LUMO+2 (–0.18336)
M-TAz	$S_0 \rightarrow S_1$	2.2655	547.27	1.2620	HOMO → LUMO (0.70020)
M-TAz-PA	$S_0 \rightarrow S_1$	2.3835	520.19	1.2420	HOMO → LUMO (0.69848)
M-TAz-EDA	$S_0 \rightarrow S_1$	2.3922	518.29	1.1089	HOMO → LUMO (0.70013)
M-TAz-Phen	$S_0 \rightarrow S_1$	2.3661	523.99	0.1325	HOMO → LUMO (0.35217)
					HOMO → LUMO+1 (0.60514)
	$S_0 \rightarrow S_2$	2.3931	518.08	0.8591	HOMO → LUMO (0.59847)
					HOMO → LUMO+1 (–0.35809)

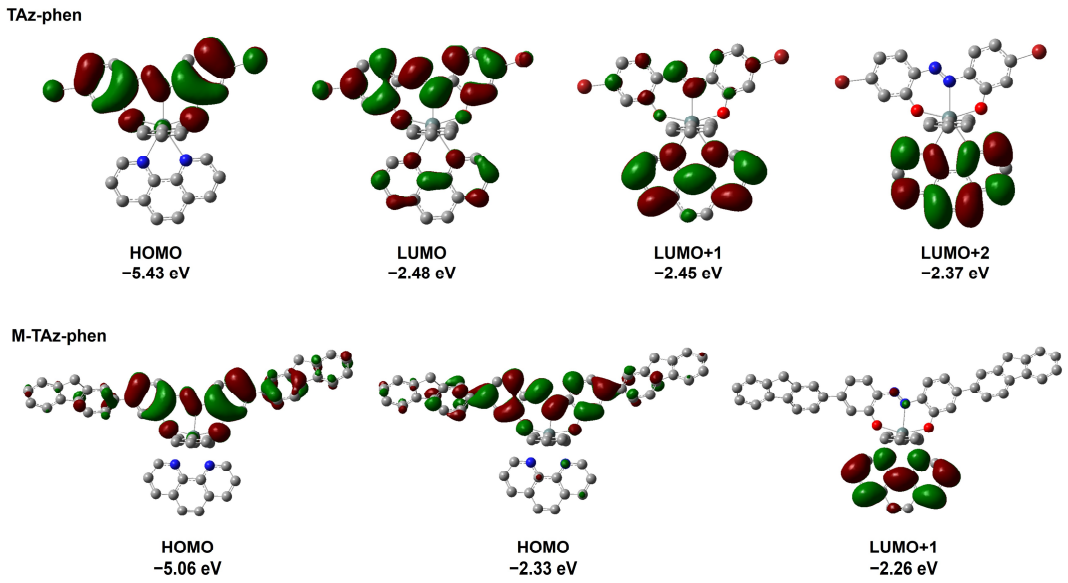


Figure S7. Selected MOs of **TAz-phen** and **M-TAz-phen** obtained with DFT calculations (isovalue = 0.02). Hydrogen atoms are omitted for clarity.

NBO calculation

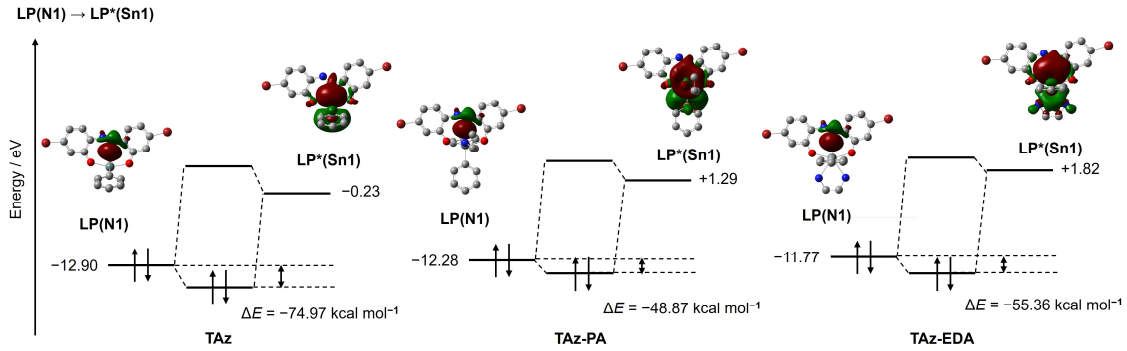


Figure S8. The results of the NBO calculations of the **TAz** complexes focused on the free energy of the donor–acceptor interactions of LP(N1)→LP*(Sn1). The figure shows representative energy diagrams and NBOs of **TAz** (isovalue = 0.02). Δ*E*: The second-order perturbation stabilization energy. Hydrogen atoms are omitted for clarity.

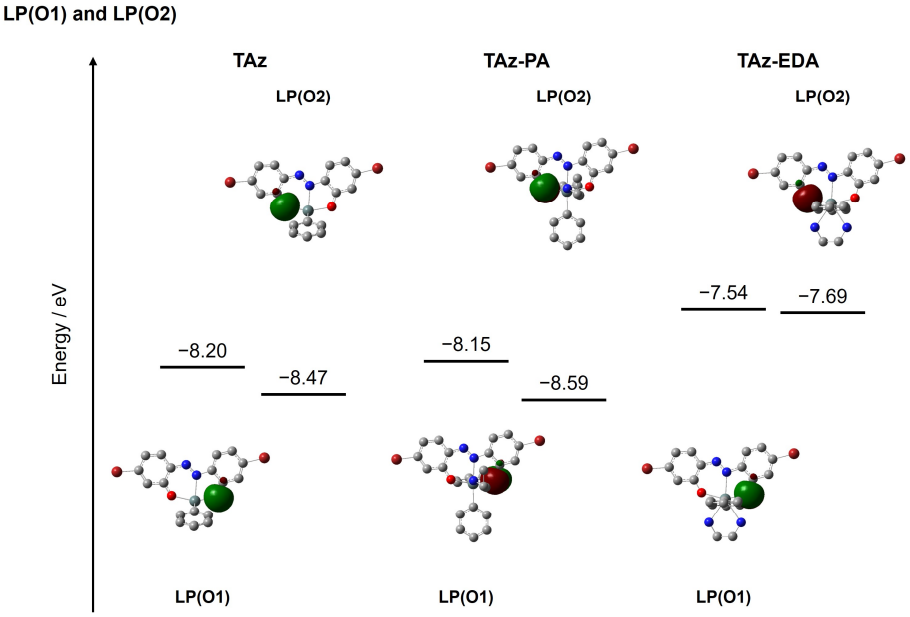


Figure S9. The results of NBO calculations of the **TAz** focused on the energy levels of LP(O1) and LP(O2). The figure shows representative energy diagrams and NBOs of **TAz**, **TAz-PA** and **TAz-EDA** (isovalue = 0.02). Hydrogen atoms are omitted for clarity.

Detailed information on vapochromism

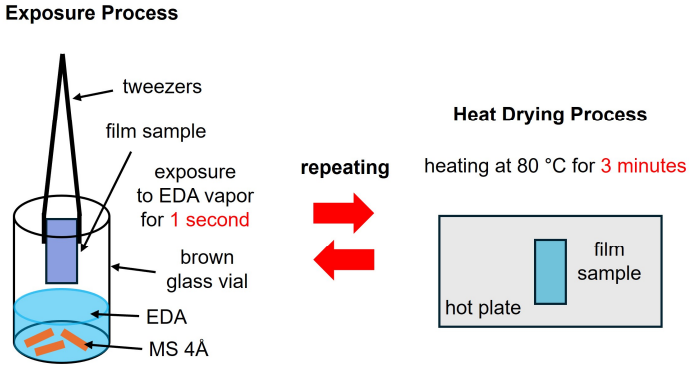


Figure S10. Illustration of the exposure to EDA vapor and the heat drying process. All processes were performed under atmospheric conditions. The molecular sieve (MS 4Å) was used for dehydration of EDA. New EDA was used each time to prevent EDA degradation due to moisture.

Table S5. Spectroscopic data of vapochromism with the **P-TAz** film and EDA vapor.

Number of cycles	λ_{abs} / nm	λ_{PL} [a] / nm	Φ_{PL} [a,b] / %
Initial	643	702	2.1
1st EDA exposure	600	696	0.3
1st heat dry	642	701	1.7
2nd EDA exposure	598	696	0.3
2nd heat dry	641	702	1.6
3rd EDA exposure	598	697	0.3
3rd heat dry	641	701	1.4
4th EDA exposure	598	699	0.2
4th heat dry	640	702	1.5
5th EDA exposure	598	694	0.3
5th heat dry	639	700	1.6

[a] Excited at λ_{abs}.

[b] Absolute PL quantum yield.

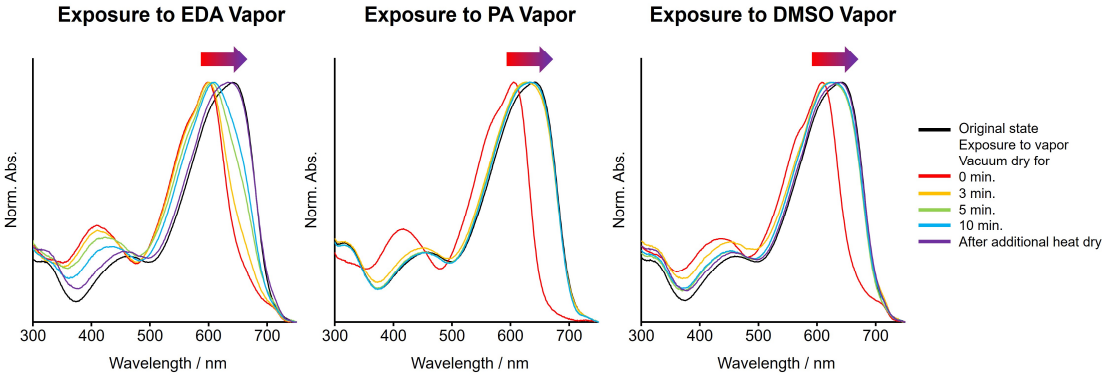


Figure S11. Time dependency of recovery behavior. After exposure to each vapor (EDA, PA and DMSO), the films were vacuum dried at room temperature and UV–vis absorption spectra were measured after certain time (3, 5, and 10 min.). Additional drying procedures (100 ℃ for 3 min) were performed for films after exposure to EDA and DMSO vapor.

Detailed information on thermochromism

Table S6. Spectroscopic data of thermochromism with the **P-TAz** and phen film.

Temp.	λ_{abs} / nm	λ_{PL} [a] / nm
30 °C	587	651
60 °C	587	655
90 °C	587	669
120 °C	607	707
150 °C	617	727

[a] Excited at 593 nm.

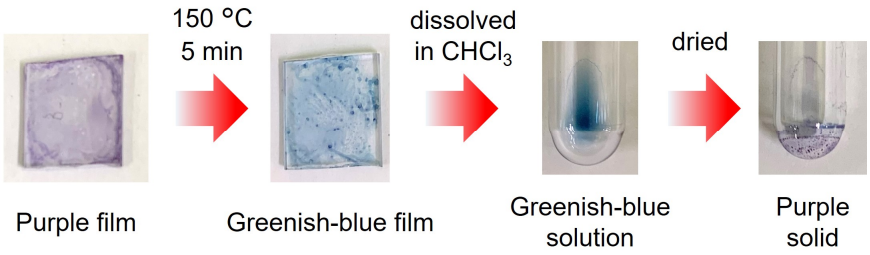


Figure S12. Changes in the film appearance by consecutive heating, dissolution in $CHCl_3$, and drying. Finally, the purple solid was recovered after the heating process causing color change.

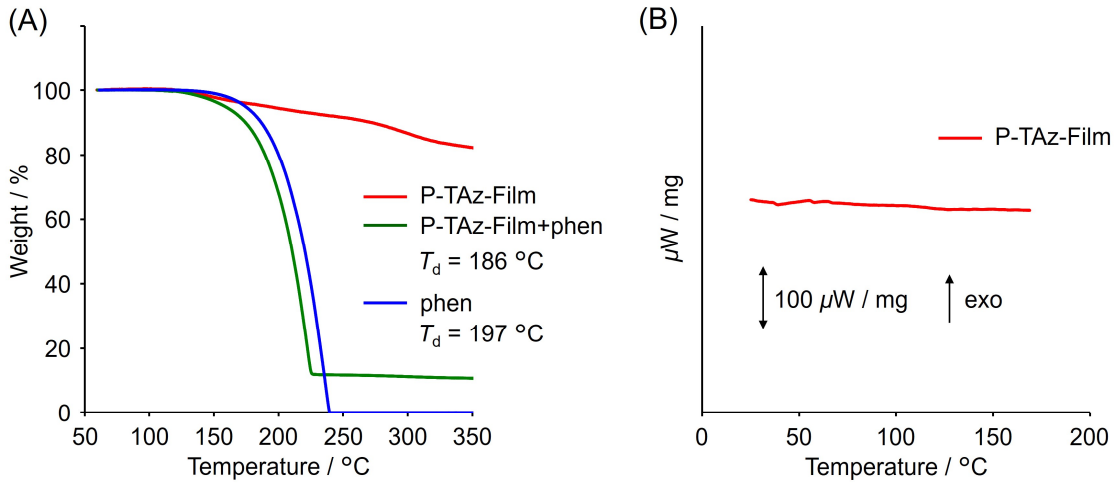


Figure S13. (A) Thermogravimetric analysis (TGA) of **P-TAz** in film, **P-TAz**/phen (1/8 w/w) in film, and phen under air (scan rate, 2 °C min^{-1}). T_d: Onset temperature of the degradation curve calculated from an extrapolation method. (B) The first scan of the differential scanning calorimetry (DSC) curve of **P-TAz** in film (scan rate, 2 °C min^{-1}) under N_2. All of the films were prepared by a drop-casting method from $CHCl_3$ solution at 60 °C.

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Coordinates for optimized structures with theoretical calculation

TAz

Center Number	Atomic Number	Atom	Coordinates (Angstroms)		
			X	Y	Z
1	50	Sn	-0.105809	1.177153	-0.000029
2	7	N	0.395384	-2.024487	0.000101
3	6	C	1.752901	-1.852813	0.000084
4	6	C	2.483158	-3.068255	0.00013
5	6	C	2.466988	-0.609363	0.000027
6	6	C	3.85668	-3.096644	0.000122
7	1	H	1.907429	-3.985638	0.000173
8	6	C	3.879609	-0.655607	0.000018
9	6	C	4.538674	-1.866626	0.000065
10	1	H	4.401399	-4.030013	0.000159
11	1	H	4.416468	0.283163	-0.000026
12	6	C	-1.795058	-1.370821	0.000083
13	6	C	-2.667341	-0.250384	0.000057
14	6	C	-2.304348	-2.675663	0.000113
15	6	C	-4.055945	-0.480309	0.000063
16	6	C	-3.669242	-2.891402	0.000117
17	1	H	-1.610336	-3.505165	0.000132
18	6	C	-4.525709	-1.779827	0.000091
19	1	H	-4.723912	0.369802	0.000044
20	1	H	-4.07278	-3.894291	0.000139
21	7	N	-0.427732	-1.049709	0.000069
22	8	O	1.877768	0.554558	-0.000015
23	8	O	-2.17655	0.97247	0.000028
24	35	Br	-6.418143	-2.082428	0.000094
25	35	Br	6.451268	-1.882809	0.000051
26	6	C	0.009708	2.110429	-1.901916
27	6	C	1.2474	2.329473	-2.520602
28	6	C	-1.159127	2.536592	-2.547081
29	6	C	1.314318	2.96152	-3.760758
30	1	H	2.159145	2.002498	-2.034587
31	6	C	-1.089153	3.167799	-3.787665
32	1	H	-2.12298	2.370206	-2.08054
33	6	C	0.146567	3.380743	-4.395004
34	1	H	2.277608	3.124783	-4.231547
35	1	H	-1.999865	3.491451	-4.27962
36	1	H	0.199608	3.87159	-5.36058
37	6	C	0.009767	2.110676	1.901732
38	6	C	1.247471	2.32977	2.520376
39	6	C	-1.15905	2.536963	2.546849

40	6	C	1.314419	2.961988	3.760443
41	1	H	2.159202	2.0027	2.034397
42	6	C	-1.089046	3.168341	3.787344
43	1	H	-2.122911	2.370538	2.080339
44	6	C	0.146686	3.381334	4.394642
45	1	H	2.277718	3.125289	4.2312
46	1	H	-1.999744	3.492089	4.279262
47	1	H	0.199751	3.872314	5.360148

TAz-PA

Center Number	Atomic Number	Atom	Coordinates (Angstroms)		
			X	Y	Z
1	50	Sn	0.001321	1.03334	0.346997
2	35	Br	6.404577	-2.034358	-0.040159
3	35	Br	-6.467116	-1.875664	-0.742492
4	8	O	-1.869058	0.475705	-0.352186
5	8	O	2.065284	0.845015	0.33754
6	6	C	-0.322401	0.582482	2.430439
7	6	C	-2.465338	-0.695202	-0.380027
8	6	C	-4.559897	-1.910639	-0.570731
9	6	C	-3.870738	-0.71572	-0.516964
10	1	H	-4.383233	0.23526	-0.568571
11	6	C	-0.189766	3.145649	0.043167
12	6	C	-3.911746	-3.151919	-0.504895
13	1	H	-4.472449	-4.074766	-0.549005
14	6	C	4.501119	-1.800753	-0.055047
15	6	C	3.981769	-0.535585	0.14441
16	1	H	4.61686	0.322653	0.315418
17	6	C	-2.539652	-3.149748	-0.389371
18	1	H	-1.986311	-4.079955	-0.345954
19	6	C	3.689997	-2.925275	-0.268978
20	1	H	4.132333	-3.90029	-0.418931
21	6	C	-1.783333	-1.957157	-0.320793
22	6	C	2.584795	-0.350753	0.139233
23	6	C	2.318529	-2.755571	-0.283382
24	1	H	1.654725	-3.594632	-0.445788
25	6	C	1.756635	-1.486908	-0.086192
26	7	N	-0.420324	-2.178816	-0.249182
27	7	N	0.384625	-1.208017	-0.105358
28	6	C	-1.40012	3.710686	-0.381602
29	6	C	0.889079	4.000945	0.308972
30	6	C	0.763784	5.380518	0.146671
31	6	C	-1.526702	5.090456	-0.544654
32	6	C	-0.444403	5.927244	-0.28154
33	1	H	1.837862	3.590393	0.639221

34	1	H	1.60873	6.027772	0.356661
35	1	H	-2.253383	3.070878	-0.581878
36	1	H	-2.471556	5.511378	-0.87212
37	1	H	-0.542875	7.00017	-0.405326
38	6	C	0.754025	0.393296	3.308636
39	6	C	-1.621644	0.509326	2.952357
40	6	C	-1.839959	0.247774	4.304558
41	6	C	0.539516	0.131406	4.661312
42	6	C	-0.758591	0.056572	5.161542
43	1	H	-2.478274	0.657361	2.303006
44	1	H	-2.853652	0.193124	4.687355
45	1	H	1.77204	0.45426	2.939086
46	1	H	1.386284	-0.013153	5.32409
47	1	H	-0.926436	-0.14744	6.213488
48	1	H	-0.604949	1.31135	-2.405488
49	1	H	0.354415	-0.000993	-2.390457
50	6	C	1.390816	1.755959	-2.728972
51	1	H	2.336874	1.344613	-2.369985
52	1	H	1.317472	2.772301	-2.338955
53	6	C	1.358382	1.772663	-4.260851
54	1	H	2.139571	2.461868	-4.599621
55	1	H	0.407274	2.203567	-4.597185
56	6	C	1.572237	0.403304	-4.913877
57	1	H	1.591924	0.488042	-6.002899
58	1	H	2.521096	-0.040829	-4.597841
59	1	H	0.773318	-0.302027	-4.664448
60	7	N	0.303833	0.970947	-2.094641

TAz-EDA

Center Number	Atomic Number	Atom	Coordinates (Angstroms)		
			X	Y	Z
1	50	Sn	-0.090464	1.175017	0.005141
2	7	N	0.404121	-2.150029	-0.011228
3	6	C	1.770499	-1.970936	-0.012578
4	6	C	2.492519	-3.186899	-0.010937
5	6	C	2.490066	-0.730415	-0.01715
6	6	C	3.869014	-3.234843	-0.012605
7	1	H	1.907899	-4.098902	-0.008114
8	6	C	3.906084	-0.798657	-0.019117
9	6	C	4.557612	-2.013544	-0.016741
10	1	H	4.402116	-4.174884	-0.011022
11	1	H	4.454265	0.133972	-0.022065
12	6	C	-1.771449	-1.504646	-0.007215
13	6	C	-2.66011	-0.396008	0.008441
14	6	C	-2.267326	-2.815129	-0.021175

15	6	C	-4.04786	-0.654334	0.009671
16	6	G	-3.628783	-3.057315	-0.019774
17	1	H	-1.559207	-3.632711	-0.033066
18	6	C	-4.499318	-1.959277	-0.004059
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20	1	H	-4.015619	-4.066799	-0.030792
21	7	N	-0.405305	-1.171887	-0.007285
22	8	O	1.929427	0.446058	-0.02112
23	8	O	-2.205233	0.836672	0.022011
24	6	C	-0.075008	1.379432	-2.144973
25	6	C	1.120363	1.339798	-2.875579
26	6	C	-1.270169	1.560865	-2.856272
27	6	C	1.126082	1.494792	-4.262312
28	1	H	2.058046	1.159987	-2.361594
29	6	C	-1.269951	1.714437	-4.243086
30	1	H	-2.215157	1.556451	-2.323835
31	6	C	-0.069966	1.687089	-4.94978
32	1	H	2.064457	1.454353	-4.805604
33	1	H	-2.208722	1.845125	-4.771241
34	1	H	-0.0679	1.802827	-6.028095
35	6	C	-0.037794	1.347982	2.157563
36	6	C	1.17284	1.302527	2.863465
37	6	C	-1.218528	1.512305	2.895431
38	6	C	1.206474	1.434919	4.25207
39	1	H	2.100807	1.137475	2.326741
40	6	C	-1.190317	1.644277	4.284257
41	1	H	-2.174484	1.509805	2.383681
42	6	C	0.023671	1.611	4.966305
43	1	H	2.155866	1.389389	4.775436
44	1	H	-2.118583	1.763029	4.833392
45	1	H	0.046831	1.70962	6.046072
46	1	H	-1.67952	3.471642	-0.918118
47	1	H	-2.076903	3.237638	0.648009
48	1	H	1.897819	3.139776	0.95375
49	1	H	2.24136	2.869709	-0.620335
50	6	C	-0.467421	4.535525	0.382061
51	1	H	-0.939709	5.491333	0.128486
52	1	H	-0.324587	4.515427	1.465732
53	6	C	0.886255	4.422975	-0.319983
54	1	H	0.743096	4.449204	-1.403481
55	1	H	1.518229	5.276336	-0.049324
56	7	N	-1.294109	3.375732	0.017358
57	7	N	1.49826	3.129446	0.019419
58	35	Br	-6.392989	-2.287314	-0.002101
59	35	Br	6.477116	-2.038828	-0.019149

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Center Number	Atomic Number	Atom	Coordinates (Angstroms)		
			X	Y	Z
1	50	Sn	-0.11742	0.34168	0.00926
2	6	C	0.07819	0.56381	-2.11519
3	6	C	-1.05708	0.7119	-2.92186
4	6	C	1.33157	0.5253	-2.73773
5	6	C	-0.94247	0.82802	-4.30683
6	1	H	-2.04024	0.72549	-2.46795
7	6	C	1.44961	0.64325	-4.12217
8	1	H	2.22589	0.3905	-2.14214
9	6	C	0.31205	0.7974	-4.91082
10	1	H	-1.83543	0.93743	-4.91341
11	1	H	2.4309	0.60823	-4.58381
12	1	H	0.40215	0.88549	-5.98814
13	6	C	-0.20172	0.60349	2.13668
14	6	C	-1.41182	0.91422	2.76914
15	6	C	0.93697	0.43452	2.93363
16	6	C	-1.48003	1.06299	4.15405
17	1	H	-2.31299	1.02706	2.17959
18	6	C	0.8721	0.58331	4.31863
19	1	H	1.88167	0.17365	2.47318
20	6	C	-0.33689	0.90107	4.93278
21	1	H	-2.42898	1.29985	4.62381
22	1	H	1.76636	0.44479	4.91734
23	1	H	-0.38928	1.01385	6.0103
24	6	C	1.57975	-2.91521	0
25	6	C	2.24224	-4.16244	-0.05879
26	6	C	2.35283	-1.71147	0.07515
27	6	C	3.61508	-4.2752	-0.05311
28	1	H	1.61494	-5.0441	-0.1109
29	6	C	3.76427	-1.84665	0.08331
30	6	C	4.35856	-3.08929	0.01943
31	1	H	4.10414	-5.23767	-0.10113
32	1	H	4.36279	-0.94758	0.13948
33	8	O	1.83899	-0.51647	0.14687
34	6	C	-1.92794	-2.27131	-0.00673
35	6	C	-2.75603	-1.12093	-0.06397
36	6	C	-2.49004	-3.55361	0.04022
37	6	C	-4.15506	-1.30542	-0.07233
38	6	C	-3.8624	-3.72508	0.03105
39	1	H	-1.82525	-4.40568	0.08451
40	6	C	-4.67406	-2.58468	-0.02612
41	1	H	-4.79702	-0.43623	-0.11573
42	1	H	-4.30134	-4.71234	0.06929
43	8	O	-2.23186	0.08283	-0.11373

44	7	N	-0.54838	-2.00391	-0.00072
45	7	N	0.20728	-3.02369	-0.012
46	6	C	1.06633	3.68026	0.05834
47	6	C	2.86133	2.25082	0.26393
48	6	C	-0.36207	3.86971	-0.07769
49	6	C	1.91116	4.81993	0.11476
50	6	C	3.77384	3.31587	0.3329
51	1	H	3.18614	1.22011	0.31645
52	6	C	-0.87721	5.18993	-0.16057
53	6	C	1.34965	6.13482	0.02875
54	6	C	3.29649	4.60307	0.25578
55	1	H	4.83105	3.10952	0.44332
56	6	C	-2.2718	5.34229	-0.29472
57	6	C	0.01104	6.31227	-0.10497
58	6	C	-2.47254	2.95779	-0.24626
59	1	H	2.01944	6.98645	0.07272
60	1	H	3.96764	5.45393	0.3024
61	6	C	-3.0715	4.22475	-0.33849
62	1	H	-2.69563	6.33858	-0.36128
63	1	H	-0.41137	7.30882	-0.17069
64	1	H	-3.05805	2.04768	-0.27312
65	1	H	-4.1467	4.30163	-0.44096
66	7	N	1.55364	2.42002	0.12931
67	7	N	-1.16396	2.78058	-0.11958
68	35	Br	-6.58225	-2.81316	-0.03846
69	35	Br	6.27507	-3.20319	0.03127

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Center Number	Atomic Number	Atom	Coordinates (Angstroms)		
			X	Y	Z
1	50	Sn	0.064769	1.93778	0.236796
2	7	N	-0.326804	-1.207378	-0.392169
3	6	C	-1.686767	-1.081798	-0.368142
4	6	C	-2.382539	-2.297754	-0.594366
5	6	C	-2.446716	0.114046	-0.148462
6	6	C	-3.752075	-2.358995	-0.604444
7	1	H	-1.778281	-3.179425	-0.771006
8	6	C	-3.851357	0.018594	-0.168768
9	6	C	-4.517329	-1.183059	-0.390183
10	1	H	-4.250857	-3.297005	-0.810853
11	1	H	-4.402224	0.929261	0.031501
12	6	C	1.841214	-0.487518	-0.254643
13	6	C	2.676157	0.637528	-0.026325
14	6	C	2.402527	-1.746198	-0.509987
15	6	C	4.066881	0.456948	-0.058812

16	6	C	3.773173	-1.897893	-0.536345
17	1	H	1.740412	-2.581525	-0.693997
18	6	C	4.630152	-0.793548	-0.310432
19	1	H	4.688613	1.318598	0.149417
20	1	H	4.198678	-2.866713	-0.765723
21	7	N	0.465359	-0.22208	-0.200611
22	8	O	-1.894498	1.279824	0.076829
23	8	O	2.138209	1.819853	0.22108
24	6	0	-0.098426	2.474175	2.285741
25	6	C	-1.347905	2.528359	2.916979
26	6	C	1.049274	2.798531	3.02164
27	6	C	-1.447467	2.899101	4.256759
28	1	H	-2.243223	2.275985	2.360737
29	6	C	0.947427	3.168367	4.361648
30	1	H	2.021993	2.756136	2.545577
31	6	C	-0.300173	3.21926	4.979964
32	1	H	-2.420052	2.936066	4.735558
33	1	H	1.842566	3.414919	4.922376
34	1	H	-0.378257	3.5067	6.022864
35	6	C	-0.072529	3.258268	-1.422108
36	6	C	-1.312673	3.561712	-1.998734
37	6	C	1.082978	3.856763	-1.942229
38	6	C	-1.395346	4.445124	-3.073503
39	1	H	-2.213367	3.10222	-1.608605
40	6	C	0.998047	4.73949	-3.017572
41	1	H	2.048567	3.626193	-1.507476
42	6	C	-0.240379	5.034602	-3.583722
43	1	H	-2.360786	4.671521	-3.51313
44	1	H	1.899181	5.195082	-3.413687
45	1	H	-0.305348	5.721233	-4.420779
46	6	C	-5.996509	-1.238269	-0.404665
47	6	C	-6.67624	-2.358027	0.109661
48	6	C	-6.751621	-0.174344	-0.931774
49	6	C	-8.060122	-2.393048	0.096988
50	1	H	-6.112314	-3.177215	0.54212
51	6	C	-8.140966	-0.208134	-0.953938
52	1	H	-6.235299	0.678314	-1.356363
53	6	C	-8.997273	-3.469283	0.603632
54	6	C	-8.802417	-1.321315	-0.435102
55	1	H	-8.69497	0.622047	-1.377971
56	1	H	-8.831022	-4.427028	0.097276
57	6	C	-10.363859	-2.896026	0.292945
58	1	H	-8.865462	-3.651639	1.676363
59	6	C	-10.230238	-1.633351	-0.317233
60	6	C	-11.621491	-3.435367	0.525307
61	6	C	-11.360851	-0.908398	-0.69551

62	6	C	-12.751444	-2.707524	0.145436
63	1	H	-11.731341	-4.407421	0.994892
64	6	C	-12.620357	-1.455064	-0.459589
65	1	H	-11.266771	0.064293	-1.165779
66	1	H	-13.73955	-3.117519	0.321461
67	1	H	-13.508395	-0.903963	-0.748048
68	6	C	6.101486	-0.967493	-0.345211
69	6	C	6.69767	-2.13691	0.161003
70	6	C	6.931735	0.032378	-0.883925
71	6	C	8.074285	-2.28318	0.12667
72	1	H	6.075986	-2.907801	0.603242
73	6	C	8.314011	-0.111278	-0.92491
74	1	H	6.478407	0.923777	-1.301116
75	6	C	8.929448	-3.431623	0.620132
76	6	C	8.892213	-1.274066	-0.416035
77	1	H	8.926245	0.673099	-1.356307
78	1	H	8.798773	-3.604141	1.694674
79	6	C	10.333267	-2.969535	0.290218
80	1	H	8.680074	-4.37255	0.116262
81	6	C	10.29235	-1.699562	-0.318246
82	6	C	11.546677	-3.608116	0.505143
83	6	C	11.472342	-1.06769	-0.71205
84	6	C	12.726377	-2.973198	0.109591
85	1	H	11.584467	-4.586346	0.973407
86	6	C	12.687383	-1.713827	-0.493637
87	1	H	11.450144	-0.090024	-1.180974
88	1	H	13.680766	-3.461365	0.271943
89	1	H	13.612571	-1.235128	-0.794589

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Center Number	Atomic Number	Atom	Coordinates (Angstroms)		
			X	Y	Z
1	50	Sn	-0.02264	1.735355	0.28532
2	8	O	-1.870519	1.061121	-0.349912
3	8	O	2.042366	1.617939	0.310833
4	6	C	-0.35631	1.55755	2.410085
5	6	C	-2.439826	-0.123278	-0.233826
6	6	C	-4.545143	-1.397068	-0.264366
7	6	C	-3.83912	-0.199852	-0.361104
8	1	H	-4.361102	0.73908	-0.499541
9	6	C	-0.262781	3.789919	-0.282435
10	6	C	-3.823009	-2.593275	-0.042701
11	1	H	-4.3441	-3.540885	0.003129
12	6	C	4.600057	-0.983477	0.225037
13	6	C	3.996889	0.272944	0.277521

14	1	H	4.591908	1.176871	0.316977
15	6	C	-2.453815	-2.555155	0.065399
16	1	H	-1.877952	-3.461327	0.21099
17	6	C	3.780041	-2.134763	0.142414
18	1	H	4.235826	-3.116944	0.13611
19	6	C	-1.721871	-1.346951	-0.016519
20	6	C	2.600235	0.419255	0.256394
21	6	C	2.405879	-2.020291	0.111825
22	1	H	1.768346	-2.893339	0.060373
23	6	C	1.801913	-0.755498	0.163076
24	7	N	-0.356397	-1.523856	0.080739
25	7	N	0.424819	-0.520651	0.112884
26	6	C	-1.48818	4.272167	-0.762742
27	6	C	0.798775	4.694981	-0.139683
28	6	C	0.642344	6.040019	-0.474264
29	6	C	-1.646421	5.617158	-1.098328
30	6	C	-0.580871	6.503198	-0.955215
31	1	H	1.758853	4.348274	0.228859
32	1	H	1.474861	6.725995	-0.357537
33	1	H	-2.327793	3.593491	-0.872067
34	1	H	-2.602898	5.973431	-1.466717
35	1	H	-0.703792	7.549528	-1.213138
36	6	C	0.716545	1.520524	3.311948
37	6	C	-1.657394	1.511822	2.930531
38	6	C	-1.880591	1.425042	4.304393
39	6	C	0.497623	1.433594	4.686374
40	6	C	-0.80227	1.384437	5.185343
41	1	H	-2.51146	1.542938	2.261864
42	1	H	-2.895863	1.38853	4.685584
43	1	H	1.735178	1.562716	2.941239
44	1	H	1.342082	1.404735	5.367248
45	1	H	-0.973821	1.316512	6.254282
46	1	H	-0.615123	1.630839	-2.489831
47	1	H	0.402948	0.377179	-2.293891
48	6	C	1.363243	2.116732	-2.865952
49	1	H	2.32229	1.802939	-2.447515
50	1	H	1.239895	3.172742	-2.620387
51	6	C	1.351018	1.922985	-4.38628
52	1	H	2.105493	2.594287	-4.811094
53	1	H	0.386161	2.259658	-4.785397
54	6	C	1.633579	0.488413	-4.843967
55	1	H	1.664505	0.423951	-5.934277
56	1	H	2.59631	0.135183	-4.462035
57	1	H	0.863188	-0.211273	-4.505244
58	7	N	0.306289	1.377344	-2.136818
59	6	C	6.076196	-1.115838	0.258872

60	6	C	6.725392	-2.104876	-0.502498
61	6	C	6.858134	-0.25639	1.052067
62	6	C	8.105414	-2.213974	-0.464755
63	1	H	6.141664	-2.76177	-1.138259
64	6	C	8.243639	-0.364017	1.096686
65	1	H	6.364214	0.489317	1.663658
66	6	C	9.011867	-3.179535	-1.199555
67	6	C	8.874501	-1.34645	0.333734
68	1	H	8.817562	0.306816	1.726586
69	1	H	8.786139	-4.222432	-0.948852
70	6	C	10.390804	-2.771141	-0.725247
71	1	H	8.9104	-3.086755	-2.287042
72	6	C	10.290963	-1.692531	0.175483
73	6	C	11.630811	-3.300378	-1.054797
74	6	C	11.438646	-1.142558	0.747355
75	6	C	12.778096	-2.747815	-0.480567
76	1	H	11.713954	-4.131323	-1.747813
77	6	C	12.680671	-1.678171	0.412596
78	1	H	11.371073	-0.312289	1.441828
79	1	H	13.75276	-3.152157	-0.729672
80	1	H	13.581278	-1.261325	0.849439
81	6	C	-6.020575	-1.419808	-0.392241
82	6	C	-6.792156	-2.304785	0.383116
83	6	C	-6.680125	-0.559221	-1.288813
84	6	C	-8.171122	-2.312124	0.258556
85	1	H	-6.303442	-2.957611	1.098047
86	6	C	-8.063853	-0.567039	-1.422405
87	1	H	-6.091368	0.106471	-1.908741
88	6	C	-9.195935	-3.153108	0.99062
89	6	C	-8.817049	-1.446082	-0.644236
90	1	H	-8.542385	0.100906	-2.130194
91	1	H	-9.038221	-4.225082	0.82526
92	6	C	-10.505098	-2.676746	0.397326
93	1	H	-9.15608	-2.991172	2.073946
94	6	C	-10.263439	-1.673401	-0.561593
95	6	C	-11.801632	-3.087458	0.674403
96	6	C	-11.325225	-1.079448	-1.244704
97	6	C	-12.862557	-2.491282	-0.011218
98	1	H	-11.994272	-3.859618	1.412101
99	6	C	-12.624408	-1.496019	-0.9622
100	1	H	-11.148176	-0.306103	-1.98416
101	1	H	-13.880065	-2.802951	0.196191
102	1	H	-13.459748	-1.043757	-1.484978

M-TAz-EDA

Center Number	Atomic Number	Atom	Coordinates (Angstroms)		
			X	Y	Z
1	50	Sn	0.049673	1.934817	0.002191
2	7	N	-0.322159	-1.389867	-0.00261
3	6	C	-1.690473	-1.25999	0.055988
4	6	C	-2.373639	-2.499703	0.057111
5	6	C	-2.457326	-0.050314	0.118675
6	6	C	-3.744003	-2.585016	0.111807
7	1	H	-1.758392	-3.390996	0.022562
8	6	C	-3.863162	-0.174579	0.179652
9	6	C	-4.518324	-1.402122	0.177354
10	1	H	-4.227808	-3.552939	0.14164
11	1	H	-4.428672	0.749838	0.195744
12	6	C	1.827573	-0.661172	-0.08337
13	6	C	2.674955	0.477706	-0.129997
14	6	C	2.378447	-1.950744	-0.09534
15	6	C	4.065251	0.269656	-0.185521
16	6	C	3.746023	-2.126725	-0.148412
17	1	H	1.704514	-2.796607	-0.071945
18	6	C	4.614585	-1.011127	-0.195484
19	1	H	4.700892	1.147001	-0.189315
20	1	H	4.156503	-3.128141	-0.188184
21	7	N	0.453136	-0.381612	-0.026362
22	8	O	-1.936862	1.149591	0.115511
23	8	O	2.168855	1.694894	-0.112213
24	6	C	0.121871	2.141398	2.153286
25	6	C	-1.037533	2.059004	2.936453
26	6	C	1.34016	2.363287	2.811986
27	6	C	-0.987431	2.213216	4.32247
28	1	H	-1.989342	1.845382	2.462714
29	6	C	1.396152	2.516283	4.197815
30	1	H	2.259644	2.391213	2.237202
31	6	C	0.230318	2.447256	4.957007
32	1	H	-1.898774	2.139424	4.907023
33	1	H	2.352401	2.679098	4.684295
34	1	H	0.271895	2.562648	6.034671
35	6	C	-0.107306	2.142906	-2.144238
36	6	C	-1.345506	2.057395	-2.796589
37	6	C	1.030938	2.366774	-2.931562
38	6	C	-1.447569	2.209968	-4.17988
39	1	H	-2.240017	1.844805	-2.221017
40	6	C	0.934616	2.519461	-4.315267
41	1	H	2.007971	2.39449	-2.461861
42	6	C	-0.306684	2.446828	-4.943151
43	1	H	-2.417099	2.132799	-4.661181
44	1	H	1.831414	2.685177	-4.90344

45	1	H	-0.382792	2.56168	-6.018981
46	1	H	1.584158	4.298495	0.882369
47	1	H	1.92813	4.088871	-0.700333
48	1	H	-2.049188	3.843121	-0.844216
49	1	H	-2.313991	3.549879	0.741259
50	6	C	0.284017	5.326112	-0.360784
51	1	H	0.728557	6.298924	-0.120333
52	1	H	0.097283	5.306424	-1.437861
53	6	C	-1.035413	5.158722	0.394529
54	1	H	-0.8488	5.185484	1.471474
55	1	H	-1.708478	5.990323	0.155509
56	7	N	1.166945	4.19712	-0.038542
57	7	N	-1.61124	3.84556	0.072556
58	6	C	6.083478	-1.205095	-0.255429
59	6	C	6.70047	-2.24187	0.467915
60	6	C	6.891569	-0.357648	-1.03537
61	6	C	8.074137	-2.408437	0.406452
62	1	H	6.09673	-2.890499	1.093296
63	6	C	8.27074	-0.521869	-1.103136
64	1	H	6.420482	0.425483	-1.617687
65	6	C	8.94794	-3.432394	1.100888
66	6	H	8.869312	-1.551833	-0.377847
67	1	H	8.864682	0.142042	-1.722037
68	1	H	8.864441	-3.366803	2.191881
69	6	C	10.337057	-3.069642	0.619099
70	1	H	8.674626	-4.457214	0.824257
71	6	C	10.271687	-1.962199	-0.24952
72	6	C	11.557384	-3.660104	0.916259
73	6	C	11.434852	-1.44579	-0.821413
74	6	C	12.720313	-3.140879	0.341981
75	1	H	11.613389	-4.513328	1.584581
76	6	C	12.657193	-2.043047	-0.519283
77	1	H	11.394129	-0.593804	-1.491358
78	1	H	13.679817	-3.59335	0.566121
79	1	H	13.56917	-1.652381	-0.956973
80	6	C	-5.997329	-1.473328	0.24258
81	6	C	-6.699512	-2.453354	-0.482357
82	6	C	-6.729563	-0.566036	1.029985
83	6	C	-8.081847	-2.50625	-0.416634
84	1	H	-6.153443	-3.147263	-1.11207
85	6	C	-8.117089	-0.617763	1.103773
86	1	H	-6.193659	0.17247	1.614475
87	6	C	-9.039533	-3.451548	-1.111681
88	6	C	-8.800768	-1.591355	0.375735
89	1	H	-8.652219	0.088485	1.729297
90	1	H	-8.955861	-3.38702	-2.202696

91	6	C	-10.391915	-2.978965	-0.620979
92	1	H	-8.8495	-4.496692	-0.841568
93	6	C	-10.232464	-1.885119	0.252527
94	6	C	-11.657809	-3.466527	-0.914424
95	6	C	-11.346579	-1.278369	0.833334
96	6	C	-12.771361	-2.857061	-0.331323
97	1	H	-11.78665	-4.3089	-1.586337
98	6	C	-12.614878	-1.772441	0.534917
99	1	H	-11.233186	-0.436208	1.50729
100	1	H	-13.765655	-3.228648	-0.55234
101	1	H	-13.489838	-1.311246	0.979349

M-TAz-phen

Center Number	Atomic Number	Atom	Coordinates (Angstroms)		
			X	Y	Z
1	50	Sn	0.09798	1.1629	-0.00056
2	6	C	0.22844	1.44866	2.12274
3	6	C	1.45804	1.7311	2.73036
4	6	C	-0.89916	1.31745	2.9422
5	6	C	1.556	1.89031	4.11239
6	1	H	2.35004	1.8137	2.12207
7	6	C	-0.80491	1.47712	4.32434
8	1	H	-1.85794	1.07693	2.50002
9	6	C	0.42341	1.76731	4.91348
10	1	H	2.51969	2.10507	4.5626
11	1	H	-1.69133	1.36856	4.94088
12	1	H	0.49871	1.88863	5.98883
13	6	C	-0.15103	1.42882	-2.11553
14	6	C	0.96163	1.61974	-2.94431
15	6	C	-1.41671	1.37094	-2.71109
16	6	C	0.81304	1.76096	-4.32375
17	1	H	1.95377	1.64638	-2.51088
18	6	C	-1.569	1.51337	-4.08997
19	1	H	-2.29301	1.20185	-2.09762
20	6	C	-0.45379	1.71182	-4.90044
21	1	H	1.68908	1.90441	-4.94788
22	1	H	-2.55943	1.46303	-4.53044
23	1	H	-0.57041	1.81956	-5.97353
24	6	C	-1.60479	-2.06492	0.03185
25	6	C	-2.27651	-3.30968	-0.00875
26	6	C	-2.37704	-0.86405	0.14515
27	6	C	-3.64584	-3.40762	0.05098
28	1	H	-1.65394	-4.19364	-0.08028
29	6	C	-3.78147	-1.0018	0.21481
30	6	C	-4.4269	-2.23382	0.16956

31	1	H	-4.12334	-4.37913	0.04605
32	1	H	-4.36187	-0.08856	0.2718
33	8	O	-1.85682	0.33464	0.18675
34	6	C	1.90135	-1.42597	-0.09727
35	6	C	2.73239	-0.2791	-0.16915
36	6	C	2.46727	-2.7086	-0.08313
37	6	C	4.12502	-0.46878	-0.22315
38	6	C	3.83706	-2.86802	-0.13489
39	1	H	1.80405	-3.56203	-0.03972
40	6	C	4.69056	-1.74271	-0.20719
41	1	H	4.75332	0.41354	-0.24557
42	1	H	4.26089	-3.86449	-0.15233
43	8	O	2.20486	0.92904	-0.17862
44	7	N	0.52519	-1.15796	-0.04143
45	7	N	-0.23659	-2.17644	-0.03228
46	6	C	-1.08392	4.5418	0.08193
47	6	C	-2.87949	3.11406	0.28844
48	6	C	0.34441	4.72979	-0.06481
49	6	C	-1.92634	5.68289	0.15056
50	6	C	-3.79055	4.18019	0.36643
51	1	H	-3.20408	2.08255	0.33678
52	6	C	0.86139	6.05007	-0.13915
53	6	C	-1.36272	6.99743	0.07158
54	6	C	-3.31138	5.46723	0.29628
55	1	H	-4.848	3.97524	0.47821
56	6	C	2.25536	6.20075	-0.28181
57	6	C	-0.02447	7.17352	-0.06797
58	6	C	2.45064	3.81514	-0.2601
59	1	H	-2.03064	7.85006	0.12588
60	1	H	-3.98093	6.31898	0.3512
61	6	C	3.05228	5.0819	-0.34265
62	1	H	2.68083	7.19687	-0.34141
63	1	H	0.39936	8.16996	-0.12765
64	1	H	3.03249	2.90274	-0.30206
65	1	H	4.12701	5.15795	-0.45157
66	7	N	-1.57253	3.28247	0.14995
67	7	N	1.14307	3.63988	-0.12556
68	6	C	6.16179	-1.9187	-0.26473
69	6	C	-5.90477	-2.31803	0.24581
70	6	C	-6.63344	-1.4611	1.09073
71	6	C	-6.60849	-3.26045	-0.52573
72	6	C	-7.98983	-3.32525	-0.44937
73	6	C	-8.01991	-1.52571	1.17562
74	6	C	-8.70555	-2.46071	0.40043
75	1	H	-6.06452	-3.91462	-1.19838
76	6	C	-8.94946	-4.23565	-1.18699

77	1	H	-6.09507	-0.75468	1.71164
78	1	H	-8.55247	-0.86002	1.84622
79	6	C	-10.13683	-2.75578	0.27519
80	6	C	-10.29928	-3.79954	-0.65703
81	6	C	-11.24816	-2.18951	0.9005
82	6	C	-12.51678	-2.67348	0.58727
83	6	C	-11.56549	-4.27727	-0.96499
84	6	C	-12.67627	-3.70832	-0.33736
85	1	H	-11.13239	-1.38627	1.62004
86	1	H	-13.38961	-2.24347	1.06585
87	1	H	-11.69668	-5.08113	-1.68209
88	1	H	-13.67075	-4.07278	-0.56914
89	1	H	-8.87722	-4.10938	-2.2734
90	1	H	-8.75097	-5.29315	-0.978
91	6	C	6.95697	-1.08432	-1.07148
92	6	C	6.79356	-2.92503	0.48814
93	6	C	8.1693	-3.07467	0.42933
94	6	C	8.33822	-1.23193	-1.13681
95	6	C	8.95168	-2.23124	-0.38171
96	1	H	6.19922	-3.56261	1.1336
97	1	H	6.47413	-0.32632	-1.67707
98	1	H	8.92225	-0.57942	-1.77692
99	6	C	10.35974	-2.61834	-0.24331
100	6	C	10.44132	-3.69805	0.65822
101	6	C	11.51506	-2.10348	-0.83226
102	6	C	12.74586	-2.67444	-0.51404
103	6	C	11.67	-4.2624	0.97128
104	6	C	12.82504	-3.74477	0.3799
105	1	H	11.46186	-1.27284	-1.52766
106	1	H	13.6519	-2.28469	-0.9647
107	6	C	9.05789	-4.06517	1.15285
108	1	H	11.73848	-5.09418	1.66498
109	1	H	13.79093	-4.17702	0.61619
110	1	H	8.79835	-5.10148	0.90751
111	1	H	8.97466	-3.96794	2.24149