Synthesis and the optical and electrochemical properties of indium(III) bis(arylimino)acenaphthene complexes

Jingyi Wang,[a] Rakesh Ganguly,[a] Li Yongxin,[a] Jesus Díaz,*[b] Han Sen Soo[a,c,d*] and Felipe García[a*]

Division of Chemistry and Biological Chemistry, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link 637371, Singapore.
Departamento de Química Orgánica e Inorgánica, Facultad de Veterinaria, Universidad de Extremadura, Cáceres 10071, Spain
Singapore-Berkeley Research Initiative for Sustainable Energy (SinBeRISE), 1 Create Way, Singapore 138602.
Solar Fuels Laboratory, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798.

Table of contents

1. Experimental section

General considerations

All reactions with $InCl_3$ and the recrystallization of products were performed under dry and inert atmospheres by using a combination of standard Schlenk line techniques and a Vacuum Atmospheres N_2 glovebox. Solvents including tetrahydrofuran (THF), diethyl ether (Et_2O), and pentane were distilled over Na/benzophenone and degassed using freeze-pump-thaw cycles prior to use. Anhydrous acetonitrile (ACN) was collected from a PURE SOLV MD-5 solvent purification system and stored in a glovebox. Anhydrous 1,2-dimethoxyethane (DME) and dichloromethane (DCM) were distilled over calcium hydride (CaH_2) and stored in a glovebox. Anhydrous *N*,*N*-dimethylformamide (DMF) in a Sure-Seal bottle was purchased from Sigma-Aldrich and used as received. Deuterated chloroform ($CDCl_3$) and acetonitrile (CD_3CN) were distilled over CaH_2 and stored over 4 Å molecular sieves. Deuterated acetone was distilled over K_2CO_3. All reagents were purchased from commercial sources and were used without further purification.

The ^1H and $^{13}C\{^1H\}$ NMR spectra were recorded at 298 K on a Bruker Avance DPX400 and DPX300 spectrometer. The chemical shift values are reported in parts per million (ppm) relative to TMS, using residual protonated solvents as the internal standards (^1H: δ = 7.26 for $CDCl_3$ and δ = 1.94 for CD_3CN; ^{13}C: δ = 77.2 for $CDCl_3$, and δ = 118.3 for CD_3CN). We attempted to record the ^{115}In spectra on a JEOL ECA400 spectrometer, using a 0.5 M D_2O solution of $In(NO_3)_3$ as the external standard. No internal standards were used for the ^{115}In NMR spectra. However, in solution, we observed dissociation and isomerization of the complexes. Moreover, we could not detect any signals by solid-state ^{115}In NMR spectroscopy due to the large quadrupolar moments of the nuclei, which result in broad and essentially unobservable NMR signals. Thus, we have not reported any ^{115}In data. UV-Vis absorption measurements were carried out on a Shimadzu UV-3600 spectrophotometer. Melting points were measured using an OptiMelt automated melting pointing system. Crystallographic data were recorded on a Bruker X8 CCD diffractometer. High-resolution ESI mass spectra were obtained using a Waters Q-Tof Premier mass spectrometer.

Synthesis of bis(arylimino)acenapthenes (Ar-BIANs)

(a) Dipp-BIAN (1a)

The procedure was similar to the one from Tu and co-workers,[1] with the following reagent quantities: acenaphthoquinone (0.21 g, 1.1 mmol), 2,6-diisopropylaniline (0.51 mL, 2.7 mmol) and acetic acid (1.90 mL). The yield was 0.48 g (85%). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 1.00 (d, J = 6.8 Hz, 12 H), 1.22 (d, J = 7.2 Hz, 12 H), 2.97 (sept, J = 6.8 Hz, 4 H), 6.67 (d, J = 7.2 Hz, 2 H), 7.22–7.30 (m, 6 H), 7.37 (d, J = 7.6 Hz, 2 H), 7.90 (d, J = 8.0 Hz, 2 H). HRMS (ESI+, *m/z*) calculated for $C_{36}H_{41}N_2$ $[M+H]^+$ *m/z* = 501.3270, found 501.3269.

(b) 2,6-Me_2Ar-BIAN (2a)

The procedure was similar to the one from Minnaard and co-workers,[2] with the following reagent quantities: acenaphthoquinone (0.48 g, 2.6 mmol), 2,6-dimethylaniline (0.74 mL, 6.0 mmol), $ZnCl_2$ (0.97 g, 7.1 mmol), sodium oxalate (0.46 g, 3.4 mmol). The yield was 0.74 g (73%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 2.14 (s, 12 H), 6.71 (d, J = 7.2 Hz, 2 H), 7.06-7.10 (m, 2 H), 7.16-7.17 (m, 4 H), 7.39 (t, J = 7.8 Hz, 2 H), 7.90 (d, J = 8.0 Hz, 2 H). HRMS (ESI+, *m/z*) calculated for $C_{28}H_{25}N_2$ $[M+H]^+$ *m/z* = 389.2018, found 389.2028.

(c) *p*-NO_2Ar-BIAN (3a)

The procedure was adapted from the one reported by Cenini and co-workers,[5] with the following reagent quantities: acenaphthoquinone (0.50 g, 2.7 mmol), *p*-nitroaniline (0.86 g, 6.2 mmol), $ZnCl_2$ (1.00 g, 7.3 mmol) and sodium oxalate (1.29 g, 9.7 mmol). The yield was 0.69 g (60%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 6.91 (d, J = 7.2 Hz, 2 H), 7.25-7.27 (m, 4 H), 7.48 (t, J = 7.6 Hz, 2 H), 8.02 (d, J = 8.4 Hz, 2 H), 8.41 (d, J = 8.4 Hz, 4 H). HRMS (ESI+, m/z) calculated for $C_{24}H_{15}N_4O_4$ $[M + H]^+$ *m/z* = 423.1093, found 423.1086.

(d) *p*-NMe_2Ar-BIAN (4a)

The synthesis was carried out by a mechanochemical approach. A stainless steel grinder jar was charged with acenaphthoquinone (0.055 g, 0.30 mmol), *N*,*N*-dimethyl-1,4-phenylenediamine (0.094 g, 0.69 mmol), catalytic amounts of acetic acid (4.3 μL, 0.075 mmol, 25 mol%), and Na_2SO_4 (0.043 g, 0.30 mmol), and a 10 mm stainless steel ball. The jar was then grinded for 5.0 h at 30 Hz. The resultant dark purple solid was washed with Et_2O and the isolated yield was 0.11 g (85%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.03 (s, 12 H), 6.84-6.86 (m, 4 H), 7.11-7.13 (m, 4 H), 7.24-7.26 (d, overlapping with $CDCl_3$ signal, 2 H) 7.39 (t, J = 7.8 Hz, 2 H), 7.86 (d, J = 8.4 Hz, 2 H). HRMS (ESI+, m/z) calculated for $C_{28}H_{27}N_4$ $[M + H]^+$ m/z = 419.2236, found 419.2229.

(e) *p*-MeOAr-BIAN (5a)

The procedure was adapted from the one reported by Djurišic and co-workers,[3] with the following amounts of reagents used: acenaphthoquinone (0.68 g, 3.7 mmol), *p*-anisidine (1.2 g, 9.4 mmol), $ZnCl_2$ (1.0 g, 7.5 mmol) and K_2CO_3 (10.0 g, 0.072 mmol). The yield was 1.40 g (61%). ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.90 (s, 6 H), 7.01-7.04 (m, 6 H), 7.09-7.11 (m, 4 H), 7.39 (t, J = 8.0 Hz, 2 H), 7.89 (d, J = 8.4 Hz, 2 H). HRMS (ESI+, m/z) calculated for $C_{26}H_{21}N_2O_2$ $[M + H]^+$ m/z = 393.1603, found 393.1595.

2. Spectroscopic data

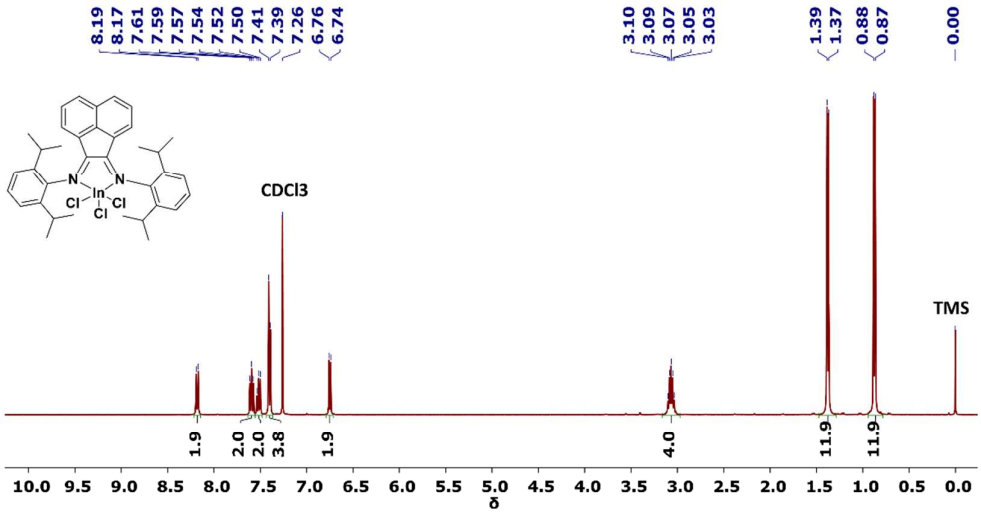

Fig. S1 The ^{1}H NMR spectrum of **1b** recorded in $CDCl_3$.

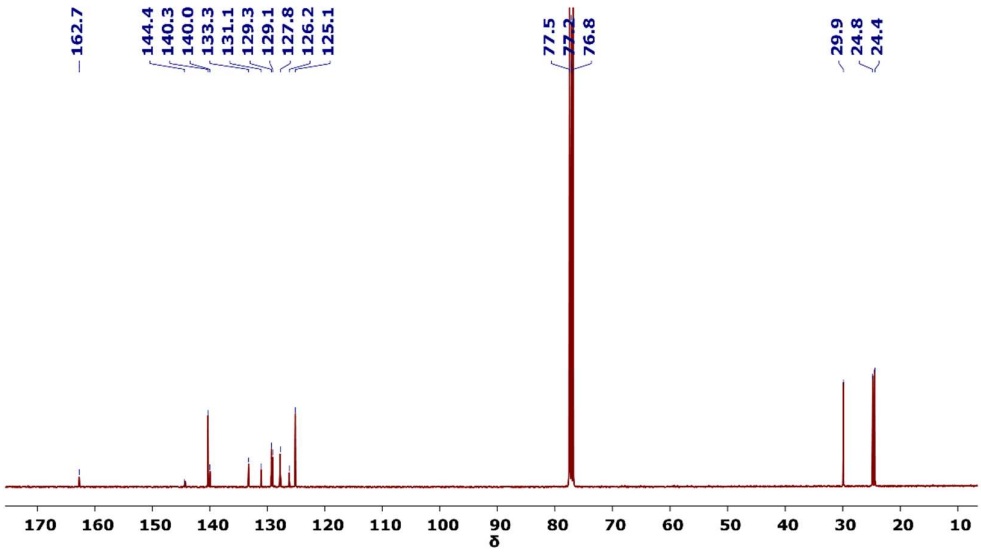

Fig. S2 The ^{13}C NMR spectrum of **1b** recorded in $CDCl_3$.

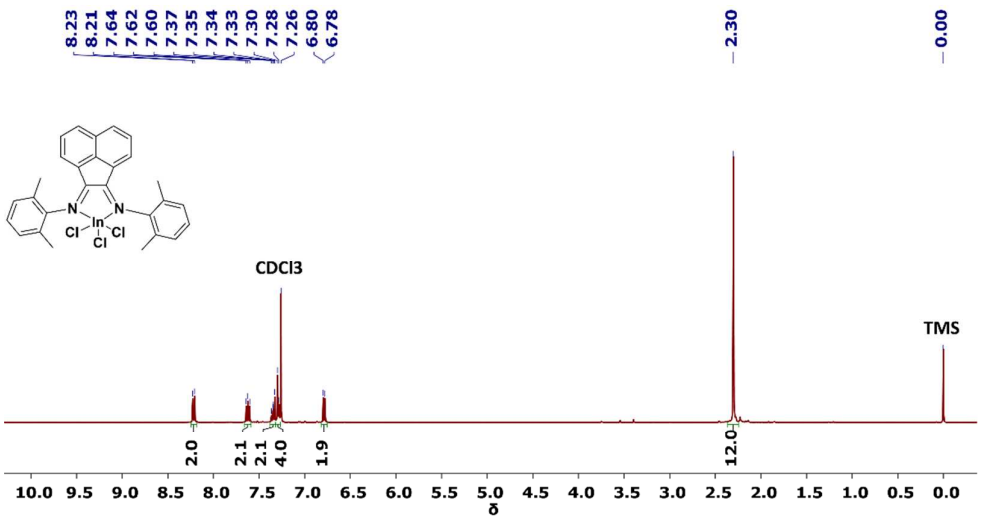

Fig. S3 The ^{1}H NMR spectrum of **2b** recorded in $CDCl_3$.

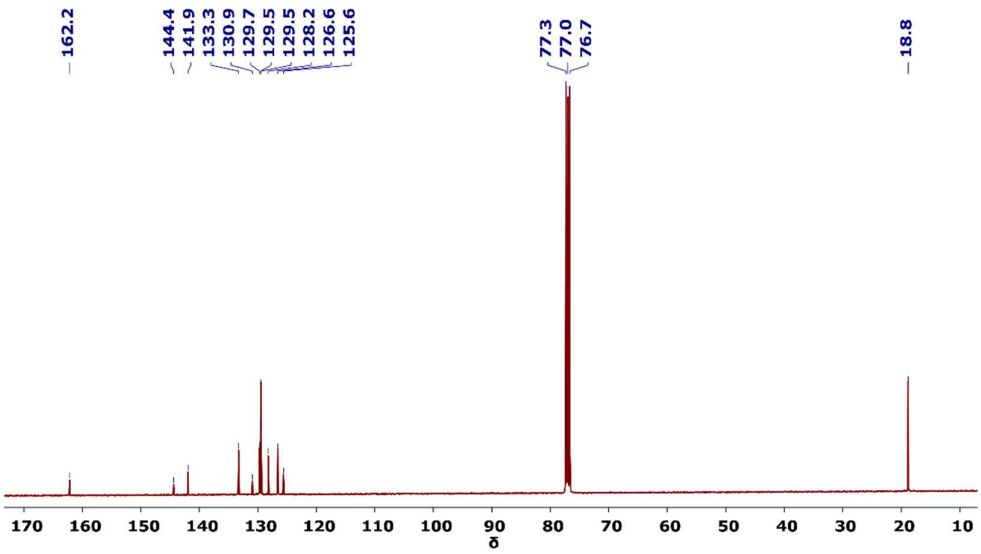

Fig. S4 The ^{13}C NMR spectrum of **2b** recorded in $CDCl_3$.

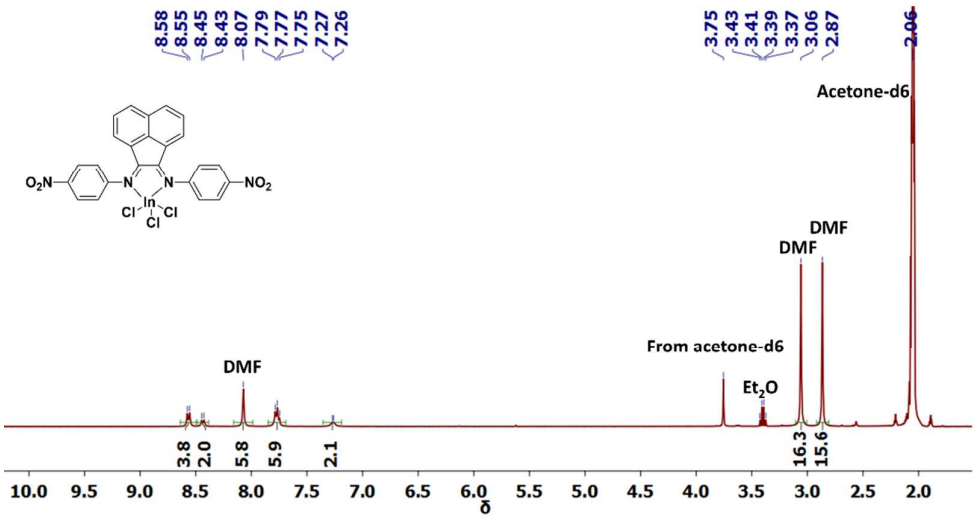

Fig. S5 The ^{1}H NMR spectrum of **3b** recorded in acetone-d_6.

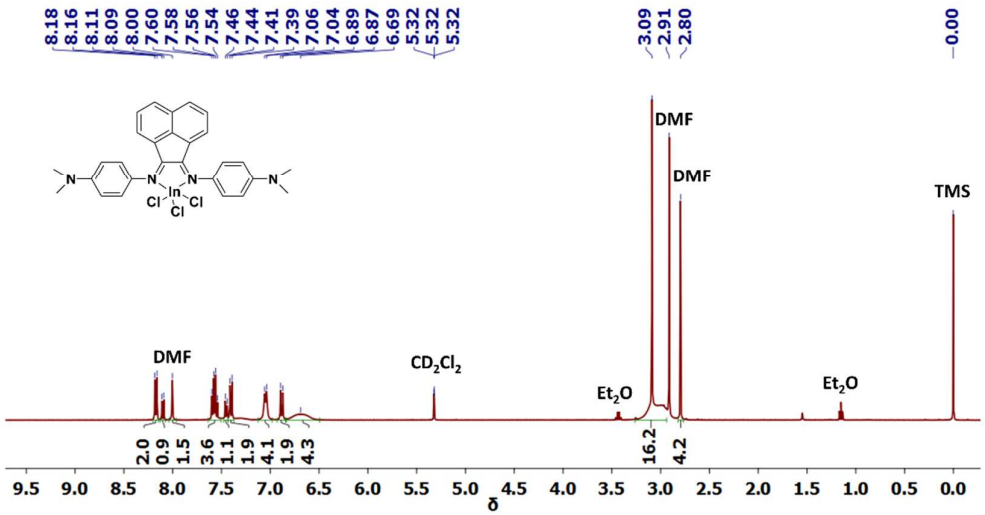

Fig. S6 The ^{1}H NMR spectrum of **4b** recorded in CD_2Cl_2.

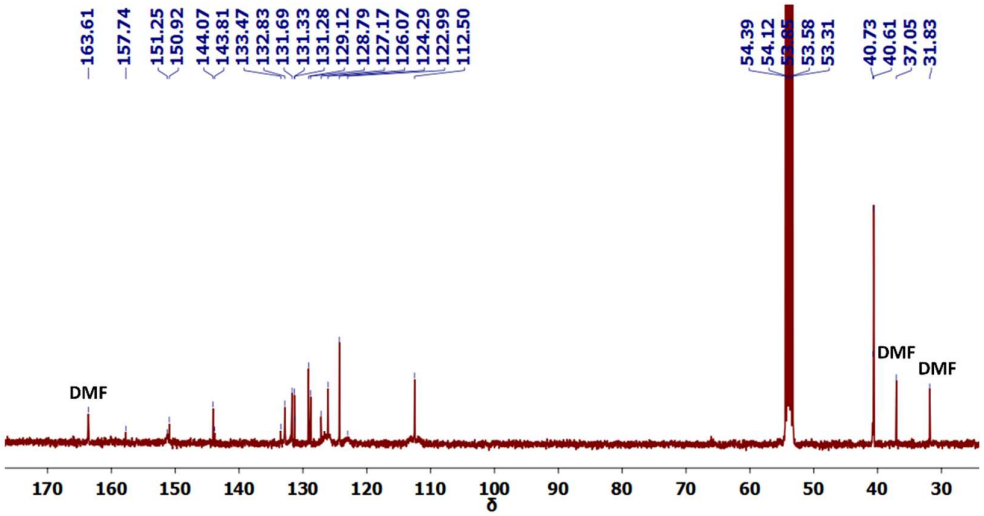

Fig. S7 The ^{13}C NMR spectrum of **4b** recorded in CD_2Cl_2.

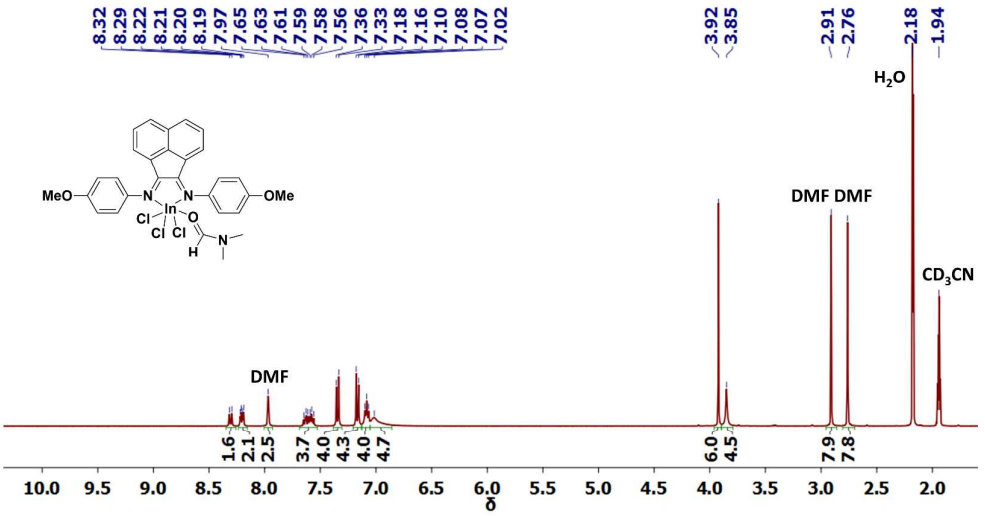

Fig. S8 The ^{1}H NMR spectrum of **5b** recorded in CD_3CN.

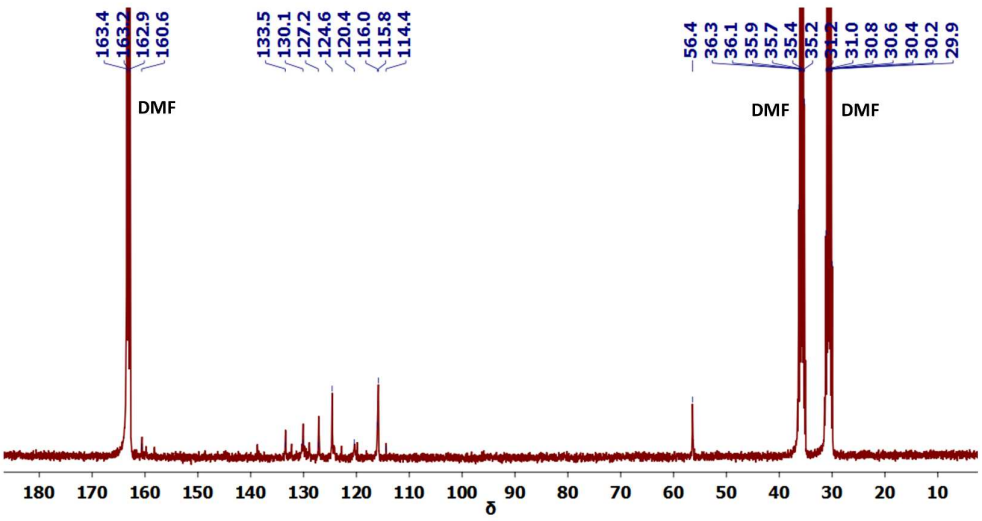

Fig. S9 The ^{13}C NMR spectrum of **5b** recorded in DMF-d_7.

3. Cyclic voltammetry studies

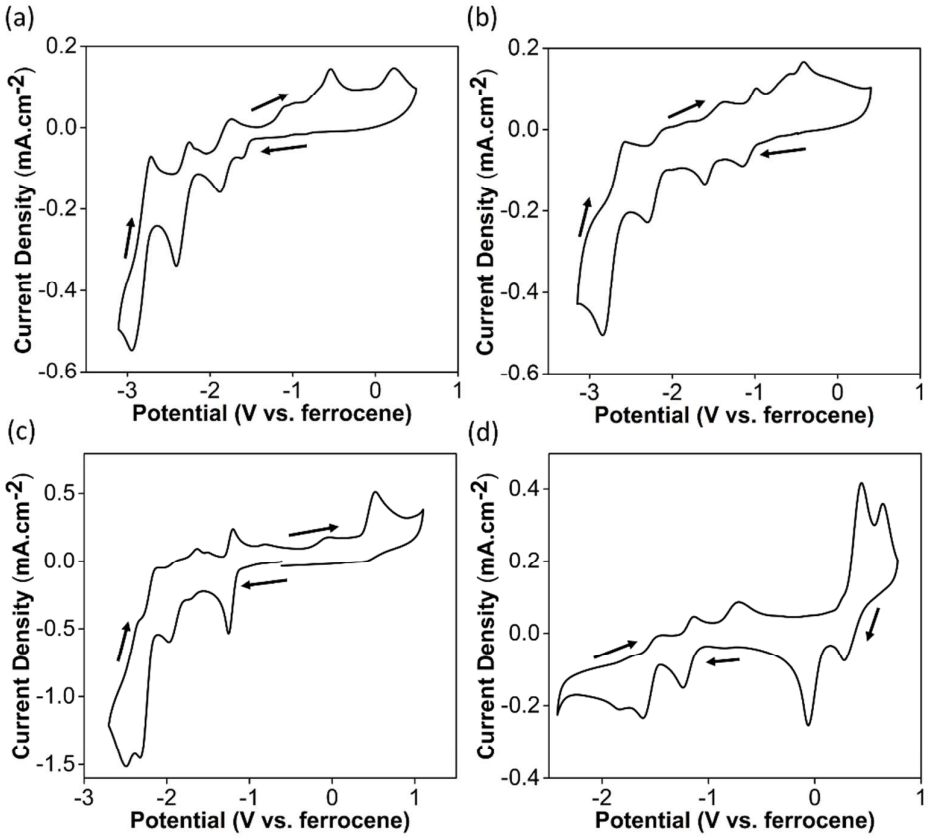

Fig. S10 Cyclic voltammograms for (a) **1b** in THF, (b) **2b** in THF, (c) **3b** in DMF, and (d) **4b** in DCM, each at a scan rate of 100 mV s^{-1} with 0.10 M *n*-Bu_4NPF_6 as the electrolyte.

4. Reduction reactions of Ar-BIAN indium(III) complex 1b

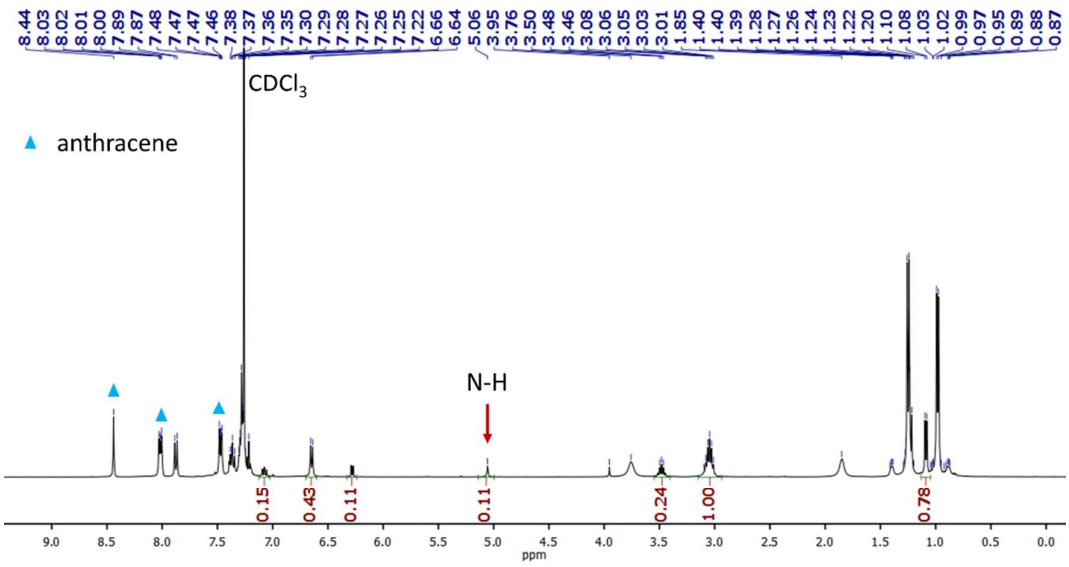

Fig. S11 The ^{1}H NMR spectrum of the crude reduction reaction mixture of **1b** using magnesium anthracene. The solvent is $CDCl_3$.

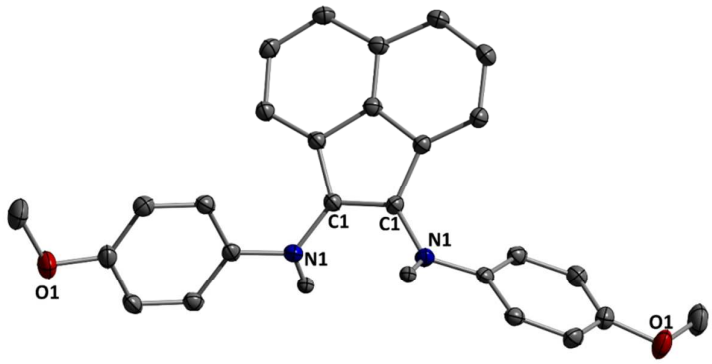

Fig. S12 Crystal structure of **8**. Thermal ellipsoids are drawn at the 50% probability level. Hydrogen atoms have been omitted for clarity.

5. Single crystal X-ray diffraction studies

Complexes **1b** to **5b** reported herein have been deposited with the Cambridge Crystallographic Data Centre (CCDC), under deposition numbers CCDC 1535077-1535081. These data can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

Complex 1b

An orange needle-like specimen of $C_{36}H_{40}Cl_3InN_2$, with approximate dimensions 0.040 mm x 0.060 mm x 0.420 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 0.62 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 11216 reflections to a maximum θ angle of 28.34° (0.75 Å resolution), of which 5953 were independent (average redundancy = 1.884, completeness = 99.6%, R_{int} = 3.73%, R_{sig} = 5.48%) and 5373 (90.26%) were greater than $2\sigma(F^2)$. The final cell constants of a = 9.6585(3) Å, b = 21.4348(8) Å, c = 16.7319(7) Å, β = 101.7562(15)°, volume = 3391.3(2) $Å^3$, are based upon the refinement of the XYZ-centroids of 5075 reflections above 20 σ(I) with 4.541° < 2θ < 55.37°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.725. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6880 and 0.9630. The final anisotropic full-matrix least-squares refinement on F^2 with 387 variables converged at R1 = 3.99% for the observed data and wR2 = 10.93% for all data. The goodness-of-fit was 1.056. The largest peak in the final difference electron density synthesis was 1.430 $e^-/Å^3$ and the largest hole was -1.834 $e^-/Å^3$ with a RMS deviation of 0.144 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.414 g/cm^3 and F(000) was 1480 e^-.

Complex 2b

An orange block-like specimen of $C_{28}H_{24}Cl_3InN_2$, with approximate dimensions 0.280 mm x 0.320 mm x 0.420 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 3 seconds per frame.

The integration of the data using a monoclinic unit cell yielded a total of 10810 reflections to a maximum θ angle of 31.10° (0.69 Å resolution), of which 5569 were independent (average redundancy = 1.941, completeness = 99.7%, R_{int} = 4.37%, R_{sig} = 7.80%) and 4264 (76.57%) were greater than $2\sigma(F^2)$. The final cell constants of a = 8.5861(9) Å, b = 17.7036(19) Å, c = 11.4783(13) Å, β = 105.462(2)°, volume = 1681.6(3) $Å^3$, are based upon the refinement of the XYZ-centroids of reflections above 20 σ(I). The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6880 and0.7740. The final anisotropic full-matrix least-squares refinement on F^2 with 165 variables converged at R1 = 3.09% for the observed data and wR2 = 5.91% for all data. The goodness-of-fit was 0.866. The largest peak in the final difference electron density synthesis was 0.923 $e^-/Å^3$ and the largest hole was -0.609 $e^-/Å^3$ with a RMS deviation of 0.089 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.251 g/cm^3 and F(000) was 636 e^-.

Complex 3b

A yellow block-like specimen of $C_{28}H_{22}Cl_3InN_6O_5$, with approximate dimensions 0.120 mm x 0.240 mm x 0.300 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 0.53 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 47312 reflections to a maximum θ angle of 31.14° (0.69 Å resolution), of which 10012 were independent (average redundancy = 4.726, completeness = 99.7%, R_{int} = 5.25%, R_{sig} = 4.08%) and 8691 (86.81%) were greater than $2\sigma(F^2)$. The final cell constants of a = 9.2235(8) Å, b = 13.9416(11) Å, c = 24.3021(19) Å, β = 96.327(4)°, volume = 3106.0(4) $Å^3$, are based upon the refinement of the XYZ-centroids of 9970 reflections above 20 σ(I) with 4.462° < 2θ < 61.79°. Data were corrected for absorption effects using the multi-scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.857. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7400 and 0.8830. The final anisotropic full-matrix least-squares refinement on F^2 with 425 variables converged at R1 = 3.01% for the observed data and wR2 = 6.69% for all data. The goodness-of-fit was 1.043. The largest peak in the final difference electron density synthesis was 0.564 $e^-/Å^3$ and the

largest hole was -0.671 $e^-/Å^3$ with a RMS deviation of 0.088 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.590 g/cm^3 and F(000) was 1488 e^-.

Complex 4b

A purple needle-like specimen of $C_{34}H_{40}Cl_3InN_6O_2$, with approximate dimensions 0.140 mm x 0.160 mm x 0.420 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 0.70 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a triclinic unit cell yielded a total of 43022 reflections to a maximum θ angle of 31.26° (0.68 Å resolution), of which 12623 were independent (average redundancy = 3.408, completeness = 99.6%, R_{int} = 10.08%, R_{sig} = 9.95%) and 9555 (75.70%) were greater than $2\sigma(F^2)$. The final cell constants of a = 8.9217(3) Å, b = 14.6932(6) Å, c = 16.1692(7) Å, α = 112.451(2)°, β = 92.719(2)°, γ = 95.175(2)°, volume = 1943.22(14) $Å^3$, are based upon the refinement of the XYZ-centroids of 7120 reflections above 20 σ(I) with 4.799° < 2θ < 53.46°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.848. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7170 and 0.8900. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 2 for the formula unit, $C_{34}H_{40}Cl_3InN_6O_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 471 variables converged at R1 = 5.76% for the observed data and wR2 = 17.28% for all data. The goodness-of-fit was 1.080. The largest peak in the final difference electron density synthesis was 1.595 $e^-/Å^3$ and the largest hole was -0.884 $e^-/Å^3$ with an RMS deviation of 0.166 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.343 g/cm^3 and F(000) was 804 e^-.

Complex 5b

A red block-like specimen of $C_{30.50}H_{30.50}Cl_3InN_{3.50}O_{3.50}$, with approximate dimensions 0.200 mm x 0.210 mm x 0.400 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 0.31 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame

algorithm. The integration of the data using a triclinic unit cell yielded a total of 50446 reflections to a maximum θ angle of 35.11° (0.62 Å resolution), of which 13260 were independent (average redundancy = 3.804, completeness = 99.4%, R_{int} = 5.21%, R_{sig} = 5.27%) and 11004 (82.99%) were greater than $2\sigma(F^2)$. The final cell constants of a = 8.9265(5) Å, b = 12.3564(7) Å, c = 14.3910(8) Å, α = 99.6119(15)°, β = 90.3519(14)°, γ = 106.1023(14)°, volume = 1501.33(15) $Å^3$, are based upon the refinement of the XYZ-centroids of 9913 reflections above 20 σ(I) with 4.756° < 2θ < 66.01°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum apparent transmission was 0.867. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.6690 and 0.8110. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group P -1, with Z = 2 for the formula unit, $C_{30.50}H_{30.50}Cl_3InN_{3.50}O_{3.50}$. The final anisotropic full-matrix least-squares refinement on F^2 with 403 variables converged at R1 = 3.46% for the observed data and wR2 = 7.37% for all data. The goodness-of-fit was 1.050. The largest peak in the final difference electron density synthesis was 0.918 $e^-/Å^3$ and the largest hole was -0.910 $e^-/Å^3$ with an RMS deviation of 0.117 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.600 g/cm^3 and F(000) was 732 e^-.

Compound 8

A red plate-like specimen of $C_{26}H_{22}N_2O_2$, approximate dimensions 0.020 mm x 0.060 mm x 0.380 mm, was used for the X-ray crystallographic analysis. The X-ray intensity data were measured. The total exposure time was 1.01 hours. The frames were integrated with the Bruker SAINT software package using a narrow-frame algorithm. The integration of the data using a monoclinic unit cell yielded a total of 5667 reflections to a maximum θ angle of 66.79° (0.84 Å resolution), of which 1714 were independent (average redundancy = 3.306, completeness = 98.3%, R_{int} = 6.22%, R_{sig} = 5.92%) and 1461 (85.24%) were greater than $2\sigma(F^2)$. The final cell constants of a = 27.3734(9) Å, b = 9.3669(3) Å, c = 7.7757(3) Å, β = 100.331(2)°, volume = 1961.40(12) $Å^3$, are based upon the refinement of the XYZ-centroids of 2642 reflections above 20 σ(I) with 6.564° < 2θ < 133.0°. Data were corrected for absorption effects using the Multi-Scan method (SADABS). The ratio of minimum to maximum

apparent transmission was 0.734. The calculated minimum and maximum transmission coefficients (based on crystal size) are 0.7840 and 0.9870. The structure was solved and refined using the Bruker SHELXTL Software Package, using the space group C 1 2/c 1, with Z = 4 for the formula unit, $C_{26}H_{22}N_2O_2$. The final anisotropic full-matrix least-squares refinement on F^2 with 142 variables converged at R1 = 4.79% for the observed data and wR2 = 13.66% for all data. The goodness-of-fit was 1.045. The largest peak in the final difference electron density synthesis was 0.253 $e^-/Å^3$ and the largest hole was -0.214 $e^-/Å^3$ with an RMS deviation of 0.055 $e^-/Å^3$. On the basis of the final model, the calculated density was 1.336 g/cm^3 and F(000) was 832 e^-.

X-ray data of compounds

Table S1. X-ray crystallographic and refinement data for complex **1b**.

Chemical formula	$C_{36}H_{40}Cl_3InN_2$
Formula weight	721.87 g/mol
Temperature	103(2) K
Wavelength	0.71073 Å
Crystal size	0.040 x 0.060 x 0.420 mm
Crystal habit	Orange needle
Crystal system	monoclinic
Space group	C 1 c 1
Unit cell dimensions	a = 9.6585(3) Å α = 90°
	b = 21.4348(8) Å β = 101.7562(15)°
	c = 16.7319(7) Å γ = 90°
Volume	3391.3(2) $Å^3$
Z	4
Density (calculated)	1.414 g/cm^3
Absorption coefficient	0.960 mm^{-1}
F(000)	1480

Theta range for data collection	1.90 to 28.34°
Index ranges	-12<=h<=12, -28<=k<=28, -11<=l<=22
Reflections collected	11216
Independent reflections	5953 [R(int) = 0.0373]
Coverage of independent reflections	99.6%
Absorption correction	multi-scan
Max. and min. transmission	0.9630 and 0.6880
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/6 (Sheldrick, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	5953 / 2 / 387
Goodness-of-fit on F^2	1.056
Δ/σ_{max}	0.001
	5373
Final R indices	data; R1 = 0.0399, wR2 = 0.0957
	$I>2\sigma(I)$
	all data R1 = 0.0473, wR2 = 0.1093
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0690P)^2]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	1.430 and -1.834 eÅ^{-3}
R.M.S. deviation from mean	0.144 eÅ^{-3}

Table S2. Selected bond lengths (Å) for complex **1b**.

In1-N1	2.342(5)	In1-N2	2.339(5)
In1-Cl1	2.3835(16)	In1-Cl2	2.3800(17)
In1-Cl3	2.3643(17)	C1-N1	1.279(7)
C2-N2	1.279(8)	C1-C2	1.535(8)

Table S3. Selected bond angles (°) for complex **1b**.

N2-In1-N1	72.28(17)	N2-In1-Cl3	95.89(13)
N1-In1-Cl3	99.03(15)	N2-In1-Cl2	88.11(13)
N1-In1-Cl2	146.42(15)	Cl3-In1-Cl2	110.12(6)
N2-In1-Cl1	150.06(13)	N1-In1-Cl1	87.61(13)
Cl3-In1-Cl1	109.30(7)	Cl2-In1-Cl1	97.76(6)

Table S4. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for complex **1b**.

	x/a	**y/b**	**z/c**	**U(eq)**
In1	0.39200(3)	0.64194(2)	0.92202(2)	0.01143(11)
C1	0.1315(6)	0.5686(3)	0.8310(4)	0.0108(11)
C2	0.2247(6)	0.5192(3)	0.8822(4)	0.0108(11)
C3	0.1542(6)	0.4588(3)	0.8632(4)	0.0123(12)
C4	0.1806(7)	0.3983(3)	0.8912(4)	0.0162(13)
C5	0.0843(7)	0.3511(3)	0.8573(5)	0.0197(14)
C6	0.9666(7)	0.3631(3)	0.7982(5)	0.0183(14)
C7	0.9368(6)	0.4244(3)	0.7676(4)	0.0145(12)
C8	0.8206(7)	0.4440(3)	0.7073(4)	0.0183(13)
C9	0.8001(7)	0.5057(3)	0.6872(4)	0.0204(14)
C10	0.8931(7)	0.5531(3)	0.7251(4)	0.0178(13)
C11	0.0096(6)	0.5356(3)	0.7817(4)	0.0115(11)
C12	0.0322(6)	0.4712(3)	0.8024(4)	0.0113(12)
C13	0.0631(6)	0.6742(3)	0.8089(4)	0.0150(13)
C14	0.0541(7)	0.6942(3)	0.7284(5)	0.0219(15)
C15	0.1570(8)	0.6752(3)	0.6763(4)	0.0223(15)
C16	0.2742(8)	0.7237(3)	0.6836(5)	0.0267(16)
C17	0.0885(11)	0.6657(4)	0.5864(5)	0.041(2)

C18	0.9465(8)	0.7374(3)	0.6985(6)	0.0314(19)
C19	0.8570(9)	0.7582(4)	0.7479(7)	0.043(2)
C20	0.8727(9)	0.7389(4)	0.8281(7)	0.039(2)
C21	0.9801(7)	0.6972(3)	0.8617(5)	0.0247(16)
C22	0.9979(8)	0.6778(3)	0.9499(5)	0.0253(16)
C23	0.8939(10)	0.6266(4)	0.9595(6)	0.039(2)
C24	0.9860(16)	0.7318(4)	0.0074(7)	0.064(4)
C25	0.4054(7)	0.4909(3)	0.9920(4)	0.0132(12)
C26	0.3620(7)	0.4885(3)	0.0671(4)	0.0163(13)
C27	0.2518(7)	0.5330(3)	0.0884(4)	0.0199(14)
C28	0.1078(8)	0.5016(4)	0.0791(5)	0.0291(17)
C29	0.2991(9)	0.5603(4)	0.1736(5)	0.037(2)
C30	0.4187(7)	0.4407(3)	0.1201(4)	0.0222(15)
C31	0.5167(7)	0.3989(3)	0.1011(5)	0.0234(15)
C32	0.5617(7)	0.4042(3)	0.0285(4)	0.0199(14)
C33	0.5082(6)	0.4514(3)	0.9716(4)	0.0140(12)
C34	0.5666(7)	0.4575(3)	0.8943(4)	0.0181(13)
C35	0.7152(8)	0.4841(4)	0.9159(5)	0.0299(17)
C36	0.5633(8)	0.3958(3)	0.8486(5)	0.0263(16)
Cl1	0.33268(19)	0.74953(7)	0.92803(12)	0.0251(4)
Cl2	0.54218(19)	0.63419(7)	0.05340(11)	0.0223(4)
Cl3	0.52447(17)	0.62718(8)	0.81926(10)	0.0219(3)
N1	0.1647(5)	0.6261(2)	0.8435(3)	0.0134(11)
N2	0.3347(5)	0.5367(2)	0.9335(3)	0.0097(9)

Table S5. Anisotropic atomic displacement parameters ($Å^2$) for complex **1b**.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
In1	0.01512(18)	0.01206(16)	0.00649(17)	-0.0009(2)	0.00072(13)	-0.0035(2)
C1	0.011(3)	0.017(3)	0.006(3)	0.001(2)	0.005(2)	0.001(2)
C2	0.015(3)	0.013(3)	0.006(3)	0.000(2)	0.006(2)	0.003(2)
C3	0.014(3)	0.016(3)	0.008(3)	-0.004(2)	0.006(2)	0.000(2)
C4	0.016(3)	0.018(3)	0.014(3)	0.001(3)	0.000(3)	0.001(2)
C5	0.020(3)	0.012(3)	0.027(4)	0.004(3)	0.006(3)	-0.002(2)
C6	0.016(3)	0.017(3)	0.022(4)	-0.005(3)	0.004(3)	-0.008(2)
C7	0.014(3)	0.019(3)	0.009(3)	-0.002(2)	0.002(2)	-0.005(2)
C8	0.015(3)	0.025(3)	0.014(3)	-0.006(3)	0.002(3)	-0.004(2)
C9	0.012(3)	0.031(3)	0.014(3)	0.001(3)	-0.007(3)	0.000(3)
C10	0.015(3)	0.018(3)	0.020(3)	0.004(3)	0.002(3)	0.000(2)
C11	0.015(3)	0.013(3)	0.007(3)	0.001(2)	0.004(2)	-0.003(2)
C12	0.013(3)	0.014(3)	0.007(3)	-0.002(2)	0.002(2)	-0.003(2)
C13	0.011(3)	0.011(3)	0.022(4)	-0.002(3)	0.001(3)	-0.003(2)
C14	0.026(3)	0.013(3)	0.025(4)	0.005(3)	0.001(3)	0.003(3)
C15	0.040(4)	0.013(3)	0.013(3)	0.002(3)	0.003(3)	0.004(3)
C16	0.035(4)	0.025(3)	0.020(4)	0.007(3)	0.006(3)	0.003(3)
C17	0.062(6)	0.033(4)	0.020(4)	-0.006(4)	-0.009(4)	0.010(4)
C18	0.023(3)	0.020(3)	0.049(5)	0.012(4)	0.002(4)	0.005(3)
C19	0.032(4)	0.023(4)	0.075(8)	0.022(4)	0.011(5)	0.014(3)
C20	0.035(4)	0.025(4)	0.065(7)	0.017(4)	0.027(5)	0.014(3)
C21	0.025(4)	0.013(3)	0.041(5)	-0.001(3)	0.017(3)	-0.001(3)
C22	0.025(3)	0.018(3)	0.036(5)	-0.008(3)	0.013(3)	-0.002(3)
C23	0.036(4)	0.041(4)	0.042(6)	0.017(4)	0.010(5)	-0.011(4)
C24	0.123(11)	0.032(5)	0.055(7)	-0.013(5)	0.057(8)	-0.003(6)
C25	0.015(3)	0.016(3)	0.006(3)	0.002(2)	-0.003(2)	-0.006(2)
C26	0.021(3)	0.020(3)	0.008(3)	0.001(2)	0.003(3)	-0.010(2)

C27	0.026(3)	0.026(3)	0.008(3)	0.000(3)	0.006(3)	-0.002(3)
C28	0.025(4)	0.037(4)	0.027(4)	0.001(3)	0.011(3)	0.001(3)
C29	0.044(5)	0.051(5)	0.019(4)	-0.006(4)	0.017(4)	-0.006(4)
C30	0.021(3)	0.032(4)	0.012(3)	0.009(3)	-0.001(3)	-0.008(3)
C31	0.022(3)	0.023(3)	0.020(4)	0.012(3)	-0.007(3)	-0.005(3)
C32	0.018(3)	0.018(3)	0.019(4)	0.002(3)	-0.005(3)	-0.002(2)
C33	0.014(3)	0.013(3)	0.013(3)	-0.001(2)	-0.002(3)	-0.007(2)
C34	0.020(3)	0.018(3)	0.017(3)	0.003(3)	0.005(3)	0.002(2)
C35	0.024(4)	0.034(4)	0.032(5)	-0.007(4)	0.009(3)	-0.012(3)
C36	0.034(4)	0.024(3)	0.022(4)	-0.006(3)	0.007(3)	0.003(3)
Cl1	0.0313(8)	0.0121(6)	0.0278(10)	-0.0026(6)	-0.0042(8)	-0.0033(6)
Cl2	0.0287(9)	0.0213(7)	0.0122(8)	-0.0012(6)	-0.0071(7)	-0.0056(6)
Cl3	0.0230(8)	0.0332(8)	0.0109(8)	0.0004(7)	0.0067(7)	-0.0035(7)
N1	0.014(2)	0.013(2)	0.012(3)	-0.003(2)	0.001(2)	-0.0010(19)
N2	0.012(2)	0.012(2)	0.005(2)	-0.002(2)	0.0020(19)	-0.0013(18)

Table S6. X-ray crystallographic and refinement data for complex **2b**.

Chemical formula	$C_{28}H_{24}Cl_3InN_2$
Formula weight	609.66 g/mol
Temperature	103(2) K
Wavelength	0.71073 Å
Crystal size	0.280 x 0.320 x 0.420 mm
Crystal habit	Orange block
Crystal system	monoclinic
Space group	P 1 21/m 1
Unit cell dimensions	a = 8.5861(9) Å α = 90°
	b = 17.7036(19) Å β = 105.462(2)°

	c = 11.4783(13) Å γ = 90°
Volume	1681.6(3) $Å^3$
Z	2
Density (calculated)	1.251 g/cm^3
Absorption coefficient	0.956 mm^{-1}
F(000)	636
Theta range for data collection	2.17 to 24.67°
Index ranges	-12<=h<=12, -25<=k<=25, 0<=l<=16
Reflections collected	10810
Independent reflections	5569 [R(int) = 0.0437]
Coverage of independent reflections	99.7%
Absorption correction	multi-scan
Max. and min. transmission	0.7740 and 0.6880
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/7 (Sheldrick, 2014)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	5569 / 0 / 165
Goodness-of-fit on F^2	0.866
Δ/σ_{max}	0.002
	4264
Final R indices	data; R1 = 0.0309, wR2 = 0.0562
	I>2σ(I)
	all data R1 = 0.0453, wR2 = 0.0591
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0172P)^2]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.923 and -0.609 $eÅ^{-3}$
R.M.S. deviation from mean	0.089 $eÅ^{-3}$

Table S7. Selected bond lengths (Å) for complex **2b**.

In1-N1	2.3196(15)	In1-Cl1	2.3897(5)
C1-N1	1.280(2)	In1-Cl2	2.3769(7)
C1-C1	1.517(3)		

Table S8. Selected bond angles (°) for complex **2b**.

N1-In1-N1	72.32(7)	N1-In1-Cl2	100.86(4)
N1-In1-Cl1	87.99(4)	N1-In1-Cl1	148.15(4)
Cl2-In1-Cl1	107.421(19)	Cl1-In1-Cl1	97.09(3)

Table S9. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for complex **2b**.

	x/a	**y/b**	**z/c**	**U(eq)**
In1	0.17055(2)	0.25	0.02214(2)	0.01440(5)
C1	0.1187(2)	0.29284(9)	0.75377(17)	0.0137(4)
C2	0.0976(2)	0.31705(10)	0.62916(18)	0.0172(4)
C3	0.0903(2)	0.38582(11)	0.57179(19)	0.0253(5)
C4	0.0713(3)	0.38659(12)	0.4466(2)	0.0345(6)
C5	0.0600(3)	0.32180(11)	0.3792(2)	0.0339(6)
C6	0.0669(4)	0.25	0.4357(3)	0.0274(7)
C7	0.0864(3)	0.25	0.5602(3)	0.0186(6)
C8	0.1765(2)	0.40820(9)	0.85672(17)	0.0142(4)
C9	0.3332(2)	0.43204(10)	0.86256(18)	0.0190(4)
C10	0.4672(2)	0.37621(11)	0.8691(2)	0.0274(5)
C11	0.3597(3)	0.50951(11)	0.8611(2)	0.0253(5)
C12	0.2357(3)	0.56006(11)	0.85581(19)	0.0263(5)
C13	0.0829(2)	0.53458(10)	0.85171(18)	0.0208(4)

C14	0.0488(2)	0.45763(10)	0.85192(17)	0.0165(4)
C15	0.8801(2)	0.42986(11)	0.8419(2)	0.0232(5)
Cl1	0.30831(6)	0.35117(3)	0.14518(5)	0.02578(12)
Cl2	0.89933(8)	0.25	0.03621(7)	0.02103(15)
N1	0.14797(17)	0.32731(8)	0.85529(14)	0.0135(3)

Table S10. Anisotropic atomic displacement parameters ($Å^2$) for complex **2b**.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
In1	0.01907(10)	0.01240(9)	0.01184(10)	0	0.00431(8)	0
C1	0.0127(9)	0.0133(8)	0.0147(10)	0.0001(7)	0.0027(8)	-0.0004(7)
C2	0.0226(10)	0.0148(9)	0.0133(10)	0.0003(7)	0.0030(8)	0.0000(8)
C3	0.0410(13)	0.0164(10)	0.0181(12)	-0.0002(8)	0.0075(10)	0.0009(9)
C4	0.0691(17)	0.0176(10)	0.0167(12)	0.0046(9)	0.0116(12)	0.0006(11)
C5	0.0621(16)	0.0262(11)	0.0134(12)	0.0039(9)	0.0099(11)	0.0017(11)
C6	0.0436(19)	0.0211(15)	0.0160(17)	0	0.0053(15)	0
C7	0.0260(15)	0.0165(13)	0.0115(15)	0	0.0020(12)	0
C8	0.0200(10)	0.0105(8)	0.0105(10)	0.0003(7)	0.0016(8)	-0.0014(7)
C9	0.0213(10)	0.0178(9)	0.0180(11)	-0.0007(8)	0.0054(9)	-0.0022(8)
C10	0.0186(10)	0.0240(11)	0.0411(16)	-0.0034(10)	0.0105(10)	-0.0025(9)
C11	0.0266(11)	0.0222(10)	0.0271(13)	-0.0015(9)	0.0071(10)	-0.0106(9)
C12	0.0401(13)	0.0134(9)	0.0241(13)	0.0001(8)	0.0066(10)	-0.0048(9)
C13	0.0324(11)	0.0140(9)	0.0150(11)	0.0009(8)	0.0042(9)	0.0053(8)
C14	0.0223(10)	0.0165(9)	0.0095(10)	0.0012(7)	0.0019(8)	0.0012(8)
C15	0.0218(10)	0.0228(10)	0.0251(13)	0.0019(9)	0.0065(9)	0.0037(8)
Cl1	0.0349(3)	0.0217(2)	0.0179(3)	-0.0026(2)	0.0021(2)	-0.0090(2)
Cl2	0.0218(3)	0.0200(3)	0.0242(4)	0	0.0112(3)	0

N1	0.0138(8)	0.0116(7)	0.0149(9)	0.0001(6)	0.0037(7)	-0.0007(6)

Table S11. X-ray crystallographic and refinement data for complex **3b**.

Chemical formula	$C_{28}H_{22}Cl_3InN_6O_5$
Formula weight	743.68 g/mol
Temperature	103(2) K
Wavelength	0.71073 Å
Crystal size	0.120 x 0.240 x 0.300 mm
Crystal habit	Yellow block
Crystal system	monoclinic
Space group	P 1 21/n 1
Unit cell dimensions	a = 9.2235(8) Å α = 90°
	b = 13.9416(11) Å β = 96.327(4)°
	c = 24.3021(19) Å γ = 90°
Volume	3106.0(4) $Å^3$
Z	4
Density (calculated)	1.590 g/cm^3
Absorption coefficient	1.066 mm^{-1}
F(000)	1488
Theta range for data collection	2.66 to 31.14°
Index ranges	-11<=h<=13, -20<=k<=20, -35<=l<=31
Reflections collected	47312
Independent reflections	10012 [R(int) = 0.0525]
Coverage of independent reflections	99.7%
Absorption correction	multi-scan
Max. and min. transmission	0.8830 and 0.7400
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/6 (Sheldrick, 2014)

Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	10012 / 107 / 425
Goodness-of-fit on F^2	1.043
Δ/σ_{max}	0.002
	8691
Final R indices	data; R1 = 0.0301, wR2 = 0.0638
	$I>2\sigma(I)$
	all data R1 = 0.0377, wR2 = 0.0669
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0209P)^2+1.9021P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.564 and -0.671 eÅ^{-3}
R.M.S. deviation from mean	0.088 eÅ^{-3}

Table S12. Selected bond lengths (Å) for complex **3b**.

In1-Cl1	2.4013(4)	In1-Cl2	2.4722(5)
In1-Cl3	2.4032(5)	In1-N1	2.3230(14)
In1-N2	2.3114(14)	In1-O5	2.2733(13)
C1-N1	1.274(2)	C11-N2	1.276(2)
C1-C11	1.519(2)		

Table S13. Selected bond angles (°) for complex **3b**.

O5-In1-N1	84.24(5)	O5-In1-N2	82.46(5)
N2-In1-N1	72.64(5)	O5-In1-Cl1	90.81(3)
N2-In1-Cl1	94.01(4)	N1-In1-Cl1	166.23(4)
O5-In1-Cl3	86.33(3)	N2-In1-Cl3	161.33(4)
N1-In1-Cl3	91.46(4)	Cl1-In1-Cl3	101.061(16)
O5-In1-Cl2	166.45(4)	N2-In1-Cl2	86.39(4)
N1-In1-Cl2	85.11(4)	Cl1-In1-Cl2	97.652(16)

Cl3-In1-Cl2	102.296(17)

Table S14. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for complex **3b**.

	x/a	y/b	z/c	U(eq)
C1	0.04459(17)	0.75574(12)	0.34671(7)	0.0113(3)
C2	0.15084(18)	0.72088(12)	0.39159(7)	0.0130(3)
C3	0.26953(19)	0.66005(13)	0.39443(8)	0.0178(3)
C4	0.3445(2)	0.64051(14)	0.44721(8)	0.0226(4)
C5	0.3039(2)	0.68047(15)	0.49494(8)	0.0236(4)
C6	0.1823(2)	0.74324(15)	0.49329(8)	0.0194(4)
C7	0.1280(2)	0.79108(16)	0.53842(8)	0.0258(4)
C8	0.0088(2)	0.85004(16)	0.53001(8)	0.0251(4)
C9	0.9320(2)	0.86524(14)	0.47699(7)	0.0187(4)
C10	0.98203(18)	0.81932(13)	0.43259(7)	0.0137(3)
C11	0.93306(17)	0.81504(11)	0.37338(7)	0.0104(3)
C12	0.10799(18)	0.76073(13)	0.44099(7)	0.0144(3)
C13	0.12245(18)	0.68458(12)	0.26671(7)	0.0111(3)
C14	0.07843(18)	0.59230(12)	0.25173(7)	0.0136(3)
C15	0.16387(18)	0.53718(12)	0.22081(7)	0.0135(3)
C16	0.28987(17)	0.57716(12)	0.20495(7)	0.0119(3)
C17	0.33750(18)	0.66793(13)	0.22053(7)	0.0149(3)
C18	0.25186(19)	0.72308(13)	0.25207(8)	0.0154(3)
C19	0.70365(17)	0.88850(12)	0.36900(7)	0.0116(3)
C20	0.61245(19)	0.83017(13)	0.39669(8)	0.0166(3)
C21	0.50043(19)	0.87151(13)	0.42195(8)	0.0169(3)
C22	0.48197(18)	0.96960(13)	0.41784(7)	0.0133(3)

C23	0.56942(19)	0.02808(13)	0.38977(8)	0.0161(3)
C24	0.68240(19)	0.98672(12)	0.36479(7)	0.0147(3)
C25	0.3139(3)	0.38943(17)	0.36337(10)	0.0312(5)
C26	0.2369(3)	0.3229(2)	0.39605(11)	0.0445(6)
Cl1	0.57172(4)	0.87365(3)	0.22763(2)	0.01649(8)
Cl2	0.70607(5)	0.64226(3)	0.28425(2)	0.02064(9)
Cl3	0.86790(5)	0.75357(3)	0.16215(2)	0.02053(9)
In1	0.80186(2)	0.79551(2)	0.25201(2)	0.01073(3)
N1	0.02541(14)	0.74250(10)	0.29454(6)	0.0107(3)
N2	0.81910(15)	0.84397(10)	0.34346(6)	0.0113(3)
N3	0.37429(16)	0.52076(11)	0.16875(6)	0.0146(3)
N4	0.36291(16)	0.01385(12)	0.44450(6)	0.0172(3)
N5	0.3732(2)	0.44067(16)	0.33755(10)	0.0426(5)
N6A	0.2549(10)	0.4025(5)	0.5340(3)	0.0639(19)
C27A	0.1980(11)	0.4514(7)	0.5615(4)	0.0428(17)
C28A	0.1081(14)	0.5091(8)	0.5963(5)	0.062(3)
N6B	0.178(4)	0.4085(15)	0.5223(8)	0.086(6)
C27B	0.152(3)	0.454(2)	0.5578(9)	0.050(4)
C28B	0.152(3)	0.5245(14)	0.6027(7)	0.045(4)
O1	0.48501(14)	0.55645(10)	0.15381(5)	0.0203(3)
O2	0.32895(14)	0.44062(10)	0.15438(6)	0.0200(3)
O3	0.33058(16)	0.09716(11)	0.43311(6)	0.0276(3)
O4	0.30057(15)	0.96487(11)	0.47658(6)	0.0252(3)
O5	0.92254(14)	0.93553(9)	0.24205(5)	0.0151(2)

Table S15. Anisotropic atomic displacement parameters ($Å^2$) for complex **3b**.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0100(7)	0.0091(7)	0.0148(8)	-0.0005(6)	0.0019(6)	-0.0007(6)
C2	0.0121(7)	0.0120(8)	0.0148(8)	0.0009(6)	0.0005(6)	0.0011(6)
C3	0.0169(8)	0.0159(8)	0.0204(9)	0.0020(7)	0.0016(7)	0.0039(7)
C4	0.0184(9)	0.0212(9)	0.0273(10)	0.0055(8)	-0.0019(7)	0.0066(7)
C5	0.0199(9)	0.0289(11)	0.0205(9)	0.0108(8)	-0.0039(7)	0.0029(8)
C6	0.0178(8)	0.0252(10)	0.0146(8)	0.0052(7)	-0.0014(6)	-0.0011(7)
C7	0.0237(9)	0.0411(12)	0.0119(8)	0.0029(8)	-0.0011(7)	-0.0001(9)
C8	0.0241(9)	0.0389(12)	0.0129(9)	-0.0047(8)	0.0046(7)	0.0012(8)
C9	0.0177(8)	0.0253(10)	0.0135(8)	-0.0039(7)	0.0034(6)	0.0013(7)
C10	0.0120(7)	0.0167(8)	0.0124(8)	0.0002(6)	0.0016(6)	-0.0003(6)
C11	0.0114(7)	0.0090(7)	0.0111(7)	-0.0007(6)	0.0028(6)	-0.0013(5)
C12	0.0132(7)	0.0168(8)	0.0132(8)	0.0010(6)	0.0010(6)	-0.0003(6)
C13	0.0123(7)	0.0109(7)	0.0099(7)	-0.0008(6)	0.0008(6)	0.0022(6)
C14	0.0122(7)	0.0112(7)	0.0182(8)	-0.0001(6)	0.0043(6)	-0.0004(6)
C15	0.0141(7)	0.0104(7)	0.0163(8)	-0.0024(6)	0.0028(6)	0.0010(6)
C16	0.0114(7)	0.0142(8)	0.0103(7)	0.0000(6)	0.0015(6)	0.0042(6)
C17	0.0106(7)	0.0153(8)	0.0191(8)	0.0008(7)	0.0033(6)	-0.0003(6)
C18	0.0133(7)	0.0119(8)	0.0208(9)	-0.0033(6)	0.0015(6)	-0.0031(6)
C19	0.0104(7)	0.0132(8)	0.0115(7)	-0.0014(6)	0.0020(6)	0.0008(6)
C20	0.0169(8)	0.0115(8)	0.0227(9)	0.0010(7)	0.0071(7)	0.0015(6)
C21	0.0161(8)	0.0151(8)	0.0206(9)	0.0011(7)	0.0070(7)	-0.0008(6)
C22	0.0112(7)	0.0175(8)	0.0114(7)	-0.0019(6)	0.0022(6)	0.0024(6)
C23	0.0164(8)	0.0132(8)	0.0194(9)	0.0006(7)	0.0050(6)	0.0025(6)
C24	0.0149(7)	0.0122(8)	0.0179(8)	0.0018(6)	0.0062(6)	0.0010(6)
C25	0.0369(12)	0.0280(11)	0.0307(12)	0.0001(9)	0.0121(9)	0.0105(9)
C26	0.0668(18)	0.0359(14)	0.0332(13)	0.0032(11)	0.0163(13)	-0.0031(13)
Cl1	0.01200(17)	0.01382(19)	0.0229(2)	-0.00004(16)	-0.00121(15)	0.00293(14)

Cl2	0.01772(19)	0.01144(18)	0.0321(2)	0.00089(17)	-0.00048(17)	-0.00260(15)
Cl3	0.0249(2)	0.0222(2)	0.0136(2)	-0.00729(16)	-0.00147(16)	0.00556(17)
In1	0.01024(5)	0.00934(6)	0.01212(6)	-0.00242(4)	-0.00099(4)	0.00115(4)
N1	0.0098(6)	0.0086(6)	0.0139(7)	-0.0018(5)	0.0017(5)	0.0004(5)
N2	0.0113(6)	0.0104(6)	0.0124(7)	-0.0010(5)	0.0021(5)	0.0003(5)
N3	0.0142(6)	0.0189(7)	0.0107(7)	0.0015(6)	0.0011(5)	0.0068(5)
N4	0.0142(7)	0.0222(8)	0.0156(7)	-0.0031(6)	0.0035(5)	0.0030(6)
N5	0.0438(12)	0.0367(12)	0.0516(14)	0.0072(10)	0.0241(10)	0.0082(10)
N6A	0.073(4)	0.067(3)	0.053(3)	-0.009(2)	0.012(3)	0.026(3)
C27A	0.056(4)	0.035(2)	0.037(3)	-0.0001(19)	0.006(3)	0.005(3)
C28A	0.089(6)	0.044(4)	0.055(5)	-0.013(3)	0.019(4)	0.010(4)
N6B	0.121(14)	0.075(9)	0.066(9)	-0.042(7)	0.034(9)	-0.012(10)
C27B	0.068(10)	0.049(7)	0.034(6)	-0.006(5)	0.017(7)	-0.009(8)
C28B	0.092(12)	0.025(6)	0.017(5)	-0.004(4)	0.002(6)	0.006(7)
O1	0.0164(6)	0.0273(7)	0.0184(7)	0.0047(5)	0.0081(5)	0.0049(5)
O2	0.0204(6)	0.0185(7)	0.0208(7)	-0.0071(5)	0.0003(5)	0.0064(5)
O3	0.0266(7)	0.0236(7)	0.0349(8)	0.0030(6)	0.0136(6)	0.0120(6)
O4	0.0238(7)	0.0307(8)	0.0239(7)	0.0012(6)	0.0144(6)	0.0021(6)
O5	0.0170(6)	0.0119(6)	0.0166(6)	-0.0002(5)	0.0032(5)	0.0006(5)

Table S16. X-ray crystallographic and refinement data for complex **4b**.

Chemical formula	$C_{34}H_{40}Cl_3InN_6O_2$
Formula weight	785.89 g/mol
Temperature	103(2) K
Wavelength	0.71073 Å

Crystal size	0.140 x 0.160 x 0.420 mm
Crystal habit	purple needle
Crystal system	triclinic
Space group	P -1
Unit cell dimensions	a = 8.9217(3) Å α = 112.451(2)°
	b = 14.6932(6) Å β = 92.719(2)°
	c = 16.1692(7) Å γ = 95.175(2)°
Volume	1943.22(14) $Å^3$
Z	2
Density (calculated)	1.343 g/cm^3
Absorption coefficient	0.850 mm^{-1}
F(000)	804
Theta range for data collection	1.37 to 31.26°
Index ranges	-13<=h<=12, -21<=k<=21, -23<=l<=23
Reflections collected	43022
Independent reflections	12623 [R(int) = 0.1008]
Coverage of independent reflections	99.6%
Absorption correction	multi-scan
Max. and min. transmission	0.8900 and 0.7170
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/6 (Sheldrick, 2014)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	12623 / 56 / 471
Goodness-of-fit on F^2	1.080
Δ/σ_{max}	0.001
	9555
Final R indices	data; R1 = 0.0576, wR2 = 0.1546

	I>2σ(I)
	all data R1 = 0.0814, wR2 = 0.1728
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0743P)^2+1.0122P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	1.595 and -0.884 eÅ^{-3}
R.M.S. deviation from mean	0.166 eÅ^{-3}

Table S17. Selected bond lengths (Å) for complex **4b**.

In1-O1	2.259(3)	In1-N1	2.317(3)
In1-N2	2.331(3)	In1-Cl1	2.4029(10)
In1-Cl2	2.4241(9)	In1-Cl3	2.4408(10)
C1-N1	1.288(4)	C1-C11	1.503(5)
C11-N2	1.276(4)		

Table S18. Selected bond angles (°) for complex **4b**.

O1-In1-N1	83.45(11)	O1-In1-N2	75.35(10)
N1-In1-N2	72.85(10)	O1-In1-Cl1	87.34(8)
N1-In1-Cl1	168.35(8)	N2-In1-Cl1	97.94(8)
O1-In1-Cl2	93.64(7)	N1-In1-Cl2	91.33(8)
N2-In1-Cl2	161.45(8)	Cl1-In1-Cl2	96.37(4)
O1-In1-Cl3	164.01(7)	N1-In1-Cl3	88.41(8)
N2-In1-Cl3	89.12(8)	Cl1-In1-Cl3	98.76(4)
Cl2-In1-Cl3	100.31(4)		

Table S19. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for complex **4b**.

	x/a	**y/b**	**z/c**	**U(eq)**

In1	0.38338(2)	0.37124(2)	0.15101(2)	0.01830(8)
C1	0.1838(4)	0.2080(3)	0.9952(2)	0.0196(6)
C2	0.1017(4)	0.1248(3)	0.9190(2)	0.0231(7)
C3	0.1276(5)	0.0745(3)	0.8312(3)	0.0346(9)
C4	0.0212(6)	0.9927(4)	0.7766(3)	0.0435(12)
C5	0.8949(5)	0.9630(3)	0.8094(3)	0.0393(11)
C6	0.8635(4)	0.0141(3)	0.8997(3)	0.0305(9)
C7	0.7399(4)	0.9928(3)	0.9426(3)	0.0365(10)
C8	0.7252(4)	0.0499(3)	0.0306(3)	0.0348(10)
C9	0.8313(4)	0.1323(3)	0.0827(3)	0.0266(8)
C10	0.9544(4)	0.1544(3)	0.0429(3)	0.0209(7)
C11	0.0920(4)	0.2265(3)	0.0745(2)	0.0181(6)
C12	0.9699(4)	0.0957(3)	0.9519(3)	0.0242(7)
C13	0.4004(4)	0.2443(3)	0.9306(2)	0.0213(7)
C14	0.4047(4)	0.3057(3)	0.8840(2)	0.0225(7)
C15	0.4947(4)	0.2897(3)	0.8133(3)	0.0248(7)
C16	0.5846(4)	0.2118(3)	0.7885(3)	0.0280(8)
C17	0.5811(5)	0.1519(3)	0.8390(3)	0.0330(9)
C18	0.4912(5)	0.1687(3)	0.9086(3)	0.0291(8)
C19	0.7775(7)	0.1208(5)	0.6994(4)	0.0639(19)
C20	0.6794(6)	0.2586(4)	0.6687(3)	0.0485(13)
C21	0.0626(4)	0.3173(3)	0.2274(2)	0.0200(7)
C22	0.9218(4)	0.3512(3)	0.2259(2)	0.0221(7)
C23	0.8418(4)	0.3785(3)	0.3010(2)	0.0244(7)
C24	0.8999(4)	0.3714(3)	0.3807(3)	0.0258(8)
C25	0.0434(4)	0.3387(3)	0.3816(3)	0.0259(8)
C26	0.1250(4)	0.3140(3)	0.3069(2)	0.0215(7)
C27	0.8840(5)	0.3928(4)	0.5371(3)	0.0387(10)

C28	0.6758(6)	0.4315(5)	0.4528(3)	0.0580(17)
C32	0.8000(12)	0.1301(7)	0.4243(6)	0.042(2)
C33	0.5786(13)	0.0272(11)	0.4075(9)	0.065(4)
C34	0.6121(13)	0.1226(8)	0.3173(8)	0.053(3)
C71	0.2242(4)	0.5279(3)	0.0880(3)	0.0232(7)
C72	0.1219(5)	0.6573(4)	0.0518(4)	0.0402(11)
C73	0.9917(5)	0.5851(4)	0.1484(4)	0.0406(11)
Cl1	0.40743(11)	0.48864(8)	0.30416(6)	0.0313(2)
Cl2	0.59486(10)	0.44860(8)	0.10310(7)	0.0307(2)
Cl3	0.50005(10)	0.23755(7)	0.17362(8)	0.0313(2)
N1	0.3090(3)	0.2633(2)	0.00429(19)	0.0200(6)
N2	0.1466(3)	0.2901(2)	0.1513(2)	0.0188(6)
N3	0.6769(5)	0.1962(3)	0.7189(3)	0.0465(11)
N4	0.8208(4)	0.3966(3)	0.4549(2)	0.0378(9)
N5	0.1180(3)	0.5876(3)	0.0959(2)	0.0286(7)
N6	0.6686(8)	0.0913(5)	0.3836(4)	0.0281(14)
O1	0.2172(3)	0.4643(2)	0.1211(2)	0.0270(6)
O3	0.8617(8)	0.1126(7)	0.4838(5)	0.060(2)
C29	0.2090(13)	0.1463(11)	0.4746(9)	0.064(3)
C30	0.1616(16)	0.1874(13)	0.6294(9)	0.097(5)
O2	0.2536(11)	0.1504(8)	0.4109(6)	0.075(3)
N7	0.2236(10)	0.2117(9)	0.5558(7)	0.071(3)
C31	0.2606(17)	0.3071(11)	0.5912(13)	0.111(5)

Table S20. Anisotropic atomic displacement parameters (Å^2) for complex **4b**.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}

In1	0.01601(12)	0.01999(13)	0.02022(13)	0.00890(9)	0.00364(8)	0.00269(8)
C1	0.0195(15)	0.0224(17)	0.0197(16)	0.0103(13)	0.0031(12)	0.0058(12)
C2	0.0249(17)	0.0240(18)	0.0188(17)	0.0059(14)	-0.0004(13)	0.0076(14)
C3	0.037(2)	0.039(2)	0.026(2)	0.0083(18)	0.0003(17)	0.0116(18)
C4	0.050(3)	0.044(3)	0.023(2)	-0.0027(19)	-0.0075(19)	0.017(2)
C5	0.041(2)	0.028(2)	0.036(2)	-0.0005(18)	-0.0127(19)	0.0090(18)
C6	0.0310(19)	0.0178(18)	0.038(2)	0.0066(16)	-0.0103(17)	0.0057(15)
C7	0.0233(18)	0.0206(19)	0.063(3)	0.015(2)	-0.0120(19)	-0.0010(15)
C8	0.0183(16)	0.027(2)	0.060(3)	0.018(2)	0.0031(18)	0.0011(15)
C9	0.0205(16)	0.0226(18)	0.039(2)	0.0134(16)	0.0044(15)	0.0041(14)
C10	0.0192(15)	0.0169(16)	0.0272(18)	0.0089(14)	0.0010(13)	0.0044(12)
C11	0.0165(14)	0.0196(16)	0.0207(16)	0.0097(13)	0.0033(12)	0.0059(12)
C12	0.0226(16)	0.0201(17)	0.0285(19)	0.0085(14)	-0.0063(14)	0.0042(13)
C13	0.0217(15)	0.0240(18)	0.0201(17)	0.0089(14)	0.0081(13)	0.0072(13)
C14	0.0258(17)	0.0233(18)	0.0220(17)	0.0113(14)	0.0045(13)	0.0077(14)
C15	0.0322(18)	0.0278(19)	0.0219(18)	0.0149(15)	0.0116(14)	0.0120(15)
C16	0.0338(19)	0.029(2)	0.028(2)	0.0149(16)	0.0142(16)	0.0135(16)
C17	0.043(2)	0.034(2)	0.036(2)	0.0237(19)	0.0205(18)	0.0233(19)
C18	0.036(2)	0.033(2)	0.031(2)	0.0231(17)	0.0171(16)	0.0163(17)
C19	0.085(4)	0.069(4)	0.075(4)	0.052(3)	0.062(4)	0.054(3)
C20	0.070(3)	0.052(3)	0.043(3)	0.033(3)	0.035(3)	0.025(3)
C21	0.0195(15)	0.0251(18)	0.0160(15)	0.0082(13)	0.0056(12)	0.0027(13)
C22	0.0208(15)	0.0271(18)	0.0183(16)	0.0084(14)	0.0000(13)	0.0051(13)
C23	0.0179(15)	0.032(2)	0.0219(18)	0.0075(15)	0.0051(13)	0.0066(14)
C24	0.0243(17)	0.031(2)	0.0209(18)	0.0087(15)	0.0059(14)	0.0031(15)
C25	0.0261(17)	0.037(2)	0.0188(17)	0.0157(16)	0.0013(14)	0.0044(15)
C26	0.0184(15)	0.0272(18)	0.0213(17)	0.0115(14)	0.0047(13)	0.0041(13)
C27	0.046(2)	0.046(3)	0.028(2)	0.016(2)	0.0151(19)	0.013(2)
C28	0.040(3)	0.104(5)	0.033(3)	0.023(3)	0.018(2)	0.029(3)
C32	0.068(6)	0.030(5)	0.022(4)	0.003(3)	0.024(4)	0.000(4)
C33	0.047(6)	0.101(11)	0.060(8)	0.051(8)	-0.008(5)	-0.015(6)
C34	0.079(8)	0.047(6)	0.058(7)	0.039(5)	0.022(6)	0.032(6)
C71	0.0181(15)	0.0270(19)	0.0272(19)	0.0133(15)	0.0019(13)	0.0040(13)
C72	0.040(2)	0.038(3)	0.055(3)	0.029(2)	0.005(2)	0.0118(19)
C73	0.0260(19)	0.047(3)	0.060(3)	0.030(2)	0.019(2)	0.0163(19)
Cl1	0.0348(5)	0.0313(5)	0.0213(4)	0.0034(4)	0.0041(4)	0.0018(4)
Cl2	0.0251(4)	0.0321(5)	0.0383(5)	0.0177(4)	0.0106(4)	-0.0018(4)
Cl3	0.0241(4)	0.0223(4)	0.0474(6)	0.0146(4)	-0.0068(4)	0.0025(3)
N1	0.0252(14)	0.0210(15)	0.0152(13)	0.0080(11)	0.0049(11)	0.0043(11)
N2	0.0161(12)	0.0234(15)	0.0192(14)	0.0102(12)	0.0043(10)	0.0041(11)
N3	0.063(3)	0.050(3)	0.050(2)	0.035(2)	0.042(2)	0.035(2)
N4	0.0318(18)	0.059(3)	0.0246(18)	0.0154(17)	0.0129(14)	0.0150(17)
N5	0.0212(14)	0.0297(18)	0.041(2)	0.0190(15)	0.0043(13)	0.0075(13)
N6	0.039(4)	0.034(4)	0.017(3)	0.014(3)	0.007(3)	0.010(3)
O1	0.0236(12)	0.0283(14)	0.0368(16)	0.0196(12)	0.0071(11)	0.0085(11)
O3	0.048(4)	0.079(6)	0.035(4)	0.008(4)	0.008(3)	-0.011(4)
C29	0.048(5)	0.078(6)	0.055(5)	0.013(5)	0.004(4)	0.011(5)
C30	0.061(7)	0.120(11)	0.072(8)	-0.002(8)	0.014(7)	0.002(7)

O2	0.104(7)	0.095(7)	0.044(5)	0.036(5)	0.019(4)	0.053(5)
N7	0.038(4)	0.085(5)	0.061(5)	-0.004(4)	-0.009(4)	0.015(4)
C31	0.086(8)	0.082(9)	0.164(11)	0.057(8)	-0.080(8)	0.006(7)

Table S21. X-ray crystallographic and refinement data for complex **5b**.

Chemical formula	$C_{30.50}H_{30.50}Cl_3InN_{3.50}O_{3.50}$
Formula weight	723.25 g/mol
Temperature	103(2) K
Wavelength	0.71073 Å
Crystal size	0.200 x 0.210 x 0.400 mm
Crystal habit	red block
Crystal system	triclinic
Space group	P -1
Unit cell dimensions	a = 8.9265(5) Å α = 99.6119(15)°
	b = 12.3564(7) Å β = 90.3519(14)°
	c = 14.3910(8) Å γ = 106.1023(14)°
Volume	1501.33(15) $Å^3$
Z	2
Density (calculated)	1.600 g/cm^3
Absorption coefficient	1.095 mm^{-1}
F(000)	732
Theta range for data collection	1.44 to 35.11°
Index ranges	-14<=h<=14, -20<=k<=19, -23<=l<=23
Reflections collected	50446
Independent reflections	13260 [R(int) = 0.0521]
Coverage of independent reflections	99.4%
Absorption correction	multi-scan
Max. and min. transmission	0.8110 and 0.6690
Refinement method	Full-matrix least-squares on F^2

Refinement program	SHELXL-2014/6 (Sheldrick, 2014)
Function minimized	$\Sigma\, w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	13260 / 0 / 403
Goodness-of-fit on F^2	1.050
Δ/σ_{max}	0.003
	11004
Final R indices	data; R1 = 0.0346, wR2 = 0.0684
	$I>2\sigma(I)$
	all data R1 = 0.0487, wR2 = 0.0737
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0224P)^2+0.8558P]$ where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.918 and -0.910 eÅ^{-3}
R.M.S. deviation from mean	0.117 eÅ^{-3}

Table S22. Selected bond lengths (Å) for complex **5b**.

C1-C2	1.522(2)	C1-N1	1.283(2)
C2-N2	1.282(2)	O1-In1	2.2306(13)
Cl1-In1	2.4417(4)	Cl2-In1	2.4301(4)
Cl3-In1	2.4058(5)	In1-N1	2.3182(14)
In1-N2	2.3444(13)		

Table S23. Selected bond angles (°) for complex **5b**.

O1-In1-N1	82.45(5)	O1-In1-N2	74.40(5)
N1-In1-N2	72.68(5)	O1-In1-Cl3	90.02(4)
N1-In1-Cl3	168.35(4)	N2-In1-Cl3	96.77(4)
O1-In1-Cl2	93.94(4)	N1-In1-Cl2	92.88(4)
N2-In1-Cl2	162.28(3)	Cl3-In1-Cl2	96.515(16)
O1-In1-Cl1	162.18(4)	N1-In1-Cl1	86.17(4)

N2-In1-Cl1	89.16(3)	Cl3-In1-Cl1	98.866(17)
Cl2-In1-Cl1	100.306(15)		

Table S24. Atomic coordinates and equivalent isotropic atomic displacement parameters ($Å^2$) for complex **5b**.

	x/a	y/b	z/c	U(eq)
C1	0.76562(18)	0.44303(13)	0.78457(11)	0.0098(3)
C2	0.90629(18)	0.54355(13)	0.82226(11)	0.0093(3)
C3	0.01660(18)	0.49684(14)	0.86833(11)	0.0100(3)
C4	0.15866(19)	0.54309(15)	0.91822(12)	0.0120(3)
C5	0.2271(2)	0.46912(15)	0.95720(12)	0.0137(3)
C6	0.1587(2)	0.35274(16)	0.94551(12)	0.0148(3)
C7	0.0131(2)	0.30250(15)	0.89391(12)	0.0130(3)
C8	0.94426(19)	0.37728(14)	0.85777(11)	0.0104(3)
C9	0.79656(19)	0.34005(14)	0.80840(11)	0.0110(3)
C10	0.7172(2)	0.22498(15)	0.79151(13)	0.0152(3)
C11	0.7866(2)	0.14825(15)	0.82526(13)	0.0177(3)
C12	0.9290(2)	0.18473(15)	0.87490(13)	0.0163(3)
C13	0.52207(19)	0.36565(14)	0.70102(12)	0.0113(3)
C14	0.4153(2)	0.31232(15)	0.76016(12)	0.0148(3)
C15	0.2908(2)	0.21766(17)	0.72273(13)	0.0188(3)
C16	0.2739(2)	0.17888(17)	0.62574(13)	0.0194(4)
C17	0.0491(3)	0.0228(2)	0.63823(17)	0.0361(6)
C18	0.3792(2)	0.23530(16)	0.56627(13)	0.0176(3)
C19	0.5021(2)	0.32898(15)	0.60386(12)	0.0142(3)
C20	0.04089(18)	0.74001(13)	0.83246(11)	0.0100(3)
C21	0.18316(19)	0.73736(14)	0.79295(12)	0.0121(3)

C22	0.3110(2)	0.83213(14)	0.81217(12)	0.0136(3)
C23	0.2999(2)	0.93109(14)	0.87214(12)	0.0133(3)
C24	0.4314(2)	0.11678(16)	0.95643(14)	0.0210(4)
C25	0.1577(2)	0.93457(14)	0.91001(12)	0.0144(3)
C26	0.0277(2)	0.83915(14)	0.88873(12)	0.0129(3)
C27	0.8207(2)	0.61609(16)	0.53227(12)	0.0155(3)
C28	0.0993(3)	0.6739(3)	0.52168(18)	0.0424(7)
C29	0.9241(3)	0.6174(2)	0.37688(14)	0.0289(5)
N3	0.94139(18)	0.63591(15)	0.47921(11)	0.0183(3)
O1	0.83505(15)	0.62518(13)	0.61987(9)	0.0190(3)
C30	0.6265(7)	0.0754(5)	0.5141(4)	0.0386(11)
C31	0.3788(7)	0.9564(5)	0.4376(4)	0.0401(13)
C32	0.4497(7)	0.9465(5)	0.6015(3)	0.0387(12)
N4	0.4924(15)	0.9933(8)	0.5162(4)	0.0401(15)
O4	0.7392(6)	0.1201(3)	0.5778(3)	0.0504(11)
Cl1	0.55343(5)	0.65316(4)	0.88638(3)	0.01508(8)
Cl2	0.44665(5)	0.60463(4)	0.62799(3)	0.01656(8)
Cl3	0.75431(6)	0.85350(4)	0.73388(4)	0.02210(9)
In1	0.67586(2)	0.65111(2)	0.73509(2)	0.00931(3)
N1	0.65433(16)	0.46033(12)	0.73769(10)	0.0103(2)
N2	0.90565(16)	0.64401(11)	0.81046(9)	0.0093(2)
O2	0.15762(17)	0.08770(14)	0.58119(10)	0.0298(4)
O3	0.43376(15)	0.01914(11)	0.88790(10)	0.0190(3)

Table S25. Anisotropic atomic displacement parameters ($Å^2$) for complex **5b**.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}

C1	0.0095(7)	0.0089(6)	0.0097(6)	-0.0002(5)	0.0005(5)	0.0018(5)
C2	0.0086(6)	0.0104(6)	0.0090(6)	0.0012(5)	0.0005(5)	0.0030(5)
C3	0.0097(7)	0.0111(7)	0.0100(6)	0.0028(5)	0.0011(5)	0.0036(5)
C4	0.0090(7)	0.0146(7)	0.0126(7)	0.0037(6)	0.0008(5)	0.0027(6)
C5	0.0099(7)	0.0202(8)	0.0126(7)	0.0048(6)	0.0009(6)	0.0057(6)
C6	0.0153(8)	0.0202(8)	0.0128(7)	0.0052(6)	0.0021(6)	0.0098(6)
C7	0.0154(8)	0.0143(7)	0.0121(7)	0.0037(6)	0.0035(6)	0.0076(6)
C8	0.0113(7)	0.0104(6)	0.0101(6)	0.0013(5)	0.0026(5)	0.0042(5)
C9	0.0108(7)	0.0103(6)	0.0121(7)	0.0012(5)	0.0010(5)	0.0035(5)
C10	0.0153(8)	0.0114(7)	0.0180(8)	0.0008(6)	0.0006(6)	0.0034(6)
C11	0.0206(9)	0.0096(7)	0.0225(9)	0.0024(6)	0.0032(7)	0.0037(6)
C12	0.0207(9)	0.0136(7)	0.0181(8)	0.0059(6)	0.0049(7)	0.0088(6)
C13	0.0081(7)	0.0113(7)	0.0133(7)	-0.0001(5)	-0.0007(5)	0.0024(5)
C14	0.0128(7)	0.0169(8)	0.0118(7)	-0.0006(6)	0.0007(6)	0.0011(6)
C15	0.0131(8)	0.0213(9)	0.0163(8)	-0.0007(7)	0.0035(6)	-0.0023(7)
C16	0.0131(8)	0.0203(9)	0.0183(8)	-0.0026(7)	0.0005(6)	-0.0025(6)
C17	0.0234(11)	0.0346(12)	0.0316(12)	-0.0034(10)	0.0043(9)	-0.0169(9)
C18	0.0149(8)	0.0204(8)	0.0129(7)	-0.0013(6)	0.0009(6)	-0.0005(6)
C19	0.0114(7)	0.0161(8)	0.0124(7)	0.0006(6)	0.0004(6)	0.0009(6)
C20	0.0095(7)	0.0089(6)	0.0111(6)	0.0020(5)	-0.0003(5)	0.0016(5)
C21	0.0120(7)	0.0113(7)	0.0126(7)	0.0004(5)	0.0019(6)	0.0039(6)
C22	0.0099(7)	0.0123(7)	0.0182(8)	0.0015(6)	0.0020(6)	0.0030(6)
C23	0.0119(7)	0.0100(7)	0.0164(7)	0.0012(6)	-0.0006(6)	0.0011(6)
C24	0.0189(9)	0.0136(8)	0.0250(9)	-0.0031(7)	-0.0018(7)	-0.0008(7)
C25	0.0147(8)	0.0097(7)	0.0168(8)	-0.0016(6)	0.0012(6)	0.0024(6)
C26	0.0118(7)	0.0128(7)	0.0140(7)	0.0008(6)	0.0024(6)	0.0043(6)
C27	0.0142(8)	0.0199(8)	0.0131(7)	0.0019(6)	0.0026(6)	0.0063(6)
C28	0.0134(10)	0.077(2)	0.0334(13)	0.0089(13)	0.0045(9)	0.0066(11)

C29	0.0291(11)	0.0419(13)	0.0139(8)	0.0049(8)	0.0074(8)	0.0067(10)
N3	0.0151(7)	0.0254(8)	0.0145(7)	0.0034(6)	0.0044(5)	0.0059(6)
O1	0.0154(6)	0.0323(8)	0.0124(6)	0.0047(5)	0.0032(5)	0.0113(5)
C30	0.048(3)	0.035(3)	0.034(3)	0.003(2)	0.001(2)	0.014(2)
C31	0.064(4)	0.030(3)	0.026(2)	0.000(2)	-0.009(2)	0.017(3)
C32	0.062(4)	0.034(3)	0.023(2)	0.0043(19)	0.000(2)	0.019(2)
N4	0.072(4)	0.028(3)	0.023(4)	0.000(3)	-0.009(4)	0.021(3)
O4	0.071(3)	0.036(2)	0.038(2)	0.0001(17)	-0.019(2)	0.010(2)
Cl1	0.01262(18)	0.02163(19)	0.01182(17)	0.00232(14)	0.00283(13)	0.00651(15)
Cl2	0.01428(18)	0.0223(2)	0.01377(17)	0.00191(15)	-0.00335(14)	0.00718(15)
Cl3	0.0196(2)	0.01129(18)	0.0363(3)	0.00912(17)	-0.00006(18)	0.00307(15)
In1	0.00829(5)	0.00974(5)	0.01045(5)	0.00219(3)	0.00071(3)	0.00316(4)
N1	0.0113(6)	0.0096(6)	0.0096(6)	0.0000(5)	-0.0004(5)	0.0033(5)
N2	0.0087(6)	0.0091(6)	0.0097(6)	0.0012(4)	0.0011(4)	0.0023(5)
O2	0.0208(7)	0.0319(8)	0.0202(7)	-0.0060(6)	0.0028(6)	-0.0133(6)
O3	0.0128(6)	0.0119(6)	0.0271(7)	-0.0022(5)	0.0017(5)	-0.0017(5)

Table S26. X-ray crystallographic and refinement data for **8**.

Chemical formula	$C_{26}H_{22}N_2O_2$
Formula weight	394.45 g/mol
Temperature	103(2) K
Wavelength	1.54178 Å
Crystal size	0.020 x 0.060 x 0.380 mm
Crystal habit	red plate

Crystal system	monoclinic
Space group	C 1 2/c 1
Unit cell dimensions	a = 27.3734(9) Å α = 90°
	b = 9.3669(3) Å β = 100.331(2)°
	c = 7.7757(3) Å γ = 90°
Volume	1961.40(12) $Å^3$
Z	4
Density (calculated)	1.336 g/cm^3
Absorption coefficient	0.674 mm^{-1}
F(000)	832
Theta range for data collection	3.28 to 66.79°
Index ranges	-31<=h<=32, -10<=k<=11, -8<=l<=9
Reflections collected	5667
Independent reflections	1714 [R(int) = 0.0622]
Coverage of independent reflections	98.3%
Absorption correction	multi-scan
Max. and min. transmission	0.9870 and 0.7840
Refinement method	Full-matrix least-squares on F^2
Refinement program	SHELXL-2014/6 (Sheldrick, 2014)
Function minimized	$\Sigma w(F_o^2 - F_c^2)^2$
Data / restraints / parameters	1714 / 0 / 142
Goodness-of-fit on F^2	1.045
Δ/σ_{max}	0.003
	1461
Final R indices	data; R1 = 0.0479, wR2 = 0.1295
	I>2σ(I)
	all data R1 = 0.0553, wR2 = 0.1366
Weighting scheme	$w=1/[\sigma^2(F_o^2)+(0.0812P)^2+0.8405P]$

	where $P=(F_o^2+2F_c^2)/3$
Largest diff. peak and hole	0.253 and -0.214 eÅ^{-3}
R.M.S. deviation from mean	0.055 eÅ^{-3}

Table S27. Selected bond lengths (Å) for **8**.

C1-C1	1.378(3)	C1-N1	1.391(2)
C1-C2	1.473(2)	C8-N1	1.397(2)

Table S28. Selected bond angles (°) for **8**.

C1-N1-C8	126.55(14)	C1-C1-N1	123.91(9)
C1-C1-C2	108.92(8)		

Table S29. Atomic coordinates and equivalent isotropic atomic displacement parameters (Å^2) for **8**.

	x/a	y/b	z/c	U(eq)
H3	0.5971	0.3358	0.0751	0.024
H4	0.5989	0.0837	0.0702	0.027
H5	0.5415	-0.0525	0.1811	0.026
H9	0.5893	0.8065	0.0073	0.024
H10	0.6734	0.8541	0.0320	0.028
H12	0.7057	0.5308	0.3789	0.028
H13	0.6209	0.4875	0.3617	0.025
H14A	0.7792	0.6485	0.4378	0.059
H14B	0.8163	0.6872	0.3073	0.059
H14C	0.7798	0.5532	0.2673	0.059
H1N	0.5264(8)	0.681(2)	0.110(3)	0.03

Table S30. Anisotropic atomic displacement parameters (Å^2) for **8**.
The anisotropic atomic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}\ ]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C1	0.0182(8)	0.0162(8)	0.0199(8)	0.0001(6)	0.0056(6)	-0.0015(6)
C2	0.0183(8)	0.0170(8)	0.0186(9)	0.0004(6)	0.0046(6)	-0.0010(6)
C3	0.0195(8)	0.0195(9)	0.0223(9)	-0.0006(6)	0.0065(6)	-0.0017(6)
C4	0.0221(8)	0.0205(9)	0.0256(9)	-0.0034(7)	0.0081(7)	0.0032(6)
C5	0.0242(8)	0.0153(8)	0.0260(10)	-0.0020(6)	0.0054(7)	0.0013(6)
C6	0.0209(11)	0.0149(11)	0.0220(12)	0	0.0036(9)	0
C7	0.0196(11)	0.0167(11)	0.0182(12)	0	0.0042(9)	0
C8	0.0205(8)	0.0144(8)	0.0211(8)	-0.0042(6)	0.0085(6)	-0.0010(6)
C9	0.0240(8)	0.0155(8)	0.0217(9)	-0.0014(6)	0.0069(7)	-0.0002(6)
C10	0.0260(9)	0.0188(8)	0.0286(10)	0.0013(7)	0.0115(7)	-0.0045(6)
C11	0.0192(8)	0.0249(9)	0.0324(10)	-0.0029(7)	0.0093(7)	-0.0023(7)
C12	0.0221(8)	0.0214(8)	0.0272(10)	-0.0005(7)	0.0051(7)	0.0020(7)
C13	0.0243(8)	0.0169(8)	0.0227(9)	0.0005(6)	0.0090(6)	-0.0004(6)
C14	0.0191(9)	0.0480(13)	0.0506(13)	0.0023(10)	0.0070(8)	0.0014(8)
N1	0.0184(7)	0.0150(7)	0.0263(8)	0.0035(6)	0.0057(6)	0.0006(5)
O1	0.0191(6)	0.0398(8)	0.0515(9)	0.0082(6)	0.0091(6)	-0.0039(5)

6. Theoretical Studies

The initial energy and geometry optimization was carried out at the B3LYP[6-8] level with the 6-31+G* basis set for non-metal atoms[9] together with the LANL2DZ[10] for In, and Cl atoms. Frequency calculations were carried out at this level to confirm that a minimum had been achieved. To account for solvent effects, a reaction field calculation

with radii and non-electrostatic terms with the SMD solvation model was used.[11] All the TD-DFT calculations were carried out using the Gaussian 09 program package.[6-8, 12]

- **Geometry optimization**

The crystallized structure of **1b** and the computationally optimized structure match and a symmetric scaffold is shown including a plane symmetry. Both 2,2´-isopropyl rings are placed orthogonal to the Ar-BIAN ligand (95.5º in the crystallographic data versus 90.5º in the computational geometry optimization) and the isopropyl moieties are perfectly eclipsed. The smaller hydrogen atoms of the isopropyl groups are directed to the indium, thus keeping away the bulkier methyl groups.

Similar to **1b**, the optimized structure for **2b** has a symmetric structure, as observed experimentally. The thermal ellipsoid plots of **2b** can be compared with the optimized structure shown in Figure S18(b), where the aromatic rings are almost orthogonal (92º) to the Ar-BIAN ligand versus the 95º seen in the X-ray structure. Also, in both cases, the symmetry is so high that the methyl groups are completely eclipsed, which is also verified by the crystallographic symmetric plane observed in Figure 1 of the main text.

The calculated geometry for **3b** (either including water molecule or not) also matches the geometry observed from the X-ray crystallographic data. The In-Cl and In-N distances are summarized in Table S26, where the experimental data are juxtaposed with the calculated distances. Water coordination leads to an octahedral arrangement. This water molecule is coordinated at an 83º angle to the ligand (81º from the theoretical optimization). The *p*-NO_2 aromatic rings in the single crystal data are twisted from each other by 26º, in contrast with the theoretical calculations, where a perfect coplanar geometry to the Ar-BIAN ligand is observed. Also a hypothetical complex (**c3**) with two coordinated Ar-BIAN ligands has been simulated and another symmetric structure was located (Figure S18).

The crystal structure of **4b** has an octahedral geometry due to the DMF molecule coordinated to the indium atom. The optimized geometries are now different from the crystallized version, since the two *p*-aminoaromatic rings are twisted 40º from one another in the experimental data, whereas the computational results predicted coplanarity. It is notable that the arylimino rings are not orthogonal with the

acenaphthene bay region of the ligand, in contrast to the structures in **1b**-**3b**. Here, we observe in the experimental data that one ring has a dihedral angle of 78º and the other one at an angle of 128º with the acenaphthene bay region.

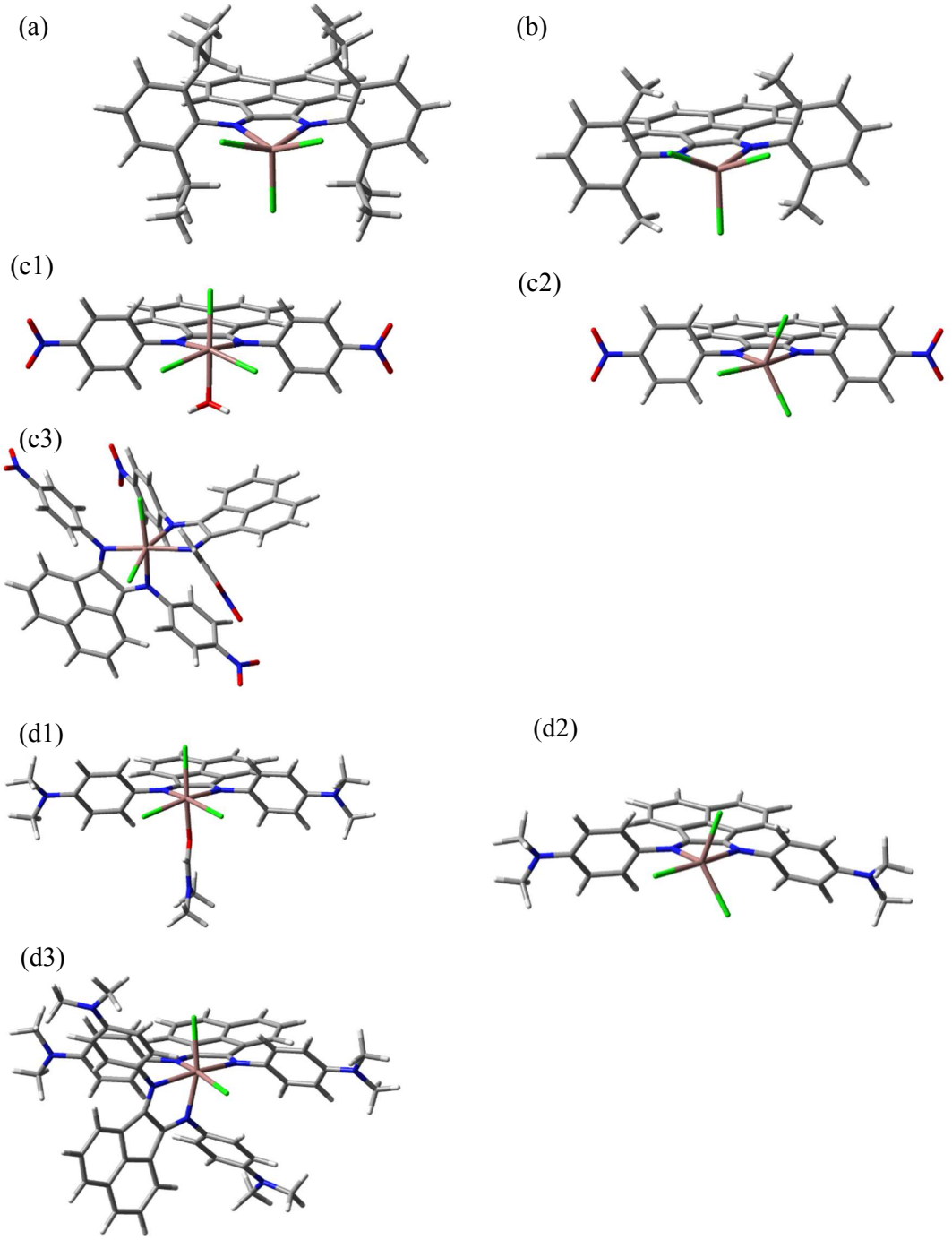

Figure S13. Geometry optimization at the B3LYP/6-31+G*/LANL2DZ level of theory for (a) **1b**, (b) **2b**, (c) **3b**, and (d) **4b**. Structures (c3) and (d3) are the corresponding hypothetical analogues for complexes **3b** and **4b** respectively, containing two Ar-BIAN ligands each.

Table S31. Comparison of the experimental and calculated bond lengths (Å). The geometries were each calculated at a 6-31+G* theory level. (**t1**, **t2**, and **t3** represent structures with a solvent coordinated, no solvent coordinated, and a hypothetical analogue coordinated by two Ar-BIAN ligands for the corresponding complexes, respectively)

1b				**2b**			
In-N		In-Cl		In-N		In-Cl	
Exp.	Calc.	Exp.	Calc.	Exp.	Calc.	Exp.	Calc.
2.343	2.384	2.365	2.424	2.320	2.431	2.377	2.421
2.340	2.383	2.383	2.428	2.320	2.365	2.389	2.423
		2.380	2.424			2.389	2.423

3bt1				**3bt2**		**3bt3**	
In-N		In-Cl		In-N	In-Cl	In-N	In-Cl
Exp.	Calc.	Exp.	Calc.	Calc.	Calc.	Calc.	Calc.
2.311	2.374	2.473	2.459	2.311	2.420	2.355	2.444
2.323	2.374	2.401	2.459	2.449	2.417	2.301	2.444
		2.403	2.458		2.415	2.355	
						2.301	

4bt1				**4bt2**		**4bt3**	
In-N		In-Cl		In-N	In-Cl	In-N	In-Cl
Exp.	Calc.	Exp.	Calc.	Calc.	Calc.	Calc.	Calc.
2.318	2.355	2.424	2.484	2.270	2.434	2.313	2.469
2.332	2.356	2.402	2.480	2.417	2.442	2.318	2.469
		2.440	2.481		2.430	2.318	
						2.313	

- **UV-Vis Spectral Simulations**

TD-DFT calculations were used to predict the electronic absorption spectra of the isolated complexes. The calculations were carried out at the B3LYP/6-31+G* level and the spectra have been calculated either in vacuum or with the polarizable continuum model to account for solvent effects.

Comparisons of the experimental and theoretical spectra for **1b** indicate that the TD-DFT calculations correctly describe the electronic absorption bands. It was necessary to include solvation effects in our theoretical studies.

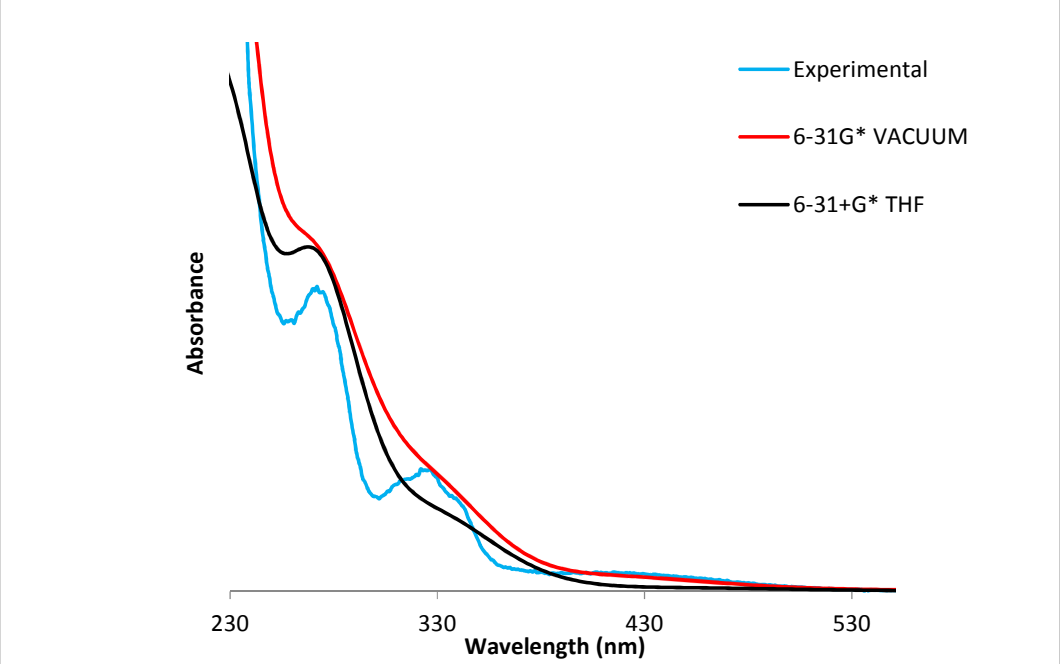

Figure S14. Experimental and calculated absorption spectra in different media for **1b**.

Table S32. Orbital contributions to the electronic absorption transitions of **1b** using a B3LYP/6-31+G* level of theory; only transitions with oscillator strengths >0.03 have been taken into account.

Transition	λ_{max} (nm)	*f*	Orbital contributions (%)

HOMO-13 →LUMO	332	0.1340	4.64
HOMO-3 →LUMO+1			90.93
HOMO-15 →LUMO	278	0.3319	23.39
HOMO-12 → LUMO			66.92
HOMO-10 → LUMO			2.16
HOMO-3 → LUMO+1			2.70
HOMO-16 → LUMO	273	0.2111	3.38
HOMO-15 → LUMO			63.86
HOMO-12 → LUMO			23.69
HOMO-10 → LUMO			2.26

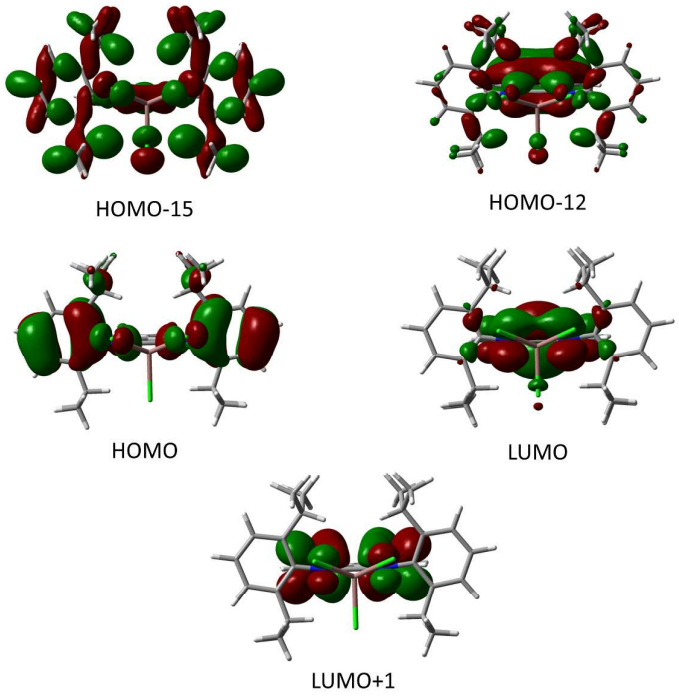

Figure S15. The MOs involved in the transitions that contribute most to the calculated absorption spectrum of **1b.**

Similarly, for **2b**, comparisons of the experimental and theoretical spectra indicate that the TD-DFT calculations correctly approximate the electronic absorption bands.

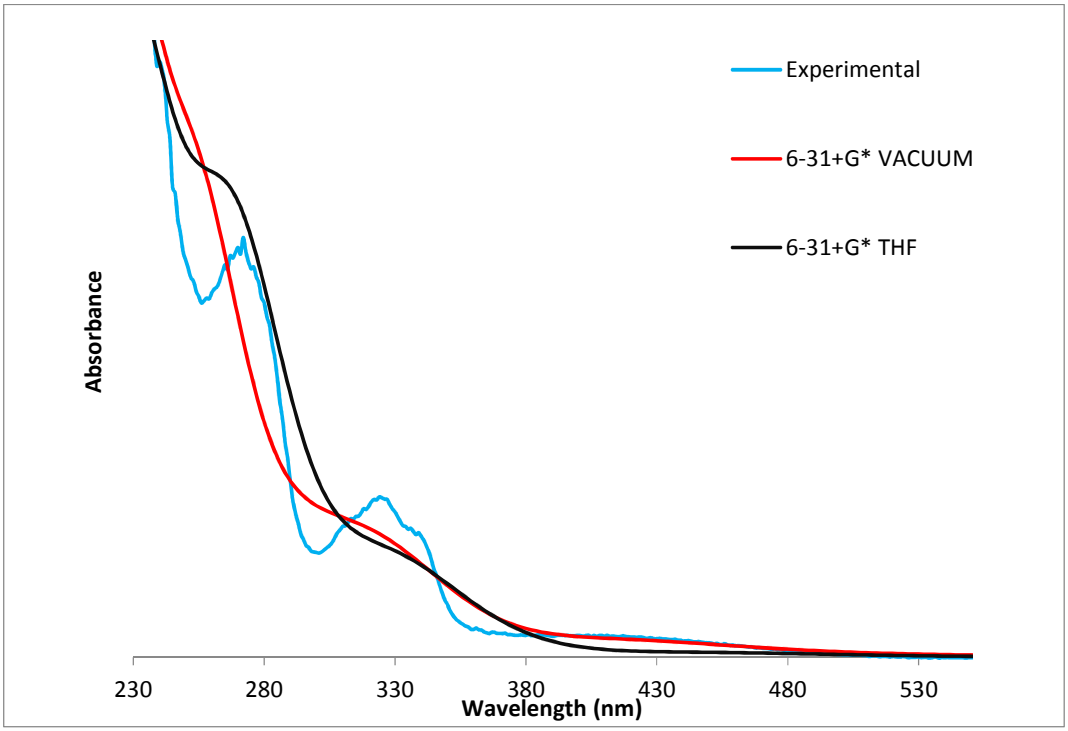

Figure S16. Experimental and calculated absorption spectra in different media for **2b**.

Table S33. Orbital contributions to the electronic absorption transitions of **2b** using a B3LYP/6-31+G* level of theory; only transitions with oscillator strengths >0.03 have been taken into account.

Transition	λ_{max} (nm)	*f*	Orbital contributions (%)
HOMO-14 →LUMO	271	0.2925	2.24
HOMO-12 →LUMO			36.1
HOMO → LUMO+2			54.46
HOMO-12 →LUMO	270	0.3986	53.27
HOMO-3 →LUMO+1			2.01
HOMO → LUMO+2			36.38
HOMO-12 →LUMO	330	0.1492	4.49

HOMO-4 → LUMO+1			18.33
HOMO-3 →LUMO+1			69.74
HOMO-1 → LUMO+1			2.34

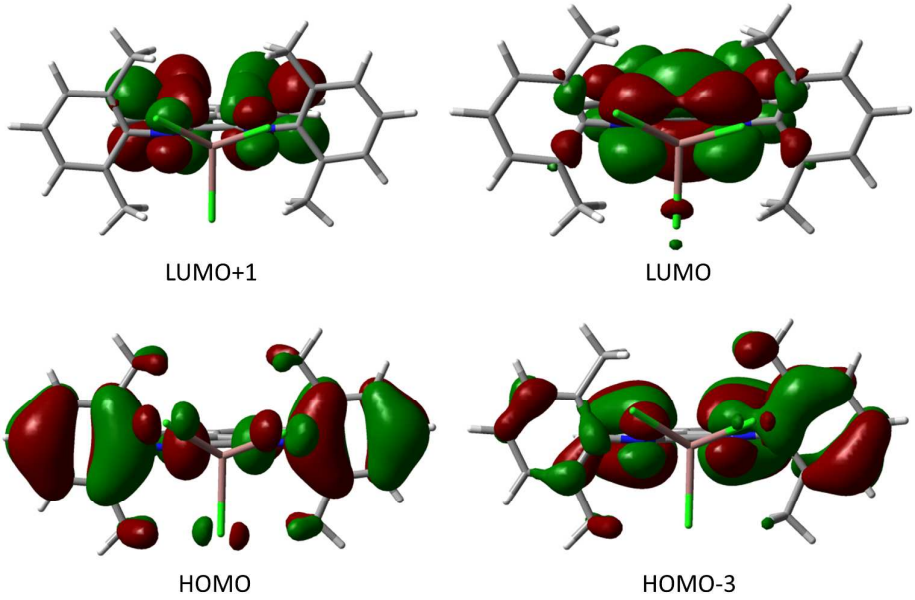

Figure S17. The MOs involved in the transitions that contribute predominantly to the calculated absorption spectrum of **2b.**

For **3b**, the spectra have been simulated in vacuum and in DMF. There is better agreement between the calculated and the experimental data when solvation is included in the computational studies. Moreover, we have also computed the hypothetical complex that arises from coordination of two Ar-BIAN ligands to one indium center.

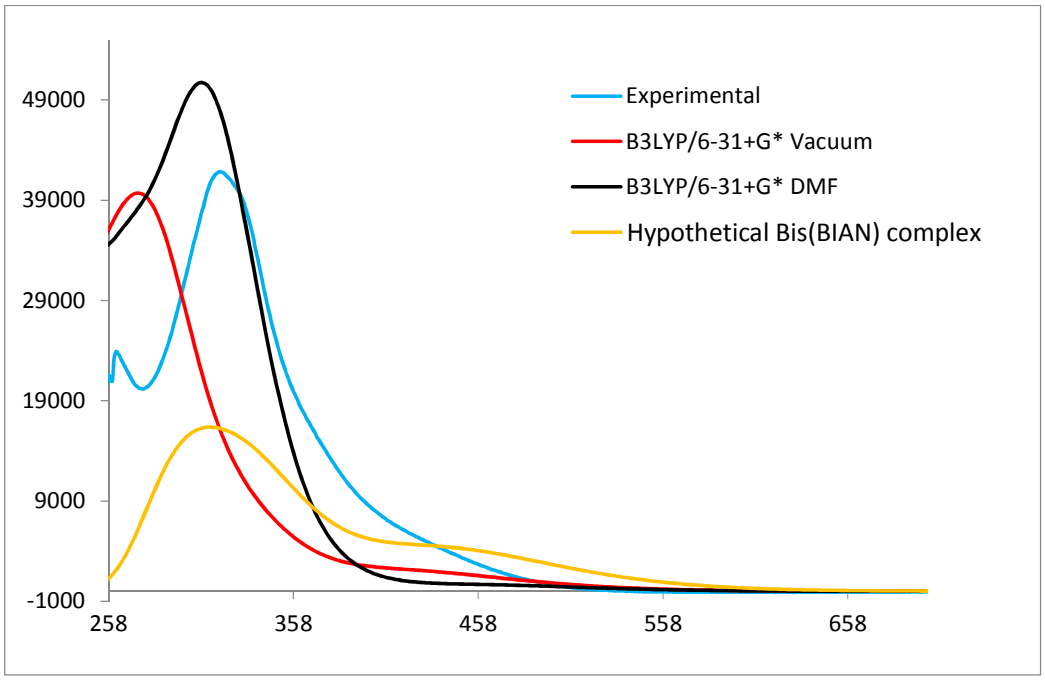

Figure S18. Experimental and calculated absorption spectra in different media for **3b**.

Table S34. Orbital contributions to the electronic absorption transitions of **3b** using a B3LYP/6-31+G* level of theory; only transitions with oscillator strengths >0.03 have been taken into account.

Transition	λ_{max} (nm)	*f*	Orbital contributions (%)
HOMO-1 → LUMO	391	0.1017	94.6
HOMO-1 → LUMO+2			2.40
HOMO-6 → LUMO	334	0.1113	2.79
HOMO → LUMO+3			87.7
HOMO-5 → LUMO+1	313	0.4282	6.58
HOMO-4 → LUMO+2			8.46
HOMO-3 → LUMO+1			6.04
HOMO-2 → LUMO+1			14.5
HOMO-1 → LUMO+2			56.5

HOMO-8 → LUMO	308	0.1450	53.37
HOMO-5 → LUMO+1			2.80
HOMO-4 → LUMO+2			5.37
HOMO-3 → LUMO+1			3.42
HOMO-2 → LUMO+1			13.97
HOMO-1 → LUMO+2			18.4
HOMO-15 → LUMO	275	0.3316	7.12
HOMO-14 → LUMO			23.03
HOMO-12 → LUMO			46.72
HOMO-11 → LUMO			6.60
HOMO-3 → LUMO+2			2.65
HOMO → LUMO+3			3.06

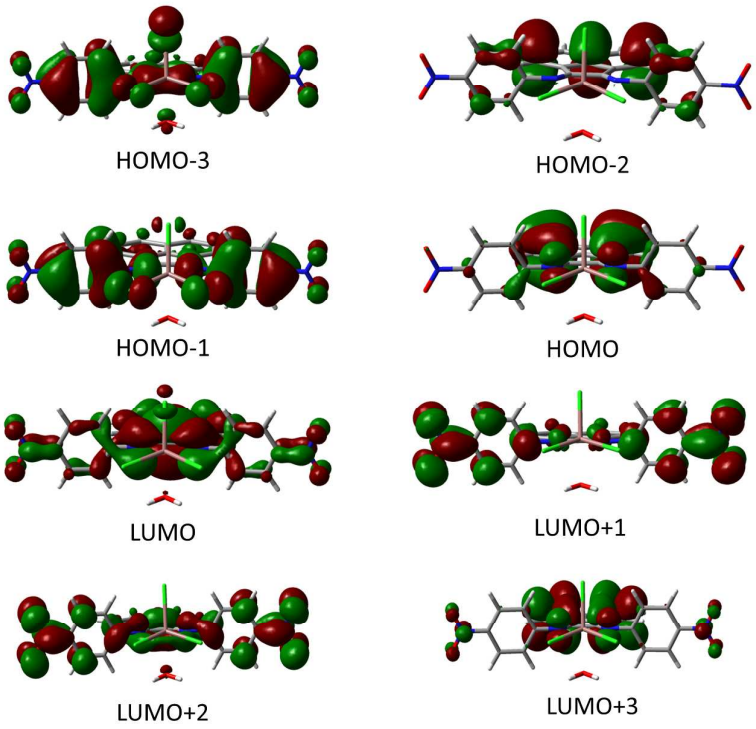

Figure S19. The MOs involved in the transitions that contribute most to the calculated absorption spectrum of **3b.**

In the case of **4b**, the calculated spectra have been modeled based on an octahedral complex with a DMF molecule coordinated to indium (either in vacuum or in DCM). A hypothetical structure with two Ar-BIAN ligands has been also computed. We can see that the predicted and experimental spectra match approximately, and no major differences are observed when solvents are included or excluded in the calculations. Gratifyingly, the calculated spectrum containing a coordinated DMF molecule most accurately matches the experimental spectrum as expected, since the crystallized compounds include coordinated DMF.

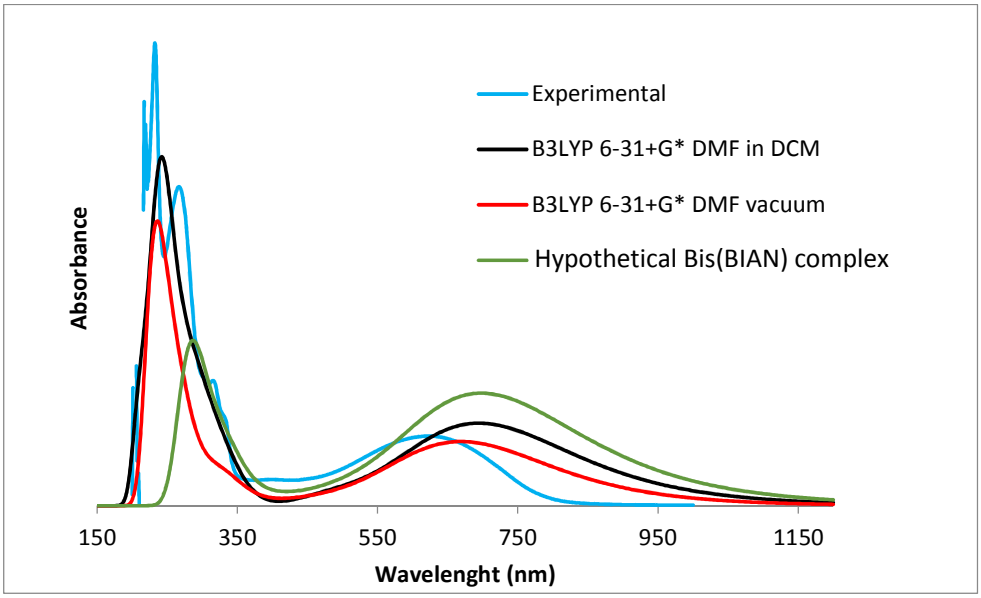

Figure S20. Experimental and calculated absorption spectra in different media for **4b**.

Table S35: Orbital contributions to the electronic absorption transitions of **4b** using a B3LYP/6-31+G* level of theory; only transitions with oscillator strengths >0.1 have been taken into account.

Transition	λ_{max} (nm)	*f*	Orbital contributions (%)
HOMO → LUMO	709	0.3773	99
HOMO-15 → LUMO	288	0.1201	3.1
HOMO-14 → LUMO			79.7
HOMO-1 → LUMO+3			5.8
HOMO → LUMO+4			4.1
HOMO-15 → LUMO	281	0.1223	76.7
HOMO-14 → LUMO			5.96
HOMO-1 → LUMO+3			9.48
HOMO-16 → LUMO	270	0.1668	18.50
HOMO-8 → LUMO+1			2.58

HOMO-1 → LUMO+4			10.34
HOMO-1 → LUMO+8			5.75
HOMO-1 → LUMO+9			5.17
HOMO → LUMO+5			2.88
HOMO → LUMO+7			48.03
HOMO-14 → LUMO+1	252	0.2707	4.16
HOMO-8 → LUMO+1			3.54
HOMO-1 → LUMO+8			8.86
HOMO → LUMO+10			71.05
HOMO-19 → LUMO	236	0.3420	25.97
HOMO-14 → LUMO+1			5.90
HOMO-6 → LUMO+1			9.49
HOMO-2 → LUMO+2			36.4
HOMO-2 → LUMO+3			2.87
HOMO-1 → LUMO+9			5.46
HOMO → LUMO+12			2.69

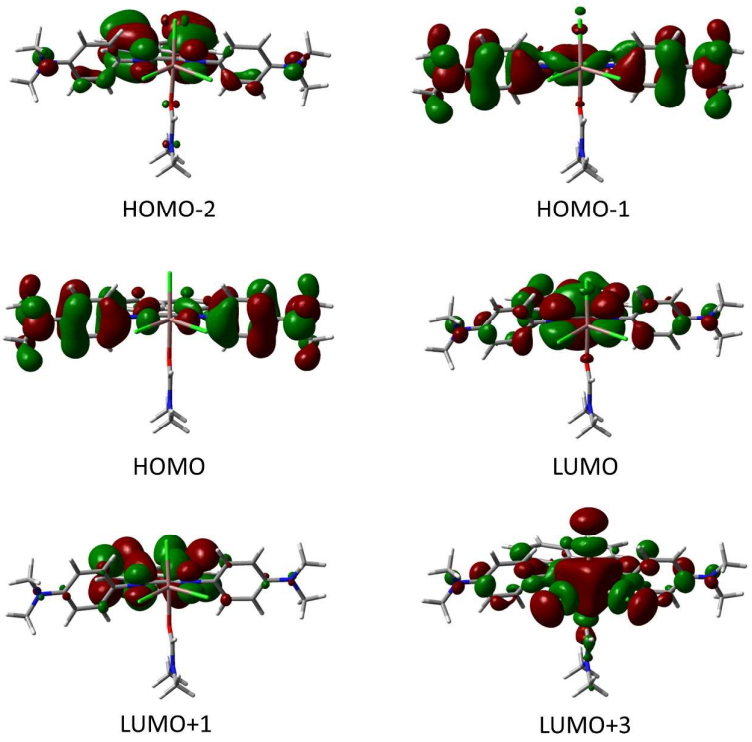

Figure S21. The MOs involved in the transitions that contribute to the calculated absorption spectrum of **4b**.

Table S36. B3LYP/6-31+G(d) optimized cartesian coordinates of the structures located in the present work.

1b

Energy: -1552.41391372

Imaginary vibrational frequency: None

C	0.761923	1.017248	-0.141722
C	-0.762529	1.017091	-0.141724
C	-1.191646	2.423343	-0.211650
C	-2.417952	3.068288	-0.233268
C	-2.436759	4.485495	-0.310423
C	-1.274384	5.240079	-0.358292
C	-0.000630	4.606842	-0.329906
C	1.273004	5.240309	-0.358137
C	2.435525	4.485937	-0.310153
C	2.416980	3.068743	-0.233046
C	1.190789	2.423540	-0.211599
C	-0.000502	3.197636	-0.259887
C	2.825312	-0.094452	0.170602
C	3.684723	-0.143928	-0.946772
C	3.184583	-0.288449	-2.381293
C	3.645421	-1.630832	-2.986301
C	3.612230	0.892071	-3.277162
C	5.064032	-0.086113	-0.699817
C	5.570391	0.001995	0.594380
C	4.696087	0.005770	1.679779
C	3.309384	-0.056279	1.498139
C	2.386783	-0.078481	2.716148
C	2.317160	1.301224	3.405204
C	2.784253	-1.173535	3.725436
C	-2.825588	-0.095043	0.170620
C	-3.309593	-0.056391	1.498158
C	-2.387040	-0.078116	2.716205
C	-2.318955	1.301290	3.405986
C	-2.783593	-1.174160	3.724826
C	-4.696303	0.005420	1.679880
C	-5.570705	0.000895	0.594566
C	-5.064414	-0.087705	-0.699627
C	-3.685110	-0.145239	-0.946651
C	-3.185037	-0.290258	-2.381127
C	-3.645494	-1.633052	-2.985508
C	-3.613145	0.889725	-3.277495
N	1.387800	-0.095712	-0.016168
N	-1.388162	-0.095957	-0.016223
H	-3.350705	2.518474	-0.192417
H	-3.398580	4.989836	-0.330635
H	-1.333334	6.324324	-0.414785
H	1.331772	6.324565	-0.414606
H	3.397250	4.990466	-0.330236
H	3.349835	2.519110	-0.192166
H	2.092297	-0.309583	-2.370677
H	4.736992	-1.665696	-3.093459
H	3.199939	-1.767162	-3.978005
H	3.335161	-2.472854	-2.360403

H	3.193496	0.767262	-4.282920
H	4.703107	0.951155	-3.377916
H	3.259049	1.852482	-2.882682
H	5.751494	-0.119834	-1.540386
H	6.643981	0.046196	0.758656
H	5.097645	0.043512	2.688243
H	1.376794	-0.324264	2.370037
H	3.300789	1.596103	3.791451
H	1.621266	1.270525	4.252701
H	1.981957	2.086561	2.717967
H	2.830488	-2.152501	3.240224
H	2.042539	-1.223517	4.532109
H	3.756755	-0.966076	4.187779
H	-1.376720	-0.322593	2.370138
H	-3.302838	1.594929	3.792518
H	-1.984646	2.087317	2.719087
H	-1.622940	1.270910	4.253399
H	-2.828572	-2.152933	3.239109
H	-3.756537	-0.967981	4.186824
H	-2.042146	-1.223718	4.531780
H	-5.097770	0.043551	2.688377
H	-6.644292	0.044906	0.758913
H	-5.751910	-0.122015	-1.540146
H	-2.092745	-0.311026	-2.370605
H	-3.200080	-1.769668	-3.977200
H	-4.737074	-1.668289	-3.092525
H	-3.334890	-2.474683	-2.359262
H	-4.704030	0.948108	-3.378574
H	-3.194062	0.764840	-4.283104
H	-3.260670	1.850479	-2.883215
Cl	1.853090	-3.301877	0.703258
Cl	0.000390	-2.082374	-2.627844
Cl	-1.851614	-3.302036	0.702255
In	0.000971	-2.025063	-0.200352

2b

Energy: -1237.91481103

Imaginary vibrational frequency: None

C	0.692134	1.034949	-0.024650
C	-0.828356	0.967583	-0.039516
C	-1.319843	2.355735	-0.041732
C	-2.573411	2.945386	-0.052273
C	-2.653901	4.363051	-0.058040
C	-1.525817	5.169237	-0.050057
C	-0.225187	4.591676	-0.037693
C	1.020196	5.279750	-0.022062
C	2.214603	4.575104	-0.005317
C	2.258042	3.156356	-0.003595
C	1.060342	2.459110	-0.020960
C	-0.163899	3.182610	-0.035865
C	2.812440	0.006446	0.122456
C	3.582058	0.063101	-1.054707
C	2.952386	0.071492	-2.427502
C	4.975352	0.116708	-0.912587
C	5.576635	0.111745	0.345800
C	4.785586	0.049413	1.492814

C	3.389620	-0.011613	1.406455
C	2.546333	-0.108545	2.655037
C	-2.843048	-0.252166	0.097835
C	-3.407769	-0.261810	1.389196
C	-2.555325	-0.173471	2.632606
C	-4.800964	-0.353652	1.490733
C	-5.604076	-0.434321	0.353298
C	-5.017134	-0.413206	-0.911148
C	-3.627000	-0.321470	-1.069728
C	-3.021252	-0.274416	-2.452044
N	1.371682	-0.052947	0.026207
N	-1.404734	-0.176554	-0.008928
H	-3.481299	2.353439	-0.056594
H	-3.636742	4.825388	-0.067663
H	-1.632360	6.251292	-0.053100
H	1.032274	6.367005	-0.022902
H	3.153210	5.121597	0.006999
H	3.213938	2.646001	0.009138
H	2.291656	0.936328	-2.572887
H	5.590709	0.154068	-1.808131
H	6.659417	0.146517	0.432042
H	5.251644	0.031218	2.474837
H	-1.985782	0.764254	2.678714
H	-5.253726	-0.374470	2.478922
H	-6.683269	-0.515801	0.452251
H	-5.640126	-0.473885	-1.800115
H	-2.450043	0.648697	-2.617141
Cl	2.100529	-3.236462	0.664410
Cl	0.025799	-2.277584	-2.535168
Cl	-1.572859	-3.305907	1.065808
In	0.128629	-2.059823	-0.124255
H	-3.808204	-0.314052	-3.211440
H	-2.333486	-1.106690	-2.629990
H	-3.182526	-0.219951	3.527954
H	-1.845107	-1.005879	2.679297
H	2.007622	-1.063314	2.685434
H	3.177097	-0.055902	3.547516
H	1.806735	0.699106	2.724646
H	3.726976	0.117312	-3.199016
H	2.348477	-0.823964	-2.607597

3b (3bt1)

Energy: -1566.10560922

Imaginary vibrational frequency: None

C	-2.802923	-0.038636	-0.088393
C	-3.512449	0.207595	-1.271754
C	-4.898993	0.084539	-1.284524
C	-5.550989	-0.281827	-0.106410
C	-4.854816	-0.546397	1.073621
C	-3.466467	-0.436833	1.079161
C	-0.761086	1.163321	-0.096651
C	-1.191768	2.568393	-0.043917
C	-2.416959	3.212700	0.016921
C	-2.436300	4.628714	0.106210
C	-1.273322	5.383235	0.138212
C	0.000002	4.750498	0.088571

C	1.273358	5.383187	0.138015
C	2.436311	4.628630	0.105845
C	2.416911	3.212615	0.016616
C	1.191684	2.568356	-0.044035
C	0.760950	1.163312	-0.096699
C	-0.000029	3.343086	-0.007819
C	2.802804	-0.038657	-0.088445
C	3.466356	-0.436219	1.079317
C	4.854711	-0.545767	1.073818
C	5.550860	-0.281758	-0.106349
C	4.898855	0.084009	-1.284639
C	3.512303	0.207010	-1.271931
N	-1.378927	0.038276	-0.087218
N	1.378786	0.038262	-0.087304
H	-2.977777	0.478271	-2.177392
H	-5.472646	0.264276	-2.185951
H	-5.394647	-0.846538	1.963763
H	-2.895430	-0.664576	1.973527
H	-3.351803	2.665447	-0.000099
H	-3.397596	5.131907	0.153130
H	-1.331923	6.466443	0.209526
H	1.332008	6.466394	0.209312
H	3.397628	5.131798	0.152604
H	3.351730	2.665323	-0.000513
H	2.895322	-0.663533	1.973796
H	5.394559	-0.845442	1.964107
H	5.472499	0.263324	-2.186155
H	2.977613	0.477207	-2.177700
In	0.000156	-1.882916	0.122026
Cl	0.000058	-1.488559	2.547959
Cl	1.930356	-3.304422	-0.425490
Cl	-1.930189	-3.304369	-0.424995
N	7.020141	-0.394223	-0.112800
N	-7.020249	-0.394347	-0.112914
O	-7.575237	-0.713890	0.938490
O	-7.607540	-0.154117	-1.169673
O	7.607418	-0.154468	-1.169669
O	7.575137	-0.713260	0.938751
O	-0.000133	-1.698503	-2.253343
H	-0.775840	-2.256400	-2.465764
H	0.775441	-2.256593	-2.465757

3b (3bt2)

Energy: -1489.65966079

Imaginary vibrational frequency: None

C	-2.771274	-0.078043	-0.006043
C	-3.461721	-0.136140	-1.221408
C	-4.853566	-0.185196	-1.218369
C	-5.524265	-0.185486	0.004819
C	-4.845416	-0.154870	1.223045
C	-3.453564	-0.104700	1.215310
C	-0.698165	1.068918	-0.003998
C	-1.115471	2.474516	-0.005115
C	-2.337167	3.131181	-0.013329
C	-2.343528	4.548918	-0.011373
C	-1.172501	5.293706	-0.000434

C	0.096345	4.650576	0.008427
C	1.375826	5.274327	0.022862
C	2.531422	4.508540	0.032448
C	2.499326	3.088816	0.025632
C	1.268334	2.455811	0.009394
C	0.824335	1.052838	0.006326
C	0.084349	3.240557	0.003441
C	2.843051	-0.178632	0.016633
C	3.525504	-0.361171	1.227190
C	4.914714	-0.469249	1.221828
C	5.593462	-0.409830	0.004382
C	4.921738	-0.263432	-1.210101
C	3.533815	-0.150375	-1.203413
N	-1.337954	-0.049273	-0.009884
N	1.420338	-0.078880	0.021448
H	-2.913078	-0.159814	-2.157676
H	-5.415862	-0.232399	-2.143252
H	-5.401508	-0.178591	2.152591
H	-2.898642	-0.102701	2.148299
H	-3.276508	2.591409	-0.020240
H	-3.299845	5.063431	-0.017931
H	-1.223226	6.379700	0.001995
H	1.444165	6.359214	0.027149
H	3.497307	5.004875	0.044647
H	3.428268	2.530562	0.031743
H	2.967492	-0.436209	2.153562
H	5.467865	-0.605501	2.143462
H	5.480272	-0.246000	-2.138385
H	2.982916	-0.067243	-2.133500
In	-0.107320	-1.998364	-0.009663
Cl	-2.099023	-3.361567	-0.076212
Cl	0.802966	-2.390964	2.197385
Cl	0.927080	-2.375471	-2.162951
N	7.063664	-0.510334	-0.000287
N	-6.998660	-0.222824	0.010420
O	-7.565974	-0.219171	1.103346
O	-7.573609	-0.245945	-1.078198
O	7.638414	-0.445830	-1.088120
O	7.631978	-0.644701	1.084278

3b (3bt3)

Energy: -2917.20069860

Imaginary vibrational frequency: None

C	5.225599	-0.613218	3.324754
C	4.196800	0.159713	3.860726
C	3.181303	0.609151	3.018191
C	3.230680	0.296356	1.654484
C	4.265782	-0.487726	1.129922
C	5.274730	-0.949885	1.972371
C	2.322642	1.693895	-0.044999
C	3.440627	2.568935	-0.403556
C	4.758559	2.697765	0.011784
C	5.555551	3.719488	-0.563140
C	5.060700	4.591382	-1.522286
C	3.710802	4.492705	-1.961998
C	3.058947	5.321441	-2.917482

C	1.722797	5.119768	-3.234892	C	-2.322644	-1.694025	-0.045677
C	0.951461	4.096036	-2.630595	C	-3.231125	-0.296822	1.653860
C	1.561069	3.267085	-1.699120	C	-3.181727	-0.609060	3.017701
C	2.932806	3.470951	-1.380614	C	-4.197435	-0.159681	3.860007
C	1.118710	2.146598	-0.869183	C	-5.226465	0.612719	3.323706
C	-1.196864	2.006357	-1.353154	C	-5.275617	0.948875	1.971191
C	-1.565587	1.455018	-2.588317	C	-4.266488	0.486721	1.128967
C	-2.738949	1.873018	-3.214211	N	2.161957	0.740870	0.807415
C	-3.529548	2.833788	-2.584413	N	-0.011995	1.556087	-0.690165
C	-3.180967	3.386850	-1.352171	N	0.012034	-1.555596	-0.690636
C	-2.008208	2.963940	-0.726848	N	-2.162213	-0.741232	0.807052
C	3.530032	-2.833131	-2.584180	H	4.190121	0.392263	4.919113
C	3.180722	-3.386924	-1.352473	H	2.357972	1.197156	3.411629
C	2.007806	-2.964070	-0.727400	H	4.277880	-0.740466	0.074316
C	1.197042	-2.005811	-1.353421	H	6.087924	-1.560536	1.597406
C	1.566491	-1.453760	-2.588048	H	5.190560	2.042204	0.758137
C	2.740006	-1.871703	-3.213693	H	6.586622	3.817794	-0.237583
C	-1.118559	-2.146302	-0.869826	H	5.706202	5.360446	-1.938358
C	-1.560593	-3.266698	-1.700052	H	3.613035	6.123255	-3.398551
C	-0.950737	-4.095273	-2.631701	H	1.246654	5.768311	-3.963922
C	-1.721786	-5.119037	-3.236302	H	-0.091528	3.984404	-2.902816
C	-3.057892	-5.321147	-2.918981	H	-0.931081	0.714980	-3.065307
C	-3.709999	-4.492809	-1.963326	H	-3.041253	1.470648	-4.174165
C	-5.059877	-4.591983	-1.523662	H	-3.820989	4.132675	-0.894450
C	-5.554993	-3.720435	-0.564345	H	-1.722001	3.360634	0.242185
C	-4.758321	-2.698565	0.010773	H	3.820287	-4.133259	-0.894951
C	-3.440421	-2.569255	-0.404504	H	1.721039	-3.361345	0.241232
C	-2.932307	-3.470960	-1.381699	H	0.932407	-0.713225	-3.064829

H	3.042845	-1.468798	-4.173254
H	0.092234	-3.983314	-2.903853
H	-1.245442	-5.767268	-3.965479
H	-3.611748	-6.123002	-3.400250
H	-6.586035	-3.819108	-0.238806
H	-5.190562	-2.043252	0.757204
H	-2.358237	-1.196661	3.411404
H	-4.190733	-0.391854	4.918476
H	-5.705135	-5.361156	-1.939909
H	-6.088978	1.559138	1.595956
H	-4.278615	0.739100	0.073270
Cl	0.572517	-1.877109	2.534538
Cl	-0.573267	1.876650	2.534896
In	-0.000139	-0.000011	1.076928
N	6.300334	-1.096771	4.218232
N	-4.776938	3.275007	-3.245096
N	-6.301396	1.096250	4.216936
N	4.777585	-3.274259	-3.244583
O	-5.049304	2.768710	-4.332939
O	-5.460168	4.113244	-2.661334
O	-7.188463	1.783823	3.712780
O	-6.239624	0.776389	5.401937
O	6.238524	-0.776562	5.403134
O	7.187282	-1.784684	3.714336
O	5.460306	-4.113092	-2.661069
O	5.050597	-2.767270	-4.331945

4b (4bt1)

Energy: -1597.13428713

Imaginary vibrational frequency: None

C	2.801253	0.261237	-0.306747
C	3.550253	0.511793	0.849606
C	4.930575	0.338716	0.858938
C	5.622031	-0.075617	-0.307322
C	4.843682	-0.345165	-1.460665
C	3.462868	-0.205308	-1.452152
C	0.756847	1.447434	-0.022071
C	1.190618	2.839389	0.219246
C	2.413153	3.490703	0.261774
C	2.433422	4.899746	0.436126
C	1.273565	5.647193	0.560120
C	0.001994	5.012291	0.501582
C	-1.268957	5.648488	0.559621
C	-2.429506	4.902205	0.435171
C	-2.410585	3.493124	0.260919
C	-1.188709	2.840544	0.218901
C	-0.756233	1.448167	-0.022247
C	0.001321	3.609526	0.339058
C	-2.801393	0.262977	-0.306975
C	-3.463002	-0.206274	-1.451341
C	-4.843790	-0.346066	-1.459639
C	-5.622205	-0.073943	-0.306938
C	-4.930814	0.343032	0.858454
C	-3.550527	0.516119	0.848792
N	1.386721	0.360783	-0.311364
N	-1.386959	0.362044	-0.311776

H	3.043563	0.808420	1.764310
H	5.463919	0.509086	1.786617
H	5.312425	-0.699912	-2.370171
H	2.886920	-0.448391	-2.339409
H	3.347761	2.952421	0.164354
H	3.396173	5.402533	0.469777
H	1.330486	6.725501	0.689127
H	-1.324832	6.726854	0.688598
H	-3.391766	5.405955	0.468427
H	-3.345705	2.955800	0.163142
H	-2.887074	-0.451191	-2.338085
H	-5.312463	-0.702895	-2.368363
H	-5.464206	0.515427	1.785731
H	-3.043894	0.814687	1.762893
In	-0.000574	-1.488135	-0.763667
Cl	0.000339	-0.813547	-3.154433
Cl	-1.877804	-3.100447	-0.590955
Cl	1.875389	-3.101306	-0.586972
N	-7.002070	-0.215457	-0.317936
N	7.001981	-0.217000	-0.318606
C	7.643349	-0.873502	-1.450000
H	7.447679	-0.329141	-2.381112
H	8.723753	-0.877763	-1.292113
H	7.306003	-1.913804	-1.581136
C	7.738107	-0.143375	0.933380
H	7.585549	0.826638	1.421886
H	7.449108	-0.936106	1.643324
H	8.805512	-0.241811	0.725643
C	-7.738443	-0.138188	0.933682
H	-7.586092	0.833290	1.419357
H	-8.805792	-0.237419	0.726060
H	-7.449459	-0.928769	1.646010
C	-7.643535	-0.873992	-1.448092
H	-8.723912	-0.878089	-1.290050
H	-7.448017	-0.331287	-2.380212
H	-7.306096	-1.914481	-1.577385
O	-0.002027	-1.468267	1.525711
C	-0.003669	-2.561130	2.133141
H	-0.007850	-3.509084	1.588541
N	-0.000835	-2.673238	3.467456
C	-0.003157	-3.983302	4.107979
H	-0.006638	-4.765632	3.345777
H	0.889637	-4.102143	4.733668
H	-0.894178	-4.097420	4.737077
C	0.004664	-1.501491	4.334005
H	0.005562	-0.605200	3.713803
H	-0.885249	-1.504061	4.975194
H	0.897852	-1.509040	4.970591

4b (4bt2)

Energy: -1348.59179137

Imaginary vibrational frequency: None

C	-2.755245	-0.075126	-0.043844
C	-3.398181	0.353352	-1.211072
C	-4.775374	0.225633	-1.352793
C	-5.569474	-0.327526	-0.315887

C	-4.895519	-0.773142	0.848827	H	-1.448375	6.423475	0.472894
C	-3.515878	-0.669887	0.969641	H	1.208328	6.504965	0.504258
C	-0.716394	1.142506	0.069534	H	3.312631	5.225702	0.459303
C	-1.190717	2.535947	0.116760	H	3.339505	2.767653	0.231296
C	-2.435024	3.143721	0.194265	H	3.026609	-1.363779	1.737712
C	-2.496765	4.555391	0.321135	H	5.435168	-1.665723	1.504407
C	-1.357903	5.344384	0.373143	H	5.369200	0.804247	-2.055472
C	-0.066787	4.751155	0.310827	H	2.976903	1.122083	-1.767195
C	1.184408	5.422753	0.402166	In	-0.034109	-1.854346	0.172128
C	2.365526	4.699680	0.376291	Cl	-1.883738	-3.427784	0.001010
C	2.388206	3.285605	0.243993	Cl	0.651189	-2.204489	2.489807
C	1.187297	2.603520	0.135639	Cl	1.183761	-2.422352	-1.852538
C	0.791655	1.180998	0.089210	N	7.000418	-0.591875	-0.415628
C	-0.023842	3.347243	0.173184	N	-6.944746	-0.434243	-0.438698
C	2.835444	-0.043567	0.044612	C	-7.692559	-1.214400	0.538380
C	3.552482	-0.868711	0.928024	H	-7.570201	-0.801264	1.546595
C	4.922704	-1.034467	0.788821	H	-8.754835	-1.169409	0.290755
C	5.638201	-0.421493	-0.272063	H	-7.384317	-2.271439	0.557874
C	4.890772	0.365043	-1.188404	C	-7.572918	-0.158090	-1.722284
C	3.527091	0.554357	-1.022525	H	-7.368940	0.869737	-2.045792
N	-1.334844	0.003831	0.076061	H	-7.233813	-0.843777	-2.515464
N	1.435285	0.064185	0.163862	H	-8.654691	-0.261768	-1.618617
H	-2.812757	0.761487	-2.030825	C	7.673862	-0.081924	-1.601146
H	-5.226024	0.536425	-2.287568	H	7.542042	1.003276	-1.693196
H	-5.443890	-1.238626	1.658251	H	8.743903	-0.279269	-1.516100
H	-3.026783	-1.053166	1.859221	H	7.308320	-0.554357	-2.526258
H	-3.352686	2.569855	0.158610	C	7.703537	-1.547658	0.429837
H	-3.473537	5.027377	0.380477	H	8.767483	-1.521313	0.188070

H	7.596115	-1.288916	1.490173
H	7.340965	-2.576964	0.286739

4b (4bt3)

Energy: -2635.09604499

Imaginary vibrational frequency: None

C	5.326917	3.424903	0.474313
C	4.099294	3.951881	-0.008777
C	3.067365	3.120836	-0.412503
C	3.225535	1.723507	-0.409840
C	4.427445	1.184753	0.076366
C	5.452413	2.008935	0.519395
C	2.261930	-0.049509	-1.690733
C	3.345573	-0.482326	-2.591394
C	4.646223	-0.068561	-2.838475
C	5.378793	-0.687130	-3.885034
C	4.840955	-1.691976	-4.672215
C	3.502521	-2.125453	-4.461980
C	2.798139	-3.100960	-5.220191
C	1.470134	-3.382686	-4.940826
C	0.762198	-2.728387	-3.900183
C	1.427888	-1.787251	-3.129246
C	2.790458	-1.501812	-3.415062
C	1.037998	-0.866400	-2.048210
C	-1.289379	-1.306847	-1.808547
C	-1.450230	-2.654365	-1.463062
C	-2.627386	-3.335580	-1.759163
C	-3.699130	-2.690040	-2.428992
C	-3.516735	-1.324226	-2.767995
C	-2.347713	-0.643195	-2.443837
C	3.698590	-2.690778	2.429516
C	3.517261	-1.324400	2.766956
C	2.348330	-0.643184	2.442951
C	1.289091	-1.307041	1.809320
C	1.449062	-2.655028	1.465126
C	2.626097	-3.336495	1.760997
C	-1.038275	-0.866161	2.048826
C	-1.428524	-1.786730	3.129985
C	-0.763139	-2.727655	3.901456
C	-1.471361	-3.381468	4.942207
C	-2.799393	-3.099507	5.221184
C	-3.503476	-2.124183	4.462463
C	-4.841889	-1.690446	4.672299
C	-5.379428	-0.685771	3.884702
C	-4.646547	-0.067621	2.838113
C	-3.345910	-0.481653	2.591426
C	-2.791116	-1.501006	3.415468
C	-2.261971	-0.049148	1.690961
C	-3.225121	1.723740	0.409550
C	-3.066937	3.121066	0.412019
C	-4.098739	3.952066	0.007876
C	-5.326215	3.425013	-0.475501
C	-5.451746	2.009035	-0.520324
C	-4.426903	1.184913	-0.076906
N	2.145265	0.905316	-0.820974
N	-0.094542	-0.591674	-1.491009

N	0.094482	-0.591577	1.491885	H	-6.348083	1.549363	-0.919676
N	-2.144989	0.905614	0.821146	H	-4.543367	0.107656	-0.148020
H	3.940310	5.022131	-0.051688	Cl	0.584536	2.707193	1.850662
H	2.138087	3.554548	-0.766359	Cl	-0.583668	2.706926	-1.850381
H	4.543891	0.107505	0.147636	In	0.000226	1.180451	0.000396
H	6.348837	1.549311	0.918602	N	6.344809	4.248188	0.891150
H	5.116054	0.714547	-2.257117	N	-4.870579	-3.358285	-2.727149
H	6.396579	-0.354984	-4.068928	N	-6.343926	4.248230	-0.892865
H	5.434806	-2.142340	-5.463603	N	4.869568	-3.359379	2.728002
H	3.303925	-3.616665	-6.032759	C	6.155630	5.694308	0.912356
H	0.946028	-4.122038	-5.539689	H	5.336006	5.988331	1.582512
H	-0.278786	-2.973172	-3.730042	H	7.071708	6.168698	1.266378
H	-0.642596	-3.181841	-0.963466	H	5.940288	6.083892	-0.091034
H	-2.706278	-4.376066	-1.467514	C	-5.874758	-2.717530	-3.566248
H	-4.294340	-0.779767	-3.290011	H	-5.483827	-2.460885	-4.562788
H	-2.238175	0.404628	-2.708671	H	-6.718315	-3.397350	-3.695061
H	4.295626	-0.779788	3.287692	H	-6.255813	-1.800185	-3.100293
H	2.239488	0.404981	2.706740	C	-6.155060	5.694399	-0.913395
H	0.640853	-3.182588	0.966546	H	-5.334558	5.988687	-1.582328
H	2.704444	-4.377258	1.470169	H	-7.070693	6.168677	-1.268710
H	0.277836	-2.972691	3.731646	H	-5.941192	6.083855	0.090385
H	-0.947446	-4.120645	5.541454	C	4.965484	-4.792563	2.489068
H	-3.305422	-3.614855	6.033827	H	5.965986	-5.133731	2.759114
H	-6.397205	-0.353425	4.068281	H	4.234975	-5.366019	3.081103
H	-5.116147	0.715377	2.256424	H	4.810562	-5.028315	1.428802
H	-2.137763	3.554833	0.766084	C	7.574731	3.681063	1.425755
H	-3.939794	5.022326	0.050733	H	7.394904	3.099895	2.342252
H	-5.435947	-2.140476	5.463722	H	8.065854	3.027776	0.692430

H	8.265813	4.489143	1.668551
C	5.876498	-2.716966	3.562445
H	6.258580	-1.802300	3.091939
H	5.487672	-2.455281	4.558453
H	6.718860	-3.397918	3.692966
C	-7.574306	3.681050	-1.426334
H	-7.395059	3.098899	-2.342306
H	-8.065413	3.028669	-0.692167
H	-8.265148	4.489151	-1.669736
C	-4.966115	-4.791738	-2.489372
H	-4.237030	-5.364950	-3.083472
H	-4.808975	-5.028234	-1.429674
H	-5.967360	-5.132406	-2.757330

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