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Supporting Information

Palladium-Catalysed Cross-Coupling Reactions Controlled by Noncovalent Zn...N Interactions

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S1. General methods.

All commercial reagents were used as supplied from commercial sources. All syntheses were performed in Schlenk-type flasks under argon atmosphere. Solvents were purified by solvent purification system equipped with a serie of activated filter columns or dried by conventional methods and distilled immediately prior to use. All reagents were weighed and handled in air, and refilled with an inert atmosphere of argon at room temperature. **A**^[1] and **B**^[2] were prepared according to literature procedures and dried under high vacuum overnight prior to be used. CDCl₃ was passed down a 5 cm-thick alumina column and stored under nitrogen over molecular sieves (4 Å). ¹H NMR spectra were recorded on Bruker GPX (400 MHz) spectrometer and ³¹P NMR spectra were recorded at 162 MHz on the same spectrometer. ¹H NMR spectra were referenced to residual protiated solvent (($\delta = 7.26$ ppm for CDCl₃, $\delta = 6.97$ ppm for toluene-*d*₈) and the ³¹P NMR data are given relative to external H₃PO₄. UV-vis absorption spectra were recorded using Specord 205 UV-vis-NIR spectrophotometer using quartz cuvettes of 1 cm pathlength. The catalytic reactions were monitored using a Shimadzu 2014 gas chromatography equipped with EquityTM-1 Fused Silica capillary column (30 m x 0.25 mm x 0.25 μ m) and a FID detector (Method: Initial temp = 60 °C, Ramp = 10 °C/min to 220 °C, hold 10 min); and the conversions were determined using dodecane as internal standard. Molecular modelling calculations were performed using PM3-Spartan molecular modelling program.

Synthesis of substrates 3 and 6. The corresponding 4-halorpyridine hydrochloride salts (1 equivalent) were treated with potassium carbonate (10 equivalents) in acetonitrile as solvent at room temperature during six hours. The reaction mixture was then filtered over magnesium sulphate and evaporation of the solvents at room temperature followed by overnight drying under high vacuum yielded **3** and **6** respectively in virtually quantitative yield. ¹H NMR data match those found in the literature.^[3]

Table S1. Response factors (*f*) of halopyridines with dodecane internal standard.

$$(\text{Area}_{\text{substrate}}/\text{Area}_{\text{dodecane}}) = f(\text{mol}_{\text{substrate}}/\text{mol}_{\text{dodecane}})$$

Substrate	<i>f</i>
2-chloropyridine (1)	0.5034
3-chloropyridine (2)	0.4765
4-chloropyridine (3)	0.4836
2-bromopyridine (4)	0.4798
3-bromopyridine (5)	0.5001
4-bromopyridine (6)	0.5047

S2. ^1H NMR studies of A and B with 1-6.

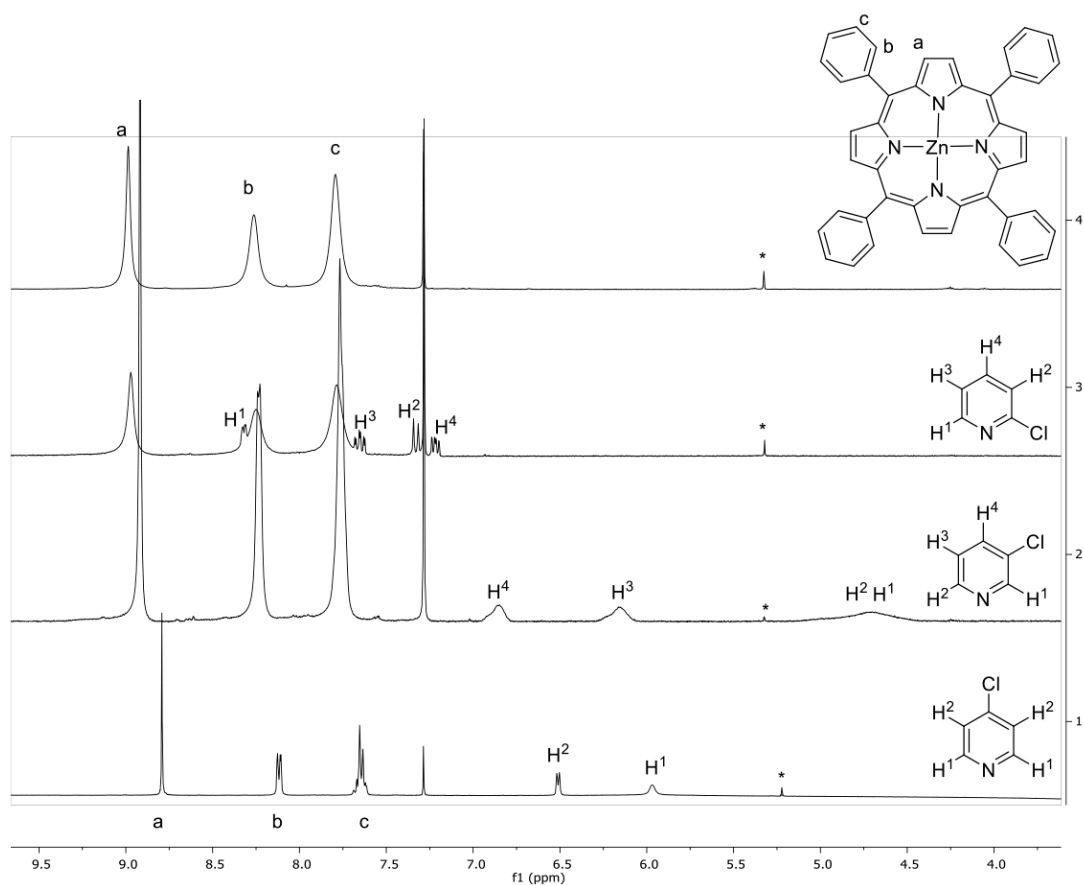


Figure S1. ^1H NMR (400.1 MHz, CDCl_3 , 298 K) spectra obtained upon stoichiometric combination of A with 1, 2 and 3, respectively. * denotes traces of dichloromethane.

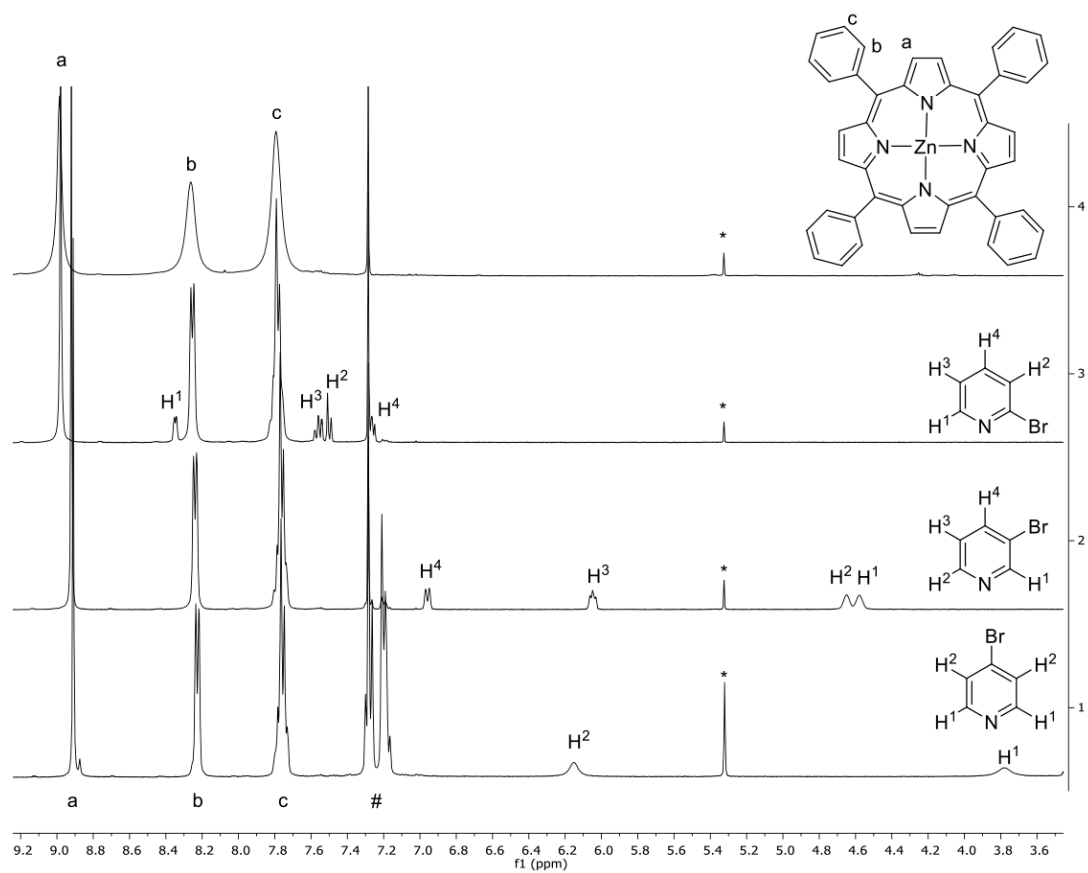


Figure S2. ^1H NMR (400.1 MHz, CDCl_3 , 298 K) spectra obtained upon stoichiometric combination of **A** with **4**, **5** and **6**, respectively. * denotes traces of dichloromethane, # denotes traces of toluene.

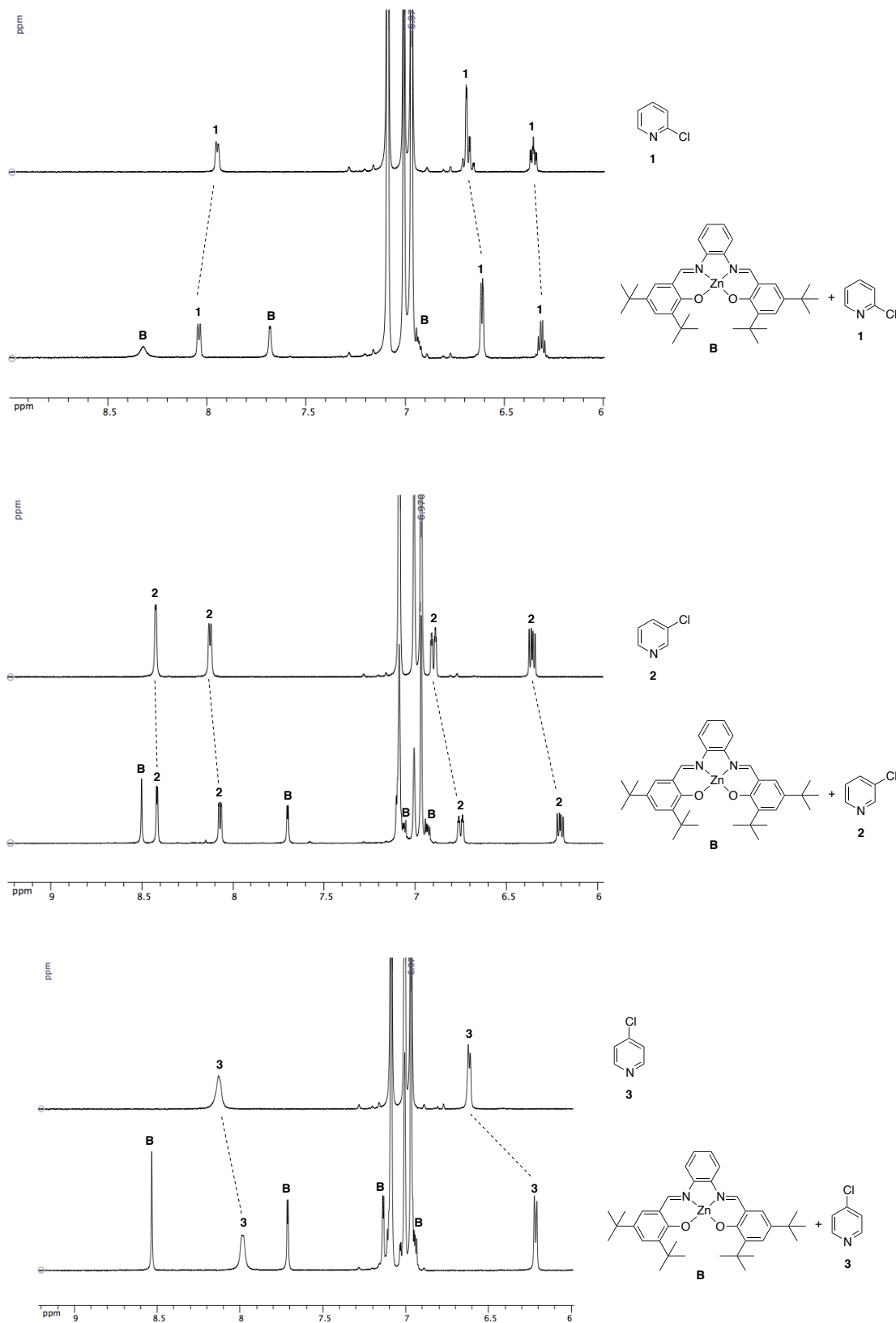


Figure S3. ^1H NMR (400.1 MHz, toluene- d_8 , 298 K) spectra obtained upon stoichiometric combination of **B** with **1** (top), **2** (middle) and **3** (bottom).

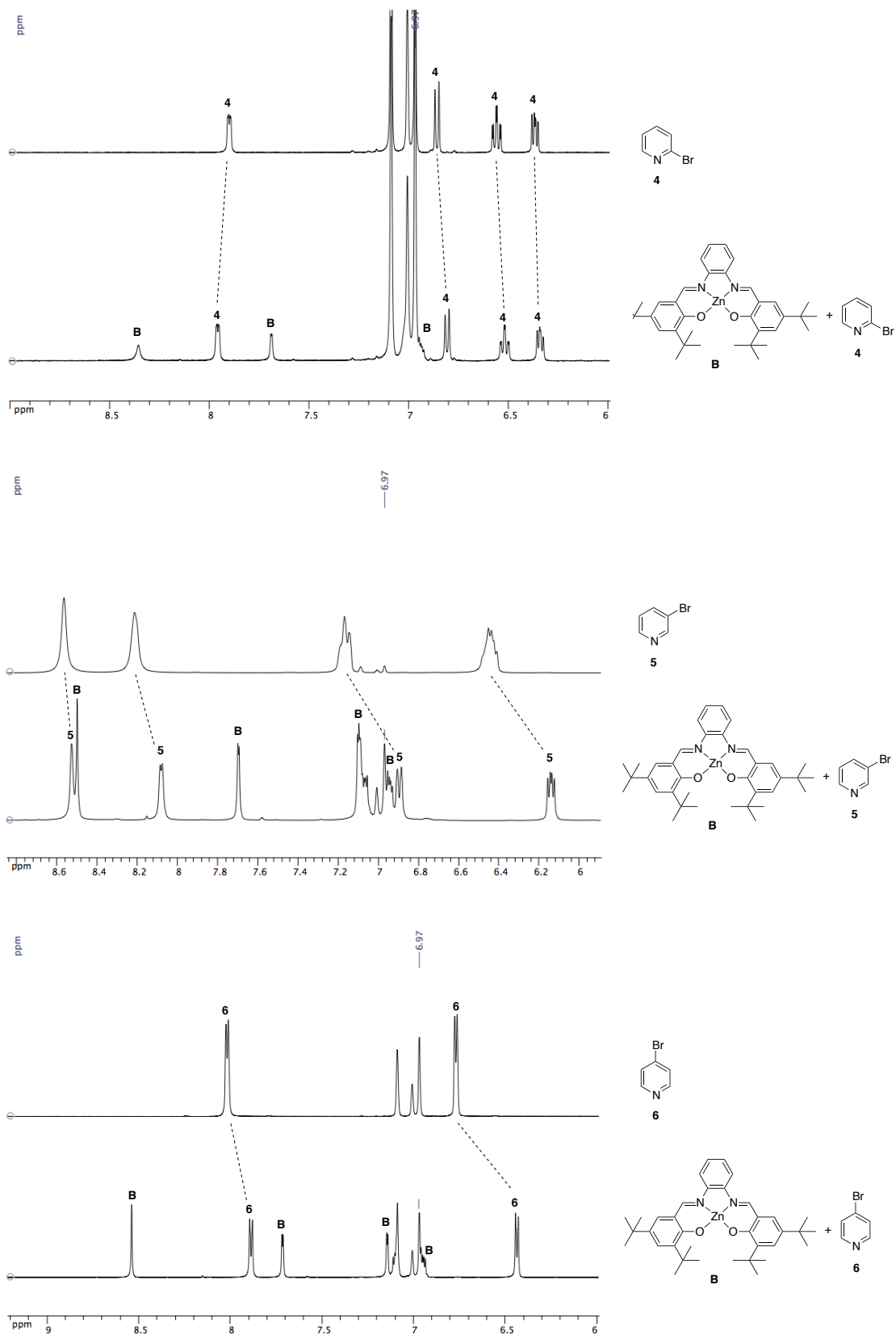


Figure S4. ^1H NMR (400.1 MHz, $\text{toluene-}d_8$, 298 K) spectra obtained upon stoichiometric combination of **B** with **4** (top), **5** (middle) and **6** (bottom).

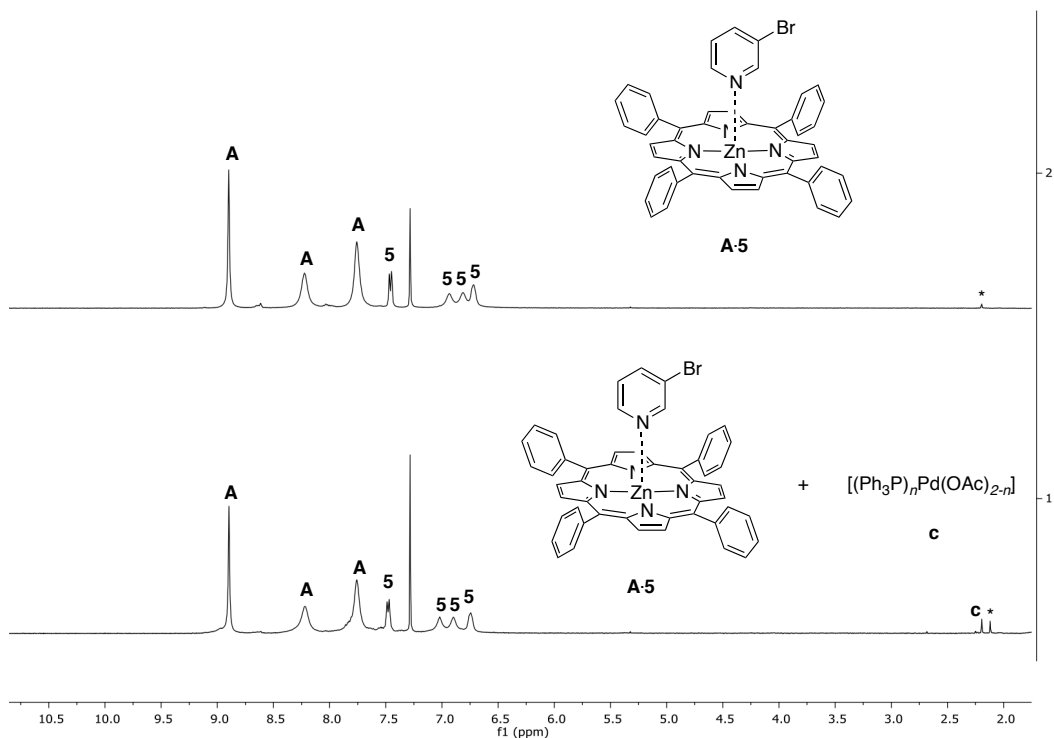


Figure S5. ^1H NMR (400.1 MHz, CDCl_3 , 298 K) spectra of **5•A** (top) and of **5•A** in the presence of a mixture of 1 mol% $\text{Pd}(\text{OAc})_2$ and 2 mol% of PPh_3 (bottom). * denotes traces of acetone. At this stage we cannot differentiate between palladium-ligated acetate ligand or free acetate ligand (c).

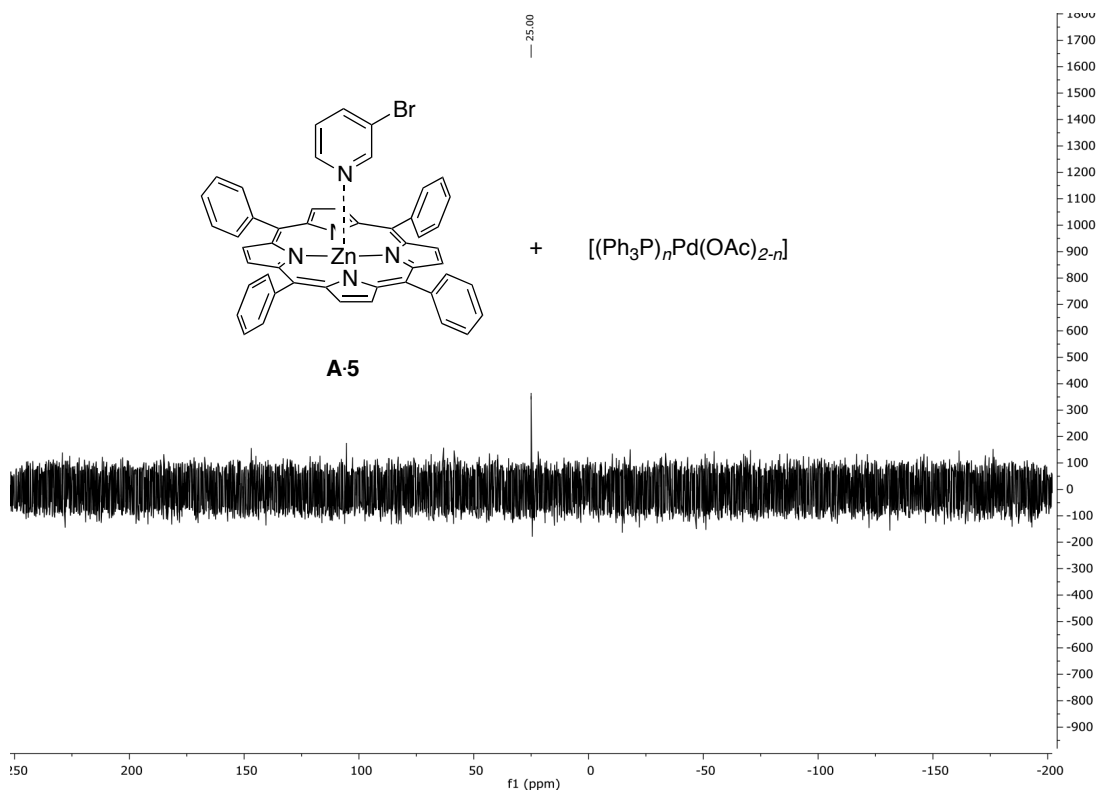
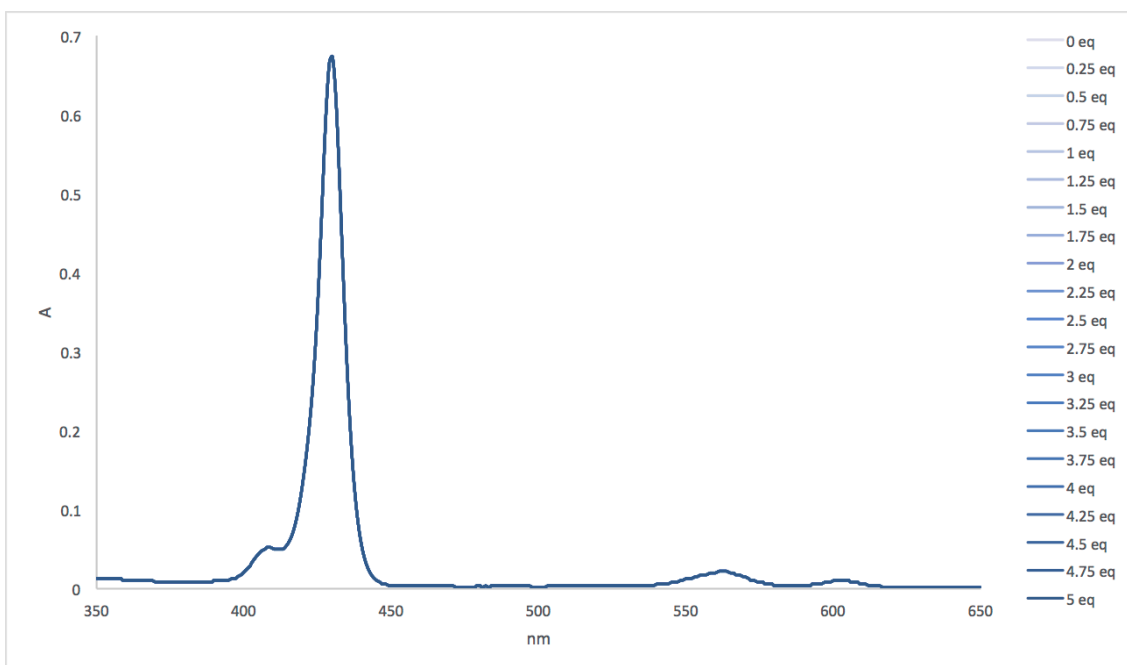


Figure S6. $^{31}\text{P}\{^1\text{H}\}$ NMR (162.0 MHz, CDCl_3 , 298 K) spectra of **5•A** in the presence of a mixture of 1 mol% $\text{Pd}(\text{OAc})_2$ and 2 mol% of PPh_3 . The peak at 25 ppm belongs to palladium-ligated triphenylphosphine species.

S3. UV-vis titration studies of A and B with 1-6.

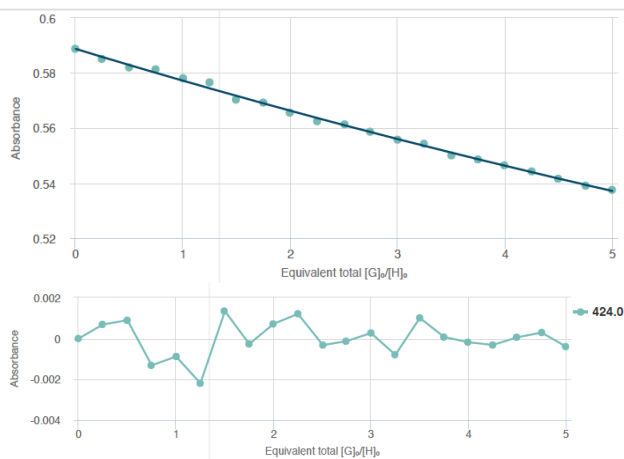
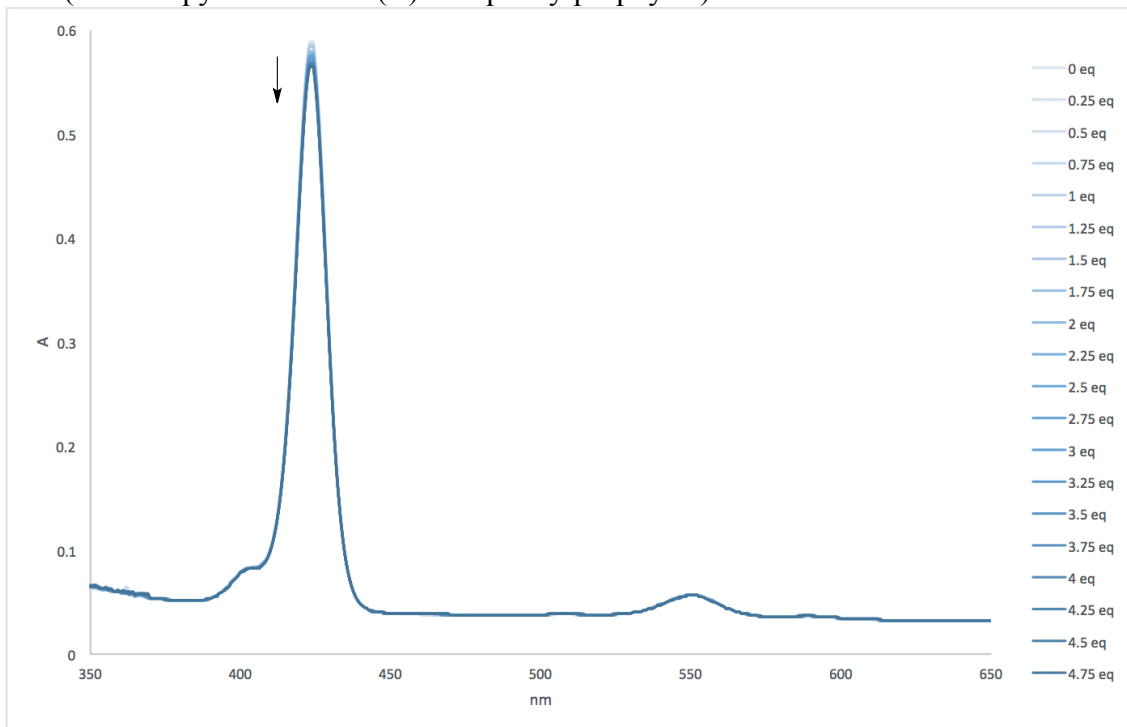
General procedure for UV-vis titrations. Host-guest interactions in solution were studied by UV-vis spectroscopy. Solutions of **A** (10^{-6} M), **B** (5×10^{-5} M) and of the different substrates tested **1-6** (10^{-4} M for titration with **A** and 5×10^{-3} M for titration with **B**) were prepared using toluene as solvent. An increasing number of substrate equivalents were added to a solution of **A** -or **B**- (2 mL in a 1 cm cuvette cell). The host concentration was kept constant. The stoichiometry of the self-assembly substrates was studied using the method of continuous variations, by adding different ratios of guest solution, in order to add an increasing number of substrate equivalents. The association constants were calculated from the changes in absorbance at the wavelengths near to λ_{max} . Nonlinear curve fitting for 1:1 binding model was found the most suitable for all cases studied in this work. Association constants $K_{1,1}$ and asymptotic changes in absorbance ΔA were set as free parameters for fitting.^[4]

1•A (2-chloropyridine + zinc(II)-tetraphenylporphyrin):

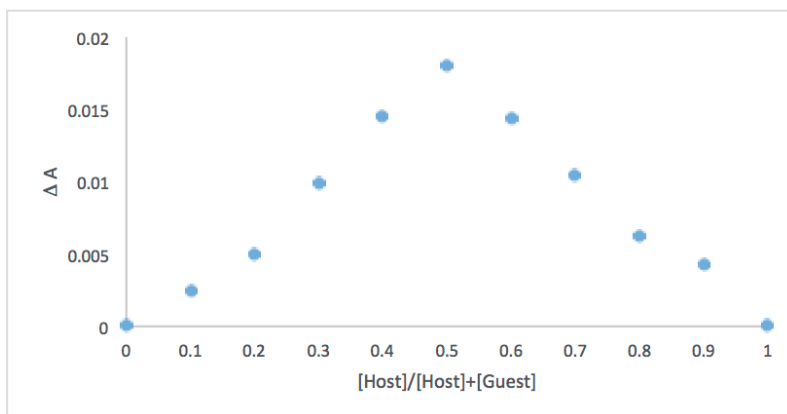


Increasing the number of substrate equivalents does not change the UV-vis spectrum, a feature that indicates no binding between **1** and **A**.

2•A (3-chloropyridine + zinc(II)-tetraphenylporphyrin):

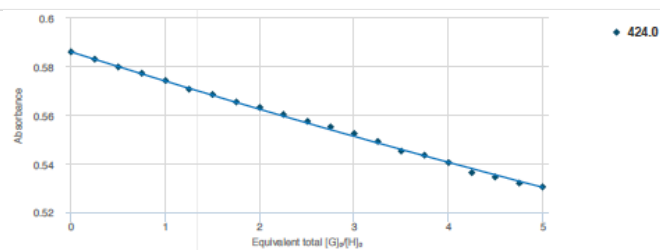
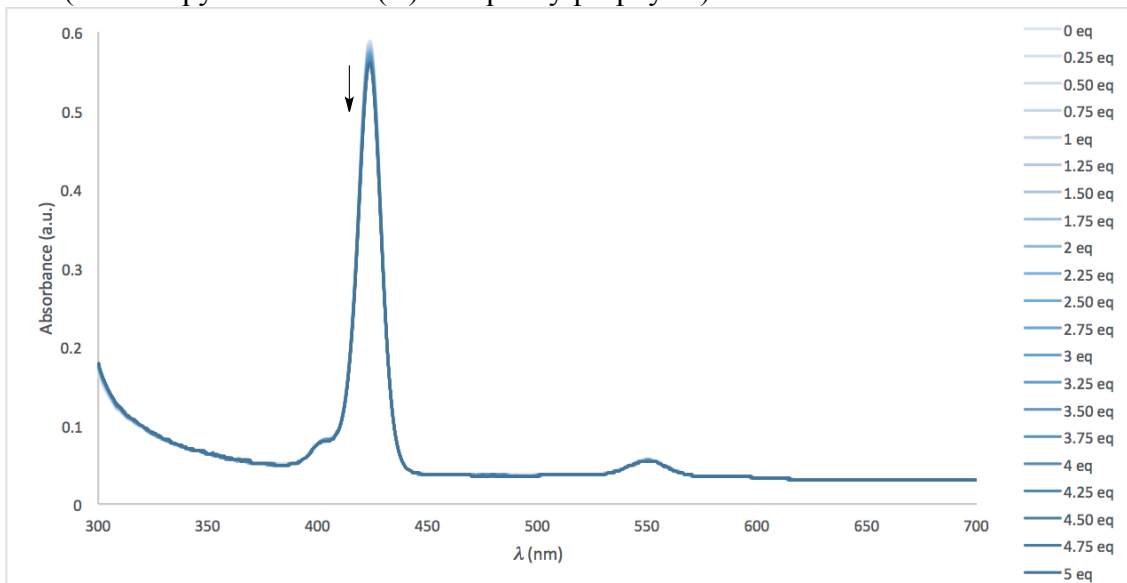


Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	10095.94	± 1.3844	100.00
	M ⁻¹	%	M ⁻¹

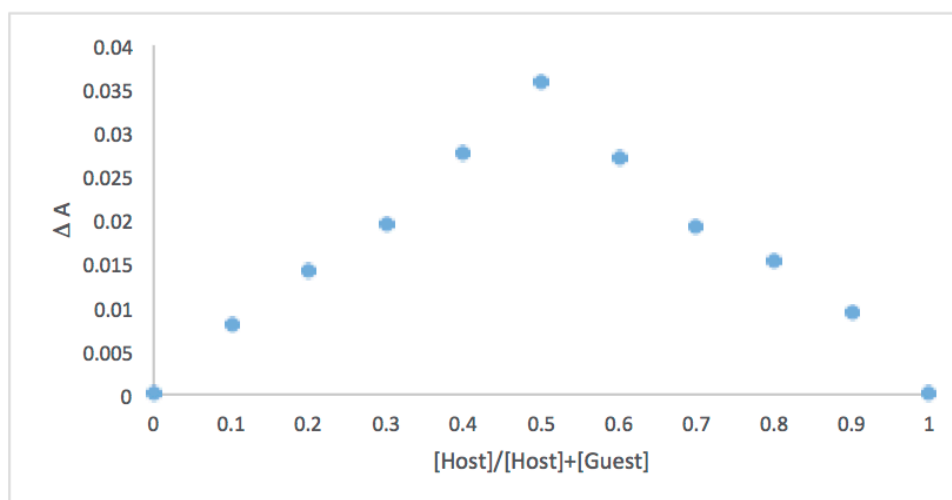


Job-Plot analysis indicating a 1:1 stoichiometry for **2•A**.

3•A (4-chloropyridine + zinc(II)-tetraphenylporphyrin):

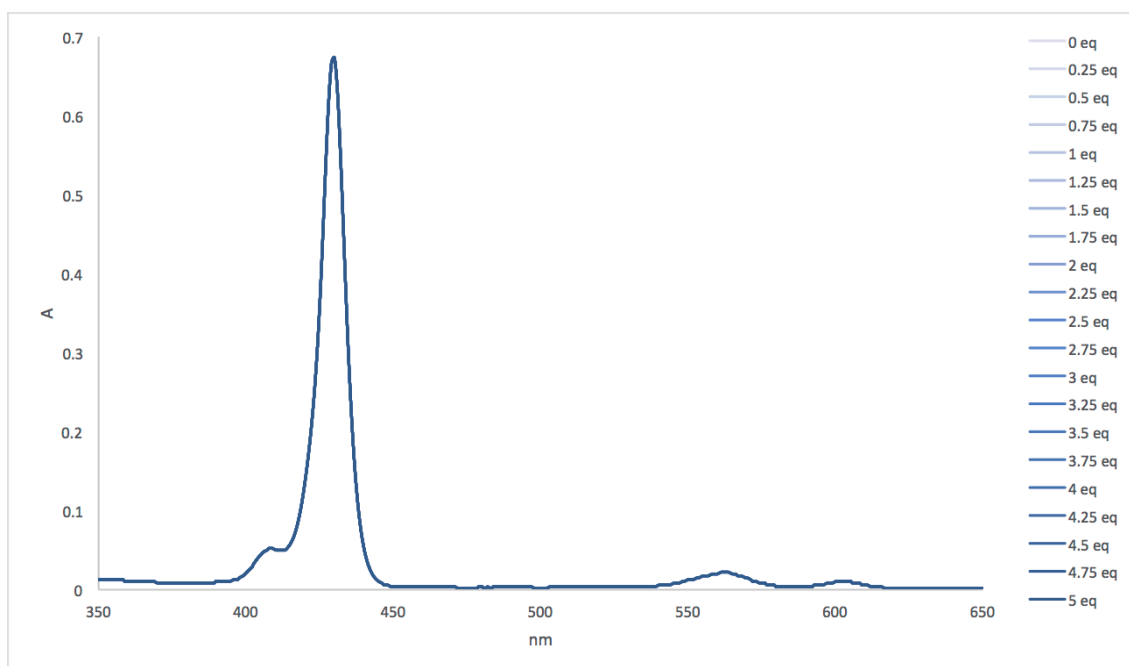


Parameter (bounds)	Optimised	Error	Initial
K ($0 \rightarrow \infty$)	9021.80 M ⁻¹	± 1.0086 %	100.00 M ⁻¹



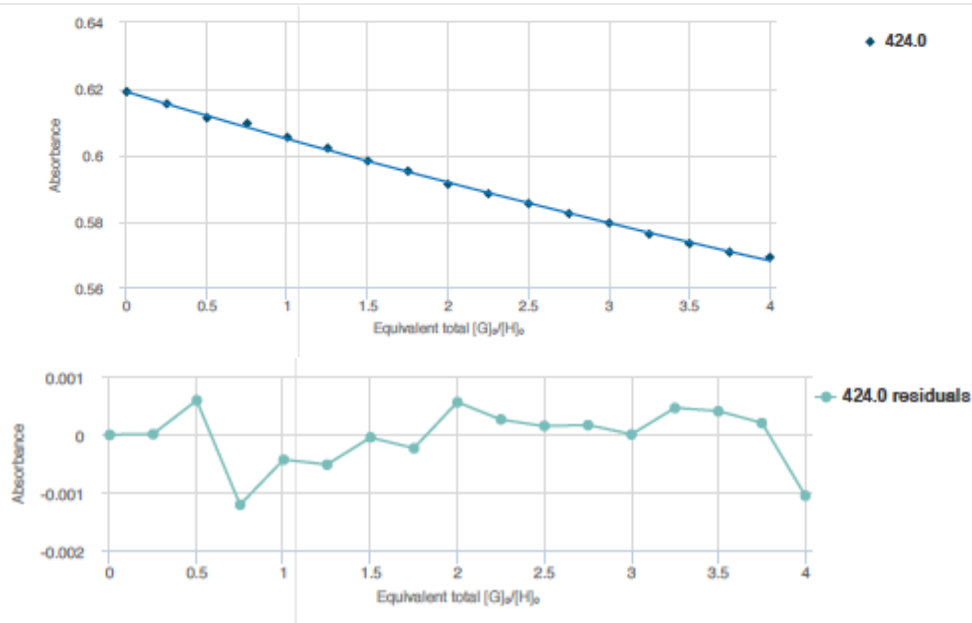
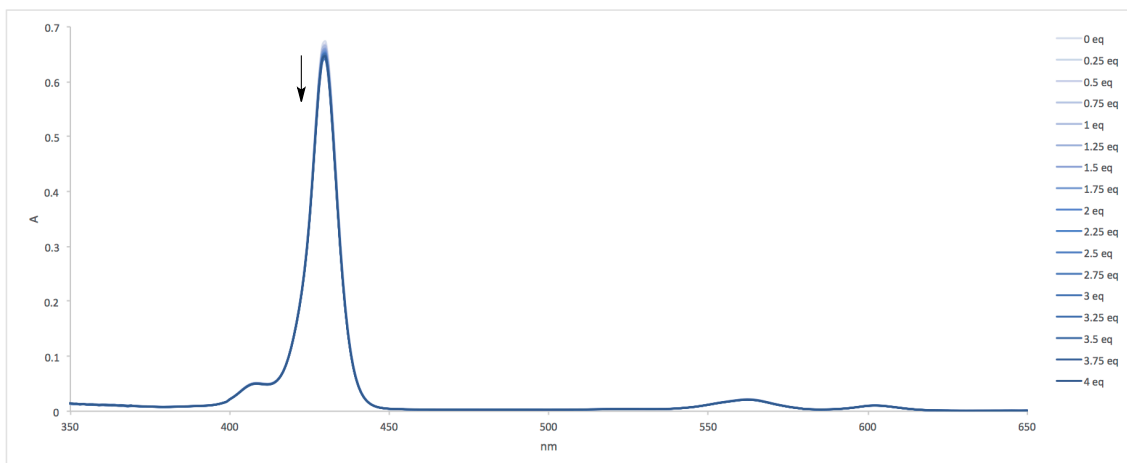
Job-Plot analysis indicating a 1:1 stoichiometry for **3•A**.

4•A (2-bromopyridine + zinc(II)-tetraphenylporphyrin):

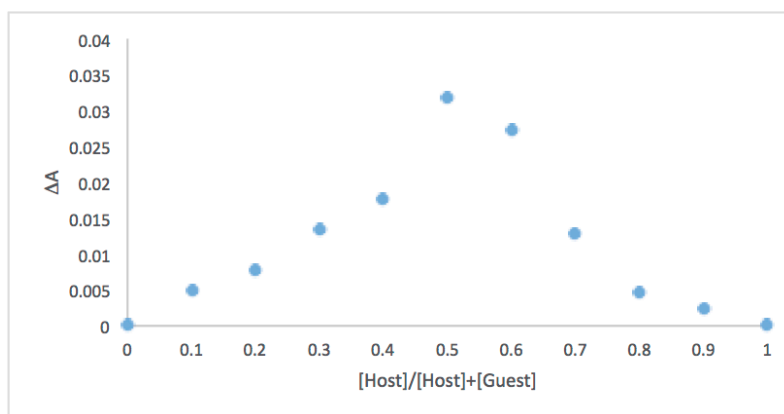


Increasing the number of substrate equivalents does not change the UV-vis spectrum, a feature that indicates no binding between **4** and **A**.

5•A (3-bromopyridine + zinc(II)-tetraphenylporphyrin):

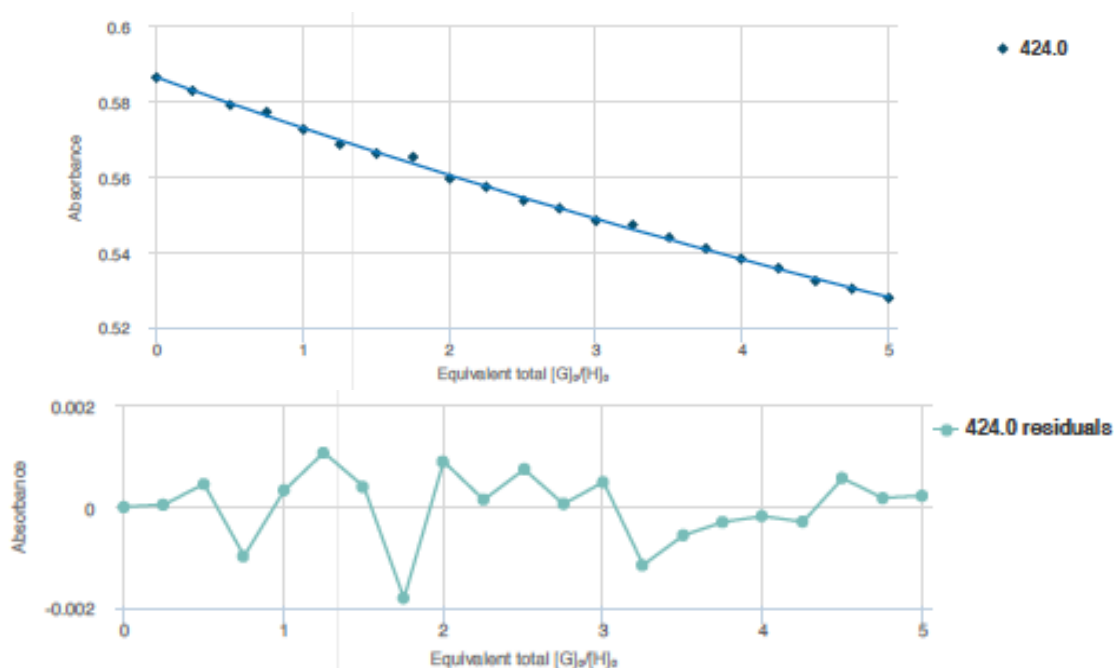
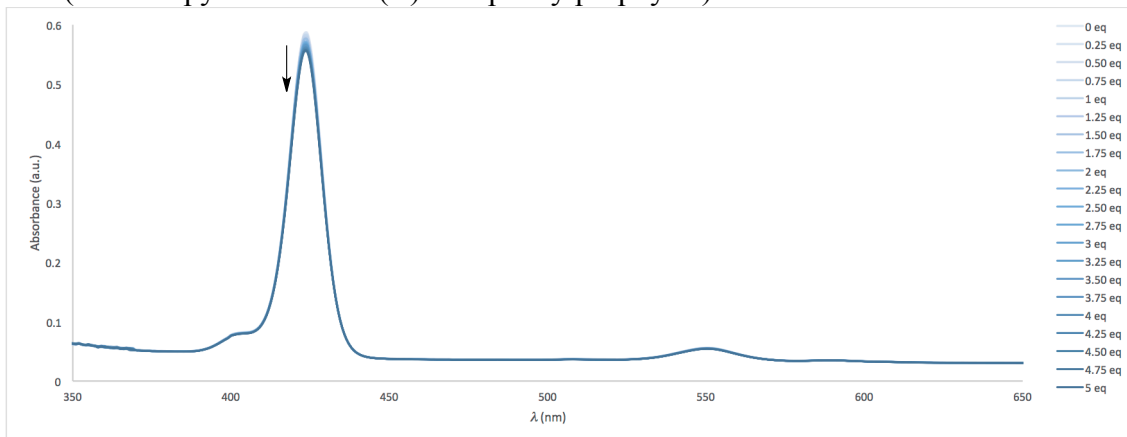


Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	18580.12	± 0.9856	100.00
	M⁻¹	%	M⁻¹

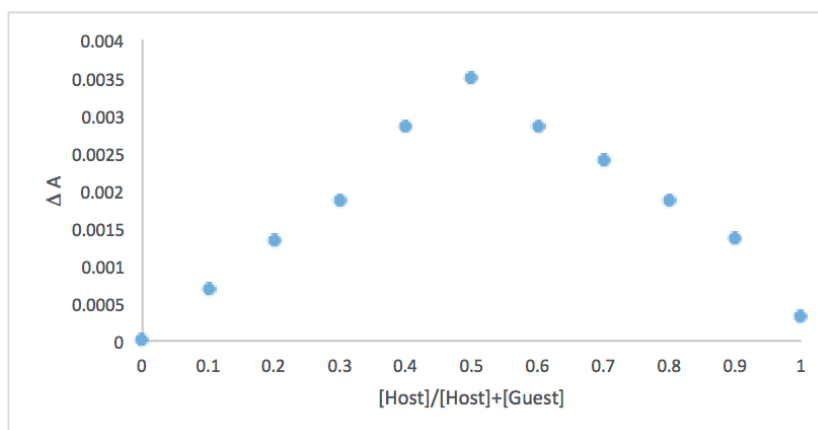


Job-Plot analysis indicating a 1:1 stoichiometry for 5•A.

6•A (4-bromopyridine + zinc(II)-tetraphenylporphyrin):

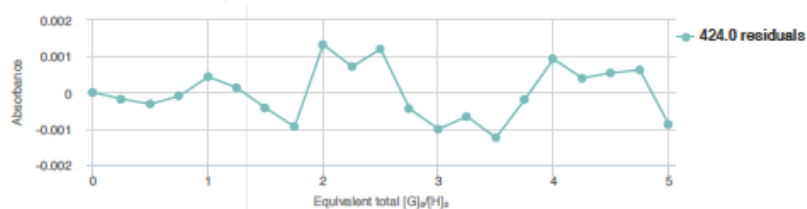
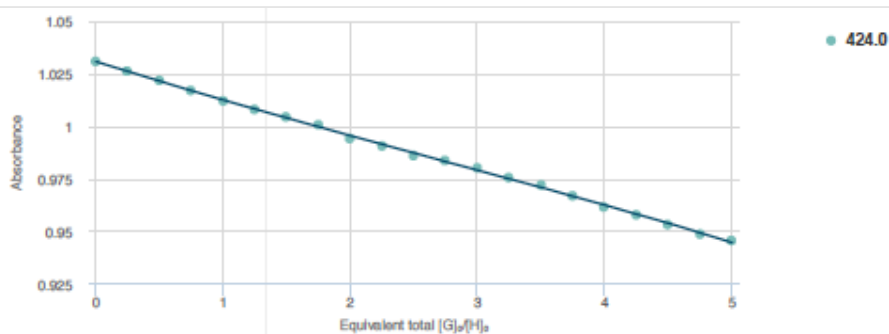
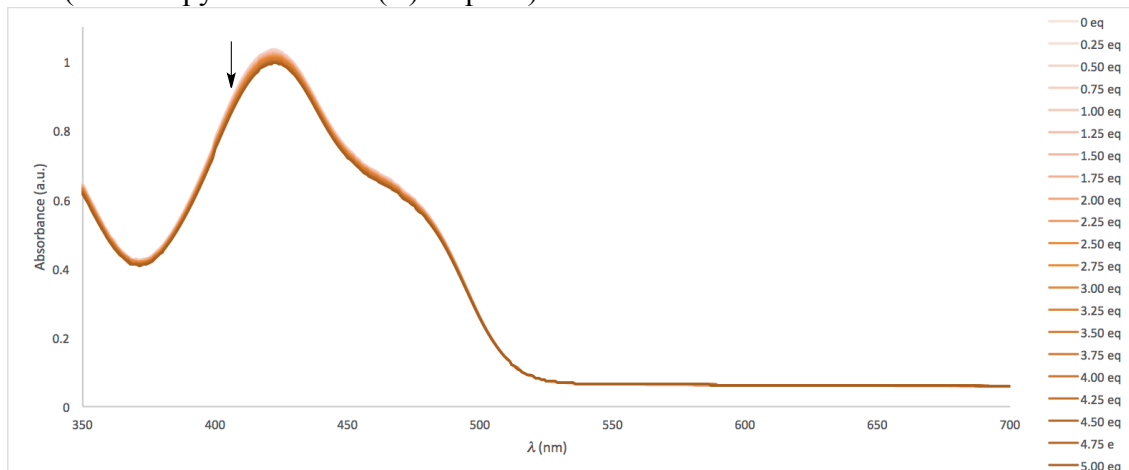


Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	19271.13 M ⁻¹	± 1.0284 %	100.00 M ⁻¹

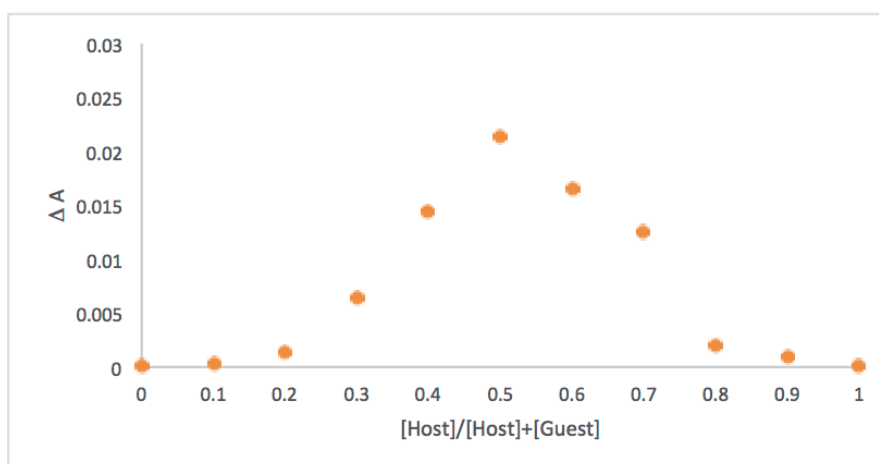


Job-Plot analysis indicating a 1:1 stoichiometry for **6•A**.

1•B (2-chloropyridine + zinc(II)-salphen):

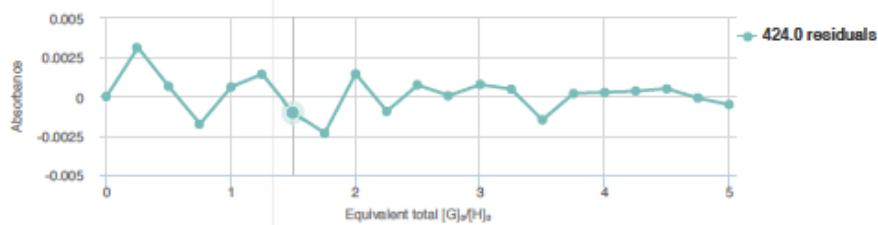
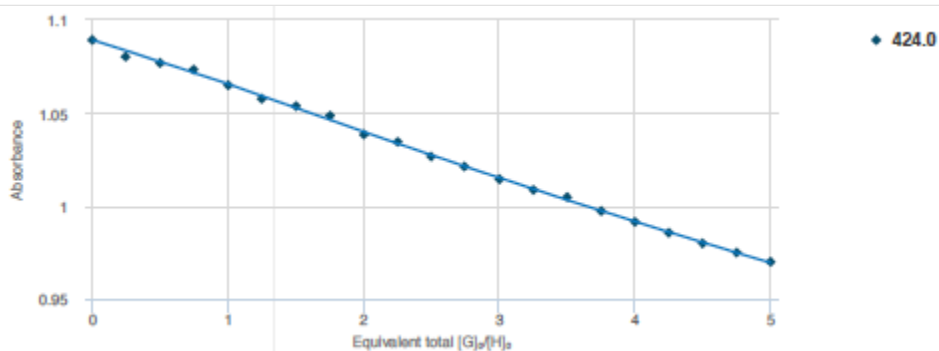
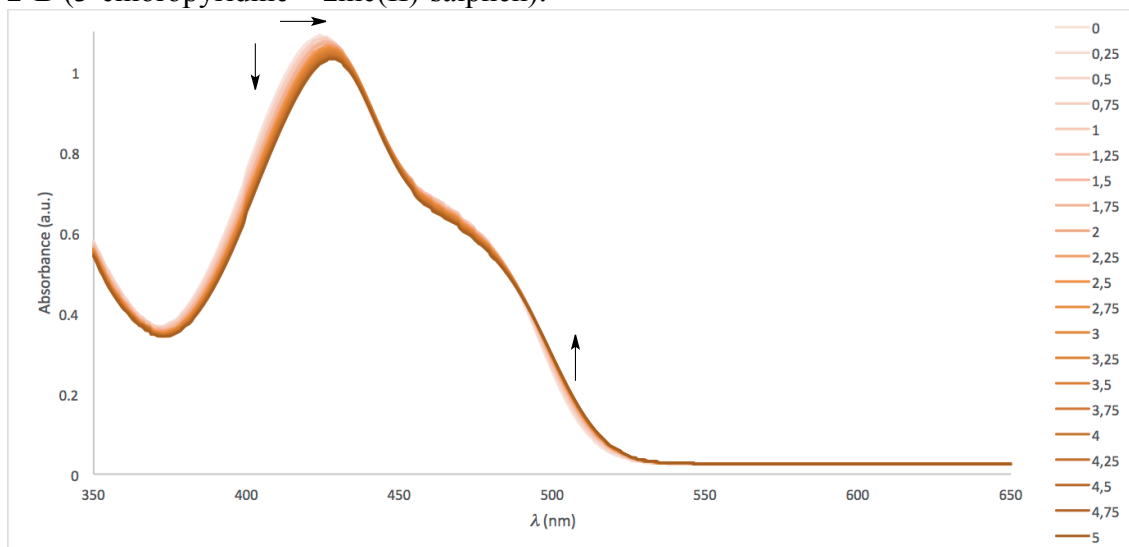


Parameter (bounds)	Optimised	Error	Initial
K ($0 \rightarrow \infty$)	2504.94 M^{-1}	± 7.1617 %	1000.00 M^{-1}



Job-Plot analysis indicating a 1:1 stoichiometry for **1•B**.

2•B (3-chloropyridine + zinc(II)-salphen):



**Parameter
(bounds)**

Optimised

Error

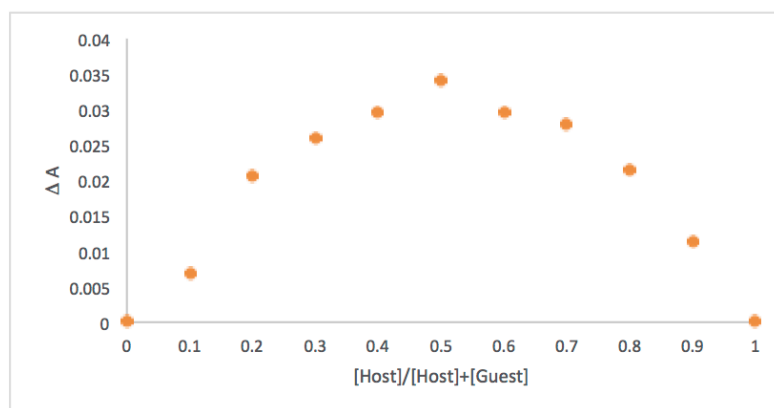
Initial

K (0 → ∞)

621488.59
M⁻¹

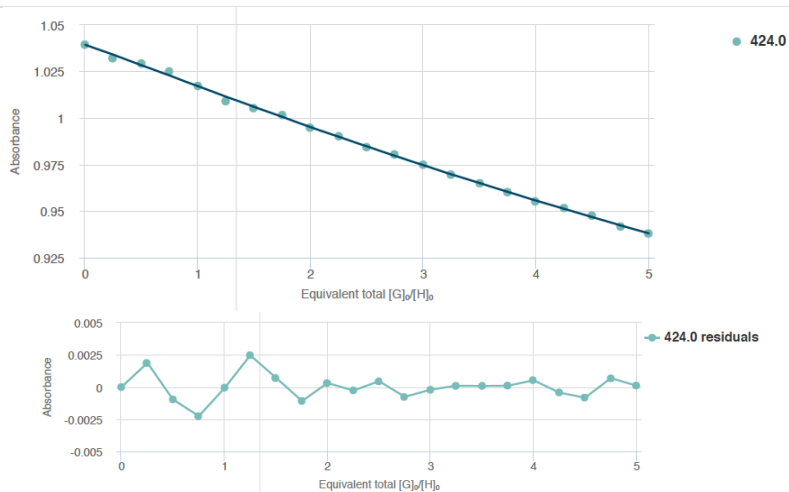
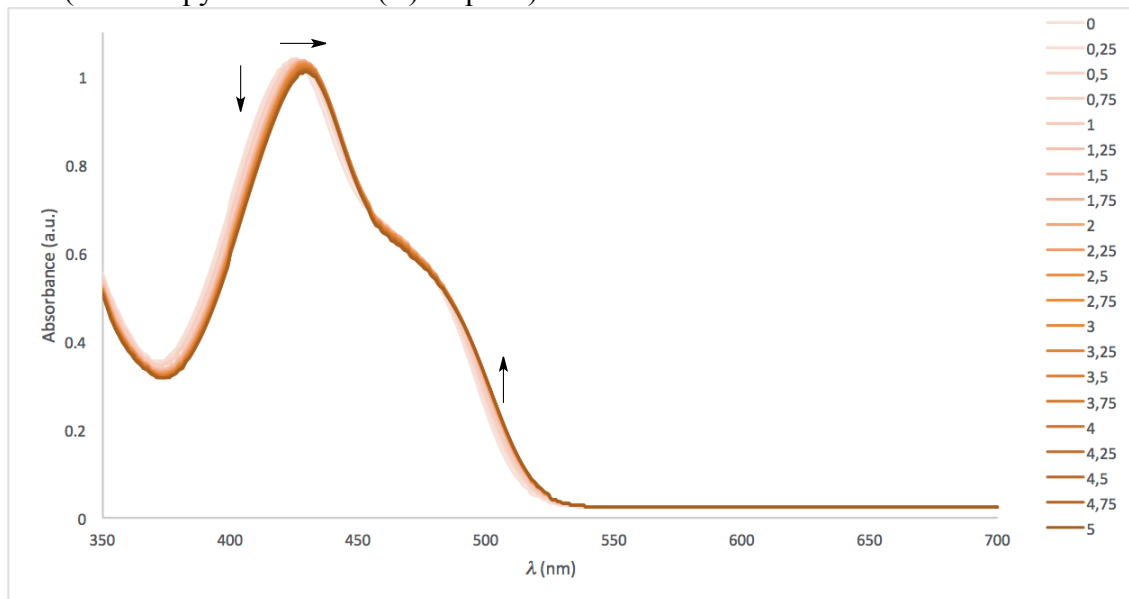
± 2.7907 %

1000.00
M⁻¹

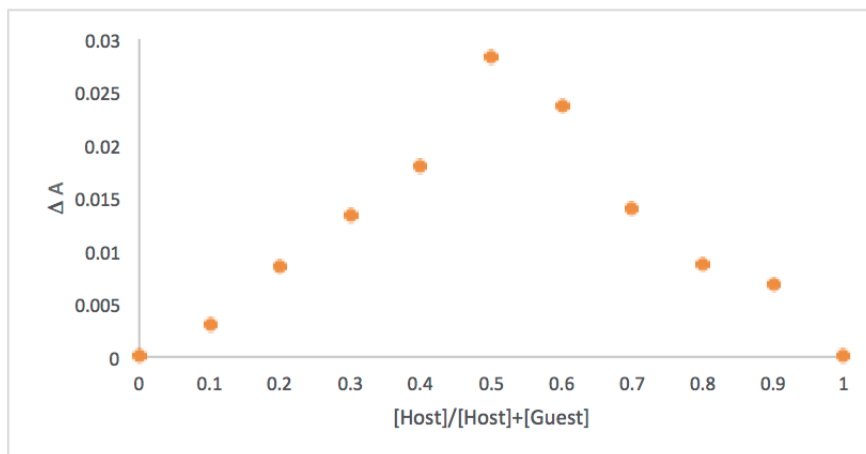


Job-Plot analysis indicating a 1:1 stoichiometry for **2•B**.

3•B (4-chloropyridine + zinc(II)-salphen):

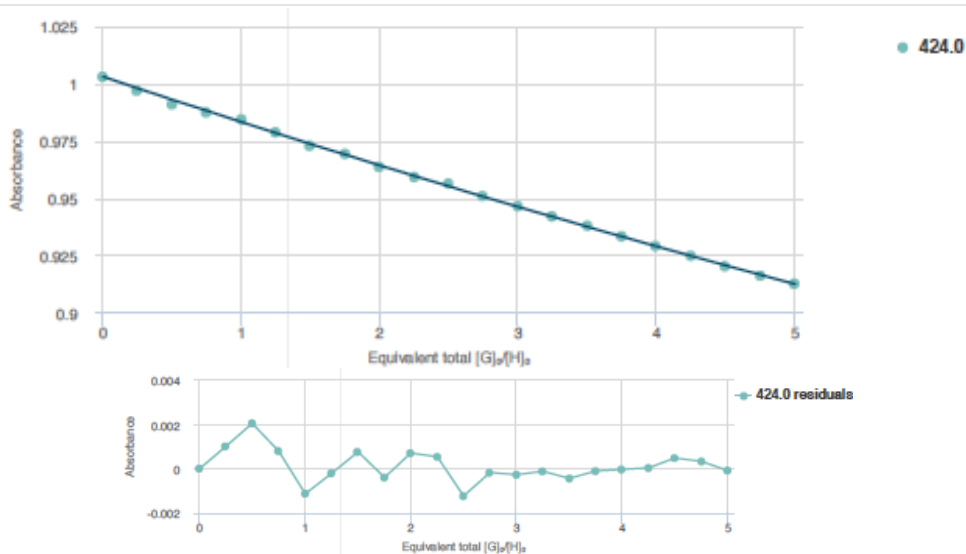
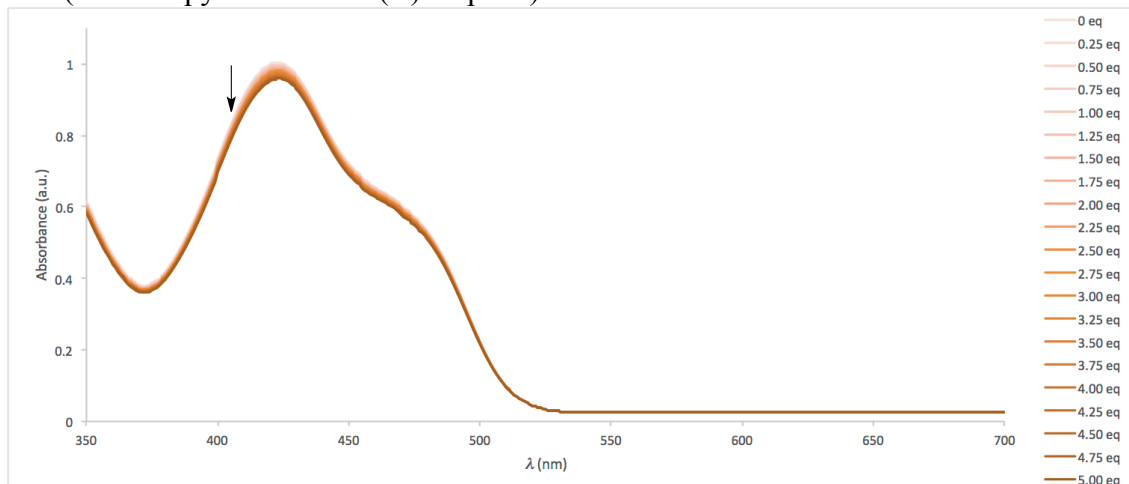


Parameter (bounds)	Optimised	Error	Initial
K ($0 \rightarrow \infty$)	2875395.76	± 12.4680	1000.00
	M^{-1}	%	M^{-1}



Job-Plot analysis indicating a 1:1 stoichiometry for **3•B**.

4•B (2-bromopyridine + zinc(II)-salphen):



**Parameter
(bounds)**

Optimised

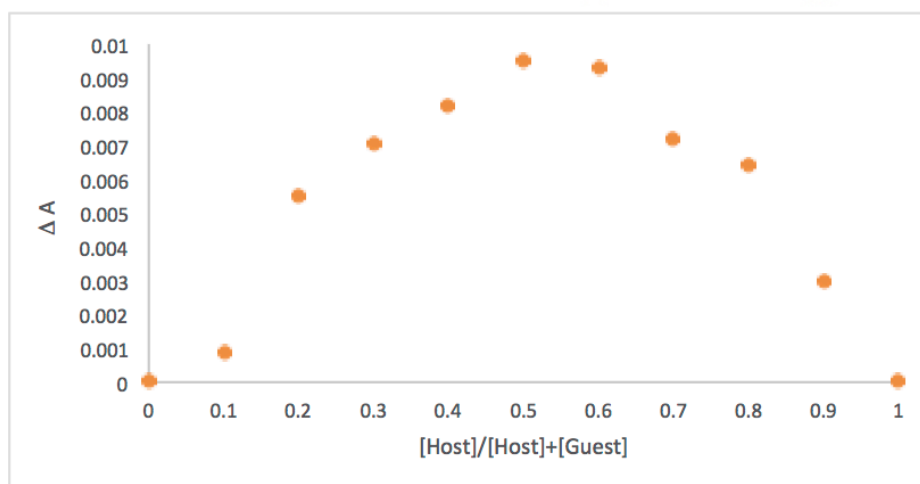
Error

Initial

K (0 → ∞)

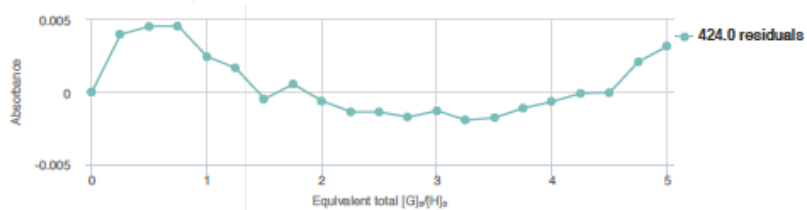
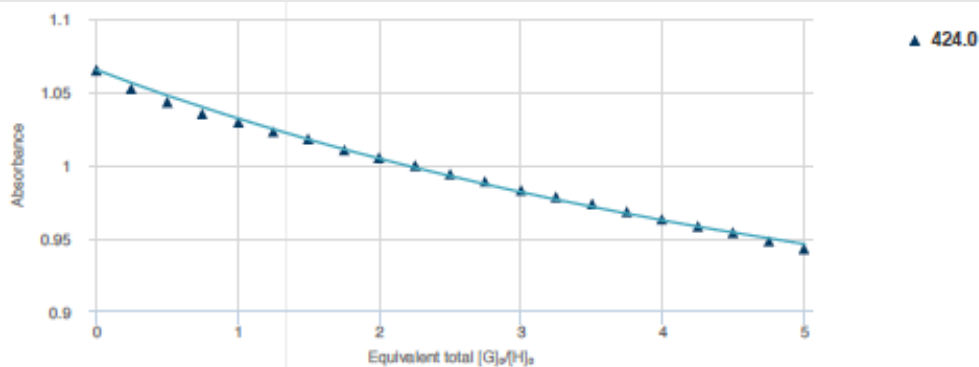
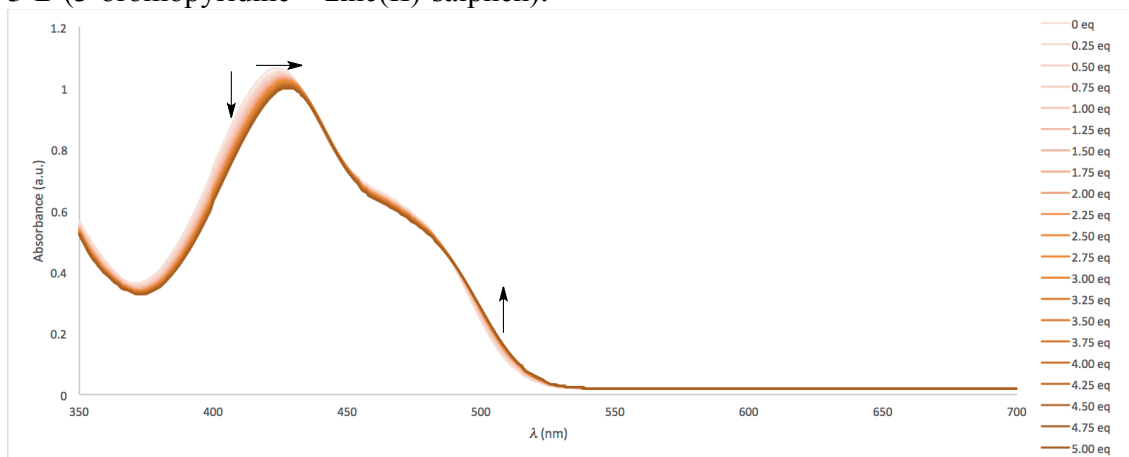
5166.87 M⁻¹ ± 0.6643 %

100.00 M⁻¹

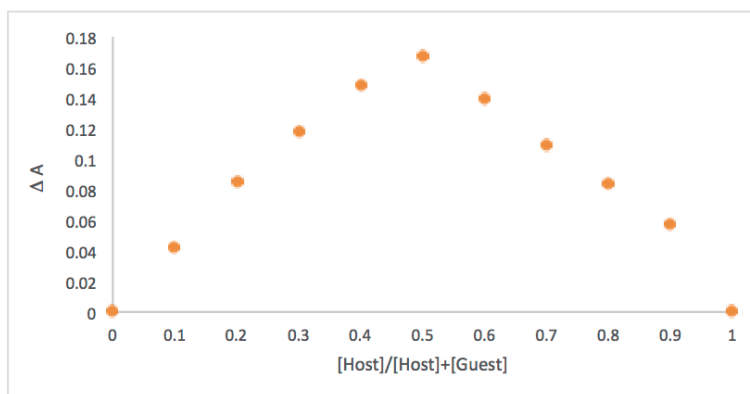


Job-Plot analysis indicating a 1:1 stoichiometry for **4•B**.

5•B (3-bromopyridine + zinc(II)-salphen):

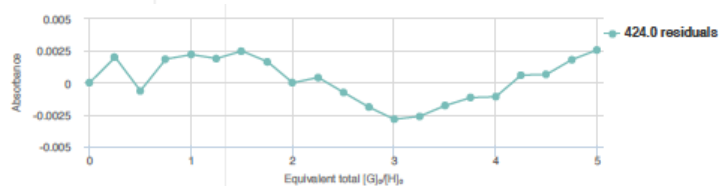
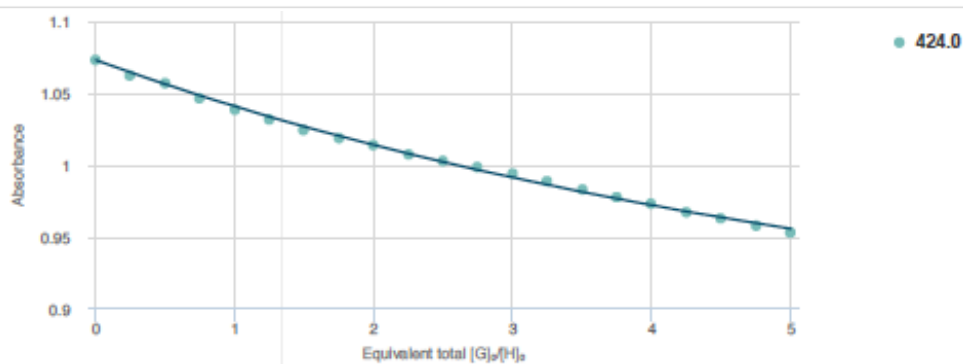
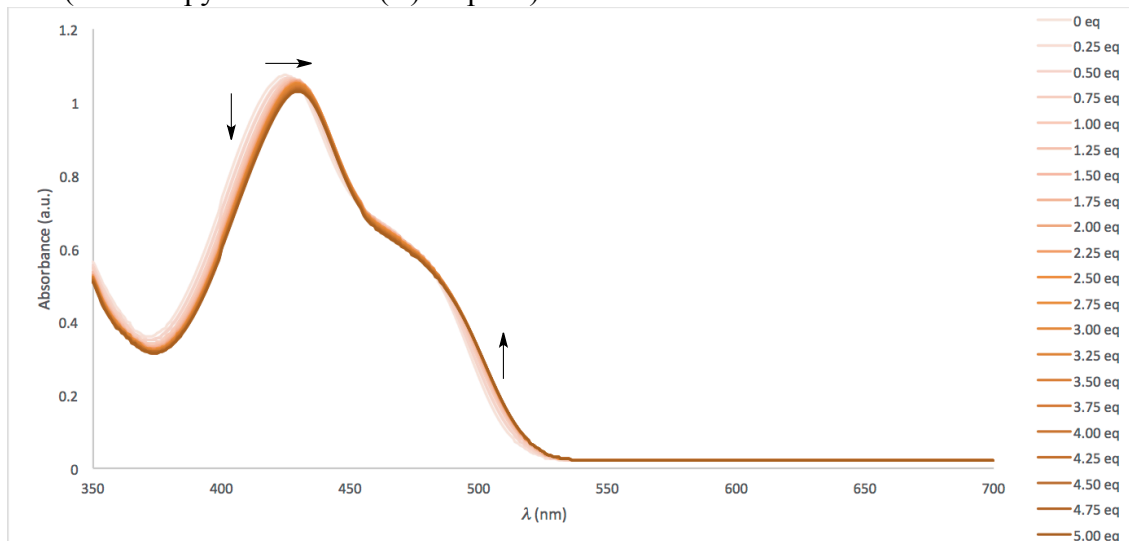


Parameter (bounds)	Optimised	Error	Initial
$K (0 \rightarrow \infty)$	3731966.54	± 1.9345	100.00
	M^{-1}	%	M^{-1}

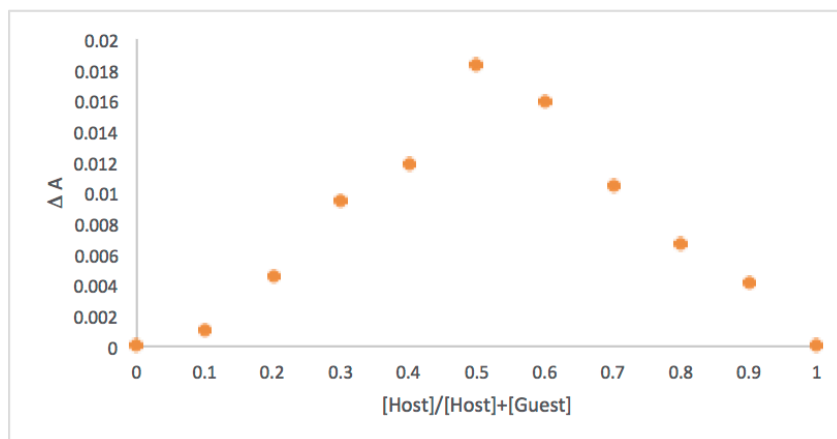


Job-Plot analysis indicating a 1:1 stoichiometry for **5•B**.

6•B (4-bromopyridine + zinc(II)-salphen):



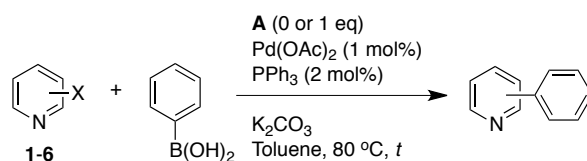
Parameter (bounds)	Optimised	Error	Initial
K (0 → ∞)	2851790.55	± 1.5133	100.00
	M ⁻¹	%	M ⁻¹



Job-Plot analysis indicating a 1:1 stoichiometry for **6•B**.

S4. Palladium-catalyzed experiments.

Table S2. Conversion of halopyridine derivatives **1-6** under palladium-catalyzed Suzuki-Miyaura reaction conditions with and without the presence of catalytically inert building block **A**.^[a]



Entry	Substrate	t (h)	Conv. (%) ^[b]
1	1	4	50
2	1•A	4	50
3	2	2	9
4	2•A	2	20
5	3	4	37
6	3•A	4	63
7	4	5	78
8	4•A	5	78
9	5	4	78
10	5•A	4	>99
11 ^[c]	5	2	85
12 ^[c]	5•A	2	85
13	6	2	62
14	6•A	2	73

[a] Reaction conditions: $[\text{Pd}(\text{OAc})_2]$ (2.5×10^{-3} mmol, 1 mol%), PPh_3 (5×10^{-3} mmol, 2 mol%), halopyridine (0.25 mmol), **A** (0.170 g, 0.25 mmol) -when applied-, $\text{PhB}(\text{OH})_2$ (0.061 g, 0.5 mmol), K_2CO_3 (0.069 g, 0.5 mmol), toluene (1.25 mL), dodecane (0.057 mL), 80 °C, argon atmosphere. [b] Conv. = conversion. The conversions were determined by GC; the calibrations were based on dodecane. Reactions were performed 2-3 times. [c] DMF was used instead of toluene.

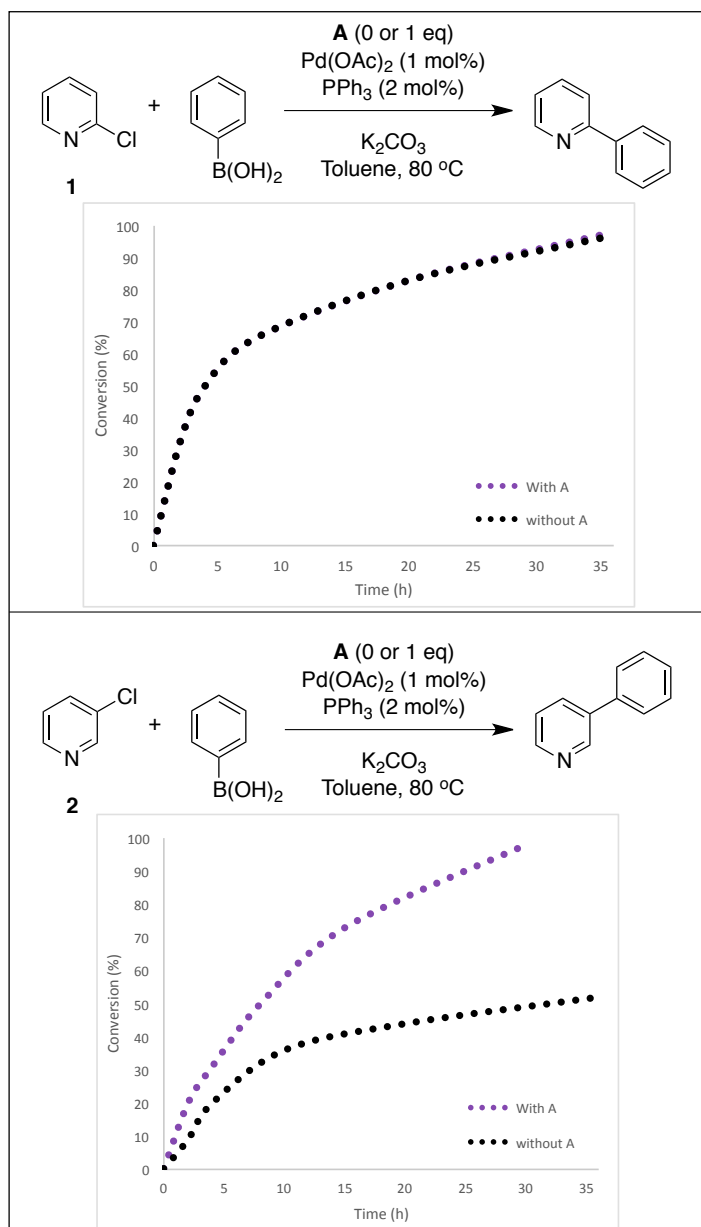
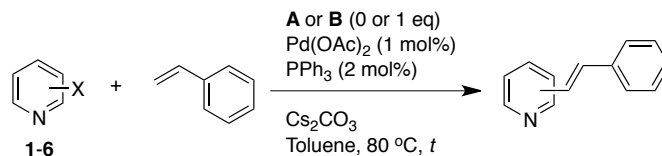


Figure S7. Top: Plot of conversion of **1** versus time under Suzuki-Miyaura conditions with the presence of **A** (purple points) and without the presence of **A** (black points). Bottom: Plot of conversion of **2** versus time under Suzuki-Miyaura conditions with the presence of **A** (purple points) and without the presence of **A** (black points).

Table S3. Conversion of halopyridine derivatives **1-6** under palladium-catalyzed Mizoroki-Heck reaction conditions with and without the presence of catalytically inert building blocks **A** and **B**.^[a]



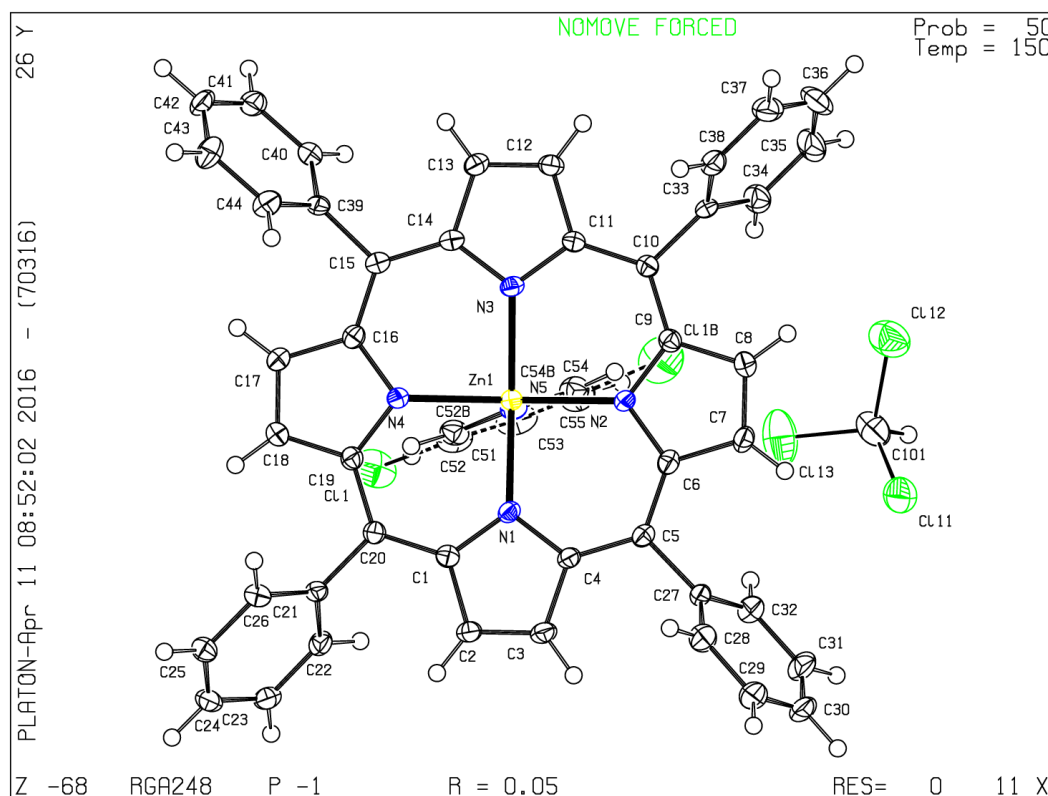
Entry	Substrate	<i>t</i> (h)	Conv. (%) ^[b]
1	1	3	0
2	1•A	3	0
3	1•B	3	12
4	2	4	0
5	2•A	4	17
6	2•B	4	33
7	3	3	4
8	3•A	3	6
9	3•B	3	36
10	4	3	0
11	4•A	3	0
12	4•B	3	16
13	5	3	0
14	5•A	3	21
15	5•B	3	45
16	6	4	18
17	6•A	4	29
18	6•B	4	47

[a] Reaction conditions: [Pd(OAc)₂] (2.5 × 10⁻³ mmol, 1 mol%), PPh₃ (5 × 10⁻³ mmol, 2 mol%), halopyridine (0.25 mmol), **A** (0.170 g, 0.25 mmol) -when applied-, **B** (0.151 g, 0.25 mmol) -when applied-, styrene (0.052 g, 0.5 mmol), anhydrous Cs₂CO₃ (0.163 g, 0.5 mmol), toluene (1.25 mL), dodecane (0.057 mL), 80 °C, argon atmosphere. [b] Conv. = conversion. The conversions were determined by GC; the calibrations were based on dodecane. Reactions were performed 2-3 times.

S5. X-ray crystallographic data for 2•A (CCDC-1509179).

(C₉₉ H₆₅ Cl₅ N₁₀ Zn₂); $M = 1702.60$. APEXII, Bruker-AXS diffractometer, Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$), $T = 150(2) \text{ K}$; Triclinic $P -1$ (I.T.#2), $a = 10.9080(6)$, $b = 12.6139(7)$, $c = 14.8574(8) \text{ \AA}$, $\alpha = 97.770(2)$, $\beta = 94.757(2)$, $\gamma = 102.284(2)^\circ$, $V = 1965.91(19) \text{ \AA}^3$. $Z = 1$, $d = 1.438 \text{ g.cm}^{-3}$, $\mu = 0.839 \text{ mm}^{-1}$. The structure was solved by direct methods using the *SIR97* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [2]. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. Except 2 linked hydrogen atoms (H55 and H101) that were introduced in the structural model through Fourier difference maps analysis, H atoms were finally included in their calculated positions. A final refinement on F^2 with 8920 unique intensities and 533 parameters converged at $\omega R(F^2) = 0.0924$ ($R(F) = 0.0483$) for 6320 observed reflections with $I > 2\sigma(I)$.

- [1] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, *J. Appl. Cryst.* (1999) 32, 115-119
- [2] Sheldrick G.M., *Acta Cryst. A*64 (2008), 112-122



S5.1. Structural data.

Empirical formula	C ₉₉ H ₆₅ Cl ₅ N ₁₀ Zn ₂
Formula weight	1702.60
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system, space group	Triclinic, <i>P</i> -1
Unit cell dimensions	a = 10.9080(6) Å, α = 97.770(2) ° b = 12.6139(7) Å, β = 94.757(2) ° c = 14.8574(8) Å, γ = 102.284(2) °
Volume	1965.91(19) Å ³
Z, Calculated density	1, 1.438 (g.cm ⁻³)
Absorption coefficient	0.839 mm ⁻¹
<i>F</i> (000)	874
Crystal size	0.430 x 0.350 x 0.120 mm
Crystal color	purple
Theta range for data collection	2.925 to 27.456 °
h_min, h_max	-11, 14
k_min, k_max	-16, 15
l_min, l_max	-19, 18
Reflections collected / unique	29869 / 8920 [R(int) ^a = 0.0695]
Reflections [I>2σ]	6320
Completeness to theta_max	0.992
Absorption correction type	multi-scan
Max. and min. transmission	0.904, 0.790
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	8920 / 0 / 533
^b Goodness-of-fit	1.024
Final <i>R</i> indices [I>2σ]	<i>R</i> 1 ^c = 0.0483, <i>wR</i> 2 ^d = 0.0924
<i>R</i> indices (all data)	<i>R</i> 1 ^c = 0.0810, <i>wR</i> 2 ^d = 0.1048
Largest diff. peak and hole	0.536 and -0.507 e ⁻ .Å ⁻³
^a <i>R</i> _{int} = ∑ <i>F</i> _o ² - < <i>F</i> _o ² > / ∑ [<i>F</i> _o ²]	
^b <i>S</i> = {∑ [w(<i>F</i> _o ² - <i>F</i> _c ²) ²] / (n - p)} ^{1/2}	
^c <i>R</i> 1 = ∑ <i>F</i> _o - <i>F</i> _c / ∑ [<i>F</i> _o]	
^d <i>wR</i> 2 = {∑ [w(<i>F</i> _o ² - <i>F</i> _c ²) ²] / ∑ [w(<i>F</i> _o ²) ²]} ^{1/2}	
w = 1 / [σ(<i>F</i> _o ²) + a <i>P</i> ² + b <i>P</i>] where <i>P</i> = [2 <i>F</i> _c ² + MAX(<i>F</i> _o ² , 0)] / 3	

S5.2. Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters (Å²). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
Zn1	0.57624(3)	0.43855(2)	0.27946(2)	1	0.01607(9)
Cl1	0.21709(8)	0.59783(8)	0.05984(6)	0.935(2)	0.0491(3)
Cl1B	0.4306(16)	0.2648(13)	-0.0940(9)	0.065(2)	0.064(5)
N1	0.42810(19)	0.37804(16)	0.34990(13)	1	0.0168(5)
N2	0.60654(19)	0.28175(16)	0.25073(13)	1	0.0161(5)
N3	0.75415(19)	0.50112(16)	0.24487(13)	1	0.0171(5)
N4	0.57053(19)	0.59568(16)	0.33767(14)	1	0.0175(5)
N5	0.46178(19)	0.43504(17)	0.14999(14)	1	0.0210(5)

C1	0.3541(2)	0.4378(2)	0.39518(16)	1	0.0174(5)
C2	0.2567(2)	0.3655(2)	0.43172(17)	1	0.0214(6)
H2	0.1944	0.3864	0.4669	1	0.026
C3	0.2707(2)	0.2622(2)	0.40642(17)	1	0.0223(6)
H3	0.2193	0.1968	0.4199	1	0.027
C4	0.3780(2)	0.2696(2)	0.35515(17)	1	0.0178(5)
C5	0.4236(2)	0.1797(2)	0.31634(16)	1	0.0173(5)
C6	0.5322(2)	0.1866(2)	0.27016(17)	1	0.0183(6)
C7	0.5879(2)	0.0954(2)	0.24281(17)	1	0.0215(6)
H7	0.5555	0.0209	0.2487	1	0.026
C8	0.6959(2)	0.1358(2)	0.20694(17)	1	0.0210(6)
H8	0.7528	0.0949	0.1828	1	0.025
C9	0.7071(2)	0.2529(2)	0.21262(16)	1	0.0177(6)
C10	0.8120(2)	0.3260(2)	0.18901(16)	1	0.0169(5)
C11	0.8332(2)	0.4413(2)	0.20504(16)	1	0.0163(5)
C12	0.9422(2)	0.5154(2)	0.18223(17)	1	0.0201(6)
H12	1.0100	0.4954	0.1530	1	0.024
C13	0.9297(2)	0.6187(2)	0.21034(17)	1	0.0195(6)
H13	0.9880	0.6848	0.2056	1	0.023
C14	0.8114(2)	0.6102(2)	0.24885(16)	1	0.0169(5)
C15	0.7625(2)	0.6996(2)	0.28396(16)	1	0.0177(6)
C16	0.6471(2)	0.6911(2)	0.32153(16)	1	0.0174(5)
C17	0.5909(2)	0.7825(2)	0.34791(17)	1	0.0229(6)
H17	0.6245	0.8572	0.3432	1	0.028
C18	0.4811(2)	0.7419(2)	0.38067(17)	1	0.0218(6)
H18	0.4231	0.7826	0.4030	1	0.026
C19	0.4691(2)	0.6253(2)	0.37517(16)	1	0.0179(6)
C20	0.3680(2)	0.5524(2)	0.40335(16)	1	0.0171(5)
C21	0.2656(2)	0.5992(2)	0.44356(17)	1	0.0172(5)
C22	0.1416(2)	0.5666(2)	0.40160(17)	1	0.0204(6)
H22	0.1224	0.5143	0.3471	1	0.024
C23	0.0455(2)	0.6090(2)	0.43775(18)	1	0.0230(6)
H23	-0.0389	0.5853	0.4089	1	0.028
C24	0.0745(2)	0.6865(2)	0.51674(18)	1	0.0236(6)
H24	0.0098	0.7168	0.5418	1	0.028
C25	0.1966(2)	0.7195(2)	0.55890(17)	1	0.0225(6)
H25	0.2156	0.7723	0.6130	1	0.027
C26	0.2917(2)	0.6762(2)	0.52299(17)	1	0.0202(6)
H26	0.3755	0.6993	0.5528	1	0.024
C27	0.3528(2)	0.0676(2)	0.32755(18)	1	0.0196(6)
C28	0.3436(3)	0.0379(2)	0.41419(19)	1	0.0288(7)
H28	0.3865	0.0875	0.4667	1	0.035
C29	0.2718(3)	-0.0642(2)	0.4240(2)	1	0.0335(7)
H29	0.2638	-0.0829	0.4834	1	0.040
C30	0.2124(3)	-0.1383(2)	0.3486(2)	1	0.0364(8)
H30	0.1643	-0.2082	0.3557	1	0.044
C31	0.2229(3)	-0.1104(2)	0.2627(2)	1	0.0348(7)
H31	0.1824	-0.1618	0.2104	1	0.042
C32	0.2921(3)	-0.0080(2)	0.2516(2)	1	0.0279(7)
H32	0.2981	0.0105	0.1920	1	0.033

C33	0.9112(2)	0.2769(2)	0.14646(17)	1	0.0184(6)
C34	0.8849(3)	0.2146(2)	0.05899(18)	1	0.0272(6)
H34	0.8032	0.2028	0.0266	1	0.033
C35	0.9763(3)	0.1698(2)	0.0190(2)	1	0.0365(8)
H35	0.9571	0.1282	-0.0407	1	0.044
C36	1.0946(3)	0.1853(3)	0.0652(2)	1	0.0422(9)
H36	1.1570	0.1542	0.0374	1	0.051
C37	1.1234(3)	0.2461(2)	0.1522(2)	1	0.0334(7)
H37	1.2052	0.2569	0.1842	1	0.040
C38	1.0317(2)	0.2910(2)	0.19211(19)	1	0.0247(6)
H38	1.0515	0.3322	0.2519	1	0.030
C39	0.8377(2)	0.8137(2)	0.28413(17)	1	0.0181(6)
C40	0.8638(2)	0.8557(2)	0.20370(18)	1	0.0219(6)
H40	0.8357	0.8101	0.1462	1	0.026
C41	0.9300(2)	0.9627(2)	0.20660(19)	1	0.0262(6)
H41	0.9474	0.9896	0.1512	1	0.031
C42	0.9711(3)	1.0311(2)	0.2893(2)	1	0.0281(7)
H42	1.0158	1.1048	0.2909	1	0.034
C43	0.9466(3)	0.9914(2)	0.3694(2)	1	0.0307(7)
H43	0.9748	1.0379	0.4264	1	0.037
C44	0.8805(3)	0.8831(2)	0.36740(18)	1	0.0259(6)
H44	0.8646	0.8565	0.4231	1	0.031
C51	0.3850(2)	0.5043(2)	0.14390(18)	1	0.0251(6)
H51	0.3809	0.5554	0.1962	1	0.030
C52	0.3116(3)	0.5032(2)	0.0634(2)	0.935(2)	0.0310(7)
C52B	0.3116(3)	0.5032(2)	0.0634(2)	0.065(2)	0.0310(7)
H52B	0.2582	0.5535	0.0608	0.065(2)	0.037
C53	0.3151(3)	0.4295(3)	-0.01350(19)	1	0.0349(8)
H53	0.2652	0.4280	-0.0694	1	0.042
C54	0.3940(3)	0.3584(3)	-0.00600(19)	0.935(2)	0.0348(7)
H54	0.3989	0.3061	-0.0572	0.935(2)	0.042
C54B	0.3940(3)	0.3584(3)	-0.00600(19)	0.065(2)	0.0348(7)
C55	0.4658(3)	0.3633(2)	0.07605(19)	1	0.0276(7)
H55	0.524(3)	0.317(3)	0.083(2)	1	0.050
C101	0.4827(6)	-0.0711(5)	0.0029(4)	0.5	0.041
C111	0.44216(16)	-0.14741(14)	0.08758(12)	0.5	0.048
C112	0.64874(19)	-0.04408(16)	-0.00189(12)	0.5	0.053
C113	0.4320(3)	0.05281(17)	0.01630(14)	0.5	0.065
H101	0.442(6)	-0.121(5)	-0.058(4)	0.5	0.050

S5.3. Anisotropic displacement parameters (\AA^2).

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

Atom	U11	U22	U33	U23	U13	U12
Zn1	0.01536(17)	0.01508(16)	0.01812(16)	0.00307(12)	0.00348(12)	0.00331(12)
C11	0.0426(6)	0.0663(7)	0.0510(6)	0.0291(5)	0.0031(4)	0.0284(5)

C11B	0.086(12)	0.065(11)	0.034(8)	0.005(7)	0.002(7)	0.007(9)
N1	0.0166(12)	0.0145(11)	0.0193(11)	0.0049(9)	0.0024(9)	0.0023(9)
N2	0.0159(11)	0.0136(11)	0.0188(11)	0.0039(9)	0.0031(9)	0.0025(9)
N3	0.0136(11)	0.0173(12)	0.0199(11)	0.0048(9)	0.0021(9)	0.0013(9)
N4	0.0165(11)	0.0155(11)	0.0194(11)	0.0011(9)	0.0046(9)	0.0014(9)
N5	0.0202(12)	0.0221(12)	0.0210(12)	0.0063(10)	0.0043(9)	0.0025(10)
C1	0.0165(14)	0.0189(14)	0.0170(13)	0.0033(11)	0.0016(10)	0.0042(11)
C2	0.0166(14)	0.0195(14)	0.0295(15)	0.0078(12)	0.0066(11)	0.0034(11)
C3	0.0196(15)	0.0204(14)	0.0284(15)	0.0095(12)	0.0075(12)	0.0024(11)
C4	0.0158(14)	0.0157(13)	0.0219(14)	0.0052(11)	0.0034(11)	0.0020(11)
C5	0.0167(14)	0.0151(13)	0.0196(13)	0.0044(10)	0.0003(10)	0.0022(11)
C6	0.0183(14)	0.0150(13)	0.0207(14)	0.0022(11)	-0.0007(11)	0.0028(11)
C7	0.0236(15)	0.0132(13)	0.0275(15)	0.0034(11)	0.0025(12)	0.0036(11)
C8	0.0217(15)	0.0188(14)	0.0235(14)	0.0017(11)	0.0039(11)	0.0073(11)
C9	0.0175(14)	0.0187(14)	0.0165(13)	0.0016(11)	0.0018(10)	0.0044(11)
C10	0.0169(14)	0.0172(14)	0.0171(13)	0.0028(10)	0.0031(10)	0.0043(11)
C11	0.0158(13)	0.0181(14)	0.0154(13)	0.0034(10)	0.0034(10)	0.0036(11)
C12	0.0165(14)	0.0222(15)	0.0238(14)	0.0077(11)	0.0061(11)	0.0054(11)
C13	0.0170(14)	0.0179(14)	0.0227(14)	0.0052(11)	0.0018(11)	0.0010(11)
C14	0.0150(13)	0.0192(14)	0.0157(13)	0.0043(10)	0.0017(10)	0.0013(11)
C15	0.0161(14)	0.0185(14)	0.0177(13)	0.0041(11)	0.0018(10)	0.0013(11)
C16	0.0184(14)	0.0164(14)	0.0162(13)	0.0021(10)	0.0001(10)	0.0025(11)
C17	0.0244(15)	0.0159(14)	0.0285(15)	0.0042(11)	0.0089(12)	0.0021(11)
C18	0.0207(15)	0.0194(14)	0.0269(15)	0.0031(11)	0.0073(12)	0.0068(12)
C19	0.0202(14)	0.0169(14)	0.0158(13)	0.0008(10)	0.0031(11)	0.0033(11)
C20	0.0170(14)	0.0173(14)	0.0159(13)	0.0005(10)	0.0015(10)	0.0027(11)
C21	0.0170(14)	0.0166(13)	0.0197(13)	0.0061(11)	0.0057(10)	0.0040(11)
C22	0.0212(15)	0.0162(14)	0.0210(14)	0.0004(11)	0.0009(11)	0.0005(11)
C23	0.0171(14)	0.0216(15)	0.0311(16)	0.0100(12)	0.0032(12)	0.0023(11)
C24	0.0203(15)	0.0270(16)	0.0275(15)	0.0081(12)	0.0101(12)	0.0087(12)
C25	0.0251(16)	0.0241(15)	0.0190(14)	0.0022(11)	0.0066(11)	0.0063(12)
C26	0.0176(14)	0.0248(15)	0.0182(13)	0.0040(11)	0.0027(11)	0.0045(11)
C27	0.0155(14)	0.0138(13)	0.0301(15)	0.0040(11)	0.0048(11)	0.0034(11)
C28	0.0335(17)	0.0250(16)	0.0315(16)	0.0096(13)	0.0101(13)	0.0087(13)
C29	0.0388(19)	0.0248(17)	0.0457(19)	0.0198(15)	0.0192(15)	0.0122(14)
C30	0.0269(17)	0.0177(16)	0.069(2)	0.0168(16)	0.0168(16)	0.0044(13)
C31	0.0222(16)	0.0201(16)	0.057(2)	0.0009(15)	0.0013(14)	-0.0029(13)
C32	0.0250(16)	0.0216(15)	0.0351(17)	0.0024(13)	0.0046(13)	0.0020(12)
C33	0.0193(14)	0.0143(13)	0.0225(14)	0.0068(11)	0.0084(11)	0.0014(11)
C34	0.0331(17)	0.0267(16)	0.0239(15)	0.0051(12)	0.0083(12)	0.0090(13)
C35	0.053(2)	0.0344(18)	0.0282(17)	0.0043(14)	0.0213(15)	0.0161(16)
C36	0.042(2)	0.044(2)	0.056(2)	0.0207(17)	0.0325(17)	0.0266(16)
C37	0.0228(16)	0.0313(17)	0.052(2)	0.0180(15)	0.0127(14)	0.0095(13)
C38	0.0238(16)	0.0193(15)	0.0319(16)	0.0077(12)	0.0053(12)	0.0040(12)
C39	0.0106(13)	0.0180(14)	0.0256(14)	0.0038(11)	0.0030(10)	0.0029(10)
C40	0.0219(15)	0.0218(15)	0.0229(14)	0.0024(11)	0.0077(11)	0.0056(12)
C41	0.0263(16)	0.0236(16)	0.0335(17)	0.0127(13)	0.0101(13)	0.0084(12)
C42	0.0226(16)	0.0143(14)	0.0480(19)	0.0103(13)	0.0059(13)	0.0016(12)
C43	0.0319(17)	0.0212(16)	0.0333(17)	-0.0002(13)	-0.0034(13)	-0.0013(13)
C44	0.0273(16)	0.0233(15)	0.0249(15)	0.0050(12)	0.0031(12)	0.0001(12)

C51	0.0256(16)	0.0287(16)	0.0227(15)	0.0073(12)	0.0068(12)	0.0064(13)
C52	0.0256(16)	0.0393(18)	0.0314(17)	0.0197(14)	0.0018(13)	0.0066(14)
C52B	0.0256(16)	0.0393(18)	0.0314(17)	0.0197(14)	0.0018(13)	0.0066(14)
C53	0.0297(18)	0.048(2)	0.0224(16)	0.0138(14)	-0.0050(13)	-0.0033(15)
C54	0.0378(19)	0.0393(19)	0.0204(15)	-0.0009(13)	0.0007(13)	-0.0022(15)
C54B	0.0378(19)	0.0393(19)	0.0204(15)	-0.0009(13)	0.0007(13)	-0.0022(15)
C55	0.0248(16)	0.0281(17)	0.0267(16)	0.0015(13)	0.0009(12)	0.0017(13)
C101	0.028	0.049	0.038	-0.012	-0.001	0.010
C111	0.046	0.041	0.051	-0.009	0.011	0.004
C112	0.050	0.064	0.042	-0.001	0.012	0.011
C113	0.087	0.058	0.054	-0.005	-0.016	0.040

S5.4. Bond lengths [Å].

Zn1 - N1	= 2.064(2)	Zn1 - N2	= 2.068(2)
Zn1 - N3	= 2.068(2)	Zn1 - N4	= 2.068(2)
Zn1 - N5	= 2.195(2)	Cl1 - C52	= 1.739(3)
Cl1B - C54B	= 1.770(16)	N1 - C1	= 1.372(3)
N1 - C4	= 1.376(3)	N2 - C9	= 1.369(3)
N2 - C6	= 1.379(3)	N3 - C14	= 1.376(3)
N3 - C11	= 1.380(3)	N4 - C16	= 1.374(3)
N4 - C19	= 1.377(3)	N5 - C55	= 1.336(3)
N5 - C51	= 1.339(3)	C1 - C20	= 1.408(3)
C1 - C2	= 1.440(3)	C2 - C3	= 1.350(4)
C2 - H2	= 0.9500	C3 - C4	= 1.442(3)
C3 - H3	= 0.9500	C4 - C5	= 1.406(3)
C5 - C6	= 1.410(3)	C5 - C27	= 1.498(3)
C6 - C7	= 1.439(3)	C7 - C8	= 1.361(3)
C7 - H7	= 0.9500	C8 - C9	= 1.446(3)
C8 - H8	= 0.9500	C9 - C10	= 1.411(3)
C10 - C11	= 1.406(3)	C10 - C33	= 1.499(3)
C11 - C12	= 1.443(3)	C12 - C13	= 1.353(3)
C12 - H12	= 0.9500	C13 - C14	= 1.443(3)
C13 - H13	= 0.9500	C14 - C15	= 1.405(3)
C15 - C16	= 1.408(3)	C15 - C39	= 1.497(3)
C16 - C17	= 1.441(3)	C17 - C18	= 1.355(3)
C17 - H17	= 0.9500	C18 - C19	= 1.439(3)
C18 - H18	= 0.9500	C19 - C20	= 1.409(3)
C20 - C21	= 1.500(3)	C21 - C26	= 1.391(3)
C21 - C22	= 1.394(3)	C22 - C23	= 1.388(3)
C22 - H22	= 0.9500	C23 - C24	= 1.389(4)
C23 - H23	= 0.9500	C24 - C25	= 1.376(4)
C24 - H24	= 0.9500	C25 - C26	= 1.383(3)
C25 - H25	= 0.9500	C26 - H26	= 0.9500
C27 - C32	= 1.392(4)	C27 - C28	= 1.394(4)
C28 - C29	= 1.390(4)	C28 - H28	= 0.9500
C29 - C30	= 1.374(4)	C29 - H29	= 0.9500
C30 - C31	= 1.377(4)	C30 - H30	= 0.9500
C31 - C32	= 1.388(4)	C31 - H31	= 0.9500
C32 - H32	= 0.9500	C33 - C38	= 1.393(4)

C33 - C34	= 1.398(4)	C34 - C35	= 1.382(4)
C34 - H34	= 0.9500	C35 - C36	= 1.373(4)
C35 - H35	= 0.9500	C36 - C37	= 1.386(4)
C36 - H36	= 0.9500	C37 - C38	= 1.386(4)
C37 - H37	= 0.9500	C38 - H38	= 0.9500
C39 - C44	= 1.398(4)	C39 - C40	= 1.398(3)
C40 - C41	= 1.382(3)	C40 - H40	= 0.9500
C41 - C42	= 1.383(4)	C41 - H41	= 0.9500
C42 - C43	= 1.377(4)	C42 - H42	= 0.9500
C43 - C44	= 1.397(4)	C43 - H43	= 0.9500
C44 - H44	= 0.9500	C51 - C52B	= 1.380(4)
C51 - H51	= 0.9500	C52 - C53	= 1.380(4)
C52B - C53	= 1.380(4)	C52B - H52B	= 0.9500
C53 - C54B	= 1.378(4)	C53 - C54	= 1.378(4)
C53 - H53	= 0.9500	C54 - C55	= 1.380(4)
C54 - H54	= 0.9500	C54B - C55	= 1.380(4)
C55 - H55	= 0.96(3)	C101 - C111	= 1.716(7)
C101 - C113	= 1.758(7)	C101 - C112	= 1.779(7)
C101 - H101	= 1.04(6)		

S5.5. Angles [°].

N1 - Zn1 - N2	= 89.30(8)
N1 - Zn1 - N3	= 163.45(8)
N2 - Zn1 - N3	= 89.30(8)
N1 - Zn1 - N4	= 88.73(8)
N2 - Zn1 - N4	= 166.30(8)
N3 - Zn1 - N4	= 88.73(8)
N1 - Zn1 - N5	= 96.61(8)
N2 - Zn1 - N5	= 96.77(8)
N3 - Zn1 - N5	= 99.93(8)
N4 - Zn1 - N5	= 96.92(8)
C1 - N1 - C4	= 106.4(2)
C1 - N1 - Zn1	= 126.46(16)
C4 - N1 - Zn1	= 126.99(16)
C9 - N2 - C6	= 106.7(2)
C9 - N2 - Zn1	= 126.76(16)
C6 - N2 - Zn1	= 126.53(16)
C14 - N3 - C11	= 106.7(2)
C14 - N3 - Zn1	= 126.73(16)
C11 - N3 - Zn1	= 126.34(16)
C16 - N4 - C19	= 106.3(2)
C16 - N4 - Zn1	= 125.57(16)
C19 - N4 - Zn1	= 125.44(16)
C55 - N5 - C51	= 118.5(2)
C55 - N5 - Zn1	= 121.00(19)
C51 - N5 - Zn1	= 120.45(17)
N1 - C1 - C20	= 125.7(2)
N1 - C1 - C2	= 109.9(2)
C20 - C1 - C2	= 124.4(2)

C3	- C2	- C1	= 106.9(2)
C3	- C2	- H2	= 126.5
C1	- C2	- H2	= 126.5
C2	- C3	- C4	= 107.4(2)
C2	- C3	- H3	= 126.3
C4	- C3	- H3	= 126.3
N1	- C4	- C5	= 125.5(2)
N1	- C4	- C3	= 109.4(2)
C5	- C4	- C3	= 125.1(2)
C4	- C5	- C6	= 125.5(2)
C4	- C5	- C27	= 117.1(2)
C6	- C5	- C27	= 117.4(2)
N2	- C6	- C5	= 125.7(2)
N2	- C6	- C7	= 109.5(2)
C5	- C6	- C7	= 124.6(2)
C8	- C7	- C6	= 107.3(2)
C8	- C7	- H7	= 126.4
C6	- C7	- H7	= 126.4
C7	- C8	- C9	= 106.7(2)
C7	- C8	- H8	= 126.6
C9	- C8	- H8	= 126.6
N2	- C9	- C10	= 125.8(2)
N2	- C9	- C8	= 109.8(2)
C10	- C9	- C8	= 124.1(2)
C11	- C10	- C9	= 125.3(2)
C11	- C10	- C33	= 117.4(2)
C9	- C10	- C33	= 117.2(2)
N3	- C11	- C10	= 125.8(2)
N3	- C11	- C12	= 109.4(2)
C10	- C11	- C12	= 124.8(2)
C13	- C12	- C11	= 107.1(2)
C13	- C12	- H12	= 126.5
C11	- C12	- H12	= 126.5
C12	- C13	- C14	= 107.5(2)
C12	- C13	- H13	= 126.3
C14	- C13	- H13	= 126.3
N3	- C14	- C15	= 125.6(2)
N3	- C14	- C13	= 109.3(2)
C15	- C14	- C13	= 125.1(2)
C14	- C15	- C16	= 125.0(2)
C14	- C15	- C39	= 118.9(2)
C16	- C15	- C39	= 116.1(2)
N4	- C16	- C15	= 125.8(2)
N4	- C16	- C17	= 109.7(2)
C15	- C16	- C17	= 124.5(2)
C18	- C17	- C16	= 107.2(2)
C18	- C17	- H17	= 126.4
C16	- C17	- H17	= 126.4
C17	- C18	- C19	= 107.0(2)
C17	- C18	- H18	= 126.5

C19	- C18	- H18	= 126.5
N4	- C19	- C20	= 125.2(2)
N4	- C19	- C18	= 109.8(2)
C20	- C19	- C18	= 125.0(2)
C1	- C20	- C19	= 124.9(2)
C1	- C20	- C21	= 117.0(2)
C19	- C20	- C21	= 118.0(2)
C26	- C21	- C22	= 118.4(2)
C26	- C21	- C20	= 121.1(2)
C22	- C21	- C20	= 120.5(2)
C23	- C22	- C21	= 121.3(2)
C23	- C22	- H22	= 119.3
C21	- C22	- H22	= 119.3
C22	- C23	- C24	= 119.0(2)
C22	- C23	- H23	= 120.5
C24	- C23	- H23	= 120.5
C25	- C24	- C23	= 120.3(2)
C25	- C24	- H24	= 119.9
C23	- C24	- H24	= 119.9
C24	- C25	- C26	= 120.4(2)
C24	- C25	- H25	= 119.8
C26	- C25	- H25	= 119.8
C25	- C26	- C21	= 120.6(2)
C25	- C26	- H26	= 119.7
C21	- C26	- H26	= 119.7
C32	- C27	- C28	= 118.7(2)
C32	- C27	- C5	= 120.5(2)
C28	- C27	- C5	= 120.8(2)
C29	- C28	- C27	= 120.2(3)
C29	- C28	- H28	= 119.9
C27	- C28	- H28	= 119.9
C30	- C29	- C28	= 120.6(3)
C30	- C29	- H29	= 119.7
C28	- C29	- H29	= 119.7
C29	- C30	- C31	= 119.6(3)
C29	- C30	- H30	= 120.2
C31	- C30	- H30	= 120.2
C30	- C31	- C32	= 120.6(3)
C30	- C31	- H31	= 119.7
C32	- C31	- H31	= 119.7
C31	- C32	- C27	= 120.3(3)
C31	- C32	- H32	= 119.9
C27	- C32	- H32	= 119.9
C38	- C33	- C34	= 117.7(2)
C38	- C33	- C10	= 121.7(2)
C34	- C33	- C10	= 120.6(2)
C35	- C34	- C33	= 120.9(3)
C35	- C34	- H34	= 119.5
C33	- C34	- H34	= 119.5
C36	- C35	- C34	= 120.3(3)

C36 - C35 - H35 = 119.8
C34 - C35 - H35 = 119.8
C35 - C36 - C37 = 120.1(3)
C35 - C36 - H36 = 119.9
C37 - C36 - H36 = 119.9
C36 - C37 - C38 = 119.5(3)
C36 - C37 - H37 = 120.3
C38 - C37 - H37 = 120.3
C37 - C38 - C33 = 121.4(3)
C37 - C38 - H38 = 119.3
C33 - C38 - H38 = 119.3
C44 - C39 - C40 = 118.0(2)
C44 - C39 - C15 = 119.4(2)
C40 - C39 - C15 = 122.6(2)
C41 - C40 - C39 = 120.9(2)
C41 - C40 - H40 = 119.5
C39 - C40 - H40 = 119.5
C40 - C41 - C42 = 120.7(3)
C40 - C41 - H41 = 119.7
C42 - C41 - H41 = 119.7
C43 - C42 - C41 = 119.4(3)
C43 - C42 - H42 = 120.3
C41 - C42 - H42 = 120.3
C42 - C43 - C44 = 120.5(3)
C42 - C43 - H43 = 119.8
C44 - C43 - H43 = 119.8
C43 - C44 - C39 = 120.6(2)
C43 - C44 - H44 = 119.7
C39 - C44 - H44 = 119.7
N5 - C51 - C52B = 121.5(3)
N5 - C51 - H51 = 119.3
C52B - C51 - H51 = 119.3
C53 - C52 - C11 = 120.6(2)
C53 - C52B - C51 = 120.5(3)
C53 - C52B - H52B = 119.8
C51 - C52B - H52B = 119.8
C54 - C53 - C52 = 117.3(3)
C54B - C53 - C52B = 117.3(3)
C54 - C53 - H53 = 121.3
C52 - C53 - H53 = 121.3
C53 - C54 - C55 = 119.8(3)
C53 - C54 - H54 = 120.1
C55 - C54 - H54 = 120.1
C53 - C54B - C55 = 119.8(3)
C53 - C54B - C11B = 127.9(6)
C55 - C54B - C11B = 111.9(6)
N5 - C55 - C54B = 122.3(3)
N5 - C55 - H55 = 115.4(18)
C54B - C55 - H55 = 122.3(19)
C54 - C55 - H55 = 122.3(19)

C111	- C101	- C113	= 112.4(4)
C111	- C101	- C112	= 110.6(4)
C113	- C101	- C112	= 110.1(4)
C111	- C101	- H101	= 106(3)
C113	- C101	- H101	= 111(3)
C112	- C101	- H101	= 106(3)

S5.6. Torsion angles [°].

C4	- N1	- C1	- C20	= -177.1(2)
Zn1	- N1	- C1	- C20	= -1.5(4)
C4	- N1	- C1	- C2	= 1.4(3)
Zn1	- N1	- C1	- C2	= 177.02(16)
N1	- C1	- C2	- C3	= -1.4(3)
C20	- C1	- C2	- C3	= 177.1(2)
C1	- C2	- C3	- C4	= 0.8(3)
C1	- N1	- C4	- C5	= 178.9(2)
Zn1	- N1	- C4	- C5	= 3.3(4)
C1	- N1	- C4	- C3	= -0.8(3)
Zn1	- N1	- C4	- C3	= -176.46(16)
C2	- C3	- C4	- N1	= 0.0(3)
C2	- C3	- C4	- C5	= -179.8(2)
N1	- C4	- C5	- C6	= 3.7(4)
C3	- C4	- C5	- C6	= -176.6(2)
N1	- C4	- C5	- C27	= -178.2(2)
C3	- C4	- C5	- C27	= 1.5(4)
C9	- N2	- C6	- C5	= 175.0(2)
Zn1	- N2	- C6	- C5	= -2.4(4)
C9	- N2	- C6	- C7	= -0.3(3)
Zn1	- N2	- C6	- C7	= -177.62(16)
C4	- C5	- C6	- N2	= -4.2(4)
C27	- C5	- C6	- N2	= 177.7(2)
C4	- C5	- C6	- C7	= 170.4(2)
C27	- C5	- C6	- C7	= -7.7(4)
N2	- C6	- C7	- C8	= 0.0(3)
C5	- C6	- C7	- C8	= -175.3(2)
C6	- C7	- C8	- C9	= 0.3(3)
C6	- N2	- C9	- C10	= -174.6(2)
Zn1	- N2	- C9	- C10	= 2.7(4)
C6	- N2	- C9	- C8	= 0.5(3)
Zn1	- N2	- C9	- C8	= 177.78(15)
C7	- C8	- C9	- N2	= -0.5(3)
C7	- C8	- C9	- C10	= 174.7(2)
N2	- C9	- C10	- C11	= 3.3(4)
C8	- C9	- C10	- C11	= -171.1(2)
N2	- C9	- C10	- C33	= -179.0(2)
C8	- C9	- C10	- C33	= 6.5(4)
C14	- N3	- C11	- C10	= 179.0(2)
Zn1	- N3	- C11	- C10	= -6.7(4)
C14	- N3	- C11	- C12	= -0.9(3)

Zn1	- N3	- C11	- C12	= 173.47(15)
C9	- C10	- C11	- N3	= -1.1(4)
C33	- C10	- C11	- N3	= -178.8(2)
C9	- C10	- C11	- C12	= 178.7(2)
C33	- C10	- C11	- C12	= 1.0(4)
N3	- C11	- C12	- C13	= 1.5(3)
C10	- C11	- C12	- C13	= -178.4(2)
C11	- C12	- C13	- C14	= -1.4(3)
C11	- N3	- C14	- C15	= 179.4(2)
Zn1	- N3	- C14	- C15	= 5.1(3)
C11	- N3	- C14	- C13	= 0.0(3)
Zn1	- N3	- C14	- C13	= -174.31(15)
C12	- C13	- C14	- N3	= 0.9(3)
C12	- C13	- C14	- C15	= -178.5(2)
N3	- C14	- C15	- C16	= 0.7(4)
C13	- C14	- C15	- C16	= -180.0(2)
N3	- C14	- C15	- C39	= 179.4(2)
C13	- C14	- C15	- C39	= -1.3(4)
C19	- N4	- C16	- C15	= 179.5(2)
Zn1	- N4	- C16	- C15	= -18.4(3)
C19	- N4	- C16	- C17	= -1.2(3)
Zn1	- N4	- C16	- C17	= 160.90(16)
C14	- C15	- C16	- N4	= 6.5(4)
C39	- C15	- C16	- N4	= -172.2(2)
C14	- C15	- C16	- C17	= -172.7(2)
C39	- C15	- C16	- C17	= 8.6(4)
N4	- C16	- C17	- C18	= 0.5(3)
C15	- C16	- C17	- C18	= 179.9(2)
C16	- C17	- C18	- C19	= 0.3(3)
C16	- N4	- C19	- C20	= -179.1(2)
Zn1	- N4	- C19	- C20	= 18.8(3)
C16	- N4	- C19	- C18	= 1.3(3)
Zn1	- N4	- C19	- C18	= -160.75(16)
C17	- C18	- C19	- N4	= -1.0(3)
C17	- C18	- C19	- C20	= 179.4(2)
N1	- C1	- C20	- C19	= -7.7(4)
C2	- C1	- C20	- C19	= 174.1(2)
N1	- C1	- C20	- C21	= 171.1(2)
C2	- C1	- C20	- C21	= -7.1(4)
N4	- C19	- C20	- C1	= -1.7(4)
C18	- C19	- C20	- C1	= 177.8(2)
N4	- C19	- C20	- C21	= 179.5(2)
C18	- C19	- C20	- C21	= -1.0(4)
C1	- C20	- C21	- C26	= 120.0(3)
C19	- C20	- C21	- C26	= -61.1(3)
C1	- C20	- C21	- C22	= -60.3(3)
C19	- C20	- C21	- C22	= 118.6(3)
C26	- C21	- C22	- C23	= -0.3(4)
C20	- C21	- C22	- C23	= 180.0(2)
C21	- C22	- C23	- C24	= 0.8(4)

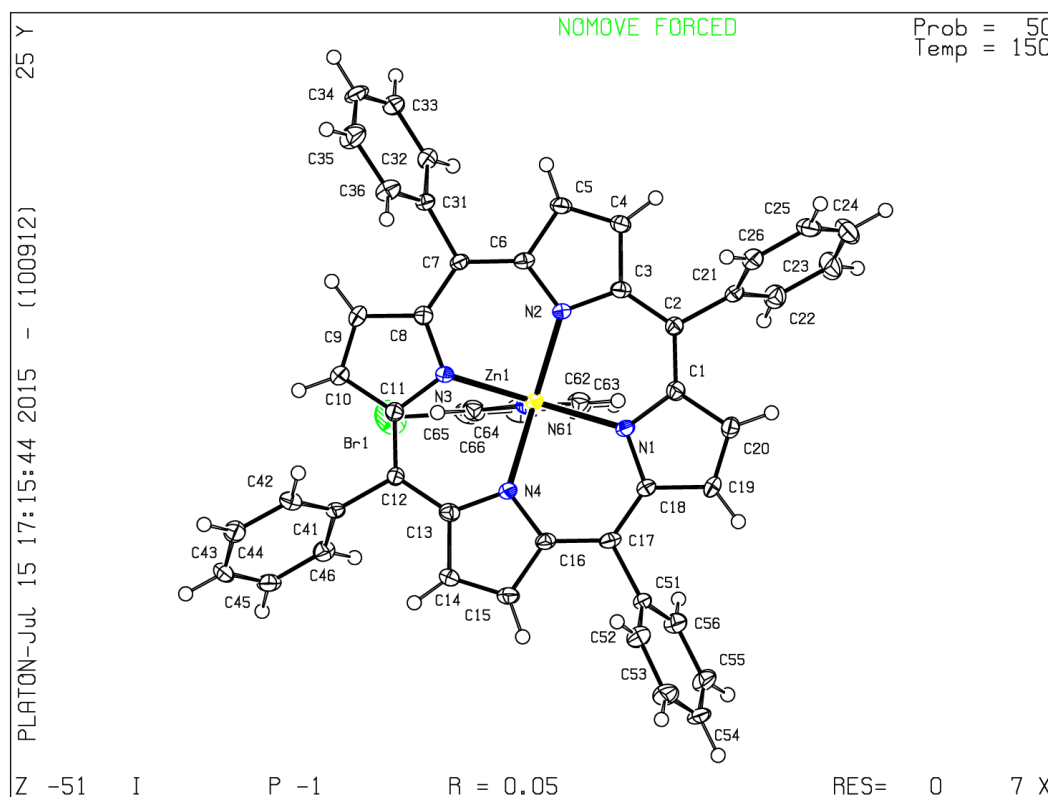
C22	- C23	- C24	- C25	= -0.8(4)
C23	- C24	- C25	- C26	= 0.2(4)
C24	- C25	- C26	- C21	= 0.3(4)
C22	- C21	- C26	- C25	= -0.3(4)
C20	- C21	- C26	- C25	= 179.4(2)
C4	- C5	- C27	- C32	= 116.1(3)
C6	- C5	- C27	- C32	= -65.7(3)
C4	- C5	- C27	- C28	= -62.3(3)
C6	- C5	- C27	- C28	= 116.0(3)
C32	- C27	- C28	- C29	= -2.0(4)
C5	- C27	- C28	- C29	= 176.4(2)
C27	- C28	- C29	- C30	= 2.0(4)
C28	- C29	- C30	- C31	= -0.8(4)
C29	- C30	- C31	- C32	= -0.5(4)
C30	- C31	- C32	- C27	= 0.6(4)
C28	- C27	- C32	- C31	= 0.7(4)
C5	- C27	- C32	- C31	= -177.7(2)
C11	- C10	- C33	- C38	= 65.9(3)
C9	- C10	- C33	- C38	= -111.9(3)
C11	- C10	- C33	- C34	= -114.3(3)
C9	- C10	- C33	- C34	= 67.8(3)
C38	- C33	- C34	- C35	= -0.8(4)
C10	- C33	- C34	- C35	= 179.4(2)
C33	- C34	- C35	- C36	= 0.5(4)
C34	- C35	- C36	- C37	= -0.1(5)
C35	- C36	- C37	- C38	= 0.1(4)
C36	- C37	- C38	- C33	= -0.4(4)
C34	- C33	- C38	- C37	= 0.8(4)
C10	- C33	- C38	- C37	= -179.5(2)
C14	- C15	- C39	- C44	= -117.4(3)
C16	- C15	- C39	- C44	= 61.3(3)
C14	- C15	- C39	- C40	= 64.8(3)
C16	- C15	- C39	- C40	= -116.4(3)
C44	- C39	- C40	- C41	= 0.0(4)
C15	- C39	- C40	- C41	= 177.8(2)
C39	- C40	- C41	- C42	= -0.5(4)
C40	- C41	- C42	- C43	= 0.6(4)
C41	- C42	- C43	- C44	= -0.2(4)
C42	- C43	- C44	- C39	= -0.4(4)
C40	- C39	- C44	- C43	= 0.5(4)
C15	- C39	- C44	- C43	= -177.4(2)
C55	- N5	- C51	- C52B	= -0.4(4)
Zn1	- N5	- C51	- C52B	= -179.62(19)
N5	- C51	- C52B	- C53	= 0.3(4)
C11	- C52	- C53	- C54	= 178.8(2)
C51	- C52B	- C53	- C54B	= 0.1(4)
C52	- C53	- C54	- C55	= -0.4(4)
C52B	- C53	- C54B	- C55	= -0.4(4)
C52B	- C53	- C54B	- C11B	= -173.3(7)
C51	- N5	- C55	- C54B	= 0.2(4)

$$\begin{array}{rclcl} \text{Zn1} & - \text{N5} & - \text{C55} & - \text{C54B} & = 179.3(2) \\ \text{C53} & - \text{C54B} & - \text{C55} & - \text{N5} & = 0.3(4) \\ \text{C11B} & - \text{C54B} & - \text{C55} & - \text{N5} & = 174.2(6) \end{array}$$

S6. X-ray crystallographic data for 5•A (CCDC-1509180).

(C₄₉ H₃₂ Br N₅ Zn); $M = 836.08$. APEXII, Bruker-AXS diffractometer, Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$), $T = 150(2) \text{ K}$; triclinic $P -1$ (I.T.#2), $a = 10.9267(3)$, $b = 12.6185(4)$, $c = 14.8621(5) \text{ \AA}$, $\alpha = 98.294(2)$, $\beta = 94.653(2)$, $\gamma = 102.3130(10)^\circ$, $V = 1967.78(11) \text{ \AA}^3$. $Z = 2$, $d = 1.411 \text{ g.cm}^{-3}$, $\mu = 1.681 \text{ mm}^{-1}$. The structure was solved by direct methods using the *SIR97* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [2] with the aid of the *WINGX* [3] program. The contribution of the disordered solvents to the calculated structure factors was estimated following the *BYPASS* algorithm [4], implemented as the *SQUEEZE* option in *PLATON* [5]. A new data set, free of solvent contribution, was then used in the final refinement. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 8868 unique intensities and 505 parameters converged at $\omega R(F^2) = 0.1298$ ($R(F) = 0.0494$) for 6400 observed reflections with $I > 2\sigma(I)$.

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- [2] Sheldrick G.M., *Acta Cryst. A* 64 (2008), 112-122
- [3] L. J. Farrugia, *J. Appl. Cryst.*, 2012, 45, 849-854
- [4] P. v.d. Sluis and A.L. Spek, *Acta Cryst.* (1990) A46, 194-201
- [5] A. L. Spek, *J. Appl. Cryst.* (2003), 36, 7-13



S6.1. Structural data.

Empirical formula	C ₄₉ H ₃₂ Br N ₅ Zn
Formula weight	836.08
Temperature	150(2) K
Wavelength	0.71073 Å
Crystal system, space group	triclinic, <i>P</i> -1
Unit cell dimensions	a = 10.9267(3) Å, α = 98.294(2) ° b = 12.6185(4) Å, β = 94.653(2) ° c = 14.8621(5) Å, γ = 102.3130(10) °
Volume	1967.78(11) Å ³
Z, Calculated density	2, 1.411 (g.cm ⁻³)
Absorption coefficient	1.681 mm ⁻¹
<i>F</i> (000)	852
Crystal size	0.34 x 0.19 x 0.12 mm
Crystal color	red
Theta range for data collection	2.92 to 27.54 °
h_min, h_max	-14, 8
k_min, k_max	-16, 16
l_min, l_max	-19, 19
Reflections collected / unique	16128 / 8868 [R(int) ^a = 0.0342]
Reflections [I>2σ]	6400
Completeness to theta_max	0.977
Absorption correction type	multi-scan
Max. and min. transmission	0.817, 0.677
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	8868 / 0 / 505
^b Goodness-of-fit	1.05
Final <i>R</i> indices [I>2σ]	<i>R</i> 1 ^c = 0.0494, <i>wR</i> 2 ^d = 0.1298
<i>R</i> indices (all data)	<i>R</i> 1 ^c = 0.0714, <i>wR</i> 2 ^d = 0.1395
Largest diff. peak and hole	1.039 and -0.879 e ⁻ .Å ⁻³
^a <i>R</i> _{int} = ∑ <i>F</i> _o ² - < <i>F</i> _o ² > / ∑ [<i>F</i> _o ²]	
^b <i>S</i> = {∑ [w(<i>F</i> _o ² - <i>F</i> _c ²) ²] / (n - p)} ^{1/2}	
^c <i>R</i> 1 = ∑ <i>F</i> _o - <i>F</i> _c / ∑ [<i>F</i> _o]	
^d <i>wR</i> 2 = {∑ [w(<i>F</i> _o ² - <i>F</i> _c ²) ²] / ∑ [w(<i>F</i> _o ²) ²]} ^{1/2}	
<i>w</i> = 1 / [σ(<i>F</i> _o ²) + a <i>P</i> ² + b <i>P</i>] where <i>P</i> = [2 <i>F</i> _c ² + MAX(<i>F</i> _o ² , 0)] / 3	

S6.2. Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters (Å²). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
Zn1	0.57544(3)	0.43598(3)	0.28032(2)	1	0.01552(11)
N1	0.6057(2)	0.2792(2)	0.25179(18)	1	0.0177(5)
N2	0.7531(2)	0.4977(2)	0.24601(18)	1	0.0174(5)
N3	0.5691(2)	0.5939(2)	0.33769(18)	1	0.0164(5)
N4	0.4272(2)	0.3768(2)	0.35037(18)	1	0.0172(5)
C1	0.7065(3)	0.2493(3)	0.2147(2)	1	0.0183(6)
C2	0.8114(3)	0.3225(2)	0.1915(2)	1	0.0172(6)
C3	0.8327(3)	0.4382(3)	0.2077(2)	1	0.0173(6)

C4	0.9406(3)	0.5110(3)	0.1845(2)	1	0.0207(7)
H4	1.0081	0.4902	0.1553	1	0.025
C5	0.9288(3)	0.6154(3)	0.2117(2)	1	0.0203(7)
H5	0.9871	0.6813	0.2068	1	0.024
C6	0.8102(3)	0.6066(3)	0.2497(2)	1	0.0167(6)
C7	0.7608(3)	0.6964(2)	0.2846(2)	1	0.0161(6)
C8	0.6457(3)	0.6884(3)	0.3218(2)	1	0.0193(7)
C9	0.5894(3)	0.7798(3)	0.3475(2)	1	0.0245(7)
H9	0.6229	0.8544	0.3425	1	0.029
C10	0.4800(3)	0.7400(3)	0.3802(2)	1	0.0223(7)
H10	0.4218	0.781	0.4022	1	0.027
C11	0.4688(3)	0.6234(3)	0.3753(2)	1	0.0180(6)
C12	0.3674(3)	0.5510(2)	0.4028(2)	1	0.0158(6)
C13	0.3532(3)	0.4360(3)	0.3947(2)	1	0.0180(6)
C14	0.2570(3)	0.3655(3)	0.4323(2)	1	0.0227(7)
H14	0.1957	0.3876	0.4679	1	0.027
C15	0.2699(3)	0.2621(3)	0.4077(2)	1	0.0234(7)
H15	0.2184	0.1971	0.4216	1	0.028
C16	0.3777(3)	0.2686(3)	0.3558(2)	1	0.0173(6)
C17	0.4235(3)	0.1783(2)	0.3172(2)	1	0.0181(6)
C18	0.5309(3)	0.1846(2)	0.2720(2)	1	0.0187(6)
C19	0.5868(3)	0.0929(3)	0.2446(2)	1	0.0220(7)
H19	0.554	0.0185	0.2503	1	0.026
C20	0.6945(3)	0.1324(3)	0.2095(2)	1	0.0215(7)
H20	0.7514	0.0911	0.1859	1	0.026
C21	0.9109(3)	0.2737(3)	0.1503(2)	1	0.0206(7)
C22	0.8844(3)	0.2088(3)	0.0627(2)	1	0.0258(7)
H22	0.8021	0.1952	0.031	1	0.031
C23	0.9756(4)	0.1640(3)	0.0215(3)	1	0.0358(9)
H23	0.9562	0.121	-0.038	1	0.043
C24	1.0956(4)	0.1829(4)	0.0682(3)	1	0.0448(11)
H24	1.1584	0.1523	0.0405	1	0.054
C25	1.1245(3)	0.2457(3)	0.1545(3)	1	0.0335(9)
H25	1.2068	0.2588	0.1861	1	0.04
C26	1.0306(3)	0.2899(3)	0.1947(3)	1	0.0260(7)
H26	1.0503	0.3322	0.2544	1	0.031
C31	0.8368(3)	0.8110(3)	0.2843(2)	1	0.0193(7)
C32	0.8616(3)	0.8514(3)	0.2040(2)	1	0.0220(7)
H32	0.833	0.8048	0.1468	1	0.026
C33	0.9274(3)	0.9586(3)	0.2061(3)	1	0.0273(8)
H33	0.9439	0.9851	0.1506	1	0.033
C34	0.9690(3)	1.0270(3)	0.2893(3)	1	0.0280(8)
H34	1.0152	1.1002	0.2908	1	0.034
C35	0.9442(3)	0.9900(3)	0.3692(3)	1	0.0335(8)
H35	0.9706	1.038	0.4261	1	0.04
C36	0.8793(3)	0.8804(3)	0.3672(2)	1	0.0251(7)
H36	0.8644	0.8539	0.4229	1	0.03
C41	0.2647(3)	0.5983(2)	0.4433(2)	1	0.0186(6)
C42	0.2915(3)	0.6757(3)	0.5221(2)	1	0.0204(7)
H42	0.3755	0.6986	0.5514	1	0.024

C43	0.1972(3)	0.7209(3)	0.5593(2)	1	0.0247(7)
H43	0.2169	0.7745	0.6133	1	0.03
C44	0.0742(3)	0.6869(3)	0.5167(2)	1	0.0256(8)
H44	0.0093	0.7172	0.5415	1	0.031
C45	0.0462(3)	0.6082(3)	0.4375(2)	1	0.0244(7)
H45	-0.0379	0.5838	0.4084	1	0.029
C46	0.1422(3)	0.5656(3)	0.4015(2)	1	0.0217(7)
H46	0.1232	0.5128	0.3469	1	0.026
C51	0.3516(3)	0.0660(3)	0.3281(2)	1	0.0216(7)
C52	0.3439(3)	0.0369(3)	0.4143(3)	1	0.0293(8)
H52	0.3881	0.0868	0.4666	1	0.035
C53	0.2720(4)	-0.0647(3)	0.4246(3)	1	0.0374(10)
H53	0.2645	-0.0829	0.4841	1	0.045
C54	0.2110(3)	-0.1397(3)	0.3479(3)	1	0.0360(10)
H54	0.1627	-0.2096	0.3548	1	0.043
C55	0.2209(3)	-0.1123(3)	0.2626(3)	1	0.0345(9)
H55	0.1805	-0.1639	0.21	1	0.041
C56	0.2899(3)	-0.0089(3)	0.2522(3)	1	0.0291(8)
H56	0.2946	0.0101	0.1928	1	0.035
N61	0.4637(2)	0.4322(2)	0.15088(18)	1	0.0213(6)
C62	0.4679(3)	0.3591(3)	0.0759(2)	1	0.0267(7)
H62	0.5213	0.3093	0.0805	1	0.032
C63	0.3980(4)	0.3533(3)	-0.0072(2)	1	0.0326(8)
H63	0.4031	0.3006	-0.0585	1	0.039
C64	0.3209(3)	0.4254(3)	-0.0141(3)	1	0.0332(9)
H64	0.2726	0.4246	-0.0704	1	0.04
C65	0.3155(3)	0.4988(3)	0.0627(3)	1	0.0306(8)
C66	0.3867(3)	0.5008(3)	0.1438(2)	1	0.0233(7)
H66	0.3811	0.5519	0.1959	1	0.028
Br1	0.21400(4)	0.60237(4)	0.05721(3)	1	0.04814(15)

S6.3. Anisotropic displacement parameters (\AA^2).

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

Atom	U11	U22	U33	U23	U13	U12
Zn1	0.01475(18)	0.01307(18)	0.0195(2)	0.00501(14)	0.00417(14)	0.00242(13)
N1	0.0151(12)	0.0138(13)	0.0243(14)	0.0054(11)	0.0033(11)	0.0016(10)
N2	0.0169(13)	0.0140(13)	0.0217(14)	0.0044(11)	0.0068(11)	0.0016(10)
N3	0.0122(12)	0.0151(13)	0.0211(14)	0.0027(11)	0.0029(10)	0.0015(10)
N4	0.0159(13)	0.0136(13)	0.0229(14)	0.0055(11)	0.0045(11)	0.0028(10)
C1	0.0192(15)	0.0177(16)	0.0197(16)	0.0051(13)	0.0038(13)	0.0061(12)
C2	0.0187(15)	0.0157(15)	0.0186(16)	0.0045(12)	0.0042(12)	0.0051(12)
C3	0.0137(14)	0.0183(16)	0.0197(16)	0.0052(13)	0.0026(12)	0.0015(12)
C4	0.0163(15)	0.0209(17)	0.0278(18)	0.0092(14)	0.0076(13)	0.0050(13)
C5	0.0138(15)	0.0206(17)	0.0278(18)	0.0091(14)	0.0051(13)	0.0024(12)
C6	0.0141(14)	0.0167(15)	0.0183(16)	0.0050(12)	0.0004(12)	0.0003(12)
C7	0.0156(15)	0.0127(15)	0.0198(16)	0.0048(12)	0.0026(12)	0.0010(12)
C8	0.0213(16)	0.0172(16)	0.0206(16)	0.0044(13)	0.0065(13)	0.0050(13)

C9	0.0276(18)	0.0131(16)	0.035(2)	0.0051(14)	0.0093(15)	0.0058(13)
C10	0.0216(16)	0.0154(16)	0.0310(19)	0.0048(14)	0.0071(14)	0.0042(13)
C11	0.0213(16)	0.0165(16)	0.0175(16)	0.0040(13)	0.0056(13)	0.0056(13)
C12	0.0174(15)	0.0141(15)	0.0164(15)	0.0026(12)	0.0031(12)	0.0043(12)
C13	0.0133(14)	0.0202(16)	0.0199(16)	0.0039(13)	0.0002(12)	0.0026(12)
C14	0.0180(16)	0.0206(17)	0.0319(19)	0.0071(14)	0.0110(14)	0.0046(13)
C15	0.0199(16)	0.0210(17)	0.0319(19)	0.0112(15)	0.0098(14)	0.0032(13)
C16	0.0130(14)	0.0163(15)	0.0220(16)	0.0057(13)	0.0003(12)	0.0010(12)
C17	0.0145(15)	0.0155(15)	0.0228(16)	0.0069(13)	0.0000(12)	-0.0011(12)
C18	0.0194(15)	0.0144(15)	0.0234(17)	0.0063(13)	0.0058(13)	0.0029(12)
C19	0.0266(17)	0.0118(15)	0.0289(18)	0.0043(13)	0.0064(14)	0.0058(13)
C20	0.0198(16)	0.0162(16)	0.0284(18)	0.0018(13)	0.0021(14)	0.0057(13)
C21	0.0205(16)	0.0138(15)	0.0301(18)	0.0093(13)	0.0082(14)	0.0042(12)
C22	0.0312(19)	0.0239(18)	0.0230(18)	0.0037(14)	0.0052(15)	0.0074(15)
C23	0.048(2)	0.035(2)	0.029(2)	0.0028(17)	0.0191(18)	0.0144(18)
C24	0.043(2)	0.043(3)	0.065(3)	0.024(2)	0.037(2)	0.024(2)
C25	0.0211(18)	0.029(2)	0.056(3)	0.0186(19)	0.0162(17)	0.0066(15)
C26	0.0240(17)	0.0194(17)	0.036(2)	0.0067(15)	0.0069(15)	0.0052(14)
C31	0.0149(15)	0.0143(15)	0.0282(18)	0.0041(13)	0.0041(13)	0.0011(12)
C32	0.0246(17)	0.0175(16)	0.0243(17)	0.0036(13)	0.0056(14)	0.0048(13)
C33	0.0295(18)	0.0207(17)	0.037(2)	0.0140(16)	0.0137(16)	0.0078(14)
C34	0.0208(17)	0.0147(16)	0.049(2)	0.0133(16)	0.0054(16)	-0.0005(13)
C35	0.036(2)	0.0226(19)	0.037(2)	0.0004(16)	0.0014(17)	-0.0008(16)
C36	0.0289(18)	0.0208(17)	0.0236(18)	0.0061(14)	0.0014(14)	0.0002(14)
C41	0.0187(16)	0.0159(15)	0.0241(17)	0.0094(13)	0.0089(13)	0.0041(12)
C42	0.0157(15)	0.0244(17)	0.0210(16)	0.0056(14)	0.0029(13)	0.0032(13)
C43	0.0296(18)	0.0221(17)	0.0233(18)	0.0047(14)	0.0079(15)	0.0056(14)
C44	0.0216(17)	0.0259(18)	0.035(2)	0.0108(15)	0.0148(15)	0.0095(14)
C45	0.0162(16)	0.0233(17)	0.035(2)	0.0122(15)	0.0045(14)	0.0015(13)
C46	0.0209(16)	0.0200(16)	0.0233(17)	0.0040(14)	0.0010(13)	0.0030(13)
C51	0.0164(15)	0.0131(15)	0.037(2)	0.0071(14)	0.0089(14)	0.0031(12)
C52	0.034(2)	0.0219(18)	0.036(2)	0.0120(16)	0.0111(16)	0.0059(15)
C53	0.038(2)	0.027(2)	0.056(3)	0.024(2)	0.020(2)	0.0099(17)
C54	0.0237(18)	0.0171(18)	0.072(3)	0.0191(19)	0.0183(19)	0.0028(14)
C55	0.0254(18)	0.0170(17)	0.057(3)	0.0008(17)	0.0052(18)	-0.0017(14)
C56	0.0225(17)	0.0207(18)	0.044(2)	0.0063(16)	0.0071(16)	0.0021(14)
N61	0.0195(14)	0.0237(15)	0.0202(14)	0.0085(12)	0.0021(11)	0.0008(11)
C62	0.0277(18)	0.0268(19)	0.0253(18)	0.0049(15)	0.0046(14)	0.0042(15)
C63	0.038(2)	0.031(2)	0.0224(18)	-0.0031(16)	0.0025(16)	-0.0003(17)
C64	0.0256(19)	0.044(2)	0.0248(19)	0.0090(17)	-0.0060(15)	-0.0022(17)
C65	0.0249(18)	0.040(2)	0.032(2)	0.0204(17)	0.0057(15)	0.0074(16)
C66	0.0228(17)	0.0264(18)	0.0239(17)	0.0098(14)	0.0061(14)	0.0077(14)
Br1	0.0456(3)	0.0627(3)	0.0485(3)	0.0259(2)	0.0038(2)	0.0290(2)

S6.4. Bond lengths [Å].

Zn1 - N4 = 2.061(2)
 Zn1 - N2 = 2.065(2)
 Zn1 - N61 = 2.182(3)
 N1 - C18 = 1.382(4)

Zn1 - N1 = 2.065(3)
 Zn1 - N3 = 2.069(3)
 N1 - C1 = 1.368(4)
 N2 - C3 = 1.371(4)

N2 - C6	= 1.373(4)	N3 - C8	= 1.366(4)
N3 - C11	= 1.366(4)	N4 - C13	= 1.360(4)
N4 - C16	= 1.373(4)	C1 - C2	= 1.411(4)
C1 - C20	= 1.443(4)	C2 - C3	= 1.410(4)
C2 - C21	= 1.490(4)	C3 - C4	= 1.432(4)
C4 - C5	= 1.357(5)	C4 - H4	= 0.95
C5 - C6	= 1.444(4)	C5 - H5	= 0.95
C6 - C7	= 1.408(4)	C7 - C8	= 1.405(4)
C7 - C31	= 1.507(4)	C8 - C9	= 1.438(4)
C9 - C10	= 1.351(5)	C9 - H9	= 0.95
C10 - C11	= 1.441(4)	C10 - H10	= 0.95
C11 - C12	= 1.406(4)	C12 - C13	= 1.412(4)
C12 - C41	= 1.507(4)	C13 - C14	= 1.431(4)
C14 - C15	= 1.343(5)	C14 - H14	= 0.95
C15 - C16	= 1.454(4)	C15 - H15	= 0.95
C16 - C17	= 1.406(4)	C17 - C18	= 1.393(4)
C17 - C51	= 1.505(4)	C18 - C19	= 1.443(4)
C19 - C20	= 1.353(4)	C19 - H19	= 0.95
C20 - H20	= 0.95	C21 - C26	= 1.377(5)
C21 - C22	= 1.407(5)	C22 - C23	= 1.388(5)
C22 - H22	= 0.95	C23 - C24	= 1.389(6)
C23 - H23	= 0.95	C24 - C25	= 1.380(6)
C24 - H24	= 0.95	C25 - C26	= 1.402(5)
C25 - H25	= 0.95	C26 - H26	= 0.95
C31 - C36	= 1.387(5)	C31 - C32	= 1.387(4)
C32 - C33	= 1.385(4)	C32 - H32	= 0.95
C33 - C34	= 1.384(5)	C33 - H33	= 0.95
C34 - C35	= 1.364(5)	C34 - H34	= 0.95
C35 - C36	= 1.407(5)	C35 - H35	= 0.95
C36 - H36	= 0.95	C41 - C42	= 1.379(5)
C41 - C46	= 1.380(4)	C42 - C43	= 1.395(4)
C42 - H42	= 0.95	C43 - C44	= 1.389(5)
C43 - H43	= 0.95	C44 - C45	= 1.393(5)
C44 - H44	= 0.95	C45 - C46	= 1.387(5)
C45 - H45	= 0.95	C46 - H46	= 0.95
C51 - C56	= 1.384(5)	C51 - C52	= 1.387(5)
C52 - C53	= 1.389(5)	C52 - H52	= 0.95
C53 - C54	= 1.392(6)	C53 - H53	= 0.95
C54 - C55	= 1.369(6)	C54 - H54	= 0.95
C55 - C56	= 1.397(5)	C55 - H55	= 0.95
C56 - H56	= 0.95	N61 - C66	= 1.338(4)
N61 - C62	= 1.351(4)	C62 - C63	= 1.383(5)
C62 - H62	= 0.95	C63 - C64	= 1.374(5)
C63 - H63	= 0.95	C64 - C65	= 1.376(5)
C64 - H64	= 0.95	C65 - C66	= 1.375(5)
C65 - Br1	= 1.891(4)	C66 - H66	= 0.95

S6.5. Angles [°].

N4	- Zn1	- N1	= 89.48(10)
N4	- Zn1	- N2	= 163.53(10)
N1	- Zn1	- N2	= 89.16(10)
N4	- Zn1	- N3	= 88.67(10)
N1	- Zn1	- N3	= 166.66(10)
N2	- Zn1	- N3	= 88.88(10)
N4	- Zn1	- N61	= 97.03(10)
N1	- Zn1	- N61	= 96.99(10)
N2	- Zn1	- N61	= 99.42(10)
N3	- Zn1	- N61	= 96.35(10)
C1	- N1	- C18	= 106.7(2)
C1	- N1	- Zn1	= 127.1(2)
C18	- N1	- Zn1	= 126.1(2)
C3	- N2	- C6	= 106.4(2)
C3	- N2	- Zn1	= 126.7(2)
C6	- N2	- Zn1	= 126.7(2)
C8	- N3	- C11	= 106.7(2)
C8	- N3	- Zn1	= 125.5(2)
C11	- N3	- Zn1	= 125.4(2)
C13	- N4	- C16	= 106.3(2)
C13	- N4	- Zn1	= 126.8(2)
C16	- N4	- Zn1	= 126.7(2)
N1	- C1	- C2	= 125.3(3)
N1	- C1	- C20	= 109.8(3)
C2	- C1	- C20	= 124.7(3)
C3	- C2	- C1	= 125.4(3)
C3	- C2	- C21	= 117.2(3)
C1	- C2	- C21	= 117.3(3)
N2	- C3	- C2	= 125.6(3)
N2	- C3	- C4	= 109.9(3)
C2	- C3	- C4	= 124.6(3)
C5	- C4	- C3	= 107.4(3)
C5	- C4	- H4	= 126.3
C3	- C4	- H4	= 126.3
C4	- C5	- C6	= 106.5(3)
C4	- C5	- H5	= 126.7
C6	- C5	- H5	= 126.7
N2	- C6	- C7	= 125.4(3)
N2	- C6	- C5	= 109.7(3)
C7	- C6	- C5	= 124.9(3)
C8	- C7	- C6	= 125.2(3)
C8	- C7	- C31	= 116.4(3)
C6	- C7	- C31	= 118.4(3)
N3	- C8	- C7	= 125.9(3)
N3	- C8	- C9	= 109.6(3)
C7	- C8	- C9	= 124.5(3)
C10	- C9	- C8	= 107.3(3)
C10	- C9	- H9	= 126.4

C8	- C9	- H9	= 126.4
C9	- C10	- C11	= 106.7(3)
C9	- C10	- H10	= 126.7
C11	- C10	- H10	= 126.7
N3	- C11	- C12	= 125.5(3)
N3	- C11	- C10	= 109.8(3)
C12	- C11	- C10	= 124.7(3)
C11	- C12	- C13	= 125.0(3)
C11	- C12	- C41	= 118.2(3)
C13	- C12	- C41	= 116.8(3)
N4	- C13	- C12	= 125.4(3)
N4	- C13	- C14	= 110.5(3)
C12	- C13	- C14	= 124.0(3)
C15	- C14	- C13	= 107.1(3)
C15	- C14	- H14	= 126.5
C13	- C14	- H14	= 126.5
C14	- C15	- C16	= 106.9(3)
C14	- C15	- H15	= 126.5
C16	- C15	- H15	= 126.5
N4	- C16	- C17	= 125.6(3)
N4	- C16	- C15	= 109.1(3)
C17	- C16	- C15	= 125.3(3)
C18	- C17	- C16	= 125.5(3)
C18	- C17	- C51	= 117.6(3)
C16	- C17	- C51	= 116.8(3)
N1	- C18	- C17	= 126.1(3)
N1	- C18	- C19	= 109.1(3)
C17	- C18	- C19	= 124.7(3)
C20	- C19	- C18	= 107.5(3)
C20	- C19	- H19	= 126.3
C18	- C19	- H19	= 126.3
C19	- C20	- C1	= 106.9(3)
C19	- C20	- H20	= 126.5
C1	- C20	- H20	= 126.5
C26	- C21	- C22	= 117.5(3)
C26	- C21	- C2	= 122.4(3)
C22	- C21	- C2	= 120.1(3)
C23	- C22	- C21	= 121.6(3)
C23	- C22	- H22	= 119.2
C21	- C22	- H22	= 119.2
C22	- C23	- C24	= 119.2(4)
C22	- C23	- H23	= 120.4
C24	- C23	- H23	= 120.4
C25	- C24	- C23	= 120.7(3)
C25	- C24	- H24	= 119.7
C23	- C24	- H24	= 119.7
C24	- C25	- C26	= 119.1(4)
C24	- C25	- H25	= 120.5
C26	- C25	- H25	= 120.5
C21	- C26	- C25	= 122.0(4)

C21	- C26	- H26	= 119
C25	- C26	- H26	= 119
C36	- C31	- C32	= 118.6(3)
C36	- C31	- C7	= 118.9(3)
C32	- C31	- C7	= 122.5(3)
C33	- C32	- C31	= 121.1(3)
C33	- C32	- H32	= 119.5
C31	- C32	- H32	= 119.5
C34	- C33	- C32	= 119.7(3)
C34	- C33	- H33	= 120.1
C32	- C33	- H33	= 120.1
C35	- C34	- C33	= 120.5(3)
C35	- C34	- H34	= 119.8
C33	- C34	- H34	= 119.8
C34	- C35	- C36	= 119.8(4)
C34	- C35	- H35	= 120.1
C36	- C35	- H35	= 120.1
C31	- C36	- C35	= 120.3(3)
C31	- C36	- H36	= 119.8
C35	- C36	- H36	= 119.8
C42	- C41	- C46	= 118.9(3)
C42	- C41	- C12	= 120.8(3)
C46	- C41	- C12	= 120.3(3)
C41	- C42	- C43	= 121.0(3)
C41	- C42	- H42	= 119.5
C43	- C42	- H42	= 119.5
C44	- C43	- C42	= 119.5(3)
C44	- C43	- H43	= 120.3
C42	- C43	- H43	= 120.3
C43	- C44	- C45	= 119.8(3)
C43	- C44	- H44	= 120.1
C45	- C44	- H44	= 120.1
C46	- C45	- C44	= 119.5(3)
C46	- C45	- H45	= 120.3
C44	- C45	- H45	= 120.3
C41	- C46	- C45	= 121.3(3)
C41	- C46	- H46	= 119.4
C45	- C46	- H46	= 119.4
C56	- C51	- C52	= 119.1(3)
C56	- C51	- C17	= 120.4(3)
C52	- C51	- C17	= 120.5(3)
C51	- C52	- C53	= 120.4(4)
C51	- C52	- H52	= 119.8
C53	- C52	- H52	= 119.8
C52	- C53	- C54	= 120.0(4)
C52	- C53	- H53	= 120
C54	- C53	- H53	= 120
C55	- C54	- C53	= 119.7(3)
C55	- C54	- H54	= 120.2
C53	- C54	- H54	= 120.2

C54	- C55	- C56	= 120.4(4)
C54	- C55	- H55	= 119.8
C56	- C55	- H55	= 119.8
C51	- C56	- C55	= 120.3(4)
C51	- C56	- H56	= 119.8
C55	- C56	- H56	= 119.8
C66	- N61	- C62	= 117.8(3)
C66	- N61	- Zn1	= 121.0(2)
C62	- N61	- Zn1	= 121.1(2)
N61	- C62	- C63	= 123.0(3)
N61	- C62	- H62	= 118.5
C63	- C62	- H62	= 118.5
C64	- C63	- C62	= 118.6(3)
C64	- C63	- H63	= 120.7
C62	- C63	- H63	= 120.7
C63	- C64	- C65	= 118.3(3)
C63	- C64	- H64	= 120.9
C65	- C64	- H64	= 120.9
C66	- C65	- C64	= 120.7(3)
C66	- C65	- Br1	= 118.8(3)
C64	- C65	- Br1	= 120.4(3)
N61	- C66	- C65	= 121.5(3)
N61	- C66	- H66	= 119.2
C65	- C66	- H66	= 119.2

S6.6. Torsion angles [°].

N4	- Zn1	- N1	- C1	= -169.9(3)
N2	- Zn1	- N1	- C1	= -6.3(3)
N3	- Zn1	- N1	- C1	= -87.9(5)
N61	- Zn1	- N1	- C1	= 93.0(3)
N4	- Zn1	- N1	- C18	= 5.7(3)
N2	- Zn1	- N1	- C18	= 169.3(3)
N3	- Zn1	- N1	- C18	= 87.7(5)
N61	- Zn1	- N1	- C18	= -91.3(3)
N4	- Zn1	- N2	- C3	= 93.3(4)
N1	- Zn1	- N2	- C3	= 8.0(3)
N3	- Zn1	- N2	- C3	= 174.8(3)
N61	- Zn1	- N2	- C3	= -89.0(3)
N4	- Zn1	- N2	- C6	= -92.8(4)
N1	- Zn1	- N2	- C6	= -178.1(3)
N3	- Zn1	- N2	- C6	= -11.3(3)
N61	- Zn1	- N2	- C6	= 85.0(3)
N4	- Zn1	- N3	- C8	= -179.2(3)
N1	- Zn1	- N3	- C8	= 98.6(5)
N2	- Zn1	- N3	- C8	= 17.0(3)
N61	- Zn1	- N3	- C8	= -82.3(3)
N4	- Zn1	- N3	- C11	= -19.2(2)
N1	- Zn1	- N3	- C11	= -101.3(4)
N2	- Zn1	- N3	- C11	= 177.1(2)

N61	- Zn1	- N3	- C11	= 77.7(3)
N1	- Zn1	- N4	- C13	= 178.8(3)
N2	- Zn1	- N4	- C13	= 93.6(4)
N3	- Zn1	- N4	- C13	= 12.0(3)
N61	- Zn1	- N4	- C13	= -84.2(3)
N1	- Zn1	- N4	- C16	= -6.3(3)
N2	- Zn1	- N4	- C16	= -91.6(4)
N3	- Zn1	- N4	- C16	= -173.1(3)
N61	- Zn1	- N4	- C16	= 90.7(3)
C18	- N1	- C1	- C2	= -174.4(3)
Zn1	- N1	- C1	- C2	= 2.0(5)
C18	- N1	- C1	- C20	= 1.2(4)
Zn1	- N1	- C1	- C20	= 177.5(2)
N1	- C1	- C2	- C3	= 4.0(5)
C20	- C1	- C2	- C3	= -170.9(3)
N1	- C1	- C2	- C21	= -179.0(3)
C20	- C1	- C2	- C21	= 6.1(5)
C6	- N2	- C3	- C2	= 179.6(3)
Zn1	- N2	- C3	- C2	= -5.5(4)
C6	- N2	- C3	- C4	= -1.6(3)
Zn1	- N2	- C3	- C4	= 173.3(2)
C1	- C2	- C3	- N2	= -2.1(5)
C21	- C2	- C3	- N2	= -179.1(3)
C1	- C2	- C3	- C4	= 179.2(3)
C21	- C2	- C3	- C4	= 2.3(5)
N2	- C3	- C4	- C5	= 2.1(4)
C2	- C3	- C4	- C5	= -179.1(3)
C3	- C4	- C5	- C6	= -1.7(4)
C3	- N2	- C6	- C7	= -179.9(3)
Zn1	- N2	- C6	- C7	= 5.2(4)
C3	- N2	- C6	- C5	= 0.6(3)
Zn1	- N2	- C6	- C5	= -174.4(2)
C4	- C5	- C6	- N2	= 0.8(4)
C4	- C5	- C6	- C7	= -178.8(3)
N2	- C6	- C7	- C8	= 0.7(5)
C5	- C6	- C7	- C8	= -179.9(3)
N2	- C6	- C7	- C31	= 179.4(3)
C5	- C6	- C7	- C31	= -1.1(5)
C11	- N3	- C8	- C7	= 179.1(3)
Zn1	- N3	- C8	- C7	= -17.8(5)
C11	- N3	- C8	- C9	= -2.0(4)
Zn1	- N3	- C8	- C9	= 161.1(2)
C6	- C7	- C8	- N3	= 6.2(5)
C31	- C7	- C8	- N3	= -172.6(3)
C6	- C7	- C8	- C9	= -172.5(3)
C31	- C7	- C8	- C9	= 8.7(5)
N3	- C8	- C9	- C10	= 1.0(4)
C7	- C8	- C9	- C10	= 179.9(3)
C8	- C9	- C10	- C11	= 0.3(4)
C8	- N3	- C11	- C12	= -179.5(3)

Zn1	- N3	- C11	- C12	= 17.3(4)
C8	- N3	- C11	- C10	= 2.2(4)
Zn1	- N3	- C11	- C10	= -160.9(2)
C9	- C10	- C11	- N3	= -1.6(4)
C9	- C10	- C11	- C12	= -179.9(3)
N3	- C11	- C12	- C13	= -0.7(5)
C10	- C11	- C12	- C13	= 177.3(3)
N3	- C11	- C12	- C41	= 179.9(3)
C10	- C11	- C12	- C41	= -2.2(5)
C16	- N4	- C13	- C12	= -177.5(3)
Zn1	- N4	- C13	- C12	= -1.8(4)
C16	- N4	- C13	- C14	= 2.1(4)
Zn1	- N4	- C13	- C14	= 177.8(2)
C11	- C12	- C13	- N4	= -7.7(5)
C41	- C12	- C13	- N4	= 171.7(3)
C11	- C12	- C13	- C14	= 172.7(3)
C41	- C12	- C13	- C14	= -7.9(5)
N4	- C13	- C14	- C15	= -2.2(4)
C12	- C13	- C14	- C15	= 177.4(3)
C13	- C14	- C15	- C16	= 1.3(4)
C13	- N4	- C16	- C17	= 178.6(3)
Zn1	- N4	- C16	- C17	= 2.9(4)
C13	- N4	- C16	- C15	= -1.2(3)
Zn1	- N4	- C16	- C15	= -177.0(2)
C14	- C15	- C16	- N4	= -0.1(4)
C14	- C15	- C16	- C17	= -179.9(3)
N4	- C16	- C17	- C18	= 4.1(5)
C15	- C16	- C17	- C18	= -176.1(3)
N4	- C16	- C17	- C51	= -177.5(3)
C15	- C16	- C17	- C51	= 2.3(5)
C1	- N1	- C18	- C17	= 174.7(3)
Zn1	- N1	- C18	- C17	= -1.7(5)
C1	- N1	- C18	- C19	= -1.2(4)
Zn1	- N1	- C18	- C19	= -177.6(2)
C16	- C17	- C18	- N1	= -4.7(5)
C51	- C17	- C18	- N1	= 176.9(3)
C16	- C17	- C18	- C19	= 170.5(3)
C51	- C17	- C18	- C19	= -7.9(5)
N1	- C18	- C19	- C20	= 0.7(4)
C17	- C18	- C19	- C20	= -175.2(3)
C18	- C19	- C20	- C1	= 0.0(4)
N1	- C1	- C20	- C19	= -0.7(4)
C2	- C1	- C20	- C19	= 174.9(3)
C3	- C2	- C21	- C26	= 64.1(4)
C1	- C2	- C21	- C26	= -113.1(4)
C3	- C2	- C21	- C22	= -115.6(3)
C1	- C2	- C21	- C22	= 67.2(4)
C26	- C21	- C22	- C23	= -1.1(5)
C2	- C21	- C22	- C23	= 178.6(3)
C21	- C22	- C23	- C24	= 0.6(5)

C22	- C23	- C24	- C25	= -0.2(6)
C23	- C24	- C25	- C26	= 0.3(6)
C22	- C21	- C26	- C25	= 1.2(5)
C2	- C21	- C26	- C25	= -178.5(3)
C24	- C25	- C26	- C21	= -0.8(5)
C8	- C7	- C31	- C36	= 61.6(4)
C6	- C7	- C31	- C36	= -117.3(3)
C8	- C7	- C31	- C32	= -115.6(3)
C6	- C7	- C31	- C32	= 65.5(4)
C36	- C31	- C32	- C33	= 0.1(5)
C7	- C31	- C32	- C33	= 177.3(3)
C31	- C32	- C33	- C34	= -0.2(5)
C32	- C33	- C34	- C35	= -0.9(5)
C33	- C34	- C35	- C36	= 2.0(5)
C32	- C31	- C36	- C35	= 1.0(5)
C7	- C31	- C36	- C35	= -176.3(3)
C34	- C35	- C36	- C31	= -2.1(5)
C11	- C12	- C41	- C42	= -60.3(4)
C13	- C12	- C41	- C42	= 120.2(3)
C11	- C12	- C41	- C46	= 119.0(3)
C13	- C12	- C41	- C46	= -60.5(4)
C46	- C41	- C42	- C43	= -0.2(5)
C12	- C41	- C42	- C43	= 179.2(3)
C41	- C42	- C43	- C44	= 0.4(5)
C42	- C43	- C44	- C45	= 0.1(5)
C43	- C44	- C45	- C46	= -0.8(5)
C42	- C41	- C46	- C45	= -0.6(5)
C12	- C41	- C46	- C45	= -179.9(3)
C44	- C45	- C46	- C41	= 1.0(5)
C18	- C17	- C51	- C56	= -66.6(4)
C16	- C17	- C51	- C56	= 114.9(4)
C18	- C17	- C51	- C52	= 114.7(4)
C16	- C17	- C51	- C52	= -63.8(4)
C56	- C51	- C52	- C53	= -2.1(5)
C17	- C51	- C52	- C53	= 176.6(3)
C51	- C52	- C53	- C54	= 2.5(5)
C52	- C53	- C54	- C55	= -0.8(6)
C53	- C54	- C55	- C56	= -1.1(5)
C52	- C51	- C56	- C55	= 0.1(5)
C17	- C51	- C56	- C55	= -178.6(3)
C54	- C55	- C56	- C51	= 1.5(5)
N4	- Zn1	- N61	- C66	= 68.5(2)
N1	- Zn1	- N61	- C66	= 158.8(2)
N2	- Zn1	- N61	- C66	= -110.9(2)
N3	- Zn1	- N61	- C66	= -21.0(2)
N4	- Zn1	- N61	- C62	= -110.0(3)
N1	- Zn1	- N61	- C62	= -19.7(3)
N2	- Zn1	- N61	- C62	= 70.6(3)
N3	- Zn1	- N61	- C62	= 160.5(2)
C66	- N61	- C62	- C63	= 0.9(5)

Zn1	- N61	- C62	- C63	= 179.5(3)
N61	- C62	- C63	- C64	= 0.2(5)
C62	- C63	- C64	- C65	= -1.0(5)
C63	- C64	- C65	- C66	= 0.8(5)
C63	- C64	- C65	- Br1	= 178.7(3)
C62	- N61	- C66	- C65	= -1.2(5)
Zn1	- N61	- C66	- C65	= -179.7(2)
C64	- C65	- C66	- N61	= 0.3(5)
Br1	- C65	- C66	- N61	= -177.6(2)

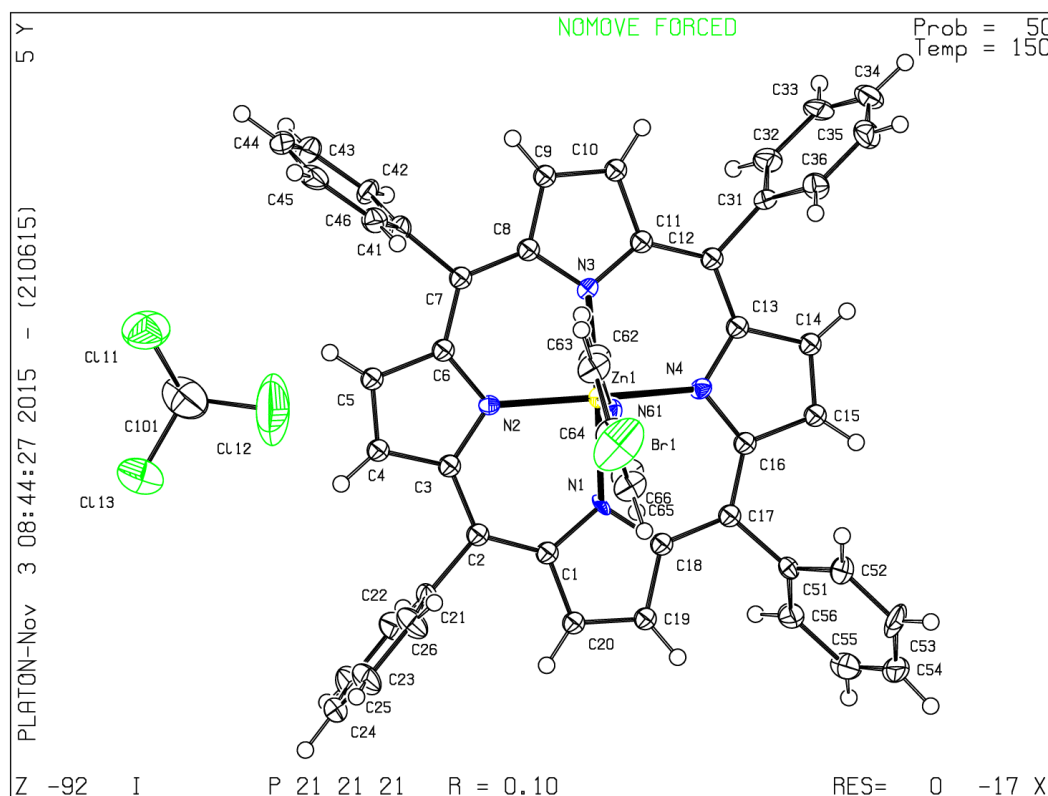
S7. X-ray crystallographic data for 6•A (CCDC-1509181).

(C₄₉ H₃₂ Br N₅ Zn, C H Cl₃); $M = 955.44$. D8 VENTURE Bruker AXS diffractometer [*], Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$), $T = 150 \text{ K}$; Orthorhombic $P 2_1 2_1 2_1$ (I.T.#19), $a = 17.5294(12)$, $b = 25.3204(17)$, $c = 9.8855(7) \text{ \AA}$, $V = 4387.7(5) \text{ \AA}^3$. $Z = 4$, $d = 1.446 \text{ g.cm}^{-3}$, $\mu = 1.695 \text{ mm}^{-1}$. The structure was solved by direct methods using the *SIR97* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [2]. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 10044 unique intensities and 403 parameters converged at $\omega R(F^2) = 0.2670$ ($R(F) = 0.1038$) for 8853 observed reflections with $I > 2\sigma(I)$.

[1] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, *J. Appl. Cryst.* (1999) 32, 115-119

[2] Sheldrick G.M., *Acta Cryst. A*64 (2008), 112-122

[*] Thanks to FEDER funds



S7.1. Structural data.

Empirical formula	C ₅₀ H ₃₃ Br Cl ₃ N ₅ Zn
Extended formula	C ₄₉ H ₃₂ Br N ₅ Zn, C H Cl ₃
Formula weight	955.44
Temperature	150 K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, <i>P</i> 2 ₁ 2 ₁ 2 ₁
Unit cell dimensions	a = 17.5294(12) Å, α = 90 ° b = 25.3204(17) Å, β = 90 ° c = 9.8855(7) Å, γ = 90 °
Volume	4387.7(5) Å ³
Z, Calculated density	4, 1.446 (g.cm ⁻³)
Absorption coefficient	1.695 mm ⁻¹
<i>F</i> (000)	1936
Crystal size	0.550 x 0.280 x 0.210 mm
Crystal color	blue
Theta range for data collection	3.106 to 27.537 °
h_min, h_max	-21, 22
k_min, k_max	-32, 32
l_min, l_max	-12, 12
Reflections collected / unique	85295 / 10044 [R(int) ^a = 0.1146]
Reflections [I > 2σ]	8853
Completeness to theta_max	0.993
Absorption correction type	multi-scan
Max. and min. transmission	0.701, 0.322
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	10044 / 0 / 403
Flack parameter	0.487(6)
^b Goodness-of-fit	1.080
Final <i>R</i> indices [I > 2σ]	<i>R</i> ^c = 0.1038, <i>wR</i> ^d = 0.2670
<i>R</i> indices (all data)	<i>R</i> ^c = 0.1160, <i>wR</i> ^d = 0.2752
Largest diff. peak and hole	2.452 and -2.465 e ⁻ .Å ⁻³
^a <i>R</i> _{int} = ∑ <i>F</i> _o ² - < <i>F</i> _o ² > / ∑ [<i>F</i> _o ²]	
^b <i>S</i> = {∑ [w(<i>F</i> _o ² - <i>F</i> _c ²) ²] / (n - p)} ^{1/2}	
^c <i>R</i> ₁ = ∑ <i>F</i> _o - <i>F</i> _c / ∑ <i>F</i> _o	
^d <i>wR</i> ₂ = {∑ [w(<i>F</i> _o ² - <i>F</i> _c ²) ²] / ∑ [w(<i>F</i> _o ²) ²]} ^{1/2}	
<i>w</i> = 1 / [σ(<i>F</i> _o ²) + a <i>P</i> ² + b <i>P</i>] where <i>P</i> = [2 <i>F</i> _c ² + MAX(<i>F</i> _o ² , 0)] / 3	

S7.2. Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters (Å²). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
Zn1	0.10005(7)	0.16933(5)	0.79038(12)	1	0.0123(3)
Br1	0.08231(15)	0.23293(10)	1.45171(17)	1	0.0699(8)
N1	-0.0174(5)	0.1664(4)	0.7642(9)	1	0.0146(18)
N2	0.0969(6)	0.2492(4)	0.7492(9)	1	0.0152(18)
N3	0.2162(5)	0.1701(4)	0.7549(8)	1	0.0130(17)
N4	0.1023(6)	0.0879(3)	0.7813(10)	1	0.0165(18)

C1	-0.0658(7)	0.2095(5)	0.7609(12)	1	0.0187(5)
C2	-0.0420(7)	0.2618(5)	0.7515(12)	1	0.0187(5)
C3	0.0336(7)	0.2810(5)	0.7427(12)	1	0.0187(5)
C4	0.0544(6)	0.3343(5)	0.7278(12)	1	0.0187(5)
H4	0.0204	0.3634	0.7228	1	0.022
C5	0.1316(6)	0.3364(5)	0.7220(12)	1	0.0187(5)
H5	0.1621	0.3671	0.7106	1	0.022
C6	0.1585(7)	0.2820(5)	0.7367(12)	1	0.0187(5)
C7	0.2352(7)	0.2661(5)	0.7329(12)	1	0.0187(5)
C8	0.2617(7)	0.2140(5)	0.7444(12)	1	0.0187(5)
C9	0.3398(7)	0.1989(5)	0.7414(12)	1	0.0187(5)
H9	0.3823	0.2219	0.7334	1	0.022
C10	0.3422(7)	0.1449(5)	0.7523(12)	1	0.0187(5)
H10	0.3864	0.1232	0.7536	1	0.022
C11	0.2637(7)	0.1278(5)	0.7615(12)	1	0.0187(5)
C12	0.2413(7)	0.0747(5)	0.7722(13)	1	0.0187(5)
C13	0.1661(7)	0.0576(5)	0.7802(13)	1	0.0187(5)
C14	0.1433(6)	0.0022(5)	0.7857(14)	1	0.0187(5)
H14	0.1765	-0.0275	0.7848	1	0.022
C15	0.0664(6)	0.0009(4)	0.7921(14)	1	0.0187(5)
H15	0.0350	-0.0296	0.7972	1	0.022
C16	0.0409(6)	0.0560(5)	0.7897(14)	1	0.0187(5)
C17	-0.0358(6)	0.0709(5)	0.7983(14)	1	0.0187(5)
C18	-0.0625(6)	0.1232(4)	0.7867(13)	1	0.0187(5)
C19	-0.1412(6)	0.1395(4)	0.7996(13)	1	0.0187(5)
H19	-0.1838	0.1176	0.8189	1	0.022
C20	-0.1421(7)	0.1928(5)	0.7785(13)	1	0.0187(5)
H20	-0.1861	0.2147	0.7761	1	0.022
C21	-0.1045(8)	0.3028(4)	0.7473(12)	1	0.020(2)
C22	-0.1273(8)	0.3286(6)	0.8640(15)	1	0.032(3)
H22	-0.1025	0.3207	0.9470	1	0.038
C23	-0.1848(9)	0.3653(6)	0.8624(16)	1	0.032(3)
H23	-0.1989	0.3833	0.9429	1	0.039
C24	-0.2223(8)	0.3759(6)	0.7407(18)	1	0.035(4)
H24	-0.2635	0.4002	0.7384	1	0.042
C25	-0.1993(9)	0.3508(6)	0.6245(17)	1	0.036(3)
H25	-0.2237	0.3587	0.5411	1	0.043
C26	-0.1416(8)	0.3147(6)	0.6281(13)	1	0.028(3)
H26	-0.1266	0.2975	0.5469	1	0.034
C31	0.3020(6)	0.0322(5)	0.7789(13)	1	0.018(2)
C32	0.3380(8)	0.0156(6)	0.6627(16)	1	0.029(3)
H32	0.3269	0.0327	0.5795	1	0.035
C33	0.3894(8)	-0.0253(6)	0.6644(18)	1	0.036(4)
H33	0.4134	-0.0362	0.5830	1	0.043
C34	0.4062(8)	-0.0504(5)	0.7853(19)	1	0.036(3)
H34	0.4410	-0.0792	0.7867	1	0.043
C35	0.3721(8)	-0.0335(6)	0.9043(17)	1	0.032(3)
H35	0.3850	-0.0496	0.9881	1	0.038
C36	0.3193(8)	0.0069(5)	0.8997(14)	1	0.024(3)
H36	0.2944	0.0176	0.9805	1	0.029

C41	0.2922(7)	0.3097(4)	0.7169(14)	1	0.019(2)
C42	0.3273(7)	0.3197(5)	0.5960(14)	1	0.022(3)
H42	0.3187	0.2967	0.5216	1	0.026
C43	0.3753(8)	0.3628(6)	0.5800(17)	1	0.034(3)
H43	0.3979	0.3695	0.4944	1	0.041
C44	0.3902(8)	0.3956(6)	0.685(2)	1	0.039(4)
H44	0.4236	0.4247	0.6730	1	0.047
C45	0.3572(7)	0.3868(5)	0.8096(19)	1	0.034(4)
H45	0.3674	0.4101	0.8828	1	0.041
C46	0.3079(8)	0.3428(5)	0.8280(15)	1	0.026(3)
H46	0.2858	0.3358	0.9139	1	0.031
C51	-0.0947(7)	0.0296(4)	0.8261(12)	1	0.019(2)
C52	-0.0942(8)	0.0027(5)	0.9477(13)	1	0.024(2)
H52	-0.0539	0.0091	1.0099	1	0.029
C53	-0.1505(10)	-0.0334(6)	0.9821(19)	1	0.041(4)
H53	-0.1496	-0.0508	1.0672	1	0.049
C54	-0.2080(8)	-0.0434(5)	0.8901(19)	1	0.035(4)
H54	-0.2483	-0.0667	0.9136	1	0.042
C55	-0.2074(8)	-0.0197(6)	0.764(2)	1	0.038(4)
H55	-0.2449	-0.0288	0.6989	1	0.046
C56	-0.1509(7)	0.0180(5)	0.7326(17)	1	0.030(3)
H56	-0.1514	0.0354	0.6475	1	0.036
N61	0.0958(6)	0.1842(4)	1.0058(10)	1	0.0181(19)
C62	0.1553(9)	0.2037(6)	1.0664(14)	1	0.0303(13)
H62	0.2018	0.2067	1.0175	1	0.036
C63	0.1532(8)	0.2201(6)	1.1982(15)	1	0.0303(13)
H63	0.1975	0.2339	1.2408	1	0.036
C64	0.0853(8)	0.2162(6)	1.2674(13)	1	0.0303(13)
C65	0.0236(8)	0.1959(6)	1.2044(15)	1	0.0303(13)
H65	-0.0232	0.1915	1.2514	1	0.036
C66	0.0301(8)	0.1816(6)	1.0697(14)	1	0.0303(13)
H66	-0.0139	0.1698	1.0223	1	0.036
C101	0.0882(13)	0.4014(9)	0.042(3)	1	0.070(7)
H101	0.0985	0.3898	-0.0533	1	0.085
C111	0.1667(3)	0.4365(3)	0.0956(7)	1	0.0711(16)
C112	0.0747(8)	0.3450(4)	0.138(2)	1	0.227(9)
C113	0.0066(3)	0.4381(3)	0.0395(8)	1	0.0783(18)

S7.3. Anisotropic displacement parameters (\AA^2).

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

Atom	U11	U22	U33	U23	U13	U12
Zn1	0.0146(5)	0.0124(5)	0.0097(5)	-0.0001(5)	-0.0004(5)	-0.0002(5)
Br1	0.0999(18)	0.0901(16)	0.0196(7)	-0.0204(9)	0.0138(9)	-0.0374(14)
N1	0.014(4)	0.013(4)	0.017(5)	0.003(4)	-0.008(3)	0.006(4)
N2	0.013(4)	0.016(4)	0.016(4)	0.000(3)	-0.003(4)	-0.001(4)
N3	0.016(4)	0.015(4)	0.007(4)	-0.003(4)	0.003(3)	-0.002(4)
N4	0.015(4)	0.015(4)	0.019(4)	-0.004(4)	0.000(5)	-0.003(4)

C1	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C2	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C3	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C4	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C5	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C6	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C7	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C8	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C9	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C10	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C11	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C12	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C13	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C14	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C15	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C16	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C17	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C18	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C19	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C20	0.0176(12)	0.0176(12)	0.0208(13)	-0.0007(10)	-0.0006(11)	-0.0005(10)
C21	0.023(6)	0.015(5)	0.023(6)	0.001(4)	0.007(5)	0.004(5)
C22	0.037(7)	0.028(7)	0.030(7)	-0.012(6)	-0.002(6)	0.014(6)
C23	0.037(8)	0.022(7)	0.037(8)	-0.012(6)	-0.001(6)	0.011(6)
C24	0.023(7)	0.021(6)	0.062(11)	0.009(6)	0.007(6)	0.004(5)
C25	0.037(8)	0.036(8)	0.036(8)	0.016(7)	-0.013(7)	0.003(6)
C26	0.030(7)	0.039(8)	0.015(6)	0.007(5)	0.002(5)	0.008(6)
C31	0.014(5)	0.020(5)	0.022(6)	0.001(5)	0.000(5)	-0.002(4)
C32	0.023(7)	0.029(7)	0.036(8)	-0.003(6)	0.008(6)	0.003(6)
C33	0.019(7)	0.030(7)	0.059(10)	-0.004(6)	0.017(6)	0.009(6)
C34	0.020(6)	0.023(6)	0.065(10)	-0.007(7)	-0.006(8)	0.006(5)
C35	0.028(7)	0.026(7)	0.042(8)	0.004(6)	-0.013(6)	0.002(6)
C36	0.027(7)	0.024(6)	0.022(6)	-0.002(5)	0.006(5)	0.004(5)
C41	0.021(6)	0.014(5)	0.022(6)	-0.004(5)	-0.002(5)	-0.001(4)
C42	0.023(6)	0.017(6)	0.027(6)	0.000(5)	0.009(5)	-0.004(5)
C43	0.026(7)	0.034(8)	0.043(9)	0.018(7)	0.006(6)	-0.001(6)
C44	0.016(6)	0.026(6)	0.076(12)	0.015(7)	-0.015(7)	-0.006(5)
C45	0.020(6)	0.022(6)	0.060(11)	-0.012(7)	-0.015(7)	0.002(5)
C46	0.023(6)	0.021(6)	0.035(8)	-0.004(5)	0.000(5)	0.001(5)
C51	0.019(5)	0.013(5)	0.024(6)	-0.002(4)	0.003(5)	0.004(5)
C52	0.028(6)	0.019(5)	0.026(6)	-0.001(5)	0.000(6)	-0.003(5)
C53	0.046(9)	0.017(6)	0.059(11)	0.003(7)	0.036(8)	-0.006(6)
C54	0.024(7)	0.018(6)	0.064(11)	-0.008(7)	0.007(7)	-0.003(5)
C55	0.024(7)	0.021(6)	0.070(12)	-0.018(7)	-0.008(7)	0.000(5)
C56	0.022(6)	0.023(6)	0.045(9)	0.000(6)	-0.007(6)	-0.001(5)
N61	0.020(5)	0.013(4)	0.021(5)	-0.001(3)	0.001(4)	-0.001(4)
C62	0.032(3)	0.040(4)	0.018(3)	-0.001(3)	-0.001(2)	-0.006(3)
C63	0.032(3)	0.040(4)	0.018(3)	-0.001(3)	-0.001(2)	-0.006(3)
C64	0.032(3)	0.040(4)	0.018(3)	-0.001(3)	-0.001(2)	-0.006(3)
C65	0.032(3)	0.040(4)	0.018(3)	-0.001(3)	-0.001(2)	-0.006(3)
C66	0.032(3)	0.040(4)	0.018(3)	-0.001(3)	-0.001(2)	-0.006(3)

C101	0.062(14)	0.059(12)	0.091(17)	-0.027(12)	-0.029(13)	0.008(11)
C111	0.050(3)	0.092(4)	0.071(4)	0.007(3)	-0.017(3)	-0.007(3)
C112	0.172(11)	0.094(7)	0.41(3)	0.144(11)	-0.096(13)	-0.035(7)
C113	0.048(3)	0.080(4)	0.107(5)	0.008(4)	-0.008(3)	0.013(3)

S7.4. Bond lengths [Å].

Zn1 - N4	= 2.063(9)	Zn1 - N2	= 2.064(9)
Zn1 - N3	= 2.066(9)	Zn1 - N1	= 2.076(9)
Zn1 - N61	= 2.164(10)	Br1 - C64	= 1.872(13)
N1 - C18	= 1.369(15)	N1 - C1	= 1.383(15)
N2 - C6	= 1.368(15)	N2 - C3	= 1.371(15)
N3 - C11	= 1.358(15)	N3 - C8	= 1.372(15)
N4 - C16	= 1.348(14)	N4 - C13	= 1.357(15)
C1 - C2	= 1.393(16)	C1 - C20	= 1.415(16)
C2 - C3	= 1.414(16)	C2 - C21	= 1.509(17)
C3 - C4	= 1.404(17)	C4 - C5	= 1.356(15)
C4 - H4	= 0.9500	C5 - C6	= 1.464(16)
C5 - H5	= 0.9500	C6 - C7	= 1.404(16)
C7 - C8	= 1.403(17)	C7 - C41	= 1.498(16)
C8 - C9	= 1.421(17)	C9 - C10	= 1.372(16)
C9 - H9	= 0.9500	C10 - C11	= 1.445(17)
C10 - H10	= 0.9500	C11 - C12	= 1.406(16)
C12 - C13	= 1.389(16)	C12 - C31	= 1.514(16)
C13 - C14	= 1.461(16)	C14 - C15	= 1.351(15)
C14 - H14	= 0.9500	C15 - C16	= 1.465(15)
C15 - H15	= 0.9500	C16 - C17	= 1.399(16)
C17 - C18	= 1.408(16)	C17 - C51	= 1.494(16)
C18 - C19	= 1.447(15)	C19 - C20	= 1.364(16)
C19 - H19	= 0.9500	C20 - H20	= 0.9500
C21 - C26	= 1.379(18)	C21 - C22	= 1.385(17)
C22 - C23	= 1.371(19)	C22 - H22	= 0.9500
C23 - C24	= 1.40(2)	C23 - H23	= 0.9500
C24 - C25	= 1.37(2)	C24 - H24	= 0.9500
C25 - C26	= 1.36(2)	C25 - H25	= 0.9500
C26 - H26	= 0.9500	C31 - C32	= 1.377(19)
C31 - C36	= 1.388(19)	C32 - C33	= 1.37(2)
C32 - H32	= 0.9500	C33 - C34	= 1.39(2)
C33 - H33	= 0.9500	C34 - C35	= 1.39(2)
C34 - H34	= 0.9500	C35 - C36	= 1.380(19)
C35 - H35	= 0.9500	C36 - H36	= 0.9500
C41 - C42	= 1.367(18)	C41 - C46	= 1.408(18)
C42 - C43	= 1.387(19)	C42 - H42	= 0.9500
C43 - C44	= 1.36(2)	C43 - H43	= 0.9500
C44 - C45	= 1.38(3)	C44 - H44	= 0.9500
C45 - C46	= 1.423(19)	C45 - H45	= 0.9500
C46 - H46	= 0.9500	C51 - C52	= 1.382(17)
C51 - C56	= 1.382(19)	C52 - C53	= 1.388(18)
C52 - H52	= 0.9500	C53 - C54	= 1.38(3)
C53 - H53	= 0.9500	C54 - C55	= 1.38(3)

C54 - H54 = 0.9500
 C55 - H55 = 0.9500
 N61 - C62 = 1.301(18)
 C62 - C63 = 1.37(2)
 C63 - C64 = 1.376(19)
 C64 - C65 = 1.350(19)
 C65 - H65 = 0.9500
 C101 - C113 = 1.71(2)
 C101 - C112 = 1.73(3)

C55 - C56 = 1.41(2)
 C56 - H56 = 0.9500
 N61 - C66 = 1.316(17)
 C62 - H62 = 0.9500
 C63 - H63 = 0.9500
 C65 - C66 = 1.38(2)
 C66 - H66 = 0.9500
 C101 - C111 = 1.72(2)
 C101 - H101 = 1.0000

S7.5. Angles [°].

N4 - Zn1 - N2 = 166.1(4)
 N4 - Zn1 - N3 = 89.1(4)
 N2 - Zn1 - N3 = 89.0(4)
 N4 - Zn1 - N1 = 88.7(4)
 N2 - Zn1 - N1 = 89.1(4)
 N3 - Zn1 - N1 = 163.0(3)
 N4 - Zn1 - N61 = 102.5(4)
 N2 - Zn1 - N61 = 91.3(3)
 N3 - Zn1 - N61 = 101.5(4)
 N1 - Zn1 - N61 = 95.5(4)
 C18 - N1 - C1 = 106.3(9)
 C18 - N1 - Zn1 = 125.5(7)
 C1 - N1 - Zn1 = 125.7(8)
 C6 - N2 - C3 = 106.1(9)
 C6 - N2 - Zn1 = 126.3(8)
 C3 - N2 - Zn1 = 127.3(8)
 C11 - N3 - C8 = 106.6(9)
 C11 - N3 - Zn1 = 126.0(8)
 C8 - N3 - Zn1 = 126.5(8)
 C16 - N4 - C13 = 108.6(9)
 C16 - N4 - Zn1 = 125.5(8)
 C13 - N4 - Zn1 = 125.5(8)
 N1 - C1 - C2 = 124.6(11)
 N1 - C1 - C20 = 110.0(10)
 C2 - C1 - C20 = 125.3(11)
 C1 - C2 - C3 = 127.7(11)
 C1 - C2 - C21 = 115.9(11)
 C3 - C2 - C21 = 116.3(11)
 N2 - C3 - C4 = 111.1(10)
 N2 - C3 - C2 = 123.6(11)
 C4 - C3 - C2 = 125.3(11)
 C5 - C4 - C3 = 107.6(11)
 C5 - C4 - H4 = 126.2
 C3 - C4 - H4 = 126.2
 C4 - C5 - C6 = 106.2(11)
 C4 - C5 - H5 = 126.9
 C6 - C5 - H5 = 126.9
 N2 - C6 - C7 = 125.8(11)

N2	- C6	- C5	= 109.0(10)
C7	- C6	- C5	= 125.2(11)
C8	- C7	- C6	= 125.8(11)
C8	- C7	- C41	= 118.7(10)
C6	- C7	- C41	= 115.5(10)
N3	- C8	- C7	= 125.1(11)
N3	- C8	- C9	= 110.1(10)
C7	- C8	- C9	= 124.8(11)
C10	- C9	- C8	= 107.3(11)
C10	- C9	- H9	= 126.4
C8	- C9	- H9	= 126.4
C9	- C10	- C11	= 105.9(11)
C9	- C10	- H10	= 127.1
C11	- C10	- H10	= 127.1
N3	- C11	- C12	= 126.0(11)
N3	- C11	- C10	= 110.2(10)
C12	- C11	- C10	= 123.8(11)
C13	- C12	- C11	= 124.5(11)
C13	- C12	- C31	= 116.3(10)
C11	- C12	- C31	= 119.2(10)
N4	- C13	- C12	= 127.4(11)
N4	- C13	- C14	= 108.5(10)
C12	- C13	- C14	= 124.1(10)
C15	- C14	- C13	= 107.3(10)
C15	- C14	- H14	= 126.4
C13	- C14	- H14	= 126.4
C14	- C15	- C16	= 106.4(10)
C14	- C15	- H15	= 126.8
C16	- C15	- H15	= 126.8
N4	- C16	- C17	= 127.5(11)
N4	- C16	- C15	= 109.1(10)
C17	- C16	- C15	= 123.3(10)
C16	- C17	- C18	= 124.5(11)
C16	- C17	- C51	= 119.1(10)
C18	- C17	- C51	= 116.3(10)
N1	- C18	- C17	= 125.0(10)
N1	- C18	- C19	= 109.6(10)
C17	- C18	- C19	= 125.3(10)
C20	- C19	- C18	= 106.3(10)
C20	- C19	- H19	= 126.9
C18	- C19	- H19	= 126.9
C19	- C20	- C1	= 107.7(11)
C19	- C20	- H20	= 126.2
C1	- C20	- H20	= 126.2
C26	- C21	- C22	= 118.2(12)
C26	- C21	- C2	= 121.1(11)
C22	- C21	- C2	= 120.7(11)
C23	- C22	- C21	= 121.5(14)
C23	- C22	- H22	= 119.3
C21	- C22	- H22	= 119.3

C22 - C23 - C24 = 119.1(14)
C22 - C23 - H23 = 120.4
C24 - C23 - H23 = 120.4
C25 - C24 - C23 = 119.5(13)
C25 - C24 - H24 = 120.2
C23 - C24 - H24 = 120.2
C26 - C25 - C24 = 120.5(14)
C26 - C25 - H25 = 119.8
C24 - C25 - H25 = 119.8
C25 - C26 - C21 = 121.2(13)
C25 - C26 - H26 = 119.4
C21 - C26 - H26 = 119.4
C32 - C31 - C36 = 118.5(11)
C32 - C31 - C12 = 120.1(12)
C36 - C31 - C12 = 121.3(11)
C33 - C32 - C31 = 121.4(15)
C33 - C32 - H32 = 119.3
C31 - C32 - H32 = 119.3
C32 - C33 - C34 = 119.8(14)
C32 - C33 - H33 = 120.1
C34 - C33 - H33 = 120.1
C33 - C34 - C35 = 119.9(12)
C33 - C34 - H34 = 120.1
C35 - C34 - H34 = 120.1
C36 - C35 - C34 = 119.3(14)
C36 - C35 - H35 = 120.4
C34 - C35 - H35 = 120.4
C35 - C36 - C31 = 121.1(13)
C35 - C36 - H36 = 119.4
C31 - C36 - H36 = 119.4
C42 - C41 - C46 = 119.0(11)
C42 - C41 - C7 = 121.9(11)
C46 - C41 - C7 = 119.0(12)
C41 - C42 - C43 = 121.2(13)
C41 - C42 - H42 = 119.4
C43 - C42 - H42 = 119.4
C44 - C43 - C42 = 120.8(14)
C44 - C43 - H43 = 119.6
C42 - C43 - H43 = 119.6
C43 - C44 - C45 = 120.4(13)
C43 - C44 - H44 = 119.8
C45 - C44 - H44 = 119.8
C44 - C45 - C46 = 119.7(14)
C44 - C45 - H45 = 120.1
C46 - C45 - H45 = 120.1
C41 - C46 - C45 = 119.0(14)
C41 - C46 - H46 = 120.5
C45 - C46 - H46 = 120.5
C52 - C51 - C56 = 118.8(12)
C52 - C51 - C17 = 120.0(12)

C56	- C51	- C17	= 121.2(11)
C51	- C52	- C53	= 122.2(14)
C51	- C52	- H52	= 118.9
C53	- C52	- H52	= 118.9
C54	- C53	- C52	= 118.6(16)
C54	- C53	- H53	= 120.7
C52	- C53	- H53	= 120.7
C55	- C54	- C53	= 120.5(13)
C55	- C54	- H54	= 119.7
C53	- C54	- H54	= 119.7
C54	- C55	- C56	= 119.9(14)
C54	- C55	- H55	= 120.1
C56	- C55	- H55	= 120.1
C51	- C56	- C55	= 119.8(15)
C51	- C56	- H56	= 120.1
C55	- C56	- H56	= 120.1
C62	- N61	- C66	= 120.0(11)
C62	- N61	- Zn1	= 119.5(9)
C66	- N61	- Zn1	= 119.6(9)
N61	- C62	- C63	= 122.2(14)
N61	- C62	- H62	= 118.9
C63	- C62	- H62	= 118.9
C62	- C63	- C64	= 118.4(13)
C62	- C63	- H63	= 120.8
C64	- C63	- H63	= 120.8
C65	- C64	- C63	= 119.4(13)
C65	- C64	- Br1	= 120.8(11)
C63	- C64	- Br1	= 119.5(10)
C64	- C65	- C66	= 118.5(13)
C64	- C65	- H65	= 120.7
C66	- C65	- H65	= 120.7
N61	- C66	- C65	= 121.4(13)
N61	- C66	- H66	= 119.3
C65	- C66	- H66	= 119.3
Cl13	- C101	- Cl11	= 113.1(12)
Cl13	- C101	- Cl12	= 109.9(16)
Cl11	- C101	- Cl12	= 111.5(14)
Cl13	- C101	- H101	= 107.4
Cl11	- C101	- H101	= 107.4
Cl12	- C101	- H101	= 107.4

S7.6. Torsion angles [°].

C18	- N1	- C1	- C2	= 174.3(12)
Zn1	- N1	- C1	- C2	= 11.5(17)
C18	- N1	- C1	- C20	= -1.3(13)
Zn1	- N1	- C1	- C20	= -164.1(8)
N1	- C1	- C2	- C3	= 1(2)
C20	- C1	- C2	- C3	= 175.5(12)
N1	- C1	- C2	- C21	= 179.1(10)

C20	- C1	- C2	- C21	= -6.0(19)
C6	- N2	- C3	- C4	= -0.8(12)
Zn1	- N2	- C3	- C4	= 173.2(8)
C6	- N2	- C3	- C2	= 179.9(12)
Zn1	- N2	- C3	- C2	= -6.2(16)
C1	- C2	- C3	- N2	= -4(2)
C21	- C2	- C3	- N2	= 177.9(10)
C1	- C2	- C3	- C4	= 177.2(12)
C21	- C2	- C3	- C4	= -1.3(18)
N2	- C3	- C4	- C5	= 1.2(15)
C2	- C3	- C4	- C5	= -179.4(12)
C3	- C4	- C5	- C6	= -1.1(15)
C3	- N2	- C6	- C7	= -177.5(12)
Zn1	- N2	- C6	- C7	= 8.5(17)
C3	- N2	- C6	- C5	= 0.0(12)
Zn1	- N2	- C6	- C5	= -174.0(8)
C4	- C5	- C6	- N2	= 0.7(14)
C4	- C5	- C6	- C7	= 178.3(12)
N2	- C6	- C7	- C8	= -2(2)
C5	- C6	- C7	- C8	= -178.8(12)
N2	- C6	- C7	- C41	= 179.3(11)
C5	- C6	- C7	- C41	= 2.1(18)
C11	- N3	- C8	- C7	= 178.9(12)
Zn1	- N3	- C8	- C7	= -11.6(17)
C11	- N3	- C8	- C9	= 1.3(13)
Zn1	- N3	- C8	- C9	= 170.7(7)
C6	- C7	- C8	- N3	= 3(2)
C41	- C7	- C8	- N3	= -177.6(11)
C6	- C7	- C8	- C9	= -179.4(12)
C41	- C7	- C8	- C9	= -0.3(19)
N3	- C8	- C9	- C10	= -0.9(14)
C7	- C8	- C9	- C10	= -178.6(12)
C8	- C9	- C10	- C11	= 0.2(14)
C8	- N3	- C11	- C12	= -179.6(12)
Zn1	- N3	- C11	- C12	= 10.9(17)
C8	- N3	- C11	- C10	= -1.1(12)
Zn1	- N3	- C11	- C10	= -170.7(7)
C9	- C10	- C11	- N3	= 0.6(14)
C9	- C10	- C11	- C12	= 179.1(12)
N3	- C11	- C12	- C13	= -1(2)
C10	- C11	- C12	- C13	= -179.6(12)
N3	- C11	- C12	- C31	= -179.8(11)
C10	- C11	- C12	- C31	= 1.9(19)
C16	- N4	- C13	- C12	= 179.8(14)
Zn1	- N4	- C13	- C12	= -6.5(19)
C16	- N4	- C13	- C14	= 1.2(14)
Zn1	- N4	- C13	- C14	= 174.9(8)
C11	- C12	- C13	- N4	= -1(2)
C31	- C12	- C13	- N4	= 177.5(12)
C11	- C12	- C13	- C14	= 177.4(12)

C31	- C12	- C13	- C14	= -4.1(19)
N4	- C13	- C14	- C15	= -1.0(16)
C12	- C13	- C14	- C15	= -179.6(13)
C13	- C14	- C15	- C16	= 0.4(16)
C13	- N4	- C16	- C17	= 177.6(14)
Zn1	- N4	- C16	- C17	= 4(2)
C13	- N4	- C16	- C15	= -1.0(14)
Zn1	- N4	- C16	- C15	= -174.6(8)
C14	- C15	- C16	- N4	= 0.3(16)
C14	- C15	- C16	- C17	= -178.3(13)
N4	- C16	- C17	- C18	= 6(2)
C15	- C16	- C17	- C18	= -175.3(13)
N4	- C16	- C17	- C51	= -171.6(12)
C15	- C16	- C17	- C51	= 7(2)
C1	- N1	- C18	- C17	= -179.5(12)
Zn1	- N1	- C18	- C17	= -16.6(18)
C1	- N1	- C18	- C19	= -0.7(14)
Zn1	- N1	- C18	- C19	= 162.1(8)
C16	- C17	- C18	- N1	= 1(2)
C51	- C17	- C18	- N1	= 178.6(11)
C16	- C17	- C18	- C19	= -177.9(13)
C51	- C17	- C18	- C19	= 0(2)
N1	- C18	- C19	- C20	= 2.6(15)
C17	- C18	- C19	- C20	= -178.7(13)
C18	- C19	- C20	- C1	= -3.3(15)
N1	- C1	- C20	- C19	= 3.0(15)
C2	- C1	- C20	- C19	= -172.6(12)
C1	- C2	- C21	- C26	= -82.4(16)
C3	- C2	- C21	- C26	= 96.3(15)
C1	- C2	- C21	- C22	= 96.3(15)
C3	- C2	- C21	- C22	= -85.0(16)
C26	- C21	- C22	- C23	= 0(2)
C2	- C21	- C22	- C23	= -179.0(14)
C21	- C22	- C23	- C24	= 2(2)
C22	- C23	- C24	- C25	= -2(2)
C23	- C24	- C25	- C26	= 2(2)
C24	- C25	- C26	- C21	= -1(2)
C22	- C21	- C26	- C25	= 0(2)
C2	- C21	- C26	- C25	= 178.5(13)
C13	- C12	- C31	- C32	= 102.3(15)
C11	- C12	- C31	- C32	= -79.1(16)
C13	- C12	- C31	- C36	= -73.7(16)
C11	- C12	- C31	- C36	= 104.9(14)
C36	- C31	- C32	- C33	= 1(2)
C12	- C31	- C32	- C33	= -175.6(13)
C31	- C32	- C33	- C34	= 0(2)
C32	- C33	- C34	- C35	= -1(2)
C33	- C34	- C35	- C36	= 3(2)
C34	- C35	- C36	- C31	= -3(2)
C32	- C31	- C36	- C35	= 1(2)

C12	- C31	- C36	- C35	= 177.0(12)
C8	- C7	- C41	- C42	= 77.7(16)
C6	- C7	- C41	- C42	= -103.1(14)
C8	- C7	- C41	- C46	= -105.0(14)
C6	- C7	- C41	- C46	= 74.2(15)
C46	- C41	- C42	- C43	= -3(2)
C7	- C41	- C42	- C43	= 174.7(12)
C41	- C42	- C43	- C44	= 2(2)
C42	- C43	- C44	- C45	= -1(2)
C43	- C44	- C45	- C46	= 1(2)
C42	- C41	- C46	- C45	= 2.5(19)
C7	- C41	- C46	- C45	= -174.9(11)
C44	- C45	- C46	- C41	= -1.6(19)
C16	- C17	- C51	- C52	= 64.2(17)
C18	- C17	- C51	- C52	= -113.9(14)
C16	- C17	- C51	- C56	= -116.7(15)
C18	- C17	- C51	- C56	= 65.2(16)
C56	- C51	- C52	- C53	= -4(2)
C17	- C51	- C52	- C53	= 175.6(12)
C51	- C52	- C53	- C54	= 1(2)
C52	- C53	- C54	- C55	= 3(2)
C53	- C54	- C55	- C56	= -5(2)
C52	- C51	- C56	- C55	= 1.6(19)
C17	- C51	- C56	- C55	= -177.5(12)
C54	- C55	- C56	- C51	= 2(2)
C66	- N61	- C62	- C63	= 3(2)
Zn1	- N61	- C62	- C63	= 171.6(11)
N61	- C62	- C63	- C64	= -1(2)
C62	- C63	- C64	- C65	= 1(2)
C62	- C63	- C64	- Br1	= 174.9(12)
C63	- C64	- C65	- C66	= -2(2)
Br1	- C64	- C65	- C66	= -176.7(11)
C62	- N61	- C66	- C65	= -5(2)
Zn1	- N61	- C66	- C65	= -173.5(11)
C64	- C65	- C66	- N61	= 5(2)

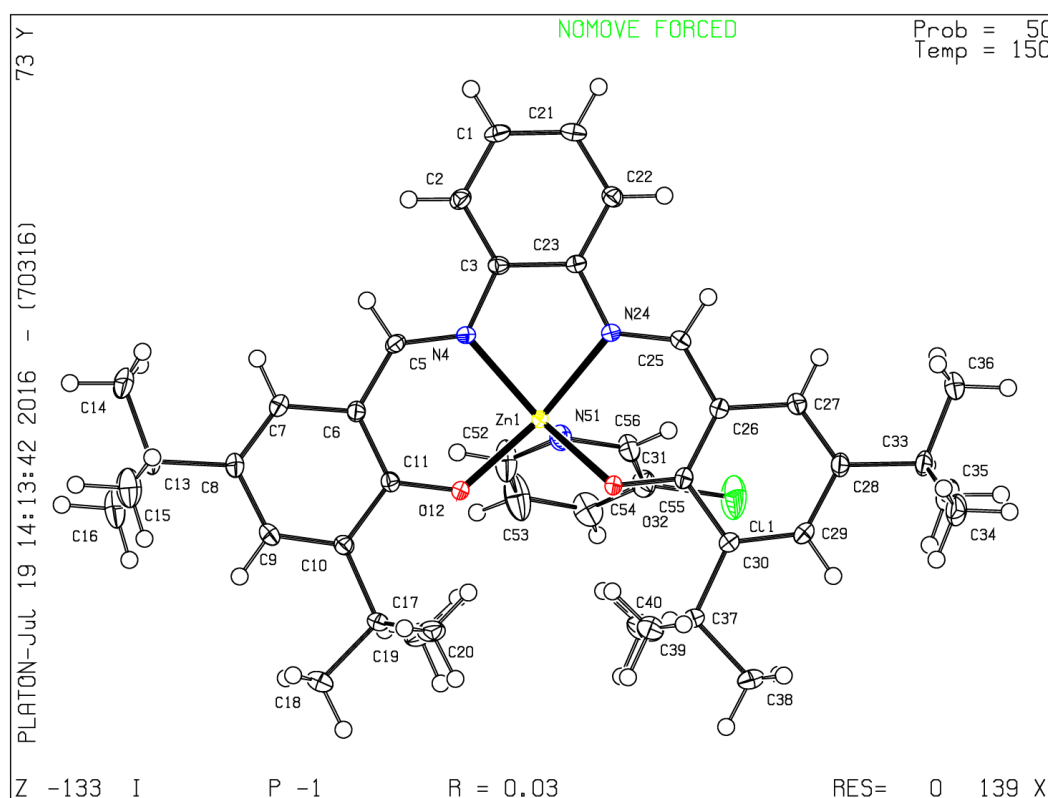
S8. X-ray crystallographic data for 2•B (CCDC-1509182).

(C₄₁ H₅₀ Cl N₃ O₂ Zn); $M = 717.66$. D8 VENTURE Bruker AXS diffractometer [*], Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$), $T = 150 \text{ K}$; triclinic $P -1$ (I.T.#2), $a = 11.6664(12)$, $b = 12.7373(13)$, $c = 13.0304(14) \text{ \AA}$, $\alpha = 92.131(4)$, $\beta = 100.274(4)$, $\gamma = 91.827(4)^\circ$, $V = 1902.5(3) \text{ \AA}^3$. $Z = 2$, $d = 1.253 \text{ g.cm}^{-3}$, $\mu = 0.753 \text{ mm}^{-1}$. The structure was solved by dual-space algorithm using the *SHELXT* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-2014*) [2]. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 8696 unique intensities and 445 parameters converged at $\omega R(F^2) = 0.0700$ ($R(F) = 0.0284$) for 7833 observed reflections with $I > 2\sigma(I)$.

[1] G. M. Sheldrick, Acta Cryst. A71 (2015) 3-8

[2] Sheldrick G.M., Acta Cryst. C71 (2015) 3-8

[*] Thanks to FEDER funds



S8.1. Structural data.

Empirical formula	C ₄₁ H ₅₀ Cl N ₃ O ₂ Zn
Formula weight	717.66
Temperature	150 K
Wavelength	0.71073 Å
Crystal system, space group	triclinic, <i>P</i> -1
Unit cell dimensions	a = 11.6664(12) Å, α = 92.131(4) ° b = 12.7373(13) Å, β = 100.274(4) ° c = 13.0304(14) Å, γ = 91.827(4) °
Volume	1902.5(3) Å ³
Z, Calculated density	2, 1.253 (g.cm ⁻³)
Absorption coefficient	0.753 mm ⁻¹
<i>F</i> (000)	760
Crystal size	0.480 x 0.340 x 0.290 mm
Crystal color	orange
Theta range for data collection	2.970 to 27.485 °
h_min, h_max	-15, 15
k_min, k_max	-16, 16
l_min, l_max	-16, 16
Reflections collected / unique	41378 / 8696 [R(int) ^a = 0.0358]
Reflections [I>2σ]	7833
Completeness to theta_max	0.999
Absorption correction type	multi-scan
Max. and min. transmission	0.804 , 0.762
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	8696 / 0 / 445
^b Goodness-of-fit	1.039
Final <i>R</i> indices [I>2σ]	<i>R</i> 1 ^c = 0.0284, <i>wR</i> 2 ^d = 0.0700
<i>R</i> indices (all data)	<i>R</i> 1 ^c = 0.0340, <i>wR</i> 2 ^d = 0.0731
Largest diff. peak and hole	0.676 and -0.532 e ⁻ .Å ⁻³
^a <i>R</i> _{int} = ∑ <i>F</i> _o ² - < <i>F</i> _o ² > / ∑ [<i>F</i> _o ²]	
^b <i>S</i> = {∑ [w(<i>F</i> _o ² - <i>F</i> _c ²) ²] / (n - p)} ^{1/2}	
^c <i>R</i> 1 = ∑ <i>F</i> _o - <i>F</i> _c / ∑ [<i>F</i> _o]	
^d <i>wR</i> 2 = {∑ [w(<i>F</i> _o ² - <i>F</i> _c ²) ²] / ∑ [w(<i>F</i> _o ²) ²]} ^{1/2}	
w = 1 / [σ(<i>F</i> _o ²) + a <i>P</i> ² + b <i>P</i>] where <i>P</i> = [2 <i>F</i> _c ² + MAX(<i>F</i> _o ² , 0)] / 3	

S8.2. Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters (Å²). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
Zn1	0.78131(2)	0.35870(2)	0.46497(2)	1	0.01265(5)
C1	0.95030(12)	0.75075(11)	0.54655(11)	1	0.0178(3)
H1	0.9875	0.8098	0.5872	1	0.021
C2	0.93998(12)	0.65544(11)	0.59250(11)	1	0.0158(3)
H2	0.9692	0.6499	0.6649	1	0.019
C3	0.88699(11)	0.56709(10)	0.53362(10)	1	0.0128(2)
N4	0.87018(10)	0.46718(8)	0.57366(9)	1	0.0127(2)
C5	0.90632(12)	0.44805(10)	0.67134(10)	1	0.0141(3)

H5	0.9393	0.5062	0.7158	1	0.017
C6	0.90178(12)	0.34879(10)	0.71898(10)	1	0.0138(3)
C7	0.95610(12)	0.34772(11)	0.82581(11)	1	0.0176(3)
H7	0.9845	0.4123	0.8615	1	0.021
C8	0.96878(13)	0.25686(11)	0.87898(11)	1	0.0182(3)
C9	0.92294(13)	0.16263(11)	0.82293(11)	1	0.0179(3)
H9	0.9321	0.0988	0.8585	1	0.022
C10	0.86602(12)	0.15727(10)	0.72039(10)	1	0.0147(3)
C11	0.85499(11)	0.25294(10)	0.66422(10)	1	0.0128(2)
O12	0.80472(9)	0.24910(7)	0.56717(7)	1	0.0161(2)
C13	1.02984(14)	0.25198(12)	0.99317(11)	1	0.0238(3)
C14	1.0617(2)	0.36200(15)	1.04341(14)	1	0.0457(5)
H14A	1.0954	0.3563	1.1174	1	0.068
H14B	0.9914	0.4032	1.0371	1	0.068
H14C	1.1187	0.3970	1.0079	1	0.068
C15	1.14086(16)	0.19000(17)	0.99776(14)	1	0.0377(4)
H15A	1.1203	0.1183	0.9690	1	0.056
H15B	1.1807	0.1875	1.0705	1	0.056
H15C	1.1926	0.2246	0.9567	1	0.056
C16	0.94875(17)	0.19788(16)	1.05742(13)	1	0.0366(4)
H16A	0.9299	0.1256	1.0298	1	0.055
H16B	0.8768	0.2365	1.0530	1	0.055
H16C	0.9878	0.1970	1.1305	1	0.055
C17	0.81380(13)	0.05304(11)	0.66539(11)	1	0.0181(3)
C18	0.83396(18)	-0.03911(12)	0.73809(13)	1	0.0335(4)
H18A	0.7967	-0.0259	0.7988	1	0.050
H18B	0.9179	-0.0462	0.7615	1	0.050
H18C	0.8002	-0.1041	0.7005	1	0.050
C19	0.68127(14)	0.06043(13)	0.62996(13)	1	0.0261(3)
H19A	0.6490	-0.0062	0.5949	1	0.039
H19B	0.6657	0.1174	0.5815	1	0.039
H19C	0.6448	0.0748	0.6909	1	0.039
C20	0.87040(15)	0.02682(11)	0.57008(12)	1	0.0238(3)
H20A	0.9534	0.0148	0.5934	1	0.036
H20B	0.8619	0.0856	0.5232	1	0.036
H20C	0.8320	-0.0367	0.5329	1	0.036
C21	0.90631(12)	0.76030(11)	0.44088(11)	1	0.0174(3)
H21	0.9111	0.8264	0.4102	1	0.021
C22	0.85566(12)	0.67366(11)	0.38045(11)	1	0.0157(3)
H22	0.8262	0.6806	0.3083	1	0.019
C23	0.84743(11)	0.57594(10)	0.42464(10)	1	0.0126(2)
N24	0.80274(10)	0.48207(9)	0.36856(9)	1	0.0133(2)
C25	0.77653(12)	0.47498(10)	0.26694(10)	1	0.0153(3)
H25	0.7886	0.5365	0.2306	1	0.018
C26	0.73096(12)	0.38230(10)	0.20518(10)	1	0.0148(3)
C27	0.68638(12)	0.39671(11)	0.09777(10)	1	0.0166(3)
H27	0.6944	0.4642	0.0707	1	0.020
C28	0.63234(12)	0.31634(11)	0.03234(10)	1	0.0168(3)
C29	0.62540(13)	0.21646(11)	0.07590(11)	1	0.0182(3)
H29	0.5864	0.1604	0.0319	1	0.022

C30	0.67131(12)	0.19483(11)	0.17779(11)	1	0.0166(3)
C31	0.72653(12)	0.27982(11)	0.24689(10)	1	0.0146(3)
O32	0.76917(9)	0.26157(7)	0.34322(7)	1	0.0180(2)
C33	0.57701(14)	0.32861(11)	-0.08241(11)	1	0.0199(3)
C34	0.62735(15)	0.24839(13)	-0.15168(12)	1	0.0271(3)
H34A	0.6150	0.1774	-0.1282	1	0.041
H34B	0.7110	0.2638	-0.1467	1	0.041
H34C	0.5880	0.2529	-0.2243	1	0.041
C35	0.44466(14)	0.30815(14)	-0.09531(12)	1	0.0276(3)
H35A	0.4285	0.2370	-0.0740	1	0.041
H35B	0.4087	0.3149	-0.1686	1	0.041
H35C	0.4123	0.3595	-0.0516	1	0.041
C36	0.60020(18)	0.43858(13)	-0.11946(12)	1	0.0319(4)
H36A	0.5672	0.4416	-0.1939	1	0.048
H36B	0.6845	0.4539	-0.1086	1	0.048
H36C	0.5638	0.4906	-0.0796	1	0.048
C37	0.66324(15)	0.08398(11)	0.21936(12)	1	0.0242(3)
C38	0.5994(2)	0.00506(14)	0.13483(15)	1	0.0446(5)
H38A	0.6414	0.0017	0.0761	1	0.067
H38B	0.5200	0.0277	0.1105	1	0.067
H38C	0.5961	-0.0646	0.1639	1	0.067
C39	0.59519(17)	0.08513(14)	0.31051(14)	1	0.0349(4)
H39A	0.5885	0.0137	0.3349	1	0.052
H39B	0.5171	0.1110	0.2867	1	0.052
H39C	0.6367	0.1314	0.3679	1	0.052
C40	0.78635(17)	0.04407(13)	0.25591(13)	1	0.0316(4)
H40A	0.8283	0.0417	0.1971	1	0.047
H40B	0.7804	-0.0266	0.2822	1	0.047
H40C	0.8287	0.0917	0.3117	1	0.047
N51	0.59863(11)	0.36793(10)	0.46988(10)	1	0.0196(2)
C52	0.56135(15)	0.34184(16)	0.55691(13)	1	0.0334(4)
H52	0.6157	0.3442	0.6207	1	0.040
C53	0.44683(15)	0.31155(19)	0.55804(14)	1	0.0416(5)
H53	0.4234	0.2935	0.6215	1	0.050
C54	0.36671(14)	0.30773(14)	0.46592(13)	1	0.0290(4)
H54	0.2879	0.2854	0.4640	1	0.035
C55	0.40511(13)	0.33732(12)	0.37724(12)	1	0.0223(3)
C56	0.52071(13)	0.36722(12)	0.38116(12)	1	0.0214(3)
H56	0.5455	0.3879	0.3191	1	0.026
Cl1	0.31064(4)	0.33458(5)	0.25887(4)	1	0.04440(13)

S8.3. Anisotropic displacement parameters (\AA^2).

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

Atom	U11	U22	U33	U23	U13	U12
Zn1	0.01563(8)	0.01105(8)	0.00992(8)	0.00067(5)	-0.00086(5)	-0.00238(5)

C1	0.0162(6)	0.0116(6)	0.0242(7)	-0.0028(5)	0.0015(5)	-0.0028(5)
C2	0.0144(6)	0.0149(6)	0.0164(6)	-0.0018(5)	-0.0010(5)	-0.0006(5)
C3	0.0119(6)	0.0109(6)	0.0157(6)	0.0003(5)	0.0023(5)	0.0011(5)
N4	0.0143(5)	0.0100(5)	0.0131(5)	0.0003(4)	0.0011(4)	-0.0003(4)
C5	0.0150(6)	0.0124(6)	0.0140(6)	-0.0024(5)	0.0005(5)	-0.0006(5)
C6	0.0154(6)	0.0145(6)	0.0113(6)	0.0003(5)	0.0014(5)	0.0013(5)
C7	0.0201(7)	0.0173(7)	0.0135(6)	-0.0014(5)	-0.0014(5)	-0.0010(5)
C8	0.0201(7)	0.0203(7)	0.0128(6)	0.0021(5)	-0.0010(5)	0.0016(5)
C9	0.0220(7)	0.0156(6)	0.0160(6)	0.0050(5)	0.0016(5)	0.0023(5)
C10	0.0181(6)	0.0130(6)	0.0135(6)	0.0014(5)	0.0040(5)	0.0008(5)
C11	0.0135(6)	0.0136(6)	0.0117(6)	0.0011(5)	0.0026(5)	0.0016(5)
O12	0.0231(5)	0.0122(4)	0.0111(4)	0.0005(3)	-0.0013(4)	-0.0019(4)
C13	0.0296(8)	0.0241(8)	0.0143(7)	0.0040(6)	-0.0059(6)	0.0025(6)
C14	0.0720(15)	0.0314(10)	0.0219(8)	-0.0004(7)	-0.0225(9)	-0.0006(9)
C15	0.0292(9)	0.0529(12)	0.0276(9)	0.0080(8)	-0.0064(7)	0.0091(8)
C16	0.0418(10)	0.0518(11)	0.0155(7)	0.0093(7)	0.0012(7)	0.0043(9)
C17	0.0268(7)	0.0117(6)	0.0157(6)	0.0023(5)	0.0035(6)	-0.0024(5)
C18	0.0567(12)	0.0158(7)	0.0253(8)	0.0061(6)	0.0003(8)	-0.0059(7)
C19	0.0253(8)	0.0233(8)	0.0291(8)	-0.0039(6)	0.0054(6)	-0.0082(6)
C20	0.0345(9)	0.0140(7)	0.0241(7)	-0.0031(6)	0.0090(6)	0.0002(6)
C21	0.0183(7)	0.0112(6)	0.0237(7)	0.0023(5)	0.0059(5)	-0.0016(5)
C22	0.0177(6)	0.0146(6)	0.0153(6)	0.0021(5)	0.0039(5)	0.0003(5)
C23	0.0123(6)	0.0108(6)	0.0144(6)	-0.0004(5)	0.0022(5)	-0.0005(5)
N24	0.0161(5)	0.0107(5)	0.0126(5)	0.0000(4)	0.0011(4)	-0.0011(4)
C25	0.0187(7)	0.0127(6)	0.0146(6)	0.0027(5)	0.0027(5)	-0.0006(5)
C26	0.0175(6)	0.0141(6)	0.0123(6)	0.0002(5)	0.0017(5)	-0.0004(5)
C27	0.0216(7)	0.0155(6)	0.0127(6)	0.0017(5)	0.0028(5)	0.0008(5)
C28	0.0201(7)	0.0187(7)	0.0110(6)	0.0003(5)	0.0007(5)	0.0031(5)
C29	0.0225(7)	0.0161(7)	0.0142(6)	-0.0031(5)	-0.0005(5)	-0.0016(5)
C30	0.0209(7)	0.0137(6)	0.0141(6)	-0.0005(5)	0.0007(5)	-0.0015(5)
C31	0.0167(6)	0.0156(6)	0.0111(6)	-0.0003(5)	0.0018(5)	0.0004(5)
O32	0.0278(5)	0.0128(4)	0.0111(4)	0.0007(4)	-0.0026(4)	-0.0012(4)
C33	0.0278(8)	0.0200(7)	0.0101(6)	-0.0013(5)	-0.0018(5)	0.0044(6)
C34	0.0363(9)	0.0317(8)	0.0131(7)	-0.0018(6)	0.0029(6)	0.0092(7)
C35	0.0271(8)	0.0316(9)	0.0209(7)	-0.0036(6)	-0.0049(6)	0.0078(7)
C36	0.0516(11)	0.0257(8)	0.0150(7)	0.0042(6)	-0.0037(7)	-0.0002(7)
C37	0.0368(9)	0.0141(7)	0.0179(7)	0.0008(5)	-0.0045(6)	-0.0068(6)
C38	0.0743(15)	0.0176(8)	0.0310(9)	0.0017(7)	-0.0172(9)	-0.0162(9)
C39	0.0415(10)	0.0299(9)	0.0334(9)	0.0094(7)	0.0076(8)	-0.0131(8)
C40	0.0465(10)	0.0180(7)	0.0272(8)	0.0020(6)	-0.0027(7)	0.0064(7)
N51	0.0170(6)	0.0231(6)	0.0180(6)	0.0028(5)	0.0007(5)	0.0011(5)
C52	0.0213(8)	0.0618(12)	0.0176(7)	0.0064(8)	0.0025(6)	0.0088(8)
C53	0.0230(9)	0.0801(15)	0.0260(9)	0.0192(9)	0.0113(7)	0.0109(9)
C54	0.0159(7)	0.0402(9)	0.0329(9)	0.0093(7)	0.0075(6)	0.0041(7)
C55	0.0169(7)	0.0261(8)	0.0221(7)	0.0028(6)	-0.0018(6)	0.0018(6)
C56	0.0186(7)	0.0272(8)	0.0180(7)	0.0064(6)	0.0017(5)	-0.0003(6)
C11	0.0241(2)	0.0755(4)	0.0286(2)	0.0114(2)	-0.00851(17)	-0.0090(2)

S8.4. Bond lengths [Å].

Zn1 - O12	= 1.9570(10)	Zn1 - O32	= 1.9570(10)
Zn1 - N4	= 2.0565(11)	Zn1 - N24	= 2.0841(11)
Zn1 - N51	= 2.1504(13)	C1 - C2	= 1.3846(19)
C1 - C21	= 1.392(2)	C1 - H1	= 0.9500
C2 - C3	= 1.3998(18)	C2 - H2	= 0.9500
C3 - N4	= 1.4144(16)	C3 - C23	= 1.4225(18)
N4 - C5	= 1.3020(17)	C5 - C6	= 1.4326(18)
C5 - H5	= 0.9500	C6 - C7	= 1.4237(18)
C6 - C11	= 1.4322(18)	C7 - C8	= 1.369(2)
C7 - H7	= 0.9500	C8 - C9	= 1.419(2)
C8 - C13	= 1.5352(19)	C9 - C10	= 1.3801(19)
C9 - H9	= 0.9500	C10 - C11	= 1.4422(18)
C10 - C17	= 1.5393(19)	C11 - O12	= 1.2941(16)
C13 - C14	= 1.530(2)	C13 - C15	= 1.532(2)
C13 - C16	= 1.534(2)	C14 - H14A	= 0.9800
C14 - H14B	= 0.9800	C14 - H14C	= 0.9800
C15 - H15A	= 0.9800	C15 - H15B	= 0.9800
C15 - H15C	= 0.9800	C16 - H16A	= 0.9800
C16 - H16B	= 0.9800	C16 - H16C	= 0.9800
C17 - C18	= 1.533(2)	C17 - C20	= 1.538(2)
C17 - C19	= 1.540(2)	C18 - H18A	= 0.9800
C18 - H18B	= 0.9800	C18 - H18C	= 0.9800
C19 - H19A	= 0.9800	C19 - H19B	= 0.9800
C19 - H19C	= 0.9800	C20 - H20A	= 0.9800
C20 - H20B	= 0.9800	C20 - H20C	= 0.9800
C21 - C22	= 1.3838(19)	C21 - H21	= 0.9500
C22 - C23	= 1.3985(18)	C22 - H22	= 0.9500
C23 - N24	= 1.4123(16)	N24 - C25	= 1.3038(17)
C25 - C26	= 1.4355(18)	C25 - H25	= 0.9500
C26 - C27	= 1.4242(18)	C26 - C31	= 1.4353(18)
C27 - C28	= 1.3692(19)	C27 - H27	= 0.9500
C28 - C29	= 1.418(2)	C28 - C33	= 1.5351(18)
C29 - C30	= 1.3814(19)	C29 - H29	= 0.9500
C30 - C31	= 1.4401(18)	C30 - C37	= 1.5369(19)
C31 - O32	= 1.2975(16)	C33 - C36	= 1.530(2)
C33 - C35	= 1.536(2)	C33 - C34	= 1.537(2)
C34 - H34A	= 0.9800	C34 - H34B	= 0.9800
C34 - H34C	= 0.9800	C35 - H35A	= 0.9800
C35 - H35B	= 0.9800	C35 - H35C	= 0.9800
C36 - H36A	= 0.9800	C36 - H36B	= 0.9800
C36 - H36C	= 0.9800	C37 - C38	= 1.535(2)
C37 - C40	= 1.539(2)	C37 - C39	= 1.542(2)
C38 - H38A	= 0.9800	C38 - H38B	= 0.9800
C38 - H38C	= 0.9800	C39 - H39A	= 0.9800
C39 - H39B	= 0.9800	C39 - H39C	= 0.9800
C40 - H40A	= 0.9800	C40 - H40B	= 0.9800
C40 - H40C	= 0.9800	N51 - C52	= 1.334(2)
N51 - C56	= 1.3367(18)	C52 - C53	= 1.382(2)

C52 - H52 = 0.9500
 C53 - H53 = 0.9500
 C54 - H54 = 0.9500
 C55 - Cl1 = 1.7268(15)

C53 - C54 = 1.382(2)
 C54 - C55 = 1.373(2)
 C55 - C56 = 1.381(2)
 C56 - H56 = 0.9500

S8.5. Angles [°].

O12 - Zn1 - O32 = 94.94(4)
 O12 - Zn1 - N4 = 90.51(4)
 O32 - Zn1 - N4 = 152.82(5)
 O12 - Zn1 - N24 = 165.13(4)
 O32 - Zn1 - N24 = 88.54(4)
 N4 - Zn1 - N24 = 80.07(4)
 O12 - Zn1 - N51 = 93.49(4)
 O32 - Zn1 - N51 = 98.47(5)
 N4 - Zn1 - N51 = 107.77(5)
 N24 - Zn1 - N51 = 100.30(5)
 C2 - C1 - C21 = 120.19(13)
 C2 - C1 - H1 = 119.9
 C21 - C1 - H1 = 119.9
 C1 - C2 - C3 = 120.81(13)
 C1 - C2 - H2 = 119.6
 C3 - C2 - H2 = 119.6
 C2 - C3 - N4 = 125.05(12)
 C2 - C3 - C23 = 118.75(12)
 N4 - C3 - C23 = 116.19(11)
 C5 - N4 - C3 = 122.05(11)
 C5 - N4 - Zn1 = 124.03(9)
 C3 - N4 - Zn1 = 113.91(8)
 N4 - C5 - C6 = 127.02(12)
 N4 - C5 - H5 = 116.5
 C6 - C5 - H5 = 116.5
 C7 - C6 - C11 = 119.99(12)
 C7 - C6 - C5 = 115.62(12)
 C11 - C6 - C5 = 124.22(12)
 C8 - C7 - C6 = 122.33(13)
 C8 - C7 - H7 = 118.8
 C6 - C7 - H7 = 118.8
 C7 - C8 - C9 = 116.74(12)
 C7 - C8 - C13 = 123.92(13)
 C9 - C8 - C13 = 119.33(13)
 C10 - C9 - C8 = 124.55(13)
 C10 - C9 - H9 = 117.7
 C8 - C9 - H9 = 117.7
 C9 - C10 - C11 = 118.41(12)
 C9 - C10 - C17 = 121.99(12)
 C11 - C10 - C17 = 119.59(12)
 O12 - C11 - C6 = 122.73(12)
 O12 - C11 - C10 = 119.34(12)
 C6 - C11 - C10 = 117.93(12)

C11 - O12 - Zn1 = 131.08(9)
 C14 - C13 - C15 = 109.27(15)
 C14 - C13 - C16 = 107.10(16)
 C15 - C13 - C16 = 109.49(14)
 C14 - C13 - C8 = 111.54(13)
 C15 - C13 - C8 = 109.21(13)
 C16 - C13 - C8 = 110.20(13)
 C13 - C14 - H14A = 109.5
 C13 - C14 - H14B = 109.5
 H14A - C14 - H14B = 109.5
 C13 - C14 - H14C = 109.5
 H14A - C14 - H14C = 109.5
 H14B - C14 - H14C = 109.5
 C13 - C15 - H15A = 109.5
 C13 - C15 - H15B = 109.5
 H15A - C15 - H15B = 109.5
 C13 - C15 - H15C = 109.5
 H15A - C15 - H15C = 109.5
 H15B - C15 - H15C = 109.5
 C13 - C16 - H16A = 109.5
 C13 - C16 - H16B = 109.5
 H16A - C16 - H16B = 109.5
 C13 - C16 - H16C = 109.5
 H16A - C16 - H16C = 109.5
 H16B - C16 - H16C = 109.5
 C18 - C17 - C20 = 107.37(13)
 C18 - C17 - C10 = 111.67(12)
 C20 - C17 - C10 = 110.57(12)
 C18 - C17 - C19 = 107.58(13)
 C20 - C17 - C19 = 109.41(12)
 C10 - C17 - C19 = 110.14(12)
 C17 - C18 - H18A = 109.5
 C17 - C18 - H18B = 109.5
 H18A - C18 - H18B = 109.5
 C17 - C18 - H18C = 109.5
 H18A - C18 - H18C = 109.5
 H18B - C18 - H18C = 109.5
 C17 - C19 - H19A = 109.5
 C17 - C19 - H19B = 109.5
 H19A - C19 - H19B = 109.5
 C17 - C19 - H19C = 109.5
 H19A - C19 - H19C = 109.5
 H19B - C19 - H19C = 109.5
 C17 - C20 - H20A = 109.5
 C17 - C20 - H20B = 109.5
 H20A - C20 - H20B = 109.5
 C17 - C20 - H20C = 109.5
 H20A - C20 - H20C = 109.5
 H20B - C20 - H20C = 109.5
 C22 - C21 - C1 = 120.14(13)

C22 - C21 - H21 = 119.9
C1 - C21 - H21 = 119.9
C21 - C22 - C23 = 120.58(13)
C21 - C22 - H22 = 119.7
C23 - C22 - H22 = 119.7
C22 - C23 - N24 = 124.76(12)
C22 - C23 - C3 = 119.40(12)
N24 - C23 - C3 = 115.84(11)
C25 - N24 - C23 = 122.80(11)
C25 - N24 - Zn1 = 124.13(9)
C23 - N24 - Zn1 = 113.06(8)
N24 - C25 - C26 = 125.68(12)
N24 - C25 - H25 = 117.2
C26 - C25 - H25 = 117.2
C27 - C26 - C31 = 120.22(12)
C27 - C26 - C25 = 116.31(12)
C31 - C26 - C25 = 123.45(12)
C28 - C27 - C26 = 122.09(13)
C28 - C27 - H27 = 119.0
C26 - C27 - H27 = 119.0
C27 - C28 - C29 = 116.76(12)
C27 - C28 - C33 = 124.34(13)
C29 - C28 - C33 = 118.88(12)
C30 - C29 - C28 = 124.71(13)
C30 - C29 - H29 = 117.6
C28 - C29 - H29 = 117.6
C29 - C30 - C31 = 118.41(12)
C29 - C30 - C37 = 122.05(12)
C31 - C30 - C37 = 119.53(12)
O32 - C31 - C26 = 122.82(12)
O32 - C31 - C30 = 119.49(12)
C26 - C31 - C30 = 117.69(12)
C31 - O32 - Zn1 = 127.31(9)
C36 - C33 - C28 = 112.29(12)
C36 - C33 - C35 = 108.64(13)
C28 - C33 - C35 = 108.93(12)
C36 - C33 - C34 = 108.12(13)
C28 - C33 - C34 = 109.51(12)
C35 - C33 - C34 = 109.30(13)
C33 - C34 - H34A = 109.5
C33 - C34 - H34B = 109.5
H34A - C34 - H34B = 109.5
C33 - C34 - H34C = 109.5
H34A - C34 - H34C = 109.5
H34B - C34 - H34C = 109.5
C33 - C35 - H35A = 109.5
C33 - C35 - H35B = 109.5
H35A - C35 - H35B = 109.5
C33 - C35 - H35C = 109.5
H35A - C35 - H35C = 109.5

H35B - C35 - H35C = 109.5
C33 - C36 - H36A = 109.5
C33 - C36 - H36B = 109.5
H36A - C36 - H36B = 109.5
C33 - C36 - H36C = 109.5
H36A - C36 - H36C = 109.5
H36B - C36 - H36C = 109.5
C38 - C37 - C30 = 111.70(12)
C38 - C37 - C40 = 107.40(15)
C30 - C37 - C40 = 109.97(13)
C38 - C37 - C39 = 107.47(15)
C30 - C37 - C39 = 110.26(13)
C40 - C37 - C39 = 109.97(14)
C37 - C38 - H38A = 109.5
C37 - C38 - H38B = 109.5
H38A - C38 - H38B = 109.5
C37 - C38 - H38C = 109.5
H38A - C38 - H38C = 109.5
H38B - C38 - H38C = 109.5
C37 - C39 - H39A = 109.5
C37 - C39 - H39B = 109.5
H39A - C39 - H39B = 109.5
C37 - C39 - H39C = 109.5
H39A - C39 - H39C = 109.5
H39B - C39 - H39C = 109.5
C37 - C40 - H40A = 109.5
C37 - C40 - H40B = 109.5
H40A - C40 - H40B = 109.5
C37 - C40 - H40C = 109.5
H40A - C40 - H40C = 109.5
H40B - C40 - H40C = 109.5
C52 - N51 - C56 = 118.18(13)
C52 - N51 - Zn1 = 118.55(10)
C56 - N51 - Zn1 = 120.09(10)
N51 - C52 - C53 = 122.64(15)
N51 - C52 - H52 = 118.7
C53 - C52 - H52 = 118.7
C52 - C53 - C54 = 119.34(16)
C52 - C53 - H53 = 120.3
C54 - C53 - H53 = 120.3
C55 - C54 - C53 = 117.64(15)
C55 - C54 - H54 = 121.2
C53 - C54 - H54 = 121.2
C54 - C55 - C56 = 120.30(14)
C54 - C55 - C11 = 120.56(12)
C56 - C55 - C11 = 119.12(12)
N51 - C56 - C55 = 121.85(14)
N51 - C56 - H56 = 119.1
C55 - C56 - H56 = 119.1

S8.6. Torsion angles [°].

C21	- C1	- C2	- C3	= 0.9(2)
C1	- C2	- C3	- N4	= -178.62(13)
C1	- C2	- C3	- C23	= 2.2(2)
C2	- C3	- N4	- C5	= -1.7(2)
C23	- C3	- N4	- C5	= 177.51(12)
C2	- C3	- N4	- Zn1	= 176.93(11)
C23	- C3	- N4	- Zn1	= -3.84(14)
C3	- N4	- C5	- C6	= -175.20(12)
Zn1	- N4	- C5	- C6	= 6.3(2)
N4	- C5	- C6	- C7	= 175.04(13)
N4	- C5	- C6	- C11	= -0.1(2)
C11	- C6	- C7	- C8	= 1.9(2)
C5	- C6	- C7	- C8	= -173.52(13)
C6	- C7	- C8	- C9	= -1.2(2)
C6	- C7	- C8	- C13	= 178.20(14)
C7	- C8	- C9	- C10	= -0.9(2)
C13	- C8	- C9	- C10	= 179.72(14)
C8	- C9	- C10	- C11	= 2.1(2)
C8	- C9	- C10	- C17	= -177.42(13)
C7	- C6	- C11	- O12	= -179.98(13)
C5	- C6	- C11	- O12	= -5.0(2)
C7	- C6	- C11	- C10	= -0.58(19)
C5	- C6	- C11	- C10	= 174.40(12)
C9	- C10	- C11	- O12	= 178.12(13)
C17	- C10	- C11	- O12	= -2.33(19)
C9	- C10	- C11	- C6	= -1.30(19)
C17	- C10	- C11	- C6	= 178.25(12)
C6	- C11	- O12	- Zn1	= 3.1(2)
C10	- C11	- O12	- Zn1	= -176.31(9)
C7	- C8	- C13	- C14	= 6.6(2)
C9	- C8	- C13	- C14	= -174.01(16)
C7	- C8	- C13	- C15	= -114.23(17)
C9	- C8	- C13	- C15	= 65.11(19)
C7	- C8	- C13	- C16	= 125.47(17)
C9	- C8	- C13	- C16	= -55.19(19)
C9	- C10	- C17	- C18	= -0.1(2)
C11	- C10	- C17	- C18	= -179.67(13)
C9	- C10	- C17	- C20	= -119.63(15)
C11	- C10	- C17	- C20	= 60.84(17)
C9	- C10	- C17	- C19	= 119.32(15)
C11	- C10	- C17	- C19	= -60.21(16)
C2	- C1	- C21	- C22	= -2.2(2)
C1	- C21	- C22	- C23	= 0.4(2)
C21	- C22	- C23	- N24	= -176.65(13)
C21	- C22	- C23	- C3	= 2.8(2)
C2	- C3	- C23	- C22	= -3.99(19)
N4	- C3	- C23	- C22	= 176.73(12)
C2	- C3	- C23	- N24	= 175.47(12)

N4	- C3	- C23	- N24	= -3.81(17)
C22	- C23	- N24	- C25	= 8.0(2)
C3	- C23	- N24	- C25	= -171.43(12)
C22	- C23	- N24	- Zn1	= -171.13(11)
C3	- C23	- N24	- Zn1	= 9.44(14)
C23	- N24	- C25	- C26	= 179.97(13)
Zn1	- N24	- C25	- C26	= -1.0(2)
N24	- C25	- C26	- C27	= 167.69(13)
N24	- C25	- C26	- C31	= -10.9(2)
C31	- C26	- C27	- C28	= 3.8(2)
C25	- C26	- C27	- C28	= -174.84(13)
C26	- C27	- C28	- C29	= -1.7(2)
C26	- C27	- C28	- C33	= 176.63(13)
C27	- C28	- C29	- C30	= -1.6(2)
C33	- C28	- C29	- C30	= -179.97(14)
C28	- C29	- C30	- C31	= 2.5(2)
C28	- C29	- C30	- C37	= -178.51(14)
C27	- C26	- C31	- O32	= 177.73(13)
C25	- C26	- C31	- O32	= -3.7(2)
C27	- C26	- C31	- C30	= -2.7(2)
C25	- C26	- C31	- C30	= 175.83(13)
C29	- C30	- C31	- O32	= 179.27(13)
C37	- C30	- C31	- O32	= 0.3(2)
C29	- C30	- C31	- C26	= -0.3(2)
C37	- C30	- C31	- C26	= -179.28(13)
C26	- C31	- O32	- Zn1	= 30.27(19)
C30	- C31	- O32	- Zn1	= -149.29(10)
C27	- C28	- C33	- C36	= 6.1(2)
C29	- C28	- C33	- C36	= -175.61(14)
C27	- C28	- C33	- C35	= -114.25(16)
C29	- C28	- C33	- C35	= 64.00(17)
C27	- C28	- C33	- C34	= 126.26(16)
C29	- C28	- C33	- C34	= -55.48(18)
C29	- C30	- C37	- C38	= -0.1(2)
C31	- C30	- C37	- C38	= 178.82(16)
C29	- C30	- C37	- C40	= 119.03(16)
C31	- C30	- C37	- C40	= -62.03(18)
C29	- C30	- C37	- C39	= -119.54(16)
C31	- C30	- C37	- C39	= 59.40(18)
C56	- N51	- C52	- C53	= 1.9(3)
Zn1	- N51	- C52	- C53	= -158.02(16)
N51	- C52	- C53	- C54	= 0.0(3)
C52	- C53	- C54	- C55	= -1.7(3)
C53	- C54	- C55	- C56	= 1.5(3)
C53	- C54	- C55	- Cl1	= 179.87(15)
C52	- N51	- C56	- C55	= -2.1(2)
Zn1	- N51	- C56	- C55	= 157.50(12)
C54	- C55	- C56	- N51	= 0.4(2)
Cl1	- C55	- C56	- N51	= -178.01(12)

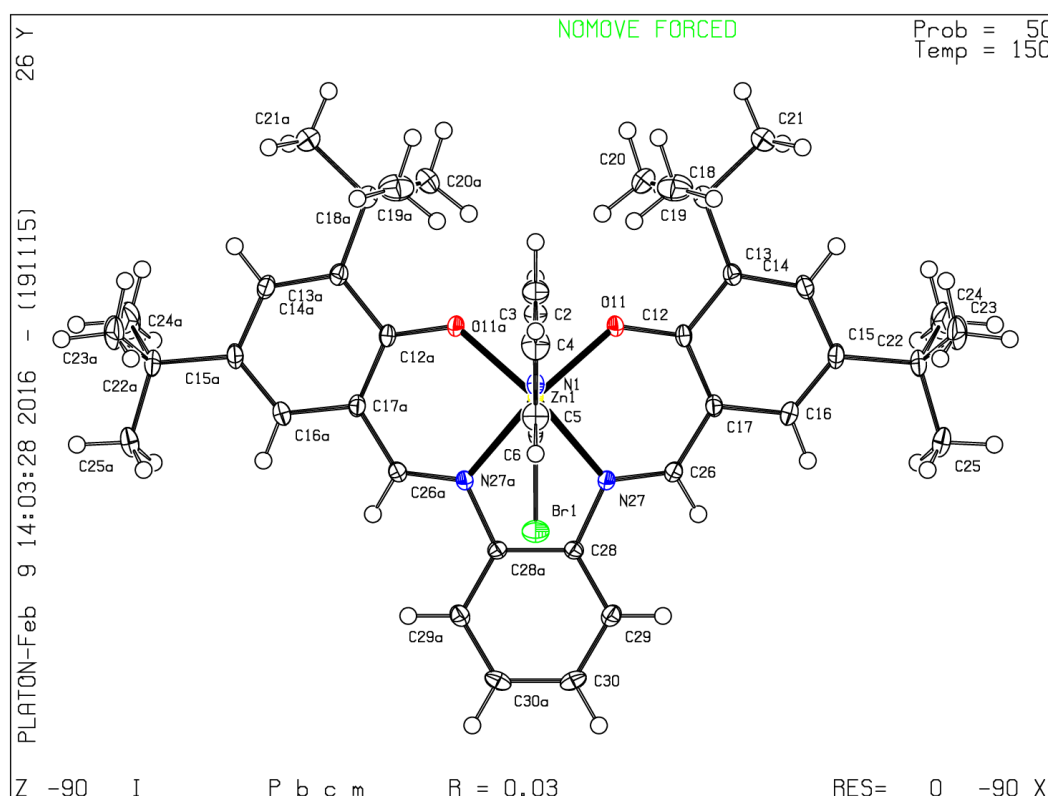
S9. X-ray crystallographic data for 4•B (CCDC-1509183).

(C₄₁ H₅₀ Br N₃ O₂ Zn); $M = 762.12$. D8 VENTURE Bruker AXS diffractometer [*], Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$), $T = 150 \text{ K}$; Orthorhombic $P b c m$ (I.T.#57), $a = 15.9728(11)$, $b = 10.2503(6)$, $c = 23.1812(18) \text{ \AA}$, $V = 3795.4(5) \text{ \AA}^3$. $Z = 4$, $d = 1.334 \text{ g.cm}^{-3}$, $\mu = 1.738 \text{ mm}^{-1}$. The structure was solved by direct methods using the *SIR97* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [2]. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 4452 unique intensities and 235 parameters converged at $\omega R(F^2) = 0.0807$ ($R(F) = 0.0298$) for 3768 observed reflections with $I > 2\sigma(I)$.

[1] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, *J. Appl. Cryst.* (1999) 32, 115-119

[2] Sheldrick G.M., *Acta Cryst. A*64 (2008), 112-122

[*] Thanks to FEDER funds



S9.1. Structural data.

Empirical formula	C ₄₁ H ₅₀ Br N ₃ O ₂ Zn
Formula weight	762.12
Temperature	150 K
Wavelength	0.71073 Å
Crystal system, space group	Orthorhombic, <i>P b c m</i>
Unit cell dimensions	a = 15.9728(11) Å, α = 90 ° b = 10.2503(6) Å, β = 90 ° c = 23.1812(18) Å, γ = 90 °
Volume	3795.4(5) Å ³
Z, Calculated density	4, 1.334 (g.cm ⁻³)
Absorption coefficient	1.738 mm ⁻¹
<i>F</i> (000)	1592
Crystal size	0.350 x 0.190 x 0.030 mm
Crystal color	yellow
Theta range for data collection	2.943 to 27.482 °
h_min, h_max	-20, 20
k_min, k_max	-13, 11
l_min, l_max	-30, 30
Reflections collected / unique	32223 / 4452 [R(int) ^a = 0.0480]
Reflections [I>2σ]	3768
Completeness to theta_max	0.998
Absorption correction type	multi-scan
Max. and min. transmission	0.949, 0.763
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	4452 / 0 / 235
^b Goodness-of-fit	1.139
Final <i>R</i> indices [I>2σ]	<i>R</i> 1 ^c = 0.0298, <i>wR</i> 2 ^d = 0.0807
<i>R</i> indices (all data)	<i>R</i> 1 ^c = 0.0420, <i>wR</i> 2 ^d = 0.0890
Largest diff. peak and hole	0.527 and -0.612 e ⁻ .Å ⁻³
^a <i>R</i> _{int} = ∑ <i>F</i> _o ² - < <i>F</i> _o ² > / ∑ [<i>F</i> _o ²]	
^b <i>S</i> = {∑ [w(<i>F</i> _o ² - <i>F</i> _c ²) ²] / (n - p)} ^{1/2}	
^c <i>R</i> 1 = ∑ <i>F</i> _o - <i>F</i> _c / ∑ [<i>F</i> _o]	
^d <i>wR</i> 2 = {∑ [w(<i>F</i> _o ² - <i>F</i> _c ²) ²] / ∑ [w(<i>F</i> _o ²) ²]} ^{1/2}	
<i>w</i> = 1 / [σ(<i>F</i> _o ²) + a <i>P</i> ² + b <i>P</i>] where <i>P</i> = [2 <i>F</i> _c ² + MAX(<i>F</i> _o ² , 0)] / 3	

S9.2. Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters (Å²). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
N1	0.76718(15)	0.8317(2)	0.2500	1	0.0135(5)
C2	0.85024(18)	0.8098(3)	0.2500	1	0.0186(6)
H2	0.8695	0.7221	0.2500	1	0.022
C3	0.9088(2)	0.9089(3)	0.2500	1	0.0245(7)
H3	0.9669	0.8895	0.2500	1	0.029
C4	0.8811(2)	1.0377(3)	0.2500	1	0.0256(7)
H4	0.9200	1.1079	0.2500	1	0.031
C5	0.7966(2)	1.0615(3)	0.2500	1	0.0216(6)

H5	0.7756	1.1482	0.2500	1	0.026
C6	0.74281(18)	0.9558(3)	0.2500	1	0.0144(5)
O11	0.76039(9)	0.56763(14)	0.31340(6)	1	0.0144(3)
C12	0.74232(12)	0.54883(18)	0.36770(8)	1	0.0123(4)
C13	0.80334(13)	0.49288(19)	0.40637(9)	1	0.0142(4)
C14	0.78363(14)	0.4808(2)	0.46411(9)	1	0.0175(4)
H14	0.8254	0.4468	0.4891	1	0.021
C15	0.70590(14)	0.5153(2)	0.48879(8)	1	0.0171(4)
C16	0.64643(13)	0.5608(2)	0.45161(9)	1	0.0172(4)
H16	0.5924	0.5808	0.4663	1	0.021
C17	0.66213(13)	0.57925(19)	0.39188(8)	1	0.0144(4)
C18	0.88944(13)	0.4499(2)	0.38367(9)	1	0.0178(4)
C19	0.93766(15)	0.5686(2)	0.36077(12)	1	0.0316(5)
H19A	0.9069	0.6071	0.3284	1	0.047
H19B	0.9933	0.5410	0.3477	1	0.047
H19C	0.9436	0.6334	0.3916	1	0.047
C20	0.87846(15)	0.3477(2)	0.33576(10)	1	0.0250(5)
H20A	0.8461	0.2737	0.3506	1	0.037
H20B	0.9336	0.3173	0.3230	1	0.037
H20C	0.8487	0.3870	0.3031	1	0.037
C21	0.94339(16)	0.3868(3)	0.43087(10)	1	0.0303(5)
H21A	0.9527	0.4497	0.4621	1	0.045
H21B	0.9974	0.3606	0.4145	1	0.045
H21C	0.9146	0.3099	0.4462	1	0.045
C22	0.69316(15)	0.5031(2)	0.55432(9)	1	0.0230(5)
C23	0.75859(17)	0.5891(3)	0.58502(10)	1	0.0365(6)
H23A	0.8149	0.5569	0.5762	1	0.055
H23B	0.7493	0.5858	0.6268	1	0.055
H23C	0.7532	0.6794	0.5716	1	0.055
C24	0.7036(2)	0.3599(3)	0.57312(11)	1	0.0403(7)
H24A	0.6615	0.3059	0.5538	1	0.060
H24B	0.6963	0.3533	0.6150	1	0.060
H24C	0.7597	0.3293	0.5626	1	0.060
C25	0.60636(16)	0.5494(3)	0.57259(10)	1	0.0309(6)
H25A	0.5990	0.6409	0.5615	1	0.046
H25B	0.6006	0.5410	0.6145	1	0.046
H25C	0.5637	0.4959	0.5535	1	0.046
C26	0.59343(12)	0.63116(19)	0.35960(8)	1	0.0143(4)
H26	0.5415	0.6381	0.3793	1	0.017
N27	0.59444(10)	0.66975(16)	0.30639(7)	1	0.0126(3)
C28	0.52117(12)	0.72130(18)	0.28044(8)	1	0.0125(4)
C29	0.45460(12)	0.77766(19)	0.31020(9)	1	0.0158(4)
H29	0.4551	0.7804	0.3512	1	0.019
C30	0.38750(13)	0.82987(19)	0.27990(9)	1	0.0182(4)
H30	0.3413	0.8658	0.3003	1	0.022
Br1	0.62667(2)	0.98707(3)	0.2500	1	0.01990(9)
Zn1	0.69569(2)	0.65168(3)	0.2500	1	0.01145(9)

S9.3. Anisotropic displacement parameters (\AA^2).

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

Atom	U11	U22	U33	U23	U13	U12
N1	0.0159(12)	0.0147(11)	0.0099(10)	0.000	0.000	-0.0015(9)
C2	0.0161(14)	0.0218(14)	0.0179(14)	0.000	0.000	0.0011(12)
C3	0.0176(15)	0.0318(17)	0.0243(16)	0.000	0.000	-0.0012(13)
C4	0.0248(17)	0.0243(16)	0.0277(17)	0.000	0.000	-0.0111(13)
C5	0.0245(16)	0.0164(14)	0.0238(15)	0.000	0.000	-0.0056(12)
C6	0.0199(14)	0.0165(13)	0.0069(12)	0.000	0.000	0.0000(11)
O11	0.0143(7)	0.0194(7)	0.0095(6)	0.0023(5)	0.0002(5)	0.0005(5)
C12	0.0159(9)	0.0115(8)	0.0094(9)	-0.0005(7)	-0.0010(7)	-0.0027(7)
C13	0.0166(10)	0.0142(9)	0.0117(9)	-0.0010(7)	-0.0019(7)	-0.0005(7)
C14	0.0224(11)	0.0188(10)	0.0112(9)	0.0004(7)	-0.0035(8)	0.0027(8)
C15	0.0240(11)	0.0183(10)	0.0090(9)	0.0000(7)	0.0011(8)	0.0011(8)
C16	0.0194(10)	0.0210(10)	0.0113(9)	0.0000(7)	0.0030(8)	0.0004(8)
C17	0.0164(9)	0.0172(9)	0.0096(9)	-0.0005(7)	-0.0008(7)	-0.0006(8)
C18	0.0180(10)	0.0209(10)	0.0146(9)	0.0003(8)	-0.0013(8)	0.0021(8)
C19	0.0195(11)	0.0313(13)	0.0441(15)	0.0049(11)	0.0026(11)	-0.0036(10)
C20	0.0265(12)	0.0293(12)	0.0190(11)	-0.0052(9)	0.0026(9)	0.0066(9)
C21	0.0271(12)	0.0435(14)	0.0204(11)	0.0000(10)	-0.0026(9)	0.0145(11)
C22	0.0294(12)	0.0308(12)	0.0089(9)	0.0011(8)	-0.0006(8)	0.0064(10)
C23	0.0376(15)	0.0585(17)	0.0133(11)	-0.0096(11)	-0.0038(10)	0.0011(13)
C24	0.0628(19)	0.0399(15)	0.0182(12)	0.0118(11)	0.0084(12)	0.0130(13)
C25	0.0327(13)	0.0480(15)	0.0119(10)	0.0001(10)	0.0052(9)	0.0061(11)
C26	0.0137(9)	0.0177(9)	0.0116(9)	-0.0013(7)	0.0012(7)	0.0004(8)
N27	0.0125(8)	0.0152(8)	0.0101(7)	-0.0011(6)	0.0002(6)	0.0003(6)
C28	0.0102(8)	0.0144(9)	0.0128(9)	-0.0011(7)	-0.0008(7)	-0.0005(7)
C29	0.0171(10)	0.0163(9)	0.0140(9)	-0.0018(7)	0.0018(7)	0.0009(8)
C30	0.0163(10)	0.0139(9)	0.0243(11)	-0.0024(8)	0.0052(8)	0.0034(8)
Br1	0.01920(16)	0.01454(14)	0.02596(17)	0.000	0.000	0.00156(11)
Zn1	0.01268(16)	0.01396(16)	0.00770(15)	0.000	0.000	-0.00044(11)

S9.4. Bond lengths [\AA].

N1 - C6	= 1.330(4)	N1 - C2	= 1.345(4)
N1 - Zn1	= 2.170(2)	C2 - C3	= 1.380(4)
C2 - H2	= 0.9500	C3 - C4	= 1.393(5)
C3 - H3	= 0.9500	C4 - C5	= 1.371(5)
C4 - H4	= 0.9500	C5 - C6	= 1.382(4)
C5 - H5	= 0.9500	C6 - Br1	= 1.883(3)
O11 - C12	= 1.306(2)	O11 - Zn1	= 1.9924(13)
C12 - C17	= 1.433(3)	C12 - C13	= 1.443(3)
C13 - C14	= 1.381(3)	C13 - C18	= 1.537(3)
C14 - C15	= 1.412(3)	C14 - H14	= 0.9500
C15 - C16	= 1.365(3)	C15 - C22	= 1.538(3)
C16 - C17	= 1.420(3)	C16 - H16	= 0.9500
C17 - C26	= 1.431(3)	C18 - C19	= 1.534(3)

C18 - C21	= 1.536(3)	C18 - C20	= 1.537(3)
C19 - H19A	= 0.9800	C19 - H19B	= 0.9800
C19 - H19C	= 0.9800	C20 - H20A	= 0.9800
C20 - H20B	= 0.9800	C20 - H20C	= 0.9800
C21 - H21A	= 0.9800	C21 - H21B	= 0.9800
C21 - H21C	= 0.9800	C22 - C25	= 1.525(3)
C22 - C24	= 1.540(3)	C22 - C23	= 1.542(3)
C23 - H23A	= 0.9800	C23 - H23B	= 0.9800
C23 - H23C	= 0.9800	C24 - H24A	= 0.9800
C24 - H24B	= 0.9800	C24 - H24C	= 0.9800
C25 - H25A	= 0.9800	C25 - H25B	= 0.9800
C25 - H25C	= 0.9800	C26 - N27	= 1.295(2)
C26 - H26	= 0.9500	N27 - C28	= 1.418(2)
N27 - Zn1	= 2.0877(16)	C28 - C29	= 1.393(3)
C28 - C28_#1	= 1.412(4)	C29 - C30	= 1.389(3)
C29 - H29	= 0.9500	C30 - C30_#1	= 1.386(4)
C30 - H30	= 0.9500	Zn1 - O11_#1	= 1.9924(13)
Zn1 - N27_#1	= 2.0878(16)		

Symmetry transformations used to generate equivalent atoms:

$$\#1 \quad x, y, -z-1/2 \quad T = [0, 0, 1]$$

S9.5. Angles [°].

C6 - N1 - C2	= 116.6(3)
C6 - N1 - Zn1	= 131.2(2)
C2 - N1 - Zn1	= 112.16(19)
N1 - C2 - C3	= 123.0(3)
N1 - C2 - H2	= 118.5
C3 - C2 - H2	= 118.5
C2 - C3 - C4	= 118.8(3)
C2 - C3 - H3	= 120.6
C4 - C3 - H3	= 120.6
C5 - C4 - C3	= 118.7(3)
C5 - C4 - H4	= 120.6
C3 - C4 - H4	= 120.6
C4 - C5 - C6	= 118.2(3)
C4 - C5 - H5	= 120.9
C6 - C5 - H5	= 120.9
N1 - C6 - C5	= 124.6(3)
N1 - C6 - Br1	= 116.8(2)
C5 - C6 - Br1	= 118.6(2)
C12 - O11 - Zn1	= 131.32(13)
O11 - C12 - C17	= 122.87(17)
O11 - C12 - C13	= 120.55(18)
C17 - C12 - C13	= 116.57(17)
C14 - C13 - C12	= 118.95(19)
C14 - C13 - C18	= 120.68(18)
C12 - C13 - C18	= 120.36(17)
C13 - C14 - C15	= 124.80(19)

C13 - C14 - H14 = 117.6
C15 - C14 - H14 = 117.6
C16 - C15 - C14 = 116.22(18)
C16 - C15 - C22 = 124.0(2)
C14 - C15 - C22 = 119.75(19)
C15 - C16 - C17 = 122.58(19)
C15 - C16 - H16 = 118.7
C17 - C16 - H16 = 118.7
C16 - C17 - C26 = 115.10(18)
C16 - C17 - C12 = 120.69(18)
C26 - C17 - C12 = 124.20(17)
C19 - C18 - C13 = 109.91(18)
C19 - C18 - C21 = 107.38(19)
C13 - C18 - C21 = 112.26(17)
C19 - C18 - C20 = 110.35(19)
C13 - C18 - C20 = 109.91(17)
C21 - C18 - C20 = 106.97(19)
C18 - C19 - H19A = 109.5
C18 - C19 - H19B = 109.5
H19A - C19 - H19B = 109.5
C18 - C19 - H19C = 109.5
H19A - C19 - H19C = 109.5
H19B - C19 - H19C = 109.5
C18 - C20 - H20A = 109.5
C18 - C20 - H20B = 109.5
H20A - C20 - H20B = 109.5
C18 - C20 - H20C = 109.5
H20A - C20 - H20C = 109.5
H20B - C20 - H20C = 109.5
C18 - C21 - H21A = 109.5
C18 - C21 - H21B = 109.5
H21A - C21 - H21B = 109.5
C18 - C21 - H21C = 109.5
H21A - C21 - H21C = 109.5
H21B - C21 - H21C = 109.5
C25 - C22 - C15 = 111.67(18)
C25 - C22 - C24 = 108.4(2)
C15 - C22 - C24 = 110.06(18)
C25 - C22 - C23 = 108.1(2)
C15 - C22 - C23 = 108.6(2)
C24 - C22 - C23 = 110.0(2)
C22 - C23 - H23A = 109.5
C22 - C23 - H23B = 109.5
H23A - C23 - H23B = 109.5
C22 - C23 - H23C = 109.5
H23A - C23 - H23C = 109.5
H23B - C23 - H23C = 109.5
C22 - C24 - H24A = 109.5
C22 - C24 - H24B = 109.5
H24A - C24 - H24B = 109.5

C22 - C24 - H24C = 109.5
 H24A - C24 - H24C = 109.5
 H24B - C24 - H24C = 109.5
 C22 - C25 - H25A = 109.5
 C22 - C25 - H25B = 109.5
 H25A - C25 - H25B = 109.5
 C22 - C25 - H25C = 109.5
 H25A - C25 - H25C = 109.5
 H25B - C25 - H25C = 109.5
 N27 - C26 - C17 = 127.01(18)
 N27 - C26 - H26 = 116.5
 C17 - C26 - H26 = 116.5
 C26 - N27 - C28 = 120.49(17)
 C26 - N27 - Zn1 = 125.36(14)
 C28 - N27 - Zn1 = 114.00(12)
 C29 - C28 - C28_#1 = 119.68(11)
 C29 - C28 - N27 = 125.07(17)
 C28_#1 - C28 - N27 = 115.10(10)
 C30 - C29 - C28 = 119.91(19)
 C30 - C29 - H29 = 120.0
 C28 - C29 - H29 = 120.0
 C30_#1 - C30 - C29 = 120.38(12)
 C30_#1 - C30 - H30 = 119.8
 C29 - C30 - H30 = 119.8
 O11_#1 - Zn1 - O11 = 95.05(8)
 O11_#1 - Zn1 - N27 = 154.42(6)
 O11 - Zn1 - N27 = 88.75(6)
 O11_#1 - Zn1 - N27_#1 = 88.76(6)
 O11 - Zn1 - N27_#1 = 154.42(6)
 N27 - Zn1 - N27_#1 = 77.54(9)
 O11_#1 - Zn1 - N1 = 95.43(6)
 O11 - Zn1 - N1 = 95.43(6)
 N27 - Zn1 - N1 = 109.40(7)
 N27_#1 - Zn1 - N1 = 109.40(7)

Symmetry transformations used to generate equivalent atoms:

#1 x, y, -z-1/2 T = [0, 0, 1]

S9.6. Torsion angles [°].

C6 - N1 - C2 - C3 = 0.0
 N1 - C2 - C3 - C4 = 0.0
 C2 - C3 - C4 - C5 = 0.0
 C3 - C4 - C5 - C6 = 0.0
 C2 - N1 - C6 - C5 = 0.0
 Zn1 - N1 - C6 - Br1 = 0.0
 C4 - C5 - C6 - N1 = 0.0
 Zn1 - O11 - C12 - C17 = 5.8(3)
 Zn1 - O11 - C12 - C13 = -175.44(13)
 O11 - C12 - C13 - C14 = 176.61(18)

C17	- C12	- C13	- C14	= -4.5(3)
O11	- C12	- C13	- C18	= -2.3(3)
C17	- C12	- C13	- C18	= 176.58(17)
C12	- C13	- C14	- C15	= 2.3(3)
C18	- C13	- C14	- C15	= -178.82(19)
C13	- C14	- C15	- C16	= 1.6(3)
C13	- C14	- C15	- C22	= -177.1(2)
C14	- C15	- C16	- C17	= -3.1(3)
C22	- C15	- C16	- C17	= 175.6(2)
C15	- C16	- C17	- C26	= -178.28(19)
C15	- C16	- C17	- C12	= 0.8(3)
O11	- C12	- C17	- C16	= -178.03(18)
C13	- C12	- C17	- C16	= 3.2(3)
O11	- C12	- C17	- C26	= 0.9(3)
C13	- C12	- C17	- C26	= -177.90(18)
C14	- C13	- C18	- C19	= -115.4(2)
C12	- C13	- C18	- C19	= 63.4(2)
C14	- C13	- C18	- C21	= 4.0(3)
C12	- C13	- C18	- C21	= -177.14(19)
C14	- C13	- C18	- C20	= 122.9(2)
C12	- C13	- C18	- C20	= -58.2(2)
C16	- C15	- C22	- C25	= -0.6(3)
C14	- C15	- C22	- C25	= 178.0(2)
C16	- C15	- C22	- C24	= 119.9(3)
C14	- C15	- C22	- C24	= -61.5(3)
C16	- C15	- C22	- C23	= -119.7(2)
C14	- C15	- C22	- C23	= 59.0(3)
C16	- C17	- C26	- N27	= 172.03(19)
C12	- C17	- C26	- N27	= -7.0(3)
C17	- C26	- N27	- C28	= -178.94(18)
C17	- C26	- N27	- Zn1	= 5.7(3)
C26	- N27	- C28	- C29	= 23.7(3)
Zn1	- N27	- C28	- C29	= -160.43(16)
C26	- N27	- C28	- C28_#1	= -160.79(14)
Zn1	- N27	- C28	- C28_#1	= 15.09(13)
C28_#1	- C28	- C29	- C30	= 2.0(2)
N27	- C28	- C29	- C30	= 177.30(18)
C28	- C29	- C30	- C30_#1	= -2.0(2)

Symmetry transformations used to generate equivalent atoms:

#1 x, y, -z-1/2 T = [0, 0, 1]

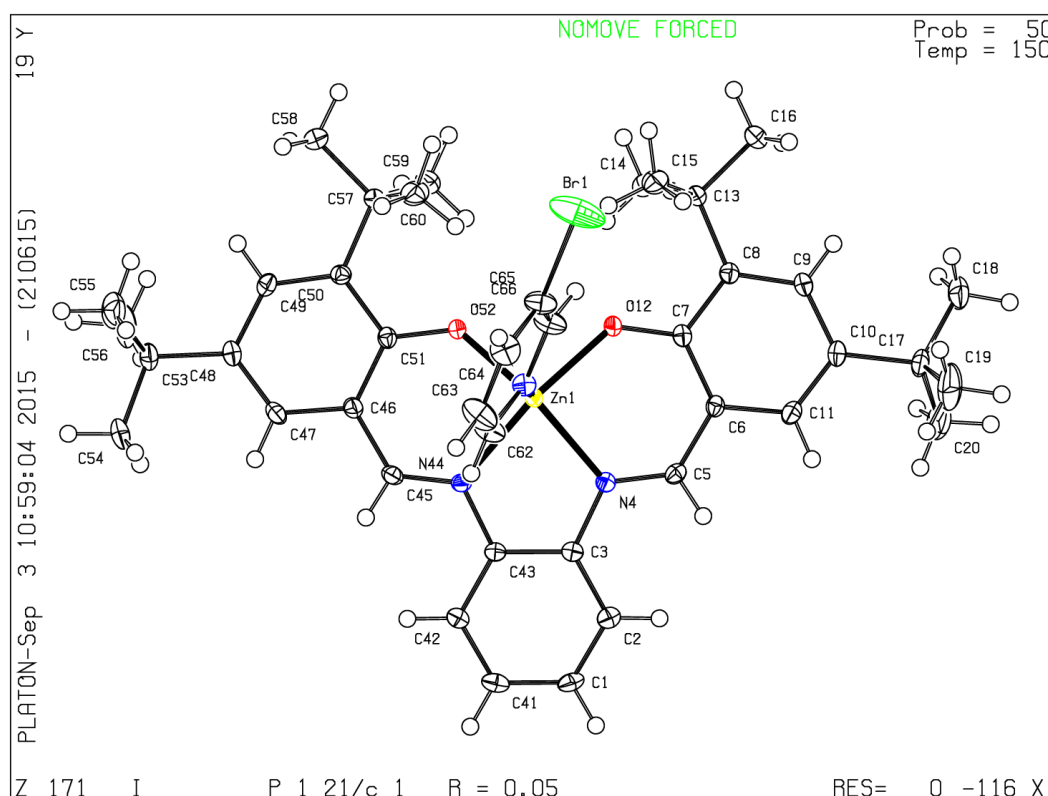
S10. X-ray crystallographic data for 5•B (CCDC-1509178).

(C₄₁ H₅₀ Br N₃ O₂ Zn); $M = 762.12$. D8 VENTURE Bruker AXS diffractometer [*], Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$), $T = 150 \text{ K}$; Monoclinic $P 1 2_1/c 1$ (I.T.#14), $a = 13.6592(4)$, $b = 13.9518(4)$, $c = 19.8686(8) \text{ \AA}$, $\beta = 93.2820(10)^\circ$, $V = 3780.2(2) \text{ \AA}^3$. $Z = 4$, $d = 1.339 \text{ g.cm}^{-3}$, $\mu = 1.745 \text{ mm}^{-1}$. The structure was solved by direct methods using the *SIR97* program [1], and then refined with full-matrix least-square methods based on F^2 (*SHELXL-97*) [2]. All non-hydrogen atoms were refined with anisotropic atomic displacement parameters. H atoms were finally included in their calculated positions. A final refinement on F^2 with 8673 unique intensities and 215 parameters converged at $\omega R(F^2) = 0.1291$ ($R(F) = 0.0596$) for 7033 observed reflections with $I > 2\sigma(I)$.

[1] A. Altomare, M. C. Burla, M. Camalli, G. Cascarano, C. Giacovazzo, A. Guagliardi, A. G. G. Moliterni, G. Polidori, R. Spagna, *J. Appl. Cryst.* (1999) 32, 115-119

[2] Sheldrick G.M., *Acta Cryst.* A64 (2008), 112-122

[*] Thanks to the FEDER funds



S10.1. Structural data.

Empirical formula	C ₄₁ H ₅₀ Br N ₃ O ₂ Zn
Formula weight	762.12
Temperature	150 K
Wavelength	0.71073 Å
Crystal system, space group	Monoclinic, <i>P</i> 1 2 ₁ / <i>c</i> 1
Unit cell dimensions	<i>a</i> = 13.6592(4) Å, α = 90 ° <i>b</i> = 13.9518(4) Å, β = 93.2820(10) ° <i>c</i> = 19.8686(8) Å, γ = 90 °
Volume	3780.2(2) Å ³
<i>Z</i> , Calculated density	4, 1.339 (g.cm ⁻³)
Absorption coefficient	1.745 mm ⁻¹
<i>F</i> (000)	1592
Crystal size	0.330 x 0.240 x 0.180 mm
Crystal color	orange
Theta range for data collection	2.920 to 27.521 °
<i>h</i> _min, <i>h</i> _max	-17, 13
<i>k</i> _min, <i>k</i> _max	-18, 18
<i>l</i> _min, <i>l</i> _max	-25, 25
Reflections collected / unique	34060 / 8673 [R(int) ^a = 0.0440]
Reflections [<i>I</i> >2 σ]	7033
Completeness to theta_max	0.996
Absorption correction type	multi-scan
Max. and min. transmission	0.730 , 0.568
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data / restraints / parameters	8673 / 0 / 215
^b Goodness-of-fit	1.023
Final <i>R</i> indices [<i>I</i> >2 σ]	<i>R</i> 1 ^c = 0.0596, <i>wR</i> 2 ^d = 0.1291
<i>R</i> indices (all data)	<i>R</i> 1 ^c = 0.0761, <i>wR</i> 2 ^d = 0.1385
Largest diff. peak and hole	3.313 and -2.697 e ⁻ .Å ⁻³

^a $R_{int} = \sum |F_o^2 - \langle F_o^2 \rangle| / \sum [F_o^2]$
^b $S = \{ \sum [w(F_o^2 - F_c^2)^2] / (n - p) \}^{1/2}$
^c $R1 = \sum ||F_o| - |F_c|| / \sum |F_o|$
^d $wR2 = \{ \sum [w(F_o^2 - F_c^2)^2] / \sum [w(F_o^2)^2] \}^{1/2}$
 $w = 1 / [\sigma(F_o^2) + aP^2 + bP]$ where $P = [2F_c^2 + \text{MAX}(F_o^2, 0)] / 3$

S10.2. Atomic coordinates, site occupancy (%) and equivalent isotropic displacement parameters (Å²). U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	x	y	z	occ.	U(eq)
Zn1	0.06153(3)	0.20061(3)	0.06450(2)	1	0.01268(10)
Br1	0.08066(5)	0.60562(3)	0.10643(3)	1	0.05587(19)
C1	0.0342(3)	-0.0165(2)	-0.15643(18)	1	0.0189(7)
H1	0.0046	-0.0458	-0.1944	1	0.023
C2	-0.0201(3)	0.0429(2)	-0.11737(17)	1	0.0173(7)
H2	-0.0855	0.0549	-0.1302	1	0.021
C3	0.0219(2)	0.0852(2)	-0.05887(16)	1	0.0126(6)
N4	-0.02744(19)	0.14521(19)	-0.01412(13)	1	0.0125(5)

C5	-0.1202(2)	0.1644(2)	-0.02330(17)	1	0.0146(6)
H5	-0.1517	0.1407	-0.0626	1	0.017
C6	-0.1798(2)	0.2183(2)	0.02060(16)	1	0.0133(6)
C7	-0.1453(2)	0.2577(2)	0.08414(16)	1	0.0127(6)
C8	-0.2165(2)	0.3028(2)	0.12460(16)	1	0.0138(6)
C9	-0.3132(2)	0.3079(2)	0.09956(16)	1	0.0154(6)
H9	-0.3583	0.3374	0.1262	1	0.018
C10	-0.3477(2)	0.2714(2)	0.03642(17)	1	0.0165(6)
C11	-0.2797(2)	0.2270(2)	-0.00135(17)	1	0.0168(7)
H11	-0.3003	0.2016	-0.0431	1	0.020
O12	-0.05431(16)	0.25381(16)	0.10635(11)	1	0.0152(5)
C13	-0.1846(2)	0.3438(2)	0.19468(17)	1	0.0165(6)
C14	-0.1452(3)	0.2635(3)	0.24162(18)	1	0.0213(7)
H14A	-0.1238	0.2903	0.2845	1	0.032
H14B	-0.0909	0.2326	0.2220	1	0.032
H14C	-0.1962	0.2176	0.2478	1	0.032
C15	-0.1048(3)	0.4203(3)	0.18890(19)	1	0.0239(8)
H15A	-0.1209	0.4604	0.1506	1	0.036
H15B	-0.0428	0.3896	0.1834	1	0.036
H15C	-0.1007	0.4587	0.2291	1	0.036
C16	-0.2700(3)	0.3918(3)	0.2284(2)	1	0.0261(8)
H16A	-0.3207	0.3454	0.2345	1	0.039
H16B	-0.2957	0.4431	0.2004	1	0.039
H16C	-0.2472	0.4170	0.2715	1	0.039
C17	-0.4553(3)	0.2831(3)	0.00937(19)	1	0.0224(7)
C18	-0.5231(3)	0.3120(3)	0.0645(2)	1	0.0390(10)
H18A	-0.5047	0.3743	0.0814	1	0.058
H18B	-0.5176	0.2662	0.1006	1	0.058
H18C	-0.5897	0.3138	0.0461	1	0.058
C19	-0.4610(4)	0.3583(4)	-0.0459(3)	1	0.0438(11)
H19A	-0.5275	0.3640	-0.0638	1	0.066
H19B	-0.4199	0.3395	-0.0813	1	0.066
H19C	-0.4391	0.4188	-0.0277	1	0.066
C20	-0.4947(4)	0.1871(3)	-0.0198(2)	1	0.0408(11)
H20A	-0.4871	0.1382	0.0141	1	0.061
H20B	-0.4585	0.1696	-0.0579	1	0.061
H20C	-0.5628	0.1939	-0.0335	1	0.061
C41	0.1328(2)	-0.0329(2)	-0.13932(17)	1	0.0171(7)
H41	0.1696	-0.0713	-0.1666	1	0.020
C42	0.1763(2)	0.0081(2)	-0.08151(16)	1	0.0156(6)
H42	0.2424	-0.0025	-0.0704	1	0.019
C43	0.1213(2)	0.0653(2)	-0.03980(16)	1	0.0123(6)
N44	0.15720(19)	0.10353(19)	0.02271(13)	1	0.0131(5)
C45	0.2388(2)	0.0736(2)	0.05213(16)	1	0.0154(6)
H45	0.2748	0.0296	0.0285	1	0.018
C46	0.2791(2)	0.1013(2)	0.11741(17)	1	0.0153(6)
C47	0.3749(2)	0.0670(2)	0.13604(17)	1	0.0174(7)
H47	0.4064	0.0281	0.1060	1	0.021

C48	0.4223(2)	0.0891(2)	0.19650(17)	1	0.0170(7)
C49	0.3706(2)	0.1472(2)	0.24085(17)	1	0.0167(6)
H49	0.4017	0.1625	0.2823	1	0.020
C50	0.2776(2)	0.1826(2)	0.22705(16)	1	0.0143(6)
C51	0.2275(2)	0.1592(2)	0.16338(16)	1	0.0136(6)
O52	0.13887(17)	0.18986(17)	0.15018(12)	1	0.0172(5)
C53	0.5262(3)	0.0554(3)	0.21795(18)	1	0.0203(7)
C54	0.5766(3)	0.0085(3)	0.1604(2)	1	0.0353(9)
H54A	0.5404	-0.0474	0.1457	1	0.053
H54B	0.6420	-0.0097	0.1755	1	0.053
H54C	0.5792	0.0529	0.1237	1	0.053
C55	0.5898(3)	0.1415(3)	0.2410(2)	1	0.0346(9)
H55A	0.6540	0.1195	0.2560	1	0.052
H55B	0.5601	0.1735	0.2775	1	0.052
H55C	0.5950	0.1852	0.2041	1	0.052
C56	0.5228(3)	-0.0140(3)	0.2775(2)	1	0.0358(10)
H56A	0.4907	-0.0722	0.2628	1	0.054
H56B	0.4871	0.0148	0.3125	1	0.054
H56C	0.5884	-0.0282	0.2945	1	0.054
C57	0.2280(2)	0.2494(2)	0.27620(17)	1	0.0165(6)
C58	0.2945(3)	0.2695(3)	0.33914(18)	1	0.0222(7)
H58A	0.3098	0.2104	0.3621	1	0.033
H58B	0.2615	0.3116	0.3686	1	0.033
H58C	0.3540	0.2992	0.3262	1	0.033
C59	0.1324(3)	0.2051(3)	0.29949(19)	1	0.0250(8)
H59A	0.0884	0.1932	0.2610	1	0.038
H59B	0.1024	0.2486	0.3295	1	0.038
H59C	0.1469	0.1458	0.3225	1	0.038
C60	0.2050(3)	0.3462(3)	0.2414(2)	1	0.0250(8)
H60A	0.2640	0.3725	0.2250	1	0.038
H60B	0.1789	0.3897	0.2732	1	0.038
H60C	0.1577	0.3367	0.2044	1	0.038
N61	0.1186(2)	0.3352(2)	0.03242(15)	1	0.0174(6)
C62	0.1868(3)	0.3472(3)	-0.0121(2)	1	0.0262(8)
H62	0.2083	0.2938	-0.0351	1	0.031
C63	0.2269(3)	0.4356(3)	-0.0256(2)	1	0.0315(9)
H63	0.2734	0.4413	-0.0578	1	0.038
C64	0.1973(3)	0.5157(3)	0.0090(2)	1	0.0261(8)
H64	0.2237	0.5759	0.0013	1	0.031
C65	0.1268(3)	0.5024(3)	0.0555(2)	1	0.0246(8)
C66	0.0879(3)	0.4123(3)	0.06516(19)	1	0.0240(8)
H66	0.0389	0.4051	0.0954	1	0.029

S10.3. Anisotropic displacement parameters (\AA^2).

The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U_{11} + \dots + 2 h k a^* b^* U_{12}]$.

Atom	U11	U22	U33	U23	U13	U12
Zn1	0.01057(17)	0.01224(17)	0.01514(18)	-0.00273(14)	-0.00004(13)	0.00091(14)
Br1	0.0939(4)	0.0161(2)	0.0622(3)	-0.0091(2)	0.0447(3)	-0.0063(2)

S10.4. Bond lengths [\AA].

Zn1 - O52	= 1.957(2)	Zn1 - O12	= 1.974(2)
Zn1 - N4	= 2.073(3)	Zn1 - N44	= 2.087(3)
Zn1 - N61	= 2.144(3)	Br1 - C65	= 1.888(4)
C1 - C2	= 1.381(5)	C1 - C41	= 1.389(5)
C1 - H1	= 0.9300	C2 - C3	= 1.397(4)
C2 - H2	= 0.9300	C3 - C43	= 1.417(4)
C3 - N4	= 1.419(4)	N4 - C5	= 1.298(4)
C5 - C6	= 1.438(4)	C5 - H5	= 0.9300
C6 - C11	= 1.415(4)	C6 - C7	= 1.431(4)
C7 - O12	= 1.296(4)	C7 - C8	= 1.442(4)
C8 - C9	= 1.386(4)	C8 - C13	= 1.545(4)
C9 - C10	= 1.410(5)	C9 - H9	= 0.9300
C10 - C11	= 1.375(5)	C10 - C17	= 1.544(5)
C11 - H11	= 0.9300	C13 - C16	= 1.532(5)
C13 - C15	= 1.534(5)	C13 - C14	= 1.535(5)
C14 - H14A	= 0.9600	C14 - H14B	= 0.9600
C14 - H14C	= 0.9600	C15 - H15A	= 0.9600
C15 - H15B	= 0.9600	C15 - H15C	= 0.9600
C16 - H16A	= 0.9600	C16 - H16B	= 0.9600
C16 - H16C	= 0.9600	C17 - C19	= 1.518(6)
C17 - C18	= 1.529(6)	C17 - C20	= 1.542(6)
C18 - H18A	= 0.9600	C18 - H18B	= 0.9600
C18 - H18C	= 0.9600	C19 - H19A	= 0.9600
C19 - H19B	= 0.9600	C19 - H19C	= 0.9600
C20 - H20A	= 0.9600	C20 - H20B	= 0.9600
C20 - H20C	= 0.9600	C41 - C42	= 1.386(5)
C41 - H41	= 0.9300	C42 - C43	= 1.399(4)
C42 - H42	= 0.9300	C43 - N44	= 1.413(4)
N44 - C45	= 1.298(4)	C45 - C46	= 1.433(5)
C45 - H45	= 0.9300	C46 - C47	= 1.422(5)
C46 - C51	= 1.434(4)	C47 - C48	= 1.367(5)
C47 - H47	= 0.9300	C48 - C49	= 1.415(5)
C48 - C53	= 1.533(5)	C49 - C50	= 1.376(5)
C49 - H49	= 0.9300	C50 - C51	= 1.441(4)
C50 - C57	= 1.535(4)	C51 - O52	= 1.296(4)
C53 - C54	= 1.516(6)	C53 - C56	= 1.532(6)
C53 - C55	= 1.537(5)	C54 - H54A	= 0.9600
C54 - H54B	= 0.9600	C54 - H54C	= 0.9600
C55 - H55A	= 0.9600	C55 - H55B	= 0.9600

C55 - H55C	= 0.9600	C56 - H56A	= 0.9600
C56 - H56B	= 0.9600	C56 - H56C	= 0.9600
C57 - C58	= 1.529(5)	C57 - C59	= 1.540(5)
C57 - C60	= 1.542(5)	C58 - H58A	= 0.9600
C58 - H58B	= 0.9600	C58 - H58C	= 0.9600
C59 - H59A	= 0.9600	C59 - H59B	= 0.9600
C59 - H59C	= 0.9600	C60 - H60A	= 0.9600
C60 - H60B	= 0.9600	C60 - H60C	= 0.9600
N61 - C62	= 1.332(5)	N61 - C66	= 1.338(5)
C62 - C63	= 1.382(6)	C62 - H62	= 0.9300
C63 - C64	= 1.385(6)	C63 - H63	= 0.9300
C64 - C65	= 1.385(5)	C64 - H64	= 0.9300
C65 - C66	= 1.382(5)	C66 - H66	= 0.9300

S10.5. Angles [°].

O52 - Zn1 - O12	= 93.91(10)
O52 - Zn1 - N4	= 152.98(10)
O12 - Zn1 - N4	= 90.47(10)
O52 - Zn1 - N44	= 88.69(10)
O12 - Zn1 - N44	= 161.23(10)
N4 - Zn1 - N44	= 79.14(10)
O52 - Zn1 - N61	= 97.95(10)
O12 - Zn1 - N61	= 96.30(10)
N4 - Zn1 - N61	= 108.06(11)
N44 - Zn1 - N61	= 101.74(11)
C2 - C1 - C41	= 120.4(3)
C2 - C1 - H1	= 119.8
C41 - C1 - H1	= 119.8
C1 - C2 - C3	= 120.9(3)
C1 - C2 - H2	= 119.6
C3 - C2 - H2	= 119.6
C2 - C3 - C43	= 118.7(3)
C2 - C3 - N4	= 125.7(3)
C43 - C3 - N4	= 115.5(3)
C5 - N4 - C3	= 121.9(3)
C5 - N4 - Zn1	= 123.7(2)
C3 - N4 - Zn1	= 114.4(2)
N4 - C5 - C6	= 127.1(3)
N4 - C5 - H5	= 116.4
C6 - C5 - H5	= 116.4
C11 - C6 - C7	= 120.1(3)
C11 - C6 - C5	= 115.3(3)
C7 - C6 - C5	= 124.5(3)
O12 - C7 - C6	= 123.0(3)
O12 - C7 - C8	= 119.5(3)
C6 - C7 - C8	= 117.4(3)
C9 - C8 - C7	= 118.8(3)
C9 - C8 - C13	= 121.2(3)
C7 - C8 - C13	= 120.0(3)

C8 - C9 - C10 = 124.3(3)
C8 - C9 - H9 = 117.8
C10 - C9 - H9 = 117.8
C11 - C10 - C9 = 116.5(3)
C11 - C10 - C17 = 121.1(3)
C9 - C10 - C17 = 122.3(3)
C10 - C11 - C6 = 122.7(3)
C10 - C11 - H11 = 118.6
C6 - C11 - H11 = 118.6
C7 - O12 - Zn1 = 130.4(2)
C16 - C13 - C15 = 106.9(3)
C16 - C13 - C14 = 107.6(3)
C15 - C13 - C14 = 109.1(3)
C16 - C13 - C8 = 111.9(3)
C15 - C13 - C8 = 110.8(3)
C14 - C13 - C8 = 110.4(3)
C13 - C14 - H14A = 109.5
C13 - C14 - H14B = 109.5
H14A - C14 - H14B = 109.5
C13 - C14 - H14C = 109.5
H14A - C14 - H14C = 109.5
H14B - C14 - H14C = 109.5
C13 - C15 - H15A = 109.5
C13 - C15 - H15B = 109.5
H15A - C15 - H15B = 109.5
C13 - C15 - H15C = 109.5
H15A - C15 - H15C = 109.5
H15B - C15 - H15C = 109.5
C13 - C16 - H16A = 109.5
C13 - C16 - H16B = 109.5
H16A - C16 - H16B = 109.5
C13 - C16 - H16C = 109.5
H16A - C16 - H16C = 109.5
H16B - C16 - H16C = 109.5
C19 - C17 - C18 = 109.2(3)
C19 - C17 - C20 = 109.0(3)
C18 - C17 - C20 = 106.6(3)
C19 - C17 - C10 = 109.4(3)
C18 - C17 - C10 = 112.5(3)
C20 - C17 - C10 = 110.1(3)
C17 - C18 - H18A = 109.5
C17 - C18 - H18B = 109.5
H18A - C18 - H18B = 109.5
C17 - C18 - H18C = 109.5
H18A - C18 - H18C = 109.5
H18B - C18 - H18C = 109.5
C17 - C19 - H19A = 109.5
C17 - C19 - H19B = 109.5
H19A - C19 - H19B = 109.5
C17 - C19 - H19C = 109.5

H19A - C19 - H19C = 109.5
 H19B - C19 - H19C = 109.5
 C17 - C20 - H20A = 109.5
 C17 - C20 - H20B = 109.5
 H20A - C20 - H20B = 109.5
 C17 - C20 - H20C = 109.5
 H20A - C20 - H20C = 109.5
 H20B - C20 - H20C = 109.5
 C42 - C41 - C1 = 119.9(3)
 C42 - C41 - H41 = 120.0
 C1 - C41 - H41 = 120.0
 C41 - C42 - C43 = 120.5(3)
 C41 - C42 - H42 = 119.8
 C43 - C42 - H42 = 119.8
 C42 - C43 - N44 = 124.4(3)
 C42 - C43 - C3 = 119.5(3)
 N44 - C43 - C3 = 116.1(3)
 C45 - N44 - C43 = 121.3(3)
 C45 - N44 - Zn1 = 124.8(2)
 C43 - N44 - Zn1 = 113.7(2)
 N44 - C45 - C46 = 126.6(3)
 N44 - C45 - H45 = 116.7
 C46 - C45 - H45 = 116.7
 C47 - C46 - C45 = 116.4(3)
 C47 - C46 - C51 = 120.2(3)
 C45 - C46 - C51 = 123.5(3)
 C48 - C47 - C46 = 122.4(3)
 C48 - C47 - H47 = 118.8
 C46 - C47 - H47 = 118.8
 C47 - C48 - C49 = 116.6(3)
 C47 - C48 - C53 = 124.0(3)
 C49 - C48 - C53 = 119.3(3)
 C50 - C49 - C48 = 124.7(3)
 C50 - C49 - H49 = 117.6
 C48 - C49 - H49 = 117.6
 C49 - C50 - C51 = 118.7(3)
 C49 - C50 - C57 = 121.8(3)
 C51 - C50 - C57 = 119.4(3)
 O52 - C51 - C46 = 123.0(3)
 O52 - C51 - C50 = 119.6(3)
 C46 - C51 - C50 = 117.4(3)
 C51 - O52 - Zn1 = 130.7(2)
 C54 - C53 - C56 = 110.1(3)
 C54 - C53 - C48 = 112.1(3)
 C56 - C53 - C48 = 109.9(3)
 C54 - C53 - C55 = 106.8(3)
 C56 - C53 - C55 = 107.8(3)
 C48 - C53 - C55 = 110.0(3)
 C53 - C54 - H54A = 109.5
 C53 - C54 - H54B = 109.5

H54A - C54 - H54B = 109.5
 C53 - C54 - H54C = 109.5
 H54A - C54 - H54C = 109.5
 H54B - C54 - H54C = 109.5
 C53 - C55 - H55A = 109.5
 C53 - C55 - H55B = 109.5
 H55A - C55 - H55B = 109.5
 C53 - C55 - H55C = 109.5
 H55A - C55 - H55C = 109.5
 H55B - C55 - H55C = 109.5
 C53 - C56 - H56A = 109.5
 C53 - C56 - H56B = 109.5
 H56A - C56 - H56B = 109.5
 C53 - C56 - H56C = 109.5
 H56A - C56 - H56C = 109.5
 H56B - C56 - H56C = 109.5
 C58 - C57 - C50 = 111.7(3)
 C58 - C57 - C59 = 107.6(3)
 C50 - C57 - C59 = 111.1(3)
 C58 - C57 - C60 = 107.6(3)
 C50 - C57 - C60 = 109.5(3)
 C59 - C57 - C60 = 109.3(3)
 C57 - C58 - H58A = 109.5
 C57 - C58 - H58B = 109.5
 H58A - C58 - H58B = 109.5
 C57 - C58 - H58C = 109.5
 H58A - C58 - H58C = 109.5
 H58B - C58 - H58C = 109.5
 C57 - C59 - H59A = 109.5
 C57 - C59 - H59B = 109.5
 H59A - C59 - H59B = 109.5
 C57 - C59 - H59C = 109.5
 H59A - C59 - H59C = 109.5
 H59B - C59 - H59C = 109.5
 C57 - C60 - H60A = 109.5
 C57 - C60 - H60B = 109.5
 H60A - C60 - H60B = 109.5
 C57 - C60 - H60C = 109.5
 H60A - C60 - H60C = 109.5
 H60B - C60 - H60C = 109.5
 C62 - N61 - C66 = 118.2(3)
 C62 - N61 - Zn1 = 126.0(3)
 C66 - N61 - Zn1 = 115.5(2)
 N61 - C62 - C63 = 122.8(4)
 N61 - C62 - H62 = 118.6
 C63 - C62 - H62 = 118.6
 C62 - C63 - C64 = 119.6(4)
 C62 - C63 - H63 = 120.2
 C64 - C63 - H63 = 120.2
 C63 - C64 - C65 = 117.2(4)

C63	- C64	- H64	= 121.4
C65	- C64	- H64	= 121.4
C66	- C65	- C64	= 120.1(4)
C66	- C65	- Br1	= 118.5(3)
C64	- C65	- Br1	= 121.4(3)
N61	- C66	- C65	= 122.1(4)
N61	- C66	- H66	= 119.0
C65	- C66	- H66	= 119.0

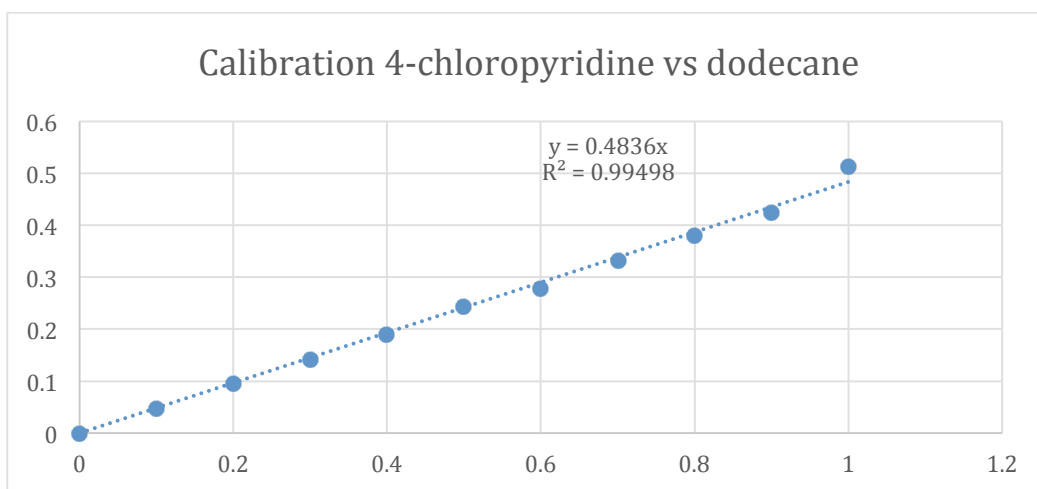
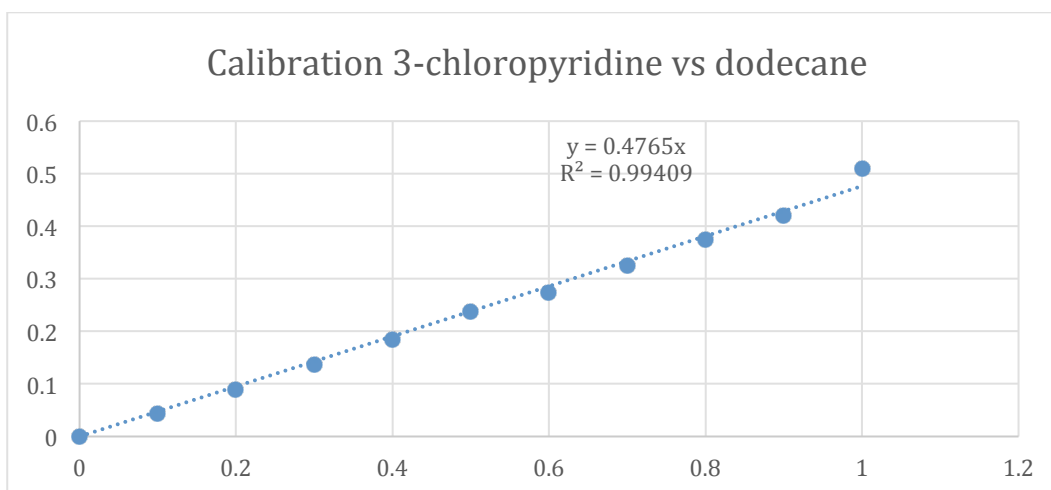
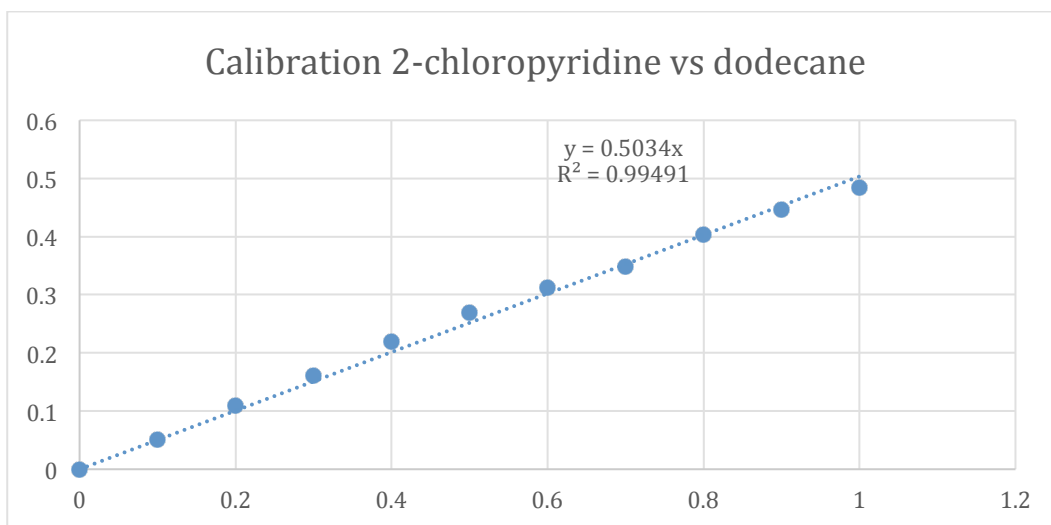
S10.6. Torsion angles [°].

C41	- C1	- C2	- C3	= -2.1(5)
C1	- C2	- C3	- C43	= -0.6(5)
C1	- C2	- C3	- N4	= -178.2(3)
C2	- C3	- N4	- C5	= 2.0(5)
C43	- C3	- N4	- C5	= -175.7(3)
C2	- C3	- N4	- Zn1	= -176.8(3)
C43	- C3	- N4	- Zn1	= 5.6(3)
C3	- N4	- C5	- C6	= 175.4(3)
Zn1	- N4	- C5	- C6	= -6.0(5)
N4	- C5	- C6	- C11	= -179.0(3)
N4	- C5	- C6	- C7	= -2.1(5)
C11	- C6	- C7	- O12	= -178.5(3)
C5	- C6	- C7	- O12	= 4.8(5)
C11	- C6	- C7	- C8	= 1.9(4)
C5	- C6	- C7	- C8	= -174.8(3)
O12	- C7	- C8	- C9	= 178.8(3)
C6	- C7	- C8	- C9	= -1.6(4)
O12	- C7	- C8	- C13	= -1.6(5)
C6	- C7	- C8	- C13	= 178.0(3)
C7	- C8	- C9	- C10	= 0.2(5)
C13	- C8	- C9	- C10	= -179.4(3)
C8	- C9	- C10	- C11	= 0.9(5)
C8	- C9	- C10	- C17	= -177.1(3)
C9	- C10	- C11	- C6	= -0.6(5)
C17	- C10	- C11	- C6	= 177.5(3)
C7	- C6	- C11	- C10	= -0.8(5)
C5	- C6	- C11	- C10	= 176.2(3)
C6	- C7	- O12	- Zn1	= 1.7(5)
C8	- C7	- O12	- Zn1	= -178.7(2)
C9	- C8	- C13	- C16	= -2.4(4)
C7	- C8	- C13	- C16	= 178.0(3)
C9	- C8	- C13	- C15	= -121.7(3)
C7	- C8	- C13	- C15	= 58.7(4)
C9	- C8	- C13	- C14	= 117.4(3)
C7	- C8	- C13	- C14	= -62.2(4)
C11	- C10	- C17	- C19	= -72.1(4)
C9	- C10	- C17	- C19	= 105.8(4)
C11	- C10	- C17	- C18	= 166.4(3)
C9	- C10	- C17	- C18	= -15.7(5)

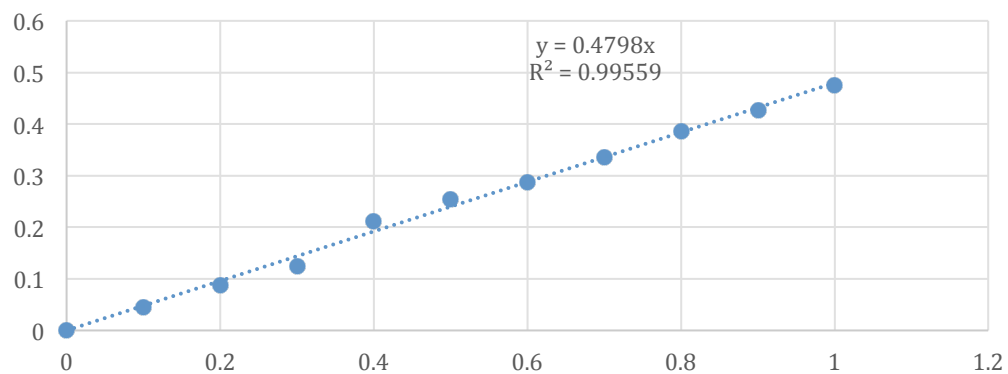
C11	- C10	- C17	- C20	= 47.6(5)
C9	- C10	- C17	- C20	= -134.4(4)
C2	- C1	- C41	- C42	= 2.1(5)
C1	- C41	- C42	- C43	= 0.6(5)
C41	- C42	- C43	- N44	= 174.7(3)
C41	- C42	- C43	- C3	= -3.3(5)
C2	- C3	- C43	- C42	= 3.3(5)
N4	- C3	- C43	- C42	= -178.9(3)
C2	- C3	- C43	- N44	= -174.8(3)
N4	- C3	- C43	- N44	= 3.0(4)
C42	- C43	- N44	- C45	= -13.1(5)
C3	- C43	- N44	- C45	= 164.9(3)
C42	- C43	- N44	- Zn1	= 171.9(3)
C3	- C43	- N44	- Zn1	= -10.1(3)
C43	- N44	- C45	- C46	= -175.1(3)
Zn1	- N44	- C45	- C46	= -0.7(5)
N44	- C45	- C46	- C47	= -173.3(3)
N44	- C45	- C46	- C51	= 7.7(5)
C45	- C46	- C47	- C48	= 179.1(3)
C51	- C46	- C47	- C48	= -1.8(5)
C46	- C47	- C48	- C49	= 1.0(5)
C46	- C47	- C48	- C53	= -178.7(3)
C47	- C48	- C49	- C50	= -0.4(5)
C53	- C48	- C49	- C50	= 179.3(3)
C48	- C49	- C50	- C51	= 0.5(5)
C48	- C49	- C50	- C57	= -176.9(3)
C47	- C46	- C51	- O52	= -177.7(3)
C45	- C46	- C51	- O52	= 1.3(5)
C47	- C46	- C51	- C50	= 1.8(5)
C45	- C46	- C51	- C50	= -179.2(3)
C49	- C50	- C51	- O52	= 178.3(3)
C57	- C50	- C51	- O52	= -4.3(5)
C49	- C50	- C51	- C46	= -1.2(5)
C57	- C50	- C51	- C46	= 176.3(3)
C46	- C51	- O52	- Zn1	= -17.7(5)
C50	- C51	- O52	- Zn1	= 162.8(2)
C47	- C48	- C53	- C54	= 9.3(5)
C49	- C48	- C53	- C54	= -170.5(3)
C47	- C48	- C53	- C56	= -113.6(4)
C49	- C48	- C53	- C56	= 66.7(4)
C47	- C48	- C53	- C55	= 128.0(4)
C49	- C48	- C53	- C55	= -51.8(4)
C49	- C50	- C57	- C58	= 0.2(4)
C51	- C50	- C57	- C58	= -177.2(3)
C49	- C50	- C57	- C59	= -119.9(3)
C51	- C50	- C57	- C59	= 62.7(4)
C49	- C50	- C57	- C60	= 119.2(3)
C51	- C50	- C57	- C60	= -58.2(4)
C66	- N61	- C62	- C63	= 0.1(6)
Zn1	- N61	- C62	- C63	= -173.6(3)

N61	- C62	- C63	- C64	= 1.3(6)
C62	- C63	- C64	- C65	= -0.9(6)
C63	- C64	- C65	- C66	= -0.9(6)
C63	- C64	- C65	- Br1	= 179.6(3)
C62	- N61	- C66	- C65	= -1.9(5)
Zn1	- N61	- C66	- C65	= 172.4(3)
C64	- C65	- C66	- N61	= 2.4(6)
Br1	- C65	- C66	- N61	= -178.1(3)

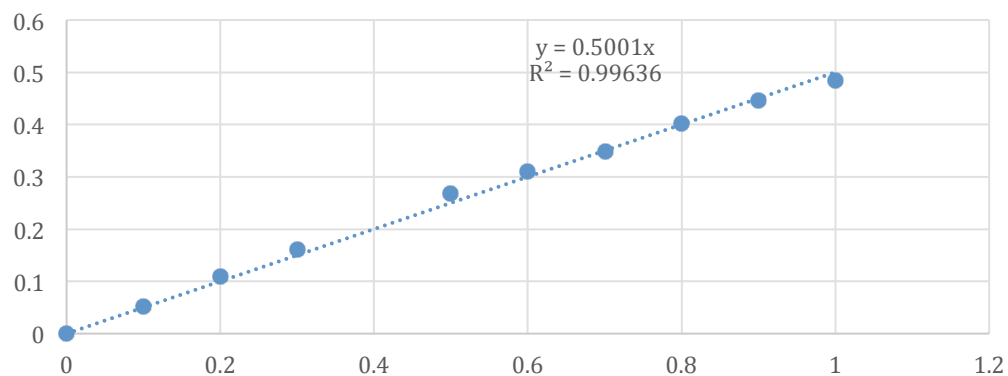
S11. Calibration curves.



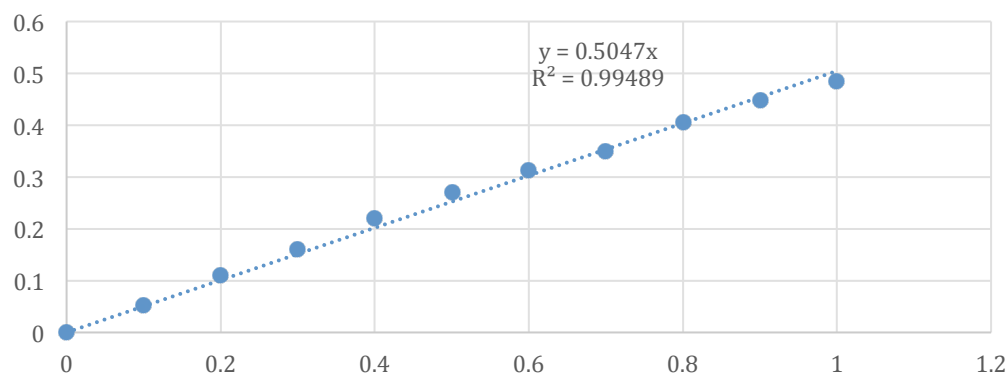
Calibration 2-bromopyridine vs dodecane



Calibration 3-bromopyridine vs dodecane



Calibration 4-bromopyridine vs dodecane



S12. References.

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[3] a) E. Busto V. Gotor-Fernández, V. Gotor, *Adv. Synth. Catal.* **2006**, *348*, 2626-2632; b) M. Mallet, G. Quéguiner, *Tetrahedron* **1982**, *38*, 3035-3042.

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