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Supplementary Information

Amido Analogues of Zincocenes and Cadmocenes

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Supplementary Information

Refinement Details and Structural Data for 1 and 2•C_7H_8 and Details of Calculations on 1, 1a and 2

Refinement Details and Structural data for **1**

Refinement Details and Structural data for **2**•C_7H_8

Details of Calculations

Refinement Details and Structural data for 1

Crystallographic Method

Crystals of **1** were mounted on a dual-stage glass fiber using YR-1800 perfluoropolyether oil (Lancaster) and cooled rapidly to 90 K in a stream of cold nitrogen using an Oxford Cryosystems low-temperature device. Data for compound **1** were collected on a Bruker SMART1000 diffractometer, equipped with a graphite-monochromated Mo-K_α radiation source (λ = 0.71073 Å). Absorption corrections were applied using a multi-scan method (SADABS).[1] All non-H atoms were located using direct methods[2] and difference Fourier syntheses. All fully occupied non-H atoms were refined with anisotropic displacement parameters. CCDC 783804 contains the supplementary data for **1**. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Refinement special details: We were unable to develop a split-atom disorder model for C52: the best description is a single atom with a prolate ellipsoid. We attribute the features which give rise to several validation Alerts to the existence of strong pseudosymmetry in the crystal structure. Although the space group indicated by analysis of systematic absences is $P2_12_12$, post-refinement analysis of the atomic positions indicates that 93% of these are compatible with *Pccn*, albeit within a wide agreement limit of 0.80 Angstroms.

Crystal data for **1**: $C_{56}H_{80}N_2Zn$, M_r = 846.59, 0.31 x 0.23 x 0.15 mm^3, orthorhombic, space group $P2_12_12$ (No. 19), a = 24.0248(12), b = 35.8255(17), c = 11.7851(6), V = 10143.4(9) Å^3, Z = 8, ρ_{calcd} = 1.109 g cm^{-3}; μ = 0.520 mm^{-1}, $Mo_{K\alpha}$ radiation, λ = 0.71073 Å, T = 90 K. 65071 reflections measured (23125 unique, R_{int} = 0.070, θ < 25°). Data were collected on a Bruker SMART1000 diffractometer and were corrected for absorption (transmission range 0.60-0.75). The structure was solved by direct methods and refined by full-matrix least-squares on F^2 to give wR_2 = 0.114 for all data and R_1 = 0.0448 for 15771 reflections with $I > 2\sigma(I)$, GooF = 1.04 for 1065 parameters. Min. and max. residual electron densities – 0.69 and 0.59 e/Å^3.

Table S1. Crystal data and structure refinement for **1**.

Identification code	ZNRMLC	
Empirical formula	C56 H80 N2 Zn	
Formula weight	846.59	
Temperature	90(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 2	
Unit cell dimensions	a = 24.0248(12) Å	α = 90°.
	b = 35.8255(17) Å	β = 90°.
	c = 11.7851(6) Å	γ = 90°.
Volume	10143.4(9) $Å^3$	
Z	8	
Density (calculated)	1.109 Mg/m^3	
Absorption coefficient	0.520 mm^{-1}	
F(000)	3680	
Crystal size	0.31 x 0.23 x 0.15 mm^3	
Theta range for data collection	1.02 to 27.48°.	
Index ranges	-27<=h<=31, -46<=k<=30, -13<=l<=15	
Reflections collected	65071	
Independent reflections	23125 [R(int) = 0.070]	
Completeness to theta = 25.03°	99.9 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.746 and 0.595	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	17883 / 1100 / 1065	
Goodness-of-fit on F^2	1.04	
Final R indices [I>2sigma(I)]	R1 = 0.0448, wR2 = 0.0947	
R indices (all data)	R1 = 0.0782, wR2 = 0.114	
Absolute structure parameter	0.464(10)	
Largest diff. peak and hole	0.59 and -0.69 $e.Å^{-3}$	

Table S2. Bond lengths [Å] and angles [°] for **1**.

Zn(1)-N(1)	1.867(3)
Zn(1)-N(2)	1.886(3)
N(1)-C(1)	1.427(4)
N(1)-C(12)	1.436(5)
C(1)-C(6)	1.405(5)
C(1)-C(2)	1.411(5)
Zn(2)-N(3)	1.870(3)
Zn(2)-N(4)	1.887(3)
N(2)-C(29)	1.430(4)
N(2)-C(40)	1.452(5)
C(2)-C(3)	1.407(5)
C(2)-C(13)	1.534(5)
N(3)-C(68)	1.431(4)
N(3)-C(57)	1.436(4)
C(3)-C(4)	1.399(5)
N(4)-C(85)	1.435(5)
N(4)-C(96)	1.435(4)
C(4)-C(5)	1.385(5)
C(4)-C(17)	1.544(5)
C(5)-C(6)	1.391(5)
C(6)-C(7)	1.437(5)
C(7)-C(8)	1.394(5)
C(7)-C(12)	1.413(5)
C(8)-C(9)	1.379(5)
C(9)-C(10)	1.401(5)
C(9)-C(21)	1.533(5)
C(10)-C(11)	1.396(5)
C(11)-C(12)	1.422(5)
C(11)-C(25)	1.544(5)
C(13)-C(16)	1.535(5)
C(13)-C(14)	1.538(5)
C(13)-C(15)	1.540(5)
C(17)-C(18)	1.524(6)
C(17)-C(19)	1.534(6)
C(17)-C(20)	1.537(5)
C(21)-C(24)	1.537(6)
C(21)-C(22)	1.537(6)
C(21)-C(23)	1.539(6)

C(25)-C(27)	1.528(5)
C(25)-C(28)	1.539(5)
C(25)-C(26)	1.553(5)
C(29)-C(30)	1.409(5)
C(29)-C(34)	1.412(5)
C(30)-C(31)	1.395(5)
C(30)-C(41)	1.539(5)
C(31)-C(32)	1.402(5)
C(32)-C(33)	1.377(5)
C(32)-C(45)	1.548(5)
C(33)-C(34)	1.389(5)
C(34)-C(35)	1.450(5)
C(35)-C(36)	1.378(5)
C(35)-C(40)	1.412(5)
C(36)-C(37)	1.389(5)
C(37)-C(38)	1.408(5)
C(37)-C(49)	1.536(5)
C(38)-C(39)	1.387(5)
C(39)-C(40)	1.407(5)
C(39)-C(53)	1.542(5)
C(41)-C(44)	1.534(5)
C(41)-C(42)	1.540(5)
C(41)-C(43)	1.542(5)
C(45)-C(46)	1.503(6)
C(45)-C(47)	1.516(6)
C(45)-C(48)	1.523(6)
C(49)-C(52)	1.527(6)
C(49)-C(50)	1.532(5)
C(49)-C(51)	1.542(5)
C(53)-C(55)	1.519(5)
C(53)-C(54)	1.529(5)
C(53)-C(56)	1.542(5)
C(57)-C(58)	1.412(5)
C(57)-C(62)	1.416(5)
C(58)-C(59)	1.387(5)
C(58)-C(69)	1.561(5)
C(59)-C(60)	1.408(5)
C(60)-C(61)	1.390(5)
C(60)-C(73)	1.530(5)
C(61)-C(62)	1.386(5)

C(62)-C(63)	1.450(5)
C(63)-C(64)	1.389(5)
C(63)-C(68)	1.400(5)
C(64)-C(65)	1.385(5)
C(65)-C(66)	1.400(5)
C(65)-C(77)	1.553(5)
C(66)-C(67)	1.404(5)
C(67)-C(68)	1.418(5)
C(67)-C(81)	1.533(5)
C(69)-C(70)	1.522(5)
C(69)-C(72)	1.536(5)
C(69)-C(71)	1.548(5)
C(73)-C(74)	1.530(6)
C(73)-C(76)	1.540(6)
C(73)-C(75)	1.541(6)
C(77)-C(80)	1.529(5)
C(77)-C(79)	1.531(5)
C(77)-C(78)	1.532(6)
C(81)-C(82)	1.533(5)
C(81)-C(83)	1.538(5)
C(81)-C(84)	1.539(5)
C(85)-C(86)	1.407(5)
C(85)-C(90)	1.408(5)
C(86)-C(87)	1.395(5)
C(86)-C(97)	1.548(5)
C(87)-C(88)	1.407(5)
C(88)-C(89)	1.389(5)
C(88)-C(101)	1.527(5)
C(89)-C(90)	1.390(5)
C(90)-C(91)	1.439(5)
C(91)-C(92)	1.396(5)
C(91)-C(96)	1.407(5)
C(92)-C(93)	1.387(5)
C(93)-C(94)	1.406(5)
C(93)-C(105)	1.537(5)
C(94)-C(95)	1.397(5)
C(95)-C(96)	1.411(5)
C(95)-C(109)	1.537(5)
C(97)-C(100)	1.527(5)
C(97)-C(99)	1.531(5)

C(97)-C(98)	1.533(5)
C(101)-C(104)	1.527(6)
C(101)-C(102)	1.532(6)
C(101)-C(103)	1.537(5)
C(105)-C(106)	1.519(6)
C(105)-C(108)	1.521(6)
C(105)-C(107)	1.547(6)
C(109)-C(111)	1.530(5)
C(109)-C(112)	1.539(5)
C(109)-C(110)	1.542(5)

N(1)-Zn(1)-N(2)	169.03(12)
C(1)-N(1)-C(12)	104.7(3)
C(1)-N(1)-Zn(1)	116.8(2)
C(12)-N(1)-Zn(1)	108.0(2)
C(6)-C(1)-C(2)	120.6(3)
C(6)-C(1)-N(1)	110.6(3)
C(2)-C(1)-N(1)	128.7(3)
N(3)-Zn(2)-N(4)	169.50(13)
C(29)-N(2)-C(40)	104.4(3)
C(29)-N(2)-Zn(1)	114.6(2)
C(40)-N(2)-Zn(1)	103.1(2)
C(3)-C(2)-C(1)	115.2(3)
C(3)-C(2)-C(13)	120.2(3)
C(1)-C(2)-C(13)	124.6(3)
C(68)-N(3)-C(57)	104.7(3)
C(68)-N(3)-Zn(2)	116.9(2)
C(57)-N(3)-Zn(2)	107.0(2)
C(4)-C(3)-C(2)	125.2(3)
C(85)-N(4)-C(96)	104.5(3)
C(85)-N(4)-Zn(2)	105.3(2)
C(96)-N(4)-Zn(2)	114.6(2)
C(5)-C(4)-C(3)	117.4(3)
C(5)-C(4)-C(17)	120.0(3)
C(3)-C(4)-C(17)	122.6(3)
C(4)-C(5)-C(6)	120.2(3)
C(5)-C(6)-C(1)	121.3(3)
C(5)-C(6)-C(7)	131.4(3)
C(1)-C(6)-C(7)	107.3(3)
C(8)-C(7)-C(12)	122.2(4)

C(8)-C(7)-C(6)	130.5(4)
C(12)-C(7)-C(6)	106.9(3)
C(9)-C(8)-C(7)	119.8(4)
C(8)-C(9)-C(10)	117.1(3)
C(8)-C(9)-C(21)	123.4(4)
C(10)-C(9)-C(21)	119.3(3)
C(11)-C(10)-C(9)	126.1(4)
C(10)-C(11)-C(12)	115.3(3)
C(10)-C(11)-C(25)	117.2(3)
C(12)-C(11)-C(25)	127.2(3)
C(7)-C(12)-C(11)	119.3(3)
C(7)-C(12)-N(1)	110.3(3)
C(11)-C(12)-N(1)	130.1(3)
C(2)-C(13)-C(16)	112.7(3)
C(2)-C(13)-C(14)	110.2(3)
C(16)-C(13)-C(14)	106.2(3)
C(2)-C(13)-C(15)	110.1(3)
C(16)-C(13)-C(15)	106.9(3)
C(14)-C(13)-C(15)	110.5(3)
C(18)-C(17)-C(19)	108.8(4)
C(18)-C(17)-C(20)	107.7(3)
C(19)-C(17)-C(20)	109.1(3)
C(18)-C(17)-C(4)	112.8(3)
C(19)-C(17)-C(4)	109.4(3)
C(20)-C(17)-C(4)	109.0(3)
C(9)-C(21)-C(24)	108.5(3)
C(9)-C(21)-C(22)	111.8(3)
C(24)-C(21)-C(22)	108.8(3)
C(9)-C(21)-C(23)	110.7(3)
C(24)-C(21)-C(23)	109.1(4)
C(22)-C(21)-C(23)	107.8(4)
C(27)-C(25)-C(28)	107.2(3)
C(27)-C(25)-C(11)	115.7(3)
C(28)-C(25)-C(11)	110.0(3)
C(27)-C(25)-C(26)	107.2(3)
C(28)-C(25)-C(26)	109.2(3)
C(11)-C(25)-C(26)	107.4(3)
C(30)-C(29)-C(34)	119.8(3)
C(30)-C(29)-N(2)	129.6(3)
C(34)-C(29)-N(2)	110.6(3)

C(31)-C(30)-C(29)	115.9(3)
C(31)-C(30)-C(41)	120.3(3)
C(29)-C(30)-C(41)	123.7(3)
C(30)-C(31)-C(32)	124.9(4)
C(33)-C(32)-C(31)	118.0(3)
C(33)-C(32)-C(45)	120.2(3)
C(31)-C(32)-C(45)	121.7(3)
C(32)-C(33)-C(34)	119.5(4)
C(33)-C(34)-C(29)	121.9(3)
C(33)-C(34)-C(35)	130.6(4)
C(29)-C(34)-C(35)	107.4(3)
C(36)-C(35)-C(40)	121.6(4)
C(36)-C(35)-C(34)	131.7(4)
C(40)-C(35)-C(34)	106.6(3)
C(35)-C(36)-C(37)	119.6(4)
C(36)-C(37)-C(38)	117.3(4)
C(36)-C(37)-C(49)	119.6(4)
C(38)-C(37)-C(49)	123.2(4)
C(39)-C(38)-C(37)	125.4(4)
C(38)-C(39)-C(40)	115.1(3)
C(38)-C(39)-C(53)	120.8(3)
C(40)-C(39)-C(53)	123.9(3)
C(39)-C(40)-C(35)	120.4(3)
C(39)-C(40)-N(2)	129.0(3)
C(35)-C(40)-N(2)	110.4(3)
C(44)-C(41)-C(30)	112.6(3)
C(44)-C(41)-C(42)	107.2(3)
C(30)-C(41)-C(42)	108.7(3)
C(44)-C(41)-C(43)	106.5(3)
C(30)-C(41)-C(43)	111.6(3)
C(42)-C(41)-C(43)	110.2(3)
C(46)-C(45)-C(47)	110.1(4)
C(46)-C(45)-C(48)	108.4(4)
C(47)-C(45)-C(48)	107.3(4)
C(46)-C(45)-C(32)	110.5(3)
C(47)-C(45)-C(32)	108.3(3)
C(48)-C(45)-C(32)	112.2(3)
C(52)-C(49)-C(50)	108.9(4)
C(52)-C(49)-C(37)	109.0(3)
C(50)-C(49)-C(37)	113.2(3)

C(52)-C(49)-C(51)	108.9(4)
C(50)-C(49)-C(51)	108.3(3)
C(37)-C(49)-C(51)	108.4(4)
C(55)-C(53)-C(54)	107.9(3)
C(55)-C(53)-C(56)	107.7(3)
C(54)-C(53)-C(56)	109.0(3)
C(55)-C(53)-C(39)	112.0(3)
C(54)-C(53)-C(39)	109.5(3)
C(56)-C(53)-C(39)	110.7(3)
C(58)-C(57)-C(62)	119.4(3)
C(58)-C(57)-N(3)	130.1(3)
C(62)-C(57)-N(3)	110.3(3)
C(59)-C(58)-C(57)	115.9(3)
C(59)-C(58)-C(69)	116.7(3)
C(57)-C(58)-C(69)	126.9(3)
C(58)-C(59)-C(60)	125.8(3)
C(61)-C(60)-C(59)	116.9(4)
C(61)-C(60)-C(73)	123.4(3)
C(59)-C(60)-C(73)	119.7(3)
C(62)-C(61)-C(60)	119.7(4)
C(61)-C(62)-C(57)	122.2(3)
C(61)-C(62)-C(63)	131.0(3)
C(57)-C(62)-C(63)	106.6(3)
C(64)-C(63)-C(68)	122.3(3)
C(64)-C(63)-C(62)	130.4(3)
C(68)-C(63)-C(62)	107.3(3)
C(65)-C(64)-C(63)	118.7(3)
C(64)-C(65)-C(66)	118.8(3)
C(64)-C(65)-C(77)	119.0(3)
C(66)-C(65)-C(77)	122.1(3)
C(65)-C(66)-C(67)	124.6(3)
C(66)-C(67)-C(68)	115.0(3)
C(66)-C(67)-C(81)	120.8(3)
C(68)-C(67)-C(81)	124.2(3)
C(63)-C(68)-C(67)	120.5(3)
C(63)-C(68)-N(3)	110.8(3)
C(67)-C(68)-N(3)	128.6(3)
C(70)-C(69)-C(72)	107.6(3)
C(70)-C(69)-C(71)	107.4(3)
C(72)-C(69)-C(71)	110.0(3)

C(70)-C(69)-C(58)	115.5(3)
C(72)-C(69)-C(58)	107.0(3)
C(71)-C(69)-C(58)	109.3(3)
C(60)-C(73)-C(74)	112.6(3)
C(60)-C(73)-C(76)	109.9(3)
C(74)-C(73)-C(76)	107.7(4)
C(60)-C(73)-C(75)	108.6(3)
C(74)-C(73)-C(75)	108.5(3)
C(76)-C(73)-C(75)	109.4(4)
C(80)-C(77)-C(79)	107.9(3)
C(80)-C(77)-C(78)	108.6(4)
C(79)-C(77)-C(78)	108.9(3)
C(80)-C(77)-C(65)	112.9(3)
C(79)-C(77)-C(65)	108.4(3)
C(78)-C(77)-C(65)	110.0(3)
C(67)-C(81)-C(82)	112.2(3)
C(67)-C(81)-C(83)	111.1(3)
C(82)-C(81)-C(83)	106.8(3)
C(67)-C(81)-C(84)	109.8(3)
C(82)-C(81)-C(84)	106.6(3)
C(83)-C(81)-C(84)	110.3(3)
C(86)-C(85)-C(90)	119.8(3)
C(86)-C(85)-N(4)	129.2(3)
C(90)-C(85)-N(4)	110.8(3)
C(87)-C(86)-C(85)	115.9(3)
C(87)-C(86)-C(97)	120.0(3)
C(85)-C(86)-C(97)	124.0(3)
C(86)-C(87)-C(88)	125.1(4)
C(89)-C(88)-C(87)	117.2(3)
C(89)-C(88)-C(101)	119.8(3)
C(87)-C(88)-C(101)	122.9(3)
C(88)-C(89)-C(90)	119.6(4)
C(89)-C(90)-C(85)	121.8(3)
C(89)-C(90)-C(91)	131.6(3)
C(85)-C(90)-C(91)	106.5(3)
C(92)-C(91)-C(96)	121.8(3)
C(92)-C(91)-C(90)	130.4(3)
C(96)-C(91)-C(90)	107.8(3)
C(93)-C(92)-C(91)	119.1(3)
C(92)-C(93)-C(94)	117.9(3)

C(92)-C(93)-C(105)	121.4(3)
C(94)-C(93)-C(105)	120.8(3)
C(95)-C(94)-C(93)	125.4(3)
C(94)-C(95)-C(96)	115.0(3)
C(94)-C(95)-C(109)	119.9(3)
C(96)-C(95)-C(109)	125.0(3)
C(91)-C(96)-C(95)	120.7(3)
C(91)-C(96)-N(4)	110.1(3)
C(95)-C(96)-N(4)	129.0(3)
C(100)-C(97)-C(99)	106.5(3)
C(100)-C(97)-C(98)	107.9(3)
C(99)-C(97)-C(98)	109.7(3)
C(100)-C(97)-C(86)	112.1(3)
C(99)-C(97)-C(86)	109.6(3)
C(98)-C(97)-C(86)	110.8(3)
C(88)-C(101)-C(104)	109.1(3)
C(88)-C(101)-C(102)	110.0(4)
C(104)-C(101)-C(102)	110.7(4)
C(88)-C(101)-C(103)	113.1(3)
C(104)-C(101)-C(103)	107.5(4)
C(102)-C(101)-C(103)	106.4(3)
C(106)-C(105)-C(108)	108.1(4)
C(106)-C(105)-C(93)	111.8(3)
C(108)-C(105)-C(93)	111.8(3)
C(106)-C(105)-C(107)	110.3(4)
C(108)-C(105)-C(107)	107.1(4)
C(93)-C(105)-C(107)	107.6(3)
C(111)-C(109)-C(95)	112.5(3)
C(111)-C(109)-C(112)	107.0(3)
C(95)-C(109)-C(112)	109.6(3)
C(111)-C(109)-C(110)	106.6(3)
C(95)-C(109)-C(110)	111.0(3)
C(112)-C(109)-C(110)	109.9(3)

Refinement Details and Structural data for 2•C_7H_8

Crystallographic Method

Crystals of **2**•C_7H_8 were mounted on a dual-stage glass fiber using YR-1800 perfluoropolyether oil (Lancaster) and cooled rapidly to 150 K in a stream of cold nitrogen using an Oxford Cryosystems low-temperature device. Data for compound **2**•C_7H_8 were collected on a Bruker SMART1000 diffractometer, equipped with a graphite-monochromated Mo-K_α radiation source (λ = 0.71073 Å). Absorption corrections were applied using a multi-scan method (SADABS).[1] All non-H atoms were located using direct methods[2] and difference Fourier syntheses. All fully occupied non-H atoms were refined with anisotropic displacement parameters. CCDC 783805 contains the supplementary data for **2**•C_7H_8. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

Refinement special details: The lattice toluene molecule was disordered over three positions. The disorder was successfully modelled using 39:33:28 occupancy levels, isotropic displacement parameters and optimised bond geometries.

Crystal data for **2**•C_7H_8: $C_{56}H_{80}CdN_2$•C_7H_8, M_r = 985.75, 0.26 x 0.16 x 0.05 mm^3, triclinic, space group *P*-1 (No. 2), a = 12.192(2), b = 14.983(3), c = 16.507(3), α = 68.19(3), β = 82.75(3), γ = 81.36(3), V = 2759.5(10) Å^3, Z = 2, ρ_{calcd} = 1.186 g cm^{-3}; μ = 0.435 mm^{-1}, $Mo_{K\alpha}$ radiation, λ = 0.71073 Å, T = 150 K. 24741 reflections measured, (12387 unique, R_{int} = 0.040, θ < 27.5°). Data were collected on a Bruker SMART1000 diffractometer and were corrected for absorption (transmission range 0.70-0.75). The structure was solved by direct methods and refined by full-matrix least-squares on F^2 to give wR_2 = 0.179 for all data and R_1 = 0.0581 for 7795 reflections with $I > 2\sigma(I)$, GooF = 1.02 for 622 parameters. Min. and max. residual electron densities –0.71 and 1.39 e/Å^3.

Table S3. Crystal data and structure refinement for **2**•C_7H_8.

Identification code	CDCBTB	
Empirical formula	C63 H88 Cd N2	
Formula weight	985.75	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 12.192(2) Å	α = 68.19(3)°.
	b = 14.983(3) Å	β = 82.75(3)°.
	c = 16.507(3) Å	γ = 81.36(3)°.
Volume	2759.5(10) $Å^3$	
Z	2	
Density (calculated)	1.186 Mg/m^3	
Absorption coefficient	0.435 mm^{-1}	
F(000)	1056	
Crystal size	0.26 x 0.16 x 0.05 mm^3	
Theta range for data collection	1.33 to 27.50°.	
Index ranges	-15<=h<=15, -19<=k<=19, -21<=l<=21	
Reflections collected	24741	
Independent reflections	12387 [R(int) = 0.040]	
Completeness to theta = 27.50°	97.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6956	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12387 / 22 / 622	
Goodness-of-fit on F^2	1.02	
Final R indices [I>2sigma(I)]	R1 = 0.0581, wR2 = 0.150	
R indices (all data)	R1 = 0.103, wR2 = 0.179	
Largest diff. peak and hole	0.71 and -1.39 e.$Å^{-3}$	

Table S4. Bond lengths [Å] and angles [°] for **2**•C_7H_8.

Cd(1)-N(1)	2.107(4)
Cd(1)-C(11)	2.703(4)
Cd(1)-C(12)	2.710(4)
N(1)-C(11)	1.419(5)
N(1)-C(12)	1.420(5)
C(1)-C(2)	1.393(6)
C(1)-C(12)	1.418(6)
C(1)-C(14)	1.530(6)
Cd(2)-N(2)	2.117(4)
Cd(2)-C(39)	2.667(4)
Cd(2)-C(40)	2.679(4)
N(2)-C(40)	1.420(5)
N(2)-C(39)	1.424(5)
C(2)-C(3)	1.398(6)
C(2)-H(2)	0.9500
C(3)-C(4)	1.381(6)
C(3)-C(17)	1.555(6)
C(4)-C(5)	1.389(6)
C(4)-H(4)	0.9500
C(5)-C(12)	1.411(6)
C(5)-C(6)	1.457(6)
C(6)-C(7)	1.388(6)
C(6)-C(11)	1.407(6)
C(7)-C(8)	1.383(6)
C(7)-H(7)	0.9500
C(8)-C(9)	1.422(6)
C(8)-C(21)	1.540(6)
C(9)-C(10)	1.383(6)
C(9)-H(9)	0.9500
C(10)-C(11)	1.411(6)
C(10)-C(25)	1.544(6)
C(13)-C(14)	1.526(7)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-C(15)	1.523(7)
C(14)-C(16)	1.534(7)
C(15)-H(15A)	0.9800

C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-H(16A)	0.9800
C(16)-H(16B)	0.9800
C(16)-H(16C)	0.9800
C(17)-C(19)	1.513(7)
C(17)-C(18)	1.524(7)
C(17)-C(20)	1.536(7)
C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(24)	1.531(6)
C(21)-C(22)	1.533(6)
C(21)-C(23)	1.542(6)
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(27)	1.521(7)
C(25)-C(28)	1.527(6)
C(25)-C(26)	1.534(6)
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-H(28A)	0.9800
C(28)-H(28B)	0.9800

C(28)-H(28C)	0.9800
C(29)-C(30)	1.380(6)
C(29)-C(40)	1.424(5)
C(29)-C(41)	1.533(6)
C(30)-C(31)	1.423(6)
C(30)-H(30)	0.9500
C(31)-C(32)	1.382(5)
C(31)-C(45)	1.532(6)
C(32)-C(33)	1.403(6)
C(32)-H(32)	0.9500
C(33)-C(40)	1.392(6)
C(33)-C(34)	1.455(5)
C(34)-C(35)	1.390(6)
C(34)-C(39)	1.402(6)
C(35)-C(36)	1.386(6)
C(35)-H(35)	0.9500
C(36)-C(37)	1.405(6)
C(36)-C(49)	1.547(6)
C(37)-C(38)	1.391(6)
C(37)-H(37)	0.9500
C(38)-C(39)	1.416(5)
C(38)-C(53)	1.531(6)
C(41)-C(42)	1.513(6)
C(41)-C(43)	1.534(6)
C(41)-C(44)	1.539(6)
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(44)-H(44A)	0.9800
C(44)-H(44B)	0.9800
C(44)-H(44C)	0.9800
C(45)-C(47)	1.523(6)
C(45)-C(48)	1.528(6)
C(45)-C(46)	1.533(6)
C(46)-H(46A)	0.9800
C(46)-H(46B)	0.9800
C(46)-H(46C)	0.9800

C(47)-H(47A)	0.9800
C(47)-H(47B)	0.9800
C(47)-H(47C)	0.9800
C(48)-H(48A)	0.9800
C(48)-H(48B)	0.9800
C(48)-H(48C)	0.9800
C(49)-C(51)	1.519(7)
C(49)-C(50)	1.523(7)
C(49)-C(52)	1.529(7)
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-H(51A)	0.9800
C(51)-H(51B)	0.9800
C(51)-H(51C)	0.9800
C(52)-H(52A)	0.9800
C(52)-H(52B)	0.9800
C(52)-H(52C)	0.9800
C(53)-C(55)	1.520(7)
C(53)-C(54)	1.528(6)
C(53)-C(56)	1.531(7)
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(56)-H(56A)	0.9800
C(56)-H(56B)	0.9800
C(56)-H(56C)	0.9800
C(100)-C(101)	1.3900
C(100)-C(105)	1.3900
C(100)-C(106)	1.474(12)
C(101)-C(102)	1.3900
C(101)-H(10A)	0.9500
C(102)-C(103)	1.3900
C(102)-H(10B)	0.9500
C(103)-C(104)	1.3900
C(103)-H(10C)	0.9500
C(104)-C(105)	1.3900

C(104)-H(10D)	0.9500
C(105)-H(10E)	0.9500
C(106)-H(10F)	0.9800
C(106)-H(10G)	0.9800
C(106)-H(10H)	0.9800
C(110)-C(115)	1.28(3)
C(110)-C(116)	1.473(16)
C(110)-C(111)	1.48(2)
C(111)-C(112)	1.4416
C(111)-H(11A)	0.9500
C(112)-C(113)	1.28(3)
C(112)-H(11C)	0.9501
C(113)-C(114)	1.44(4)
C(113)-H(11D)	0.9500
C(114)-C(115)	1.39(3)
C(114)-H(11F)	0.9500
C(115)-H(11G)	0.9500
C(116)-H(11H)	0.9800
C(116)-H(11I)	0.9800
C(116)-H(11J)	0.9800
C(200)-C(201)	1.3900
C(200)-C(205)	1.3900
C(200)-C(206)	1.469(12)
C(201)-C(202)	1.3900
C(201)-H(20D)	0.9500
C(202)-C(203)	1.3900
C(202)-H(20E)	0.9500
C(203)-C(204)	1.3900
C(203)-H(20F)	0.9500
C(204)-C(205)	1.3900
C(204)-H(20G)	0.9500
C(205)-H(20H)	0.9500
C(206)-H(20I)	0.9800
C(206)-H(20J)	0.9800
C(206)-H(20K)	0.9800

N(1)-Cd(1)-C(11)	31.30(12)
N(1)#1-Cd(1)-C(11)	148.70(12)
N(1)-Cd(1)-C(12)	31.20(12)
N(1)#1-Cd(1)-C(12)	148.80(12)

C(11)-Cd(1)-C(12)	49.02(12)
C(11)#1-Cd(1)-C(12)	130.98(12)
C(11)-N(1)-C(12)	104.6(3)
C(11)-N(1)-Cd(1)	98.2(2)
C(12)-N(1)-Cd(1)	98.5(3)
C(2)-C(1)-C(12)	114.4(4)
C(2)-C(1)-C(14)	122.1(4)
C(12)-C(1)-C(14)	123.3(4)
N(2)-Cd(2)-C(39)	32.08(12)
N(2)#2-Cd(2)-C(39)	147.92(12)
N(2)-Cd(2)-C(40)	31.79(12)
N(2)#2-Cd(2)-C(40)	148.21(12)
C(39)-Cd(2)-C(40)	49.64(12)
C(39)#2-Cd(2)-C(40)	130.36(12)
C(40)-N(2)-C(39)	104.2(3)
C(40)-N(2)-Cd(2)	96.5(2)
C(39)-N(2)-Cd(2)	95.8(2)
C(1)-C(2)-C(3)	125.0(4)
C(1)-C(2)-H(2)	117.5
C(3)-C(2)-H(2)	117.5
C(4)-C(3)-C(2)	119.0(4)
C(4)-C(3)-C(17)	121.8(4)
C(2)-C(3)-C(17)	119.1(4)
C(3)-C(4)-C(5)	118.7(4)
C(3)-C(4)-H(4)	120.6
C(5)-C(4)-H(4)	120.6
C(4)-C(5)-C(12)	121.3(4)
C(4)-C(5)-C(6)	132.4(4)
C(12)-C(5)-C(6)	106.2(4)
C(7)-C(6)-C(11)	120.7(4)
C(7)-C(6)-C(5)	132.9(4)
C(11)-C(6)-C(5)	106.3(4)
C(8)-C(7)-C(6)	119.7(4)
C(8)-C(7)-H(7)	120.2
C(6)-C(7)-H(7)	120.2
C(7)-C(8)-C(9)	118.2(4)
C(7)-C(8)-C(21)	122.9(4)
C(9)-C(8)-C(21)	118.9(4)
C(10)-C(9)-C(8)	124.2(4)
C(10)-C(9)-H(9)	117.9

C(8)-C(9)-H(9)	117.9
C(9)-C(10)-C(11)	115.4(4)
C(9)-C(10)-C(25)	121.9(4)
C(11)-C(10)-C(25)	122.5(4)
C(6)-C(11)-C(10)	121.4(4)
C(6)-C(11)-N(1)	111.4(3)
C(10)-C(11)-N(1)	127.2(4)
C(6)-C(11)-Cd(1)	107.8(3)
C(10)-C(11)-Cd(1)	109.7(3)
N(1)-C(11)-Cd(1)	50.5(2)
C(5)-C(12)-C(1)	121.2(4)
C(5)-C(12)-N(1)	111.3(3)
C(1)-C(12)-N(1)	127.5(4)
C(5)-C(12)-Cd(1)	107.9(3)
C(1)-C(12)-Cd(1)	109.0(3)
N(1)-C(12)-Cd(1)	50.3(2)
C(14)-C(13)-H(13A)	109.5
C(14)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(14)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(15)-C(14)-C(13)	108.1(4)
C(15)-C(14)-C(1)	113.6(4)
C(13)-C(14)-C(1)	107.9(4)
C(15)-C(14)-C(16)	106.1(4)
C(13)-C(14)-C(16)	109.9(5)
C(1)-C(14)-C(16)	111.2(4)
C(14)-C(15)-H(15A)	109.5
C(14)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(14)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(14)-C(16)-H(16A)	109.5
C(14)-C(16)-H(16B)	109.5
H(16A)-C(16)-H(16B)	109.5
C(14)-C(16)-H(16C)	109.5
H(16A)-C(16)-H(16C)	109.5
H(16B)-C(16)-H(16C)	109.5

C(19)-C(17)-C(18)	110.0(4)
C(19)-C(17)-C(20)	109.2(5)
C(18)-C(17)-C(20)	107.6(5)
C(19)-C(17)-C(3)	108.9(4)
C(18)-C(17)-C(3)	110.2(4)
C(20)-C(17)-C(3)	110.9(4)
C(17)-C(18)-H(18A)	109.5
C(17)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
C(17)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(17)-C(19)-H(19A)	109.5
C(17)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(17)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(17)-C(20)-H(20A)	109.5
C(17)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5
C(17)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(24)-C(21)-C(22)	108.5(4)
C(24)-C(21)-C(8)	108.7(4)
C(22)-C(21)-C(8)	111.7(4)
C(24)-C(21)-C(23)	109.4(4)
C(22)-C(21)-C(23)	107.7(4)
C(8)-C(21)-C(23)	110.9(3)
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
H(22A)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
H(22A)-C(22)-H(22C)	109.5
H(22B)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5

H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(21)-C(24)-H(24A)	109.5
C(21)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(21)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(27)-C(25)-C(28)	107.9(4)
C(27)-C(25)-C(26)	108.5(4)
C(28)-C(25)-C(26)	108.0(4)
C(27)-C(25)-C(10)	112.5(3)
C(28)-C(25)-C(10)	112.2(4)
C(26)-C(25)-C(10)	107.5(4)
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(25)-C(28)-H(28A)	109.5
C(25)-C(28)-H(28B)	109.5
H(28A)-C(28)-H(28B)	109.5
C(25)-C(28)-H(28C)	109.5
H(28A)-C(28)-H(28C)	109.5
H(28B)-C(28)-H(28C)	109.5
C(30)-C(29)-C(40)	115.0(4)
C(30)-C(29)-C(41)	123.3(4)
C(40)-C(29)-C(41)	121.6(4)
C(29)-C(30)-C(31)	124.8(4)
C(29)-C(30)-H(30)	117.6
C(31)-C(30)-H(30)	117.6
C(32)-C(31)-C(30)	118.0(4)
C(32)-C(31)-C(45)	122.2(4)

C(30)-C(31)-C(45)	119.8(3)
C(31)-C(32)-C(33)	119.3(4)
C(31)-C(32)-H(32)	120.3
C(33)-C(32)-H(32)	120.3
C(40)-C(33)-C(32)	121.0(4)
C(40)-C(33)-C(34)	106.7(3)
C(32)-C(33)-C(34)	132.3(4)
C(35)-C(34)-C(39)	120.9(4)
C(35)-C(34)-C(33)	133.0(4)
C(39)-C(34)-C(33)	106.1(3)
C(36)-C(35)-C(34)	119.0(4)
C(36)-C(35)-H(35)	120.5
C(34)-C(35)-H(35)	120.5
C(35)-C(36)-C(37)	118.9(4)
C(35)-C(36)-C(49)	121.8(4)
C(37)-C(36)-C(49)	119.3(4)
C(38)-C(37)-C(36)	124.4(4)
C(38)-C(37)-H(37)	117.8
C(36)-C(37)-H(37)	117.8
C(37)-C(38)-C(39)	114.9(4)
C(37)-C(38)-C(53)	122.1(4)
C(39)-C(38)-C(53)	123.0(4)
C(34)-C(39)-C(38)	121.7(4)
C(34)-C(39)-N(2)	111.2(3)
C(38)-C(39)-N(2)	127.1(4)
C(34)-C(39)-Cd(2)	105.3(3)
C(38)-C(39)-Cd(2)	110.4(3)
N(2)-C(39)-Cd(2)	52.1(2)
C(33)-C(40)-N(2)	111.5(3)
C(33)-C(40)-C(29)	121.6(4)
N(2)-C(40)-C(29)	126.9(4)
C(33)-C(40)-Cd(2)	105.2(3)
N(2)-C(40)-Cd(2)	51.7(2)
C(29)-C(40)-Cd(2)	110.9(3)
C(42)-C(41)-C(29)	108.8(4)
C(42)-C(41)-C(43)	109.3(4)
C(29)-C(41)-C(43)	112.1(3)
C(42)-C(41)-C(44)	108.1(4)
C(29)-C(41)-C(44)	111.9(3)
C(43)-C(41)-C(44)	106.6(4)

C(41)-C(42)-H(42A)	109.5
C(41)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(41)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(41)-C(43)-H(43A)	109.5
C(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5
C(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
C(41)-C(44)-H(44A)	109.5
C(41)-C(44)-H(44B)	109.5
H(44A)-C(44)-H(44B)	109.5
C(41)-C(44)-H(44C)	109.5
H(44A)-C(44)-H(44C)	109.5
H(44B)-C(44)-H(44C)	109.5
C(47)-C(45)-C(48)	107.3(4)
C(47)-C(45)-C(31)	111.6(4)
C(48)-C(45)-C(31)	111.9(3)
C(47)-C(45)-C(46)	109.3(4)
C(48)-C(45)-C(46)	108.0(4)
C(31)-C(45)-C(46)	108.6(4)
C(45)-C(46)-H(46A)	109.5
C(45)-C(46)-H(46B)	109.5
H(46A)-C(46)-H(46B)	109.5
C(45)-C(46)-H(46C)	109.5
H(46A)-C(46)-H(46C)	109.5
H(46B)-C(46)-H(46C)	109.5
C(45)-C(47)-H(47A)	109.5
C(45)-C(47)-H(47B)	109.5
H(47A)-C(47)-H(47B)	109.5
C(45)-C(47)-H(47C)	109.5
H(47A)-C(47)-H(47C)	109.5
H(47B)-C(47)-H(47C)	109.5
C(45)-C(48)-H(48A)	109.5
C(45)-C(48)-H(48B)	109.5
H(48A)-C(48)-H(48B)	109.5
C(45)-C(48)-H(48C)	109.5

H(48A)-C(48)-H(48C)	109.5
H(48B)-C(48)-H(48C)	109.5
C(51)-C(49)-C(50)	108.5(4)
C(51)-C(49)-C(52)	109.9(4)
C(50)-C(49)-C(52)	107.9(4)
C(51)-C(49)-C(36)	108.2(4)
C(50)-C(49)-C(36)	111.4(3)
C(52)-C(49)-C(36)	110.9(4)
C(49)-C(50)-H(50A)	109.5
C(49)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(49)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
C(49)-C(51)-H(51A)	109.5
C(49)-C(51)-H(51B)	109.5
H(51A)-C(51)-H(51B)	109.5
C(49)-C(51)-H(51C)	109.5
H(51A)-C(51)-H(51C)	109.5
H(51B)-C(51)-H(51C)	109.5
C(49)-C(52)-H(52A)	109.5
C(49)-C(52)-H(52B)	109.5
H(52A)-C(52)-H(52B)	109.5
C(49)-C(52)-H(52C)	109.5
H(52A)-C(52)-H(52C)	109.5
H(52B)-C(52)-H(52C)	109.5
C(55)-C(53)-C(54)	106.9(4)
C(55)-C(53)-C(38)	112.8(4)
C(54)-C(53)-C(38)	111.9(4)
C(55)-C(53)-C(56)	107.8(4)
C(54)-C(53)-C(56)	109.1(5)
C(38)-C(53)-C(56)	108.3(4)
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
H(54A)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
H(54A)-C(54)-H(54C)	109.5
H(54B)-C(54)-H(54C)	109.5
C(53)-C(55)-H(55A)	109.5
C(53)-C(55)-H(55B)	109.5

H(55A)-C(55)-H(55B)	109.5
C(53)-C(55)-H(55C)	109.5
H(55A)-C(55)-H(55C)	109.5
H(55B)-C(55)-H(55C)	109.5
C(53)-C(56)-H(56A)	109.5
C(53)-C(56)-H(56B)	109.5
H(56A)-C(56)-H(56B)	109.5
C(53)-C(56)-H(56C)	109.5
H(56A)-C(56)-H(56C)	109.5
H(56B)-C(56)-H(56C)	109.5
C(101)-C(100)-C(105)	120.0
C(101)-C(100)-C(106)	119.7(4)
C(105)-C(100)-C(106)	120.3(4)
C(102)-C(101)-C(100)	120.0
C(102)-C(101)-H(10A)	120.0
C(100)-C(101)-H(10A)	120.0
C(100)-C(101)-H(11C)	103.3
C(101)-C(102)-C(103)	120.0
C(101)-C(102)-H(10B)	120.0
C(103)-C(102)-H(10B)	120.0
C(104)-C(103)-C(102)	120.0
C(104)-C(103)-H(10C)	120.0
C(102)-C(103)-H(10C)	120.0
C(103)-C(104)-C(105)	120.0
C(103)-C(104)-H(10D)	120.0
C(105)-C(104)-H(10D)	120.0
C(104)-C(105)-C(100)	120.0
C(104)-C(105)-H(10E)	120.0
C(100)-C(105)-H(10E)	120.0
C(115)-C(110)-C(116)	128(2)
C(115)-C(110)-C(111)	118.4(19)
C(116)-C(110)-C(111)	113.8(15)
C(112)-C(111)-C(110)	112.0(9)
C(112)-C(111)-H(11A)	124.0
C(110)-C(111)-H(11A)	124.0
C(113)-C(112)-C(111)	132.4(15)
C(113)-C(112)-H(11C)	115.6
C(111)-C(112)-H(11C)	112.1
C(112)-C(113)-C(114)	111(2)
C(112)-C(113)-H(11D)	124.7

C(114)-C(113)-H(11D)	124.7
C(115)-C(114)-C(113)	123(2)
C(115)-C(114)-H(11F)	118.7
C(113)-C(114)-H(11F)	118.7
C(110)-C(115)-C(114)	124(3)
C(110)-C(115)-H(11G)	118.0
C(114)-C(115)-H(11G)	118.0
C(110)-C(116)-H(11H)	109.5
C(110)-C(116)-H(11I)	109.5
H(11H)-C(116)-H(11I)	109.5
C(110)-C(116)-H(11J)	109.5
H(11H)-C(116)-H(11J)	109.5
H(11I)-C(116)-H(11J)	109.5
C(201)-C(200)-C(205)	120.0
C(201)-C(200)-C(206)	119.4(4)
C(205)-C(200)-C(206)	120.5(4)
C(202)-C(201)-C(200)	120.0
C(202)-C(201)-H(20D)	120.0
C(200)-C(201)-H(20D)	120.0
C(201)-C(202)-C(203)	120.0
C(201)-C(202)-H(20E)	120.0
C(203)-C(202)-H(20E)	120.0
C(202)-C(203)-C(204)	120.0
C(202)-C(203)-H(20F)	120.0
C(204)-C(203)-H(20F)	120.0
C(203)-C(204)-C(205)	120.0
C(203)-C(204)-H(20G)	120.0
C(205)-C(204)-H(20G)	120.0
C(204)-C(205)-C(200)	120.0
C(204)-C(205)-H(20H)	120.0
C(200)-C(205)-H(20H)	120.0

Symmetry transformations used to generate equivalent atoms:

#1 -x+1,-y+1,-z+1 #2 -x+2,-y,-z

References

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DFT Calculations

Restricted geometry optimisations were performed for models of **1**, **1a** and **2** using coordinates derived from the X-ray crystal structures of these compounds. **1** was geometry optimised without constraints whereas **1a** and **2** were geometry optimised in C_i symmetry (the molecular symmetry of **2** as derived from X-ray crystallography). The calculations were performed using the Amsterdam Density Functional (ADF) suite version 2009.01.[1,2] The DFT geometry optimisations employed all-electron Slater type orbital (STO) triple-ζ-plus polarisation basis sets (from the ZORA/TZP database of the ADF suite for the Zn, Cd, C, N, and H atoms. Scalar relativistic approaches were used within the ZORA Hamiltonian for the inclusion of relativistic effects and the local density approximation (LDA) with the correlation potential due to Vosko et al.[3] was used in all of the calculations. Gradient corrections were performed using the functionals of Becke[4] and Perdew.[5] The bond orders between molecular fragments were calculated using the AOMix program.[6,7]

References

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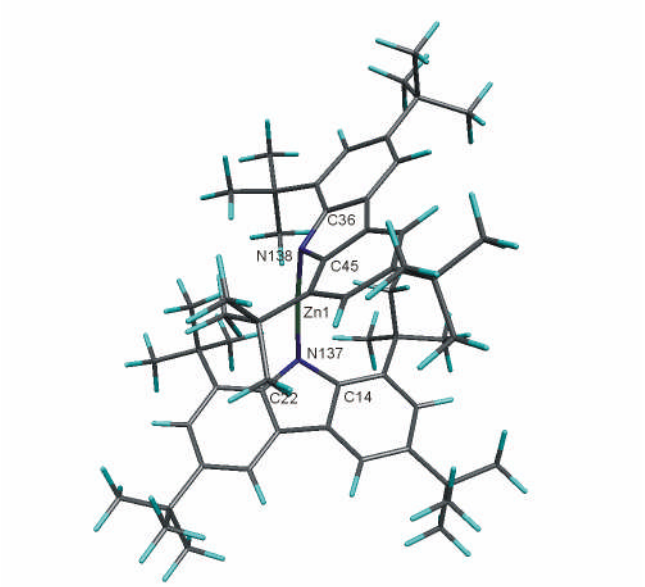
Geometry Optimised Structure and Coordinates for **1**



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3.C	3.746344	3.433029	-4.733844
4.C	0.143588	-2.027801	-3.717836
5.C	2.436376	3.599334	-3.928783
6.C	-0.421993	-0.622791	-3.401482
7.C	1.029103	1.479306	-3.480938
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10.C	2.610034	4.757812	-2.920161
11.C	-7.264117	-0.535630	-1.585467
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21.C	7.793335	-0.501104	0.063010
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45.C	-1.579170	0.678620	1.566001
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49.C	-1.064767	2.925171	2.188083
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55.C	0.610243	1.245161	2.995580
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62.H	3.986650	4.361484	-5.276015
63.H	0.915622	-1.968785	-4.498803
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65.H	0.348432	4.102807	-4.389435
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67.H	0.393931	1.791620	-4.303072
68.H	4.593604	3.196435	-4.074852
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71.H	2.830013	5.697660	-3.450422
72.H	-8.322404	-0.614730	-1.879343
73.H	-2.440829	-1.271851	-2.864510
74.H	-7.064997	0.516290	-1.340510
75.H	1.696823	4.901075	-2.325052
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77.H	3.924343	2.389986	-1.943636
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79.H	3.436840	4.565367	-2.222724
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81.H	-1.316035	-1.363035	-1.529676
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85.H	-1.951397	-4.042255	-1.128448
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90.H	-7.245313	-3.609338	0.040497
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99.H	-3.942228	-5.149727	-0.109722
100.H	-0.965893	-4.933559	0.064069
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116.H	1.181934	-4.604646	1.950789
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121.H	6.236716	0.670339	2.955517
122.H	1.643164	3.139990	2.541383
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133.H	-1.446229	5.291664	3.597254
134.H	0.124268	2.693730	4.587412
135.H	-0.465721	1.049399	4.902877
136.H	1.271471	1.422175	5.072676

137.N	1.499242	-1.237573	-0.892078
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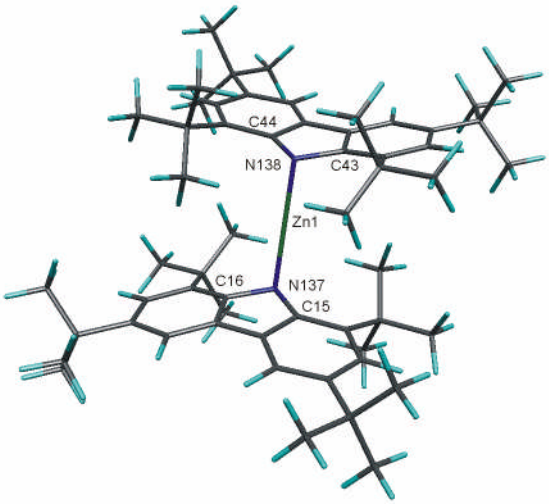
Energy = -804.91905621 eV

Geometry Optimised Structure and Coordinates for **1a**



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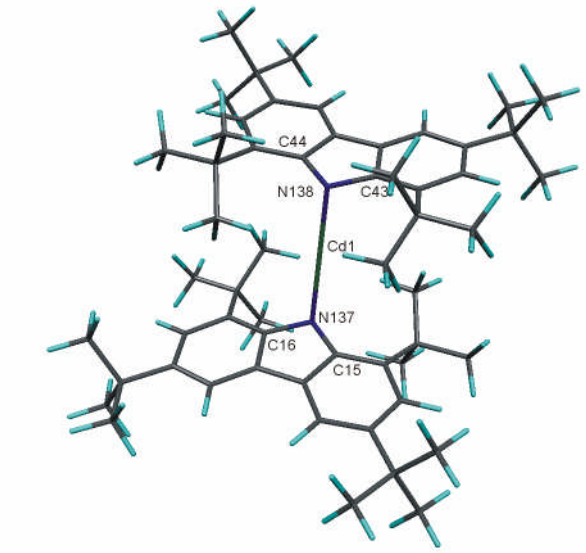
29.C	4.306335	2.793895	0.048852
30.C	3.988320	-3.225414	0.011852
31.C	-6.029213	-4.478927	0.701064
32.C	-5.523684	5.076650	0.756703
33.C	4.428908	1.430762	0.317247
34.C	4.250532	-1.886577	0.301427
35.C	-3.372977	0.898731	0.166527
36.C	-3.450394	-0.547114	0.158928
37.C	4.904183	-4.374452	0.475060
38.C	5.339005	3.833997	0.524208
39.C	-2.867472	3.524373	0.799019
40.C	-3.220001	-3.219941	0.752632
41.C	4.081522	-5.406966	1.280155
42.C	6.426059	3.202413	1.412216
43.C	-2.203177	1.241737	0.890134
44.C	-2.321065	-1.020746	0.873888
45.C	-1.964528	2.577416	1.298997
46.C	-2.221843	-2.379945	1.262616
47.C	6.050806	-3.870204	1.369467
48.C	4.630519	4.939941	1.340686
49.C	0.229564	-2.479891	2.045485
50.C	0.480420	2.405166	2.086959
51.C	-0.792035	4.493861	2.524959
52.C	-0.926364	2.965425	2.375130
53.C	-1.255663	-4.426256	2.461182
54.C	-1.228435	-2.890187	2.330435
55.C	-1.416210	2.390172	3.727485
56.C	-1.651383	-2.282887	3.691237
57.H	0.964380	2.618148	-4.484772
58.H	0.700426	-2.640722	-4.526831
59.H	2.670967	2.594290	-3.960799
60.H	2.397867	-2.804998	-3.998596
61.H	1.506816	-1.297163	-3.674455
62.H	1.625139	1.185855	-3.651702
63.H	0.514130	4.736621	-3.211451
64.H	0.023841	-4.714687	-3.279946
65.H	2.234167	4.796205	-2.797372
66.H	1.726792	-4.960898	-2.864740
67.H	-1.189560	-2.767085	-2.846760
68.H	-0.896900	2.925351	-2.798698
69.H	-5.670679	3.361224	-2.266895
70.H	-6.665309	4.719917	-1.700737
71.H	-4.143419	-4.519158	-2.232279
72.H	-5.358487	-5.697754	-1.670312
73.H	-5.993997	-2.726764	-2.304271
74.H	-0.490002	-1.308628	-2.147587
75.H	-0.356964	1.391599	-2.120354
76.H	-7.126579	-3.979100	-1.752235
77.H	-3.641936	4.946111	-2.176604
78.H	-4.724470	6.241532	-1.601035
79.H	-6.710094	3.174065	-0.831524

80.H	1.001785	4.923744	-1.513690
81.H	-3.859963	-5.450549	-0.746914
82.H	0.484969	-4.973354	-1.584032
83.H	4.750015	-5.500518	-1.411740
84.H	6.545943	3.719205	-1.305398
85.H	-0.863096	-2.726548	-1.107118
86.H	-0.574133	2.826849	-1.060367
87.H	2.718962	-4.564057	-1.082878
88.H	3.180388	4.273245	-1.021975
89.H	6.118428	-4.369708	-1.353303
90.H	5.303760	4.988017	-1.350575
91.H	-7.008832	-2.446805	-0.866257
92.H	-5.138114	1.594660	-0.860625
93.H	-5.283736	-1.039522	-0.866665
94.H	-3.261015	5.825640	-0.681346
95.H	-6.770892	-5.225140	0.374885
96.H	6.182373	-5.899776	-0.437589
97.H	-6.182373	5.899776	0.437589
98.H	6.770892	5.225140	-0.374885
99.H	3.261015	-5.825640	0.681346
100.H	7.008832	2.446805	0.866257
101.H	-6.118428	4.369708	1.353303
102.H	-5.303760	-4.988017	1.350575
103.H	-6.545943	-3.719205	1.305398
104.H	5.283736	1.039522	0.866665
105.H	5.138114	-1.594660	0.860625
106.H	-4.750015	5.500518	1.411740
107.H	-3.180388	-4.273245	1.021975
108.H	-2.718962	4.564057	1.082878
109.H	6.710094	-3.174065	0.831524
110.H	7.126579	3.979100	1.752235
111.H	4.724470	-6.241532	1.601035
112.H	3.859963	5.450549	0.746914
113.H	0.574133	-2.826849	1.060367
114.H	0.863096	2.726548	1.107118
115.H	-0.484969	4.973354	1.584032
116.H	-1.001785	-4.923744	1.513690
117.H	3.641936	-4.946111	2.176604
118.H	5.993997	2.726764	2.304271
119.H	5.358487	5.697754	1.670312
120.H	6.665309	-4.719917	1.700737
121.H	5.670679	-3.361224	2.266895
122.H	0.356964	-1.391599	2.120354
123.H	0.490002	1.308628	2.147587
124.H	4.143419	4.519158	2.232279
125.H	-1.726792	4.960898	2.864740
126.H	-2.234167	-4.796205	2.797372
127.H	0.896900	-2.925351	2.798698
128.H	1.189560	2.767085	2.846760
129.H	-0.023841	4.714687	3.279946
130.H	-0.514130	-4.736621	3.211451
131.H	-1.625139	-1.185855	3.651702

132.H	-1.506816	1.297163	3.674455
133.H	-2.397867	2.804998	3.998596
134.H	-2.670967	-2.594290	3.960799
135.H	-0.700426	2.640722	4.526831
136.H	-0.964380	-2.618148	4.484772
137.N	1.460054	-0.066133	-1.231113
138.N	-1.460054	0.066133	1.231113
139.Zn	0.000000	0.000000	0.000000

Energy = -804.87863635 eV

Geometry Optimised Structure and Coordinates for **2**



1.C	1.717644	2.341265	-3.769292
2.C	1.469814	-2.436998	-3.803892
3.C	1.347786	4.455697	-2.481880
4.C	0.895875	-4.532097	-2.562225
5.C	1.324393	2.917114	-2.386448
6.C	1.021623	-3.001037	-2.432902
7.C	-6.118440	3.868701	-1.365445
8.C	-0.384498	-2.451183	-2.115706
9.C	-0.129030	2.499760	-2.080951
10.C	-4.678921	-4.902170	-1.360189
11.C	-6.505083	-3.194629	-1.384981
12.C	-4.121306	5.371727	-1.306909
13.C	2.336586	2.384155	-1.347718
14.C	2.079517	-2.591780	-1.383725
15.C	2.458624	1.011880	-1.007910
16.C	2.341404	-1.244524	-1.023357
17.C	-5.411744	-3.836706	-0.512050
18.C	-4.971280	4.382029	-0.476530
19.C	3.313785	3.225430	-0.801489

20.C	2.960949	-3.537521	-0.845394
21.C	5.590333	-5.137759	-0.723313
22.C	6.097319	4.534952	-0.686480
23.C	3.581450	0.541034	-0.278610
24.C	3.505274	-0.902938	-0.286845
25.C	-4.362654	1.890557	-0.217631
26.C	-4.539705	-1.426965	-0.233099
27.C	-4.081876	3.232607	0.035085
28.C	-4.401250	-2.794034	0.003270
29.C	4.401250	2.794034	-0.003270
30.C	4.081876	-3.232607	-0.035085
31.C	-6.097319	-4.534952	0.686480
32.C	-5.590333	5.137759	0.723313
33.C	4.539705	1.426965	0.233099
34.C	4.362654	-1.890557	0.217631
35.C	-3.505274	0.902938	0.286845
36.C	-3.581450	-0.541034	0.278610
37.C	4.971280	-4.382029	0.476530
38.C	5.411744	3.836706	0.512050
39.C	-2.960949	3.537521	0.845394
40.C	-3.313785	-3.225430	0.801489
41.C	4.121306	-5.371727	1.306909
42.C	6.505083	3.194629	1.384981
43.C	-2.341404	1.244524	1.023357
44.C	-2.458624	-1.011880	1.007910
45.C	-2.079517	2.591780	1.383725
46.C	-2.336586	-2.384155	1.347718
47.C	6.118440	-3.868701	1.365445
48.C	4.678921	4.902170	1.360189
49.C	0.129030	-2.499760	2.080951
50.C	0.384498	2.451183	2.115706
51.C	-0.895875	4.532097	2.562225
52.C	-1.021623	3.001037	2.432902
53.C	-1.347786	-4.455697	2.481880
54.C	-1.324393	-2.917114	2.386448
55.C	-1.469814	2.436998	3.803892
56.C	-1.717644	-2.341265	3.769292
57.H	1.012576	2.690584	-4.540702
58.H	0.734277	-2.699446	-4.581249
59.H	2.729663	2.663653	-4.053765
60.H	2.445501	-2.850806	-4.096850
61.H	1.557584	-1.343415	-3.762922
62.H	1.697956	1.243664	-3.751402
63.H	0.600446	4.782490	-3.219242
64.H	0.123658	-4.768385	-3.308472
65.H	2.323837	4.833756	-2.815946
66.H	1.832282	-4.995572	-2.902218
67.H	-1.114806	-2.847334	-2.837103
68.H	-0.815947	2.979764	-2.794009
69.H	-5.738887	3.323868	-2.241714
70.H	-6.714784	4.717576	-1.730661
71.H	-4.193635	-4.443021	-2.233734

72.H	-5.391321	-5.660985	-1.720307
73.H	-6.077049	-2.683901	-2.259462
74.H	-0.410683	-1.357420	-2.216390
75.H	-0.260585	1.415971	-2.203972
76.H	-7.191426	-3.971279	-1.752842
77.H	-3.679504	4.872345	-2.181454
78.H	-4.745476	6.205755	-1.664414
79.H	-6.795069	3.202282	-0.811695
80.H	1.100949	4.930932	-1.521182
81.H	-3.903360	-5.419284	-0.778628
82.H	0.599504	-5.002382	-1.613121
83.H	4.814951	-5.566840	-1.372923
84.H	6.631633	3.805361	-1.312219
85.H	-0.731730	-2.746090	-1.113207
86.H	-0.448308	2.807095	-1.072801
87.H	2.793948	-4.583647	-1.092514
88.H	3.255287	4.286718	-1.033315
89.H	6.206580	-4.463713	-1.335857
90.H	5.366376	5.051848	-1.323587
91.H	-7.102214	-2.465968	-0.818341
92.H	-5.245447	1.596247	-0.783080
93.H	-5.388910	-1.034730	-0.790620
94.H	-3.300600	5.797284	-0.713238
95.H	-6.823129	-5.283482	0.330934
96.H	6.227771	-5.963395	-0.369069
97.H	-6.227771	5.963395	0.369069
98.H	6.823129	5.283482	-0.330934
99.H	3.300600	-5.797284	0.713238
100.H	7.102214	2.465968	0.818341
101.H	-6.206580	4.463713	1.335857
102.H	-5.366376	-5.051848	1.323587
103.H	-6.631633	-3.805361	1.312219
104.H	5.388910	1.034730	0.790620
105.H	5.245447	-1.596247	0.783080
106.H	-4.814951	5.566840	1.372923
107.H	-3.255287	-4.286718	1.033315
108.H	-2.793948	4.583647	1.092514
109.H	6.795069	-3.202282	0.811695
110.H	7.191426	3.971279	1.752842
111.H	4.745476	-6.205755	1.664414
112.H	3.903360	5.419284	0.778628
113.H	0.448308	-2.807095	1.072801
114.H	0.731730	2.746090	1.113207
115.H	-0.599504	5.002382	1.613121
116.H	-1.100949	-4.930932	1.521182
117.H	3.679504	-4.872345	2.181454
118.H	6.077049	2.683901	2.259462
119.H	5.391321	5.660985	1.720307
120.H	6.714784	-4.717576	1.730661
121.H	5.738887	-3.323868	2.241714
122.H	0.260585	-1.415971	2.203972
123.H	0.410683	1.357420	2.216390

124.H	4.193635	4.443021	2.233734
125.H	-1.832282	4.995572	2.902218
126.H	-2.323837	-4.833756	2.815946
127.H	0.815947	-2.979764	2.794009
128.H	1.114806	2.847334	2.837103
129.H	-0.123658	4.768385	3.308472
130.H	-0.600446	-4.782490	3.219242
131.H	-1.697956	-1.243664	3.751402
132.H	-1.557584	1.343415	3.762922
133.H	-2.445501	2.850806	4.096850
134.H	-2.729663	-2.663653	4.053765
135.H	-0.734277	2.699446	4.581249
136.H	-1.012576	-2.690584	4.540702
137.N	1.619428	-0.073070	-1.404016
138.N	-1.619428	0.073070	1.404016
139.Cd	0.000000	0.000000	0.000000

Energy = -804.16338982 eV