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Supporting Information

Reaction of L_2Zn_2 with Ph_2E_2 – Synthesis of LZnEPh and reactions with oxygen and H-acidic substrates

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Experimental Section

Manipulations were performed in a glove box under an Ar-atmosphere or with standard Schlenk techniques. Dry solvents were obtained from a solvent purification system (MBraun) and degassed prior to use. $Mesnacnac_2Zn_2$[1] were prepared according to literature methods, whereas Te_2Ph_2 and Se_2Ph_2 were commercially available (Acros Organics; Sigma-Aldrich) and used as received. A Bruker Avance 300 spectrometer was used for NMR spectroscopy. ^1H and $^{13}C\{^1H\}$ NMR spectra were referenced to internal C_6D_5H (^1H: δ = 7.154; ^{13}C: δ = 128.0). ^{125}Te NMR spectra were referenced to Na_2TeO_3 in D_2O and ^{77}Se NMR spectra were referenced to Me_2Se_2 in C_6D_6. IR spectra were recorded on an Alpha-T FT-IR spectrometer with a single reflection ATR sampling module. Melting points were measured in sealed capillaries and were not corrected. Elemental analyses were performed at the *Elementaranalyse Labor* of the University of Duisburg-Essen.

[(Mesnacnac)ZnSePh] (1)

$Mesnacnac_2Zn_2$ (160 mg, 200 µmol) was dissolved in 15 mL of fluorobenzene at – 35 °C. A solution of Se_2Ph_2 (60 mg, 200 µmol) in 10 mL of fluorobenzene was slowly added. The reaction vessel was stirred over night. After evaporation of the solvent in vacuum, a colorless solid was obtained, that was recrystallized from a mixture of hexane / toluene. A colorless solid was obtained after storage for 24h at -30 °C. Yield: 108 mg (98 %). – M.p. 162 °C. – $C_{29}H_{34}N_2SeZn$ (553.971): calcd. C 62.82, H 6.13, N 5.05; found C 62.60, H 6.24, N 4.87. – IR: ν = 3054, 2961, 2913, 2854, 1547, 1517, 1473, 1450, 1435, 1372, 1259, 1198, 1147, 1092, 1071, 1018, 959, 857, 798, 767, 731, 689, 667, 628, 567, 500, 463, 388 cm^{-1}. – ^1H NMR (300 MHz, C_6D_6, 20 °C): δ= 1.55 (s, 6 H, C*CH₃*), 2.07 (s, 12 H, *o-CH₃*), 2.12 (s, 6 H, *p-CH₃*), 4.91 (s, 1 H, *CH*), 6.60 (m, 2 H, Ph-*o-H*), 6.68 (s, 4 H, Mes-*H*), 6.80 (m, 2 H, Ph-*m-H*), 6.88 (m, 1 H, Ph-*p-H*). – ^{13}C NMR (75 MHz, C_6D_6, 20 °C): δ = 18.98 (*o-CH₃*), 21.26 (*p-C*H₃), 23.01 (C*C*H₃), 96.31 (*γ–C*), 124.45 (*p*-Ph), 129.30 (*m*-Ph), 130.00 (*m*-Ar), 131.33 (*o*-Ar), 132.31 (*o*-Ph), 134.78 (*p*-Ar), 136.23 (*i*-Ph), 144.62 (*i*-Ar), 168.99 (*ß-C*). – ^{77}Se NMR (57 MHz, C_6D_6, 20 °C): δ= -218.

[(Mesnacnac)ZnTePh] (2)

$Mesnacnac_2Zn_2$ (80 mg, 100 µmol) and Te_2Ph_2 (50 mg, 100µmol) were dissolved in 15 mL of fluorobenzene. The reaction vessel was stirred over night at room temperature, yielding an orange suspension. After evaporation of the solvent in vacuum, an orange solid was obtained,

that was recrystallized from from a mixture of hexane / toluene. An orange solid was obtained after storage for 24h at -30 °C. Yield: 55 mg (91 %). – M.p. 198 °C. – $C_{29}H_{34}N_2TeZn$ (602.6): calcd. C 57.75, H 5.64, N 4.64; found C 56.60, H 5.71, N 4.54. – IR: ν = 3062, 2963, 2909, 2851, 1548, 1522, 1471, 1447, 1430, 1372, 1259, 1202, 1148, 1090, 1060, 1014, 862, 799, 763, 753, 726, 691, 651, 568, 502, 454, 390 cm^{-1}. – ^{1}H NMR (300 MHz, C_6D_6, 20 °C): δ = 1.55 (s, 6 H, C*CH₃*), 2.09 (s, 12 H, *o-CH₃*), 2.10 (s, 6 H, *p-CH₃*), 4.94 (s, 1 H, *CH*), 6.53 (m, 2 H, Ph-*o-H*), 6.67 (s, 4 H, Mes-*H*), 7.33 (m, 2 H, Ph-*m-H*), 7.70 (m, 1 H, Ph-*p-H*). – ^{13}C NMR (75 MHz, C_6D_6, 20 °C): δ = 18.44 (*o-CH₃*), 20.62 (*p-*CH_3), 22.39 (CCH_3), 95.95 (*γ–C*), 124.70 (*p*-Ph), 129.16 (*m*-Ph), 129.36 (*m*-Ar), 130.63 (*o*-Ar), 134.18 (*o*-Ph), 137.53 (*p*-Ar), 140.90 (*i*-Ph), 144.04 (*i*-Ar), 168.12 (*ß-C*). – ^{125}Te NMR (95 MHz, C_6D_6, 20 °C): δ = 416.

[(Mesnacnac)ZnOH]$_2$ (3)

1 (50 mg, 90 µmol) was dissolved in 15 mL fluorbenzene and water (1.7 µL, 90 µmol) was slowly added via an Eppendorf pipette. The reaction vessel was stirred over night at room temperature. The flask was stored at 4 °C, yielded colorless crystals over night, which were isolated by filtration and clearly identified by NMR spectroscopy. An analogous experiment using **2** (55 mg, 90 µmol) also resulted in the formation of **3**.

^{1}H NMR (300 MHz, C_6D_6, 20 °C): δ = - 0.2 (s, 2H, O*H*), 1.46 (s, 6 H, C*CH₃*), 1.95 (s, 12 H, *o-CH₃*), 2.34 (s, 6 H, *p-CH₃*), 4.73 (s, 1 H, *CH*), 6.75 (s, 4 H, Ar-*H*). – ^{13}C NMR (75 MHz, C_6D_6, 20 °C): δ = 17.90 (*o-CH₃*), 21.00 (*p-*CH_3), 22.80 (CCH_3), 93.80 (*γ–C*), 128.70 (*m*-Ar), 131.10 (*o*-Ar), 132.10 (*p*-Ar), 145.60 (*i*-Ar), 167.30 (*ß-C*).

The hydrolysis reaction of **1** in an NMR-tube was also monitored by ^{77}Se NMR. Immediately after addition of water, the ^{77}Se NMR spectra showed a signal at 144.6 ppm, which corresponds very well with the value reported for PhSeH (145 ppm).[3] In contrast, hydrolysis of **2** gave a new signal in the ^{125}Te NMR spectrum at 3210 ppm, which fairly corresponds to the resonance reported for $[Te_4]^{2+}$ (3008 ppm).[2] This resonance steadily increased over the next 12h and the solution intensified its color, finally forming a dark-red solution as is typical for $[Te_4]^{2+}$ dications. We couldn't see any other resonance indicating the formation of either PhTeH (161.8 ppm)[4] or Ph_2Te_2 (422 ppm)!

^{77}Se NMR (57 MHz, C_6D_6, 20 °C): δ = 144.6.

^{125}Te NMR (95 MHz, C_6D_6, 20 °C): δ = - 3210.

[(Mesnacnac)ZnOEt]$_2$ (4)

2 (55 mg, 90 µmol) was dissolved in 15 mL of fluorbenzene and ethanol (5.3 µL, 90 µmol) was slowly added via an Eppendorf pipette. The reaction vessel was stirred over night at room temperature. The flask was stored at 18 °C, yielded colorless crystals of **4** after 5 h, which were isolated by filtration. Yield: 0.27 mg (68 %). – M.p. > 230 °C – IR: ν = 2964, 2913, 2834, 2853, 1544, 1523, 1403, 1261, 1202, 1148, 1021, 856, 798, 724, 685, 661, 632, 573, 532, 484, 453, 388 cm^{-1}. – ^{1}H NMR (300 MHz, C_6D_6, 20 °C): δ = 1.18 (t, 3 H, *CH₃*), 1.48 (s, 6 H, C*CH₃*), 1.92 (s, 12 H, *o*-*CH₃*), 2.38 (s, 6 H, *p*-*CH₃*), 3.79 (q, 2 H, *CH₂*), 4.77 (s, 1 H, *CH*), 6.89 (s, 4 H, Ar-*H*). – ^{13}C NMR (75 MHz, C_6D_6, 20 °C): δ = 18.32 (*o*-*CH₃*), 20.93 (OCH₂*CH₃*), 21.37 (*p*-*C*H₃), 22.96 (C*C*H₃), 60.05 (O*CH₂*CH₃), 94.78 (*γ–C*), 128.85 (*m*-Ar), 130.26 (*o*-Ar), 132.12 (*p*-Ar), 145.63 (*i*-Ar), 167.67 (*ß-C*).

The analogous reaction of or **1** (50 mg, 90 µmol) also gave **4** in comparable yield (71%).

The reaction of **1** with EtOH in an NMR-tube was also monitored by ^{77}Se NMR. Immediately after addition of EtOH, the ^{77}Se NMR spectra showed a signal at 144.7 ppm, which again corresponds with the value reported for PhSeH (145 ppm).[3] In addition, the reaction of **2** with EtOH again gave a new signal in the ^{125}Te NMR spectrum at 3210 ppm. Again, no other resonance indicating the formation of either PhTeH (161.8 ppm)[4] or Ph_2Te_2 (422 ppm) was observed!

^{77}Se NMR (57 MHz, C_6D_6, 20 °C): δ = 144.7.

^{125}Te NMR (95 MHz, C_6D_6, 20 °C): δ = - 3210.

[(Mesnacnac)ZnO₂TePh]₂ (5)

2 (55 mg, 90 µmol) was dissolved in 15 mL fluorbenzene. The reaction vessel was filled up with an oxygen atmosphere and stirred over night at room temperature. The flask was stored at 18 °C, yielding colorless crystals after 24 h, which were isolated by filtration. Yield: 50 mg (38 %). – M.p. 246 °C. – $C_{70}H_{78}N_4O_4F_2Te_2Zn_2$ (1463.30):calcd. C 57.40, H 5.33, N 3.82; found C 56.87, H 5.28, N 3.92. – IR: ν = 2962, 2915, 2855, 1592, 1555, 1518, 1493, 1451, 1400, 1376, 1265, 1214, 1198, 1147, 1062, 997, 959, 859, 803, 744, 685, 661, 632, 595, 582, 567, 518, 497, 464, 404, 387 cm^{-1}. – ^{1}H NMR (300 MHz, C_6D_6, 20 °C): δ = 1.56 (s, 6 H, C*CH₃*), 1.95 (s, 6 H, *p*-*CH₃*), 2.30 (s, 6 H, *o*-*CH₃*), 2.34 (s, 6 H, o-*CH₃*), 4.72 (s, 1 H, *CH*), 6.65 (s, 2 H, Ar-*H*), 6.78 (s, 2 H, Ar-*H*), 7.01 (m, 1 H, Ph-p-*H*), 7.28 (m, 2 H, Ph-m-*H*), 7.78 (d, 2 H, Ph-o-*H*). – ^{13}C NMR (75 MHz, C_6D_6, 20 °C): δ = 18.17 (*o*-*CH₃*), 19.97 (*p*-*C*H₃), 20.66 (C*C*H₃), 94.12 (*γ–C*), 115.05 (*p*-Ph), 115.33 (*m*-Ph), 128.66 (*m*-Ar), 129.82 (*o*-Ar), 129.92 (*o*-Ph), 131.72 (*p*-Ar), 133.34 (*i*-Ph), 141.57 (*i*-Ar), 160.77 (*ß-C*). – ^{125}Te NMR (95 MHz, C_6D_6, 20 °C): δ = 1681.

Crystal structure determination

The crystals of **4** and **5** were mounted on nylon loops in inert oil. Data were collected on a Bruker AXS D8 Kappa diffractometer with APEX2 detector (mono-chromated $Mo_{K\alpha}$ radiation, λ = 0.71073 Å) at 170(1) K (**4**) and 180(1) K (**5**). The structure was solved by Direct Methods (SHELXS-97)[7] and refined anisotropically by full-matrix least-squares on F^2 (SHELXL-97).[8] Absorption corrections was performed semi-empirically from equivalent reflections on basis of multi-scans (Buker AXS APEX2). Hydrogen atoms were refined using a riding model or rigid methyl groups. CCDC 970723 (**1**), 964285 (**4**) and CCDC 964286 (**5**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre *via* www.ccdc.cam.ac.uk/data_request/cif.

References

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Compound 1

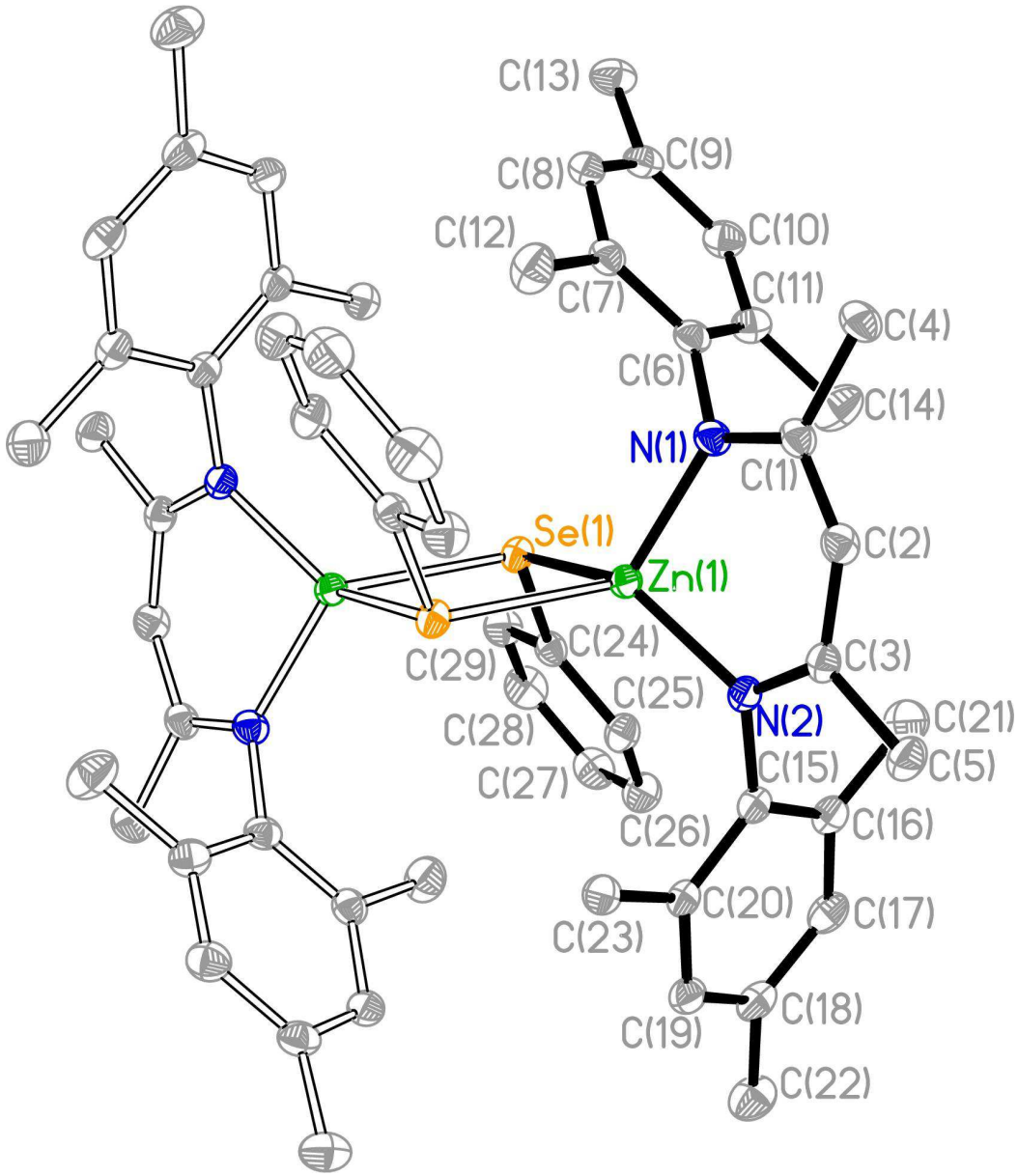


Table 1: Crystal structure data

Identification code	**sg_555m**
Empirical formula	C58 H68 N4 Se2 Zn2
Formula weight	1109.82
Density (calculated)	1.410 g · cm^{-1}
F(000)	1144
Temperature	100(1) K
Crystal size	0.150 × 0.070 × 0.050 mm
Crystal colour	colourless
Crystal description	prism
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	*P 21/n*
Unit cell dimensions	
a [Å]	12.812(3)
b [Å]	15.463(4)
c [Å]	14.313(3)
α [°]	90
β [°]	112.843(12)
γ [°]	90
Volume	2613.3(10) Å^3
Z	2
Cell measurement reflections used	9174
Cell measurement θ min/max	2.63°/38.19°
Diffractometer control software	BRUKER D8 KAPPA APEX 2 (3.0-2009)
Diffractometer measurement device	Bruker D8 KAPPA series II with APEX II area detector system
Diffractometer measurement method	Data collection strategy APEX 2/COSMO
θ range for data collection	1.814°- 34.573°
Completeness to θ = 25.242°	100.0%
Index ranges	$-15 \leq h \leq 20$
	$-21 \leq k \leq 24$
	$-22 \leq l \leq 22$
Computing data reduction	BRUKER D8 KAPPA APEX 2 (3.0-2009)
Absorption coefficient	2.352 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Computation absorption correction	BRUKER AXS SMART APEX 2 Vers. 3.0-2009

Max./min. Transmission	0.75/0.65
R_{merg} before/after correction	0.0609/0.0431
Computing structure solution	BRUKER D8 KAPPA APEX 2 (3.0-2009)
Computing structure refinement	SHELXL-2013 (Sheldrick, 2013)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	57134
Independent reflections	10912
R_{int}	0.0382
Data	8020
Restraints	0
Parameter	306
GooF	1.028
Weighting details	$w = 1/[\sigma^2(F_{obs}^2) + (0.0476P)^2 + 1.2180P]$ where $P = (F_{obs}^2 + 2F_{calc}^2)/3$
R_1 [$I > 2\sigma(I)$]	0.0348
wR_2 [$I > 2\sigma(I)$]	0.0828
R_1 [all data]	0.0615
wR_2 [all data]	0.0945
Absolute structure parameter	
Largest diff. peak and hole	1.516/-0.857

Table 2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for sg_555m. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
Se(1)	4096(1)	507(1)	8874(1)	17(1)
Zn(2)	5803(1)	984(1)	10262(1)	16(1)
N(1)	5468(1)	2004(1)	10937(1)	18(1)
N(2)	7316(1)	1340(1)	10368(1)	17(1)
C(1)	6318(1)	2445(1)	11604(1)	19(1)
C(2)	7459(1)	2294(1)	11767(1)	20(1)
H(2)	8001	2520	12381	24
C(3)	7907(1)	1853(1)	11143(1)	18(1)
C(4)	6074(2)	3171(1)	12198(1)	24(1)
H(4A)	5799	3677	11759	36
H(4B)	6770	3323	12776	36
H(4C)	5496	2984	12445	36
C(5)	9145(2)	2000(1)	11364(1)	25(1)
H(5A)	9522	1442	11404	38
H(5B)	9498	2307	12010	38
H(5C)	9218	2348	10820	38
C(6)	4327(1)	2301(1)	10667(1)	18(1)
C(7)	3648(1)	1960(1)	11147(1)	19(1)
C(8)	2521(1)	2217(1)	10811(1)	20(1)
H(8)	2065	2005	11148	24
C(9)	2044(1)	2776(1)	9994(1)	21(1)
C(10)	2739(2)	3109(1)	9531(1)	24(1)
H(10)	2425	3496	8976	28
C(11)	3877(2)	2888(1)	9861(1)	22(1)
C(12)	4092(2)	1303(1)	11981(2)	29(1)
H(12A)	3719	1382	12457	44
H(12B)	4911	1379	12339	44
H(12C)	3934	720	11690	44
C(13)	803(2)	2982(1)	9597(2)	28(1)
H(13A)	682	3580	9349	41
H(13B)	526	2915	10142	41
H(13C)	390	2587	9040	41
C(14)	4601(2)	3251(2)	9334(2)	33(1)

H(14A)	4148	3649	8796	49
H(14B)	4879	2777	9038	49
H(14C)	5246	3564	9827	49
C(15)	7789(1)	1089(1)	9639(1)	17(1)
C(16)	7707(1)	1665(1)	8845(1)	21(1)
C(17)	8040(1)	1377(1)	8071(1)	23(1)
H(17)	7981	1761	7535	27
C(18)	8454(2)	544(1)	8067(1)	23(1)
C(19)	8591(1)	13(1)	8894(1)	21(1)
H(19)	8916	-544	8922	25
C(20)	8269(1)	266(1)	9687(1)	18(1)
C(21)	7234(2)	2560(1)	8801(2)	30(1)
H(21A)	7279	2872	8222	45
H(21B)	7674	2870	9428	45
H(21C)	6442	2523	8725	45
C(22)	8740(2)	231(2)	7187(1)	31(1)
H(22A)	9538	60	7439	47
H(22B)	8603	699	6691	47
H(22C)	8261	-266	6864	47
C(23)	8440(2)	-337(1)	10560(1)	22(1)
H(23A)	8578	2	11176	32
H(23B)	9092	-712	10665	32
H(23C)	7761	-692	10409	32
C(24)	4134(1)	514(1)	7540(1)	18(1)
C(25)	5105(2)	712(1)	7370(1)	22(1)
H(25)	5790	842	7927	26
C(26)	5079(2)	720(1)	6382(1)	27(1)
H(26)	5749	848	6276	32
C(27)	4090(2)	545(1)	5564(1)	28(1)
H(27)	4071	558	4894	34
C(28)	3118(2)	349(1)	5737(1)	29(1)
H(28)	2432	226	5178	35
C(29)	3137(2)	330(1)	6721(1)	23(1)
H(29)	2469	191	6828	28

Table 3: Anisotropic displacement parameters (Å^2 × 10^3) for sg_555m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Se(1)	17(1)	18(1)	16(1)	-1(1)	6(1)	-3(1)
Zn(2)	16(1)	16(1)	18(1)	-4(1)	8(1)	-3(1)
N(1)	18(1)	18(1)	18(1)	-4(1)	6(1)	-1(1)
N(2)	17(1)	17(1)	18(1)	-1(1)	8(1)	-2(1)
C(1)	22(1)	17(1)	17(1)	-2(1)	7(1)	-1(1)
C(2)	19(1)	20(1)	19(1)	-3(1)	5(1)	-2(1)
C(3)	16(1)	17(1)	18(1)	1(1)	5(1)	-1(1)
C(4)	27(1)	22(1)	24(1)	-9(1)	10(1)	-2(1)
C(5)	19(1)	27(1)	30(1)	-4(1)	10(1)	-6(1)
C(6)	17(1)	18(1)	18(1)	-5(1)	6(1)	0(1)
C(7)	21(1)	17(1)	19(1)	-3(1)	8(1)	-1(1)
C(8)	22(1)	19(1)	22(1)	-4(1)	11(1)	-1(1)
C(9)	20(1)	22(1)	21(1)	-5(1)	8(1)	2(1)
C(10)	25(1)	25(1)	21(1)	1(1)	9(1)	4(1)
C(11)	22(1)	24(1)	21(1)	-1(1)	10(1)	1(1)
C(12)	25(1)	30(1)	32(1)	8(1)	9(1)	1(1)
C(13)	22(1)	32(1)	28(1)	-3(1)	9(1)	5(1)
C(14)	27(1)	44(1)	30(1)	12(1)	14(1)	3(1)
C(15)	16(1)	19(1)	16(1)	-1(1)	7(1)	-2(1)
C(16)	18(1)	23(1)	22(1)	3(1)	8(1)	-1(1)
C(17)	20(1)	31(1)	18(1)	5(1)	8(1)	-1(1)
C(18)	18(1)	32(1)	18(1)	-4(1)	8(1)	-6(1)
C(19)	21(1)	22(1)	23(1)	-4(1)	11(1)	-3(1)
C(20)	16(1)	19(1)	18(1)	-1(1)	7(1)	-3(1)
C(21)	35(1)	26(1)	33(1)	10(1)	18(1)	6(1)
C(22)	33(1)	42(1)	23(1)	-6(1)	16(1)	-6(1)
C(23)	24(1)	20(1)	24(1)	2(1)	12(1)	1(1)
C(24)	21(1)	15(1)	16(1)	1(1)	7(1)	1(1)
C(25)	23(1)	22(1)	21(1)	3(1)	9(1)	-1(1)
C(26)	32(1)	26(1)	26(1)	4(1)	16(1)	1(1)
C(27)	40(1)	27(1)	20(1)	1(1)	14(1)	2(1)
C(28)	31(1)	32(1)	19(1)	-4(1)	4(1)	-1(1)
C(29)	23(1)	26(1)	20(1)	-4(1)	6(1)	-1(1)

Table 4: Bond lengths [Å] for sg_555m.

Se(1)-C(24)	1.9282(16)	C(9)-C(10)	1.399(2)
Se(1)-Zn(2)	2.4291(5)	C(9)-C(13)	1.500(2)
Se(1)-Zn(2)#1	2.5951(6)	C(10)-C(11)	1.389(2)
Zn(2)-N(2)	1.9635(14)	C(11)-C(14)	1.513(2)
Zn(2)-N(1)	1.9822(14)	C(15)-C(20)	1.403(2)
Zn(2)-Se(1)#1	2.5951(6)	C(15)-C(16)	1.416(2)
N(1)-C(1)	1.325(2)	C(16)-C(17)	1.405(2)
N(1)-C(6)	1.435(2)	C(16)-C(21)	1.503(3)
N(2)-C(3)	1.335(2)	C(17)-C(18)	1.394(3)
N(2)-C(15)	1.448(2)	C(18)-C(19)	1.394(2)
C(1)-C(2)	1.407(2)	C(18)-C(22)	1.521(2)
C(1)-C(4)	1.513(2)	C(19)-C(20)	1.406(2)
C(2)-C(3)	1.412(2)	C(20)-C(23)	1.506(2)
C(3)-C(5)	1.509(2)	C(24)-C(29)	1.387(2)
C(6)-C(7)	1.403(2)	C(24)-C(25)	1.392(2)
C(6)-C(11)	1.404(2)	C(25)-C(26)	1.401(2)
C(7)-C(8)	1.391(2)	C(26)-C(27)	1.377(3)
C(7)-C(12)	1.501(2)	C(27)-C(28)	1.394(3)
C(8)-C(9)	1.390(2)	C(28)-C(29)	1.400(2)

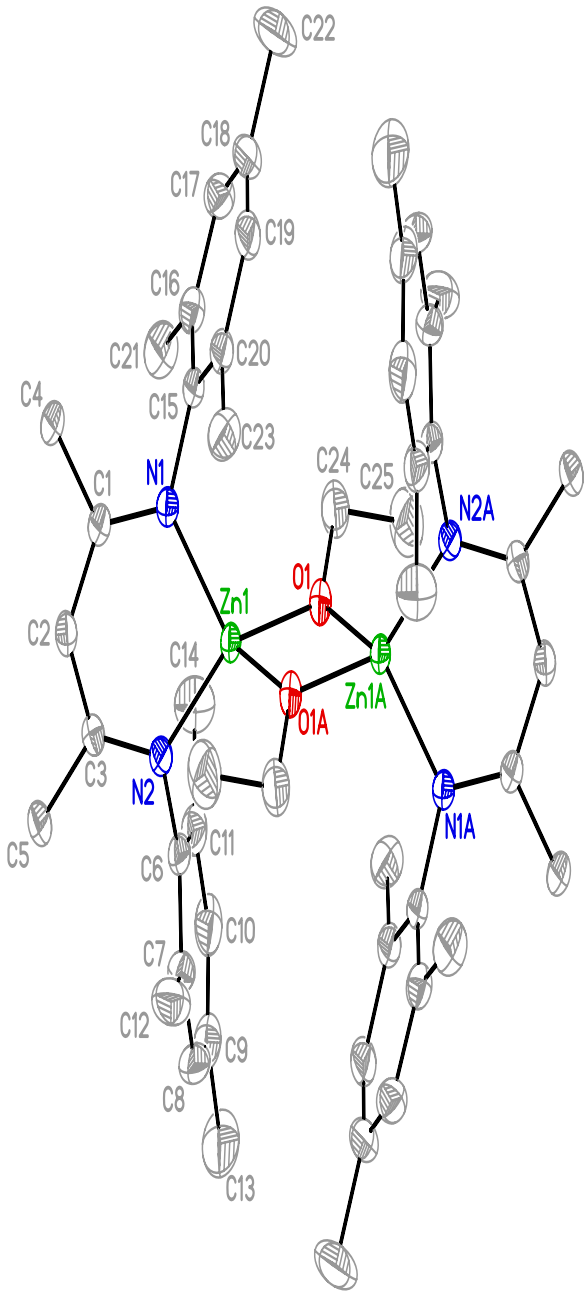
#1 -x+1,-y,-z+2

Table 5: Bond angles [°] for sg_555m.

C(24)-Se(1)-Zn(2)	116.57(5)	C(8)-C(9)-C(10)	118.31(16)
C(24)-Se(1)-Zn(2)#1	117.44(5)	C(8)-C(9)-C(13)	120.42(16)
Zn(2)-Se(1)-Zn(2)#1	90.997(14)	C(10)-C(9)-C(13)	121.21(16)
N(2)-Zn(2)-N(1)	97.66(6)	C(11)-C(10)-C(9)	121.70(16)
N(2)-Zn(2)-Se(1)	134.16(4)	C(10)-C(11)-C(6)	118.70(15)
N(1)-Zn(2)-Se(1)	110.08(4)	C(10)-C(11)-C(14)	120.33(16)
N(2)-Zn(2)-Se(1)#1	110.34(4)	C(6)-C(11)-C(14)	120.93(16)
N(1)-Zn(2)-Se(1)#1	117.06(4)	C(20)-C(15)-C(16)	120.26(14)
Se(1)-Zn(2)-Se(1)#1	89.003(14)	C(20)-C(15)-N(2)	120.45(14)
C(1)-N(1)-C(6)	119.75(14)	C(16)-C(15)-N(2)	119.20(15)
C(1)-N(1)-Zn(2)	119.17(11)	C(17)-C(16)-C(15)	118.87(16)
C(6)-N(1)-Zn(2)	120.96(10)	C(17)-C(16)-C(21)	120.00(15)
C(3)-N(2)-C(15)	119.83(13)	C(15)-C(16)-C(21)	121.09(15)
C(3)-N(2)-Zn(2)	117.09(10)	C(18)-C(17)-C(16)	121.94(15)
C(15)-N(2)-Zn(2)	123.06(10)	C(17)-C(18)-C(19)	117.61(15)
N(1)-C(1)-C(2)	123.06(15)	C(17)-C(18)-C(22)	120.76(16)
N(1)-C(1)-C(4)	119.69(15)	C(19)-C(18)-C(22)	121.62(17)
C(2)-C(1)-C(4)	117.21(15)	C(18)-C(19)-C(20)	122.77(16)
C(1)-C(2)-C(3)	128.76(15)	C(15)-C(20)-C(19)	118.29(15)
N(2)-C(3)-C(2)	125.07(15)	C(15)-C(20)-C(23)	121.41(14)
N(2)-C(3)-C(5)	118.37(14)	C(19)-C(20)-C(23)	120.30(15)
C(2)-C(3)-C(5)	116.53(15)	C(29)-C(24)-C(25)	119.28(15)
C(7)-C(6)-C(11)	120.68(15)	C(29)-C(24)-Se(1)	117.84(12)
C(7)-C(6)-N(1)	120.55(15)	C(25)-C(24)-Se(1)	122.86(13)
C(11)-C(6)-N(1)	118.59(14)	C(24)-C(25)-C(26)	120.39(17)
C(8)-C(7)-C(6)	118.73(15)	C(27)-C(26)-C(25)	120.67(17)
C(8)-C(7)-C(12)	119.36(15)	C(26)-C(27)-C(28)	118.84(17)
C(6)-C(7)-C(12)	121.87(15)	C(27)-C(28)-C(29)	121.00(18)
C(9)-C(8)-C(7)	121.83(15)	C(24)-C(29)-C(28)	119.82(17)

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

Compound 4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C18
C17
C19
C16
C21
C20
C15
C23
C4
C1
N1
C24
C25
N2A
O1
Zn1
C2
C14
Zn1A
O1A
C3
N2
N1A
C5
C11
C6
C10
C7
C12
C9
C8
C13

Table 1: Crystal structure data

Identification code	**sg_473m**
Empirical formula	C50 H68 N4 O2 Zn2
Formula weight	887.82
Density (calculated)	1.251 g · cm^{-1}
F(000)	472
Temperature	170(1) K
Crystal size	0.330 × 0.280 × 0.170 mm
Crystal colour	colourless
Crystal description	block
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	*P -1*
Unit cell dimensions	
a [Å]	10.6645(7)
b [Å]	11.1272(7)
c [Å]	11.9910(8)
α [°]	72.859(2)
β [°]	73.051(2)
γ [°]	61.825(2)
Volume	1178.84(14) Å^3
Z	1
Cell measurement reflections used	21401
Cell measurement *θ* min/max	2.51°/29.17°
Diffractometer control software	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Diffractometer measurement device	Bruker D8 KAPPA series II with APEX II area detector system
Diffractometer measurement method	Data collection strategy APEX 2/COSMO
θ range for data collection	1.807°- 29.223°
Completeness to *θ* = 25.242°	98.5%
Index ranges	$-14 \leq h \leq 13$
	$-15 \leq k \leq 15$
	$-16 \leq l \leq 16$
Computing data reduction	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Absorption coefficient	1.059 mm^{-1}
Absorption correction	Semi-empirical from equivalents
Computation absorption correction	BRUKER AXS SMART APEX 2 Vers. 3.0-2009

Max./min. Transmission	0.75/0.57
R_{merg} before/after correction	0.0676/0.0292
Computing structure solution	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Computing structure refinement	SHELXL-2013 (Sheldrick, 2013/4)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	31017
Independent reflections	6280
R_{int}	0.0224
Data	5662
Restraints	0
Parameter	262
GooF	1.050
Weighting details	$w = 1/[\sigma^2(F_{obs}^2) + (0.0656P)^2 + 0.5796P]$
	where $P = (F_{obs}^2 + 2F_{calc}^2)/3$
R_1 [$I > 2\sigma(I)$]	0.0351
wR_2 [$I > 2\sigma(I)$]	0.0985
R_1 [all data]	0.0407
wR_2 [all data]	0.1044
Absolute structure parameter	
Largest diff. peak and hole	1.896/-0.280

Table 2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for sg_473m. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
Zn(1)	4258(1)	6508(1)	5005(1)	23(1)
N(1)	2735(2)	7411(1)	6281(1)	23(1)
N(2)	4237(2)	8204(1)	3843(1)	24(1)
O(1)	5973(1)	4904(1)	5523(1)	27(1)
C(1)	1813(2)	8729(2)	6037(1)	23(1)
C(2)	1943(2)	9623(2)	4940(2)	26(1)
H(2)	1122	10485	4833	31
C(3)	3113(2)	9421(2)	3984(1)	24(1)
C(4)	547(2)	9363(2)	6988(2)	30(1)
H(4A)	55	8750	7347	44
H(4B)	-132	10270	6632	44
H(4C)	900	9480	7600	44
C(5)	3073(2)	10720(2)	3080(2)	31(1)
H(5A)	3927	10859	3042	47
H(5B)	2196	11524	3316	47
H(5C)	3070	10612	2298	47
C(6)	5454(2)	8217(2)	2925(1)	26(1)
C(7)	5465(2)	8266(2)	1737(2)	34(1)
C(8)	6641(3)	8382(2)	880(2)	45(1)
H(8)	6645	8448	71	55
C(9)	7793(3)	8404(2)	1163(2)	47(1)
C(10)	7788(2)	8285(2)	2345(2)	41(1)
H(10)	8592	8261	2558	49
C(11)	6630(2)	8199(2)	3235(2)	32(1)
C(12)	4287(3)	8184(3)	1366(2)	48(1)
H(12A)	4147	8754	576	72
H(12B)	3385	8525	1936	72
H(12C)	4558	7218	1342	72
C(13)	9039(3)	8545(3)	208(3)	73(1)
H(13A)	8718	9497	-245	109
H(13B)	9356	7897	-325	109
H(13C)	9845	8334	578	109
C(14)	6661(3)	8097(3)	4507(2)	47(1)
H(14A)	5850	8904	4809	71
H(14B)	7574	8073	4556	71

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H(14C)	6578	7247	4985	71
C(15)	2612(2)	6675(2)	7483(1)	25(1)
C(16)	3218(2)	6829(2)	8298(2)	31(1)
C(17)	3118(2)	6074(2)	9454(2)	40(1)
H(17)	3536	6162	10009	48
C(18)	2424(2)	5197(2)	9816(2)	43(1)
C(19)	1828(2)	5072(2)	8991(2)	38(1)
H(19)	1345	4481	9231	45
C(20)	1919(2)	5791(2)	7816(2)	30(1)
C(21)	3955(2)	7792(2)	7938(2)	41(1)
H(21A)	4431	7666	8577	61
H(21B)	3233	8755	7788	61
H(21C)	4677	7581	7215	61
C(22)	2301(4)	4411(4)	11075(2)	71(1)
H(22A)	3198	4092	11364	106
H(22B)	2136	3608	11098	106
H(22C)	1488	5020	11581	106
C(23)	1285(2)	5619(2)	6941(2)	38(1)
H(23A)	526	6514	6660	56
H(23B)	870	4946	7324	56
H(23C)	2045	5285	6266	56
C(24)	6605(3)	4671(2)	6502(2)	42(1)
H(24A)	5963	4484	7248	50
H(24B)	6690	5520	6501	50
C(25)	8079(3)	3466(3)	6463(3)	55(1)
H(25A)	8032	2667	6320	83
H(25B)	8392	3221	7222	83
H(25C)	8771	3728	5822	83

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Table 3: Anisotropic displacement parameters ($Å^2 \times 10^3$) for sg_473m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Zn(1)	25(1)	15(1)	21(1)	-3(1)	0(1)	-6(1)
N(1)	24(1)	18(1)	21(1)	-3(1)	0(1)	-7(1)
N(2)	26(1)	19(1)	21(1)	-3(1)	0(1)	-9(1)
O(1)	29(1)	18(1)	28(1)	-6(1)	-6(1)	-5(1)
C(1)	21(1)	21(1)	24(1)	-6(1)	-2(1)	-6(1)
C(2)	24(1)	18(1)	28(1)	-3(1)	-4(1)	-4(1)
C(3)	28(1)	18(1)	22(1)	-2(1)	-5(1)	-9(1)
C(4)	24(1)	25(1)	27(1)	-7(1)	2(1)	-3(1)
C(5)	36(1)	20(1)	27(1)	1(1)	-2(1)	-9(1)
C(6)	30(1)	17(1)	24(1)	-4(1)	3(1)	-8(1)
C(7)	45(1)	26(1)	24(1)	-3(1)	2(1)	-15(1)
C(8)	63(1)	34(1)	25(1)	-6(1)	12(1)	-19(1)
C(9)	44(1)	27(1)	47(1)	-5(1)	20(1)	-13(1)
C(10)	32(1)	27(1)	54(1)	-5(1)	6(1)	-13(1)
C(11)	33(1)	24(1)	36(1)	-6(1)	1(1)	-12(1)
C(12)	72(2)	51(1)	29(1)	-5(1)	-11(1)	-32(1)
C(13)	58(2)	53(2)	68(2)	-5(1)	33(1)	-21(1)
C(14)	50(1)	60(1)	43(1)	-10(1)	-8(1)	-32(1)
C(15)	24(1)	19(1)	22(1)	-4(1)	0(1)	-4(1)
C(16)	25(1)	30(1)	29(1)	-8(1)	-4(1)	-4(1)
C(17)	33(1)	44(1)	27(1)	-6(1)	-7(1)	-2(1)
C(18)	36(1)	37(1)	26(1)	4(1)	-1(1)	-1(1)
C(19)	36(1)	24(1)	34(1)	0(1)	6(1)	-8(1)
C(20)	29(1)	21(1)	28(1)	-4(1)	3(1)	-7(1)
C(21)	39(1)	45(1)	44(1)	-14(1)	-8(1)	-18(1)
C(22)	65(2)	76(2)	32(1)	16(1)	-5(1)	-16(2)
C(23)	41(1)	37(1)	38(1)	-10(1)	3(1)	-23(1)
C(24)	50(1)	30(1)	42(1)	-8(1)	-19(1)	-7(1)
C(25)	45(1)	50(1)	62(2)	-8(1)	-26(1)	-6(1)

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Table 4: Bond lengths [Å] for sg_473m.

Zn(1)-O(1)	1.9599(12)	C(7)-C(8)	1.404(3)
Zn(1)-N(1)	1.9766(13)	C(7)-C(12)	1.498(3)
Zn(1)-N(2)	1.9833(13)	C(8)-C(9)	1.379(4)
Zn(1)-O(1)#1	1.9929(12)	C(9)-C(10)	1.383(4)
Zn(1)-Zn(1)#1	2.9594(4)	C(9)-C(13)	1.518(3)
N(1)-C(1)	1.326(2)	C(10)-C(11)	1.399(3)
N(1)-C(15)	1.435(2)	C(11)-C(14)	1.505(3)
N(2)-C(3)	1.336(2)	C(15)-C(20)	1.399(2)
N(2)-C(6)	1.440(2)	C(15)-C(16)	1.405(2)
O(1)-C(24)	1.420(2)	C(16)-C(17)	1.396(3)
O(1)-Zn(1)#1	1.9929(12)	C(16)-C(21)	1.509(3)
C(1)-C(2)	1.411(2)	C(17)-C(18)	1.391(4)
C(1)-C(4)	1.516(2)	C(18)-C(19)	1.390(3)
C(2)-C(3)	1.405(2)	C(18)-C(22)	1.509(3)
C(3)-C(5)	1.520(2)	C(19)-C(20)	1.401(2)
C(6)-C(11)	1.399(3)	C(20)-C(23)	1.500(3)
C(6)-C(7)	1.406(2)	C(24)-C(25)	1.508(3)

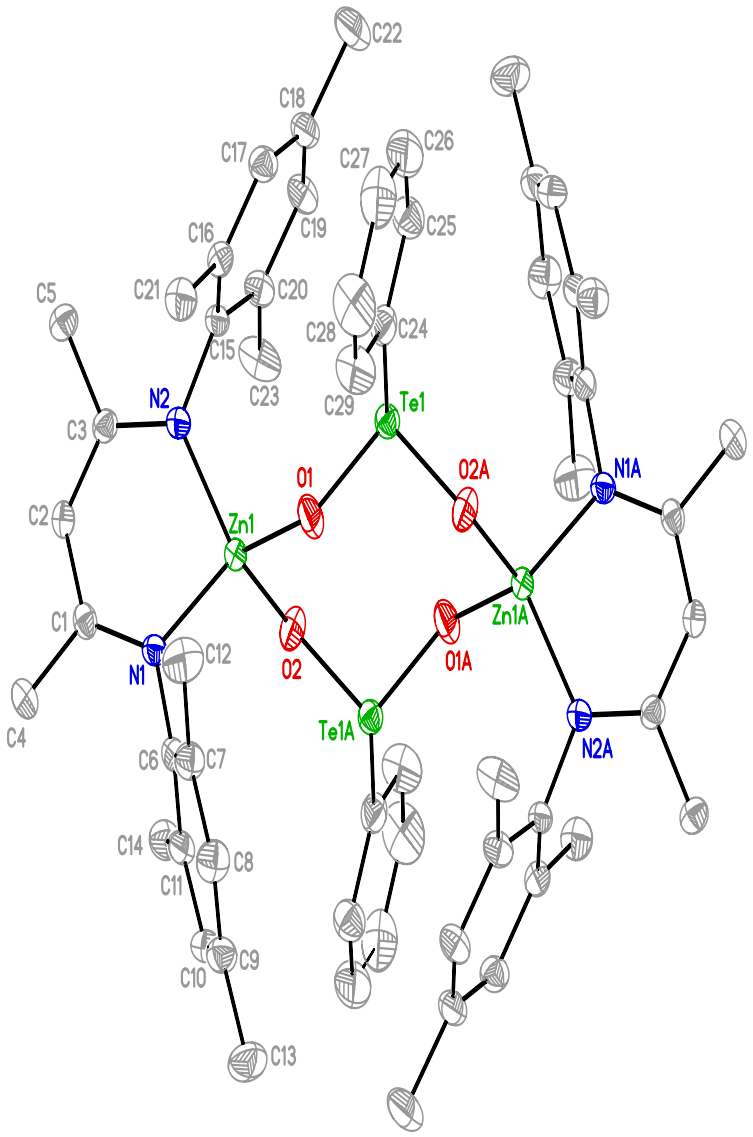
#1 -x+1,-y+1,-z+1

Table 5: Bond angles [°] for sg_473m.

O(1)-Zn(1)-N(1)	115.62(5)	C(7)-C(6)-N(2)	121.28(16)
O(1)-Zn(1)-N(2)	126.16(6)	C(8)-C(7)-C(6)	117.9(2)
N(1)-Zn(1)-N(2)	98.33(6)	C(8)-C(7)-C(12)	119.54(19)
O(1)-Zn(1)-O(1)#1	83.05(5)	C(6)-C(7)-C(12)	122.57(17)
N(1)-Zn(1)-O(1)#1	116.64(5)	C(9)-C(8)-C(7)	122.7(2)
N(2)-Zn(1)-O(1)#1	118.49(5)	C(8)-C(9)-C(10)	118.16(18)
O(1)-Zn(1)-Zn(1)#1	41.95(4)	C(8)-C(9)-C(13)	121.1(3)
N(1)-Zn(1)-Zn(1)#1	126.04(4)	C(10)-C(9)-C(13)	120.7(3)
N(2)-Zn(1)-Zn(1)#1	135.40(4)	C(9)-C(10)-C(11)	121.7(2)
O(1)#1-Zn(1)-Zn(1)#1	41.10(3)	C(6)-C(11)-C(10)	119.23(18)
C(1)-N(1)-C(15)	118.68(13)	C(6)-C(11)-C(14)	120.98(17)
C(1)-N(1)-Zn(1)	119.90(11)	C(10)-C(11)-C(14)	119.8(2)
C(15)-N(1)-Zn(1)	121.41(10)	C(20)-C(15)-C(16)	121.07(16)
C(3)-N(2)-C(6)	117.61(13)	C(20)-C(15)-N(1)	119.36(15)
C(3)-N(2)-Zn(1)	119.12(11)	C(16)-C(15)-N(1)	119.55(15)
C(6)-N(2)-Zn(1)	122.90(10)	C(17)-C(16)-C(15)	118.49(18)
C(24)-O(1)-Zn(1)	128.09(11)	C(17)-C(16)-C(21)	120.62(18)
C(24)-O(1)-Zn(1)#1	126.30(11)	C(15)-C(16)-C(21)	120.89(17)
Zn(1)-O(1)-Zn(1)#1	96.95(5)	C(18)-C(17)-C(16)	121.81(19)
N(1)-C(1)-C(2)	124.28(14)	C(19)-C(18)-C(17)	118.36(18)
N(1)-C(1)-C(4)	119.38(14)	C(19)-C(18)-C(22)	120.6(2)
C(2)-C(1)-C(4)	116.32(14)	C(17)-C(18)-C(22)	121.1(2)
C(3)-C(2)-C(1)	129.24(15)	C(18)-C(19)-C(20)	121.97(19)
N(2)-C(3)-C(2)	124.97(14)	C(15)-C(20)-C(19)	118.28(18)
N(2)-C(3)-C(5)	119.35(14)	C(15)-C(20)-C(23)	120.93(16)
C(2)-C(3)-C(5)	115.66(14)	C(19)-C(20)-C(23)	120.78(18)
C(11)-C(6)-C(7)	120.24(16)	O(1)-C(24)-C(25)	111.99(18)
C(11)-C(6)-N(2)	118.47(15)		

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

Compound 5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N1
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Te1A
N2A
C6
C7
C14
C8
C11
C9
C10
C13

Table 1: Crystal structure data

Identification code	**sg_530m**
Empirical formula	C70 H78 F2 N4 O4 Te2 Zn2
Formula weight	1463.30
Density (calculated)	1.485 g · cm^{-1}
F(000)	1480
Temperature	180(1) K
Crystal size	0.170 × 0.150 × 0.150 mm
Crystal colour	colourless
Crystal description	block
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	*P 21/c*
Unit cell dimensions	
a [Å]	12.3389(3)
b [Å]	15.5903(4)
c [Å]	17.8480(5)
α [°]	90
β [°]	107.5790(10)
γ [°]	90
Volume	3273.03(15) Å^3
Z	2
Cell measurement reflections used	36523
Cell measurement *θ* min/max	2.21°/31.55°
Diffractometer control software	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Diffractometer measurement device	Bruker D8 KAPPA series II with APEX II area detector system
Diffractometer measurement method	Data collection strategy APEX 2/COSMO
θ range for data collection	1.731°- 31.584°
Completeness to *θ* = 25.242°	98.4%
Index ranges	$-17 \leq h \leq 18$
	$-22 \leq k \leq 22$
	$-26 \leq l \leq 25$
Computing data reduction	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Absorption coefficient	1.662 mm^{-1}
Absorption correction	Semi-empirical from equivalents

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Computation absorption correction	BRUKER AXS SMART APEX 2 Vers. 3.0-2009
Max./min. Transmission	0.75/0.68
R_{merg} before/after correction	0.0452/0.0374
Computing structure solution	BRUKER D8 KAPPA APEX 2 Vers. 3.0-2009
Computing structure refinement	SHELXL-2013 (Sheldrick, 2013/4)
Refinement method	Full-matrix least-squares on F^2
Reflections collected	73231
Independent reflections	10619
R_{int}	0.0257
Data	9026
Restraints	0
Parameter	348
GooF	1.051
Weighting details	$w = 1/[\sigma^2(F_{obs}^2) + (0.0356P)^2 + 2.2306P]$ where $P = (F_{obs}^2 + 2F_{calc}^2)/3$
R_1 [$I > 2\sigma(I)$]	0.0260
wR_2 [$I > 2\sigma(I)$]	0.0659
R_1 [all data]	0.0352
wR_2 [all data]	0.0719
Largest diff. peak and hole	0.835/-0.742

Table 2: Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for sg_530m. U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	*y*	*z*	U_{eq}
Te(1)	3813(1)	10351(1)	4005(1)	20(1)
Zn(1)	3454(1)	9323(1)	5550(1)	20(1)
N(1)	3055(1)	9429(1)	6530(1)	20(1)
N(2)	2168(1)	8616(1)	4956(1)	21(1)
O(1)	3516(1)	10380(1)	4962(1)	28(1)
O(2)	4997(1)	8870(1)	5775(1)	27(1)
C(1)	2222(1)	8972(1)	6652(1)	20(1)
C(2)	1527(1)	8406(1)	6096(1)	22(1)
H(2)	1037	8056	6286	26
C(3)	1451(1)	8280(1)	5302(1)	21(1)
C(4)	1962(2)	9065(1)	7423(1)	28(1)
H(4A)	2634	8905	7857	42
H(4B)	1326	8689	7424	42
H(4C)	1759	9662	7489	42
C(5)	488(2)	7722(1)	4822(1)	32(1)
H(5A)	5	8055	4381	48
H(5B)	35	7523	5154	48
H(5C)	800	7226	4620	48
C(6)	3732(1)	9995(1)	7117(1)	21(1)
C(7)	3473(2)	10872(1)	7082(1)	26(1)
C(8)	4186(2)	11424(1)	7625(1)	31(1)
H(8)	4005	12017	7609	37
C(9)	5160(2)	11128(1)	8193(1)	30(1)
C(10)	5400(2)	10258(1)	8213(1)	27(1)
H(10)	6059	10048	8598	33
C(11)	4703(2)	9680(1)	7684(1)	22(1)
C(12)	2447(2)	11213(1)	6462(1)	40(1)
H(12A)	2412	11837	6514	59
H(12B)	1759	10954	6529	59
H(12C)	2502	11069	5941	59
C(13)	5913(2)	11753(2)	8766(1)	42(1)
H(13A)	6400	11439	9218	63
H(13B)	5440	12161	8944	63
H(13C)	6389	12065	8506	63
C(14)	4993(2)	8738(1)	7714(1)	28(1)

H(14A)	4403	8408	7849	42
H(14B)	5728	8641	8112	42
H(14C)	5038	8553	7199	42
C(15)	1895(1)	8653(1)	4120(1)	20(1)
C(16)	1120(1)	9275(1)	3710(1)	23(1)
C(17)	924(2)	9354(1)	2900(1)	26(1)
H(17)	378	9759	2616	31
C(18)	1500(2)	8860(1)	2496(1)	27(1)
C(19)	2286(2)	8266(1)	2922(1)	28(1)
H(19)	2690	7925	2655	33
C(20)	2501(2)	8154(1)	3730(1)	25(1)
C(21)	556(2)	9876(1)	4139(1)	30(1)
H(21A)	116	10307	3772	45
H(21B)	1137	10162	4564	45
H(21C)	46	9550	4361	45
C(22)	1293(2)	8981(2)	1628(1)	39(1)
H(22A)	551	9253	1397	58
H(22B)	1303	8422	1379	58
H(22C)	1890	9347	1541	58
C(23)	3382(2)	7529(2)	4182(1)	39(1)
H(23A)	3966	7836	4590	59
H(23B)	3734	7246	3823	59
H(23C)	3022	7097	4427	59
C(24)	2549(1)	11230(1)	3400(1)	26(1)
C(25)	2109(2)	11171(1)	2589(1)	32(1)
H(25)	2384	10747	2309	38
C(26)	1260(2)	11739(2)	2188(1)	42(1)
H(26)	945	11696	1634	51
C(27)	877(2)	12358(2)	2589(2)	48(1)
H(27)	305	12748	2312	57
C(28)	1323(2)	12417(2)	3397(2)	51(1)
H(28)	1061	12852	3673	62
C(29)	2151(2)	11843(2)	3809(1)	41(1)
H(29)	2440	11872	4365	49
F(1)	1553(6)	5572(5)	4303(4)	130(2)
C(31)	2169(4)	4922(2)	4555(3)	62(2)
C(32)	3187(4)	4716(3)	4415(3)	59(1)

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C(33)	3773(3)	3977(3)	4741(3)	57(1)
C(34)	3341(3)	3445(2)	5206(3)	49(1)
C(35)	2323(4)	3650(3)	5346(2)	46(1)
C(36)	1737(3)	4389(3)	5020(3)	54(1)
H(32)	3483	5080	4097	65
H(33)	4468	3837	4645	65
H(34)	3741	2940	5429	65
H(35)	2027	3286	5664	65
H(36)	1042	4529	5116	65
F(1A)	1009(6)	5504(4)	4621(4)	121(2)
C(31A)	1815(4)	4890(2)	4752(3)	49(1)
C(32A)	1728(3)	4163(3)	5180(3)	47(1)
C(33A)	2559(4)	3530(2)	5317(3)	57(2)
C(34A)	3476(4)	3625(3)	5025(3)	71(2)
C(35A)	3563(4)	4353(4)	4597(3)	74(2)
C(36A)	2733(5)	4985(3)	4460(3)	66(2)
H(32A)	1101	4098	5380	80
H(33A)	2499	3033	5610	80
H(34A)	4044	3193	5118	80
H(35A)	4190	4418	4397	80
H(36A)	2792	5483	4167	80

Table 3: Anisotropic displacement parameters ($Å^2 \times 10^3$) for sg_530m. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$

	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Te(1)	21(1)	20(1)	19(1)	2(1)	5(1)	0(1)
Zn(1)	19(1)	25(1)	16(1)	0(1)	5(1)	-4(1)
N(1)	21(1)	20(1)	16(1)	-2(1)	4(1)	-2(1)
N(2)	21(1)	24(1)	16(1)	-2(1)	4(1)	-3(1)
O(1)	35(1)	27(1)	24(1)	3(1)	13(1)	-3(1)
O(2)	20(1)	26(1)	34(1)	2(1)	7(1)	-3(1)
C(1)	22(1)	20(1)	18(1)	1(1)	6(1)	1(1)
C(2)	22(1)	24(1)	21(1)	1(1)	7(1)	-5(1)
C(3)	21(1)	21(1)	21(1)	0(1)	3(1)	-4(1)
C(4)	31(1)	35(1)	20(1)	-1(1)	11(1)	-3(1)
C(5)	33(1)	34(1)	26(1)	-2(1)	4(1)	-15(1)
C(6)	24(1)	21(1)	17(1)	-1(1)	6(1)	-3(1)
C(7)	28(1)	22(1)	24(1)	-1(1)	5(1)	1(1)
C(8)	37(1)	21(1)	31(1)	-4(1)	6(1)	-2(1)
C(9)	34(1)	30(1)	23(1)	-6(1)	5(1)	-7(1)
C(10)	26(1)	32(1)	20(1)	-1(1)	1(1)	-3(1)
C(11)	26(1)	23(1)	18(1)	1(1)	5(1)	0(1)
C(12)	40(1)	29(1)	40(1)	0(1)	-2(1)	8(1)
C(13)	44(1)	39(1)	36(1)	-14(1)	1(1)	-11(1)
C(14)	32(1)	24(1)	26(1)	4(1)	4(1)	3(1)
C(15)	22(1)	22(1)	17(1)	-1(1)	4(1)	-3(1)
C(16)	22(1)	24(1)	21(1)	-1(1)	5(1)	-2(1)
C(17)	27(1)	26(1)	22(1)	3(1)	2(1)	-1(1)
C(18)	34(1)	27(1)	18(1)	0(1)	6(1)	-4(1)
C(19)	35(1)	29(1)	20(1)	-3(1)	9(1)	2(1)
C(20)	30(1)	23(1)	20(1)	-1(1)	6(1)	3(1)
C(21)	26(1)	33(1)	31(1)	-2(1)	8(1)	6(1)
C(22)	55(1)	41(1)	19(1)	3(1)	8(1)	-2(1)
C(23)	52(1)	35(1)	27(1)	-2(1)	6(1)	20(1)
C(24)	21(1)	27(1)	27(1)	4(1)	5(1)	0(1)
C(25)	32(1)	34(1)	27(1)	6(1)	5(1)	4(1)
C(26)	37(1)	50(1)	34(1)	16(1)	3(1)	7(1)
C(27)	34(1)	47(1)	60(2)	24(1)	12(1)	16(1)
C(28)	53(2)	45(1)	58(2)	4(1)	19(1)	22(1)
C(29)	44(1)	41(1)	36(1)	0(1)	9(1)	12(1)

Table 4: Bond lengths [Å] for sg_530m.

Te(1)-O(1)	1.8524(13)	C(16)-C(17)	1.398(2)
Te(1)-O(2)#1	1.8529(12)	C(16)-C(21)	1.507(2)
Te(1)-C(24)	2.1118(17)	C(17)-C(18)	1.389(3)
Zn(1)-O(2)	1.9553(13)	C(18)-C(19)	1.389(3)
Zn(1)-N(2)	1.9589(14)	C(18)-C(22)	1.506(2)
Zn(1)-N(1)	1.9620(14)	C(19)-C(20)	1.396(2)
Zn(1)-O(1)	1.9678(13)	C(20)-C(23)	1.500(3)
N(1)-C(1)	1.322(2)	C(24)-C(29)	1.379(3)
N(1)-C(6)	1.430(2)	C(24)-C(25)	1.387(3)
N(2)-C(3)	1.330(2)	C(25)-C(26)	1.393(3)
N(2)-C(15)	1.428(2)	C(26)-C(27)	1.368(4)
O(2)-Te(1)#1	1.8529(12)	C(27)-C(28)	1.382(4)
C(1)-C(2)	1.410(2)	C(28)-C(29)	1.390(3)
C(1)-C(4)	1.511(2)	F(1)-C(31)	1.266(8)
C(2)-C(3)	1.404(2)	C(31)-C(32)	1.3900
C(3)-C(5)	1.513(2)	C(31)-C(36)	1.3900
C(6)-C(7)	1.402(2)	C(32)-C(33)	1.3900
C(6)-C(11)	1.402(2)	C(33)-C(34)	1.3900
C(7)-C(8)	1.393(2)	C(34)-C(35)	1.3900
C(7)-C(12)	1.504(3)	C(35)-C(36)	1.3900
C(8)-C(9)	1.395(3)	F(1A)-C(31A)	1.348(7)
C(9)-C(10)	1.387(3)	C(31A)-C(32A)	1.3900
C(9)-C(13)	1.512(3)	C(31A)-C(36A)	1.3900
C(10)-C(11)	1.397(2)	C(32A)-C(33A)	1.3900
C(11)-C(14)	1.509(2)	C(33A)-C(34A)	1.3900
C(15)-C(20)	1.402(2)	C(34A)-C(35A)	1.3900
C(15)-C(16)	1.402(2)	C(35A)-C(36A)	1.3900

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

Table 5: Bond angles [°] for sg_530m.

O(1)-Te(1)-O(2)#1	98.79(6)	C(20)-C(15)-C(16)	120.44(15)
O(1)-Te(1)-C(24)	97.71(7)	C(20)-C(15)-N(2)	120.24(15)
O(2)#1-Te(1)-C(24)	95.70(6)	C(16)-C(15)-N(2)	118.80(15)
O(2)-Zn(1)-N(2)	119.14(6)	C(17)-C(16)-C(15)	118.61(16)
O(2)-Zn(1)-N(1)	109.75(6)	C(17)-C(16)-C(21)	120.52(16)
N(2)-Zn(1)-N(1)	98.58(6)	C(15)-C(16)-C(21)	120.80(15)
O(2)-Zn(1)-O(1)	102.67(6)	C(18)-C(17)-C(16)	122.09(17)
N(2)-Zn(1)-O(1)	109.80(6)	C(19)-C(18)-C(17)	117.94(16)
N(1)-Zn(1)-O(1)	117.78(6)	C(19)-C(18)-C(22)	121.36(18)
C(1)-N(1)-C(6)	121.48(14)	C(17)-C(18)-C(22)	120.68(18)
C(1)-N(1)-Zn(1)	121.27(11)	C(18)-C(19)-C(20)	122.16(17)
C(6)-N(1)-Zn(1)	117.20(10)	C(19)-C(20)-C(15)	118.68(16)
C(3)-N(2)-C(15)	121.37(14)	C(19)-C(20)-C(23)	121.17(17)
C(3)-N(2)-Zn(1)	120.96(11)	C(15)-C(20)-C(23)	120.13(16)
C(15)-N(2)-Zn(1)	116.04(10)	C(29)-C(24)-C(25)	120.56(18)
Te(1)-O(1)-Zn(1)	121.46(7)	C(29)-C(24)-Te(1)	120.35(14)
Te(1)#1-O(2)-Zn(1)	117.85(7)	C(25)-C(24)-Te(1)	119.08(14)
N(1)-C(1)-C(2)	123.96(14)	C(24)-C(25)-C(26)	119.3(2)
N(1)-C(1)-C(4)	119.22(15)	C(27)-C(26)-C(25)	120.3(2)
C(2)-C(1)-C(4)	116.81(14)	C(26)-C(27)-C(28)	120.1(2)
C(3)-C(2)-C(1)	129.71(15)	C(27)-C(28)-C(29)	120.4(2)
N(2)-C(3)-C(2)	124.21(15)	C(24)-C(29)-C(28)	119.3(2)
N(2)-C(3)-C(5)	118.86(15)	F(1)-C(31)-C(32)	126.9(5)
C(2)-C(3)-C(5)	116.93(15)	F(1)-C(31)-C(36)	113.1(5)
C(7)-C(6)-C(11)	120.44(15)	C(32)-C(31)-C(36)	120.0
C(7)-C(6)-N(1)	119.61(15)	C(31)-C(32)-C(33)	120.0
C(11)-C(6)-N(1)	119.73(15)	C(34)-C(33)-C(32)	120.0
C(8)-C(7)-C(6)	118.95(16)	C(33)-C(34)-C(35)	120.0
C(8)-C(7)-C(12)	120.54(17)	C(36)-C(35)-C(34)	120.0
C(6)-C(7)-C(12)	120.50(16)	C(35)-C(36)-C(31)	120.0
C(7)-C(8)-C(9)	121.74(17)	F(1A)-C(31A)-C(32A)	119.9(5)
C(10)-C(9)-C(8)	118.18(17)	F(1A)-C(31A)-C(36A)	120.1(5)
C(10)-C(9)-C(13)	122.01(18)	C(32A)-C(31A)-C(36A)	120.0
C(8)-C(9)-C(13)	119.81(19)	C(33A)-C(32A)-C(31A)	120.0
C(9)-C(10)-C(11)	122.00(17)	C(32A)-C(33A)-C(34A)	120.0
C(10)-C(11)-C(6)	118.67(16)	C(35A)-C(34A)-C(33A)	120.0

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C(10)-C(11)-C(14)	120.84(16)	C(34A)-C(35A)-C(36A)	120.0
C(6)-C(11)-C(14)	120.49(15)	C(35A)-C(36A)-C(31A)	120.0

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