SUPPORTING INFORMATION

Structural Characterization of Zinc Bicarbonate Compounds Relevant to the Mechanism of Action of Carbonic Anhydrase

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EXPERIMENTAL SECTION

General Considerations

All manipulations were performed by using a combination of glovebox, high vacuum, and Schlenk techniques under a nitrogen or argon atmosphere,¹ unless specified otherwise. Solvents were purified and degassed by standard procedures. Solution NMR spectra were measured on Bruker 300 DRX, Bruker 400 DRX, and Bruker Avance 500 DMX spectrometers. ¹H NMR chemical shifts are reported in ppm relative to SiMe₄ ($\delta = 0$) and were referenced internally with respect to the protio solvent impurity (δ 7.16 for C₆D₅H and δ 5.32 for CHDCl₂).² ¹³C NMR spectra are reported in ppm relative to SiMe₄ ($\delta = 0$) and were referenced internally with respect to the solvent (δ 128.06 for C₆D₆ and δ 54.00 for CD₂Cl₂).² Coupling constants are given in hertz. Solid-state ¹³C{¹H} NMR experiments were performed on a Bruker 400 Cyber-enabled Avance III at a field of 9.40 T (corresponding to a ¹³C resonance frequency of 100.62 MHz) using the CP-MAS pulse sequence, with an acquisition time of 0.05 seconds and a spin rate of 10⁴ Hz. Infrared spectra were recorded on Nicolet Avatar 370 DTGS spectrometer and are reported in cm⁻¹. All chemicals were obtained from Aldrich. [κ ⁴-Tptm]ZnOSiMe₃,³ [κ ³-Tptm]ZnN(SiMe₃)₂,³ and [κ ³-Tptm]ZnH³ were prepared by the literature methods.

X-ray Structure Determinations

X-ray diffraction data were collected on a Bruker Apex II diffractometer. Crystal data, data collection and refinement parameters are summarized in Table 1. The structures were solved using direct methods and standard difference map techniques, and were refined by full-matrix least-squares procedures on F^2 with SHELXTL (Version 6.1).⁴

Synthesis of [Tp^{Bu^t,Me}]ZnOH

 $[Tp^{ButMe}]$ ZnOH was prepared by a method analogous to that previously reported.⁵ A solution of $[Tp^{ButMe}]$ Li (1.868 g, 4.34 mmol) in MeOH (*ca.* 40 mL) was treated with Zn(ClO₄)₂•6H₂O (1.864 g, 5.01 mmol) and the resulting suspension was stirred for 15 minutes, during which period most of the solid dissolved. KOH (268 mg, 4.78 mmol) was added and the suspension was stirred for 1 hour, after which the volatile components were removed *in vacuo*. Benzene (*ca.* 50 mL) was added and the mixture was washed with several portions of H₂O (300 mL total). The benzene layer was filtered and then lyophilized to give $[Tp^{ButMe}]$ ZnOH (1.73 g, 79 %) as a white solid of sufficient purity for further reactions. Large colorless crystals of $[Tp^{ButMe}]$ ZnOH can be obtained from vapor diffusion of ether into a saturated benzene solution.

Structural Characterization of [Tp^{But,Me}]ZnOCO₂H

Crystals of $[Tp^{But,Me}]$ ZnOCO₂H suitable for X-ray diffraction were obtained by treatment of $[Tp^{But,Me}]$ ZnOH with CO₂. A solution of $[Tp^{But,Me}]$ ZnOH (*ca.* 10 mg) in benzene (*ca.* 0.5 mL) was placed in a small vial that was located inside a larger vial that contained pentane and dry ice. The larger vial was lightly stoppered until the dry ice had sublimed and then sealed completely. The sample was allowed to stand at room temperature, thereby depositing colorless crystals of $[Tp^{But,Me}]$ ZnOCO₂H that were suitable for X-ray diffraction. IR Data (KBr disk, cm⁻¹): 3424 (w), 2962 (s), 2930 (m), 2868 (m), 2548 (m), 1651 (m), 1636 (m), 1588 (m), 1545 (s), 1479 (m), 1405 (m), 1425 (s), 1383 (w), 1364 (s), 1309 (s), 1245 (w), 1192 (s), 1068 (s), 1029 (w), 852 (w), 795 (w), 771 (m), 649 (m). Upon dissolving in C₆D₆, solutions of $[Tp^{But,Me}]$ ZnOCO₂H immediately release CO₂ and regenerate $[Tp^{But,Me}]$ ZnOH, as indicated by ¹H NMR spectroscopy.



Molecular Structure of [*Tp*^{Bu^t,Me}]*ZnOCO*₂*H*

Synthesis of $\{[\kappa^3 - Tptm]Zn(\mu - OH)\}_2$

A suspension of $[\kappa^3$ -Tptm]ZnH (28 mg, 0.07 mmol) in pentane (*ca*. 4 mL) was treated with H_2O (50 µL, 2.78 mmol) and ethanol (10 µL, 0.16 mmol) via syringe. Evolution of H₂ was observed, and the reaction was left open to the nitrogen manifold at room temperature for 2 days. After this period, much of the pentane has evaporated and the residue was dried *in vacuo* to give $\{[\kappa^3-Tptm]Zn(\mu-OH)\}_2$ as an off-white solid (23 mg, 79%). Colorless crystals of $\{[\kappa^3-\text{Tptm}]Zn(\mu-\text{OH})\}_2 \cdot (C_6H_6)$ suitable for X-ray diffraction were obtained from a concentrated solution in benzene, but it should be noted that $\{[\kappa^3 -$ Tptm] $Zn(\mu-OH)$ ₂ decomposes to [Tptm]H and unidentified zinc products over several hours at room temperature. In addition, crystals of composition $\{[\kappa^3-Tptm]Zn(\mu-$ OH)₂•(C₇H₈) were obtained by the slow hydrolysis of a solution of $[\kappa^4$ -Tptm]ZnN(SiMe₃)₂ in toluene with adventitious water over a period of two months at -15 °C. Anal. Calcd. for { $[\kappa^{3}$ -Tptm]Zn(μ -OH)}₂•0.30(C₇H₈): C, 48.0%; H, 3.4%; N, 9.3%. Found: C, 48.1%; H, 3.1%; N, 9.1%. IR Data (KBr disk, cm⁻¹): 3402 (w), 3078 (w), 3047 (w), 1589 (s), 1555 (s), 1453 (s), 1416 (s), 1280 (m), 1131 (s), 1090 (m), 1045 (m), 1006 (m), 759 (s), 723 (m), 637 (w). ¹H NMR (C_6D_6): Not observed [(SC₅H₄N)₃CZnO<u>H</u>], 6.20 [t, ³J_{H-H} = 6 Hz, 3H, $(SC_5H_4N)_3CZnOH]$, 6.61 [t, ${}^{3}J_{H-H} = 7$ Hz, 3H, $(SC_5H_4N)_3CZnO_2H]$, 6.74 [d, ${}^{3}J_{H-H} = 7$ Hz, 3H, $(SC_{5}H_{4}N)_{3}CZnOH$], 8.95 [s, 3H, $(SC_{5}H_{4}N)_{3}CZnOH$]. ¹³C{¹H} NMR $(C_{6}D_{6})$: Not observed, $[(SC_{5}H_{4}N)_{3}CZnOH]$, 118.7 [s, 3C, $(SC_{5}H_{4}N)_{3}CZnOH$], 120.7 [s, 3C, $(SC_{5}H_{4}N)_{3}CZnOH$], 137.0 [s, 3C, $(SC_{5}H_{4}N)_{3}CZnOH$], 149.2 [s, 3C, $(SC_{5}H_{4}N)_{3}CZnOH$], not observed [s, 3H, $(SC_{5}H_{4}N)_{3}CZnOH$].



Molecular Structure of $\{[\kappa^3 - Tptm]Zn(\mu - OH)\}_2 \bullet (C_7H_8)$



Molecular Structure of $\{[\kappa^3 - Tptm]Zn(\mu - OH)\}_2 \bullet (C_6H_6)$

Synthesis of [κ⁴-Tptm]ZnOCO₂H

(a) A solution of $[\kappa^4$ -Tptm]ZnOSiMe₃ (30 mg, 0.06 mmol) in C₆H₆ (*ca.* 2 mL) in a small Schlenk tube was treated with H_2O (40 μ L, 40 mg, 2.22 mmol). The sample was frozen, degassed and allowed to warm to room temperature. The suspension was then treated with CO_2 (1 atm) while being shaken vigorously for a brief period. The mixture was allowed to stand at room temperature, thereby depositing colorless crystals of $[\kappa^4$ -Tptm]ZnOCO₂H•(C_6H_6) over a period of 30 minutes. The mother liquor was decanted, and the precipitate was washed with benzene (*ca.* 1 mL). The precipitate was dried *in vacuo* giving $[\kappa^4$ -Tptm]ZnOCO₂H•(C₆H₆) (12 mg, 36 %) as an off white powder. Colorless crystals of $[\kappa^4$ -Tptm]ZnOCO₂H suitable for X-ray diffraction were obtained directly from the reaction mixture before drying *in vacuo*. IR Data (KBr disk, cm⁻¹): 3078 (w), 3018 (w), 2633 (w), 1628 (s)/1621 (s) [v(CO₃)], 1591 (s), 1558 (s), 1477 (m), 1459 (s), 1416 (s), 1363 (s) [v_{sym} (CO₂)], 1283 (s), 1155 (w), 1094 (m), 1047 (m), 1032 (m), 1007 (m), 975 (w), 834 (w), 757 (s), 723 (m), 692 (s), 642 (m), 611 (w). Anal. calcd. for $[\kappa^4$ -Tptm]ZnOCO₂H•0.9(C₆H₆): C, 49.9%; H, 3.4%; N, 7.8%. Found: C, 49.7%; H, 3.3%; N, 7.4%. Crystals of $[\kappa^4$ -Tptm]ZnOCO₂H were also obtained *via* the analogous reactions employing $[\kappa^3$ -Tptm]ZnN(SiMe₃)₂ and $[\kappa^3$ -Tptm]ZnH instead of $[\kappa^4$ -Tptm]ZnOSiMe₃. (b) A solution of $\{[\kappa^3-Tptm]Zn(\mu-OH)\}_2$ (8 mg, 0.01 mmol) in benzene (ca. 2 mL) was treated with H_2O (50 µL, 2.78 mmol). The sample was frozen, degassed, and allowed to warm to room temperature. The resulting suspension was treated with CO_2 (1 atm) while being shaken vigorously, thereby resulting in the formation of colorless crystals. The mixture was allowed to stand at room temperature for 30 minutes and lyophilized to give $[\kappa^4$ -Tptm]ZnOCO₂H•(C₆H₆) (7 mg, 70%) as a white solid.



Molecular Structure of $[\kappa^4$ -*Tptm*]*ZnOCO*₂*H*

Synthesis of [κ^4 -Tptm]ZnO¹³CO₂H

A degassed solution of $[\kappa^4$ -Tptm]ZnOSiMe₃ (103 mg, 0.21 mmol) in benzene (*ca.* 2.0 mL) was treated with ¹³CO₂ (1 atm). H₂O (30 mg, 1.67 mmol) was added and the sample was shaken. The sample was allowed to stand at room temperature for 1 hour, over which period colorless crystals of $[\kappa^4$ -Tptm]ZnO¹³CO₂H•(C₆H₆) were deposited. The mixture was filtered and the precipitate was dried *in vacuo* giving $[\kappa^4$ -Tptm]ZnO¹³CO₂H•(C₆H₆) (75 mg, 66%) as an off-white powder. IR Data (KBr disk, cm⁻¹): 3085 (w), 3014 (w), 2908 (w), 1591 (s), 1580 (s) $[v(CO_3)]$, 1556 (s), 1459 (s), 1417 (s), 1389 (w), 1352 (s) $[v_{sym}(CO_2)]$, 1282 (w), 1132 (s), 1095 (w), 1047 (m), 1007 (m), 808 (w), 757 (s), 724 (m), 697 (m). ¹³C{¹H} NMR (Solid state): 165.0, $[(SC_5H_4N)_3CZn^{13}CO_2H]$.

Synthesis of [κ^4 -Tptm]ZnO¹³CO₂D

A degassed solution of $[\kappa^4$ -Tptm]ZnOSiMe₃ (103 mg, 0.21 mmol) in benzene (*ca.* 2 mL) was treated with ¹³CO₂ (1 atm). D₂O (20 mg, 1.00 mmol) was added and the sample was shaken. The mixture was allowed to stand at room temperature for 1 hour, during which period colorless crystals of $[\kappa^4$ -Tptm]ZnO¹³CO₂D•(C₆H₆) were deposited. The

mixture was filtered, and the precipitate was dried in vacuo giving [κ^4 -

Tptm]ZnO¹³CO₂D•(C₆H₆) (29 mg, 25%) as an off-white powder. IR Data (KBr disk, cm⁻¹): 3085 (w), 3014 (w), 2362 (w), 2339 (w), 1590 (s) [v(CO₃)] (overlapping), 1556 (s), 1479 (w), 1458 (s), 1417 (s), 1370 (m), 1355 (s) [v_{asym} (CO₂)], 1282 (m), 1252 (m), 1131 (s), 1094 (w), 1066 (w), 1047 (m), 1007 (m), 809 (w), 758 (s), 724 (m), 693 (m), 642 (w).

Synthesis of [Tptm]Zn(µ-CO₃)Zn[Tptm]

(a) A solution of $[\kappa^4$ -Tptm]ZnOSiMe₃ (18 mg, 0.04 mmol) in benzene (*ca.* 1 mL) was treated with H₂O (10 mg, 0.56 mmol). The sample was exposed to air for 14 hours, during which period colorless crystals were deposited. The crystals were isolated, washed with benzene (3 × 1 mL) and dried *in vacuo* to give $[\kappa^3$ -Tptm]Zn(μ - κ^2 , κ^1 - OCO_2 Zn[κ^4 -Tptm]•(C₆H₆) (12 mg, 70 %). IR Data (KBr disk, cm⁻¹): 3055 (w), 2384(w), 2293 (w), 2221 (w), 1589 (s), 1554 (s), 1480 (s) [v(CO₃)], 1454 (s), 1418 (s), 1407 (s) [v(CO₃)], 1278 (m), 1131 (s), 1091 (w), 1044 (m), 1011 (m), 848 (w), 765 (m), 747 (s), 721 (m), 642 (w), 610 (w). Anal. calcd. for $[\kappa^3$ -Tptm]Zn(μ - κ^2 , κ^1 -OCO₂)Zn[κ^4 -Tptm]•0.9(C₆H₆): C, 48.6%; H, 2.7%; N, 8.6%. Found: C, 48.8%; H, 3.1%; N, 8.9%. Crystals of composition [κ³-Tptm] $Zn(\mu-\kappa^2,\kappa^1-OCO_2)Zn[\kappa^4-Tptm]$ •(THF) were obtained by performing the reaction in THF, whereas $[\kappa^4$ -Tptm]Zn(μ - κ^2 , κ^2 -OCO₂)Zn[κ^4 -Tptm] was obtained by performing the reaction in toluene. IR data (KBr disk, cm⁻¹): 3043 (w), 3002 (w), 2360(w), 2341 (w), 1585 (s), 1557 (s), 1492 (m) [v(CO₃)], 1453 (s), 1417 (s), 1385 (m) [v(CO₃)], 1280 (m), 1129 (s), 1090 (w), 1044 (m), 1010 (m), 845 (w), 756 (m), 721 (m), 638 (w), 617 (m), 485 (m). ¹H NMR (CD₂Cl₂): 6.91 [s, 6H, {(SC₅H₄N)₃CZn}₂CO₃], 7.09 [d, ${}^{3}J_{H-H} = 8$ Hz, 6H, $\{(SC_5H_4N)_3CZn\}_2CO_3\}, 7.53 [t, {}^{3}J_{H-H} = 8 Hz, 6H, \{(SC_5H_4N)_3CZn\}_2CO_3\}, 8.70 [s, 6H, 100]$ $\{(SC_5H_4N)_3CZn\}_2CO_3\}$. See below for ¹³C NMR data.



Molecular structure of $[\kappa^3 - Tptm]Zn(\mu - \kappa^2, \kappa^1 - OCO_2)Zn[\kappa^4 - Tptm] \bullet 0.5THF$



Molecular structure of $[\kappa^3 - Tptm]Zn(\mu - \kappa^2, \kappa^1 - OCO_2)Zn[\kappa^4 - Tptm] \cdot C_6H_6$



Molecular structure of $[\kappa^4$ -Tptm] $Zn(\mu - \kappa^2, \kappa^2 - OCO_2)Zn[\kappa^4 - Tptm]$

(b) A solution of $\{[\kappa^3-Tptm]Zn(\mu-OH)\}_2$ (8 mg, 0.01 mmol) in C₆H₆ (ca. 2 mL) was frozen, degassed and allowed to warm to room temperature. CO₂ (1 atm) was added and the mixture was shaken, thereby resulting in the formation of a colorless precipitate over a period of 20 minutes. The sample was lyophilized to give [κ^4 -Tptm]Zn(CO₃)Zn[κ^3 -Tptm] (6 mg, 70 %) as a white solid.

(c) A solution of $\{[\kappa^3-Tptm]Zn(\mu-OH)\}_2$ (2 mg, 0.002 mmol) in C_6H_6 (ca. 1 mL) was exposed to air for two hours, during which period colorless crystals were deposited. The mother liquor was decanted to give $[Tptm]Zn(\mu-CO_3)Zn[Tptm]$ (1 mg, 50%) as colorless crystals that was dried *in vacuo*.

Synthesis of [Tptm]Zn(µ-¹³CO₃)Zn[Tptm]

A solution of [κ^4 -Tptm]ZnOSiMe₃ (52 mg, 0.10 mmol) in benzene (*ca.* 1.0 mL) was treated with H₂O (30 mg, 1.67 mmol). The sample was shaken, then frozen, and degassed. The sample was allowed to warm to room temperature, at which point the sample was filled with a mixture of ¹³CO₂ (100 mm Hg) and N₂ (660 mm Hg). Colorless crystals of [κ^3 -Tptm]Zn(μ - κ^2 , κ^1 -O¹³CO₂)Zn[κ^4 -Tptm]•(C₆H₆) formed slowly over a period of 5 hours. The mixture was filtered, and the precipitate was dried *in vacuo* giving [κ^3 -Tptm]Zn(μ - κ^2 , κ^1 -O¹³CO₂)Zn[κ^4 -Tptm]•(C₆H₆) (31 mg, 62%) as an off white powder. IR Data (KBr disk, cm⁻¹): 3061 (w), 2949 (w), 1587 (s), 1561 (s), 1557 (s), 1556 (s), 1457 (s) [ν (CO₃)] (overlapping), 1419 (s), 1347 (w) [ν (CO₃)], 1282 (w), 1248 (w), 1131 (s), 1093 (w), 1044 (m), 1006 (m),905 (w), 837 (w), 758 (s), 722 (m), 640 (w). ¹H NMR (CD₂Cl₂): 6.91 [s, 6H, {(SC₃H₄N)₃CZn}₂CO₃], 7.09 [d, ³J_{H-H} = 8 Hz, 6H, {(SC₃H₄N)₃CZn}₂CO₃], 7.53 [t, ³J_{H-H} = 7 Hz, 6H, {(SC₃H₄N)₃CZn}₂CO₃], 8.70 [s, 6H, {(SC₃H₄N)₃CZn}₂CO₃]. ¹³C{¹H} NMR (Solid state): 171.6 and 172.1 (two isomers). ¹³C{¹H} NMR (CD₂Cl₂, 298 K): 170.5 [s, 1C, {(SC₃H₄N)₃CZn}₂CO₃].

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	$[\kappa^4 - Tptm]ZnOCO_2H \cdot (C_6H_6)$	$[Tp^{Bu^{t},Me}]ZnOCO_{2}H \cdot (C_{6}H_{6})$		
lattice	Monoclinic	Monoclinic		
formula	$C_{23}H_{19}N_3O_3S_3Zn$	$C_{31}H_{47}BN_6O_3Zn$		
formula weight	546.96	627.93		
space group	$P2_1/n$	$P2_1/n$		
a/Å	8.9280(7)	10.750(4)		
b/Å	14.6268(12)	19.725(7)		
c/Å	18.4948(15)	15.634(5)		
$lpha/\circ$	90	90		
β/°	103.8610(10)	91.283(6)		
γ/°	90	90		
$V/\text{\AA}^3$	2344.9(3)	3314(2)		
Ζ	4	4		
temperature (K)	150(2)	150(2)		
radiation (λ, Å)	0.71073	0.71073		
ho (calcd.), g cm ⁻³	1.549	1.258		
μ (Mo Kα), mm ⁻¹	1.346	0.781		
θ max, deg.	30.51	24.41		
no. of data collected	37376	33541		
no. of data used	7148	5450		
no. of parameters	302	397		
$R_1 \left[I > 2\sigma(I) \right]$	0.0412	0.0490		
$wR_2 [I > 2\sigma(I)]$	0.0799	0.0867		
R_1 [all data]	0.0778	0.1079		
wR_2 [all data]	0.0924	0.1067		
GOF	1.011	1.012		

Table 1. Crystal, intensity collection and refinement data.

Table 1(cont). Crystal, intensity collection and refinement data.

	[κ^3 -Tptm]Zn(μ - κ^2 , κ^1 - OCO ₂)Zn[κ^4 -Tptm]•(C ₄ H ₄)	[κ ³ -Tptm]Zn(μ-κ ² ,κ ¹ - OCO ₂)Zn[κ ⁴ -Tptm]•(THF)		
lattice	Monoclinic	Monoclinic		
formula	$C_{39}H_{30}N_6O_3S_6Zn_2$	$C_{35}H_{28}N_6O_{3.5}S_6Zn_2$		
formula weight	953.79	911.73		
space group	$P2_{1}/c$	<i>C</i> 2/ <i>c</i>		
a/Å	22.3176(17)	31.669(6)		
b/Å	10.4067(8)	8.7545(18)		
c/Å	17.2733(14)	28.505(6)		
$\alpha/°$	90	90		
β/°	99.2290(10)	108.802(3)		
γ/°	90	90		
$V/\text{\AA}^3$	3959.8(5)	7481(3)		
Ζ	4	8		
temperature (K)	125(2)	150(2)		
radiation (λ, Å)	0.71073	0.71073		
ho (calcd.), g cm ⁻³	1.600	1.619		
μ (Mo K α), mm ⁻¹	1.575	1.664		
θ max, deg.	30.58	31.36		
no. of data collected	60665	61941		
no. of data used	12104	12294		
no. of parameters	505	472		
$R_1[I > 2\sigma(I)]$	0.0659	0.0451		
$wR_2 [I > 2\sigma(I)]$	0.1536	0.1053		
R_1 [all data]	0.1231	0.0855		
wR_2 [all data]	0.1801	0.1219		
GOF	1.128	1.021		

Table 1(cont).	Crystal, intensity collection and refinement data.	

	$[\kappa^4$ -Tptm]Zn(μ - κ^2 , κ^2 -	${[\kappa^3-Tptm]Zn(\mu-$		
	OCO_2)Zn[κ^4 -Tptm]	OH)} ₂ •(Toluene)		
lattice	Monoclinic	Triclinic		
formula	$C_{33}H_{24}N_6O_3S_6Zn_2$	$C_{40.75}H_{36}N_6O_2S_6Zn_2$		
formula weight	875.68	964.86		
space group	$P2_1/n$	<i>P-1</i>		
a/Å	8.8656(9)	12.632(3)		
b/Å	28.048(3)	15.474(3)		
c/Å	14.4431(15)	22.903(5)		
$lpha/\circ$	90	93.590(3)		
β/°	102.816(2)	96.263(3)		
γ/°	90	107.390(3)		
$V/\text{\AA}^3$	3501.9(6)	4225.4(14)		
Ζ	4	4		
temperature (K)	150(2)	150(2)		
radiation (λ , Å)	0.71073	0.71073		
ρ (calcd.), g cm ⁻³	1.661	1.517		
μ (Mo K α), mm ⁻¹	1.773	1.475		
θ max, deg.	28.28	30.62		
no. of data collected	48636	67413		
no. of data used	8686	25729		
no. of parameters	451	1066		
$R_1[I > 2\sigma(I)]$	0.0559	0.0631		
$wR_2 [I > 2\sigma(I)]$	0.0879	0.1477		
R_1 [all data]	0.1413	0.1762		
wR_2 [all data]	0.1129	0.1867		
GOF	1.002	1.039		

Table 1(cont).	Crystal,	intensity	collection	and	refine	ment o	data.

	{[κ³–Tptm]Zn(μ-
	$\mathbf{OH})\}_{2} \cdot (\mathbf{C}_{6}\mathbf{H}_{6})$
lattice	Triclinic
formula	$C_{40.75}H_{36}N_6O_2S_6Zn_2$
formula weight	1005.90
space group	P - 1
a/Å	12.575(2)
b/Å	13.205(3)
c/Å	14.031(3)
$\alpha/^{\circ}$	112.044(3)
β/°	95.622(3)
γ/°	104.585(3)
$V/\text{\AA}^3$	2041.4(7)
Ζ	2
temperature (K)	150(2)
radiation (λ, Å)	0.71073
ρ (calcd.), g cm ⁻³	1.636
μ (Mo Kα), mm ⁻¹	1.531
θ max, deg.	30.74
no. of data collected	12639
no. of data used	12639
no. of parameters	439
$R_1\left[I > 2\sigma(I)\right]$	0.0548
$wR_2 [I > 2\sigma(I)]$	0.0878
R_1 [all data]	0.1127
wR_2 [all data]	0.0957
GOF	1.026

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