Synthesis and Characterization of a Zinc(II) Complex of Bispicen

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S U P P O R T I N G I N F O R M A T I O N

Table S1. Atomic coordinates (× 10^4) and equivalent isotropic displacement parameters (Å^2 × 10^3) for [Zn(bispicen)Cl(H_2O)]$_2$($ZnCl_4$). *U*(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Atom	*x*	*y*	*z*	*U*(eq)
C(1)	1025(1)	8820(4)	509(2)	47(1)
C(3)	893(2)	6284(4)	796(2)	54(1)
C(4)	554(2)	5929(5)	–41(3)	67(1)
C(5)	452(2)	7077(6)	–609(3)	70(1)
C(6)	683(2)	8542(5)	–336(2)	61(1)
C(7)	1308(2)	10397(4)	848(2)	59(1)
C(8)	930(2)	11057(6)	1706(3)	89(2)
C(9)	994(2)	10663(5)	2495(4)	91(2)
C(10)	1414(2)	8768(6)	3604(3)	81(1)
C(11)	2012(2)	9325(5)	4056(2)	70(1)
C(13)	2811(1)	9583(5)	4051(2)	66(1)
C(14)	3103(2)	10151(7)	4855(3)	95(2)
C(15)	2825(2)	10365(8)	5247(3)	116(2)
C(16)	2278(2)	9926(7)	4857(3)	109(2)
N(1)	1132(1)	7705(3)	1072(2)	42(1)
N(2)	1443(1)	10633(3)	1694(2)	52(1)
N(3)	1138(1)	9008(4)	2696(2)	55(1)
N(4)	2272(1)	9194(3)	3646(2)	51(1)
O(1W)	1785(1)	6052(3)	2772(2)	59(1)
Cl(1)	2513(1)	8148(1)	2163(1)	52(1)
Cl(2)	750(1)	4580(1)	2795(1)	51(1)
Cl(3)	196(1)	7622(1)	3602(1)	58(1)
Zn(1)	1744(1)	8428(1)	2360(1)	37(1)
Zn(2)	0	6103(1)	2500	37(1)

Table S2. Anisotropic displacement parameters ($Å^2 \times 10^3$) for $[Zn(bispicen)Cl(H_2O)]_2[ZnCl_4]$. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(1)	36(2)	53(2)	44(2)	3(2)	17(2)	3(1)
C(3)	55(2)	47(2)	63(2)	–13(2)	34(2)	–10(2)
C(4)	54(2)	69(3)	76(3)	–35(2)	34(2)	–19(2)
C(5)	43(2)	97(3)	53(2)	–23(2)	17(2)	1(2)
C(6)	45(2)	84(3)	45(2)	7(2)	18(2)	9(2)
C(7)	56(2)	48(2)	59(2)	13(2)	23(2)	–1(2)
C(8)	88(3)	74(3)	81(3)	2(2)	29(3)	53(3)
C(9)	72(3)	70(3)	137(5)	–14(3)	60(3)	16(2)
C(10)	72(3)	111(4)	86(3)	–39(3)	60(3)	–38(3)
C(11)	66(2)	95(3)	60(2)	–17(2)	40(2)	–35(2)
C(13)	41(2)	96(3)	49(2)	7(2)	16(2)	–17(2)
C(14)	61(3)	146(5)	48(2)	9(3)	11(2)	–41(3)
C(15)	103(4)	179(6)	45(2)	–14(3)	27(3)	–68(4)
C(16)	112(4)	173(6)	63(3)	–36(3)	60(3)	–67(4)
N(1)	37(1)	39(1)	45(1)	–6(1)	20(1)	–5(1)
N(2)	46(2)	33(2)	62(2)	–1(1)	18(2)	–1(1)
N(3)	41(2)	48(2)	83(2)	–19(2)	37(2)	–11(1)
N(4)	43(2)	61(2)	46(2)	–1(1)	23(1)	–15(1)
O(1W)	62(2)	43(2)	93(2)	19(1)	55(2)	11(1)
Cl(1)	44(1)	44(1)	79(1)	5(1)	41(1)	4(1)
Cl(2)	36(1)	47(1)	67(1)	–3(1)	27(1)	5(1)
Cl(3)	56(1)	56(1)	55(1)	–16(1)	26(1)	–1(1)
Zn(1)	30(1)	35(1)	44(1)	0(1)	18(1)	1(1)
Zn(2)	32(1)	34(1)	45(1)	0	20(1)	0

Table S3. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for $[Zn(bispicen)Cl(H_2O)]_2[ZnCl_4]$.

Atom	*x*	*y*	*z*	*U*(eq)
H(3)	959	5506	1183	65
H(4)	397	4928	–214	80
H(5)	228	6864	–1176	83
H(6)	611	9343	–716	73
H(7A)	1650	10443	846	70
H(7B)	1061	11237	492	70
H(8A)	858	12181	1604	107
H(8B)	607	10498	1260	107
H(9A)	1287	11314	2934	110
H(9B)	646	10884	2463	110
H(10A)	1404	7656	3718	97
H(10B)	1211	9350	3800	97
H(13)	3001	9467	3781	80
H(14)	3483	10383	5125	114
H(15)	3008	10808	5777	139
H(16)	2086	10028	5125	131
H(1W)	2002(16)	5300(50)	2780(20)	69(13)
H(2N)	1694(16)	11270(50)	1930(20)	63(12)
H(2W)	1542(15)	5700(40)	2760(20)	49(12)
H(3N)	842(16)	8430(40)	2410(20)	57(11)

Table S4. Full bond lengths (Å) and angles (deg) for $[Zn(bispicen)Cl(H_2O)]_2[ZnCl_4]$[a].

C(1)–N(1)	1.336(4)	N(3)–C(10)–C(11)	110.3(3)
C(1)–C(6)	1.380(5)	N(4)–C(11)–C(16)	122.2(4)
C(1)–C(7)	1.509(5)	N(4)–C(11)–C(10)	116.3(3)
C(3)–N(1)	1.339(4)	C(16)–C(11)–C(10)	121.5(4)
C(3)–C(4)	1.380(5)	N(4)–C(13)–C(14)	123.0(4)
C(4)–C(5)	1.365(6)	C(15)–C(14)–C(13)	118.9(4)
C(5)–C(6)	1.366(6)	C(14)–C(15)–C(16)	119.3(4)
C(7)–N(2)	1.457(5)	C(15)–C(16)–C(11)	119.0(5)
C(8)–C(9)	1.455(7)	C(1)–N(1)–C(3)	118.1(3)
C(8)–N(2)	1.508(6)	C(1)–N(1)–Zn(1)	113.7(2)
C(9)–N(3)	1.451(5)	C(3)–N(1)–Zn(1)	128.0(2)
C(10)–N(3)	1.480(5)	C(7)–N(2)–C(8)	111.7(3)
C(10)–C(11)	1.500(5)	C(7)–N(2)–Zn(1)	108.5(2)
C(11)–N(4)	1.337(4)	C(8)–N(2)–Zn(1)	105.8(3)
C(11)–C(16)	1.385(6)	C(9)–N(3)–C(10)	109.6(4)
C(13)–N(4)	1.326(4)	C(9)–N(3)–Zn(1)	107.0(3)
C(13)–C(14)	1.376(6)	C(10)–N(3)–Zn(1)	108.2(2)
C(14)–C(15)	1.356(7)	C(13)–N(4)–C(11)	117.4(3)
C(15)–C(16)	1.357(6)	C(13)–N(4)–Zn(1)	127.3(3)
N(1)–Zn(1)	2.193(2)	C(11)–N(4)–Zn(1)	115.2(2)
N(2)–Zn(1)	2.157(3)	O(1W)–Zn(1)–N(2)	162.88(12)
N(3)–Zn(1)	2.183(3)	O(1W)–Zn(1)–N(4)	89.87(12)
N(4)–Zn(1)	2.170(3)	N(2)–Zn(1)–N(4)	102.64(12)
O(1W)–Zn(1)	2.139(3)	O(1W)–Zn(1)–N(3)	89.93(12)
Cl(1)–Zn(1)	2.4097(8)	N(2)–Zn(1)–N(3)	81.75(12)
Cl(2)–Zn(2)	2.2761(8)	N(4)–Zn(1)–N(3)	76.78(11)
Cl(3)–Zn(2)	2.2621(9)	O(1W)–Zn(1)–N(1)	90.18(11)
Zn(2)–Cl(3)#1	2.2621(9)	N(2)–Zn(1)–N(1)	76.12(11)
Zn(2)–Cl(2)#1	2.2761(8)	N(4)–Zn(1)–N(1)	173.81(10)
		N(3)–Zn(1)–N(1)	97.03(11)
N(1)–C(1)–C(6)	122.0(3)	O(1W)–Zn(1)–Cl(1)	95.21(8)
N(1)–C(1)–C(7)	116.3(3)	N(2)–Zn(1)–Cl(1)	95.43(9)
C(6)–C(1)–C(7)	121.7(3)	N(4)–Zn(1)–Cl(1)	94.42(8)
N(1)–C(3)–C(4)	122.5(4)	N(3)–Zn(1)–Cl(1)	169.82(9)
C(5)–C(4)–C(3)	118.7(4)	N(1)–Zn(1)–Cl(1)	91.74(7)
C(6)–C(5)–C(4)	119.4(4)	Cl(3)–Zn(2)–Cl(3')	110.77(5)
C(5)–C(6)–C(1)	119.3(4)	Cl(3)–Zn(2)–Cl(2)	111.31(3)
N(2)–C(7)–C(1)	110.9(3)	Cl(3)–Zn(2)–Cl(2')	106.24(3)
C(9)–C(8)–N(2)	112.2(3)	Cl(2)–Zn(2)–Cl(2')	111.06(5)
N(3)–C(9)–C(8)	110.7(4)		

[a] Symmetry operation two-fold axis #1: $-x, y, -z+1/2$.

Table S5. H bond distances (Å) and angles (deg) in [Zn(bispicen)Cl(H_2O)]$_2$[$ZnCl_4$].

D–H	*d*(D–H)	*d*(H···A)	∠(D–H···A)	*d*(D···A)	A	Symmetry operation
O1W–H1W	0.881	2.245	171.57	3.120	Cl1	[–*x*+1/2, *y*–1/2, –*z*+1/2]
N2–H2N	0.807	2.521	173.14	3.324	Cl1	[–*x*+1/2, *y*+1/2, –*z*+1/2]
O1W–H2W	0.736	2.468	176.35	3.204	Cl2	
N3–H3N	0.864	2.587	160.69	3.414	Cl3	[–*x*, *y*, –*z*+1/2]