Electronic Supporting Information

Development of Pyridine Based o-Aminophenolate Zinc Complexes as Structurally Tunable Catalysts for CO₂ Fixation into Cyclic Carbonates

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ZnL^{APIP}-Br

Figure S1. Space filling representation of $ZnL^{APIP}X$ (X = OAc, Br, I, CI)

X-Ray Crystallography data of $ZnL^{APIP}X$ (X = OAc, Br, I)

ZnL^{APIP} OAc

In all complexes, the coordination sphere ZnN₃OX has a geometry of a distorted square pyramid, but *tau* parameters [1] of 0.31, 0.32 and 0.17 indicate the polyhedron being an intermediate between the square pyramid (SP) and the trigonal bypyramid (TB), with the deformation towards TB being smallest in ZnL^{APIP}I. The valence geometry of the L^{APIP} ligand found in ZnL^{APIP}OAc, ZnL^{APIP}Br and ZnL^{APIP}I is typical for such systems. However, the difference is found between the imine bond lengths with that involving N2 being significantly longer than that formed by N1. That difference in the bond lengths being the largest for acetate complex ZnL^{APIP}OAc and the smallest for iodide complex ZnL^{APIP}I. That also reflects the internal strain imposed by the rigidity of the four-dentate L^{APIP} ligand.

With the four-dentate coordination, the L^{APIP} ligand is not flat. In ZnL^{APIP}OAc, the dihedral angles between C1--C6 (R1), C8--C13 (R2) and C15--N3 (R3) rings being R1-R2 18.1(3), R2-R3 30.7(2) and R1-R3 46.3(2)°. The dihedral angles between these ring planes and the N₃O₁ plane of the pyramid base are 24.8(2), 12.5(3) and 21.7(2)°, respectively. The dihedral angle between the best plane of acetate ligand and the N₃O₁ pyramid base plane is 85.1(2)°, but the acetate is slightly tilted towards N1 and O1, with the Zn1-O2-C28 angle being 129.3(4)°. The L^{APIP} conformation can be described with the torsion angles C1-C6-N1-C7 177.6(4)°, N1-C7-C8-C13 -13.9(7)° and C8-C13-N2-C14 -149.8(4)°. In ZnL^{APIP}Br, the significant effect of the bulk imposed by Br ligand is clearly visible. The dihedral angles R1-R2, R2-R3 and R1-R3 are 30.03(14), 37.74(15) and 65.05(14)° and are larger than these found in ZnL^{APIP}OAc. In ZnL^{APIP}OAc. The reason for this similarity seems to be a Zn-I bond being the longest among the reported structures, and therefore minimizing the bulk of the axial ligand. In ZnL^{APIP}Br, angles between the N₃O₁ plane of the pyramid base and R1, R2 and R3 are 33.58(9), 13.7(1) and 31.7(1)°, respectively, and these values are again larger than these reported for ZnL^{APIP}OAc. In ZnL^{APIP}Br, the corresponding angles are 17.40(11), 4PIPOAc. In ZnL^{APIP}Br, angles between the N₃O₁ plane of the pyramid base and R1, R2 and R3 are 33.58(9), 13.7(1) and 31.7(1)°, respectively, and these values are again larger than these reported for ZnL^{APIP}OAc. In ZnL^{APIP}Br, the corresponding angles are 25.11(9), 11.4(1) and 21.96(8)°.

The intramolecular Cg...Cg distances between the gravity centers of Zn1-O1-C1-C6-N1 chelate and N3--C19 pyridine rings as well as between Zn1-N2-C14-C15-N3 and C1--C6 phenolic rings are 4.675(3), 5.413(3) Å for ZnL^{APIP}OAc, 4.5044(16), 5.1743(15) Å in ZnL^{APIP}Br and 4.6447(13), 5.2968(13) Å for ZnL^{APIP}I. These data indicate that the internal strain seems to be the largest for the Br complex ZnL^{APIP}Br. Analysis of the crystal packing of complexes revealed some intermolecular C-H... π interactions.

Bonds		Angles	
Zn1-01	1.978(3)	01-Zn1-O2	111.95(14)
Zn1-O2	1.991(4)	O1-Zn1-N1	81.73(12)
Zn1-N1	2.087(3)	O2-Zn1-N1	117.06(15)
Zn1-N3	2.109(4)	O1-Zn1-N3	96.71(13)
Zn1-N2	2.174(3)	O2-Zn1-N3	105.45(15)
01-C1	1.311(5)	N1-Zn1-N3	134.79(14)
C1-C2	1.431(5)	01-Zn1-N2	153.35(14)
C1-C6	1.432(5)	02-Zn1-N2	94.67(13)
C2-C3	1.392(5)	N1-ZN1-N2 N2 Zn1 N2	85.04(13)
C2-C20	1.343(3)	C1_O1_Zn1	11/ 7(2)
C4-C5	1 390(6)	01-01-211	123 0(3)
C4-C24	1.546(6)	01-C1-C6	119.8(3)
C5-C6	1.386(5)	C2-C1-C6	117.1(3)
C6-N1	1.426(5)	C3-C2-C1	119.1(3)
N1-C7	1.281(5)	C3-C2-C20	121.3(4)
C7-C8	1.471(6)	C1-C2-C20	119.6(3)
C8-C9	1.394(6)	C4-C3-C2	123.5(4)
C8-C13	1.428(6)	C5-C4-C3	117.5(4)
C10 C11	1.390(6)		121.3(4)
C11-C12	1.304(7)	C5-C4-C24 C6-C5-C4	121.1(4)
C12-C13	1.394(6)	C5-C6-N1	125 2(4)
C13-N2	1.419(5)	C5-C6-C1	121.1(4)
N2-C14	1.249(6)	N1-C6-C1	113.6(3)
C14-C15	1.465(6)	C7-N1-C6	123.5(3)
C15-N3	1.354(6)	C7-N1-Zn1	126.2(3)
C15-C16	1.374(6)	C6-N1-Zn1	110.1(2)
C16-C17	1.389(7)	N1-C7-C8	127.2(4)
C17-C18	1.400(8)	C9-C8-C13	116.8(4)
C18-C19	1.380(7)		110.5(4)
C20-C21	1.520(0)	C10-C9-C8	120.7(4)
C20-C23	1.520(7)	C11-C10-C9	120.9(4)
C20-C22	1.552(6)	C10-C11-C12	119.7(4)
C24-C27	1.493(9)	C11-C12-C13	120.6(4)
C24-C25	1.502(7)	C12-C13-N2	121.8(4)
C24-C26	1.569(8)	C12-C13-C8	120.4(4)
O2-C28	1.209(7)	N2-C13-C8	117.8(4)
C28-O3	1.246(7)	C14-N2-C13	121.6(4)
628-629	1.528(9)	C14-N2-Z01 C12 N2 Zp1	114.3(3)
		N2-C14-C15	124.0(3)
		N3-C15-C16	122.5(4)
		N3-C15-C14	115.5(4)
		C16-C15-C14	121.9(4)
		C15-C16-C17	118.6(5)
		C16-C17-C18	118.7(5)
		C19-C18-C17	119.1(5)
		N3-C19-C18	122.0(5)
		C19-N3-C15 C10 N2 7n1	119.2(4)
		C15-N3-Zn1	120.4(3)
		C21-C20-C23	109.7(4)
		C21-C20-C2	108.2(4)
		C23-C20-C2	110.4(4)
		C21-C20-C22	108.7(4)
		C23-C20-C22	108.0(4)
		C2-C20-C22	111.9(4)
		C27-C24-C25	111.7(6)
			109.9(5)
		C25-C24-C4	107.6(6)
		C25-C24-C26	105 3(5)
		C4-C24-C26	108.6(4)
		C28-O2-Zn1	129.3(4)
		O2-C28-O3	124.8(6)
		O2-C28-C29	118.7(5)
		O3-C28-C29	116.5(6)

Table S2. Bo	ond lengths [A] and angles	[°] for Zr	וL ^{APIP} Br
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Number	Atom1	Atom2	Length	Number	Atom1	Atom2	Atom3	Angle
1	Zn1	Br1	2.4003(5)	1	Br1	Zn1	01	112.25(7)
2	Zn1	O1	1.960(2)	2	Br1	Zn1	N1	111.95(7)
3	Zn1	N1	2.106(2)	3	Br1	Zn1	N2	99.24(6)
4	Zn1 Zn1	N2	2.170(2)	4	Bri	Zn1 Zn1	N3	116.74(7)
5	01	C1	2.121(2)	5	01	Z111 Zn1	IN I N2	01.12(9)
7	C1	C2	1 420(4)	7	01	Zn1	N3	93 67(9)
8	C1	C6	1.426(3)	8	N1	Zn1	N2	82.03(9)
9	C2	C3	1.378(4)	9	N1	Zn1	N3	129.02(9)
10	C2	C20	1.535(4)	10	N2	Zn1	N3	76.37(9)
11	C3	H3A	0.93	11	Zn1	01	C1	115.0(2)
12	C3	C4	1.405(4)	12	01	C1	C2	123.0(2)
14	C4	C24	1.570(4)	13	C2	C1	C6	117 1(2)
15	C5	H5A	0.93	15	C1	C2	C3	118.4(3)
16	C5	C6	1.382(4)	16	C1	C2	C20	119.5(2)
17	C6	N1	1.407(3)	17	C3	C2	C20	122.1(3)
18	C7	H7A	0.93	18	C2	C3	H3A	117.7
20	C7		1.290(3)	19		C3	C4	124.5(3)
21	C8	C9	1.393(4)	20	C3	C4	C5	116.7(3)
22	C8	C13	1.407(3)	22	C3	C4	C24	122.3(3)
23	C9	H9A	0.93	23	C5	C4	C24	121.1(2)
24	C9	C10	1.370(4)	24	C4	C5	H5A	119.4
25	C10	H10A	0.93	25		C5	C6	121.3(2)
20	C10		0.93	20 27	C1	C5	C5	122 0(2)
28	C11	C12	1.378(4)	28	C1	C6	N1	113.5(2)
29	C12	H12A	0.93	29	C5	C6	N1	124.5(2)
30	C12	C13	1.384(4)	30	H7A	C7	N1	117.3
31	C13	N2	1.421(3)	31	H7A	C7	C8	117.1
32 33	N2 C14	C14 H14Δ	1.271(4)	32	N1 7n1	07 N1		125.6(2)
34	C14	C15	1.468(3)	34	Zn1	N1	C7	124.9(2)
35	C15	C16	1.382(4)	35	C6	N1	C7	124.3(2)
36	C15	N3	1.349(4)	36	C7	C8	C9	117.0(2)
37	C16	H16A	0.93	37	C7	C8	C13	125.8(2)
38	C16	C17	1.382(4)	38	C9	C8		117.1(2)
				40	C8	C9	C10	122 5(3)
				41	H9A	C9	C10	118.7
				42	C9	C10	H10A	120.3
				43	C9	C10	C11	119.4(3)
				44	H10A	C10		120.3
				45 46	C10	C11	C12	119 9(3)
				47	H11A	C11	C12	120
				48	C11	C12	H12A	119.8
				49	C11	C12	C13	120.4(3)
				50	H12A	C12 C13	C13	119.8
				52	C8	C13	N2	118.7(2)
				53	C12	C13	N2	120.7(2)
				54	Zn1	N2	C13	122.4(2)
				55	Zn1	N2	C14	114.4(2)
				56 57	C13	N2		123.1(2)
				58	N2	C14	C15	119 0(3)
				59	H14A	C14	C15	120.5
				60	C14	C15	C16	122.6(3)
				61	C14	C15	N3	114.8(2)
				62	C16	C15	N3	122.5(3)
				63 64	C15	C16	C17	ा∠∪.७ 118 २/२)
				65	H16A	C16	C17	120.8
				66	C16	C17	H17A	120.3
				67	C16	C17	C18	119.4(3)
				68	H17A	C17	C18	120.2
				69 70	C17	C18	H18A	120.6
				70	H18A	C18	C19	120.6

Humber Atom1 Atom2 Largth 1 1 2.11 D1 1147.366 2 2.11 1 1.95(2) 3 11 2.11 N1 117.36(6) 3 2.11 N1 2.15(2) 3 11 2.11 N1 81.32(7) 4 2.71 N1 2.15(2) 6 01 2.11 N2 144.13(7) 5 2.11 N3 2.12(2) 7 01 2.11 N3 9.2(2) 6 0.1 C.1 C.2 1.35(3) 9 N1 2.11 N3 9.2(2) 7 0.1 C.2 C.2 1.35(3) 11 2.11 N3 1.32(3) 10 C.2 C.2 1.35(3) 16 C.2 C.2 1.33(7) 11 C.3 0.44 1.410(3) 14 C.2 C.2 1.33(7) 12 C.3 C.4 1.410(3) 1.410(3) 1.117(7) <th>Number</th> <th>Atom1</th> <th>Atom2</th> <th>Atom3</th> <th>Angle</th> <th>_</th> <th></th> <th></th> <th></th>	Number	Atom1	Atom2	Atom3	Angle	_			
Number Atomi Atomi Atomi Atomi 2 11 Zn1 N1 1176805 2 2.11 11 2.15640 3 11 Zn1 N2 1016216 4 Zn1 N1 2.15620 6 01 Zn1 N2 2.16420 6 01 C1 1.31830 8 N1 Zn1 N2 2.29977 7 C1 C2 C2 1.42040 9 N1 Zn1 N3 7.62277 9 C2 C2 C2 C2 C3 1.17782 7.11 N3 7.62277 9 C2 C3 C4 C5 1.377(4) 16 C1 C2 C3 117.822 11 C3 H3A 0.329 17 C3 C3 C4 C5 1.377(4) 16 C3 L377(4) 16 C1 C2 C3 1.17.822 17 C5	N	A 1 4		1	- 1	11	Zn1	01	114.73(5)
1 2n1 1 2n1 N1 2n1 N2 101 1662 2 2n1 01 12622 4 11 2n1 N3 106816 3 2n1 N12 211620 5 01 2n1 N13 122407 6 2n1 N3 212620 7 01 121 N3 133757 7 C1 C2 1.428401 9 N1 Zn1 N3 133757 8 C1 C6 1.413(3) 10 N2 Zn1 N3 133757 9 C2 C3 1.368(3) 11 Zn1 C1 C1 12147(1) 10 C3 C4 0.410(3) 13 C1 C2 C3 12200(2) 11 C4 C24 1.5354(4) 16 C1 C2 C3 C4 1176 12 C5 H5A 0.33 17 C3 C2 C3 </th <th>Number</th> <th>Atom1</th> <th>Atom2</th> <th>Length</th> <th>_ 2</th> <th>11</th> <th>Zn1</th> <th>N1</th> <th>117.60(5)</th>	Number	Atom1	Atom2	Length	_ 2	11	Zn1	N1	117.60(5)
2 2n1 01 1968(2) 4 11 2n1 N3 106.81(2) 3 2n1 N12 2.162(2) 6 01 Zn1 N3 15.23(7) 5 01 03 2.162(2) 6 01 Zn1 N3 95.23(7) 7 01 C1 C2 1.43(1) 10 N3 10.82(1) 9 C2 C3 C4 1.43(1) 10 N2 Zn1 N3 76.22(7) 9 C2 C3 C4 1.41(1) 14 C1 C2 C2 N1 Zn1 N3 76.22(7) 10 C2 C3 C4 1.41(1) 14 C1 C2 C3 C4 1.41(2) 16 C1 C2 C3 11.78(2) 11 C4 C5 C4 1.33(1) 10 C1 C3 C4 124.8(2) 12 C3 C4 <th1.42(1)< th=""> 13.77(4)<th>1</th><th>Zn1</th><th>11</th><th>2.5765(4)</th><th>3</th><th>l1</th><th>Zn1</th><th>N2</th><th>101.16(5)</th></th1.42(1)<>	1	Zn1	11	2.5765(4)	3	l1	Zn1	N2	101.16(5)
3 2n1 N1 2.116(2) 5 01 2n1 N1 8123(7) 6 C1 C1 1313(3) 8 N1 2n1 N3 8224(7) 7 C1 C1 1313(3) 8 N1 2n1 N3 8224(7) 9 C2 C3 1333(8) 10 12 11 N3 7227(1) 9 C2 C3 1343(3) 14 12 11 N1 7227(1) 10 C2 C3 134(3) 14 C2 C1 C6 1277(2) 11 C3 H3A 0.229 13 C1 C2 C3 117.8(2) 12 C3 C4 C5 1377(4) 16 C1 C2 C3 117.8(2) 13 C4 C5 C3 1377(4) 16 C1 C2 C3 1237(2) 14 C4 C4 C4 C4 C4 <th>2</th> <th>Zn1</th> <th>01</th> <th>1.962(2)</th> <th>4</th> <th>l1</th> <th>Zn1</th> <th>N3</th> <th>106.81(5)</th>	2	Zn1	01	1.962(2)	4	l1	Zn1	N3	106.81(5)
4 Zn1 N2 2.162(2) 6 O1 Zn1 N3 9.204(7) 6 O1 C1 C1 1.318(3) 8 N1 Zn1 N3 9.204(7) 7 O1 C2 C3 1.318(3) 8 N1 Zn1 N3 7.224(7) 8 O1 C2 C3 1.328(3) 11 N2 C1 C2 C3 1.327(4) 13 O1 C1 C2 C3 1.722(2) 1.722(2	3	Zn1	N1	2.116(2)	5	01	Zn1	N1	81.23(7)
5 Zn1 N3 2.128(2) 7 O1 Zn1 N3 92.04(7) 7 C1 C2 1.439(3) 6 N1 Zn1 N3 1.8222(7) 8 C1 C6 1.413(3) 10 N2 Z11 N3 1.8222(7) 9 C2 C3 C4 C5 1.346(3) 11 Zn1 C1 C1 C1 1.414(7) 9 C2 C3 C4 C5 1.377(4) 15 C1 C2 C3 1.114(7) 14 C4 C2 S3 T7 C3 C2 C3 H3A 1.178(2) 15 C5 H5A 0.93 17 C3 C2 C3 H3A 1.178(2) 16 C5 C6 1.390(3) 18 C2 C3 C4 1.244(32) 17 C6 N1 1.434(3) 20 C4 C5 C6 1.1178(2)	4	Zn1	N2	2.162(2)	6	01	Zn1	N2	144.10(7)
6 01 C1 1.318/3) 8 N1 Zn1 N2 8.2.829 7 C1 C2 1.348/3) 10 N2 Zn1 N3 133.75(7) 8 C1 C6 1.413(3) 10 N2 Zn1 N3 17.7622(7) 9 C2 C3 1.348(3) 11 C1 C1 C1 12.1447(1) 10 C2 C20 1.541(3) 12 C1 C2 C3 1.77.82(7) 112 C3 HAA 0.92(3) 18 C2 C3 C4 17.76.20 114 C4 C2 HSA 0.33 17 C3 C2 C3 C4 122.32(7) 15 C5 H5A 0.93 21 C3 C4 124.412.49(2) 16 C5 C6 1.3398(3) 22 C3 C4 124.194.23 17 C6 N1 1.417(7) 19 C4	5	Zn1	N3	2.126(2)	7	01	Zn1	N3	92.04(7)
7 C1 C2 1.4.29(4) 9 N1 Zn1 N3 1.33.767/ 1.01 8 C1 C6 1.4.13(3) 10 N2 Zn1 N3 T622(7) 9 C2 C3 1.33.86(3) 11 Zn1 O1 C1 1.4.114(3) 10 C2 C20 1.541(3) 12 O1 C1 C6 1.20.72 12 C3 C4 1.410(3) 14 C2 C1 C6 1.77.8(2) 13 C4 C5 C6 0.390(3) 16 C3 C2 C3 L4 1.72.20 16 C5 C6 0.390(3) 12 C3 C4 C3 C4 1.22.49(2) 17 C6 N1 4.417(3) 19 C2 C3 C4 C5 C6 1.167(2) 21 C6 C7 C7 R4 0.38 23 C5 C4 C5 C6 1	6	01	C1	1.318(3)	8	N1	Zn1	N2	82,99(7)
8 C1 C6 1413(3) 10 N2 Zn1 N3 7622(7) 10 C2 C2 C3 1.388(3) 11 Zn1 C1 C1 1147(1) 11 C3 H3A 0.929 13 C1 C1 C6 1.07(2) 12 C3 C4 1.410(3) 14 C2 C3 1.178(2) 14 C4 C24 1.535(4) 16 C1 C2 C3 H3A 1.78(2) 15 C3 H3A 0.93 17 C3 C2 C3 H3A 1.178(2) 16 C3 C6 1.390(3) 18 C2 C3 C4 1249(2) 17 C1 C3 C4 C3 C4 1177(6) 20 C7 C6 C1 C3 C4 C5 C6 11210(2) 21 C6 C10 1.370(4) 26 H5A C5	7	C1	C2	1.429(4)	9	N1	7n1	N3	133 75(7)
9 C2 C3 1368(3) 11 Zn1 C1 C1 1147(7) 10 C2 C20 1.541(3) 12 C1 C1 C2 124(2) 11 C3 H3A 0.929 13 O1 C1 C6 120.72) 13 C4 C5 1.377(4) 16 C1 C2 C20 120.0(2) 14 C4 C5 H53(4) 16 C1 C2 C20 120.0(2) 15 C5 H5A 0.93 17 C3 C2 C3 H3A 17.5 17 C6 C1 1.294(3) 18 C2 C3 H3A 17.5 19 C7 H7A 0.93 22 C3 C4 C5 H5A 119.5 21 C6 C9 1.399(3) 23 C5 C4 C5 C6 121.0(2) 22 C8 C10 C10 13	8	C1	C6	1.413(3)	10	N2	Zn1	N3	76 22(7)
0 C2 C20 1.541(3) 12 C11 C1 C2 1214(2) 11 C3 H3A 0.929 13 O1 C1 C2 1214(2) 12 C3 C4 C5 1.377(4) 15 C1 C2 C3 17.8(2) 14 C4 C24 1.357(4) 16 C1 C2 C3 C4 C5 1.778(2) 15 C5 H5A 0.93 17 C3 C2 C3 C4 1.47173(3) 16 C5 C6 1.390(3) 18 C2 C3 C4 C5 1167(2) 17 C6 N1 1.47173(3) 21 C3 C4 C5 C6 1194(2) 18 C7 L7A(3) 32 C4 C5 C6 1194(2) 21 C8 C10 1.370(4) 28 C4 C5 C6 N1 1244(2) 22	9	C2	C3	1.368(3)	11	7n1	01	C1	1147(1)
11 C3 H3A 0.929 13 O1 C1 C6 1077(2) 12 C3 C4 1410(3) 14 C2 C1 C6 117.8(2) 14 C4 C2 1.377(4) 15 C1 C2 C3 117.8(2) 15 C5 H5A 0.93 17 C3 C2 C20 122.3(2) 16 C5 C6 1.390(3) 18 C2 C3 C4 124.9(2) 18 N1 C7 1.244(3) 20 H3A C3 C4 116.7(2) 20 C7 C8 1.449(4) 22 C3 C4 C24 123.9(2) 21 C8 C9 1.386(3) 23 C5 C4 C24 123.9(2) 22 C8 H5A 0.33 25 C4 C5 C6 119.5 23 C10 H1A 0.33 25 C4 C5	10	C2	C20	1.541(3)	12	01	C1	C2	121 4(2)
12 C3 C4 C5 1377(4) 15 C1 C2 C3 C6 178(2) 14 C4 C24 155(5) 15 C5 145 C1 C2 C20 1200(2) 15 C5 H5A 0.93 17 C3 C2 C3 H3A 177.5 16 C5 G6 1.390(3) 18 C2 C3 C4 17.6 17 C6 N1 1.417(3) 19 C2 C3 C4 C5 116.7(2) 20 C7 C8 1.459(4) 22 C3 C4 C5 116.7(2) 21 C8 C13 1.408(4) 24 C4 C5 C6 119.5 22 C8 C10 1.39(3) 23 C5 C4 C5 C6 119.5 23 C9 C10 1.370(4) 26 H5A 0.55 C6 N1 113.5(2) <th>11</th> <th>C3</th> <th>H3A</th> <th>0.929</th> <th>13</th> <th>01</th> <th>C1</th> <th>C6</th> <th>121.4(2) 1207(2)</th>	11	C3	H3A	0.929	13	01	C1	C6	121.4(2) 1207(2)
13 C4 C5 1377(4) 15 C1 C2 C3 1178(2) 14 C4 C24 1555(4) 16 C1 C2 C3 120(2) 15 C5 H5A 0.93 17 C3 C2 C3 H3A 117,5 16 C5 C5 N1 1.417(3) 19 C2 C3 C4 124,9(2) 18 N1 C7 1.284(3) 20 H3A C3 C4 116,7(2) 20 C7 C8 1.499(4) 22 C3 C4 C24 119,4(2) 21 C8 C13 1.408(4) 24 C4 C5 H16,4 119,5 22 C8 C10 1.370(4) 26 H6A C5 C5 121,0(2) 24 C9 H9A 0.33 27 C1 C6 N1 124,8(2) 27 C10 H1A 0.33 C1	12	C3	C4	1 410(3)	14	C2	C1	60	117 8(2)
14 C4 C24 155(5) C5 C20 C30 C4 C41 C41 <thc41< th=""> <thc41< th=""> <thc41< th=""></thc41<></thc41<></thc41<>	13	C4	C5	1.377(4)	15	C1	C2	C3	117.8(2)
15 C5 H5A 0.93 17 C3 C2 C20 D1223(2) 16 C5 C6 1.390(3) 18 C2 C3 H5A 1123(2) 17 C6 N1 1.417(3) 19 C2 C3 C4 117.6 18 N1 C7 H7A 0.93 21 C3 C4 C24 119.4(2) 20 C7 C8 1.459(4) 22 C3 C4 C24 119.4(2) 21 C8 C13 1.408(4) 24 C4 C5 H5A 119.5 224 C9 C10 1.370(4) 26 H5A C5 C6 119.5 23 C9 H9A 0.93 27 C1 C6 N1 113.5(2) 24 C9 C10 1.370(4) 28 C1 C6 N1 113.5(2) 25 C10 C111 1.36(4) 28 C1 <th>14</th> <th>C4</th> <th>C24</th> <th>1 535(4)</th> <th>16</th> <th>C1</th> <th>C2</th> <th>C20</th> <th>120.0(2)</th>	14	C4	C24	1 535(4)	16	C1	C2	C20	120.0(2)
16 C5 C6 130(3) 18 C2 C3 H3A 1175 17 C6 N1 1417(3) 19 C2 C3 C4 1125 18 N1 C7 H7A 0.93 21 C3 C4 C24 11342 20 C7 C7 B 1.459(4) 21 C3 C4 C24 1133(2) 21 C8 C9 1.398(3) 23 C5 C4 C24 1133(2) 22 C8 C13 1.408(4) 23 C5 C4 C5 166 1110(2) 23 C9 H9A 0.93 25 C4 C5 C6 11117(2) 24 C9 C10 1.370(4) 28 C1 C6 N1 1248(2) 25 C10 H10A 0.93 29 C5 C6 N1 1248(2) 26 C10 C11 N2 N1	15	C5	H5A	0.93	17	C3	C2	C20	120.0(2)
17 C6 N1 1417(2) 19 C2 C3 C4 1142(2) 18 N1 C7 H7A 0.93 20 H3A C3 C4 172(6) 19 C7 H7A 0.93 21 H3A C3 C4 C24 1194(2) 20 C7 C8 1.499(4) 22 C3 C4 C24 1194(2) 21 C8 C9 1.398(3) 23 C5 C4 C5 H5A 113(14) 22 C8 C13 1.408(4) 24 C4 C5 C6 119.5 23 C9 H9A 0.93 27 C1 C6 N1 113.5(2) 24 C9 C10 1.370(4) 28 C1 C6 N1 113.5(2) 25 C10 C111 1.36(4) 33 N1 C7 123.6(2) 24 C12 H12A 0.93 31	16	C5	C6	1.390(3)	19	C2	C2	U20	117.5
16 17 124(3) 10 Class Class <thclas< th=""> <thclas< th=""> <thclass< th=""></thclass<></thclas<></thclas<>	17	C6	N1	1 417(3)	10	C2	C3	C4	124 0(2)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	18	N1	C7	1 284(3)	20	U2A	C3	C4	124.9(2)
20 C7 C8 C3 C4 C3 C4 C3 C4 C24 C194(2) 21 C6 C9 1398(3) 23 C5 C4 C24 1234(2) 22 C6 C9 H9A 0.93 25 C4 C5 C6 1210(2) 23 C9 H9A 0.93 25 C4 C5 C6 119.5 24 C9 C10 1370(4) 26 H4A C5 C6 1119.5 25 C10 C11 136(4) 28 C1 C6 N1 1135(2) 26 C10 C11 136(3) 30 Zn1 N1 C7 128 (2) 27 C11 H1A 0.93 31 Zn1 N1 C7 128 (2) 30 C12 C13 1373(3) 30 Zn1 C7 C8 125.9(2) 31 C14 C14 126(3) <	19	C7	H7A	0.93	20	П3А С2	C3	C4 C5	116 7(2)
21 CB CB CB TB TB <thtb< th=""> TB TB TB<!--</th--><th>20</th><th>C7</th><th>C8</th><th>1 459(4)</th><th>21</th><th>03</th><th>C4</th><th>C34</th><th>110.7(2)</th></thtb<>	20	C7	C8	1 459(4)	21	03	C4	C34	110.7(2)
12 C3 C4 C4 C4 C4 C4 C4 C4 C4 C4 C5 C4 C5 C6 119.5 23 C9 H9A 0.93 25 C4 C5 C6 119.5 24 C9 C10 1370(4) 26 C14 C5 C6 119.5 25 C10 H10A 0.33 27 C1 C6 N11 113.6(2) 26 C10 C11 1.360(4) 28 C5 C6 N11 113.6(2) 27 C11 H14A 0.93 31 Zn1 N1 C7 128.6(2) 28 C11 C12 L1376(3) 33 N1 C7 C18.6(2) 117.1 30 C12 C13 N2 1.448(3) 33 N1 C7 C8 125.9(2) 31 C14 H144 0.929 35 H7A C7 C8 117.1	20	C8	C0	1 308(3)	22	C3	C4	024	119.4(2)
Z2 C0 C13 1.100(4) Z4 C4 C5 C6 HPA 1195. Z4 C9 C10 1.370(4) Z6 H5A C5 C6 119.5 Z5 C10 C11 1.366(4) Z8 C1 C6 N1 113.5(2) Z6 C10 C11 1.366(4) Z8 C1 C6 N1 124.6(2) Z7 C11 C12 1.375(3) 30 Zn1 N1 C7 128.6(2) 30 C12 C13 1.383(4) 32 C6 N1 C7 128.6(2) 31 C13 N2 1.418(3) 33 N1 C7 C8 125.9(2) 33 C14 H14A 0.929 35 H7A C7 C8 117.1 34 C14 C15 1.465(3) 36 C7 C8 C13 116.7(2) 35 C15 N3 1.344(3) 38	20	C8	C13	1.000(0)	23	05	64	024	123.9(2)
23 C3 C4 C5 C6 1210(2) 24 C9 C10 H1370(4) 26 H5A C5 C6 119.5 25 C10 H10A 0.93 27 C1 C6 C5 119.5 26 C10 C11 H14A 0.93 29 C5 C6 N1 124.8(2) 28 C11 C12 H12A 0.93 31 Zn1 N1 C7 128.6(2) 30 C12 H12A 0.93 33 N1 C7 H7A 117 31 C13 N2 1.418(3) 33 N1 C7 H7A 117 32 N2 C14 H14A 0.929 35 H7A C7 C8 125.9(2) 33 C14 C16 1.465(3) 36 C7 C8 C13 1126.1(2) 34 C14 C15 N3 1.344(3) 38 C9	22	C0		0.02	24	C4	C5	H5A	119.5
Z4 C5 C10 L370(4) Z6 H5A C5 C6 T195 Z5 C10 C11 1.366(4) 28 C1 C6 N1 1135(2) Z6 C10 C11 1.366(4) 28 C1 C6 N1 1135(2) Z7 C11 C12 1.377(3) 30 Zn1 N1 C6 1095(3) Z9 C12 H12A 0.93 31 Zn1 N1 C7 128.8(2) 30 C12 C13 1.383(4) 32 C6 N1 C7 128.8(2) 31 C13 N2 L418(5) 33 N1 C7 C8 116.7(2) 33 C14 H14A 0.929 35 H7A C7 C8 C13 112.7(2) 34 C14 C15 1.465(3) 36 C7 C8 C13 112.7(2) 35 C15 N3 1.344(3) 38	23	C9	C10	0.93	25	C4	C5	C6	121.0(2)
25 C10 F10/A 0.93 27 C11 C65 C55 121.7(2) 27 C11 H11A 0.93 29 C5 C6 N1 1124.8(2) 28 C11 C12 H12A 0.93 31 Zn1 N1 C6 109.5(1) 29 C12 H12A 0.93 31 Zn1 N1 C7 128.8(2) 30 C12 C13 1.383(4) 32 C6 N1 C7 128.8(2) 31 C13 N2 1.418(3) 33 N1 C7 H7A 117.2 33 C14 H14A 0.929 35 H7A C7 C8 C13 126.1(2) 34 C16 1.379(3) 37 C7 C8 C13 117.2(2) 35 C16 N13 1.34(3) 38 C9 C8 C13 1122.0(2) 36 C15 N3 1.34(3) 39 <th>24</th> <th>C9</th> <th></th> <th>1.370(4)</th> <th>26</th> <th>H5A</th> <th>C5</th> <th>C6</th> <th>119.5</th>	24	C9		1.370(4)	26	H5A	C5	C6	119.5
26 C10 C11 1.300(4) 28 C1 C6 N1 113.8(2) 27 C11 C12 1.375(3) 30 Zn1 N1 C6 109.5(1) 28 C12 H12A 0.93 31 Zn1 N1 C6 109.5(1) 30 C12 C13 1.383(4) 32 C6 N1 C7 128.8(2) 31 C13 N2 1.418(3) 33 N1 C7 H7A 117 32 N2 C14 1.266(3) 34 N1 C7 C8 117.1 33 C14 C15 1.465(3) 36 C7 C8 C13 112.2(2) 35 C15 C16 1.379(3) 37 C7 C8 C13 117.2(2) 36 C17 C18 116A 0.93 39 C8 C9 C10 122.0(2) 39 C16 C17 C18 1.330(3) <th>20</th> <th>C10</th> <th>C11</th> <th>0.93</th> <th>27</th> <th>61</th> <th>C6</th> <th>05</th> <th>121.7(2)</th>	20	C10	C11	0.93	27	61	C6	05	121.7(2)
27 C11 F11A 0.93 29 C5 C6 N1 124.8[2] 28 C11 C12 1.375(3) 30 Zn1 N1 C6 109.5(1) 29 C12 H12A 0.93 31 Zn1 N1 C7 128.8[2] 30 C12 C13 N.2 1.418(3) 33 N1 C7 H7A 117 31 C13 N.2 1.418(3) 33 N1 C7 C8 125.9(2) 32 N2 C14 H14A 0.929 35 H7A C7 C8 117.1 34 C14 C15 1.465(3) 36 C7 C8 C9 H16.7(2) 35 C15 N3 1.344(3) 38 C9 C8 C9 H40 119 36 C16 C17 1.373(3) 40 C8 C9 C10 119 37 C16 H17A 0.9	20	010		1.300(4)	28	C1	C6	N1	113.5(2)
29 C11 C12 1.375(3) 30 Zn1 N1 C6 1095(1) 30 C12 C13 1.383(4) 32 C6 N1 C7 1228(2) 31 C13 N2 1.418(3) 33 N1 C7 H7A 117 32 N2 C14 1.266(3) 34 N1 C7 C8 1259(2) 33 C14 H14A 0.929 35 H7A C7 C8 C9 1167(2) 34 C14 C15 1.465(3) 36 C7 C8 C13 117.1 35 C15 C16 1.379(3) 30 C8 C9 C10 122.0(2) 36 C16 C17 1.373(3) 40 C8 C9 C10 122.0(2) 39 C17 H17A 0.931 41 H9A C9 C10 C10 122.0(2) 34 C19 N3 0.330(3)	27		HITA	0.93	29	C5	C6	N1	124.8(2)
29 C12 H12A 0.933 31 Zn1 N1 C7 128.8(2) 30 C12 C13 N2 1.418(3) 33 N1 C7 H7A 117 31 C13 N2 1.418(3) 33 N1 C7 H7A 117 32 N2 C14 H14A 0.929 35 H7A C7 C8 C13 125.9(2) 33 C14 H14A 0.929 35 H7A C7 C8 C13 125.1(2) 34 C15 C16 1.379(3) 37 C7 C8 C13 122.0(2) 35 C16 C17 1.373(3) 40 C8 C9 C10 119 36 C17 H17A 0.931 41 H9A C9 C10 C11 122.0(2) 37 C16 H18A 0.929 43 C9 C10 C11 122.0(2) 38 <t< th=""><th>28</th><th>010</th><th>612</th><th>1.375(3)</th><th>30</th><th>Zn1</th><th>N1</th><th>C6</th><th>109.5(1)</th></t<>	28	010	612	1.375(3)	30	Zn1	N1	C6	109.5(1)
30 C12 C13 1.4383(4) 32 C6 N1 C7 H7A H17 32 N2 C14 1.266(3) 34 N1 C7 C8 1259(2) 33 C14 H14A 0.929 35 H7A C7 C8 117,1 34 C14 C15 1.465(3) 36 C7 C8 C9 116,7(2) 35 C15 C16 1.379(3) 36 C7 C8 C13 117,2(2) 36 C15 N3 1.344(3) 38 C9 C8 C13 117,2(2) 37 C16 H16A 0.93 39 C8 C9 C10 122.0(2) 38 C16 C17 H373(3) 40 C8 C9 C10 119 40 C17 H17A 0.931 45 C10 C11 H19.8(2) 42 C18 H18A 0.929 43 C9	29	012	HIZA	0.93	31	Zn1	N1	C7	126.8(2)
31 C13 N2 1418(3) 33 N1 C7 H7A 117 32 N2 C14 144 0.929 35 H7A C7 C8 117.1 34 C14 C15 1.465(3) 36 C7 C8 C9 116.7(2) 35 C15 C16 1.379(3) 37 C7 C8 C13 117.2(2) 36 C16 H16A 0.93 39 C8 C9 H9A 119 38 C16 C17 1.373(3) 40 C8 C9 C10 1120.0(2) 39 C17 H17A 0.931 41 H9A C9 C10 119 40 C17 C18 1.364(4) 42 C9 C10 C11 119.8 41 C18 H18A 0.929 43 C9 C10 C11 119.2 42 C19 H19A 0.33 45 C10 </th <th>30</th> <th>012</th> <th>013</th> <th>1.383(4)</th> <th>32</th> <th>C6</th> <th>N1</th> <th>C7</th> <th>123.6(2)</th>	30	012	013	1.383(4)	32	C6	N1	C7	123.6(2)
32 N2 C14 1266(3) 34 N1 C7 C8 1259(2) 33 C14 C14 C15 1.465(3) 36 C7 C8 C13 126.1(2) 35 C15 C16 1.379(3) 37 C7 C8 C13 126.1(2) 36 C15 N3 1.344(3) 38 C9 C8 C13 126.1(2) 37 C16 H16A 0.93 39 C8 C9 H9A 119 38 C16 C17 1.373(3) 40 C8 C9 C10 1122.0(2) 39 C17 H17A 0.931 41 H9A C9 C10 H10A 120.1 40 C17 C18 H18A 0.929 43 C9 C10 C11 1120.2 43 C19 H19A 0.93 45 C10 C11 H1A 118.2 44 C19 N3	31	C13	N2	1.418(3)	33	N1	C7	H7A	117
33 C14 H14A 0.929 35 H7A C7 C8 117.1 34 C14 C15 1.465(3) 36 C7 C8 C9 116.7(2) 35 C15 N3 1.334(3) 37 C7 C8 C13 117.2(2) 36 C15 N3 1.334(3) 38 C9 C8 C9 H9A 119 38 C16 C17 1.373(3) 40 C8 C9 C10 122.0(2) 39 C16 C17 C18 1.364(4) 42 C9 C10 H10A 120.1 41 C18 H18A 0.929 43 C9 C10 C11 119.8 42 C18 C19 1.379(4) 44 H10A C10 C11 H12A 119.8 44 C19 N3 1.330(3) 46 C10 C11 C12 119.9 45 C20 C22	32	N2	C14	1.266(3)	34	N1	C7	C8	125.9(2)
34 C14 C15 1.46b(3) 36 C7 C8 C9 116.7(2) 35 C15 N3 1.344(3) 38 C9 C8 C13 117.2(2) 36 C15 N3 1.344(3) 38 C9 C8 C13 117.2(2) 37 C16 H16A 0.93 39 C8 C9 H9A 119 38 C17 H17A 0.931 41 H9A C9 C10 122.0(2) 39 C17 C18 1.364(4) 42 C9 C10 C11 119.8(2) 40 C17 C18 C19 1.379(4) 44 H10A C10 C11 1120.2 43 C19 N3 1.330(3) 46 C10 C11 C12 120.4(2) 44 C19 N3 1.330(3) 46 C10 C11 C12 120.4(2) 45 C20 C22 1.528(3)	33	C14	H14A	0.929	35	H7A	C7	C8	117.1
35 C15 C16 1.379(3) 37 C7 C8 C13 126.1(2) 36 C15 N3 1.344(3) 38 C9 C8 C13 117.2(2) 37 C16 H16A 0.93 39 C8 C9 H9A 119 38 C16 C17 1.373(3) 40 C8 C9 C10 1122.0(2) 39 C16 C17 H17A 0.931 41 H9A C9 C10 H10A 120.1 40 C17 C18 H18A 0.929 43 C99 C10 C11 119.8(2) 42 C18 C19 H13A 0.33 45 C10 C11 H14A 119.8(2) 43 C19 H19A 0.93 45 C10 C11 C12 120.4(2) 44 C19 N3 1.330(3) 46 C10 C11 C12 119.9 45 C20 <th>34</th> <th>C14</th> <th>C15</th> <th>1.465(3)</th> <th>36</th> <th>C7</th> <th>C8</th> <th>C9</th> <th>116.7(2)</th>	34	C14	C15	1.465(3)	36	C7	C8	C9	116.7(2)
36 C15 N3 1.344(3) 38 C9 C8 C13 117.2(2) 37 C16 C17 1.373(3) 40 C8 C9 C10 112.0(2) 38 C16 C17 1.373(3) 40 C8 C9 C10 112.0(2) 39 C17 H17A 0.931 41 H9A C9 C10 1120.1 40 C17 C18 1.384(4) 42 C9 C10 C11 122.01 41 C18 H18A 0.929 43 C9 C10 C11 119.8(2) 42 C19 H19A 0.93 45 C10 C11 C12 120.4(2) 43 C19 N3 1.330(3) 46 C10 C11 C12 119.9 44 C19 N3 1.330(3) 48 C11 C12 119.9 45 C20 C22 1.528(4) 49 C11	35	C15	C16	1.379(3)	37	C7	C8	C13	126.1(2)
37 C16 H16A 0.93 39 C8 C9 H9A 119 38 C16 C17 1.373(3) 40 C8 C9 C10 122.0(2) 39 C17 H17A 0.931 41 H9A C9 C10 119 40 C17 C18 1.364(4) 42 C9 C10 H10A 122.0(2) 42 C18 C19 1.379(4) 44 H10A C10 C11 119.8(2) 43 C19 H19A 0.93 45 C10 C11 H14A 119.8(2) 44 C19 N3 1.330(3) 46 C10 C11 C12 120.4(2) 45 C20 C21 1.528(4) 47 H11A C11 C12 119.8 47 C20 C23 1.528(3) 48 C11 C12 C13 120.4(2) 47 C20 C23 1.528(3) 48 C11 C12 C13 120.5(2) 56 C13 N2 C14<	36	C15	N3	1.344(3)	38	C9	C8	C13	117.2(2)
38 C16 C17 1.373(3) 40 C8 C9 C10 122(02) 39 C17 C18 1.364(4) 41 H9A C9 C10 H10A 120.1 40 C17 C18 1.364(4) 42 C9 C10 H10A 120.1 41 C18 H18A 0.929 43 C9 C10 C11 H19A 42 C19 H13A 0.933 45 C10 C11 H11A H198(2) 43 C19 H33 1.330(3) 46 C10 C11 H11A H198 44 C19 N3 1.330(3) 46 C10 C11 C12 H12A H198 47 C20 C23 1.528(3) 48 C11 C12 C13 120.5(2) 50 H12A C12 C13 119.7 120.8 120.9(2) 51 C8 C13 C12 C13 <th1< th=""><th>37</th><th>C16</th><th>H16A</th><th>0.93</th><th>39</th><th>C8</th><th>C9</th><th>H9A</th><th>119</th></th1<>	37	C16	H16A	0.93	39	C8	C9	H9A	119
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42 C18 C19 1.379(4) 44 H10A C10 C11 120.2 43 C19 H19A 0.93 45 C10 C11 H11A 119.8 44 C19 N3 1.330(3) 46 C10 C11 C12 120.4(2) 45 C20 C21 1.525(4) 47 H11A C11 C12 119.9 46 C20 C22 1.528(3) 48 C11 C12 C13 120.5(2) 47 C20 C23 1.528(4) 49 C11 C12 C13 120.5(2) 50 H12A C12 C13 119.7 51 C8 C13 N2 119.0(2) 53 C12 C13 N2 120.9(2) 54 Zn1 N2 C14 114.6(2) 55 Zn1 N2 C14 114.6(2) 56 C13 N2 C14 1122.1(2) 57 N2 C14 H12A C15 119.2(2) <td< th=""><th>41</th><th>C18</th><th>H18A</th><th>0.929</th><th>43</th><th>C9</th><th>C10</th><th>C11</th><th>119.8(2)</th></td<>	41	C18	H18A	0.929	43	C9	C10	C11	119.8(2)
43 C19 H19A 0.93 45 C10 C11 H11A 119.8 44 C19 N3 1.330(3) 46 C10 C11 C12 120.4(2) 45 C20 C21 1.525(4) 47 H11A C11 C12 119.9 46 C20 C22 1.528(3) 48 C11 C12 C13 120.5(2) 47 C20 C23 1.528(4) 49 C11 C12 C13 120.5(2) 50 H12A C12 C13 119.7 51 C8 C13 N2 119.0(2) 51 C8 C13 N2 119.0(2) 53 C12 C13 122.4(2) 54 Zn1 N2 C14 114.6(2) 55 Zn1 N2 C14 112.6(2) 55 Zn1 N2 C14 H14A 120.4 120.4(2) 120.4(2) 56 C13 N2 C14 114.6(2) 56 C13 N2 1414.6(2) 57 N2	42	C18	C19	1.379(4)	44	H10A	C10	C11	120.2
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45 C20 C21 1.525(4) 47 H11A C11 C12 119.9 46 C20 C22 1.528(3) 48 C11 C12 H12A 119.8 47 C20 C23 1.528(4) 49 C11 C12 C13 120.5(2) 50 H12A C12 C13 119.0(2) 52 C8 C13 N2 119.0(2) 51 C8 C13 N2 119.0(2) 53 C12 C13 120.9(2) 54 Zn1 N2 C13 123.4(1) 55 Zn1 N2 C14 114.6(2) 56 C13 N2 C14 124.6(2) 56 C13 N2 C14 122.1(2) 59 H14A C14 C15 C16 119.2(2) 59 H14A C14 C15 123.2(2) 60 C14 C15 N3 112.1(2) 62 C16 C16 123.2(2) 61 C14 C15 N3 112.0(2) 63 C15 C16	44	C19	N3	1.330(3)	46	C10	C11	C12	120.4(2)
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$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$	47	C20	C23	1.528(4)	49	C11	C12	C13	120.5(2)
$ \begin{array}{c c c c c c c c c c c c c c c c c c c $					50	H12A	C12	C13	119.7
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53 C12 C13 N2 120.9(2) 54 Zn1 N2 C13 123.4(1) 55 Zn1 N2 C14 114.6(2) 56 C13 N2 C14 122.1(2) 57 N2 C14 H14A 120.4 58 N2 C14 C15 119.2(2) 59 H14A C14 C15 123.2(2) 61 C14 C15 N3 114.7(2) 61 C14 C15 N3 112.7(2) 61 C14 C15 N3 112.7(2) 61 C14 C15 N3 112.7(2) 62 C16 C15 N3 112.7(2) 63 C15 C16 H16A 120.8 64 C15 N3 112.7(2) 8 65 H16A C16 C17 118.4(2) 65 H16A C16 C17 120.8 66 C16 C17 H17A 120.8 66 C16					52	C8	C13	N2	119.0(2)
54 Zn1 N2 C13 123.4(1) 55 Zn1 N2 C14 114.6(2) 56 C13 N2 C14 122.1(2) 57 N2 C14 H14.4 120.4 58 N2 C14 C15 119.2(2) 59 H14A C14 C15 120.4 60 C14 C15 C16 123.2(2) 61 C14 C15 N3 114.7(2) 62 C16 C15 N3 112.1(2) 63 C15 C16 C17 118.4(2) 63 C15 C16 C17 118.4(2) 64 C15 C16 C17 118.4(2) 65 H16A C16 C17 118.4(2) 65 H16A C16 C17 120.8 66 C16 C17 C18 119.9(2) 68 H17A C17 C18 119.9(2) 68 H17A C17 C18 119.9(2) 69					53	C12	C13	N2	120.9(2)
55 Zn1 N2 C14 114.6(2) 56 C13 N2 C14 122.1(2) 57 N2 C14 H14A 120.4 58 N2 C14 C15 119.2(2) 59 H14A C14 C15 120.4 60 C14 C15 C16 123.2(2) 61 C14 C15 N3 114.7(2) 62 C16 C15 N3 122.1(2) 63 C15 C16 H16A 120.8 64 C15 C16 C17 118.4(2) 65 H16A C16 C17 120.8 66 C16 C17 H18.4(2) 65 67 C16 C17 C18 119.9(2) 68 H17A C17 C18 119.9(2) 68 H17A C17 C18 120.7 69 C17 C18 H19.9(2) 68 70 C17 C18 C19 118.5(2) 71 H18A <th></th> <th></th> <th></th> <th></th> <th>54</th> <th>Zn1</th> <th>N2</th> <th>C13</th> <th>123.4(1)</th>					54	Zn1	N2	C13	123.4(1)
56 C13 N2 C14 122.1(2) 57 N2 C14 H14A 120.4 58 N2 C14 C15 119.2(2) 59 H14A C14 C15 120.4 60 C14 C15 C16 123.2(2) 61 C14 C15 N3 114.7(2) 62 C16 C15 N3 112.1(2) 63 C15 C16 H16A 120.8 64 C15 C16 C17 118.4(2) 65 H16A C16 C17 120.8 66 C16 C17 H18.4(2) 65 65 H16A C16 C17 120.8 66 C16 C17 H18.4(2) 66 67 C16 C17 C18 119.9(2) 68 H17A C17 C18 120.8 69 C17 C18 H18A 120.8 70 C17 C18 H18A 120.8 70 C17					55	Zn1	N2	C14	114.6(2)
57 N2 C14 H14A 120.4 58 N2 C14 C15 119.2(2) 59 H14A C14 C15 120.4 60 C14 C15 C16 123.2(2) 61 C14 C15 N3 114.7(2) 62 C16 C15 N3 112.1(2) 63 C15 C16 H16A 120.8 64 C15 C16 C17 118.4(2) 65 H16A C16 C17 120.8 66 C16 C17 H120.8 119.9(2) 67 C16 C17 T18.4(2) 65 H16A C16 C17 120.8 66 C16 C17 T18.4(2) 66 67 C16 C17 C18 119.9(2) 68 H17A C17 C18 120.7 69 C17 C18 H18A 120.8 70					56	C13	N2	C14	122.1(2)
58 N2 C14 C15 119.2(2) 59 H14A C14 C15 120.4 60 C14 C15 C16 123.2(2) 61 C14 C15 N3 114.7(2) 62 C16 C15 N3 112.1(2) 63 C15 C16 H16A 120.8 64 C15 C16 C17 118.4(2) 65 H16A C16 C17 120.8 66 C16 C17 H17A 120 67 C16 C17 C18 119.9(2) 68 H17A C17 C18 119.9(2) 69 C17 C18 H18A 120.8 69 C17 C18 H18A 120.7 71 H18A C18 C19 118.5(2)					57	N2	C14	H14A	120.4
59 H14A C14 C15 120.4 60 C14 C15 C16 123.2(2) 61 C14 C15 N3 114.7(2) 62 C16 C15 N3 122.1(2) 63 C15 C16 H16A 120.8 64 C15 C16 C17 118.4(2) 65 H16A C16 C17 120.8 66 C16 C17 H17A 120 67 C16 C17 C18 119.9(2) 68 H17A C17 C18 120.8 69 C17 C18 120.8 70 C17 C18 H19.9(2) 71 H18A C19 120.7					58	N2	C14	C15	119.2(2)
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64 C15 C16 C17 118.4(2) 65 H16A C16 C17 120.8 66 C16 C17 H17A 120 67 C16 C17 C18 119.9(2) 68 H17A C17 C18 120.8 69 C17 C18 H18A 120.8 70 C17 C18 C19 118.5(2) 71 H18A C18 C19 120.7					63	C15	C16	H16A	120.8
65 H16A C16 C17 120.8 66 C16 C17 H17A 120 67 C16 C17 C18 119.9(2) 68 H17A C17 C18 120.8 69 C17 C18 H18A 120.8 70 C17 C18 C19 118.5(2) 71 H18A C18 C19 120.7					64	C15	C16	C17	118.4(2)
66 C16 C17 H17A 120 67 C16 C17 C18 119.9(2) 68 H17A C17 C18 120 69 C17 C18 H18A 120.8 70 C17 C18 C19 118.5(2) 71 H18A C18 C19 120.7					65	H16A	C16	C17	120.8
67 C16 C17 C18 119.9(2) 68 H17A C17 C18 120 69 C17 C18 H18A 120.8 70 C17 C18 C19 118.5(2) 71 H18A C18 C19 120.7					66	C16	C17	H17A	120
68 H17A C17 C18 120. 69 C17 C18 H18A 120.8 70 C17 C18 C19 118.5(2) 71 H18A C18 C19 120.7					67	C16	C17	C18	119 9(2)
69 C17 C18 H18A 120.8 70 C17 C18 C19 118.5(2) 71 H18A C18 C19 120.7					68	H17A	C17	C18	120
70 C17 C18 C19 118.5(2) 71 H18A C18 C19 120.7					69	C17	C18	H18A	120.8
71 H18A C18 C19 120.7					70	C17	C18	C19	118 5(2)
					71	H18A	C18	C19	120.7

Table S3. Bond lengths [Å] and angles [°] for $ZnL^{\mbox{\scriptsize APIP}}$ I



Figure S2. GPC analysis of Styrene Carbonate reaction mixture relevant to table 4 entry 12 showing no polymer chain



Figure S3. GPC analysis of **a**) typical polyether of cyclohexane oxide identified by ¹H NMR, **b**) Cyclohexane carbonate reaction mixture (Table 5, entries 6-10), **c**) Overlap spectra of **(a)** (blue) and **(b)** (black),**d**) Cyclohexane carbonate reaction catalyzed by TBAI relevant to table 5, entry 11.



Figure S4.¹H NMR spectrum of the cyclohexane oxide polyether chain (broad signal at δ = 3.45 ppm) (It was isolated by crystallization in THF in -1 °C)







Figure S6. ¹H NMR of ZnL^{APIP}OAc



Figure S7. ¹³C NMR of ZnL^{APIP}OAc



Figure S8. FTIR of ZnLAPIPCI



Figure S10. ¹³C NMR of ZnL^{APIP}CI



Figure S12. FTIR of ZnLAPIPBr



Figure S14. ¹³C NMR of ZnL^{APIP}Br







Figure S16. FTIR of ZnLAPIPI



Figure S18. ¹³C NMR of ZnL^{APIP} I





Additional IR, ¹H and ¹³C NMR spectra of products

(1b) Styrene carbonate was isolated as a white powder. mp: 60 °C





(2b) Propylene carbonate was isolated as colorless oil.





(3b) Ethylene Carbonate was isolated as white powder.







(4b) 4-((allyloxy)methyl)-1,3-dioxolan-2-one was isolated as pale yellow oil.



(5b) (2-oxo-1,3-dioxolan-4-yl)methyl methacrylate









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(6b) 4-(isopropoxymethyl)-1,3-dioxolan-2-one







(7b) 4-(butoxymethyl)-1,3-dioxolan-2-one







(8b) 4-(chloromethyl)-1,3-dioxolan-2-one









(9b) 4-ethyl-1,3-dioxolan-2-one











(10b) 4-(phenoxymethyl)-1,3-dioxolan-2-one was isolated as a white powder. mp: 108 $^\circ\text{C}$



















(12b) hexahydrobenzo[d][1,3]dioxol-2-one









Figure S20. ¹H NMR, ¹³C NMR and FTIR-spectra of cyclic carbonates