SUPPLEMENTARY INFORMATION

A novel zinc(II) complex containing square pyramidal, octahedral and tetrahedral geometries on the same polymeric chain constructed from pyrazine-2,3-dicarboxylic acid and 1-vinylimidazole

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Table of Contents:

Table S1. Selected geometric parameters for Zn(II) complex.

Bond lengths (Å)			
Zn1-N5	2.041(2)	Zn3-N15	2.005(3)
Zn1-O7	2.0428(19)	Zn3-N15^{i}	2.005(3)
Zn1-N3	2.072(3)	Zn3-O3	2.005(2)
Zn1-O1	2.075(2)	Zn3-O3^{i}	2.005(2)
Zn1-N1	2.203(2)	Zn4-O11	1.994(2)
Zn2-N9	2.068(3)	Zn4-O11^{ii}	1.994(2)
Zn2-O5	2.086(2)	Zn4-N17	2.000(2)
Zn2-N11	2.110(3)	Zn4-N17^{ii}	2.000(2)
Zn2-O9	2.127(2)	Zn2-N7	2.270(3)
Zn2-N13	2.221(2)		
Bond angles (°)			
N5-Zn1-O7	100.40(8)	N15-Zn3-N15^{i}	116.56(17)
N5-Zn1-N3	104.56(12)	N15-Zn3-O3	114.02(10)
O7-Zn1-N3	102.60(11)	N15^{i}-Zn3-O3	107.74(9)
N5-Zn1-O1	89.19(9)	N15-Zn3-O3^{i}	107.74(9)
O7-Zn1-O1	152.00(10)	N15^{i}-Zn3-O3^{i}	114.02(10)
N3-Zn1-O1	100.27(10)	O3-Zn3-O3^{i}	94.81(12)
N5-Zn1-N1	160.10(11)	O11^{ii}-Zn4-O11	98.06(12)
O7-Zn1-N1	87.25(8)	O11^{ii}-Zn4-N17	113.62(9)
N3-Zn1-N1	91.45(10)	O11^{ii}-Zn4-N17^{ii}	105.39(9)
O1-Zn1-N1	76.18(8)	O11-Zn4-N17	105.39(9)
N9-Zn2-O5	105.77(9)	O11-Zn4-N17^{ii}	113.62(9)
N9-Zn2-N11	98.81(10)	N17-Zn4-N17^{ii}	118.95(16)
O5-Zn2-N11	86.80(9)	O9-Zn2-N13	75.05(8)
N9-Zn2-O9	88.03(9)	N9-Zn2-N7	89.19(10)
O5-Zn2-O9	163.05(9)	O5-Zn2-N7	74.48(9)
N11-Zn2-O9	101.03(10)	N11-Zn2-N7	161.06(9)
N9-Zn2-N13	162.83(9)	O9-Zn2-N7	96.35(9)
O5-Zn2-N13	90.45(9)	N13-Zn2-N7	89.80(10)
N11-Zn2-N13	87.48(10)		

i: -x+1, y, -z+2; ii: -x, y, -z+1

Table S2. Hydrogen bond interactions in Zn(II) complex.

D–H···A	**D–H (Å)**	**H···A (Å)**	**D···A (Å)**	**D–H···A (°)**
O1W—H1W1---O6	0.86(7)	2.01(7)	2.807(7)	154(8)
O1W—H2W1---O8^{vi}	0.85(4)	2.12(6)	2.862(8)	147(11)
O2W—H1W2---O7	0.87(7)	1.97(7)	2.776(6)	154(7)
C12—H12---O6	0.93	2.45	3.250(6)	145
C14—H14---O12^{vi}	0.93	2.33	3.166(5)	149
C18—H18---O2W^{v}	0.93	2.18	3.107(9)	175
C41—H41---O2^{iii}	0.93	2.26	3.180(6)	172
C42—H42---O11^{vii}	0.93	2.32	3.231(7)	168
C46—H46---O10	0.93	2.33	3.252(6)	172
C47—H47---O3^{v}	0.93	2.36	3.269(7)	167
C50—H50---O1W	0.93	2.48	3.295(11)	147
C51—H51---O2W^{viii}	0.93	1.83	2.761(10)	175
C53—H53A---O6^{iv}	0.93	2.59	3.427(12)	149

iii: 1-x, y, 2-z; iv: 1/2-x, 1/2+y, 1-z; v: 1/2-x, 1/2+y, 2-z; vi: 1/2-x, -1/2+y, 1-z; vii: 1/2+x, 1/2+y, 1+z; viii: x, y, -1+z

D: Donor, A: Acceptor

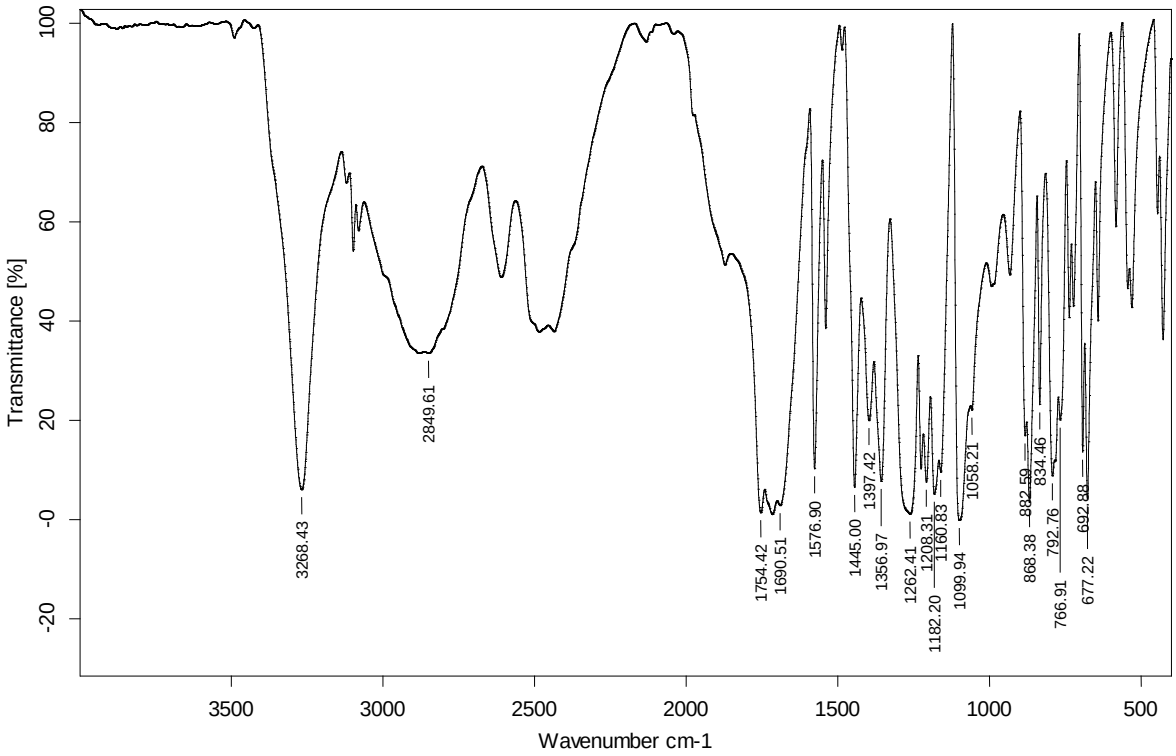

Figure S1. IR spectrum of pyrazine-2,3-dicarboxylic acid.

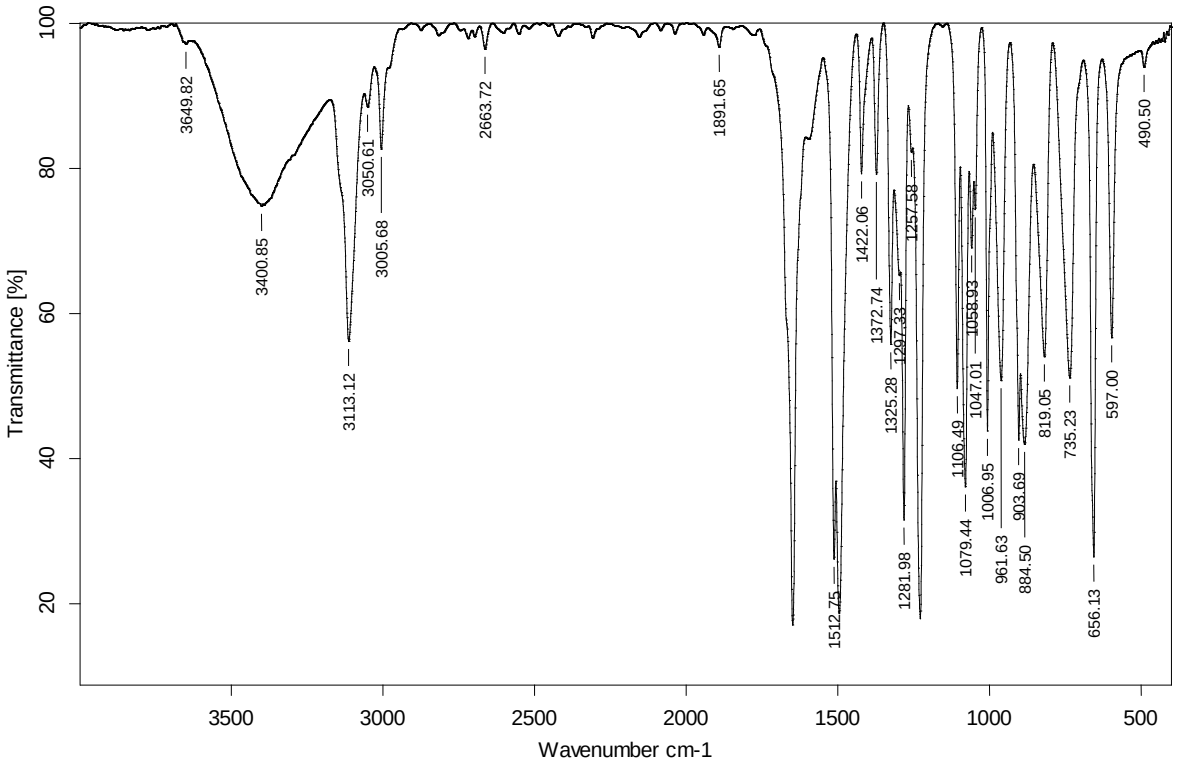

Figure S2. IR spectrum of 1-vinylimidazole.

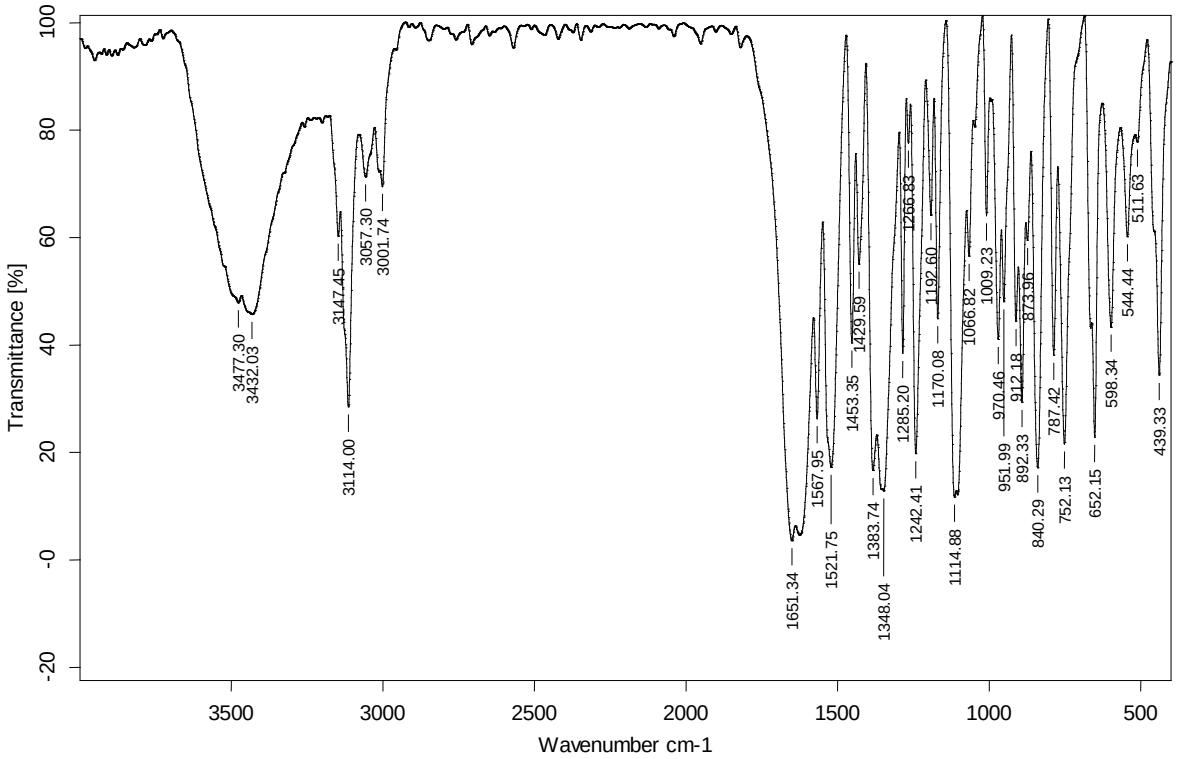

Figure S3. IR spectrum of Zn(II) complex.

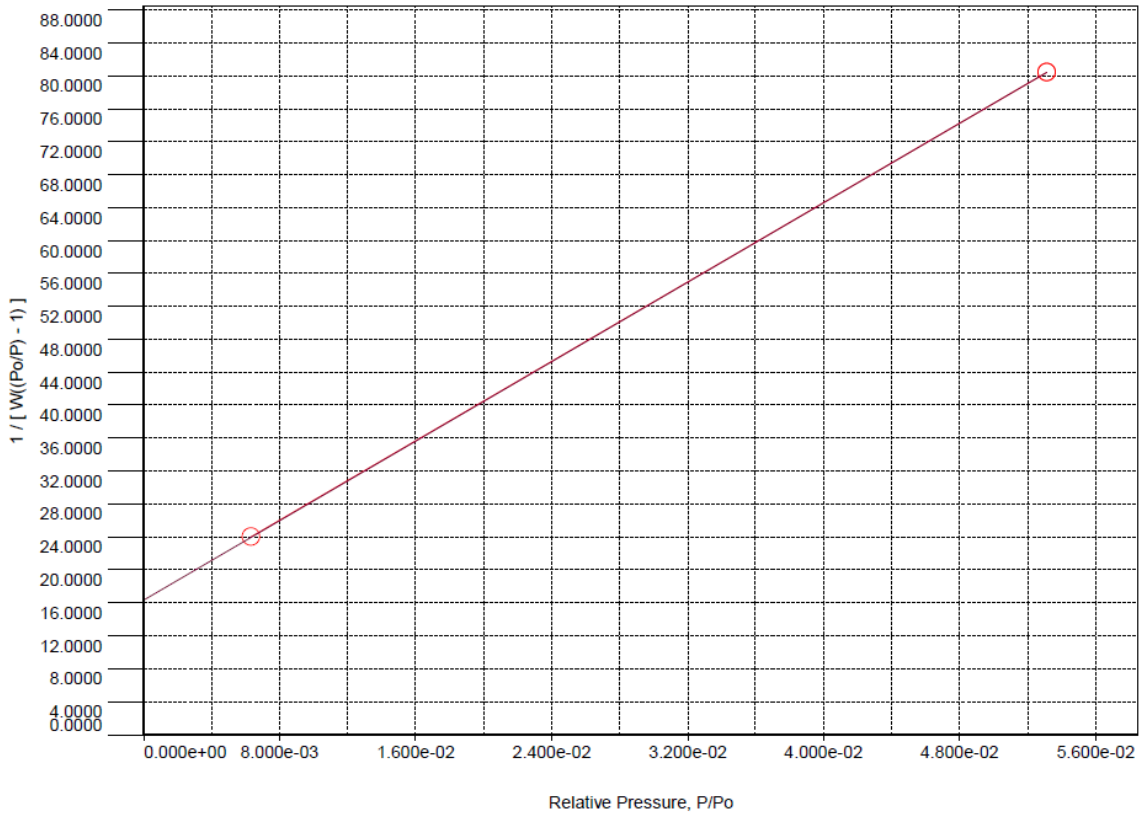

Figure S4. BET surface area isotherm of Zn(II) complex.