

**A novel octa-nuclear 32-membered zirconocene macrocycle based on
the aromatic selenite**

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Supporting Information

Table of contents

1. X-ray crystallography.....	3
Table S1. Selected bond lengths [Å] and angles [°] for complex 1.....	3
2. Figures of crystal structure.....	5
Figure S1. The asymmetric unit of complex 1 (ellipsoid figures).....	5
Figure S2. The 32-membered macrocycle structure of complex 1 (ellipsoid figures).....	6
Figure S3. 2D network structure of complex 1.....	6
Figure S4. The 3D structure of complex 1.....	7
Figure S5. The FT-IR spectrum of complex 1.....	7
Figure S6. The ¹ H NMR spectrum of complex 1 recorded in DMSO.....	8
Figure S7. The ¹³ C NMR spectrum of complex 1 recorded in DMSO/CDCl ₃	8
Figure S8. PXRD patterns of complex 1.....	9

1. X-ray crystallography

Table S1 Selected bond lengths [Å] and angles [°] for complex **1**.

Bond length			
Zr(1)-O(1)	2.112(6)	Zr(3)-C(40)	2.470(13)
Zr(1)-O(7)	2.126(6)	Zr(3)-C(36)	2.492(12)
Zr(1)-O(3)	2.129(5)	Zr(3)-C(38)	2.495(12)
Zr(1)-O(5)	2.194(5)	Zr(3)-C(43)	2.521(13)
Zr(1)-C(28)	2.537(9)	Zr(3)-C(44)	2.512(12)
Zr(1)-Cl(1)	2.540(3)	Zr(3)-C(35)	2.533(12)
Zr(1)-C(27)	2.534(10)	Zr(3)-C(42)	2.549(13)
Zr(1)-C(26)	2.548(10)	Zr(3)-C(41)	2.550(13)
Zr(1)-C(29)	2.551(9)	Zr(3)-C(39)	2.574(12)
Zr(1)-C(25)	2.570(10)	Se(1)-O(1)	1.678(6)
Zr(2)-O(8)#1	2.115(6)	Se(1)-O(2)	1.698(6)
Zr(2)-O(2)	2.138(6)	Se(1)-C(1)	1.882(6)
Zr(2)-O(6)	2.159(6)	Se(2)-O(3)	1.698(5)
Zr(2)-O(4)	2.209(5)	Se(2)-O(4)	1.698(6)
Zr(2)-C(30)	2.504(10)	Se(2)-C(7)	1.946(9)
Zr(2)-Cl(2)	2.509(3)	Se(3)-O(6)	1.687(6)
Zr(2)-C(31)	2.523(10)	Se(3)-O(5)	1.691(6)
Zr(2)-C(34)	2.546(10)	Se(3)-C(13)	1.883(5)
Zr(2)-C(32)	2.544(10)	Se(4)-O(8)	1.695(6)
Zr(2)-C(33)	2.565(10)	Se(4)-O(7)	1.711(5)
Zr(3)-O(9)	1.9503(15)	Se(4)-C(19)	1.928(10)
Zr(3)-C(37)	2.445(12)	O(8)-Zr(2)#2	2.114(6)
Zr(3)-Cl(3)	2.455(3)	O(9)-Zr(3)#3	1.9503(15)
Bond angles			
O(1)-Zr(1)-O(7)	153.9(2)	O(8)#1-Zr(2)-O(2)	85.2(2)
O(1)-Zr(1)-O(3)	86.8(2)	O(8)#1-Zr(2)-O(6)	159.2(2)
O(7)-Zr(1)-O(3)	87.7(2)	O(2)-Zr(2)-O(6)	86.5(2)
O(1)-Zr(1)-O(5)	79.1(2)	O(8)#1-Zr(2)-O(4)	78.2(2)
O(7)-Zr(1)-O(5)	74.9(2)	O(2)-Zr(2)-O(4)	77.2(2)
O(3)-Zr(1)-O(5)	79.0(2)	O(6)-Zr(2)-O(4)	81.4(2)
O(1)-Zr(1)-Cl(1)	85.78(17)	O(8)#1-Zr(2)-Cl(2)	89.67(16)
O(7)-Zr(1)-Cl(1)	90.24(16)	O(2)-Zr(2)-Cl(2)	156.39(17)
O(3)-Zr(1)-Cl(1)	158.73(16)	O(6)-Zr(2)-Cl(2)	90.30(17)
O(5)-Zr(1)-Cl(1)	80.02(15)	O(4)-Zr(2)-Cl(2)	79.20(15)
O(9)-Zr(3)-Cl(3)	98.84(17)	O(8)-Se(4)-O(7)	100.9(3)
O(1)-Se(1)-O(2)	103.6(3)	Se(1)-O(1)-Zr(1)	149.0(3)
O(1)-Se(1)-C(1)	97.2(4)	Se(1)-O(2)-Zr(2)	125.9(3)
O(2)-Se(1)-C(1)	98.6(3)	Se(2)-O(3)-Zr(1)	132.1(3)
O(3)-Se(2)-O(4)	101.5(3)	Se(2)-O(4)-Zr(2)	126.4(3)
O(3)-Se(2)-C(7)	96.3(4)	Se(3)-O(5)-Zr(1)	123.9(3)

O(4)-Se(2)-C(7)	102.0(3)	Se(3)-O(6)-Zr(2)	130.2(3)
O(6)-Se(3)-O(5)	101.4(3)	Se(4)-O(7)-Zr(1)	123.8(3)
O(6)-Se(3)-C(13)	99.9(3)	Se(4)-O(8)-Zr(2)#2	132.6(3)
O(5)-Se(3)-C(13)	100.1(3)	Zr(3)-O(9)-Zr(3)#3	168.9(6)

Symmetry code for complex 1: #1 $y+1/4, -x+3/4, -z+1/4$ #2 $-y+3/4, x-1/4, -z+1/4$ #3 $y-1/4, x+1/4, -z+1/4$

2. Figures of crystal structure

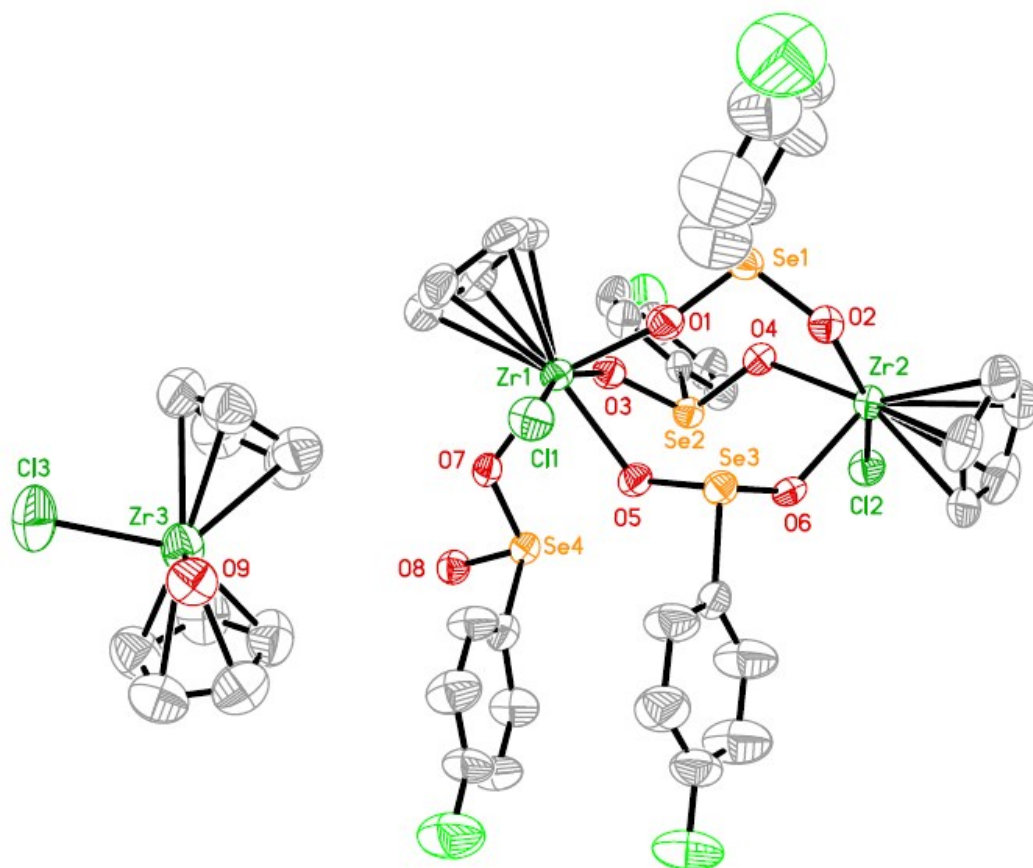


Figure S1 The asymmetric unit of complex **1**, rendered with 30% probability ellipsoids. Hydrogen atoms are omitted for clarity.

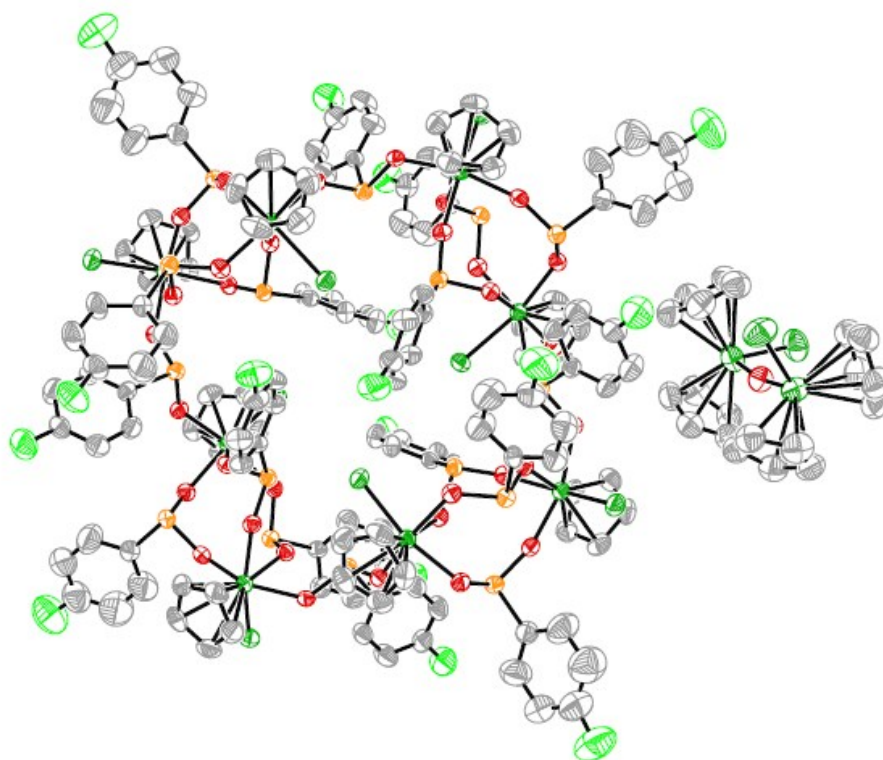


Figure S2 The 32-membered macrocycle of complex **1**, rendered with 30% probability ellipsoids. Hydrogen atoms are omitted for clarity.

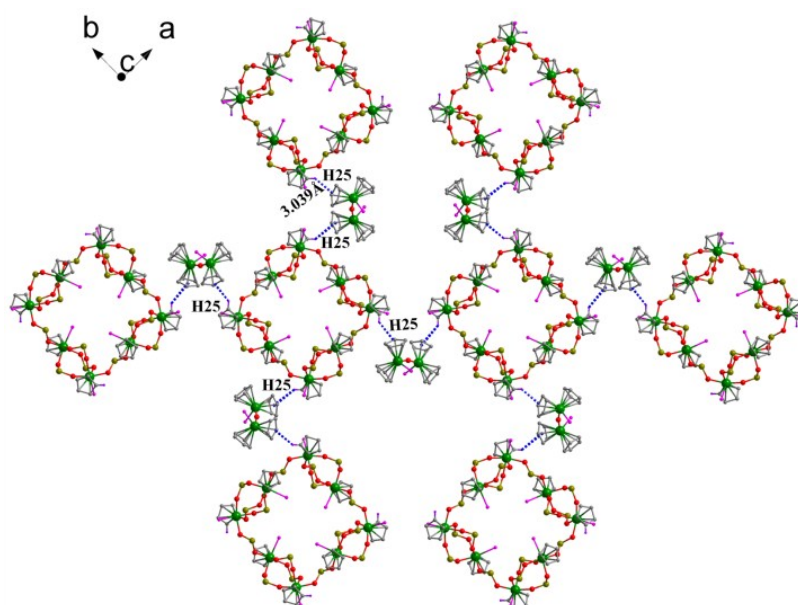


Figure S3 2D network structure of complex **1** constructed by C-H $\cdots$ π interactions (blue dashes).

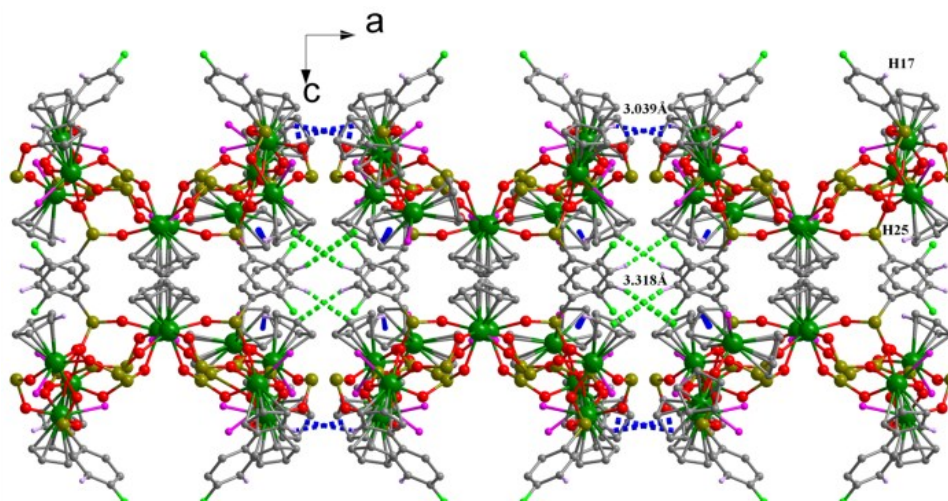


Figure S4 The 3D structure of complex **1** constructed from the interlayer C-H $\cdots\pi$ interactions (green dashes).

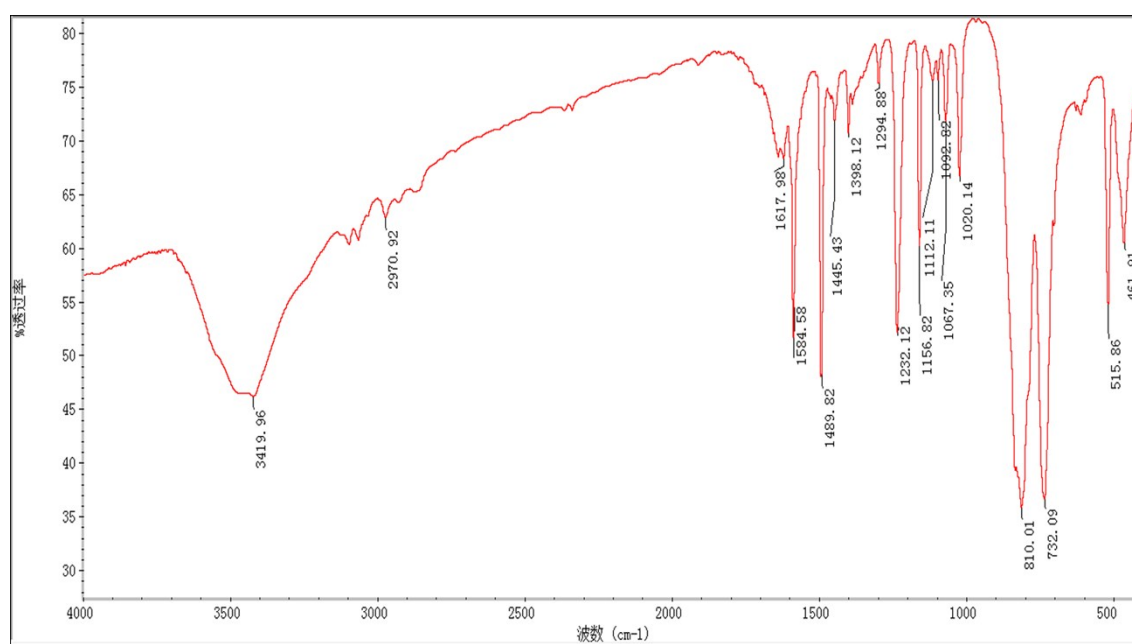


Figure S5 The FT-IR spectrum of complex **1**.

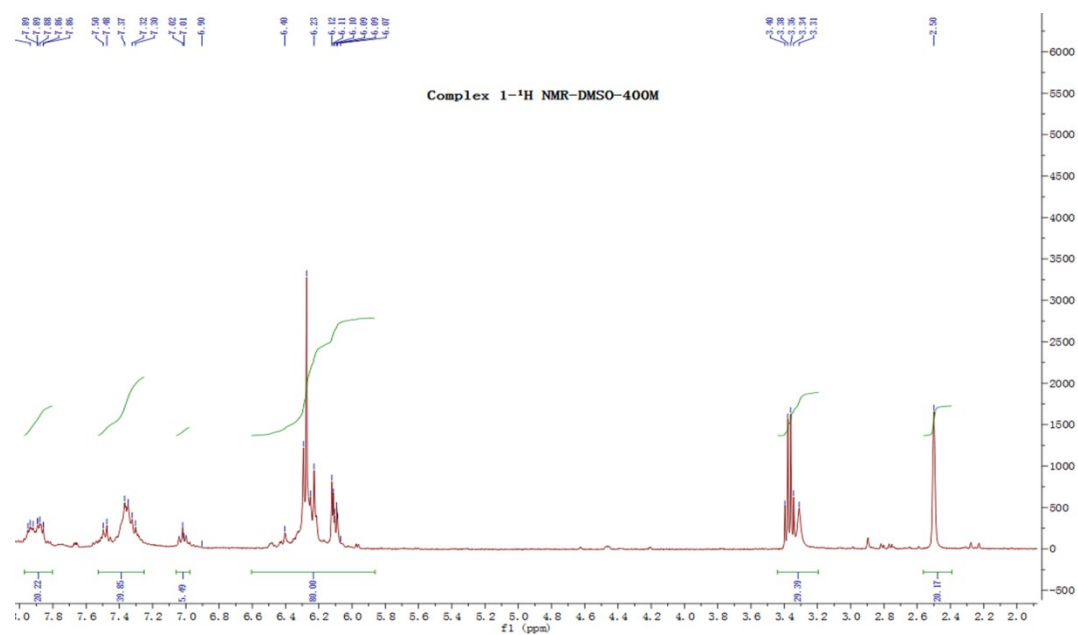


Figure S6 The ¹H NMR spectrum of complex **1** recorded in DMSO

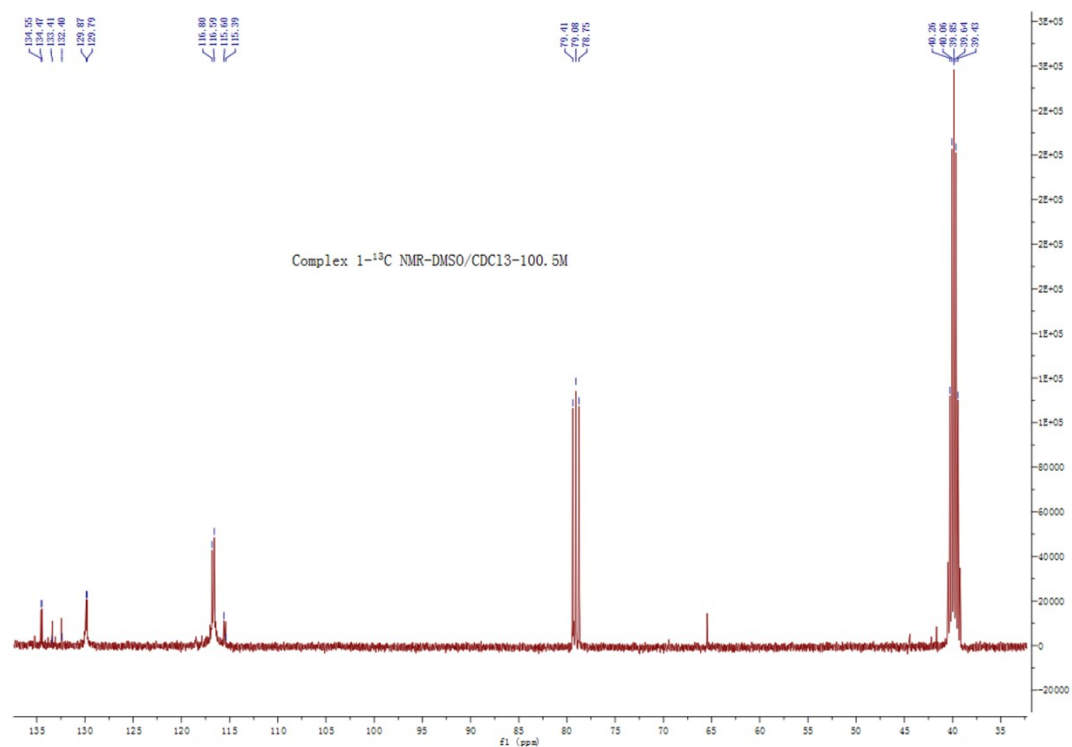


Figure S7 The ¹³C NMR spectrum of complex **1** recorded in DMSO/CDCl₃.

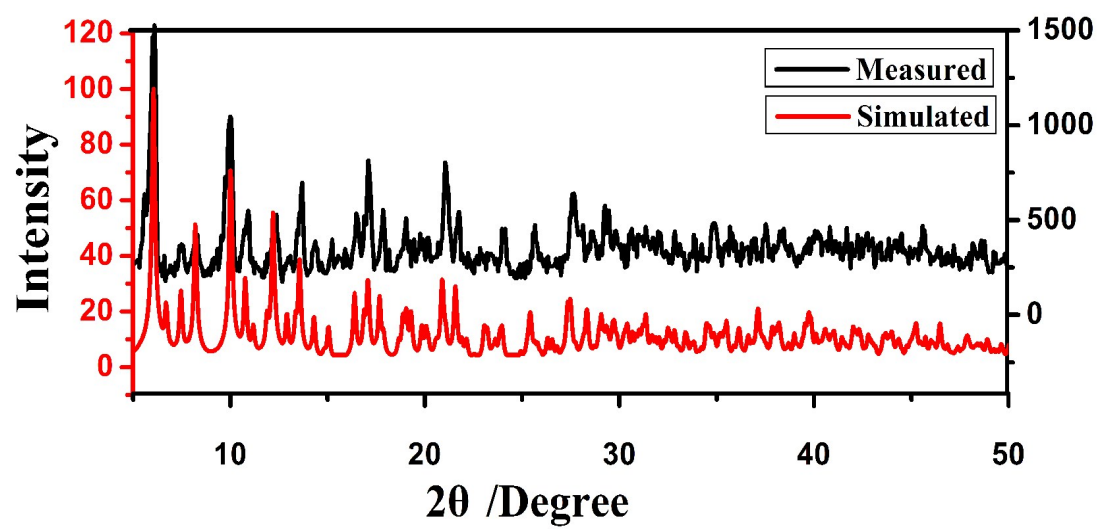


Figure S8 PXRD patterns of complex 1.