Electronic Supplementary Information (ESI)

Ligand-Directed Self-Assembly of Binuclear/Hexanuclear Lanthanide Complexes for Functional Catalysis

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Materials and reagents

3,4-diaminobenzoic acid (98%), imidazole-4-carbaldehyde (98%), imidazole-2-carbaldehyde (98%), Na_2SO_3 (≥96.5%), $La(NO_3)_3·5H_2O$ (99%), $Nd(NO_3)_3·5H_2O$ (99%), $Sm(NO_3)_3·5H_2O$ (99%), $Dy(NO_3)_3·5H_2O$ (99%), $HoCl_3·6H_2O$ (99%), $ErCl_3·6H_2O$ (99%), Na_2SO_3 (≥99.0%), EtOH (≥99.7%), Acetonitrile (99%), *N,N*-dimethylformamide (99%) were purchased from Adamas and used as received.

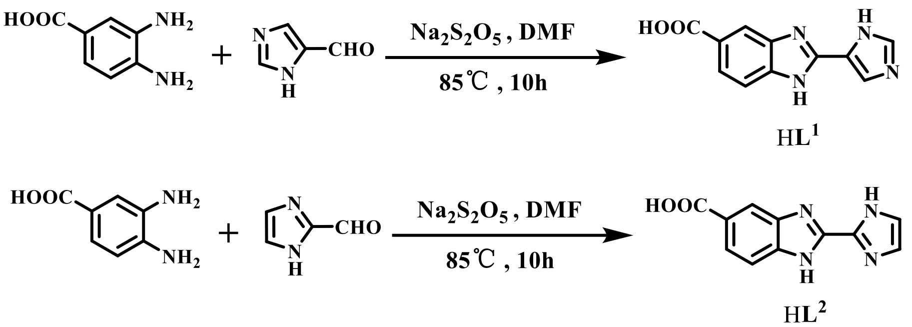
Chemicals and Physical Measurement

The FT-IR spectra were recorded on a Brucker Equinox 55 in the range of 4000–400 cm^{-1} with KBr discs. Thermogravimetric analysis (TGA) was performed using a DSC 200F3 apparatus under a N_2 atmosphere with heating rate of 10 °C/min. Powder X-ray diffraction (PXRD) was studied on a Bruker D8 with Cu radiation (Cu K*α*, λ=1.54056 Å, 293 K). ^{1}H NMR spectra were measured on a Varian 600 MHz NMR spectrometer. Inductively coupled plasma-optical emission spectroscopy (ICP-OES) data was obtained by Optima 8000.

X-ray crystallography

The crystal diffraction date of complexes **1-6** were collected using Bruker Smart Apex-II diffractometer with graphite-monochromatic Mo Kα radiation (λ = 0.71073 Å) in *φ*/*ω* scan mode. The structures of complexes **1-6** were determined by employing the crystallographic software package of SHELXL-2014/7. Anisotropic thermal displacement coefficients were used to refine non-hydrogen atoms. All hydrogen atoms were located in theoretically specific positions and were refined by a riding model.

Synthesis of ligands HL^1 and HL^2



1.91 g (10 mmol) Na_2SO_3, 0.96 g (10 mmol) imidazole-4-carbaldehyde and 1.52 g (10 mmol) 3,4-diaminobenzoic acid were added to a 100 mL round bottom flask, and 60 mL DMF was added as a solvent. After 10 hours of reaction at 85 °C, the reaction mixture was poured into 50 mL ice water, and the green solid H**L^1** was separated by suction filtration with a yield of 85%. ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.43 (s, 1H, 1,2,4-triazole), 8.34 (m, 1H, triazole), 8.21 (s, 1H, benzene), 8.12 (d, 1H, benzene), 7.70-8.88 (dd, 5H, benzene). IR (KBr, cm^{-1})：3298 (m, N-H, benzimidazole), 3123 (m), 2868 (m), 2806 (m), 2545 (m), 1897 (w), 1705 (s, C=O, carboxyl)), 1626 (m, C=C, benzene), 1613 (m, C=C, benzene), 1516 (s, C=C, benzene), 1451 (m, C=C, benzene), 1419 (m), 1366 (m), 1298 (s), 1218 (s), 1148 (s), 1051 (m), 1017 (m), 978 (s), 886 (m, C-H, benzene), 844 (s, C-H, benzene), 772 (s, C-H, benzene), 669 (m), 641 (m), 556 (w), 522 (w), 507 (w), 454 (w). Elemental Anal. Calcd(%): $C_{11}H_8N_4O_2$: C, 57.89%; H, 3.53%; N, 24.56%; O, 14.02%. Found: C, 56.55%; H, 3.72%; N, 24.08%; O, 15.65%.

The synthesis method of ligand H**L²** is similar to that of H**L¹**. Only imidazole-4-carbaldehyde in the raw material is replaced by imidazole-2-carbaldehyde, and the final product is a pale green solid H**L²** with a yield of 92%. ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.43 (s, 1H, 1,2,4-triazole), 8.34 (m, 1H, triazole), 8.21 (s, 1H, benzene), 8.12 (d, 1H, benzene), 7.70-8.88 (dd, 5H, benzene). IR (KBr, cm^{-1})：3298 (m, N-H, benzimidazole), 3123 (m), 2868(m), 2806 (m), 2545 (m), 1897 (w), 1705 (s, C=O, carboxyl), 1626 (m, C=C, benzene), 1613 (m, C=C, benzene), 1516 (s, C=C, benzene), 1451 (m, C=C, benzene), 1419 (m), 1366 (m), 1298 (s), 1218 (s), 1148 (s), 1051 (m), 1017 (m), 978 (s), 886 (m, C-H, benzene), 844 (s, C-H, benzene), 772 (s, C-H, benzene), 669 (m), 641 (m), 556 (w), 522 (w), 507 (w), 454 (w). Elemental Anal. Calcd(%): $C_{11}H_8N_4O_2$: C, 57.89%; H, 3.53%; N, 24.56%; O, 14.02%. Found: C, 57.02%; H, 3.41%; N, 25.11%; O, 14.46%.

Table S1. Crystallographic data for complexes **1-6**.

Complex	**1**	**2**	**3**
Formula	$C_{22}H_{26}N_{12}O_{22}La_2$	$C_{22}H_{26}N_{12}O_{22}Nd_2$	$C_{22}H_{26}N_{12}O_{22}Sm_2$
Molecular weight	1088.37	1099.03	1111.25
Crystal system	Triclinic	Triclinic	Triclinic
Space group	*P*-1	*P*-1	*P*-1
a/Å	296(2)	296(2)	296(2)
b/Å	8.5602(3)	8.5601(10)	8.5680(9)
c/Å	9.1168(3)	9.1050(10)	9.0880(10)
α/ (°)	11.4220(4)	11.3843(12)	11.3279(12)
β/ (°)	95.5340(10)	95.586(3)	95.682(3)
γ (°)	94.7330(10)	94.771(3)	94.776(3)
V (Å^3)	96.5840(10)	96.714(3)	97.044(3)
T (K)	877.43(5)	873.00(17)	867.03(16)
Z	1	1	1
D (mg·m^{-3})	2.060	2.090	2.128
μ (mm^{-1})	2.510	3.049	3.462
F (000)	532	538	542
Reflections collected	11623	17411	23672
Independent reflections [I>2σ(I)]	3047	3073	3051
Goodness of fit on F^2			
$R^a/wR^b[I>2\sigma (I)]$	0.0275/0.0673	0.0275/0.0510	0.0246/0.0521

$R^a = \Sigma(||F_0|-|F_C||)/\Sigma|F_0|$; $wR^b = [\Sigma w(|F_0|^2-|F_C|^2)^2/\Sigma w(F_0^2)]^{1/2}$

Complex	**4**	**5**	**6**
Formula	$C_{22}H_{26}N_{12}O_{22}Dy_2$	$C_{88}H_{96}N_{32}O_{41}Ho_6$	$C_{88}H_{96}N_{32}O_{41}Er_6$
Molecular weight	1135.55	32247.48	3261.4
Crystal system	Triclinic	Tetragonal	Tetragonal
Space group	*P*-1	*I*4₁/*a*	*I*4₁/*a*
a/Å	296(2)	296(2)	296(2)
b/Å	8.620(9)	14.7916(5)	14.8086(8)
c/Å	9.188(9)	14.7916(5)	14.8086(8)
α/ (°)	11.602(11)	53.557(3)	53.648(4)
β/ (°)	95.61(3)	90	90
γ (°)	94.86(3)	90	90
V ($Å^3$)	96.10(3)	90	90
T (K)	905.1(15)	11717.7(10)	11764.8(16)
Z	1	8	16
D ($mg·m^{-3}$)	2.083	1.836	1.832
μ (mm^{-1})	4.201	4.097	4.325
F (000)	550	6280	6272
Reflections collected	11453	50617	24852
Independent reflections [I>2σ(I)]	3107	5205	5194
Goodness of fit on F^2			
$R^a/wR^b[I>2\sigma(I)]$	0.0460/0.1175	0.0627/0.1527	0.0628/0.1623

$R^a = \Sigma(||F_0|-|F_C||)/\Sigma|F_0|$; $wR^b = [\Sigma w(|F_0|^2-|F_C|^2)^2/\Sigma w(F_0^2)]^{1/2}$

Table S2. Selected bond lengths (Å) and bond angles (°) in complexes **1-6**.

Complex **1**			
La(1)-N(1) $^{\#1}$	2.601(3)	La(1)-O(6)$^{\#1}$	2.599(3)
La(1)-N(3) $^{\#1}$	2.651(3)	La(1)-O(8)	2.621(3)
La(1)-N(6)	3.012(4)	La(1)-O(9)$^{\#1}$	2.541(3)
La(1)-O(1)	2.484(3)	N(1)-La(1) $^{\#1}$	2.451(3)
La(1)-O(2)	2.578(3)	N(3)-La(1) $^{\#1}$	2.601(3)
La(1)-O(3)	2.590(3)		
La(1)-O(5)	2.760(3)		
N(1) $^{\#1}$-La(1)-N(3) $^{\#1}$	63.95(9)	O(5)-La(1)-N(6)	86.21(10)
N(1) $^{\#1}$-La(1)-N(6)	93.18(10)	O(6)-La(1)-N(1)$^{\#1}$	72.22(9)
N(1)-La(1)-O(5)	67.04(9)	O(6)-La(1)-N(3)$^{\#1}$	69.37(9)
N(1)-La(1)-O(8)	116.87(9)	O(6)-La(1)-N(6)	24.49(9)
N(3) $^{\#1}$-La(1)-N(6)	66.95(9)	O(6)-La(1)-O(5)	66.76(10)
N(3) $^{\#1}$-La(1)-O(5)	121.45(9)	O(6)-La(1)-O(8)	48.63(9)

O(1)-La(1)-N(1)$^{\#1}$	133.11(9)	O(8)-La(1)-N(3)$^{\#1}$	75.11(10)
O(1)-La(1)-N(3)$^{\#1}$	74.52(9)	O(8)-La(1)-N(6)	24.63(9)
O(1)-La(1)-N(6)	89.71(10)	O(8)-La(1)-O(5)	101.43(10)
O(1)-La(1)-O(2)	50.69(8)	O(9)-La(1)-N(1)$^{\#1}$	74.44(10)
O(1)-La(1)-O(3)	112.81(9)	O(9)-La(1)-N(3)$^{\#1}$	70.47(9)
O(1)-La(1)-O(5)	159.70(9)	O(9)-La(1)-N(6)	136.75(9)
O(1)-La(1)-O(6)	113.17(10)	O(9)-La(1)-O(2)	95.33(10)
O(1)-La(1)-O(8)	68.95(10)	O(9)-La(1)-O(3)	145.16(10)
O(1)-La(1)-O(9)	71.87(10)	O(9)-La(1)-O(5)	123.39(10)
O(2)-La(1)-N(1)$^{\#1}$	164.05(10)	O(9)-La(1)-O(6)	135.91(9)
O(2)-La(1)-N(3)$^{\#1}$	124.79(8)	O(6)-La(1)-O(8)	133.13(10)
O(2)-La(1)-N(6)	102.56(10)	O(10)-La(1)- N(1)$^{\#1}$	84.68(10)
O(2)-La(1)-O(3)	68.08(9)	O(10)-La(1)- N(3)$^{\#1}$	132.88(9)
O(2)-La(1)-O(5)	110.98(9)	O(10)-La(1)- N(6)	153.88(10)
O(2)-La(1)-O(6)	122.41(9)	O(10)-La(1)-O(1)	110.71(10)
O(2)-La(1)-O(8)	79.06(9)	O(10)-La(1)-O(2)	80.06(9)
O(3)-La(1)-N(1)$^{\#1}$	113.55(9)	O(10)-La(1)-O(3)	79.13(10)
O(3)-La(1)-N(3)$^{\#1}$	144.27(10)	O(10)-La(1)-O(5)	68.95(10)
O(3)-La(1)-N(6)	77.92(10)	O(10)-La(1)-O(6)	135.16(10)
O(3)-La(1)-O(5)	46.91(9)	O(10)-La(1)-O(8)	151.79(10)
O(3)-La(1)-O(6)	76.01(9)	O(10)-La(1)-O(9)	67.61(9)
O(3)-La(1)-O(8)	75.59(10)		

Complex **2**

Nd(1)-O(7)	2.434(3)	Nd(1)-O(8)	2.569(3)
Nd(1)-O(1)	2.470(3)	Nd(1)-O(5)	2.582(3)
Nd(1)-O(6)	2.525(3)	Nd(1)-O(3)	2.604(3)
Nd(1)-O(2)	2.565(3)	Nd(1)-O(9)	2.762(3)
O(7)-Nd(1)-O(1)	111.19(10)	O(5)-Nd(1)-N(1)$^{\#1}$	69.60(9)
O(7)-Nd(1)-O(6)	68.47(9)	N(3)$^{\#1}$-Nd(1)-N(1)$^{\#1}$	64.37(9)
O(1)-Nd(1)-O(6)	71.78(10)	O(3)-Nd(1)-N(1)$^{\#1}$	75.22(10)
O(7)-Nd(1)-O(2)	79.76(9)	O(7)-Nd(1)-O(9)	68.18(10)
O(1)-Nd(1)-O(2)	50.99(8)	O(1)-Nd(1)-O(9)	159.82(9)

O(6)-Nd(1)-O(2)	95.38(10)	O(7)-Nd(1)-N(1)$^{\#1}$	133.81(9)
O(7)-Nd(1)-O(8)	78.19(10)	O(1)-Nd(1)-N(1)$^{\#1}$	74.32(9)
O(1)-Nd(1)-O(8)	112.89(9)	O(6)-Nd(1)-N(1)$^{\#1}$	70.60(9)
O(6)-Nd(1)-O(8)	145.05(10)	O(2)-Nd(1)-N(1)$^{\#1}$	124.86(8)
O(2)-Nd(1)-O(8)	67.87(9)	O(8)-Nd(1)-N(1)$^{\#1}$	144.26(10)
O(7)-Nd(1)-O(5)	134.38(10)	O(6)-Nd(1)-O(9)	123.33(10)
O(1)-Nd(1)-O(5)	113.27(10)	O(2)-Nd(1)-O(9)	110.77(9)
O(6)-Nd(1)-O(5)	136.21(9)	O(8)-Nd(1)-O(9)	46.93(9)
O(2)-Nd(1)-O(5)	122.25(9)	O(5)-Nd(1)-O(9)	66.63(10)
O(8)-Nd(1)-O(5)	75.81(9)	N(3)$^{\#1}$-Nd(1)-O(9)	66.95(9)
O(7)-Nd(1)-N(3)$^{\#1}$	84.56(10)	O(3)-Nd(1)-O(9)	101.54(10)
O(1)-Nd(1)-N(3)$^{\#1}$	133.11(9)	N(1)$^{\#1}$-Nd(1)-O(9)	121.57(9)
O(6)-Nd(1)-N(3)$^{\#1}$	74.31(10)	O(7)-Nd(1)-N(5)	152.83(10)
O(2)-Nd(1)-N(3)$^{\#1}$	163.62(10)	O(1)-Nd(1)-N(5)	89.65(11)
O(8)-Nd(1)-N(3)$^{\#1}$	113.52(9)	O(6)-Nd(1)-N(5)	137.12(9)
O(5)-Nd(1)-N(3)$^{\#1}$	72.64(10)	O(2)-Nd(1)-N(5)	102.27(10)
O(7)-Nd(1)-O(3)	150.80(10)	O(8)-Nd(1)-N(5)	77.65(10)
O(1)-Nd(1)-O(3)	68.84(10)	O(5)-Nd(1)-N(5)	24.68(9)
O(6)-Nd(1)-O(3)	133.20(10)	N(3)$^{\#1}$-Nd(1)-N(5)	93.84(10)
O(2)-Nd(1)-O(3)	78.83(9)	O(3)-Nd(1)-N(5)	24.65(9)
O(8)-Nd(1)-O(3)	75.48(10)	N(1)$^{\#1}$-Nd(1)-N(5)	67.21(9)
O(5)-Nd(1)-O(3)	48.87(9)	O(9)-Nd(1)-N(5)	86.20(10)
N(3)$^{\#1}$-Nd(1)-O(3)	117.53(10)		

Complex **3**

N(2)-Sm(1)$^{\#1}$	2.597(3)	O(5)-Sm(1)	2.535(3)
N(3)-Sm(1)$^{\#1}$	2.556(3)	O(6)-Sm(1)	2.776(3)
O(1)-Sm(1)	2.444(3)	O(8)-Sm(1)	2.552(3)
O(2)-Sm(1)	2.541(3)	O(10)-Sm(1)	2.573(3)
O(3)-Sm(1)	2.495(3)	Sm(1)-N(3)$^{\#1}$	2.556(3)
O(4)-Sm(1)	2.403(3)	Sm(1)-N(2)$^{\#1}$	2.596(3)
O(4)-Sm(1)-O(1)	111.67(10)	O(8)-Sm(1)-N(2)$^{\#1}$	70.00(9)
O(4)-Sm(1)-O(3)	68.60(10)	N(3)$^{\#1}$-Sm(1)-N(2)$^{\#1}$	65.13(9)

O(1)-Sm(1)-O(3)	71.41(11)	O(3)-Sm(1)-O(10)	133.33(10)
O(4)-Sm(1)-O(5)	78.26(10)	O(5)-Sm(1)-O(10)	74.90(10)
O(1)-Sm(1)-O(5)	112.93(9)	O(2)-Sm(1)-O(10)	78.82(9)
O(3)-Sm(1)-O(5)	145.02(10)	O(8)-Sm(1)-O(10)	49.33(9)
O(4)-Sm(1)-O(2)	79.68(9)	N(3)$^{\#1}$-Sm(1)-O(10)	118.58(9)
O(1)-Sm(1)-O(2)	51.36(8)	O(10)-Sm(1)-N(2)$^{\#1}$	75.52(10)
O(3)-Sm(1)-O(2)	94.76(10)	O(4)-Sm(1)-O(6)	68.05(11)
O(5)-Sm(1)-O(2)	67.84(9)	O(1)-Sm(1)-O(6)	159.81(9)
O(4)-Sm(1)-O(8)	133.39(10)	O(3)-Sm(1)-O(6)	123.83(10)
O(1)-Sm(1)-O(8)	113.71(10)	O(5)-Sm(1)-O(6)	46.88(9)
O(3)-Sm(1)-O(8)	137.09(9)	O(2)-Sm(1)-O(6)	110.58(9)
O(5)-Sm(1)-O(8)	75.04(9)	O(8)-Sm(1)-O(6)	65.75(10)
O(2)-Sm(1)-O(8)	122.41(10)	N(3)$^{\#1}$-Sm(1)-O(6)	66.53(9)
O(4)-Sm(1)-N(3)$^{\#1}$	83.45(10)	O(10)-Sm(1)-O(6)	101.14(11)
O(1)-Sm(1)-N(3)$^{\#1}$	133.54(9)	N(2)$^{\#1}$-Sm(1)-O(6)	121.32(9)
O(3)-Sm(1)-N(3)$^{\#1}$	74.69(10)	O(4)-Sm(1)-N(6)	151.90(10)
O(5)-Sm(1)-N(3)$^{\#1}$	113.12(9)	O(1)-Sm(1)-N(6)	90.08(11)
O(2)-Sm(1)-N(3)$^{\#1}$	162.52(10)	O(3)-Sm(1)-N(6)	137.89(9)
O(8)-Sm(1)-N(3)$^{\#1}$	73.14(10)	O(5)-Sm(1)-N(6)	76.87(9)
O(4)-Sm(1)-O(10)	150.39(10)	O(2)-Sm(1)-N(6)	102.59(10)
O(1)-Sm(1)-O(10)	68.80(11)	O(8)-Sm(1)-N(6)	24.68(9)

Complex **4**

Dy(1)-O(9)	2.518(6)	Dy(1)-O(7)	2.653(6)
Dy(1)-O(1)	2.552(5)	Dy(1)-O(6)	2.676(7)
Dy(1)-O(10)	2.599(6)	Dy(1)-N(1)$^{\#1}$	2.676(6)
Dy(1)-O(2)	2.635(6)	Dy(1)-N(3)$^{\#1}$	2.704(6)
Dy(1)-O(3)	2.640(6)		
O(9)-Dy(1)-O(1)	110.8(2)	O(9)-Dy(1)-N(3)$^{\#1}$	131.93(18)
O(9)-Dy(1)-O(10)	67.14(19)	O(1)-Dy(1)-N(3)$^{\#1}$	74.74(18)
O(1)-Dy(1)-O(10)	72.3(2)	O(10)-Dy(1)-N(3)$^{\#1}$	70.03(19)
O(9)-Dy(1)-O(2)	81.39(19)	O(2)-Dy(1)-N(3)$^{\#1}$	124.03(16)
O(1)-Dy(1)-O(2)	49.72(17)	O(3)-Dy(1)-N(3)$^{\#1}$	145.0(2)

O(10)-Dy(1)-O(2)	95.7(2)	O(10)-Dy(1)-N(1)#1	74.3(2)
O(9)-Dy(1)-O(3)	79.12(19)	O(2)-Dy(1)-N(1)#1	165.26(19)
O(1)-Dy(1)-O(3)	112.82(18)	O(3)-Dy(1)-N(1)#1	113.55(18)
O(10)-Dy(1)-O(3)	144.76(19)	O(7)-Dy(1)-N(1)#1	71.75(19)
O(2)-Dy(1)-O(3)	68.56(17)	O(6)-Dy(1)-N(1)#1	115.41(19)
O(9)-Dy(1)-O(7)	135.71(19)	O(7)-Dy(1)-N(3)#1	69.01(18)
O(1)-Dy(1)-O(7)	112.68(19)	O(6)-Dy(1)-N(3)#1	74.70(19)
O(10)-Dy(1)-O(7)	135.19(18)	N(1)#1-Dy(1)-N(3)#1	63.32(18)
O(2)-Dy(1)-O(7)	122.13(19)	O(9)-Dy(1)-O(5)	69.1(2)
O(3)-Dy(1)-O(7)	76.99(19)	O(1)-Dy(1)-O(5)	159.19(18)
O(9)-Dy(1)-O(6)	153.22(19)	O(10)-Dy(1)-O(5)	123.4(2)
O(1)-Dy(1)-O(6)	69.3(2)	O(2)-Dy(1)-O(5)	111.38(18)
O(10)-Dy(1)-O(6)	133.1(2)	O(3)-Dy(1)-O(5)	46.37(18)
O(2)-Dy(1)-O(6)	79.33(19)	O(7)-Dy(1)-O(5)	67.4(2)
O(3)-Dy(1)-O(6)	76.6(2)	O(6)-Dy(1)-O(5)	101.2(2)
O(7)-Dy(1)-O(6)	47.64(19)	N(1)#1-Dy(1)-O(5)	67.57(18)
O(9)-Dy(1)-N(1)#1	84.7(2)	N(3)#1-Dy(1)-O(5)	121.73(19)
O(1)-Dy(1)-N(1)#1	133.07(18)		

Complex **5**

Ho(1)-Ho(2)#1	3.7070(8)	Ho(2)-O(2)	2.397(7)
Ho(1)-Ho(2)	3.7221(8)	Ho(2)-O(3)	2.398(8)
Ho(1)-Ho(2)#2	3.7070(8)	Ho(2)-O(4)	2.398(8)
Ho(1)-O(5)#3	2.308(7)	Ho(2)-O(5)#2	2.356(7)
Ho(1)-O(5)	2.308(7)	Ho(2)-O(5)	2.391(7)
Ho(1)-O(6)	2.6846(8)	Ho(2)-O(6)	2.5674(5)
Ho(1)-O(7)#3	2.426(10)	Ho(2)-O(8)#3	2.362(8)
Ho(1)-O(7)	2.426(10)	Ho(2)-O(8)#2	2.372(8)
Ho(1)-O(8)#3	2.311(8)	O(2)-Ho(2)#1	2.451(7)
Ho(1)-O(8)	2.311(8)	O(5)-Ho(2)#1	2.356(7)
Ho(1)-O(9)#3	2.441(10)	O(6)-Ho(1)#2	2.6847(8)
Ho(1)-O(9)	2.441(10)	O(6)-Ho(2)#2	2.5673(5)
Ho(2)-Ho(1)#2	3.7071(8)	O(6)-Ho(2)#1	2.5674(5)

Ho(2)-Ho(2)$^{\#2}$	3.6308(7)	O(6)-Ho(2)$^{\#3}$	2.5673(5)
Ho(2)-Ho(2)$^{\#1}$	3.6308(7)	O(8)-Ho(2)$^{\#3}$	2.362(8)
Ho(2)-O(2)$^{\#2}$	2.451(7)	O(8)-Ho(2)$^{\#1}$	2.372(8)
Ho(2)$^{\#1}$-Ho(1)-Ho(2)	58.514(11)	Ho(2)$^{\#2}$-Ho(2)-Ho(1)$^{\#2}$	60.953(14)
Ho(2)$^{\#2}$-Ho(1)-Ho(2)$^{\#1}$	87.67(2)	Ho(2)$^{\#1}$-Ho(2)-Ho(1)$^{\#2}$	60.953(14)
Ho(2)$^{\#2}$-Ho(1)-Ho(2)	58.514(11)	Ho(2)$^{\#2}$-Ho(2)-Ho(2)$^{\#1}$	90.0
O(5)-Ho(1)-Ho(2)$^{\#1}$	37.81(18)	O(1)$^{\#2}$-Ho(2)-Ho(1)$^{\#2}$	111.4(2)
O(5)-Ho(1)-Ho(2)$^{\#2}$	93.51(18)	O(1)$^{\#2}$-Ho(2)-Ho(2)$^{\#2}$	74.51(18)
O(5)$^{\#3}$-Ho(1)-Ho(2)$^{\#2}$	37.81(18)	O(1)$^{\#2}$-Ho(2)-Ho(2)$^{\#1}$	164.36(18)
O(5)$^{\#3}$-Ho(1)-Ho(2)$^{\#1}$	93.51(18)	O(1)$^{\#2}$-Ho(2)-O(6)	119.49(18)
O(5)$^{\#3}$-Ho(1)-Ho(2)	92.99(19)	O(2)-Ho(2)-Ho(1)$^{\#2}$	108.4(2)
O(5)-Ho(1)-Ho(2)	38.4(17)	O(2)-Ho(2)-Ho(2)$^{\#2}$	162.17(17)
O(5)-Ho(1)-O(5)$^{\#3}$	119.3(4)	O(2)-Ho(2)-Ho(2)$^{\#1}$	72.17(17)
O(5)-Ho(1)-O(6)	59.66(19)	O(2)-Ho(2)-O(1)$^{\#2}$	123.3(2)
O(5)$^{\#3}$-Ho(1)-O(6)	59.66(19)	O(2)-Ho(2)-O(3)	72.8(3)
O(5)-Ho(1)-O(7)$^{\#3}$	142.5(3)	O(2)-Ho(2)-O(6)	117.17(17)
O(5)$^{\#3}$-Ho(1)-O(7)	142.5(3)	O(3)-Ho(2)-Ho(1)$^{\#2}$	87.8(2)
O(5)$^{\#3}$-Ho(1)-O(7)$^{\#3}$	79.6(3)	O(3)-Ho(2)-Ho(2)$^{\#1}$	120.9(2)
O(5)-Ho(1)-O(7)	79.6(3)	O(3)-Ho(2)-Ho(2)$^{\#2}$	118.5(2)
O(5)$^{\#3}$-Ho(1)-O(8)	75.1(3)	O(3)-Ho(2)-O(1)$^{\#2}$	70.1(3)
O(5)$^{\#3}$-Ho(1)-O(8)$^{\#3}$	75.1(3)	O(3)-Ho(2)-O(6)	134.2(2)
O(5)-Ho(1)-O(8)$^{\#3}$	75.1(3)	O(4)-Ho(2)-Ho(1)$^{\#2}$	176.7(2)
O(5)-Ho(1)-O(8)	75.1(3)	O(4)-Ho(2)-Ho(2)$^{\#2}$	119.4(2)
O(5)$^{\#3}$-Ho(1)-O(9)	79.0(3)	O(4)-Ho(2)-Ho(2)$^{\#1}$	115.8(2)
O(5)-Ho(1)-O(9)	142.3(3)	O(4)-Ho(2)-O(1)$^{\#2}$	71.6(3)
O(5)$^{\#3}$-Ho(1)-O(9)$^{\#3}$	142.3(3)	O(4)-Ho(2)-O(2)	70.4(3)
O(5)-Ho(1)-O(9)$^{\#3}$	79.1(3)	O(4)-Ho(2)-O(3)	94.7(3)
O(6)-Ho(1)-Ho(2)$^{\#1}$	43.834(12)	O(4)-Ho(2)-O(6)	131.2(2)
O(6)-Ho(1)-Ho(2)$^{\#2}$	43.834(12)	O(5)$^{\#2}$-Ho(2)-Ho(1)$^{\#2}$	36.92(18)
O(6)-Ho(1)-Ho(2)	43.610(12)	O(5)-Ho(2)-Ho(1)$^{\#2}$	97.05(18)
O(7)-Ho(1)-Ho(2)$^{\#1}$	83.5(3)	O(5)$^{\#2}$-Ho(2)-Ho(2)$^{\#1}$	94.52(18)
O(7)$^{\#3}$-Ho(1)-Ho(2)$^{\#1}$	171.2(3)	O(5)-Ho(2)-Ho(2)$^{\#1}$	39.74(18)

O(7)$^{\#3}$-Ho(1)-Ho(2)$^{\#2}$	83.5(3)	O(5)-Ho(2)-Ho(2)$^{\#2}$	94.08(18)
O(7)-Ho(1)-Ho(2)	116.2(3)	O(5)$^{\#2}$-Ho(2)-Ho(2)$^{\#2}$	40.46(18)
O(7)$^{\#3}$-Ho(1)-Ho(2)	115.9(3)	O(5)-Ho(2)-O(1)$^{\#2}$	137.4(3)
O(7)-Ho(1)-Ho(2)$^{\#2}$	171.4(3)	O(5)$^{\#2}$-Ho(2)-O(1)$^{\#2}$	75.2(3)
O(7)-Ho(1)-O(6)	127.3(3)	O(5)$^{\#2}$-Ho(2)-O(2)	138.7(3)
O(7)$^{\#3}$-Ho(1)-O(6)	127.3(3)	O(5)-Ho(2)-O(2)	72.2(3)
O(7)-Ho(1)-O(7)$^{\#3}$	105.3(6)	O(5)$^{\#2}$-Ho(2)-O(3)	82.0(3)
O(7)$^{\#3}$-Ho(1)-O(9)$^{\#3}$	69.0(4)	O(5)-Ho(2)-O(3)	144.6(3)
O(7)-Ho(1)-O(9)	69.0(4)	O(5)$^{\#2}$-Ho(2)-O(4)	145.6(3)
O(7)$^{\#3}$-Ho(1)-O(9)	68.7(4)	O(5)-Ho(2)-O(4)	79.7(3)
O(7)-Ho(1)-O(9)$^{\#3}$	68.7(4)	O(5)$^{\#2}$-Ho(2)-O(5)	121.6(3)
O(8)$^{\#3}$-Ho(1)-Ho(2)$^{\#2}$	38.2(2)	O(5)-Ho(2)-O(6)	60.56(18)
O(8)$^{\#3}$-Ho(1)-Ho(2)	37.66(19)	O(5)$^{\#2}$-Ho(2)-O(6)	60.99(17)
O(8)-Ho(1)-Ho(2)$^{\#1}$	38.2(2)	O(5)$^{\#2}$-Ho(2)-O(8)$^{\#2}$	73.1(3)
O(8)$^{\#3}$-Ho(1)-Ho(2)$^{\#1}$	92.9(2)	O(5)$^{\#2}$-Ho(2)-O(8)$^{\#3}$	79.8(3)
O(8)-Ho(1)-Ho(2)	93.2(2)	O(6)-Ho(2)-Ho(1)$^{\#2}$	46.402(12)
O(8)-Ho(1)-Ho(2)$^{\#2}$	92.9(2)	O(6)-Ho(2)-Ho(2)$^{\#1}$	45.0
O(8)-Ho(1)-O(6)	59.4(2)	O(6)-Ho(2)-Ho(2)$^{\#2}$	45.0
O(8)$^{\#3}$-Ho(1)-O(6)	59.4(2)	O(8)$^{\#3}$-Ho(2)-Ho(1)$^{\#2}$	97.3(2)
O(8)-Ho(1)-O(7)$^{\#3}$	142.3(3)	O(8)$^{\#2}$-Ho(2)-Ho(1)$^{\#2}$	37.1(19)
O(8)$^{\#3}$-Ho(1)-O(7)$^{\#3}$	80.2(4)	O(8)$^{\#2}$-Ho(2)-Ho(2)$^{\#2}$	94.44(19)
O(8)$^{\#3}$-Ho(1)-O(7)	142.1(3)	O(8)$^{\#2}$-Ho(2)-Ho(2)$^{\#1}$	39.8(19)
O(8)-Ho(1)-O(7)	80.0(4)	O(8)$^{\#3}$-Ho(2)-Ho(2)$^{\#1}$	94.01(19)
O(8)$^{\#3}$-Ho(1)-O(8)	118.8(4)	O(8)$^{\#3}$-Ho(2)-Ho(2)$^{\#2}$	40.1(2)
O(8)-Ho(1)-O(9)	79.3(4)	O(8)$^{\#2}$-Ho(2)-O(1)$^{\#2}$	141.6(3)
O(8)-Ho(1)-O(9)$^{\#3}$	142.4(3)	O(8)$^{\#3}$-Ho(2)-O(1)$^{\#2}$	72.8(3)
O(8)$^{\#3}$-Ho(1)-O(9)	142.4(3)	O(8)$^{\#3}$-Ho(2)-O(2)	138.5(3)
O(8)$^{\#3}$-Ho(1)-O(9)$^{\#3}$	79.3(4)	O(8)$^{\#2}$-Ho(2)-O(2)	72.1(3)
O(9)$^{\#3}$-Ho(1)-Ho(2)$^{\#2}$	115.7(3)	O(8)$^{\#3}$-Ho(2)-O(3)	141.8(3)
O(9)$^{\#3}$-Ho(1)-Ho(2)$^{\#1}$	115.2(3)	O(8)$^{\#2}$-Ho(2)-O(3)	84.5(3)
O(9)-Ho(1)-Ho(2)$^{\#1}$	115.8(3)	O(8)$^{\#3}$-Ho(2)-O(4)	82.2(3)
O(9)-Ho(1)-Ho(2)$^{\#2}$	115.2(3)	O(8)$^{\#2}$-Ho(2)-O(4)	140.9(3)

O(9)-Ho(1)-Ho(2)	170.3(3)	O(8)#3-Ho(2)-O(5)	72.6(2)
O(9)#3-Ho(1)-Ho(2)	83.1(3)	O(8)#2-Ho(2)-O(5)	78.9(3)
O(9)-Ho(1)-O(6)	126.7(3)	O(8)#2-Ho(2)-O(6)	60.57(19)
O(9)#3-Ho(1)-O(6)	126.7(3)	O(8)#3-Ho(2)-O(6)	60.69(19)
O(9)-Ho(1)-O(9)#3	106.7(6)	O(8)#3-Ho(2)-O(8)#2	121.3(4)

Complex **6**

Er(1)-O(5)#2	2.312(8)	Er(2)-O(3)	2.378(8)
Er(1)-O(5)	2.311(8)	Er(2)-O(4)	2.378(8)
Er(1)-O(8)#2	2.321(8)	Er(2)-O(8)	2.400(8)
Er(1)-O(8)	2.321(8)	Er(2)-O(1)#3	2.413(7)
Er(1)-O(9)#2	2.417(9)	Er(2)-O(6)	2.5978(5)
Er(1)-O(9)	2.417(9)	Er(2)-Er(2)#1	3.6739(7)
Er(1)-O(7)	2.437(9)	Er(2)-Er(2)#3	3.6739(7)
Er(1)-O(7)#2	2.437(9)	Er(2)-Er(1)#3	3.7458(8)
Er(1)-O(6)	2.7111(8)	O(1)-Er(2)#1	2.413(7)
Er(1)-Er(2)#2	3.7639(9)	O(5)-Er(2)#3	2.380(8)
Er(1)-Er(2)#3	3.7458(9)	O(6)-Er(2)#3	2.5978(5)
Er(1)-Er(2)#1	3.7458(9)	O(6)-Er(2)#2	2.5978(5)
Er(2)-O(8)#3	2.358(8)	O(6)-Er(2)#1	2.5978(5)
Er(2)-O(5)	2.352(9)	O(6)-Er(1)#3	2.7111(8)
Er(2)-O(5)#1	2.380(8)	O(8)-Er(2)#1	2.358(8)
Er(2)-O(2)	2.372(7)		
O(5)-Er(1)-O(5)#3	116.0(4)	O(8)#1-Er(2)-O(4)	83.1(3)
O(5)#3-Er(1)-O(8)	74.3(3)	O(8)#1-Er(2)-O(5)#2	72.3(2)
O(5)-Er(1)-O(8)#3	74.3(3)	O(5)-Er(2)-O(5)#2	118.3(4)
O(5)#3-Er(1)-O(8)#3	73.7(3)	O(8)#1-Er(2)-O(2)	138.3(3)
O(5)-Er(1)-O(8)	73.7(3)	O(5)-Er(2)-O(2)	138.6(3)
O(8) -Er(1)-O(8)#3	117.3(4)	Er(2)#2-O(8)-Er(2)	101.1(3)
O(5)#3-Er(1)-O(9)#3	142.4(3)	O(8)#1-Er(2)-O(3)	145.5(3)
O(5)#3-Er(1)-O(9)	81.3(3)	O(5)-Er(2)-O(3)	82.3(3)
O(8)#3-Er(1)-O(9)#3	80.3(3)	Er(1)-O(8)-Er(2)#2	106.4(3)
O(8)-Er(1)-O(9)#3	143.0(3)	O(2)-Er(2)-O(3)	71.8(3)

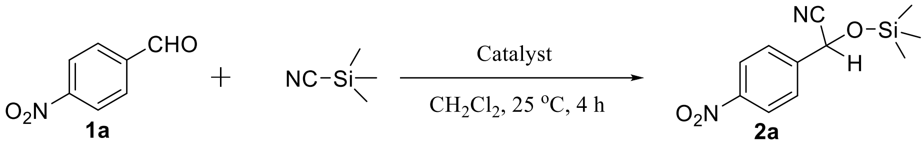
O(5) -Er(1)-O(9)#3	81.3(3)	Er(1)-O(8)-Er(2)	105.7(3)
O(5)-Er(1)-O(9)	142.4(3)	O(5)-Er(2)-O(4)	143.9(3)
O(8)#3-Er(1)-O(9)	143.0(3)	O(5)#2-Er(2)-O(8)	77.4(2)
O(8)-Er(1)-O(9)	80.3(3)	O(2)-Er(2)-O(4)	72.2(3)
O(9)-Er(1)-O(9)#3	105.5(5)	Er(2)-O(6)-Er(2)#2	90.0
O(5)#3-Er(1)-O(7)	144.0(3)	O(8)#1-Er(2)-O(8)	119.6(4)
O(5)-Er(1)-O(7)#3	144.0(3)	O(5)-Er(2)-O(8)	71.6(2)
O(8)#3-Er(1)-O(7)	141.4(3)	O(5)-Er(2)-O(8)#1	78.8(2)
O(8)-Er(1)-O(7)	79.3(3)	O(2)-Er(2)-O(8)	72.6(3)
O(9)#3-Er(1)-O(7)	69.0(3)	O(3)-Er(2)-O(8)	80.5(3)
O(9)-Er(1)-O(7)	70.3(4)	O(4)-Er(2)-O(8)	144.0(3)
O(5)-Er(1)-O(7)	78.5(3)	O(8)#1-Er(2)-O(1)#1	75.3(3)
O(5)#3-Er(1)-O(7)#3	78.5(3)	O(5)-Er(2)-O(1)#1	73.7(3)
O(8)#3-Er(1)-O(7)#3	79.3(3)	O(5)#2-Er(2)-O(1)#1	141.8(3)
O(8)-Er(1)-O(7)#3	141.4(3)	O(2)-Er(2)-O(1)#1	124.5(2)
O(9)#3-Er(1)-O(7)#3	70.3(4)	O(3)-Er(2)-O(1)#1	71.7(3)
O(9)-Er(1)-O(7)#3	69.0(3)	O(4)-Er(2)-O(1)#1	71.5(3)
O(7)#3-Er(1)-O(7)	109.9(5)	O(8)-Er(2)-O(1)#1	137.8(3)
O(5)#3-Er(1)-O(6)	58.0(2)	O(8)#1-Er(2)-O(6)	60.06(19)
O(5)-Er(1)-O(6)	58.0(2)	O(5)-Er(2)-O(6)	59.3(2)
O(8)#3-Er(1)-O(6)	58.7(2)	O(5)#2-Er(2)-O(6)	59.0(2)
O(8)-Er(1)-O(6)	58.7(2)	O(2)-Er(2)-O(6)	116.44(18)
O(9)#3-Er(1)-O(6)	127.3(2)	O(3)-Er(2)-O(6)	130.6(2)
O(9)-Er(1)-O(6)	127.3(2)	O(4)-Er(2)-O(6)	133.6(2)
O(7)-Er(1)-O(6)	125.0(2)	O(8)-Er(2)-O(6)	59.58(19)
O(7)#3-Er(1)-O(6)	125.0(2)	O(1)#1-Er(2)-O(6)	119.01(18)
O(5)#3-Er(1)-Er(2)#2	37.7(2)	O(8)#1-Er(2)-Er(2)#1	39.86(19)
O(5)-Er(1)-Er(2)#2	91.6(2)	O(5)-Er(2)-Er(2)#1	39.34(19)
O(8)#3-Er(1)-Er(2)#2	92.7(2)	O(5)#2-Er(2)-Er(2)#2	38.8(2)
O(8)-Er(1)-Er(2)#2	37.15(19)	O(2)-Er(2)-Er(2)#1	161.44(18)
O(9)#3-Er(1)-Er(2)#2	171.2(2)	O(3)-Er(2)-Er(2)#2	115.9(2)
O(9)-Er(1)-Er(2)#2	83.3(2)	O(4)-Er(2)-Er(2)#1	119.0(2)

O(7)-Er(1)-Er(2)$^{\#2}$	114.9(2)	O(8)-Er(2)-Er(2)$^{\#1}$	93.24(19)
O(7)$^{\#3}$-Er(1)-Er(2)$^{\#2}$	113.9(2)	O(1)$^{\#1}$-Er(2)-Er(2)$^{\#1}$	74.03(18)
O(6)-Er(1)-Er(2)$^{\#2}$	43.909(13)	O(6)-Er(2)-Er(2)$^{\#1}$	46.367(13)
O(5)$^{\#3}$-Er(1)-Er(2)$^{\#3}$	36.5(2)	O(8)$^{\#1}$-Er(2)-Er(2)$^{\#}$	93.79(19)
O(5)-Er(1)-Er(2)$^{\#3}$	92.1(2)	O(5)-Er(2)-Er(2)$^{\#2}$	92.7(2)
O(8)$^{\#3}$-Er(1)-Er(2)$^{\#3}$	37.85(19)	O(5)$^{\#2}$-Er(2)-Er(2)$^{\#1}$	93.2(2)
O(8)-Er(1)-Er(2)$^{\#3}$	92.1(2)	O(2)-Er(2)-Er(2)$^{\#2}$	71.44(18)
O(9)$^{\#3}$-Er(1)-Er(2)$^{\#3}$	116.1(2)	O(3)-Er(2)-Er(2)$^{\#1}$	118.5(2)
O(9)-Er(1)-Er(2)$^{\#3}$	115.9(3)	O(4)-Er(2)-Er(2)$^{\#2}$	119.6(2)
O(7)-Er(1)-Er(2)$^{\#3}$	168.7(2)	O(8)-Er(2)-Er(2)$^{\#2}$	39.03(19)
O(7)$^{\#3}$-Er(1)-Er(2)$^{\#3}$	81.4(2)	O(1)$^{\#1}$-Er(2)-Er(2)$^{\#2}$	163.90(18)
O(6)-Er(1)-Er(2)$^{\#3}$	43.645(13)	Er(2)$^{\#2}$-O(6)-Er(2)$^{\#1}$	179.45(3)
Er(2)$^{\#1}$-Er(1)-Er(2)$^{\#2}$	87.82(3)	Er(2)$^{\#1}$-Er(2)-Er(2)$^{\#2}$	90.0
O(5)$^{\#3}$-Er(1)-Er(2)$^{\#1}$	91.6(2)	O(8)$^{\#1}$-Er(2)-Er(1)$^{\#1}$	36.49(19)
O(5)-Er(1)-Er(2)$^{\#1}$	37.7(2)	O(5)-Er(2)-Er(1)$^{\#1}$	96.2(2)
O(8)$^{\#3}$-Er(1)-Er(2)$^{\#1}$	37.15(19)	O(5)$^{\#2}$-Er(2)-Er(1)$^{\#1}$	36.4(2)
O(8)-Er(1)-Er(2)$^{\#1}$	92.7(2)	O(2)-Er(2)-Er(1)$^{\#1}$	107.7(2)
O(9)$^{\#3}$-Er(1)-Er(2)$^{\#1}$	83.3(2)	O(3)-Er(2)-Er(1)$^{\#1}$	176.5(2)
O(9)-Er(1)-Er(2)$^{\#1}$	171.2(2)	O(4)-Er(2)-Er(1)$^{\#1}$	87.2(2)
O(7)-Er(1)-Er(2)$^{\#1}$	113.9(2)	O(8)-Er(2)-Er(1)$^{\#1}$	96.10(19)
O(7)$^{\#3}$-Er(1)-Er(2)$^{\#1}$	114.9(2)	O(1)$^{\#1}$-Er(2)-Er(1)$^{\#1}$	110.9(2)
O(6)-Er(1)-Er(2)$^{\#1}$	43.909(13)	Er(2)$^{\#1}$-O(6)-Er(2)$^{\#3}$	90.0
Er(2)$^{\#1}$-Er(1)-Er(2)$^{\#3}$	58.579(12)	Er(2)$^{\#1}$-Er(2)-Er(1)$^{\#1}$	60.957(15)
Er(2)$^{\#2}$-Er(1)-Er(2)$^{\#3}$	58.579(12)	Er(2)$^{\#2}$-Er(2)-Er(1)$^{\#1}$	60.957(15)
O(2)-Er(2)-O(5)$^{\#2}$	72.4(3)	O(3)-Er(2)-O(5)$^{\#2}$	142.1(3)
O(4)-Er(2)-O(3)	95.9(3)	O(4)-Er(2)-O(5)$^{\#2}$	84.7(3)
O(6)-Er(2)-Er(2)$^{\#1}$	45	O(6)-Er(2)-Er(2)$^{\#2}$	45
Er(1)-O(5)-Er(2)	107.6(3)	Er(1)-O(5)-Er(2)$^{\#1}$	106.0(3)
Er(2)-O(5)-Er(2)$^{\#1}$	101.9(3)	Er(1)-O(6)-Er(1)$^{\#1}$	180.0
Er(2)$^{\#2}$-O(6)-Er(1)	89.724(15)	Er(2)$^{\#1}$-O(6)-Er(1)	89.724(15)
Er(2)$^{\#2}$-O(6)-Er(1)$^{\#1}$	90.276(15)	Er(2)$^{\#3}$-O(6)-Er(1)	90.276(15)
Er(2)$^{\#1}$-O(6)-Er(1)$^{\#1}$	90.276(15)	Er(2)-O(6)-Er(1)	90.277(15)

Er(2)-O(6)-Er(1)♯1	89.723(15)	Er(2)♯3-O(6)-Er(1)♯1	89.724(15)
Er(2)-O(6)-Er(2)♯1	90.0	Er(2)♯2-O(6)-Er(2)♯3	90.0
Er(2)-O(6)-Er(2)♯3	179.45(3)		

for **1**: ♯1 -y+1, x-y, z; ♯2 -x+y+1, -x+1, z; ♯3 -y+1, x-y+1, z; ♯4 -y+1, x-y, -z+1/2; ♯5 -x+y+1, -x+1, -z+1/2; ♯6 x, y, -z+1/2; ♯7 -x+y, -x+1, -z+1/2; ♯8 -x+y, -x+1, z; for **2**: ♯1 -x+y+1, -x+1, z ♯2 -y+1, x-y, z; ♯3 -x+y+1, -x+2, z; ♯4 -x+y+1, -x+1, -z+1/2; ♯5 -y+1, x-y, -z+1/2; ♯6 x, y, -z+1/2; ♯7 -x+y+2, -x+2, -z+1/2; ♯8 -y+2, x-y+1, z; for **3**: ♯1 -x+y+1, -x+1, z; ♯2 -y+1, x-y, z; ♯3 -x+y+1, -x+2,z; ♯4 -x+y+1, -x+1, -z+1/2; ♯5 x, y, -z+1/2; ♯6 -y+1, x-y, -z+1/2; ♯7 -x+y+2, -x+2, -z+1/2; ♯8 -y+2, x-y+1, z; for **4**: ♯1 -x+y, -x+1, z; ♯2 -y+1, x-y+1, z; ♯3 -y+1, x-y, z; ♯4 x, y, -z+1/2; ♯5 -y+1, x-y+1, -z+1/2; for **5**: ♯1 5/4-y, -3/4+x, 5/4-z; ♯2 3/4+y, 5/4-x, 5/4-z; ♯3 2-x, 1/2-y, +z; for **6**: ♯1 -y+5/4, x-3/4, -z+5/4; ♯2-x+2, -y+1/2, z; ♯3 y+3/4, -x+5/4, -z+5/4.

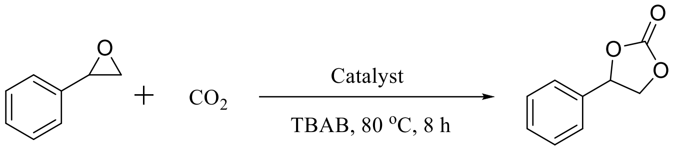
Table S3. 4-nitrobenzaldehyde cyanosilylation with TMSCN into the corresponding cyanohydrin product.[a]



Entry	Cat.	Cat. (mol%)	Solvent	Time (h)	Yield (%)[b]
1	**4**	1	CH_2Cl_2	4	92
2	**4**	1	$CHCl_3$	4	40
3	**4**	1	CH_3CN	4	52
4	**4**	1	toluene	4	22
5	**4**	0.25	CH_2Cl_2	4	58
6	**4**	0.5	CH_2Cl_2	4	76
7	**4**	2	CH_2Cl_2	4	92
8	**4**	1	CH_2Cl_2	1	33
9	**4**	1	CH_2Cl_2	2	62
10	**4**	1	CH_2Cl_2	3	78
11	**4**	1	CH_2Cl_2	5	92
12	-	-	CH_2Cl_2	4	15
13	$Dy(NO_3)_3·5H_2O$	1	CH_2Cl_2	4	9
14	H**L**¹	1	CH_2Cl_2	4	11
15	$Dy(NO_3)_3·5H_2O$+ H**L**¹	1	CH_2Cl_2	4	17
16	**1**	1	CH_2Cl_2	4	79
17	**2**	1	CH_2Cl_2	4	83
18	**3**	1	CH_2Cl_2	4	85
19	**5**	1	CH_2Cl_2	4	76
20	**6**	1	CH_2Cl_2	4	71

[a] Reaction conditions: substrates (0.5 mmol), TMSCN (1 mmol), 25 ºC, catalyst (0-2 mol%), solvent (2 mL).
[b] Isolated yield.

Table S4. Optimization of catalytic reaction conditions for the conversion of CO_2 with styrene oxide. [a]

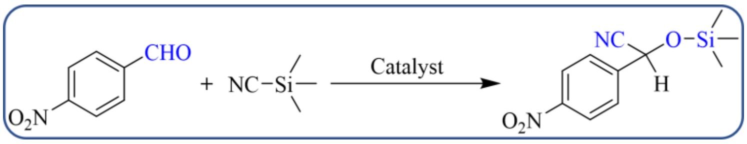


3a 4a

Entry	Cat.	Cat. (mol%)	TBAB (mol%)	Temp (°C)	Time (h)	Yield (%) [b]
1	Complex **6**	0.1	3	80	8	46
2	Complex **6**	0.3	3	80	8	74
3	Complex **6**	0.5	3	80	8	92
4	Complex **6**	1	3	80	8	92
5	Complex **6**	0.5	3	40	8	21
6	Complex **6**	0.5	3	60	8	53
7	Complex **6**	0.5	3	80	4	42
8	Complex **6**	0.5	3	80	6	76
9	Complex **6**	0.5	3	80	10	91
10[c]	Complex **6**	0.5	3	80	8	22
11[d]	Complex **6**	0.5	3	80	8	28
12[e]	Complex **6**	0.5	3	80	8	32
13	-	-	-	80	8	0
14	TBAB	-	3	80	8	15
15	Complex **6**	0.5	-	80	8	16
16	$ErCl_3 \cdot 6H_2O$	0.5	3	80	8	22
17	H**L**¹	0.5	3	80	8	10
18	Complex **1**	0.5	3	80	8	76
19	Complex **2**	0.5	3	80	8	78
20	Complex **3**	0.5	3	80	8	82
21	Complex **4**	0.5	3	80	8	85
22	Complex **5**	0.5	3	80	8	87

[a] Reaction conditions: substrates (10.0 mmol), solvent-free (entries 1-9, 13-22), CO_2 (0.1 MPa), temperature (40-80 °C), catalyst (0-0.5 mol%), TBAB (0-3.0 mol%). [b] Isolated yield. [c] CH_3OH as solvent. [d] CH_3CH_2OH as solvent. [e] CH_3CN as solvent.

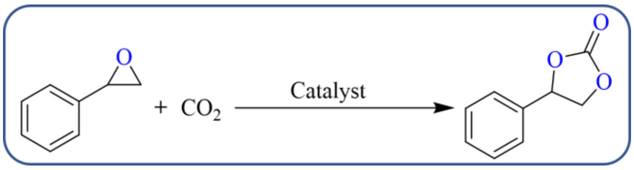
Table S5. Comparisons of the catalytic activity of various complex **4** for the cyanosilylation reaction.



Catalyst	Amount of catalysts (mol%)	atmosphere	Temp. (°C)	Time (h)	Yield (%)	Ref.
$Zn_{0.29}$-STU-2	15 mg	N_2	R.T.	12	88	[1]
Compound 8	3.0	air	35	10	99	[2]
Compound 3	4.0	air	R.T.	3	83	[3]
[Co(Hamda)(μ-Hamda)(μ-dpey)$_{0.5}$]$_n$·nH_2O	4.0	air	35	10	99	[4]
[Zn(μ-1κO^1:1κO^2-L)(H_2O)$_2$]$_n$·n(H_2O)	2.0	air	50 [a]	1.5	99	[5]
[{Cu(L^a)}$_2$(μ-L^5)$_2$]$_n$	4.0	air	R.T.	8	90	[6]
[Zn(L)(DMF)$_2$]$_n$	2.0	air	R.T.	10	81	[7]
[PbMn$_{0.5}$(L)(H_2O)]$_n$	4.0	N_2	40	6	99	[8]
Zn(H_2L^2)]$_2$	1.0	air	R.T.	12	92	[9]
Ag_7Ti_4	0.15	air	60	1.1	99	[10]
V-Zn-MOF	2.0	N_2	60	3	99	[11]
Complex **4**	**1.0**	**air**	**R.T.**	**4**	**92**	**This work**

[a] A combination of 4-nitrobenzaldehyde, trimethylsilyl cyanide and catalyst was placed in a Pyrex tube covered with a Teflon cap and stirred at 50 °C, under microwave irradiation (5 W), for 1.5 h, under solvent-free conditions.

Table S6. Comparisons of the catalytic activity of various complex **6** for the cycloaddition of CO_2 with styrene oxide.



Catalyst	Amount of catalysts (mol%)	Amount of TBAB (mol%)	CO_2 Pres. (MPa)	Temp. (°C)	Time (h)	Yield (%)	Ref.
ADES-3	2.0	2.5	1	80	8	99	[12]
$[Al(HL')(H_2O)_3](H_2O)_2Cl$	0.5	0.5	1	60	24	39	[13]
ZnMOF-1-NH_2	1.0	2.4	0.8	80	8	88	[14]
JLU-MOF200	0.5	5	2	60	6	58	[15]
$Zn_7(L_3)(H_2O)_5(NO_3)_2$	0.2	2.5	1	25	24	63	[16]
HE-LnMOF	0.5	0.5	1.2	100	6	81	[17]
NUC-30	1.0	5	1	60	12	92	[18]
MOF-1a	1.0	5	1	50	12	87	[19]
Zn-URJC-8	1.5	5	1.2	25	24	58	[20]
Cd-CP-1a	0.61	5	0.1	70	16	95	[21]
CP 4	0.5	3	0.1	45	10	44	[22]
Fe_3-MOF	0.4	5	0.1	80	12	99	[23]
Hie-Zn-MOF-TEA	0.5	2.2	1	25	16	77	[24]
Complex **6**	**0.5**	**3**	**0.1**	**80**	**8**	**92**	**This work**

Table S7. The content of metal ions tested by inductively coupled plasma-opticalemission spectroscopy.

Metallic element	Concentration (mg/L)
Dy(III)	0.038
Er(III)	0.052

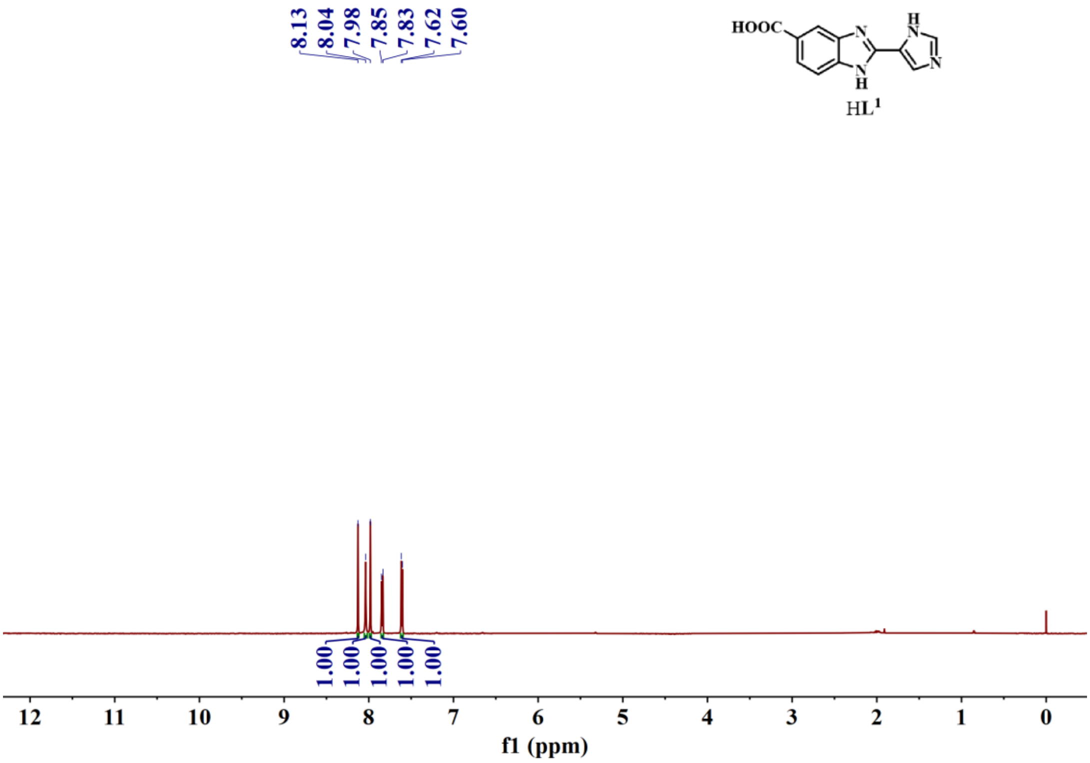


Fig. S1. ^{1}H NMR of H**L**$^{\mathbf{1}}$.

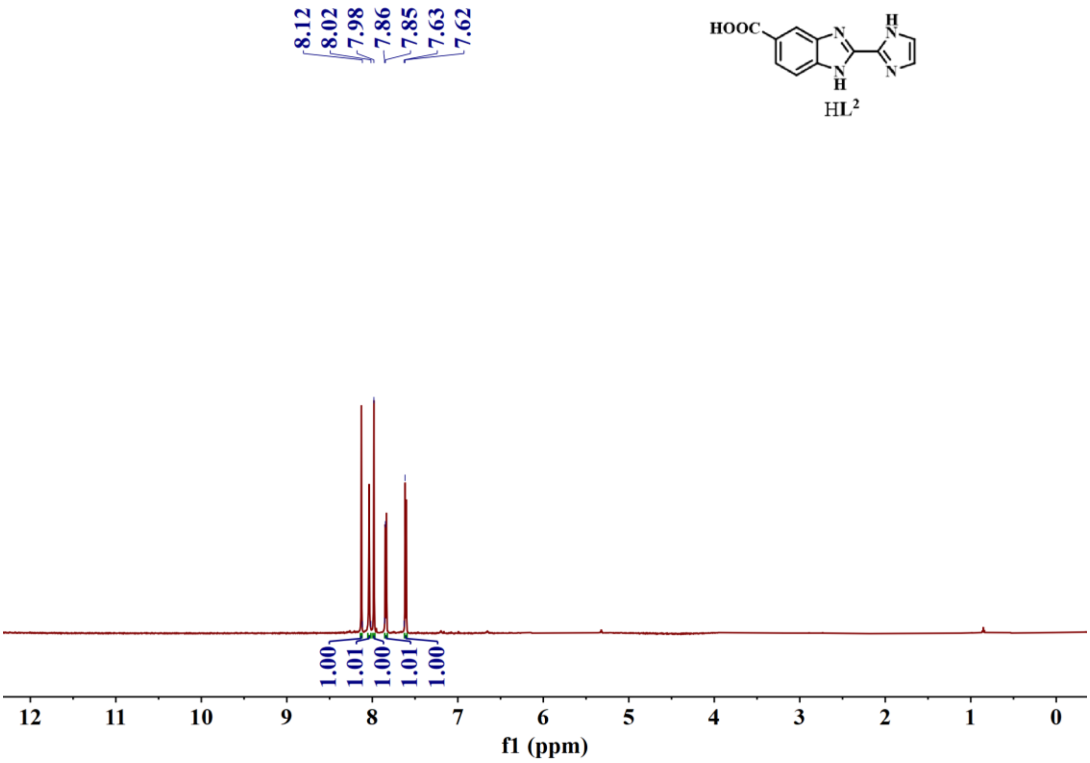


Fig. S2. ^{1}H NMR of H**L**$^{\mathbf{2}}$.

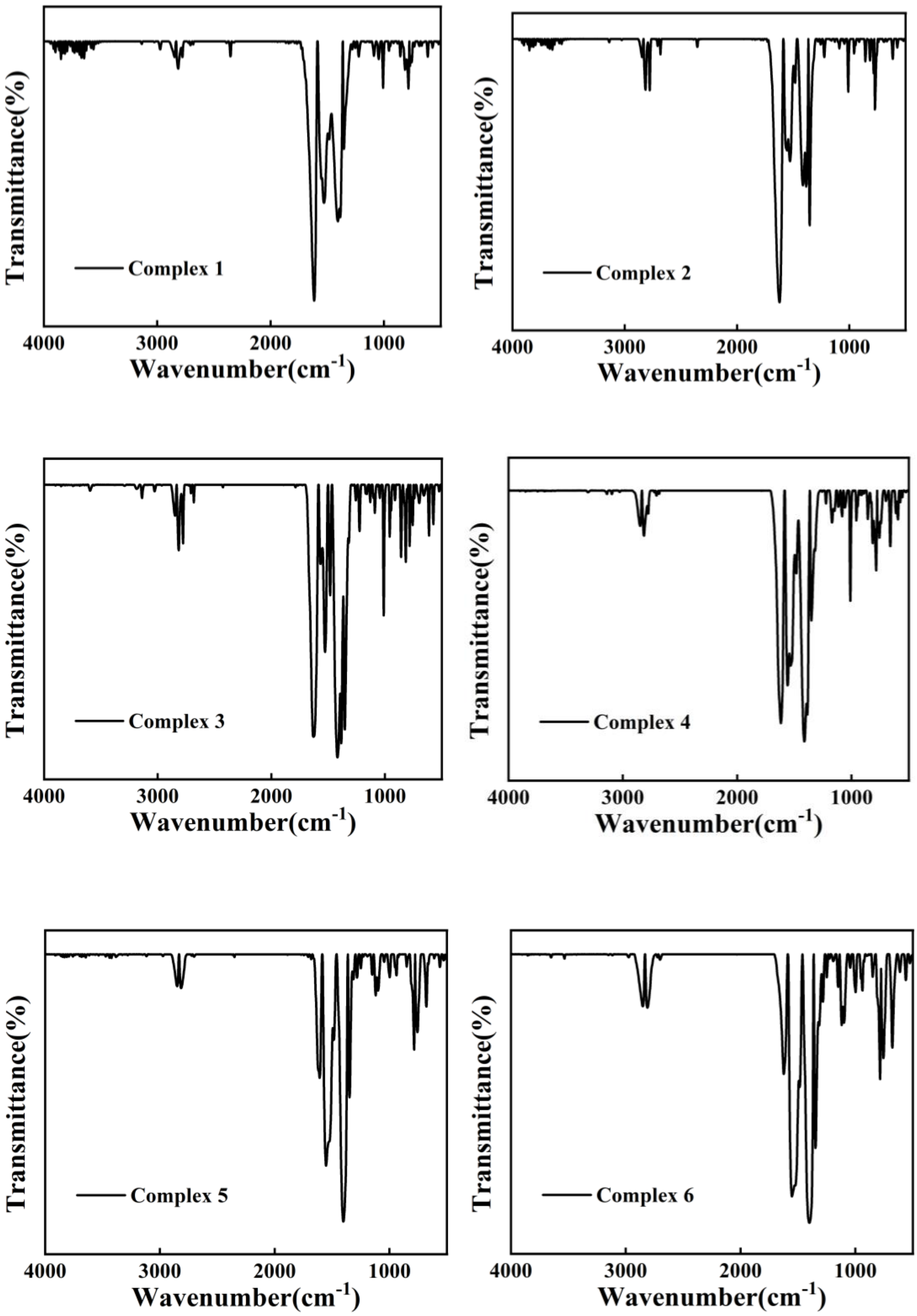


Fig. S3. IR patterns of complexes **1-6**.

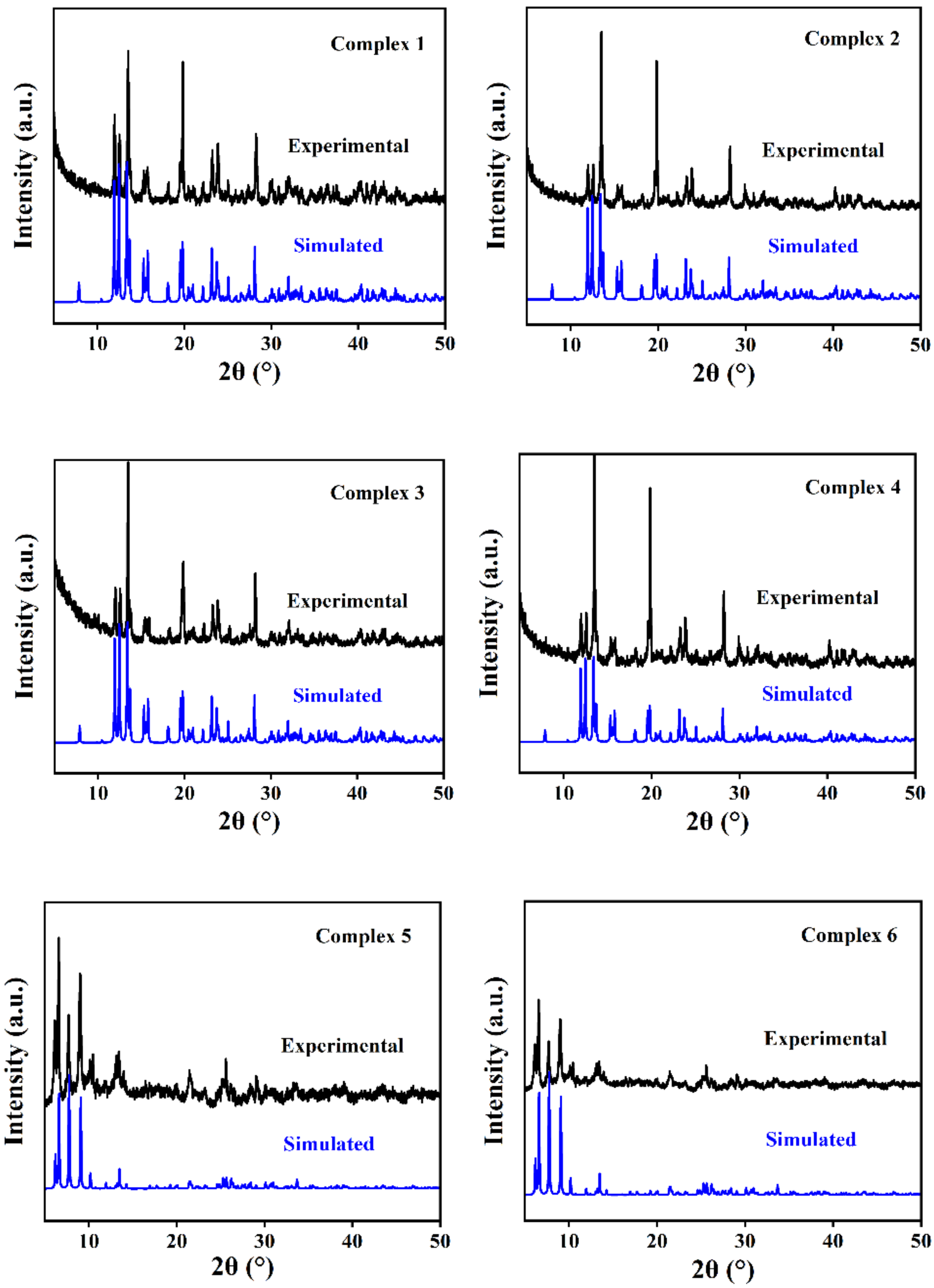


Fig. S4. PXRD spectra of complexes **1-6**.

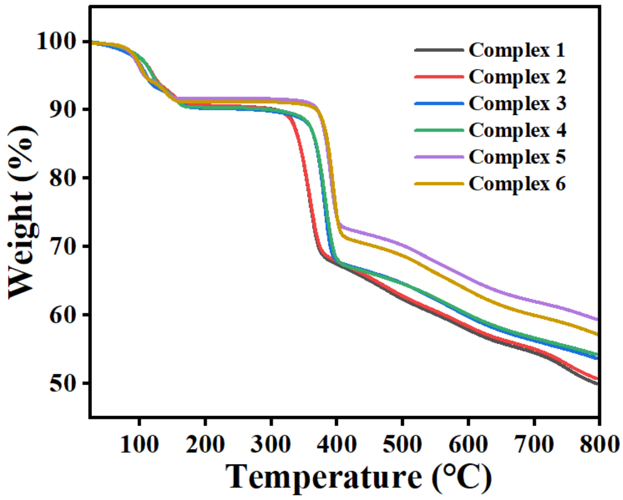


Fig. S5. TGA curves of complexes 1-6.

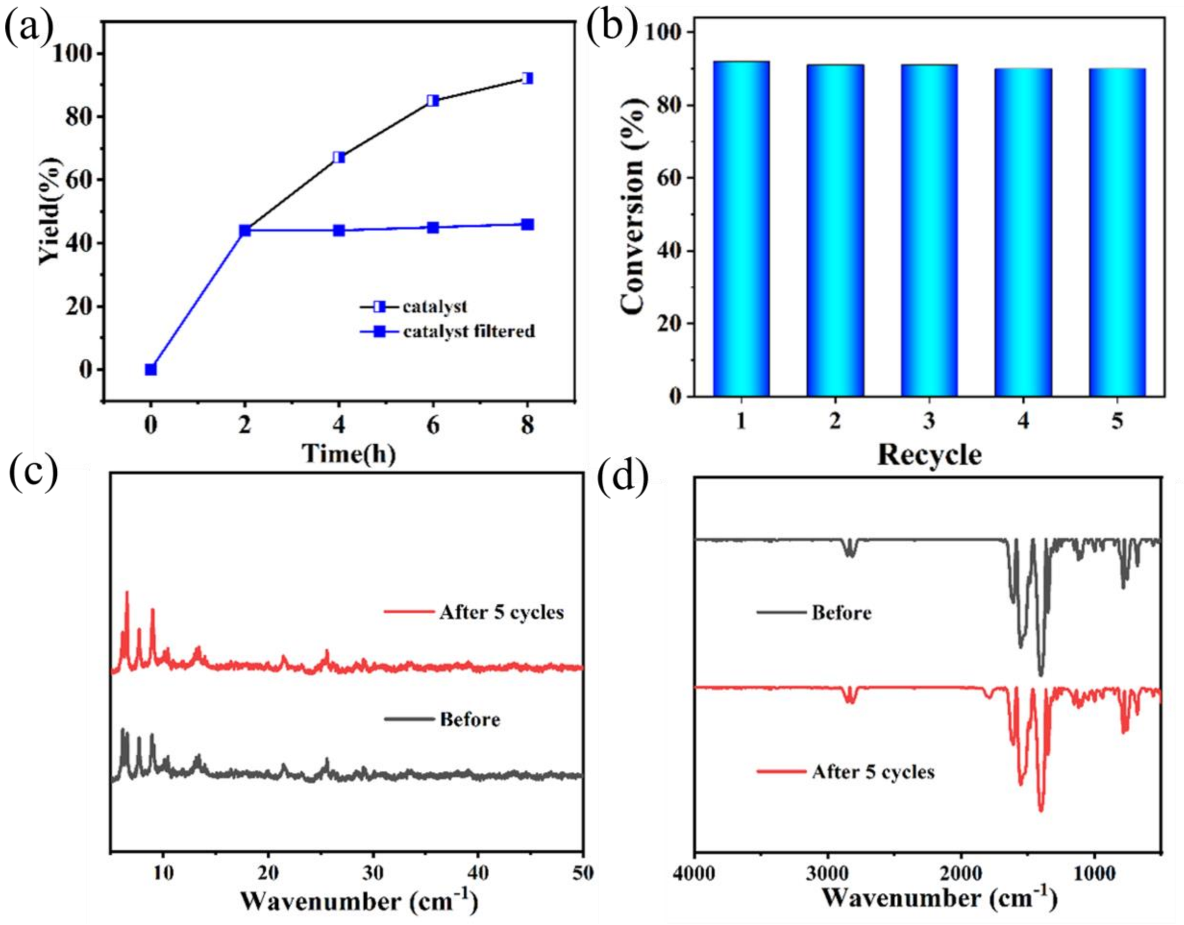


Fig. S6. (a) Thermal filtration experiment of complex **6**; (b) Cycle experiment; (c) PXRD of complex **6** after 5 cycles; (d) IR spectra of complex **6** after 5 cycles.

NMR data description

2-(1*H*-imidazol-5-yl)-1*H*-benzo[d]imidazole-5-carboxylic acid (HL^1)

^{1}H NMR (600 MHz, DMSO-d_6) δ 8.13 (s, 1H), 8.04 (s, 1H), 7.98 (s, 1H), 7.84 (d, *J* = 10.0 Hz, 1H), 7.61 (d, *J* = 8.4 Hz, 1H).

2-(1*H*-imidazol-2-yl)-1*H*-benzo[d]imidazole-5-carboxylic acid (HL^2)

^{1}H NMR (600 MHz, DMSO-d_6) δ 8.13 (d, *J* = 1.5 Hz, 1H), 8.02 (s, 1H), 7.98 (s, 1H), 7.85 (s, 1H), 7.62 (s, 1H).

2-(4-nitrophenyl)-2-((trimethylsilyl)oxy)acetonitrile (2a) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.2 Hz, 2H), 7.61 (d, *J* = 8.1 Hz, 2H), 5.54 (s, 1H), 0.28 (s, 9H).

2-(2-nitrophenyl)-2-((trimethylsilyl)oxy)acetonitrile (2b) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.17 (d, *J* = 8.2 Hz, 1H), 8.02 (d, *J* = 7.9 Hz, 1H), 7.77 (t, *J* = 7.7 Hz, 1H), 7.60 (t, *J* = 7.9 Hz, 1H), 6.22 (s, 1H), 0.29 (s, 9H).

2-(3-nitrophenyl)-2-((trimethylsilyl)oxy)acetonitrile (2c) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 8.34 (s, 1H), 8.25 (d, *J* = 9.3 Hz, 1H), 7.83 (d, *J* = 9.6 Hz, 1H), 7.63 (t, *J* = 8.0 Hz, 1H), 5.62 (s, 1H), 0.28 (s, 9H).

4-(cyano((trimethylsilyl)oxy)methyl)benzonitrile (2d) [25]

^{1}H NMR (600 MHz, Chloroform-*d*) δ 7.67 – 7.65 (m, 2H), 7.55 – 7.53 (m, 2H), 5.48 (s, 1H), 0.20 (s, 9H).

2-(4-fluorophenyl)-2-((trimethylsilyl)oxy)acetonitrile (2e) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 8.8, 5.2 Hz, 2H), 7.11 (t, *J* = 8.6 Hz, 2H), 5.47 (s, 1H), 0.23 (s, 9H).

2-(4-chlorophenyl)-2-((trimethylsilyl)oxy)acetonitrile (2f) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.42 (d, *J* = 5.8 Hz, 4H), 5.49 (s, 1H), 0.26 (s, 9H).

2-(4-bromophenyl)-2-((trimethylsilyl)oxy)acetonitrile (2g) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.48 (dd, *J* = 8.6, 5.3 Hz, 2H), 7.13 (t, *J* = 8.6 Hz, 2H), 5.50 (s, 1H), 0.26 (s, 9H).

2-(p-tolyl)-2-((trimethylsilyl)oxy)acetonitrile (2h) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.28 (d, *J* = 8.1 Hz, 2H), 7.14 (d, *J* = 7.9 Hz, 2H), 5.38 (s, 1H), 2.29 (s, 3H), 0.14 (s, 9H).

2-(4-methoxyphenyl)-2-((trimethylsilyl)oxy)acetonitrile (2i) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 (d, *J* = 8.0 Hz, 2H), 7.21 (d, *J* = 7.8 Hz, 2H), 5.45 (s, 1H), 2.36 (s, 3H), 0.22 (s, 9H).

4-phenyl-1,3-dioxolan-2-one (4a) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.45 – 7.34 (m, 5H), 5.67 (t, *J* = 8.0 Hz, 1H), 4.79 (t, *J* = 8.4 Hz, 1H), 4.34 – 4.30 (m, 1H).

4-(chloromethyl)-1,3-dioxolan-2-one (4b) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 5.00 – 4.95 (m, 1H), 4.60 (t, *J* = 8.5 Hz, 1H), 4.43 – 4.41 (m, 1H), 3.79 – 3.73 (m, 2H).

4-(bromomethyl)-1,3-dioxolan-2-one (4c) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 5.05 – 5.02 (m, 1H), 4.67 – 4.62 (m, 1H), 4.36 (dd, *J* = 8.9, 5.8 Hz, 1H), 3.66 (dd, *J* = 31.1, 4.5 Hz, 2H).

4-ethyl-1,3-dioxolan-2-one (4d) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 4.74 – 4.67 (m, 1H), 4.56 (t, *J* = 8.2 Hz, 1H), 4.13 – 4.09 (m, 1H), 1.80 (dp, *J* = 21.8, 7.1 Hz, 2H), 1.05 – 1.01 (m, 3H).

4-butyl-1,3-dioxolan-2-one(4e) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 4.72 (qd, *J* = 7.5, 5.4 Hz, 1H), 4.55 (t, *J* = 8.1 Hz, 1H), 4.10 – 4.06 (m, 1H), 1.84 – 1.77 (m, 1H), 1.73 – 1.67 (m, 1H), 1.49 – 1.34 (m, 4H), 0.93 (t, *J* = 7.1 Hz, 3H).

4-(butoxymethyl)-1,3-dioxolan-2-one (4f) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 4.82 (ddd, *J* = 8.4, 6.1, 3.8 Hz, 1H), 4.52 (s, 1H), 4.39 (dd, *J* = 8.3, 6.0 Hz, 1H), 3.69 – 3.61 (m, 2H), 3.51 (td, *J* = 6.6, 2.1 Hz, 2H), 1.57 – 1.54 (m, 2H), 1.39 – 1.35 (m, 2H), 0.92 (s, 3H).

4-((neopentyloxy)methyl)-1,3-dioxolan-2-one (4g) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 4.83 – 4.77 (m, 1H), 4.49 (t, *J* = 8.3 Hz, 1H), 4.38 (dd, *J* = 8.3, 5.7 Hz, 1H), 3.64 (dd, *J* = 10.5, 4.1 Hz, 1H), 3.52 (dd, *J* = 10.6, 3.5 Hz, 1H), 1.20 (s, 9H).

4-((allyloxy)methyl)-1,3-dioxolan-2-one (4h) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 5.88 (ddt, *J* = 16.4, 10.8, 5.6 Hz, 1H), 5.32 – 5.21 (m, 2H), 4.87 – 4.78 (m, 1H), 4.51 (t, *J* = 8.4 Hz, 1H), 4.40 (dd, *J* = 8.3, 6.1 Hz, 1H), 4.06 (t, *J* = 4.6 Hz, 2H), 3.70 (dd, *J* = 11.0, 3.7 Hz, 1H), 3.62 (dd, *J* = 11.1, 3.8 Hz, 1H).

4-((benzyloxy)methyl)-1,3-dioxolan-2-one (4i) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.35 – 7.27 (m, 5H), 4.80 – 4.74 (m, 1H), 4.59 – 4.51 (m, 2H), 4.42 (d, *J* = 8.4 Hz, 1H), 4.33 (dd, *J* = 8.4, 6.0 Hz, 1H), 3.68 (dd, *J* = 11.1, 3.6 Hz, 1H), 3.58 – 3.56 (m, 1H).

4-((benzyloxy)methyl)-1,3-dioxolan-2-one (4j) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 7.30 – 7.27 (m, 2H), 7.00 (t, *J* = 7.4 Hz, 1H), 6.89 (d, *J* = 8.0 Hz, 2H), 5.02 – 4.97 (m, 1H), 4.57 (t, *J* = 8.5 Hz, 1H), 4.49 (dd, *J* = 8.6, 5.9 Hz, 1H), 4.21 – 4.18 (m, 1H), 4.10 (dd, *J* = 10.7, 3.6 Hz, 1H).

tetrahydro-4H-cyclopenta[d][1,3]dioxol-2-one (4k) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 5.11 (dd, *J* = 3.9, 1.7 Hz, 2H), 2.19 – 2.15 (m, 2H), 1.81 (td, *J* = 12.1, 11.1, 5.2 Hz, 2H), 1.68 (ddd, *J* = 14.2, 10.0, 5.1 Hz, 2H).

hexahydrobenzo[d][1,3]dioxol-2-one (4l) [25]

^{1}H NMR (600 MHz, $CDCl_3$) δ 4.70 (q, *J* = 5.9, 5.0 Hz, 2H), 1.90 (p, *J* = 4.9 Hz, 4H), 1.66 – 1.59 (m, 2H), 1.44 (dt, *J* = 10.7, 6.1 Hz, 2H).

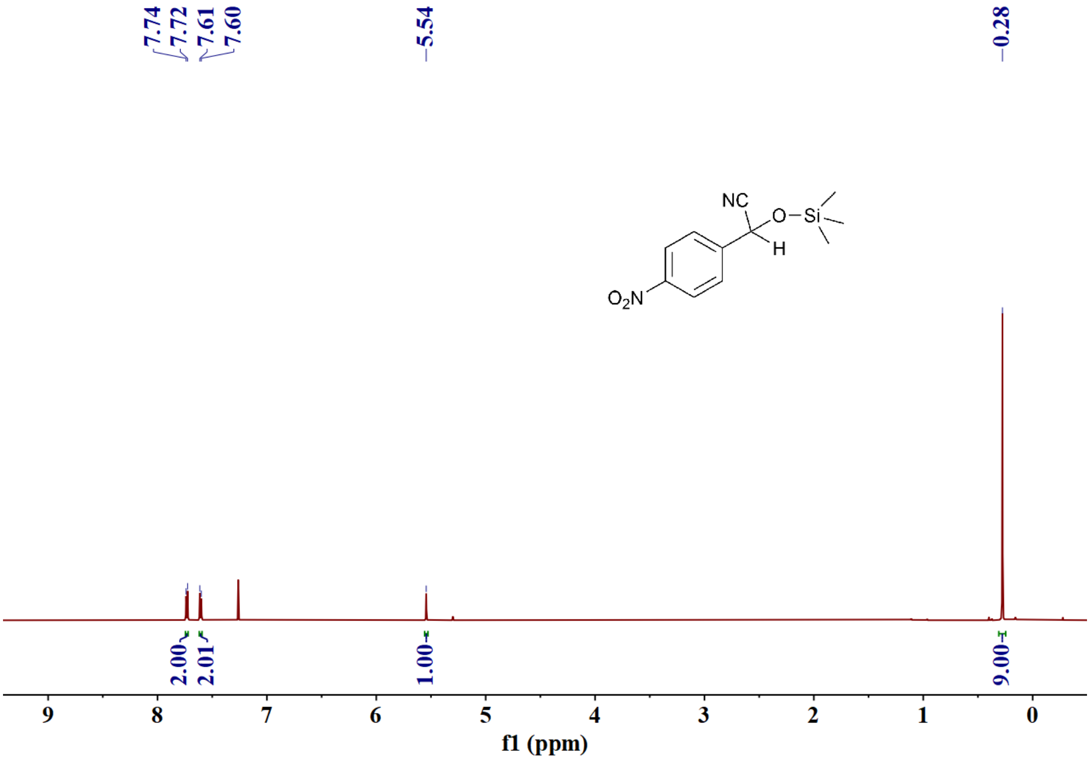


Fig. S7. ^{1}H NMR of 2a (600 MHz, $CDCl_3$)

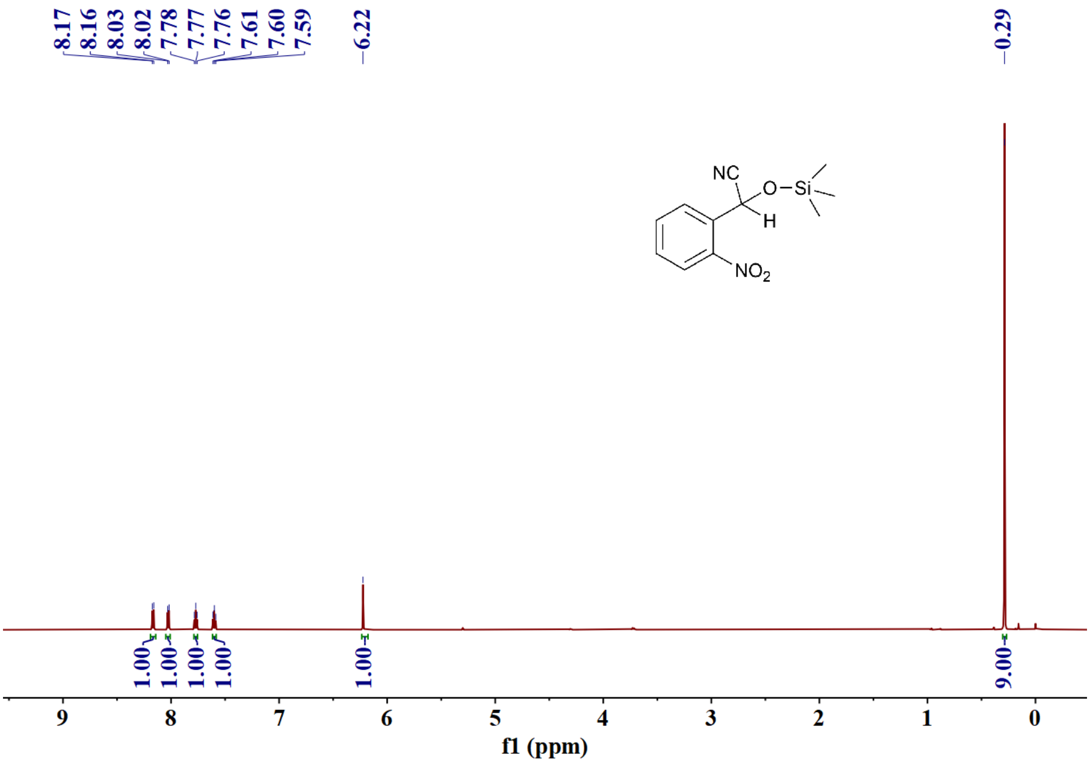


Fig. S8. ^{1}H NMR of 2b (600 MHz, $CDCl_3$)

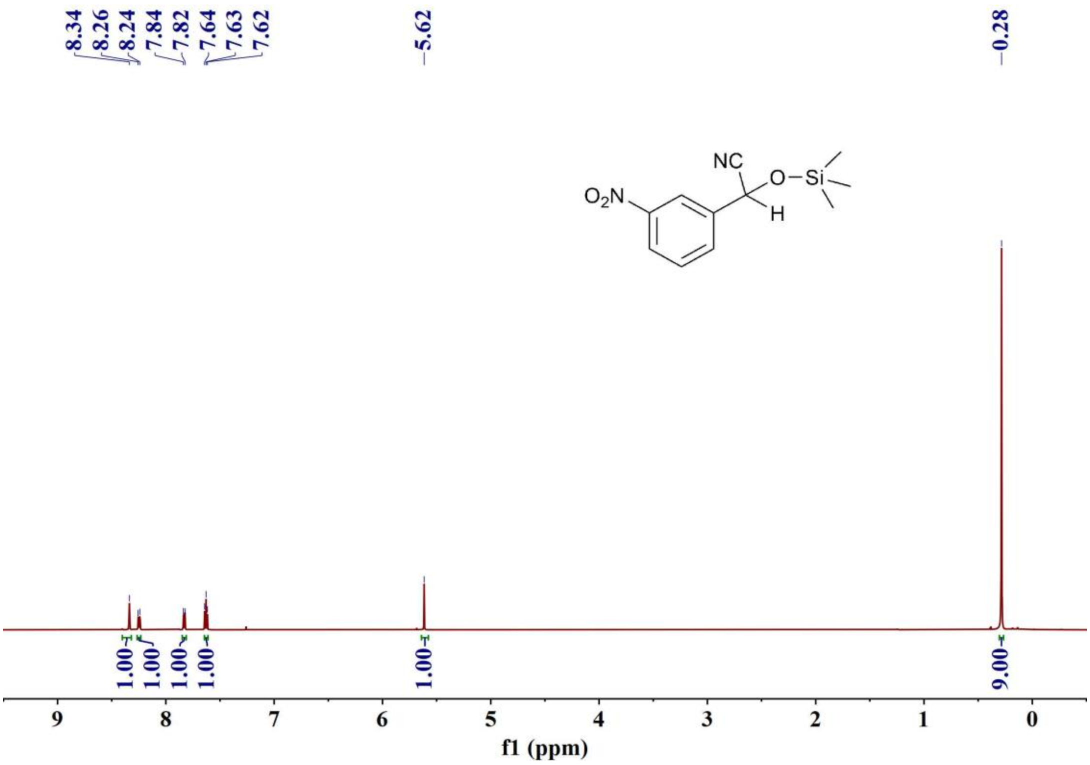


Fig. S9. ^{1}H NMR of 2c (600 MHz, $CDCl_3$)

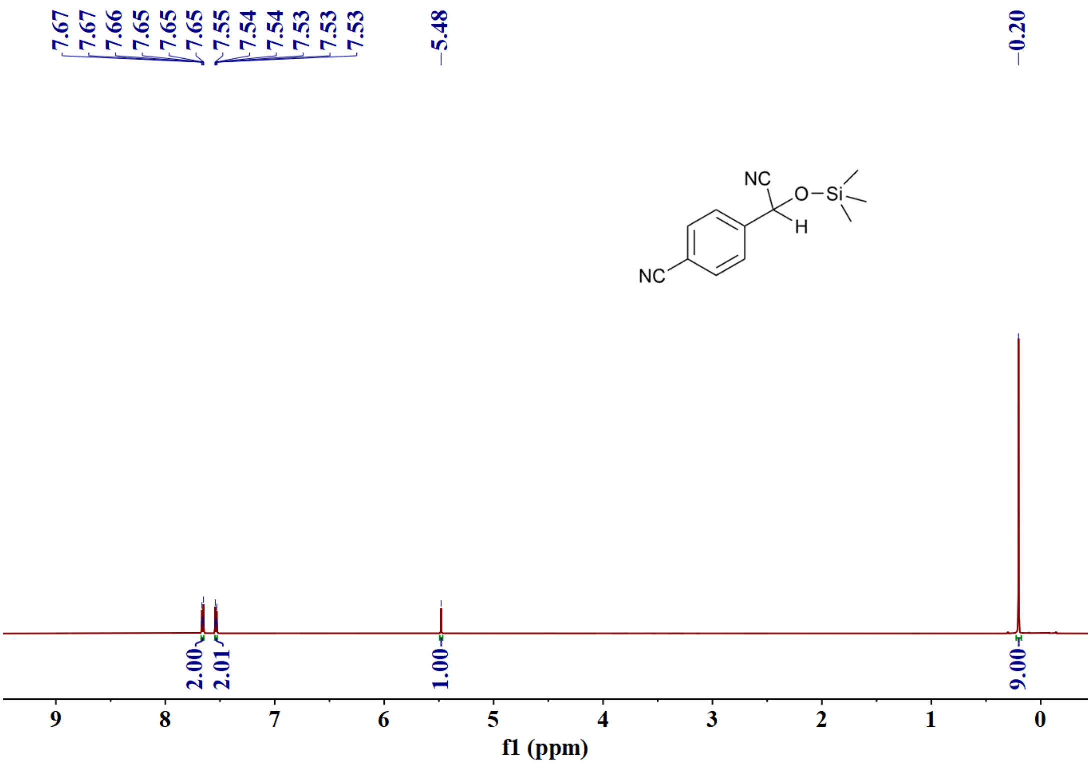


Fig. S10. ^{1}H NMR of 2d (600 MHz, CDCl3)

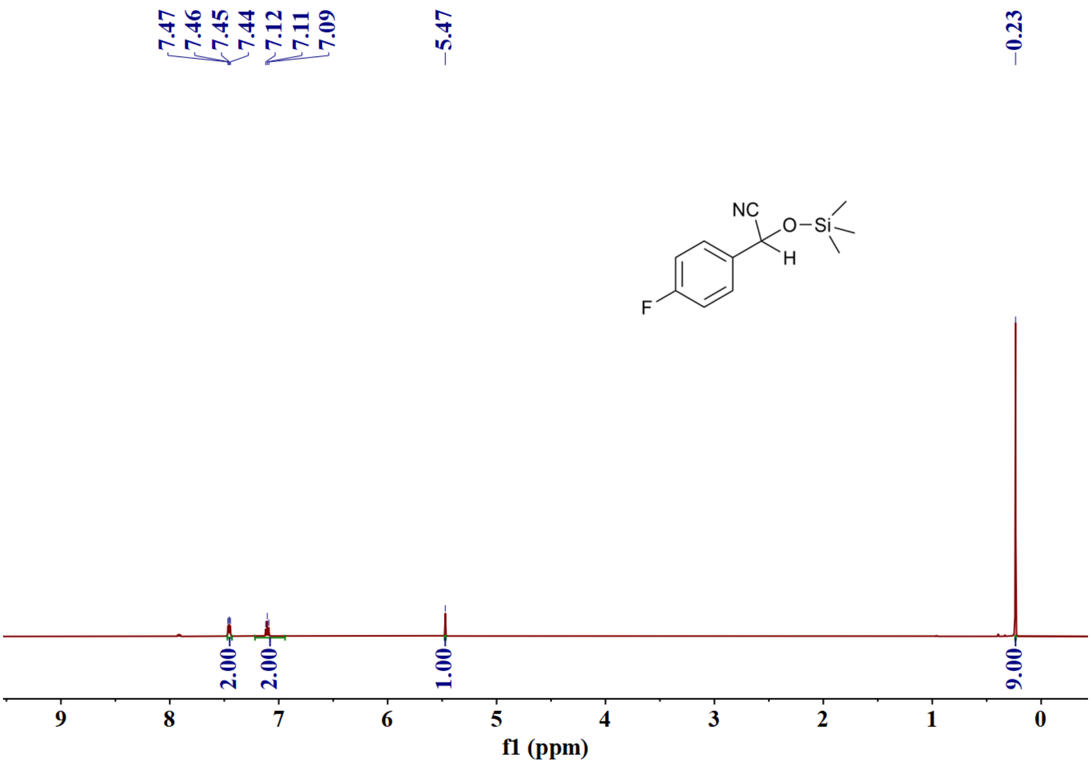


Fig. S11. ^{1}H NMR of 2e (600 MHz, $CDCl_3$)

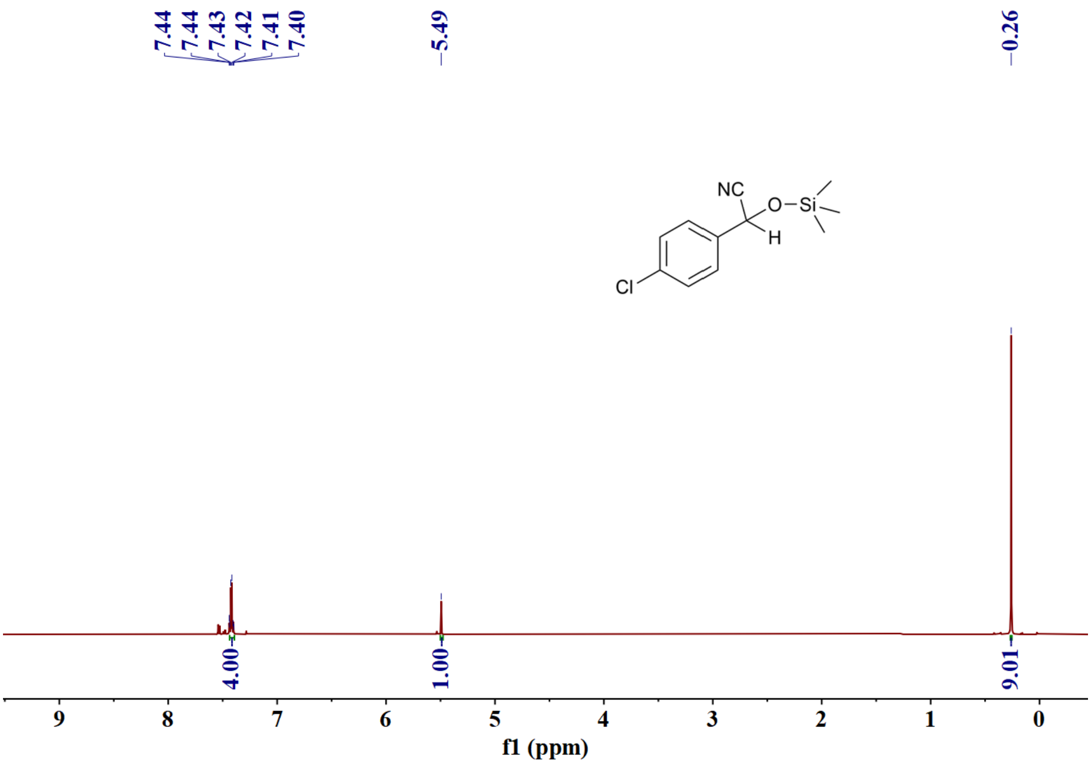


Fig. S12. ^{1}H NMR of 2f (600 MHz, $CDCl_3$)

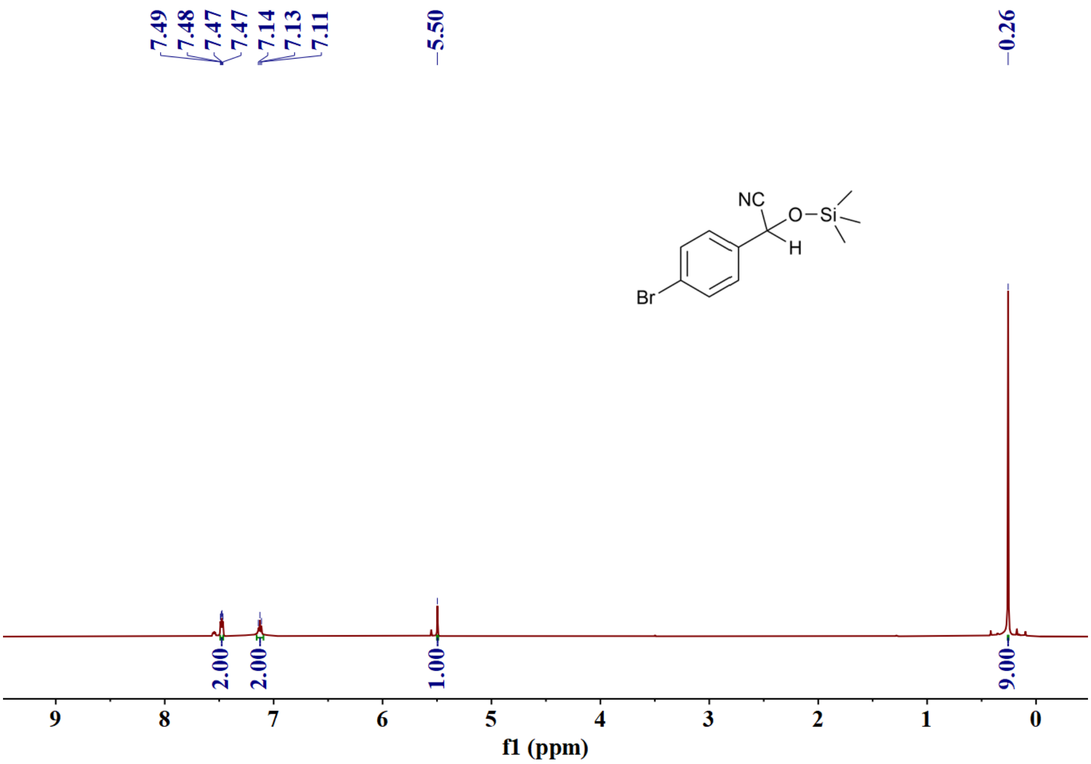


Fig. S13. ^{1}H NMR of 2g (600 MHz, $CDCl_3$)

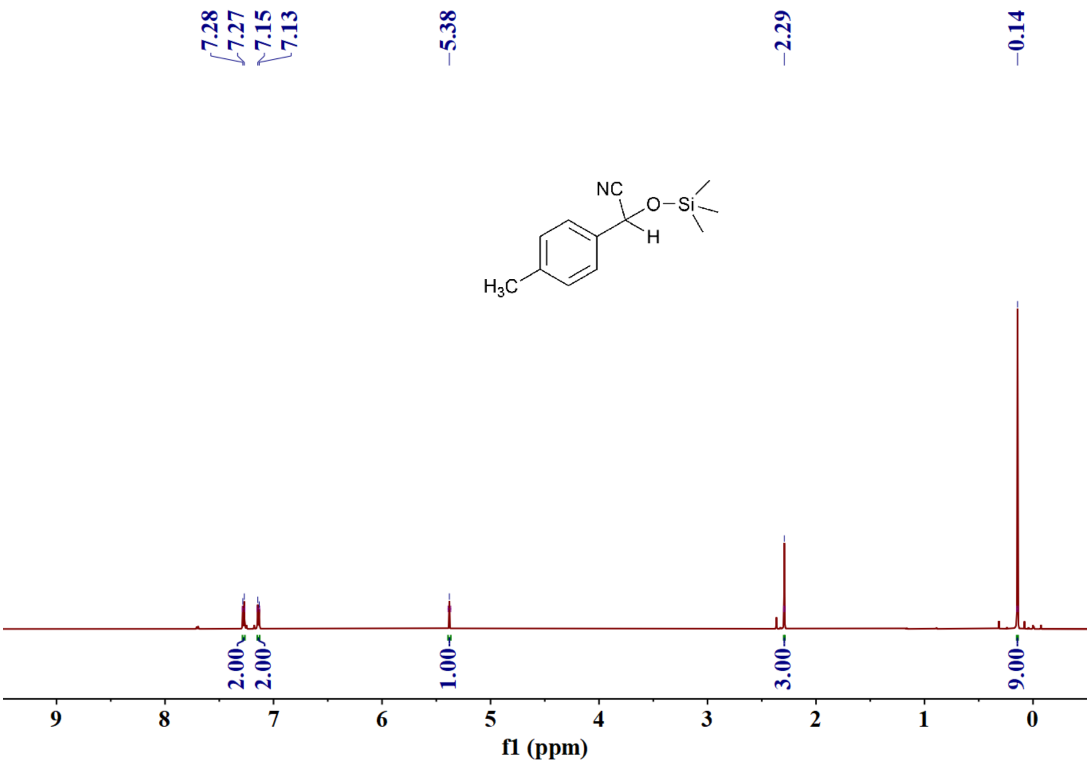


Fig. S14. ^{1}H NMR of 2h (600 MHz, $CDCl_3$)

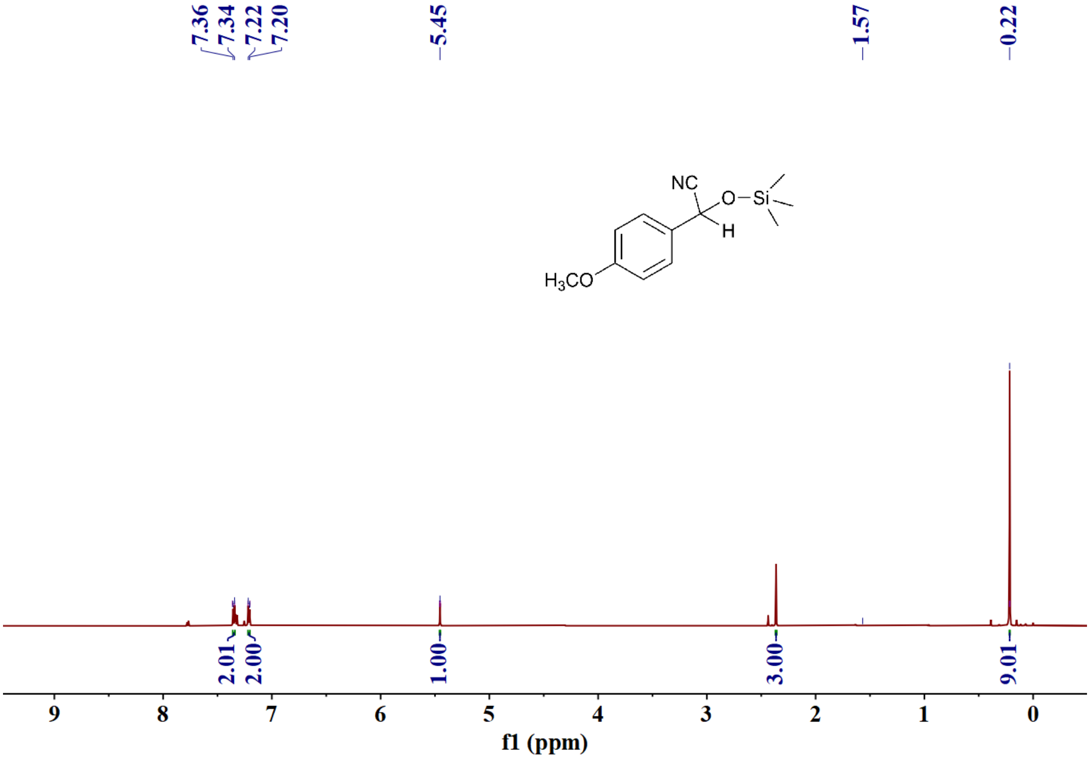


Fig. S15. ^{1}H NMR of 2i (600 MHz, $CDCl_3$)

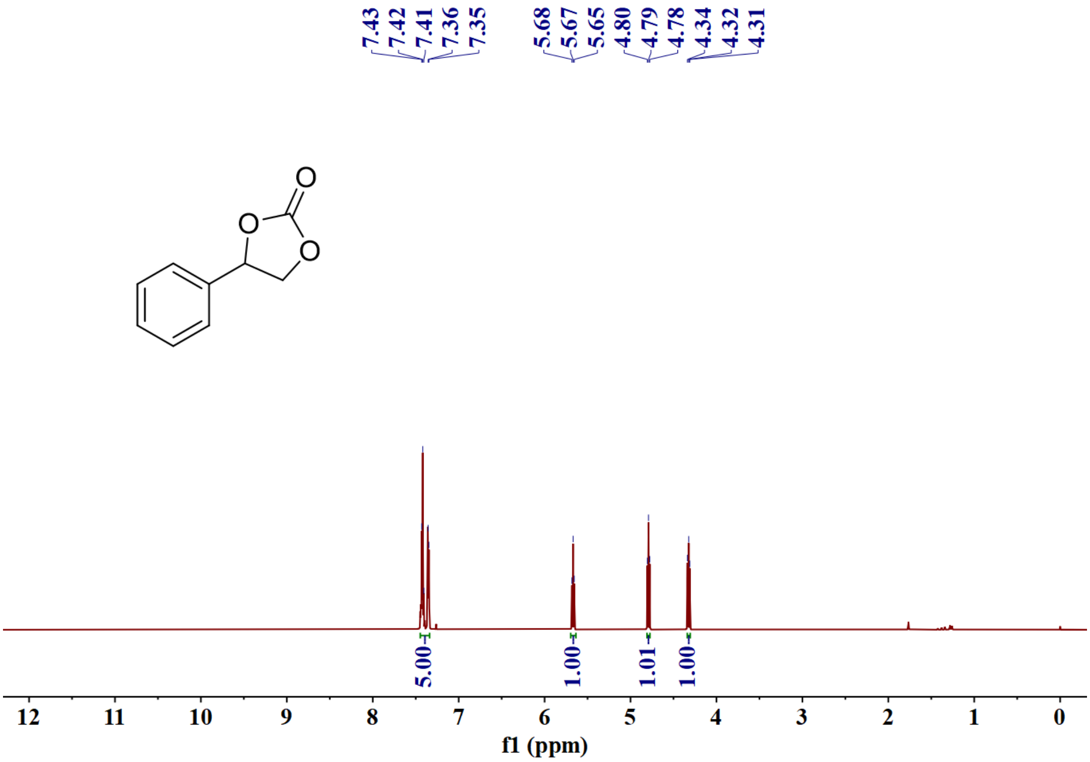


Fig. S16. ^{1}H NMR of 4a (600 MHz, $CDCl_3$)

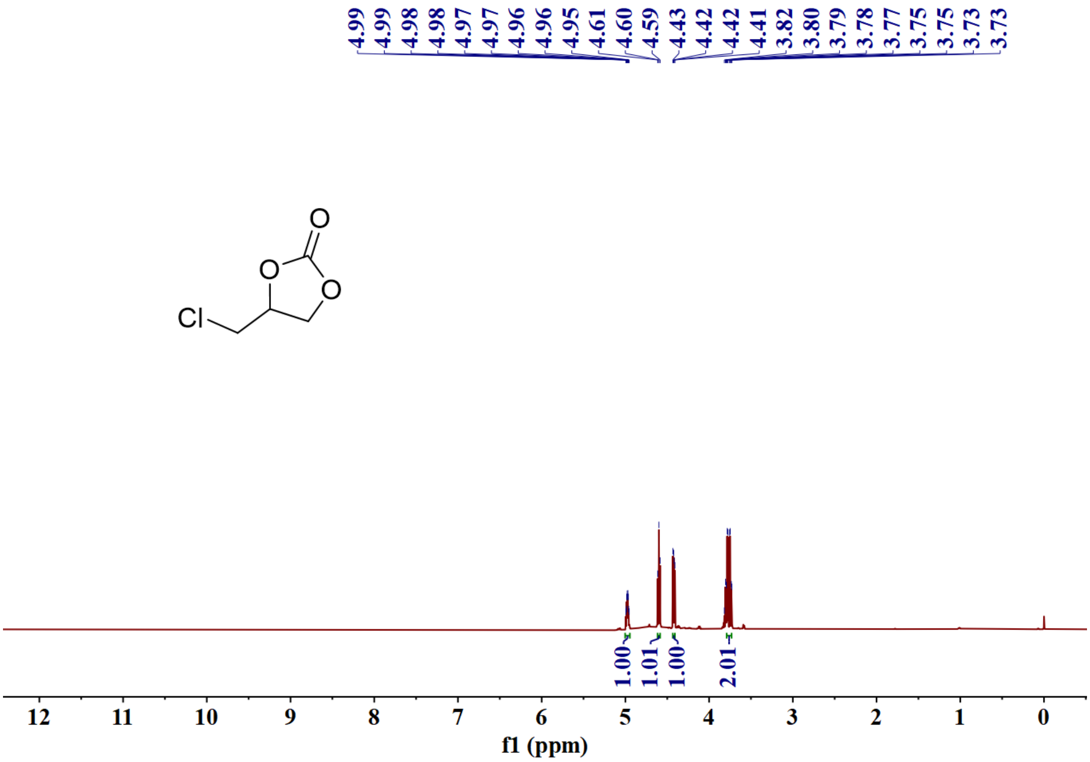


Fig. S17. ^{1}H NMR of 4b (600 MHz, $CDCl_3$)

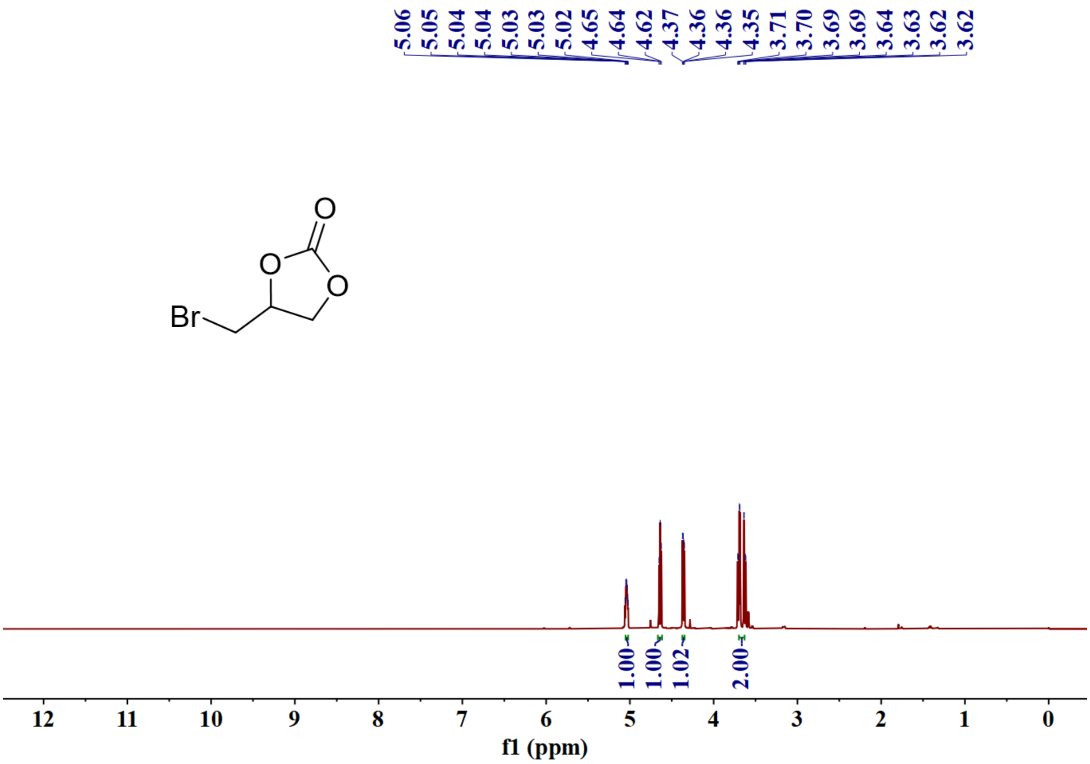


Fig. S18. ^{1}H NMR of 4c (600 MHz, $CDCl_3$)

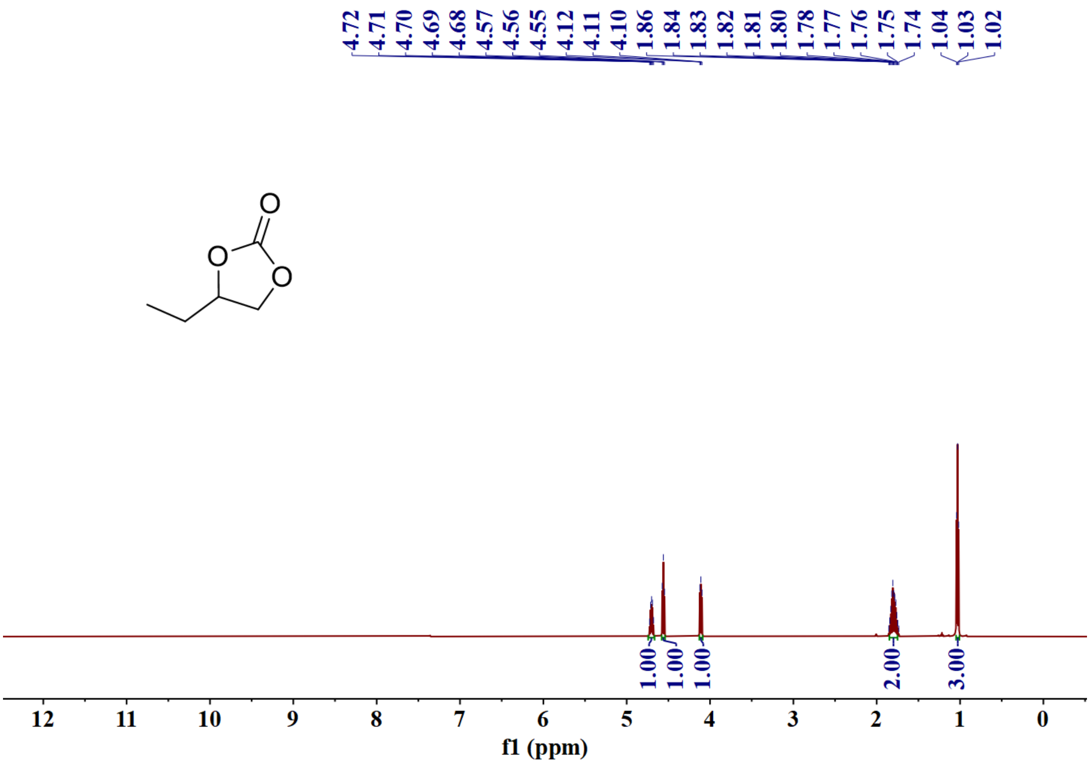


Fig. S19. ^{1}H NMR of 4d (600 MHz, CDCl3)

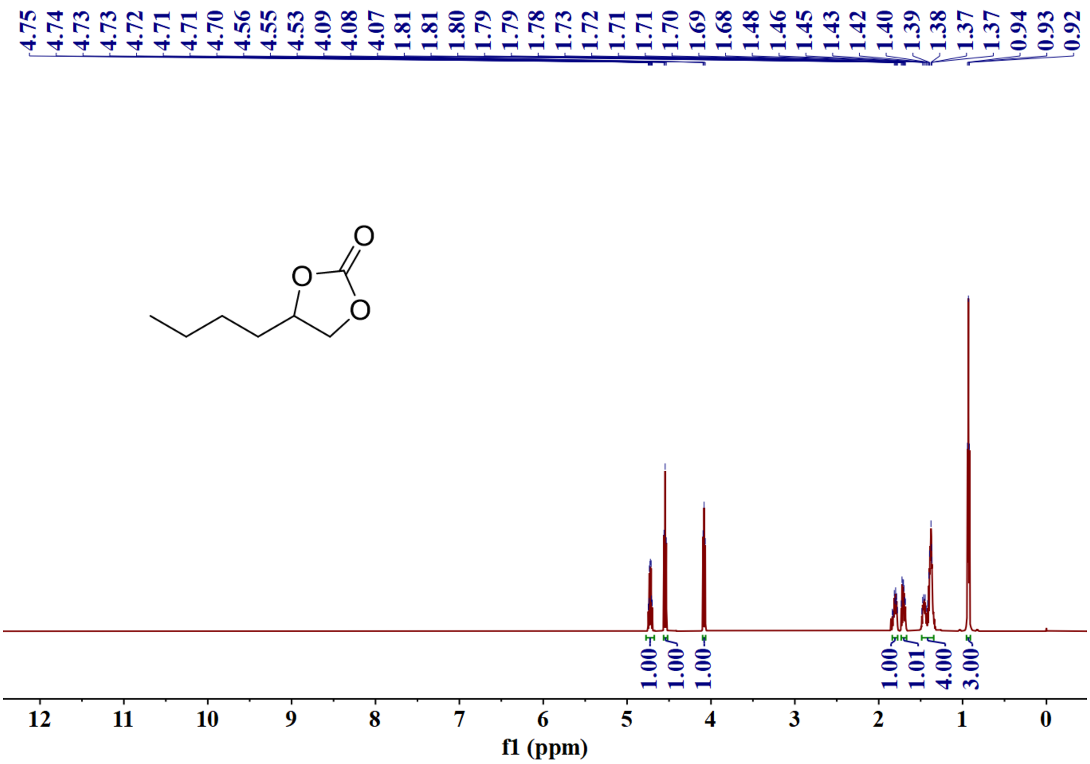


Fig. S20. ^{1}H NMR of 4e (600 MHz, $CDCl_3$)

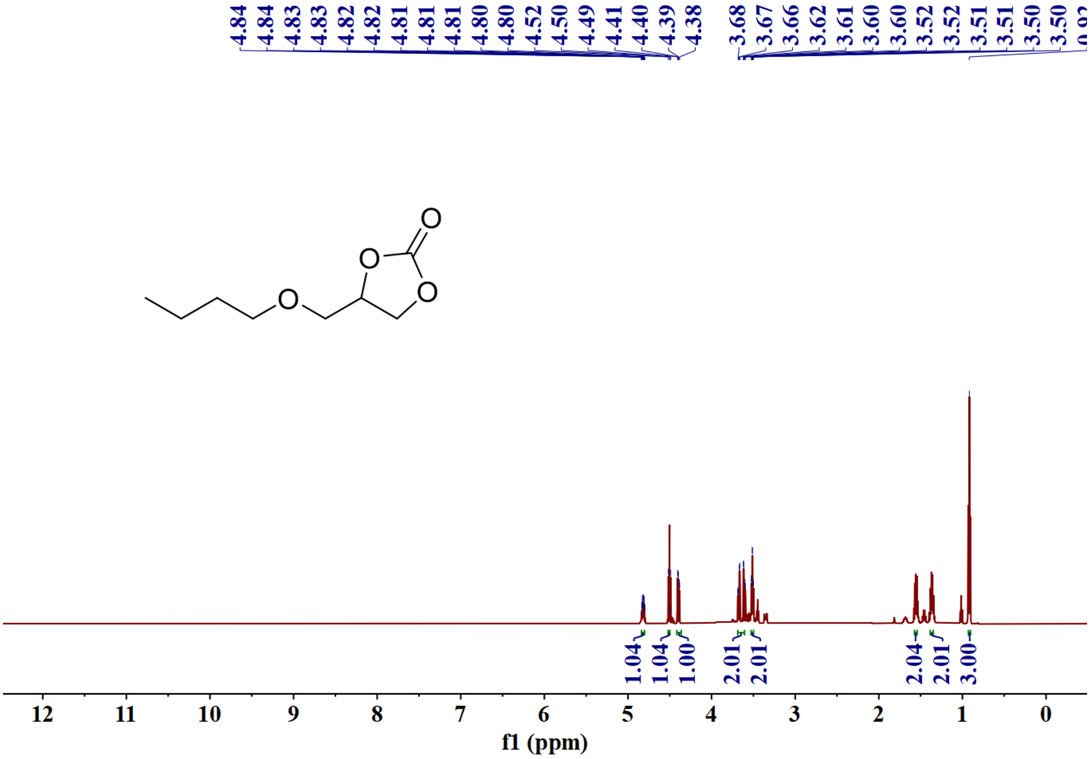


Fig. S21. ^{1}H NMR of 4f (600 MHz, $CDCl_3$)

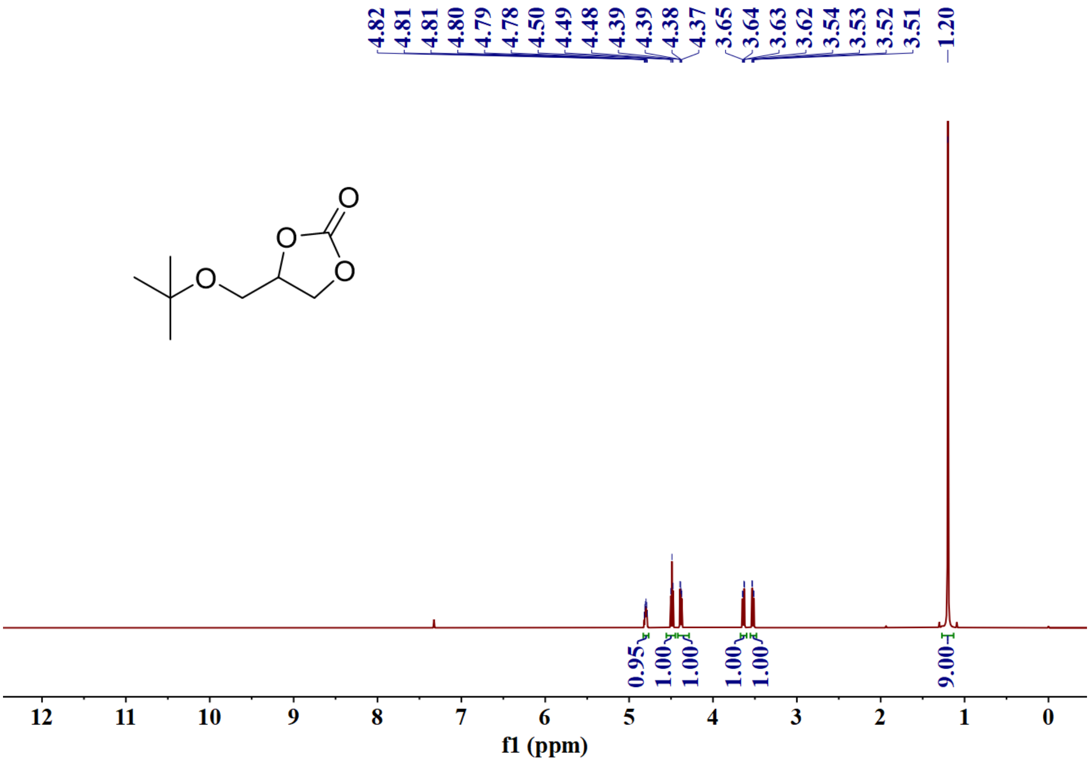


Fig. S22. ^{1}H NMR of 4g (600 MHz, $CDCl_3$)

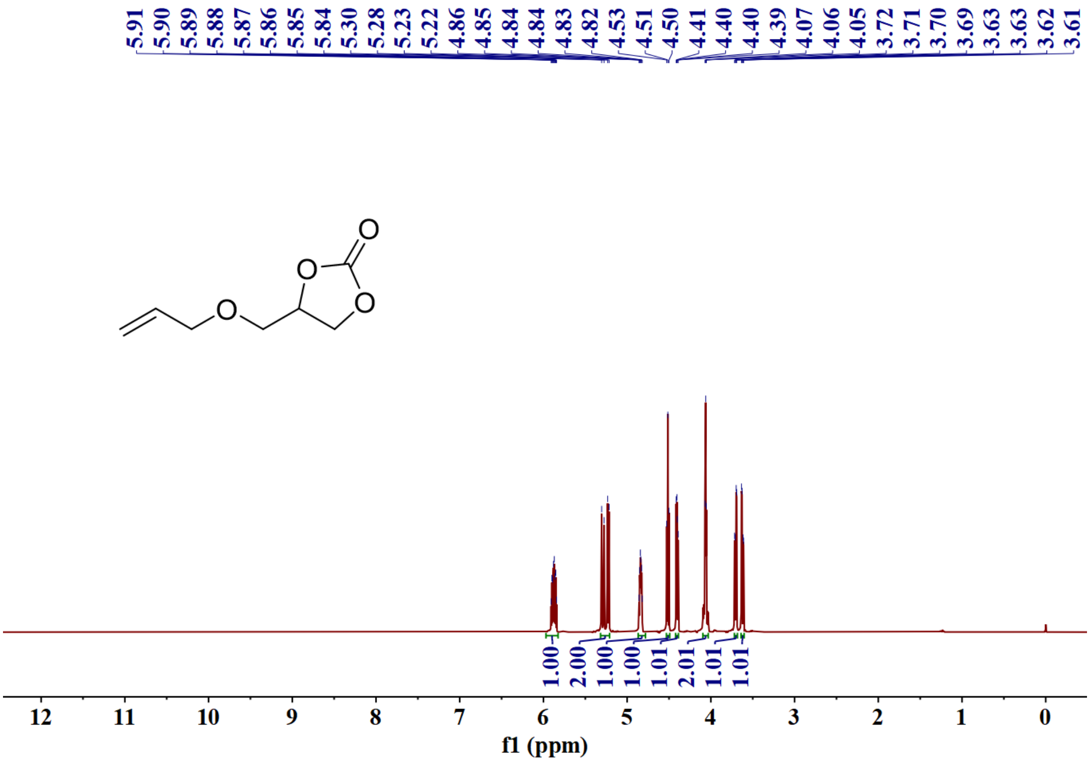


Fig. S23. ^{1}H NMR of 4h (600 MHz, $CDCl_3$)

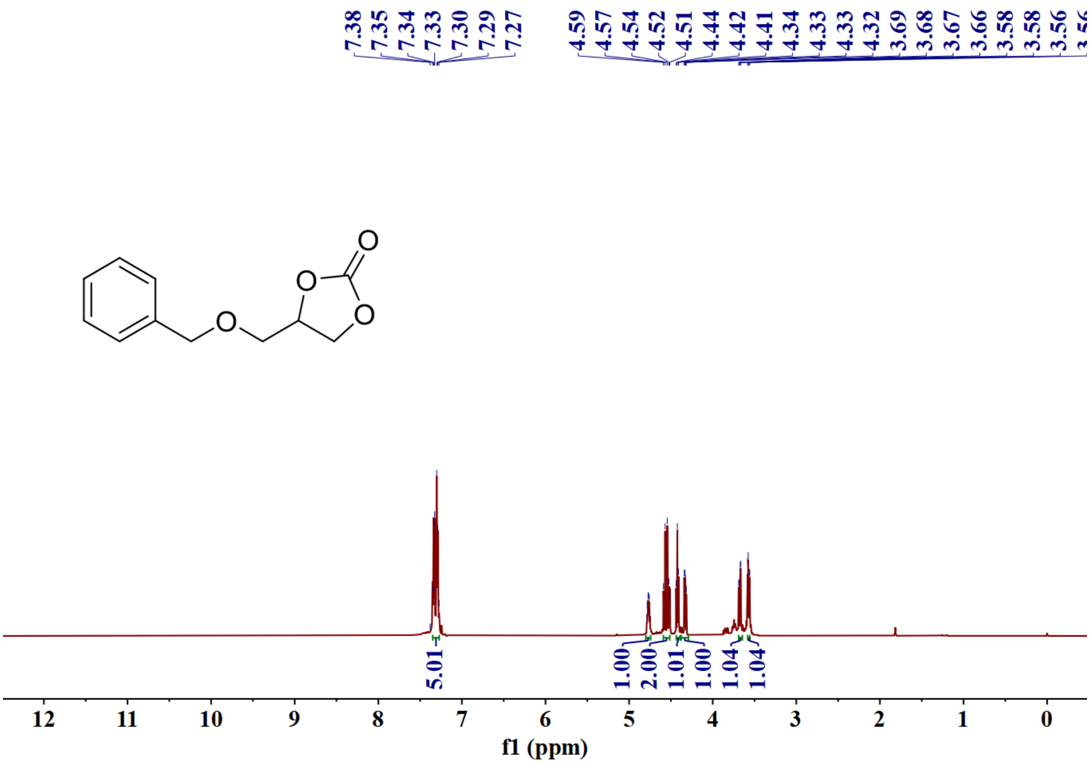


Fig. S24. ^{1}H NMR of 4i (600 MHz, $CDCl_3$)

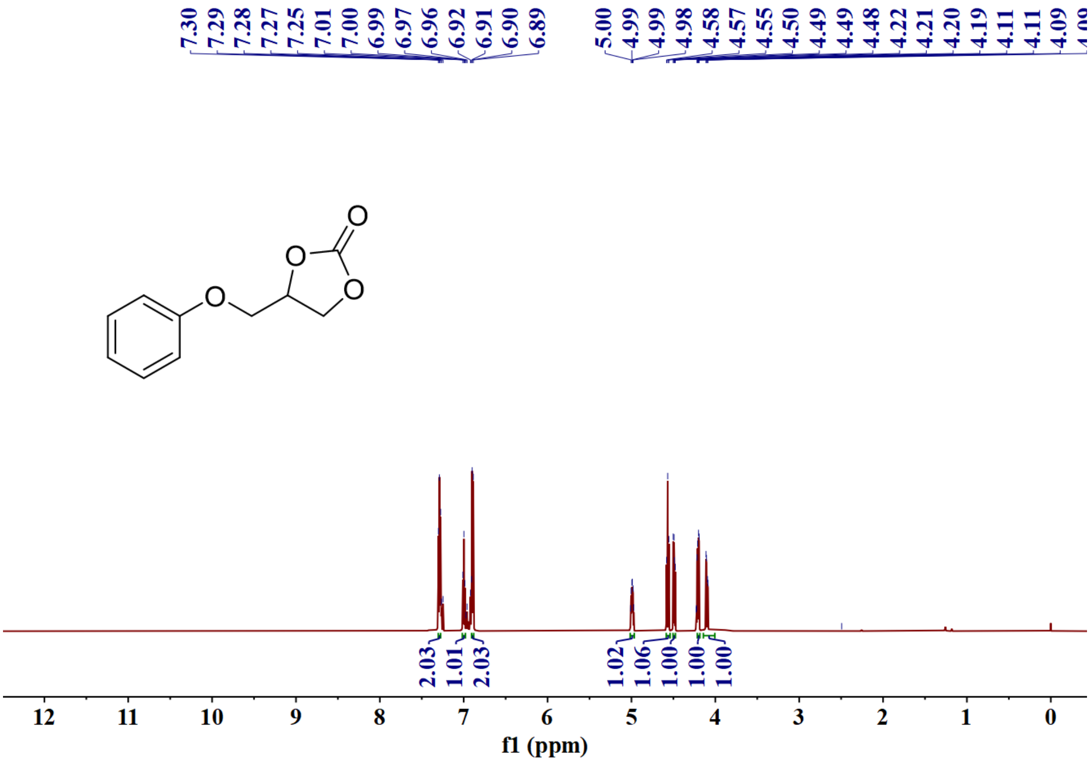


Fig. S25. ^{1}H NMR of 4j (600 MHz, $CDCl_3$)

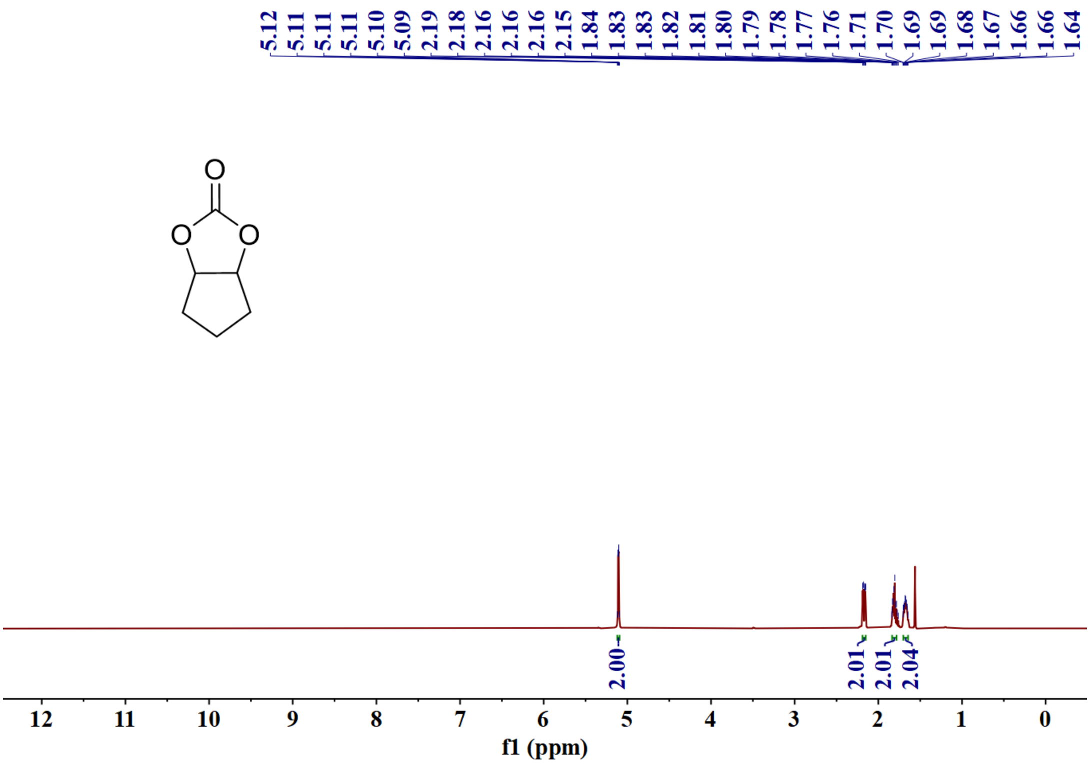


Fig. S26. ^{1}H NMR of 4k (600 MHz, $CDCl_3$)

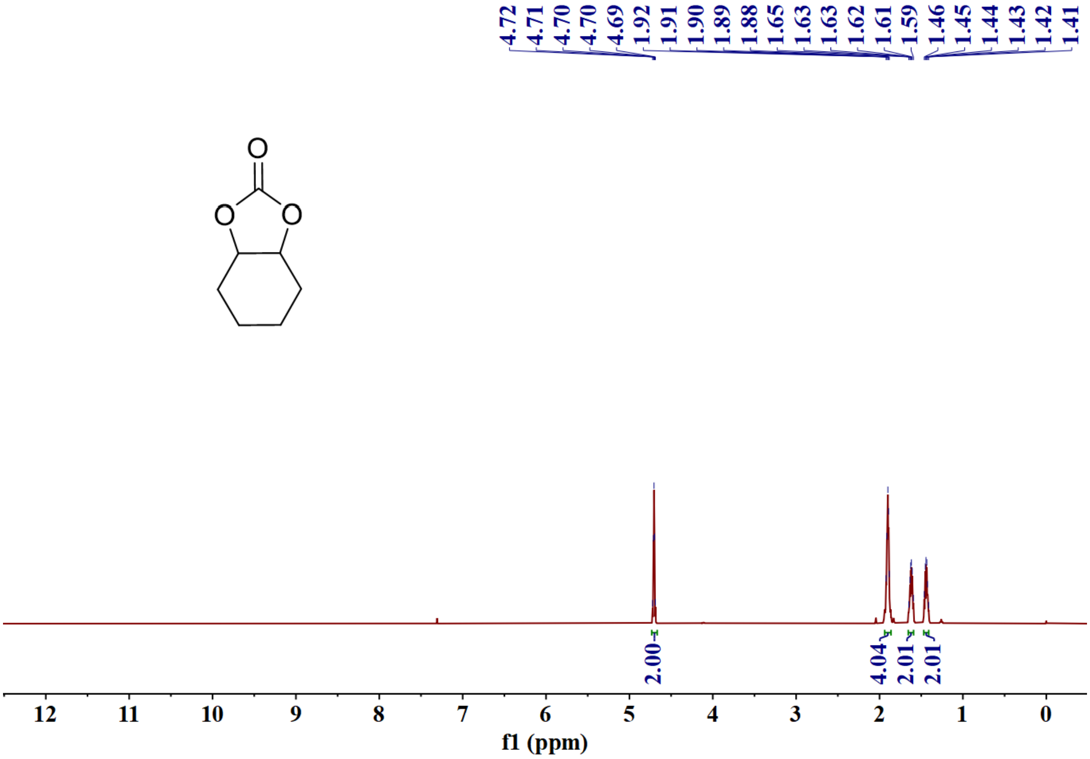


Fig. S27. ^{1}H NMR of 4l (600 MHz, $CDCl_3$)

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