Supporting Information for

Two Scandium-Based Coordination Polymers: Rapid Ultrasound-Assisted Synthesis, Crystal Transformation, and Catalytic Property

*Rui Liu[a], Yansong Jiang[a b], Yiran Gong[a], Yu Fu[a], Jieyu Shen[a], Li Wang[a], Yong Fan[a], Yupeng Guo[a], Jianing Xu[a]**

a College of Chemistry, Jilin University, Changchun, 130012, Jilin, People's Republic of China

b South China Advanced Institute for Soft Matter Science and Technology, School of Molecular Science and Engineering, South China University of Technology, Guangzhou, 510640 Guangdong Province, P. R. China

Email: xujn@jlu.edu.cn

Contents

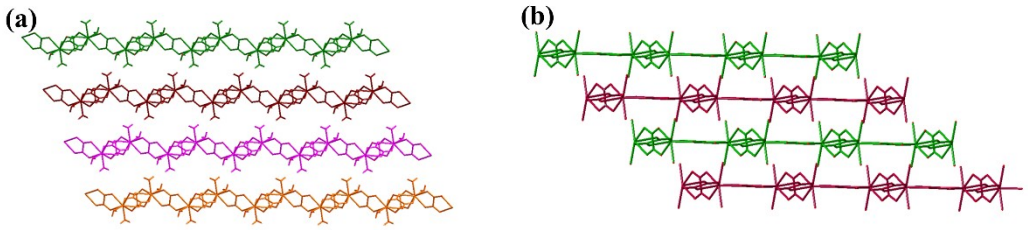

Fig. S1 Layers stacking modes of **1** (a) and **2** (b)

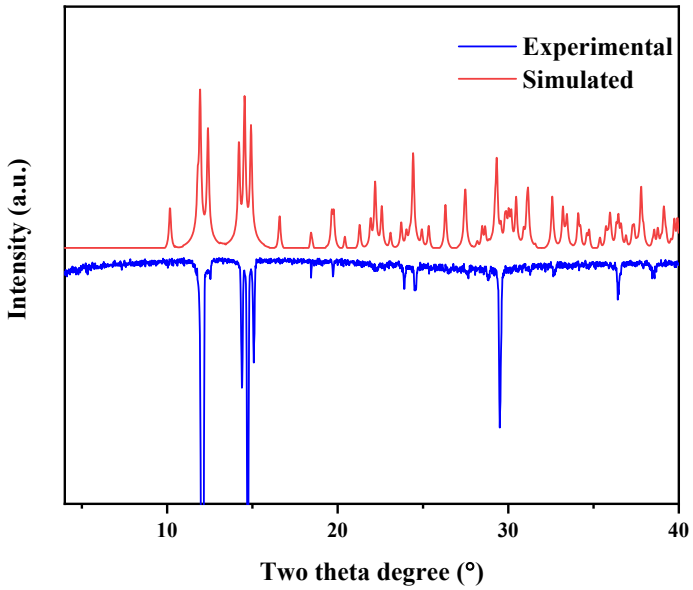

Fig. S2 PXRD pattern of **1**.

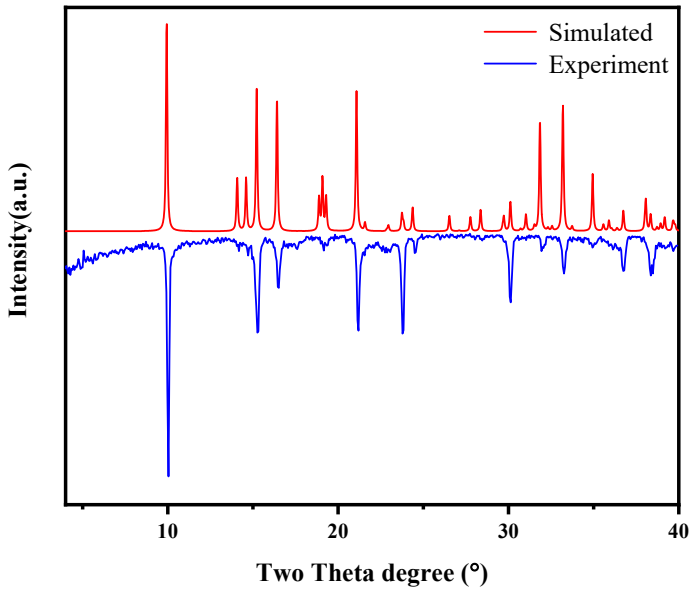

Fig. S3 PXRD pattern of **2**.

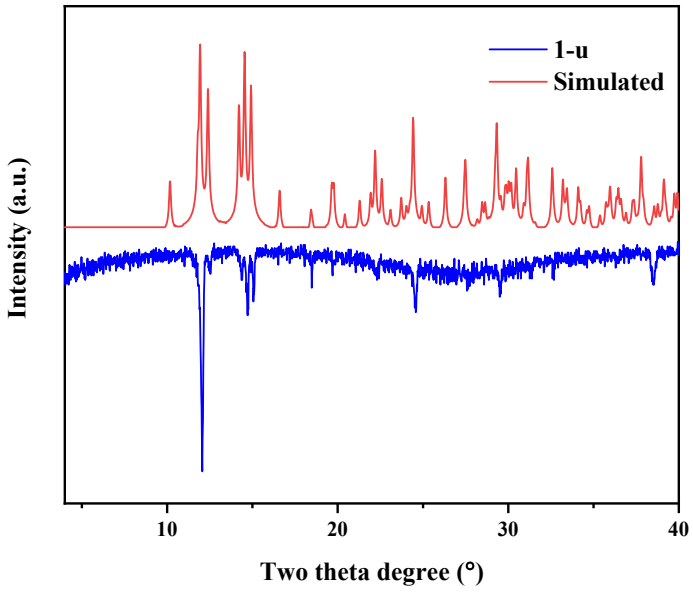

Fig. S4 PXRD patterns of **1-u**.

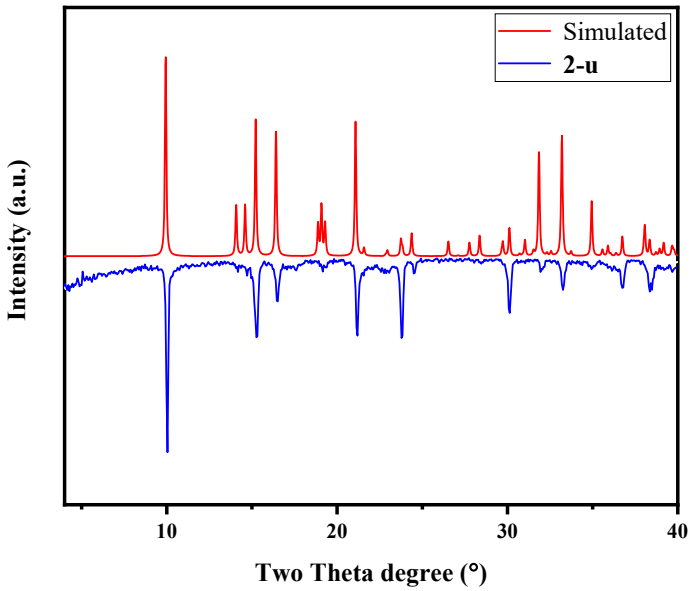

Fig. S5 PXRD patterns of **2-u**.

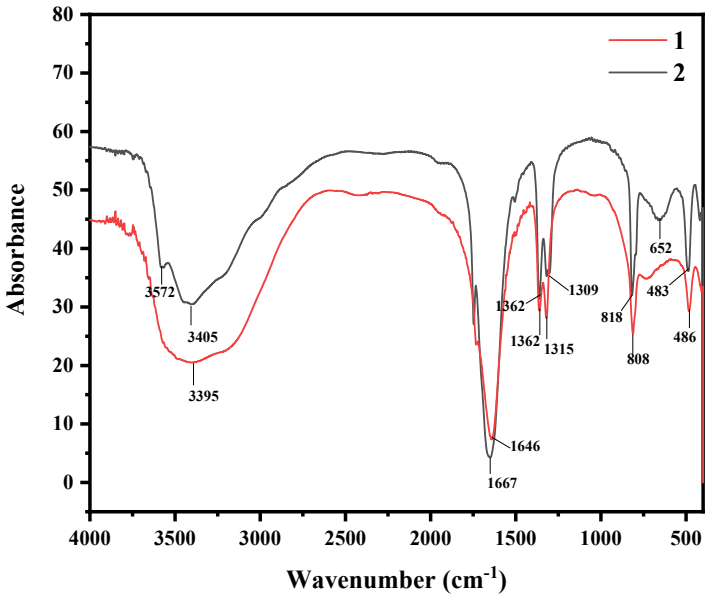

Fig. S6 FT-IR spectra.

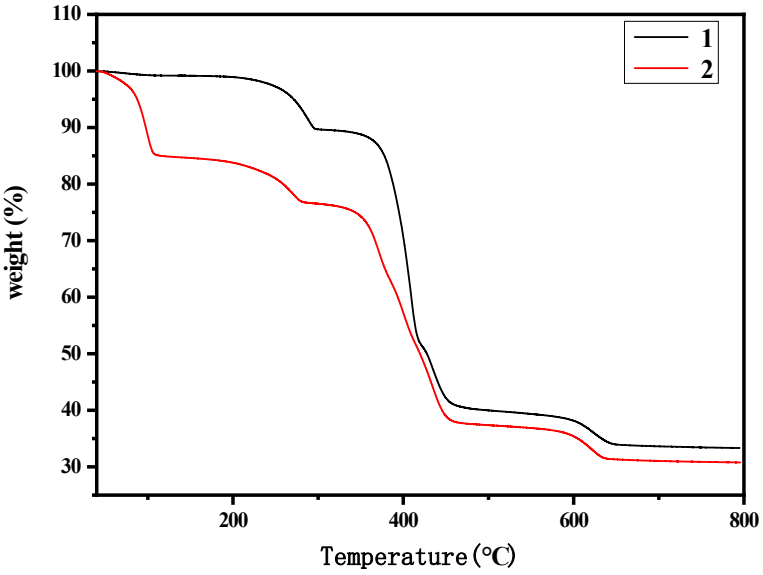

Fig. S7 TG curves.

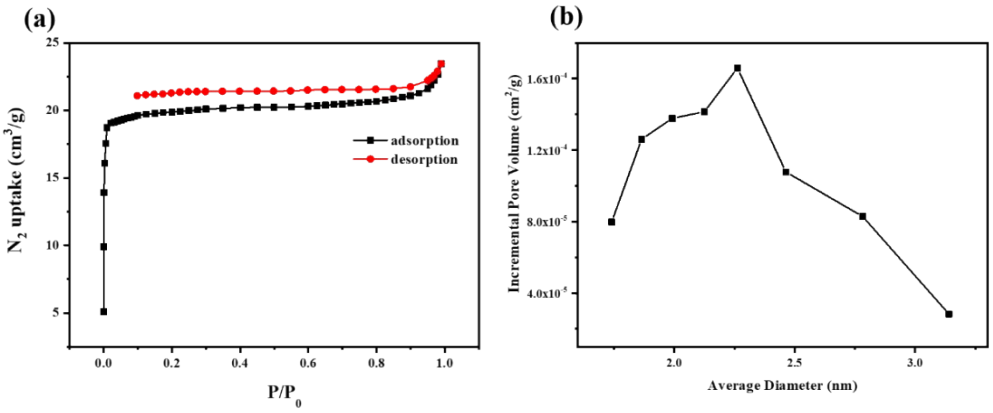

Fig. S8 pore size distribution and N_2 adsorption/desorption isomers of **2**

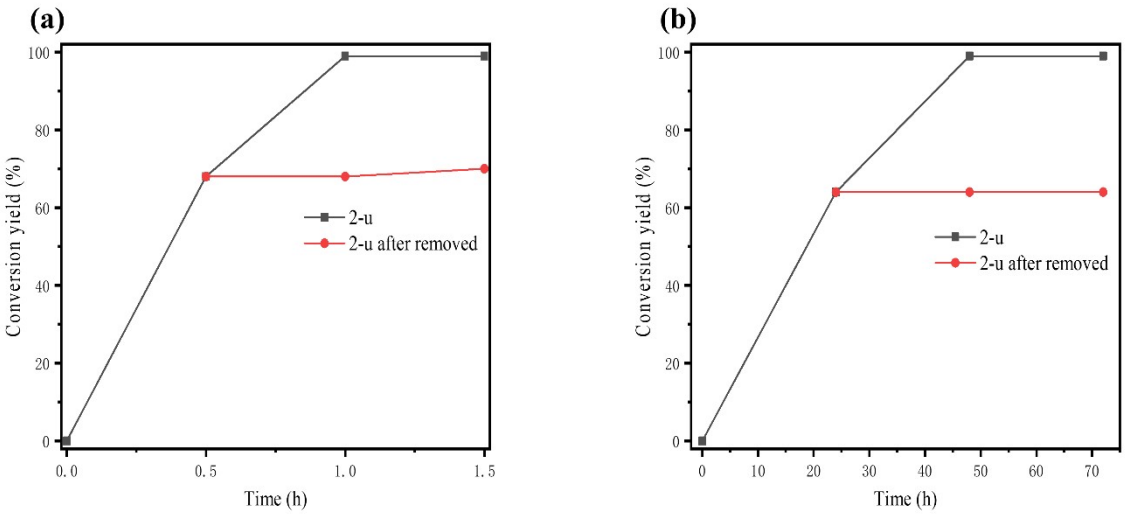

Fig. S9 Effect of conversion yield with time of (a) cyanosilyalation and (b) Stricker reaction**.**

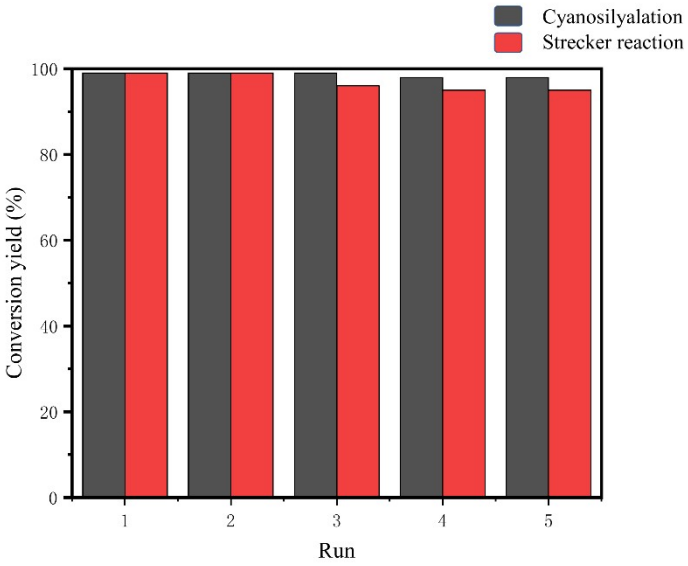

Fig. S10 Recycle studies of **2-u.**

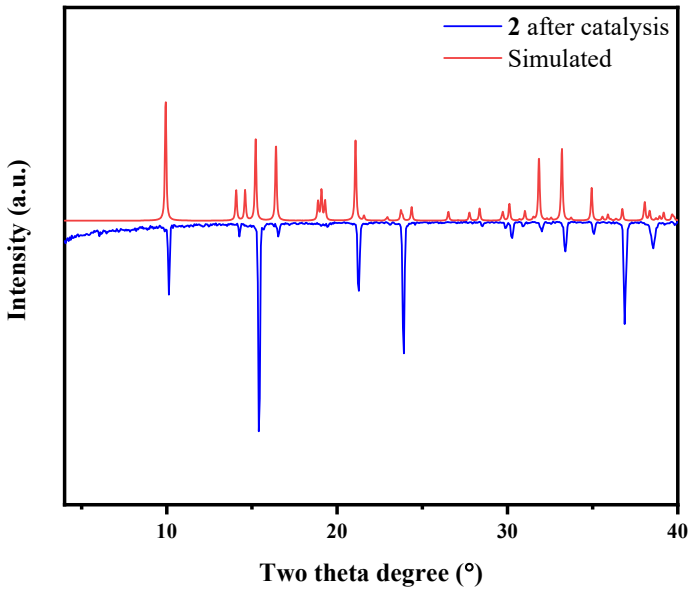

Fig. S11 PXRD patterns of **2** after catalysis of cyanosilylation.

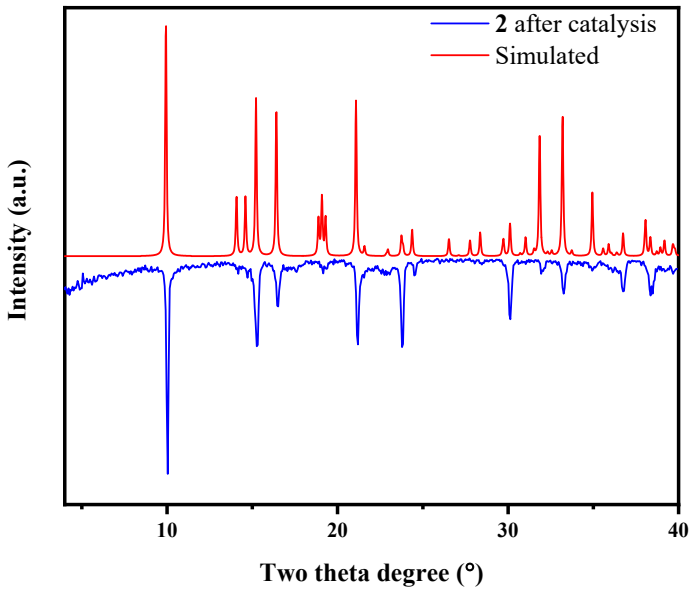

Fig. S12 PXRD patterns of **2** after catalysis of Strecker reaction.

Table S1 Crystal data and structure refinement for **1-2**.

Chemical formula	$C_3H_{12}O_{12}Sc$	$C_3H_6O_9Sc$
M_r	285.09	231.04
Crystal system, space group	Triclinic, *P*-1	Triclinic, *P*-1
Temperature (K)	298	293
a (Å)	7.8876 (5)	6.1711 (12)
b (Å)	8.3604 (6)	6.5104 (14)
c (Å)	9.6680 (7)	9.2896 (17)
a (°)	65.082 (2)	75.586 (17)
β (°)	76.419 (2)	80.143 (16)
γ (°)	73.429 (2)	83.472 (17)
V (Å^3)	549.34 (7)	355.15 (13)
Z	2	2
Radiation type	Mo *K*α	Mo *K*α
μ (mm^{-1})	0.73	1.07
Diffractometer	Bruker D8 venture	Bruker D8 venture
Absorption correction	Multi-scan	Multi-scan
T_{min}, T_{max}	0.917, 0.930	0.443, 0.633
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5795, 2034, 1767	2560, 1622, 1319
R_{int}	0.058	0.033
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.604	0.689
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.047, 0.137, 1.06	0.052, 0.146, 1.07
No. of reflections	1940	1622
No. of parameters	147	123
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.94, −0.40	0.80, −0.75

Table S2 Selected bond lengths [Å] for **1**.

Bond	Length/Å	Bond	Length/Å
Sc01—O008	2.140 (2)	O003—C00B	1.264 (3)
Sc01—O00A	2.172 (2)	O004—C00D	1.255 (3)
Sc01—O003	2.186 (2)	O005—C00D	1.244 (3)
Sc01—O007	2.206 (2)	O005—Sc01^{i}	2.2531 (19)
Sc01—O005^{i}	2.2531 (19)	O006—C00C	1.236 (4)
Sc01—O004	2.2567 (19)	O006—Sc01^{iii}	2.366 (2)
Sc01—O002^{ii}	2.2631 (19)	O007—C00C	1.260 (3)
Sc01—O006^{iii}	2.366 (2)	C00B—C00B^{ii}	1.525 (5)
O002—C00B	1.245 (3)	C00C—C00C^{iii}	1.528 (5)
O002—Sc01^{ii}	2.2632 (19)	C00D—C00D^{i}	1.536 (5)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*; (iii) −*x*+1, −*y*+1, −*z*.

Table S3 Selected bond lengths [Å] for **2**.

Bond	Length/Å	Bond	Length/Å
Sc01—O002	2.181 (2)	O005—C00B	1.251 (4)
Sc01—O009	2.207 (3)	O005—Sc01^{i}	2.239 (2)
Sc01—O007	2.207 (3)	O006—C00C	1.238 (4)
Sc01—O008	2.235 (3)	O007—H00A	0.8798
Sc01—O005^{i}	2.239 (2)	O007—H00B	0.8798
Sc01—O006	2.244 (2)	O008—H00C	0.8648
Sc01—O004^{ii}	2.258 (3)	O008—H00D	0.8652
Sc01—O003^{iii}	2.259 (2)	O009—C00A	1.240 (4)
O002—C00B	1.249 (4)	C00A—C00A^{iii}	1.534 (6)
O003—C00A	1.256 (4)	C00B—C00B^{i}	1.515 (6)
O003—Sc01^{iii}	2.259 (2)	C00C—C00C^{ii}	1.523 (7)
O004—C00C	1.267 (4)	O00D—H00E	0.8500
O004—Sc01^{ii}	2.258 (3)	O00D—H00F	0.8500

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+2, −*y*+2, −*z*; (iii) −*x*+1, −*y*+1, −*z*+1.

Table S4 Selected angles [°] for **1**.

Angel	Angel/°	Angel	Angel/°
O008—Sc01—O00A	89.52 (10)	O005^{i}—Sc01—O004	71.48 (7)
O008—Sc01—O003	144.38 (8)	O008—Sc01—O002^{ii}	80.35 (8)
O00A—Sc01—O003	103.51 (10)	O00A—Sc01—O002^{ii}	71.09 (8)
O008—Sc01—O007	99.27 (9)	O003—Sc01—O002^{ii}	73.12 (7)
O00A—Sc01—O007	150.76 (8)	O007—Sc01—O002^{ii}	137.73 (7)
O003—Sc01—O007	85.41 (8)	O005^{i}—Sc01—O002^{ii}	125.97 (7)
O008—Sc01—O005^{i}	142.95 (8)	O004—Sc01—O002^{ii}	140.43 (8)
O00A—Sc01—O005^{i}	77.86 (9)	O008—Sc01—O006^{iii}	73.35 (8)
O003—Sc01—O005^{i}	72.67 (7)	O00A—Sc01—O006^{iii}	138.97 (8)
O007—Sc01—O005^{i}	78.45 (8)	O003—Sc01—O006^{iii}	75.29 (8)
O008—Sc01—O004	72.16 (7)	O007—Sc01—O006^{iii}	70.07 (7)
O00A—Sc01—O004	80.61 (8)	O005^{i}—Sc01—O006^{iii}	136.32 (8)
O003—Sc01—O004	142.08 (7)	O004—Sc01—O006^{iii}	125.80 (7)
O007—Sc01—O004	75.78 (8)	O002^{ii}—Sc01—O006^{iii}	69.44 (7)

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) −*x*+2, −*y*+1, −*z*; (iii) −*x*+1, −*y*+1, −*z*.

Table S5 Selected angles [°] for **2**.

Angel	Angel/°	Angel	Angel/°
O002—Sc01—O009	120.32 (10)	O005^{i}—Sc01—O004^{ii}	71.93 (9)
O002—Sc01—O007	144.34 (9)	O006—Sc01—O004^{ii}	71.60 (9)
O009—Sc01—O007	77.55 (10)	O002—Sc01—O003^{iii}	76.38 (9)
O002—Sc01—O008	67.79 (9)	O009—Sc01—O003^{iii}	72.11 (9)
O009—Sc01—O008	74.27 (10)	O007—Sc01—O003^{iii}	81.51 (9)
O007—Sc01—O008	146.50 (10)	O008—Sc01—O003^{iii}	106.24 (10)
O002—Sc01—O005^{i}	72.88 (9)	O005^{i}—Sc01—O003^{iii}	73.76 (9)
O009—Sc01—O005^{i}	138.25 (9)	O006—Sc01—O003^{iii}	143.80 (9)
O007—Sc01—O005^{i}	74.27 (9)	O004^{ii}—Sc01—O003^{iii}	142.44 (9)
O008—Sc01—O005^{i}	139.19 (9)	C00B—O002—Sc01	118.4 (2)
O002—Sc01—O006	135.12 (9)	C00A—O003—Sc01^{iii}	117.3 (2)
O009—Sc01—O006	75.09 (9)	C00C—O004—Sc01^{ii}	117.6 (2)
O007—Sc01—O006	76.84 (9)	C00B—O005—Sc01^{i}	115.9 (2)
O008—Sc01—O006	78.71 (10)	C00C—O006—Sc01	118.1 (2)
O005^{i}—Sc01—O006	125.93 (9)	Sc01—O007—H00A	111.3
O002—Sc01—O004^{ii}	79.35 (9)	Sc01—O007—H00B	110.9
O009—Sc01—O004^{ii}	145.44 (9)	H00A—O007—H00B	102.9
O007—Sc01—O004^{ii}	103.20 (10)	Sc01—O008—H00C	110.3
O008—Sc01—O004^{ii}	90.28 (10)	Sc01—O008—H00D	110.1

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*; (ii) −*x*+2, −*y*+2, −*z*; (iii) −*x*+1, −*y*+1, −*z*+1.

Table S6 Specified hydrogen bonds for **1**.

D-H...A	d(D-H)	D(H...A)	D(D...A)	<(DHA)
O(008)-H(00A)...O(009)	0.86	1.95	2.746(3)	152.6
O(008)-H(00B)...O(00E)	0.86	1.91	2.714(3)	155.9
O(00A)-H(00C)...O(009)	0.85	2.10	2.830(3)	142.9
O(00F)-H(00J)...O(00E)	0.85	2.00	2.764(4)	149.6
O(00G)-H(00K)...O(00F)	0.85	2.06	2.839	152.5

Table S7 Specified hydrogen bonds for **2**.

D-H...A	D-H	H...A	D...A	<(DHA)
O007-H00B...O00D	0.88	1.87	2.718(5)	161.4
O008-H00D...O003	0.87	2.23	2.872(3)	130.5