Doubled-basic Sr-Amino containing MOF as highly stable heterogeneous catalyst

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S1. Crystallographic data of Sr(NH_2-bdc)

Table S1. Crystallographic data for Sr(NH_2-bdc).

Chemical formula	$C_{11}H_{12}N_2O_5Sr$
Molecular weight ($g.mol^{-1}$)	339,85
Temperature (K)	100
λ (Å)	0,71073
Crystallographic system	Monoclinic
Space group	$P2_1/_n$
a (Å)	9.9671 (8)
b (Å)	7.3143 (6)
c (Å)	18.1950 (16)
α (°)	90
β (°)	90.611(3)
σ (°)	90
Volume ($Å^3$)	1326.38(19)
Z	4
ρ ($g.cm^{-3}$)	1.702
μ(mm^{-1})	4.082
F(000)	680
Crystal size (mm)	0.12 x 0.11 x 0.08
Observed reflections	3106
R_{int}	0.0273
R1 [b] / wR2 [c] [I>2σ(I)]	0.0410 / 0.0919
R1 [b] / wR2 [c] (all data)	0.0458 / 0.0951
GoF	1.272
Largest diff. pk and hole [$eÅ^{-3}$]	0.583 and -0.892

S2. Selected bonds distances and angles of Sr(NH_2-bdc)

Table S2. Selected distances (Å) and angles (°) for Sr(NH_2-bdc).

Distances		Angles			
Sr1 O1	2.458(4)	O1 Sr1 O1	149.12(10)	O3 Sr1 O3	152.98(7)
Sr1 O1	2,672(4)	O1 Sr1 O2	154.11(14)	O3 Sr1 O4	155.37(15)
Sr1 O2	2.569(4)	O1 Sr1 O3	95.48(14)	O3 Sr1 O5A	68.0(2)
Sr1 O3	2.631(4)	O1 Sr1 O3	75.87(12)	O3 Sr1 O5A	71.9(3)
Sr1 O3	2.504(4)	O1 Sr1 O4	98.27(17)	O3 Sr1 O5A	85.2(3)
Sr1 O4	2.604(5)	O1 Sr1 O5A	79.6(2)	O3 Sr1 O5B	81.0(3)
Sr1 O5A	2.723(10)	O1 Sr1 O5A	75.1(2)	O3 Sr1 O5B	126.5(3)
Sr1 O5A	2.596(9)	O1 Sr1 O5A	69.7(2)	O3 Sr1 O5B	75.3(3)
Sr1 O5B	2.685(12)	O1 Sr1 O5B	66.6(3)	O4 Sr1 O1	93.02(16)
Sr1 O5B	2.639(12)	O1 Sr1 O5B	70.3(3)	O4 Sr1 O3	50.10(15)
		O1 Sr1 O5B	83.2(3)	O4 Sr1 O5A	117.7(3)
		O2 Sr1 O1	49.50(13)	O4 Sr1 O5B	122.5(3)
		O2 Sr1 O3	110.38(13)	O4 Sr1 O5B	80.2(3)
		O2 Sr1 O4	97.34(17)	O5A Sr1 O1	135.0(2)
		O2 Sr1 O5A	86.3(3)	O5A Sr1 O3	131.3(3)
		O2 Sr1 O5A	110.8(3)	O5A Sr1 O4	83.5(3)
		O2 Sr1 O5B	92.2(3)	O5A Sr1 O5A	149.2(3)
		O2 Sr1 O5B	105.4(3)	O5A Sr1 O5B	148.6(3)
		O3 Sr1 O1	70.23(11)	O5B Sr1 O1	140.3(3)
		O3 Sr1 O1	104.20(13)	C(3B)-N(1B)-C(2B)	120(2)
		O3 Sr1 O2	81.35(14)		

S3. N_2 Isotherm at 77k of Sr(NH_2-bdc)

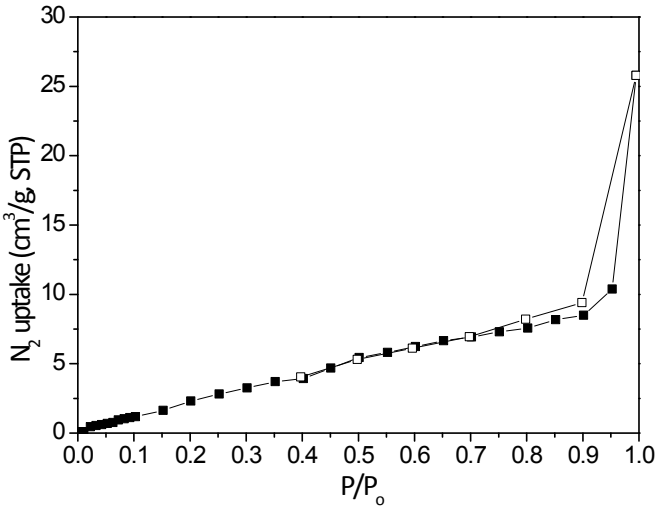

Figure S3. N_2 adsorption–desorption isotherms at 77 K.

S4. ^{1}H and ^{13}C NMR analysis of catalytic product ethyl trans-α-cyanocinnamate.

Product was confirmed by means of ^{1}H, ^{13}C NMR spectroscopy. As an example, we present here the results obtained following this reaction conditions: 80°C, using DMF as solvent, equimolar ratio of benzaldehyde/ethyl cyanoacetate, and catalyst concentration of 5 mmol of strontium. For ethyl trans-α-cyanocinnamate product different proton chemical shifts were detected in the range of 1.28 to 8.38 ppm. DMF, H_2O and starting materials were also identified in the spectra.

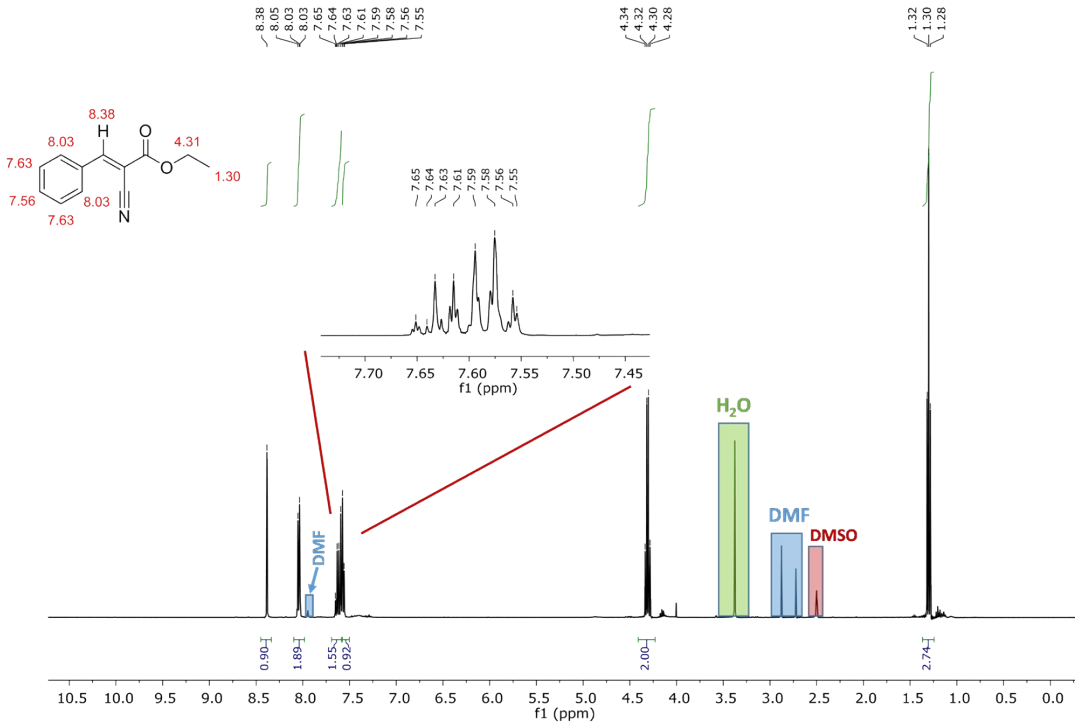

Figure S4a. ^{1}H NMR of reaction media at 300min (298 K, 400 MHz, DMSO-d6). Ethyl trans-α-cyanocinnamate product: δ 8.38 (s, 1H), 8.05-8.03 (d, J = 7.1 Hz, 2H), 7.65 – 7.55 (m, 2H), 4.31 (q, J = 7.1 Hz, 2H), 1.28 (t, J = 7.1 Hz, 3H). The following multiplicity abbreviations are used: (s) singlet, (d) doublet, (t) triplet, (q) quartet, (m) muliplet.

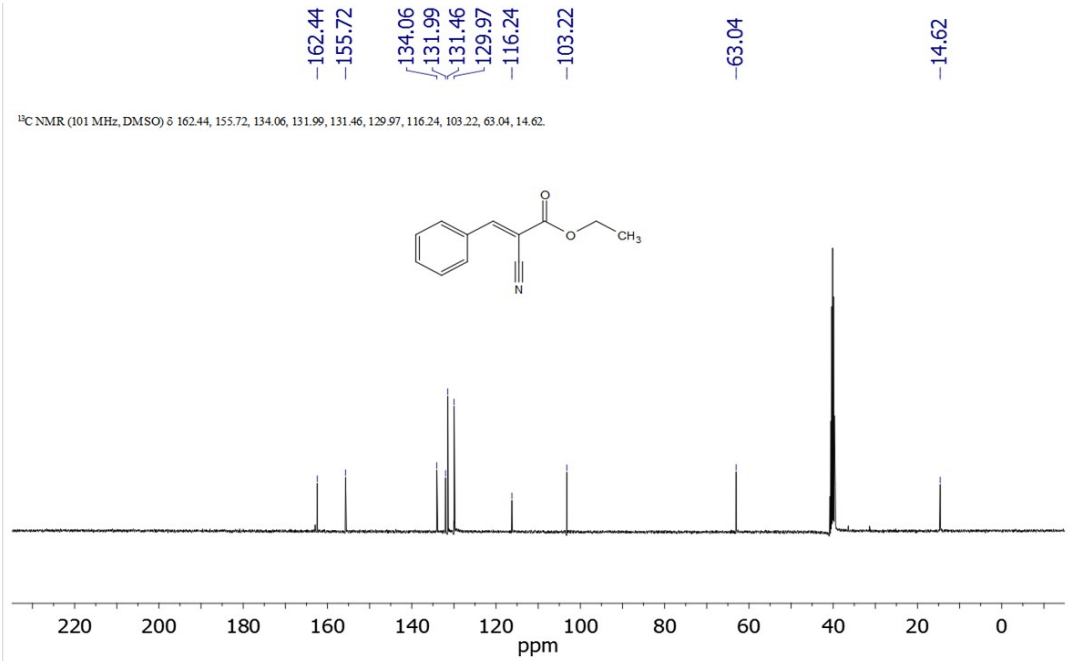

Figure S4b. ^{13}C NMR of reaction media at 300min (298 K, 100 MHz, DMSO-d6). Ethyl trans-α-cyanocinnamate product: δ 162.44, 155.72, 134.06, 131.99, 131.46, 129.97, 116.24, 103.22, 63.04, 14.62.

S5. Stability of IRMOF-3 catalyst

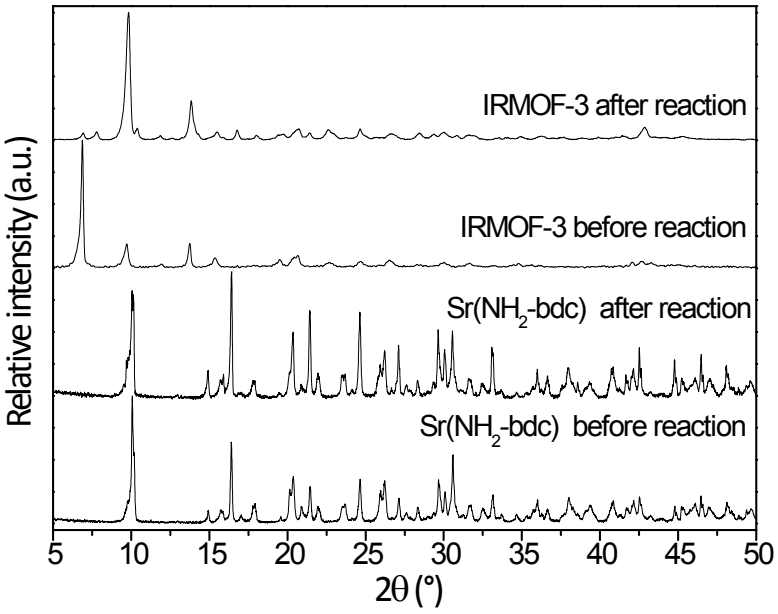

Figure S5. X-ray diffraction patterns of fresh and used IRMOF-3 and $Sr(NH_2\text{-bdc})$. Reaction conditions of the catalytic run: 80 °C, equimolar ratio of benzaldehyde and ethyl cyanoacetate and DMF as solvent.

S6. IR spectra of the Sr(NH_2-bdc) before and after catalytic activity

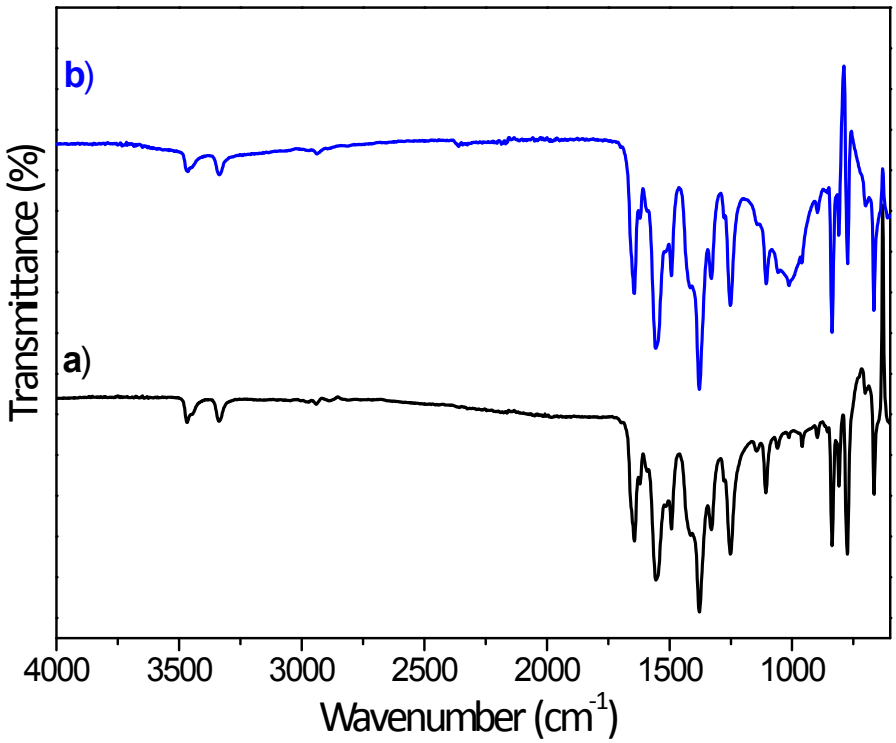

Figure S6. FT-IR spectra of the fresh (a) and used (b) Sr(NH_2-bdc). Reaction conditions of the catalytic run: 80 °C, equimolar ratio of benzaldehyde and ethyl cyanoacetate and DMF as solvent.

S7. SEM images of $Sr(NH_2\text{-bdc})$