Supporting Information

CFA-14 – a perfluorinated metal-organic framework with linear 1-D Co^{II}-chains showing temperature dependent spin-chain magnetic ordering

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1. IR- Spectrum

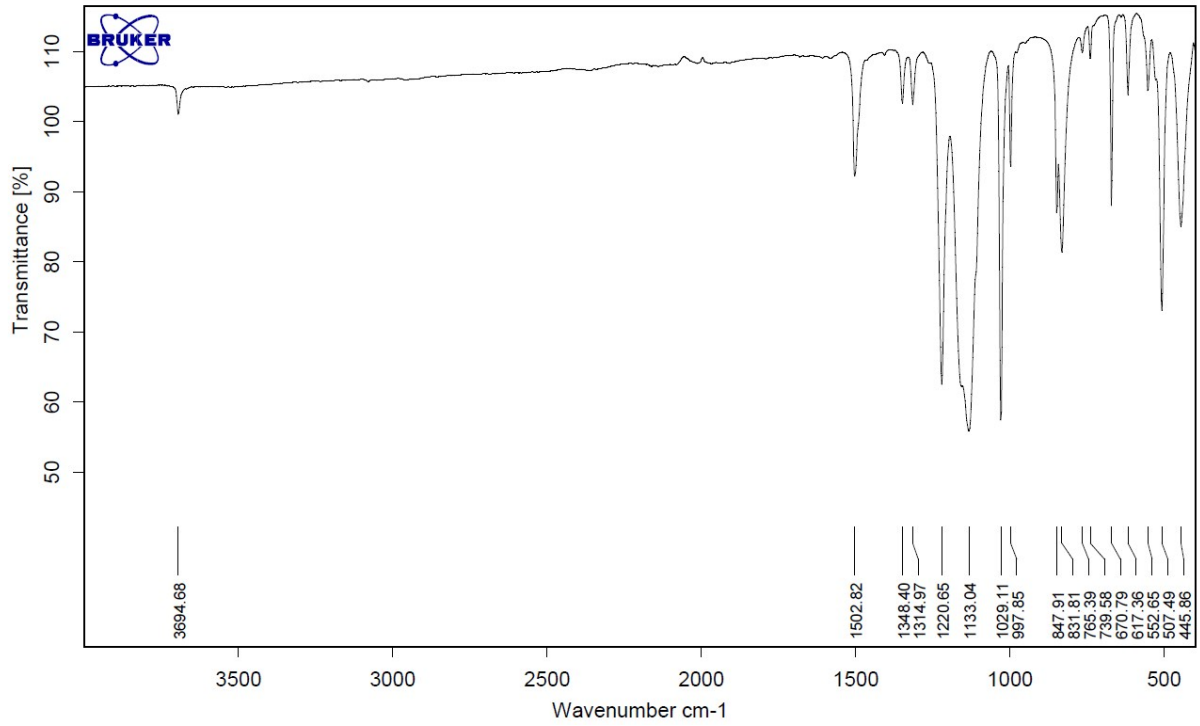

Fig. S1 Full-range IR spectrum of **CFA-14**.

2. Diffuse Reflectance Fourier-Transform IR spectra

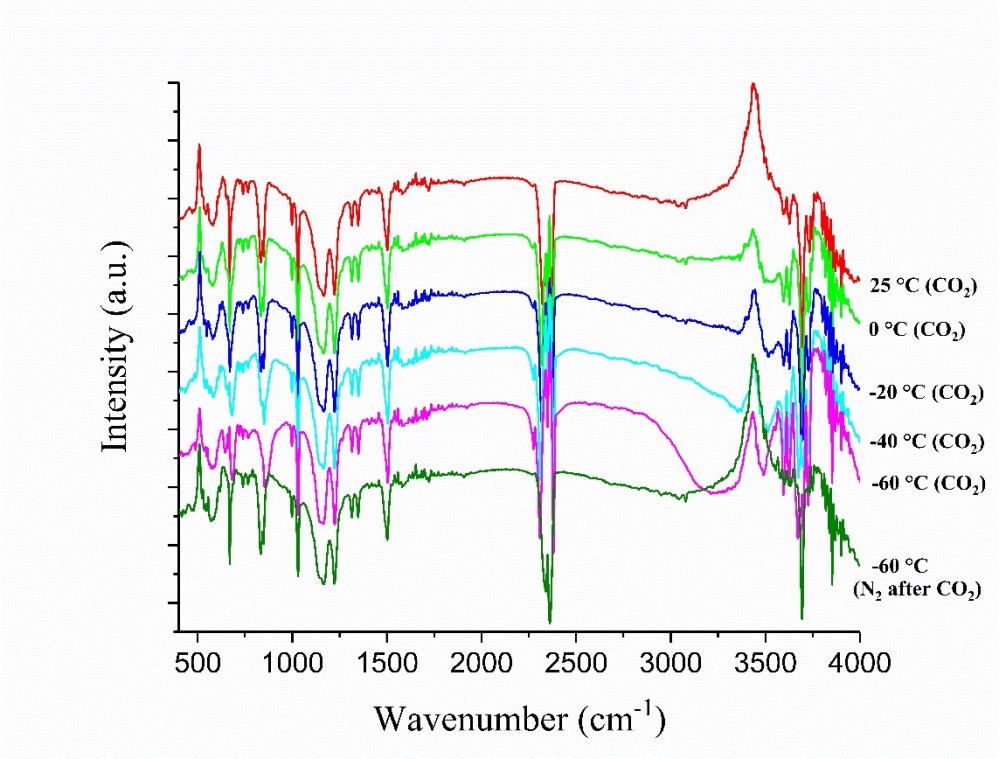

Fig. S2 In situ DRIFT spectra of **CFA-14** upon cooling from room temperature to -60 °C under CO_2 atmosphere.

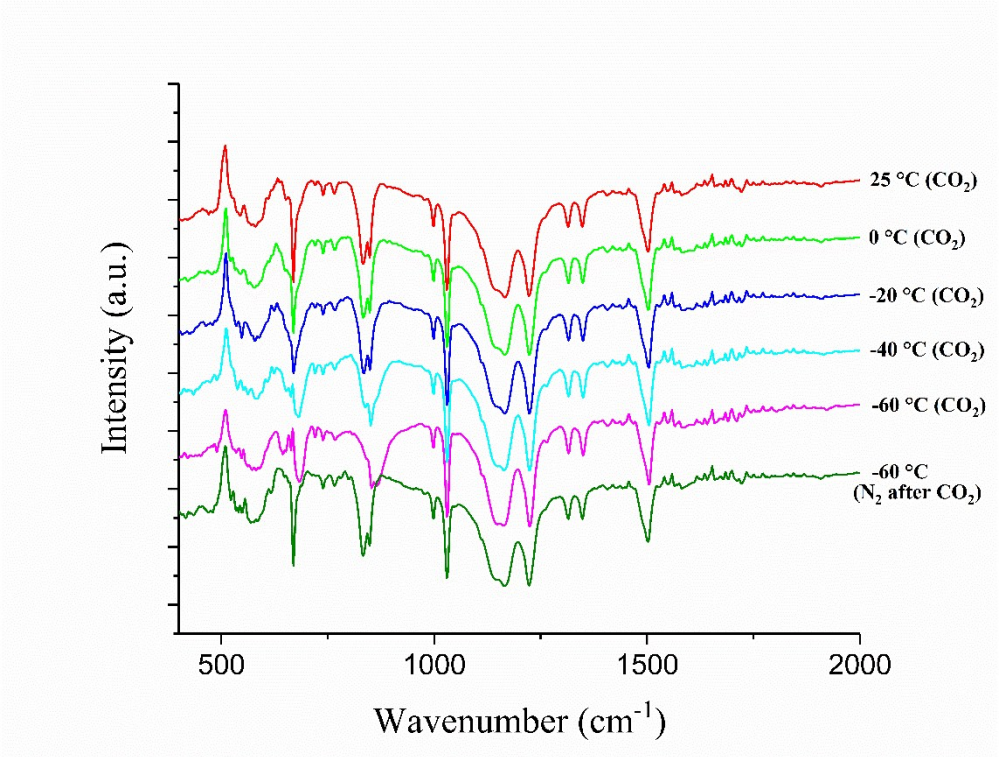

Fig. S3 In situ DRIFT spectra of **CFA-14** upon cooling from room temperature to -60 °C under CO_2 atmosphere in the range of 400 – 2000 cm^{-1}.

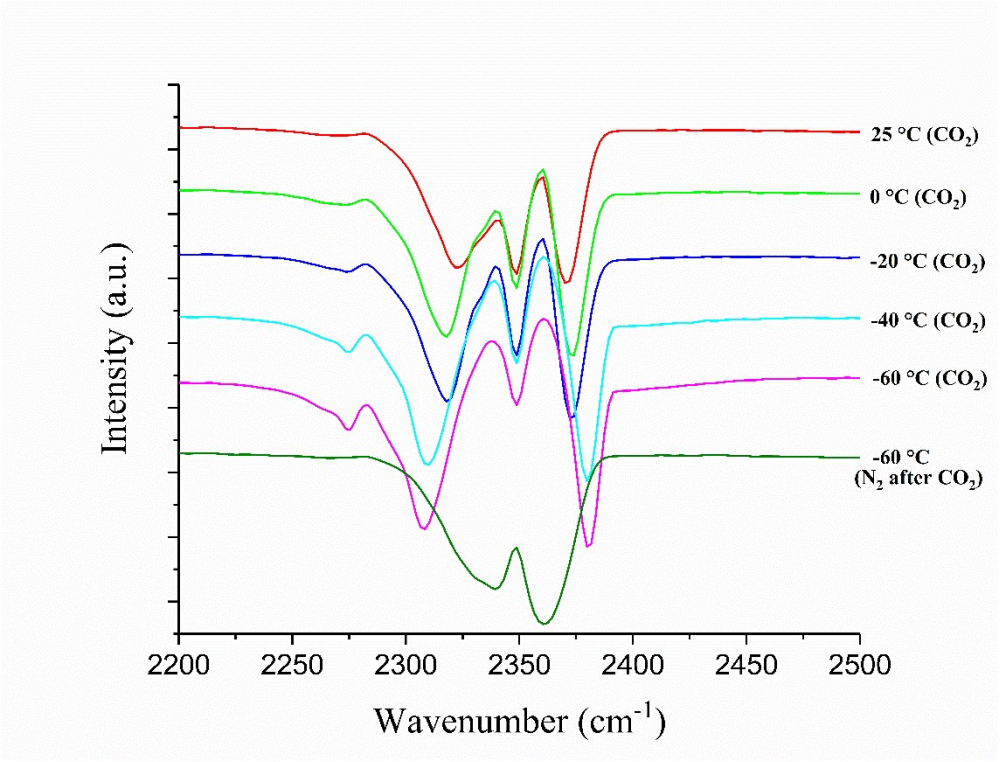

Fig. S4 In situ DRIFT spectra of **CFA-14** upon cooling from room temperature to -60 °C under CO_2 atmosphere in the range of 2200 – 2500 cm^{-1}.

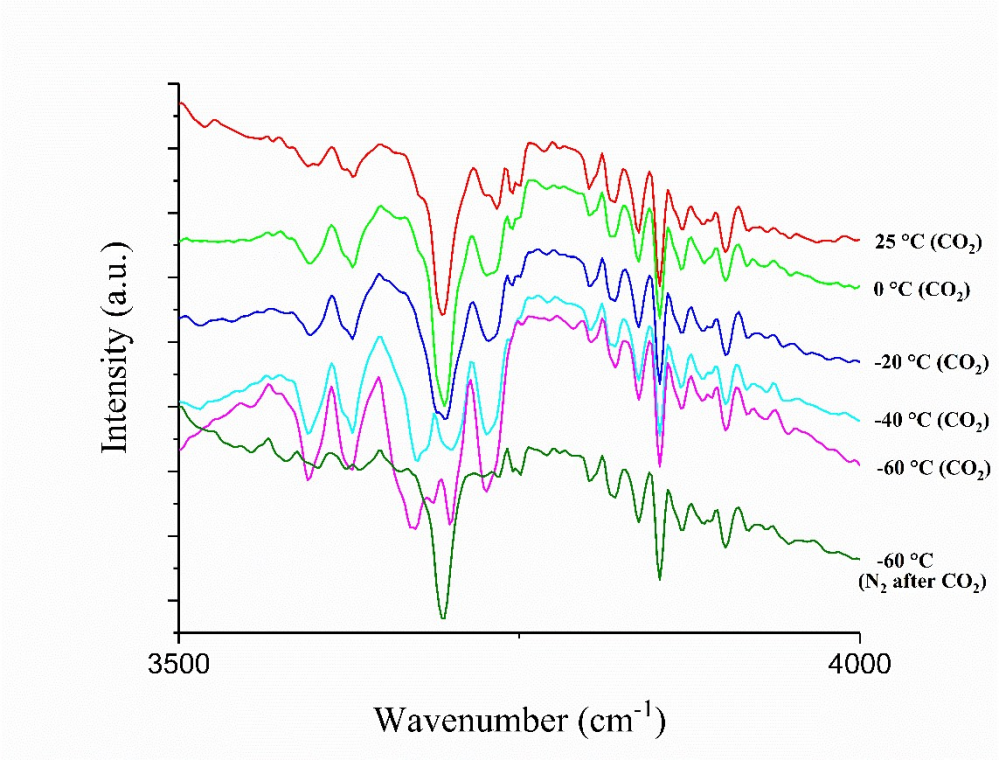

Fig. S5 In situ DRIFT spectra of **CFA-14** upon cooling from room temperature to -60 °C under CO_2 atmosphere in the range of 3500 – 4000 cm^{-1}.

3. Crystallographic data

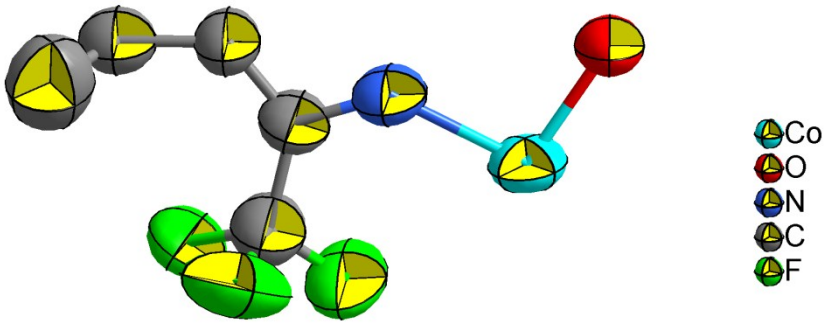

Fig. S6 ORTEP-style plot of asymmetric unit of **CFA-14**. Thermal ellipsoids probability: 50%. Hydrogen atoms have been omitted for clarity.

Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) For **CFA-14**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Co(1)	2500	4728(1)	5000	94(1)
O(1)	2727(4)	5227(4)	6250	112(4)
N(1)	1814(4)	4163(4)	5719(6)	90(2)
C(1)	1402(5)	3707(5)	5421(8)	100(3)
C(3)	495(6)	2995(6)	6250	110(5)
C(2)	1001(5)	3501(5)	6250	102(4)
C(4)	680(8)	2313(7)	6251(2)	154(6)
C(5)	1421(9)	3438(9)	4293(12)	145(5)
F(1)	1764(6)	3801(5)	3637(6)	204(5)
F(2)	893(5)	3219(6)	3914(6)	181(4)
F(3)	1768(8)	2879(7)	4249(10)	233(6)

Table S2. Bond lengths [Å] and angles [°] for **CFA-14**.

Co(1)-O(1)	1.910(6)
Co(1)-O(1)#1	1.910(6)
Co(1)-N(1)	2.015(7)
Co(1)-N(1)#2	2.015(7)
O(1)-H(1)	0.93(2)
N(1)-C(1)	1.302(12)
N(1)-N(1)#3	1.387(15)
C(1)-C(2)	1.379(13)
C(1)-C(5)	1.503(18)
C(3)-C(4)#3	1.437(16)
C(3)-C(4)	1.437(16)
C(3)-C(2)	1.45(2)
C(4)-C(4)#4	1.42(3)
C(4)-H(4)	0.9500
C(5)-F(2)	1.251(15)
C(5)-F(1)	1.301(15)
C(5)-F(3)	1.34(2)
O(1)-Co(1)-O(1)#1	115.8(3)
O(1)-Co(1)-N(1)	96.4(3)
O(1)#1-Co(1)-N(1)	119.7(2)
O(1)-Co(1)-N(1)#2	119.7(2)
O(1)#1-Co(1)-N(1)#2	96.4(3)
N(1)-Co(1)-N(1)#2	110.5(5)
Co(1)-O(1)-Co(1)#5	113.7(5)
Co(1)-O(1)-H(1)	123.1(3)
Co(1)#5-O(1)-H(1)	123.1(3)
C(1)-N(1)-N(1)#3	106.6(5)
C(1)-N(1)-Co(1)	136.4(6)
N(1)#3-N(1)-Co(1)	116.6(2)
N(1)-C(1)-C(2)	112.7(9)
N(1)-C(1)-C(5)	120.5(9)
C(2)-C(1)-C(5)	126.7(10)
C(4)#3-C(3)-C(4)	120.3(19)
C(4)#3-C(3)-C(2)	119.9(10)
C(4)-C(3)-C(2)	119.9(10)
C(1)#3-C(2)-C(1)	101.3(12)
C(1)#3-C(2)-C(3)	129.4(6)

C(1)-C(2)-C(3)	129.4(6)
C(4)#4-C(4)-C(3)	119.9(10)
C(4)#4-C(4)-H(4)	120.1
C(3)-C(4)-H(4)	120.1
F(2)-C(5)-F(1)	115.2(15)
F(2)-C(5)-F(3)	97.8(13)
F(1)-C(5)-F(3)	100.0(14)
F(2)-C(5)-C(1)	117.2(13)
F(1)-C(5)-C(1)	112.8(11)
F(3)-C(5)-C(1)	111.1(15)

Symmetry transformations used to generate equivalent atoms:

#1 -y+3/4,x+1/4,z-1/4 #2 -x+1/2,y,-z+1 #3 y-1/4,x+1/4,-z+5/4

#4 -y+1/4,-x+1/4,-z+5/4 #5 y-1/4,-x+3/4,z+1/4

Table S3. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **CFA-14**. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2 a^{*2} U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Co(1)	110(2)	114(2)	57(1)	0	8(1)	0
O(1)	136(6)	136(6)	64(6)	-19(4)	19(4)	-45(6)
N(1)	98(5)	111(6)	59(4)	9(4)	6(3)	-9(5)
C(1)	120(8)	123(8)	57(5)	-12(5)	0(5)	-28(6)
C(3)	124(8)	124(8)	82(10)	-7(6)	7(6)	-15(11)
C(2)	116(7)	116(7)	74(8)	-11(5)	11(5)	-29(9)
C(4)	147(10)	126(11)	190(16)	1(9)	45(9)	2(8)
C(5)	154(12)	179(14)	102(10)	-24(10)	26(9)	-72(11)
F(1)	283(10)	253(11)	78(5)	-39(5)	45(6)	-128(9)
F(2)	156(7)	290(12)	98(5)	-64(6)	1(4)	-52(7)
F(3)	302(14)	254(13)	142(8)	-82(9)	50(8)	21(11)

4. Gas sorption measurements

The isosteric heats of adsorption were calculated from the measured isotherms (Fig. S4) using the Clausius-Clapeyron equation (**I**). The slopes of linear plots lnP versus 1/RT for different loadings (Fig. S5) give the adsorption enthalpies, according to the equation (**II**).

$$Q_{st} = -R\left(\frac{\partial(\ln P)}{\partial(1/T)}\right)_{\theta}$$ (**I**), Θ – surface coverage

$$\ln P = -\frac{Q_{st}}{R}\left(\frac{1}{T}\right) + C$$ (**II**), C – integration constant

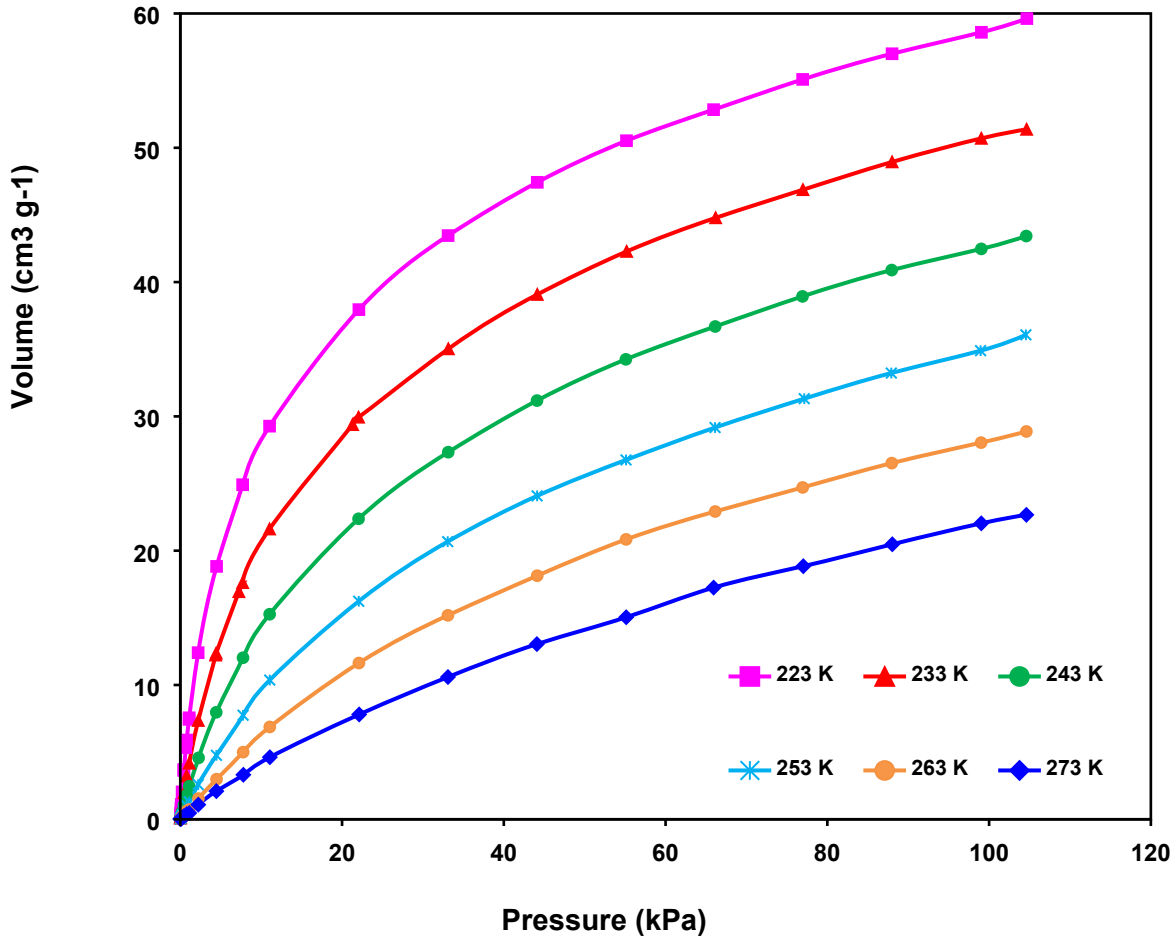

Fig. S7 CO_2 adsorption isotherms for **CFA-14** at different temperatures.

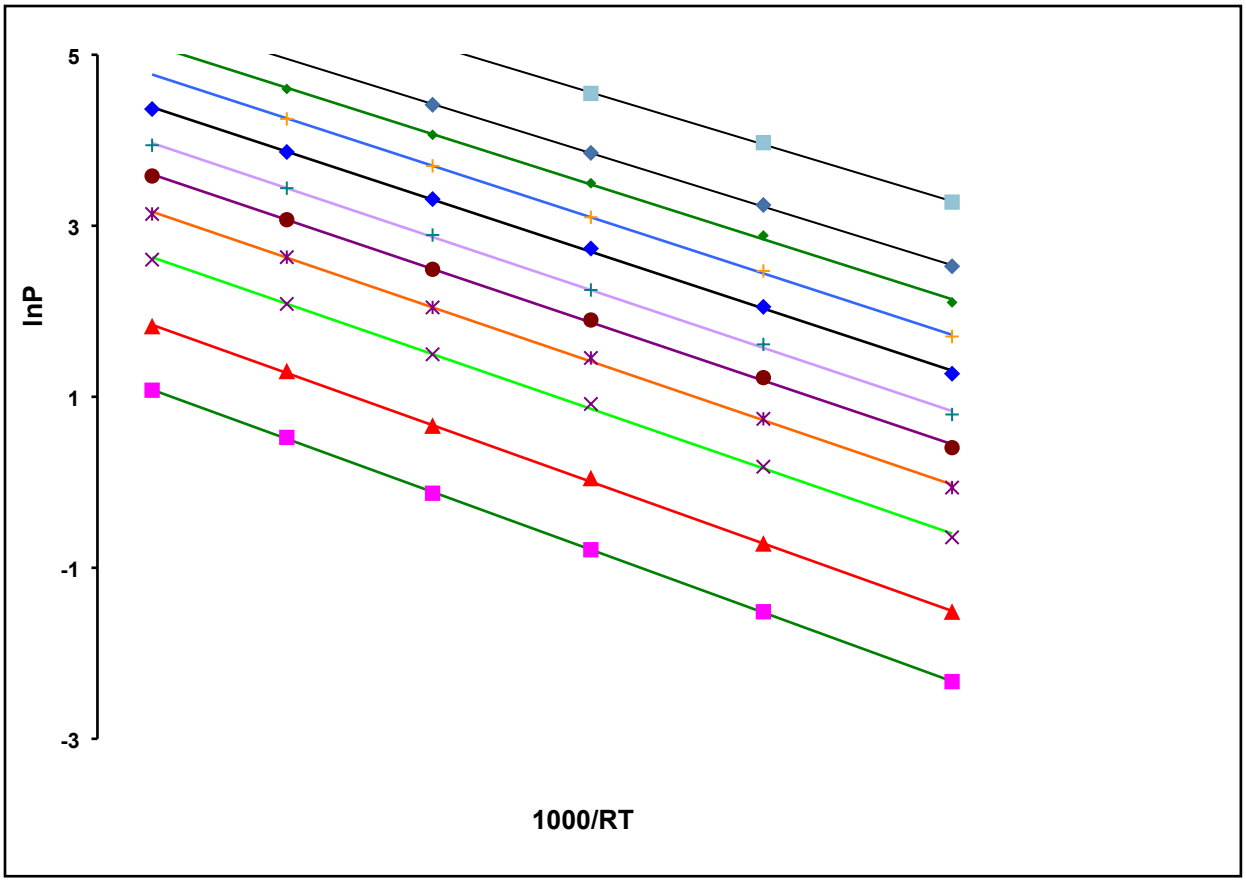

Fig. S8 lnP versus 1/RT plots for different loadings for CO_2 adsorption on **CFA-14**.