## SUPPORTING INFORMATION

A Cd mixed-ligand MOF showing Ligand-Disorder Induced Breathing Behavior at High Temperature and Stepwise, Selective Carbon Dioxide Adsorption at Low Temperature

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Hydrogen bonding	D-H / Å	H…A /	D···A / Å	D-H···A /	Symmetry
atoms		A		•	operators
104 K					
C4A-H4A…O1S1	0.95	2.60	3.472(10)	153	1-x,1-y,1-z
C12A-H12A…O1S1	0.95	2.48	3.374(10)	156	1-x,1-y,1-z
C5A-H5A…O6D	0.95	2.40	3.151(6)	136	x,-1+y,z
C9A-H9A…O4D	0.95	2.48	3.412(10)	168	1-x,2-y,1-z
298 K					
C5A-H5A···O6D	0.93	2.45	3.1749(9)	135	x,-1+y,z
C9A-H9A…O4D	0.93	2.48	3.3928(12)	166	1-x,2-y,1-z
323 K					
C5A-H5A…O6D	0.93	2.42	3.139(12)	135	x,-1+y,z

 Table S1 C-H…O hydrogen bonding parameters as obtained from PLATON







Figure S1 (a) DSC and (b) TGA thermograms of 1







**Figure S2.** (a) Adsorption and desorption isotherms for carbon dioxide at 273 K, 280 K, 290 K and 298 K and (b) heat of adsorption values calculated for load values ranging from 5.6-15.5 cm<sup>3</sup> (STP) g<sup>-1</sup>



Figure S3. PXRD patterns of 1 before and after  $CO_2$  sorption at 195 K compared to the VT-PXRD patterns at 303 K and returned to 303 K.