Supporting information

1 breakthrough setup

Fig. S.1 shows a simplified scheme of the breakthrough setup.

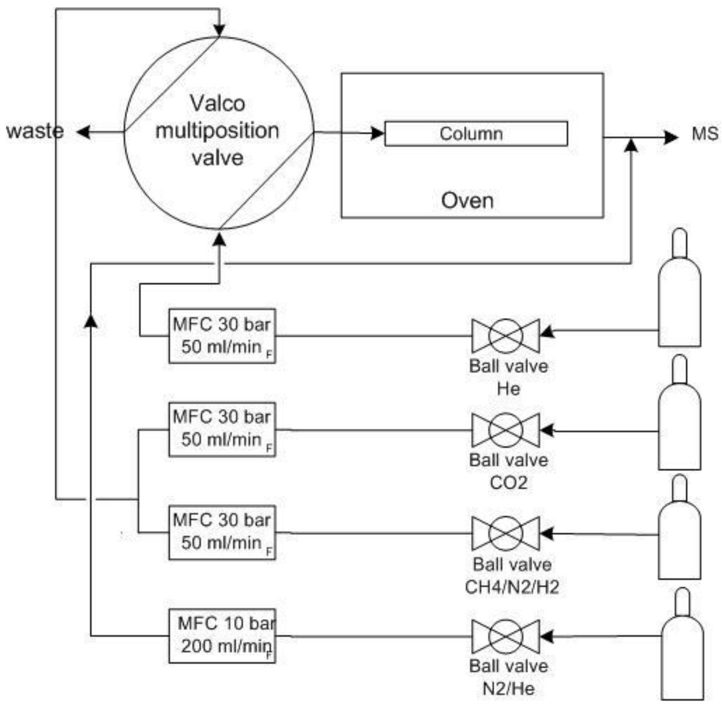

Fig. S.1 Simplified scheme of the breakthrough setup; MFC: Mass flow controller

A stainless steel column with a length of 30 cm and an internal diameter of 0.216 cm was filled with MIL-47 or NH_2-MIL-47 pellets having a diameter ranging from 500 to 650 µm. These pellets were obtained by pressing the powder of the materials into a solid disc at high pressure (740 bar), followed by crushing and sieving to obtain the desired fraction. This column was placed in a ventilated thermostatted oven. A Valco four-way valve was used to switch the gas stream flowing through the column from pure helium to a desired adsorbate mixture containing CO_2, and CH_4. Gas flows were regulated with mass flow controllers (MFCs) (Gefran Flowcor). Temperature of the experiments was 30 °C, total flow 10 Nml/min and a total pressure of 1 bar was maintained. The gas flow at the outlet of the column was measured on-line by means of a mass spectrometer (MS). In order to obtain a linear correlation between the measured MS signals and the flow rates, a permanent N_2 dilution flow of 100 Nml/min was added after the column outlet and before the MS inlet. Before every measurement, the material was regenerated by heating it in a helium flow (10 Nml/min) to 393 K and maintaining this temperature for half an hour.

The amount adsorbed for gas a, q_a, was calculated using the method of Malek and Farooq[1]:

The adsorption separation factor α between two components i and j is defined as:

$$\alpha = \frac{q_i/x_i}{q_j/x_j}$$

2 Pulse gas chromatography:

Pellets of 400-500 µm, obtained by pressing the amino-MIL-47(V) powder into a solid disc followed by crushing and sieving, were packed into a stainless steel column (1/8”) with a length of 0.30 m and an internal diameter of 0.216 cm. Pulse chromatographic experiments were performed using this column to determine low coverage adsorption properties of methane and CO_2. A HP-4890 gas chromatograph (GC) equipped with a thermal conductivity detector (TCD) was used. In situ activation of the adsorbent was performed under constant Helium flow by raising the temperature from ambient to 393 K at a rate of 1 K/min and maintaining this temperature overnight. Helium was used as the carrier gas. Henry adsorption constants were determined from the first moment of the response curve on the TCD after injection of a component. Adsorption enthalpy was obtained from the temperature dependence of the Henry adsorption constants using the van’t Hoff equation. Different temperatures were used to perform these experiments, ranging from 297K till 353K. The Henry constants of the corresponding temperatures can be found in table S1.

Table S1: Henry constants (mol/kh/Pa) of CO_2 and CH_4

	25°C	30°C	35°C	40°C	45°C	50°C	60°C	80°C
CO_2	$1.14\ 10^{-5}$	$9.83\ 10^{-6}$	$8.40\ 10^{-6}$	$7.19\ 10^{-6}$	$6.28\ 10^{-6}$	$5.47\ 10^{-6}$	$4.27\ 10^{-6}$	$2.92\ 10^{-6}$
CH_4	$2.72\ 10^{-6}$	$2.56\ 10^{-6}$	$2.23\ 10^{-6}$	$2.08\ 10^{-6}$	$1.93\ 10^{-6}$	$1.85\ 10^{-6}$		

3 Additional characterization results of NH_2-MIL-47 and MIL-47

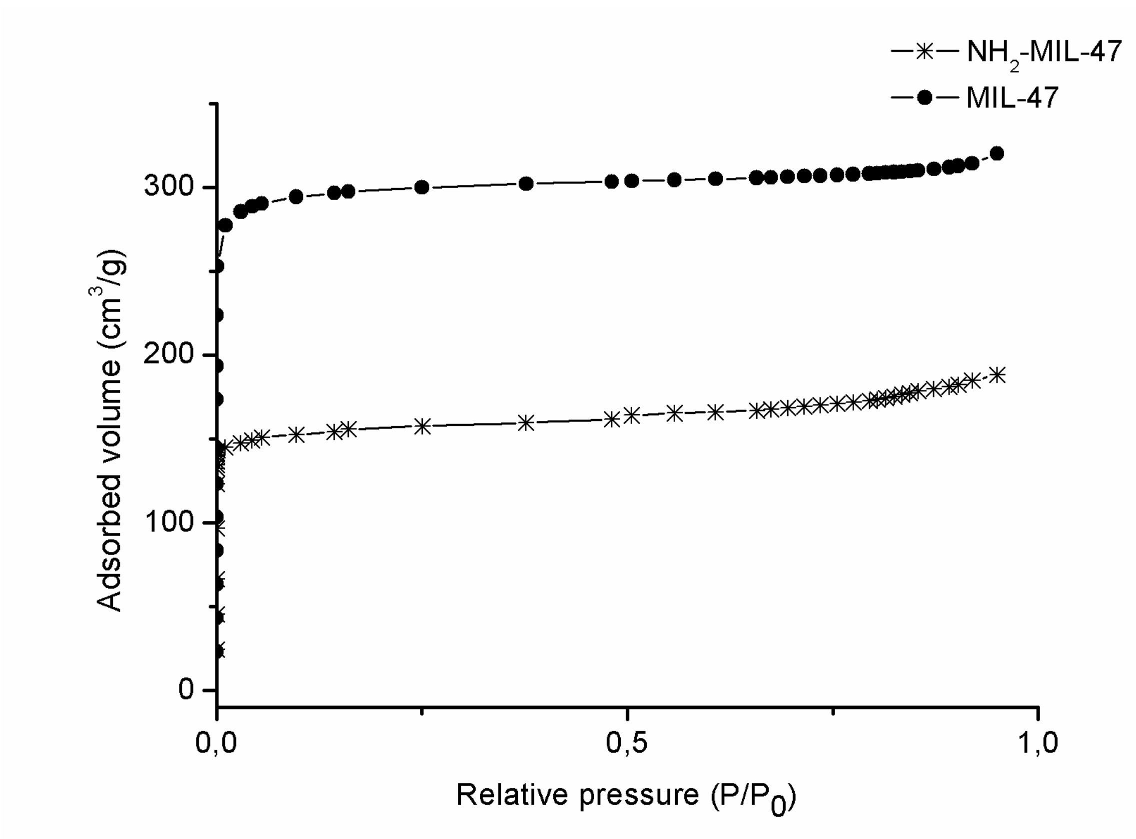

Fig. S.2 Nitrogen adsorption isotherms of MIL-47 and NH_2-MIL-47

4 Periodic VASP calculations:

The geometry of the periodic system with inclusion of the guest molecules is optimized by means of the Vienna Ab Initio Simulation Package (VASP)[2-5] making use of the PBE exchange correlation functional[6,7]. The unit cell has been doubled along the **a** direction to prevent self interactions between the adsorbates.

For those simulations, we restricted the Brillouin zone to the **Γ**-point. The projector augmented wave approximation (PAW) [8] together with a plane wave basis set was used. A kinetic energy cut off of 600 eV has been chosen for all the calculations. Throughout the different optimization steps, the convergence criterion for the electronic self-consistent field (SCF) problem is set to 10^{-6} eV. The quasi-newton algorithm has been chosen as optimizer to converge the atomic forces below 0.01 eV/Å. To improve convergence, a Gaussian smearing of 0.05 eV was also applied[5]. The van der Waals corrections for the PBE functional are used throughout the optimization, as implemented in the 5.2.11 edition of VASP. The MIL-47 and the NH_2-MIL-47, were initially constructed with similar cell parameters as the MIL-53(Fe) series and then subjected to a cell optimization with those criteria[9]. Almost orthogonal unit cells ($\alpha = \beta = \gamma = 90°$) were obtained (MIL-47: **a** = 6.752, **b** = 17.541, **c** = 12.274; NH_2-MIL-47: **a** = 6.725, **b** = 17.861, **c** = 11.836). Afterwards, the unit cell is doubled along **a** in order to prevent self interactions between the adsorbates during the adsorption study. Such interactions can occur if the adsorbate would interact too strongly with their image in the neighbouring unit cells along the channel of the pores. The exact cell vectors were maintained during the adsorption study and are given for all adsorption geometries in Section S.5 and S.6. The fact that the cell parameters resemble more the MIL-47 *as*, is due to the initial construction of MIL-47 and NH_2-MIL-47 from the MIL-53(Fe) series[9]. However this is not a disadvantage, because the slightly more narrow pores will give optimal stabilization for the adsorbates and might even represent the small unit cell contraction at low adsorbate loadings.

5 Adsorption geometries of CO_2 and CH_4 on the (amino-) terephthalate linkers

5.1 CH_4 adsorbed on terephthalic acid

23

C	-1.240634	0.411548	0.132918
C	-0.037406	1.111631	0.194383
C	1.179641	0.451217	0.027648
C	1.189068	-0.917087	-0.197954
C	-0.014180	-1.618776	-0.254762
C	-1.231743	-0.956839	-0.092616
C	-0.100960	2.572429	0.485077
H	2.105688	1.008278	0.083593
H	2.117426	-1.459335	-0.328418
C	0.051820	-3.089312	-0.494373
H	-2.157386	-1.515176	-0.139979
H	-2.168533	0.952445	0.272630
O	-1.162797	-3.667299	-0.529779
O	1.068751	-3.710555	-0.642164
H	-1.026291	-4.610716	-0.688315
O	1.114802	3.145720	0.548803
O	-1.116951	3.189415	0.657412
H	0.979296	4.081018	0.750775
C	0.119366	0.962557	3.453616
H	0.081273	-0.036662	3.019359
H	-0.775674	1.515797	3.167791
H	0.171017	0.890220	4.539338
H	1.003275	1.482012	3.081887

5.2 CO_2 adsorbed on terephthalic acid

21

C	0.513018	0.099661	0.999451
O	1.639240	0.298748	0.834661
O	-0.614709	-0.097892	1.151938
C	-1.379445	0.652116	4.365846
C	-0.177822	1.340561	4.208275
C	1.023395	0.647724	4.048554
C	1.015775	-0.740239	4.042031
C	-0.187580	-1.427634	4.195891
C	-1.386535	-0.734562	4.360719
C	-0.225734	2.831737	4.217473
H	1.949350	1.194454	3.925320
H	1.931229	-1.305734	3.915920
C	-0.142367	-2.918538	4.165807
H	-2.312444	-1.282419	4.475334
H	-2.294654	1.218591	4.485261
O	-1.348035	-3.480715	4.361913
O	0.853468	-3.564852	3.985269
H	-1.228064	-4.438833	4.322635
O	0.982159	3.392041	4.025241
O	-1.223774	3.479872	4.375644
H	0.861343	4.350630	4.046705

5.3 CH_4 adsorbed on amino-terephthalic acid

25

C	1.286667	-0.380832	-0.337777
C	0.536843	-1.530835	-0.044615
C	-0.836807	-1.489693	0.050473
C	-1.483934	-0.264649	-0.158899

C	-0.773314	0.881871	-0.449273
C	0.633817	0.858232	-0.540648
C	-2.971917	-0.237314	-0.044617
O	-3.494173	0.989065	-0.240150
N	1.302547	2.019855	-0.774163
C	2.754450	-0.464912	-0.430220
O	3.238480	-1.697394	-0.189777
O	-3.653085	-1.195612	0.197539
O	3.498383	0.453953	-0.696353
H	-1.296695	1.819418	-0.593433
H	1.066251	-2.461881	0.108461
H	-1.421935	-2.370114	0.278539
H	4.199026	-1.641783	-0.276567
H	-4.452357	0.907332	-0.146426
H	2.296944	1.994360	-0.940159
H	0.779236	2.838774	-1.030118
C	0.183467	1.130271	2.794636
H	0.443139	1.131153	3.852807
H	0.945964	1.666880	2.229620
H	0.119413	0.103343	2.433202
H	-0.780350	1.620140	2.655771

5.4 CO_2 adsorbed on amino-terephthalic acid

23

C	-1.257221	-0.172109	0.051650
C	-0.530139	-1.370941	0.055206
C	0.848584	-1.374754	0.034419
C	1.521043	-0.148127	0.016983

C	0.829080	1.048778	0.019600
C	-0.577992	1.067496	0.033221
C	3.013729	-0.173505	-0.000131
O	3.560893	1.055944	-0.032708
N	-1.228337	2.272538	0.107161
C	-2.733787	-0.206175	0.068695
O	-3.237192	-1.446658	0.190291
O	3.675861	-1.174731	0.012355
O	-3.460284	0.757369	-0.023986
H	1.371385	1.986633	0.024319
H	-1.078295	-2.303407	0.073212
H	1.417778	-2.294462	0.034537
H	-4.199410	-1.359158	0.195085
H	4.520265	0.941007	-0.037541
H	-2.220016	2.284151	-0.084855
H	-0.697378	3.096813	-0.122276
C	-0.927316	1.776866	2.975627
O	0.007968	2.455197	2.998321
O	-1.858191	1.093102	2.976657

6 Adsorption geometries of CO_2 and CH_4 within MIL-47 and MIL-47-NH_2

presented in POSCAR format, can be opened by molden[10].

6.1 CH_4 adsorbed within MIL-47

```
V O C H
  1.00000000000000
   13.5306685888651756    0.0057087870689278   -0.0003857084078472
    0.0065556329053147   16.2735692524908728    0.0003113444397211
   -0.0005690401423668    0.0000998239597547   13.9790236252066276
    8    40    65    36
Direct
  0.3409376006500007  0.2472985233615148  0.7374556019388231
  0.3985597953804295  0.7473079847899508  0.2377676806936730
  0.5909131297715451  0.2472646625040766  0.7648561169680802
  0.6485814732996348  0.7472157177821805  0.2650184845470963
  0.8409272529689035  0.2472896623729724  0.7374194454184604
  0.8985517391994642  0.7472265132427259  0.2374217311927755
  0.0909376424280735  0.2472747028326491  0.7648169922288435
  0.1485555642965539  0.7473023865373084  0.2648625464581714
  0.7251532152135308  0.2472063181294424  0.6973487509689298
  0.3980355887119510  0.1619898153556839  0.6521273514213092
  0.3149504434149739  0.1584971517856467  0.8330017591067044
  0.5143224471529050  0.7474688813948620  0.1976724133680403
  0.4751548005202984  0.2473427528851104  0.8049814830307819
  0.2642748969604196  0.7472545131494007  0.3051328181760400
  0.3416977757877714  0.8329808464273287  0.1527416943394559
  0.6475067736386154  0.3331932416307966  0.8495830849194910
  0.5917772660847270  0.6614618914949325  0.3498729968467808
  0.5917024673710463  0.8322139222217703  0.3508538104926291
  0.6481648082383876  0.1622960013619034  0.8505573358556242
```

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0.5644936298069488	0.3354248801384951	0.6686992368648880
0.6748499749064459	0.6588651553797784	0.1689878196045034
0.6746274110954036	0.8360849877993914	0.1695324908564207
0.5648510926601680	0.1581954144389498	0.6697241788796843
0.4248360170796207	0.6585153199781001	0.3331425980958020
0.3145480530071888	0.3357646983093486	0.8332502568459851
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0.8963549847510184	0.4456653211014730	0.9197789412937861
0.8431312105084213	0.5490475067872901	0.4198445669473084
0.8428346627531975	0.9461403658968005	0.4198110195319227
0.8965633763497860	0.0482542085673818	0.9197668783948395
0.0931590396250217	0.5492985460549378	0.0820477380081765
0.1464896123836991	0.4452206986430486	0.5819497060262865
0.4678287927196283	0.6232396732180846	0.6548643922608929
0.4117788301786131	0.7007274281787512	0.5817668654249378
0.4593029760571864	0.7270316930399325	0.6975534840031341
0.5425220551681366	0.7018601672647945	0.6021225921793375

6.2 CO_2 adsorbed within MIL-47

V O C H

1.00000000000000

13.5306685888651756	0.0057087870689278	-0.0003857084078472
0.0065556329053147	16.2735692524908728	0.0003113444397211
-0.0005690401423668	0.0000998239597547	13.9790236252066276

8 42 65 32

Direct

0.3398825294465189	0.2484199744291142	0.7360735852687805
0.3984230457271967	0.7487083464660749	0.2359086338479766
0.5900190338228383	0.2491163386443221	0.7637253063342218
0.6484231060808940	0.7485582000634117	0.2636625950559596
0.8400383138524337	0.2483888662791151	0.7361447742684352
0.8984961260157185	0.7485111804400951	0.2361620125611406
0.0899892366154348	0.2484106407397255	0.7637152406502412
0.1484858086612024	0.7482301015730697	0.2635900031611515
0.7241746746172824	0.2491299763682141	0.6962004531319811
0.3972054758197314	0.1620425145362406	0.6522843188765706
0.3138707551478667	0.1609131383698501	0.8331770622885515
0.5142797351517953	0.7491426969551295	0.1960224255934584
0.4742582748458943	0.2491543043791409	0.8037147947827823
0.2642856858082170	0.7483107573092558	0.3035963866668520
0.3415174749725675	0.8346724480353626	0.1516447233279875
0.6465778470046484	0.3358259608554120	0.8476501325318939
0.5914986727525992	0.6621171124845853	0.3477056276956810
0.5914426894596968	0.8330271229613677	0.3501233987893275
0.6474144386240885	0.1646409942826875	0.8501974136452584
0.3415247353226587	0.6641097864050529	0.1494269327308060

0.3966726778002973	0.3326854067250818	0.6490012275215603
0.4245868751278611	0.8365708899421818	0.3327514239213653
0.5633414570185659	0.3375280946928925	0.6677193785240287
0.6747900954362329	0.6610137924469289	0.1666581231626917
0.6745302943237309	0.8382331663129956	0.1693227805337875
0.5641843802780949	0.1597312584066002	0.6687531789173020
0.4245705281480189	0.6594074881429758	0.3306242056281982
0.3136603058905452	0.3382490026953375	0.8299171702438278
0.2241542195185693	0.2477372921658728	0.6959470086551715
0.8971638556935627	0.1636726143401780	0.6501103468768086
0.8139029503954792	0.1589284500717352	0.8306682713165802
0.0142322227446072	0.7485849778168784	0.1960480055637926
0.9741819195543417	0.2483222305867074	0.8037137782344936
0.7641875326250049	0.7480304854676276	0.3037121560463223
0.8412831433166429	0.8341942276955945	0.1512849410716179
0.1469786136203916	0.3342460952589121	0.8482753877027103
0.0917076043270254	0.6625163446227096	0.3485411734719522
0.0914429318392146	0.8335069303833681	0.3492177009450133
0.1469151203039990	0.1634788391140767	0.8495968117640494
0.8417869980888719	0.6633720996680629	0.1504384532247603
0.8966187325852328	0.3345279489414234	0.6517770102737044
0.9245497975176388	0.8367882633541514	0.3321554308854631
0.0636648234205874	0.3364542727397661	0.6674713087187429
0.1748367742811718	0.6599092921353159	0.1677203883561425
0.1745336770842683	0.8370542998838477	0.1680372648038126
0.0638510289522925	0.1592002698529962	0.6686761700143095
0.9248157534402396	0.6596815196609693	0.3315446601305134
0.8138773027411043	0.3355660924604122	0.8337414867502971

0.6840570290008917	0.5318132656078035	0.7408919310060751
0.5177605775106484	0.5208042451747501	0.7881206733215494
0.4027988371492698	0.0340782185778449	0.5207199699853124
0.5805027660574440	0.0261850740081943	0.5461412809480921
0.4888351315851094	0.0631628447634240	0.5655951599939052
0.4829330459288199	0.1333448967735170	0.6337891484841034
0.3358642279826991	0.9624511187660314	0.0198354169706868
0.6530398061964698	0.4613726042375372	0.9820180979657075
0.5859146758505311	0.5323735198702665	0.4770433125394377
0.5860620082486216	0.9607559461763169	0.4823737307178129
0.6526378007753403	0.0362467663424768	0.9820701311478908
0.3350112602514965	0.5388901338974634	0.0133014204629637
0.4016739302046886	0.4622831141143788	0.5188214317505698
0.6583174851988847	0.9709654047457433	0.0460273422862360
0.3292165980104166	0.4736402101991609	0.9493037319301373
0.4075676709610198	0.5276809692381640	0.4550755015879509
0.4083621793928923	0.9686900781195322	0.4569260733817260
0.3302241846537985	0.0279640606799766	0.9562227357072586
0.6586393215253209	0.5273517626117403	0.0449912940569869
0.5800936361202927	0.4666990097262410	0.5404029481165313
0.2498605391749676	0.9333580331323693	0.0647238310288068
0.7389503957610726	0.4324055038798246	0.9367116158751566
0.4996981282967352	0.5631202847644786	0.4340417755541664
0.5000454324440006	0.9317746249957660	0.4373820482761065
0.7384790006613594	0.0647712651484570	0.9364017625438962
0.2500532262692130	0.5652917921694145	0.0622227115889280
0.4879015068782380	0.4316099272501056	0.5619231839427891
0.2557672903918721	0.8633139134763919	0.1330250524386494

0.7327717561124846	0.3627860058676932	0.8678736410192049
0.5058086884356698	0.6332857297482825	0.3658806251515019
0.5058329696153014	0.8620895123303030	0.3684972724837294
0.7327133273761347	0.1344485199298278	0.8674941842126194
0.2560286934590438	0.6347669781079577	0.1313468184346411
0.4819799084370573	0.3622041926506719	0.6311142993284891
0.9025454496739654	0.0349954014315097	0.5190034126543090
0.0800903554318970	0.0266400352597089	0.5453144176504939
0.9884459752569446	0.0638525730750609	0.5642941581290868
0.9826554527921449	0.1339438966512342	0.6326002994578211
0.8357896483768777	0.9622660999467492	0.0194593254593909
0.1532367041781795	0.4607781301853710	0.9823307809779804
0.0861152984923466	0.5339973124460916	0.4798534424091271
0.0857861037447747	0.9612017301098251	0.4815963726773798
0.1525235738705758	0.0358516761806311	0.9818294737080003
0.8361276982209384	0.5355775934791476	0.0182764772295208
0.9021786749088305	0.4628117427150689	0.5202191741004799
0.1581528043703381	0.9703303504575818	0.0454294009031213
0.8305213084220168	0.4697536326931330	0.9551276488256898
0.9080529169815559	0.5280146823499713	0.4562032392562244
0.9082268148336413	0.9695217590369269	0.4553277464208411
0.8300994093145250	0.0275161066950642	0.9554731446683213
0.1590519422934396	0.5260943924902222	0.0461845857638010
0.0802680721970572	0.4687135692898045	0.5437559229231991
0.7499174769926445	0.9336585642261986	0.0650027946902683
0.2383318698561751	0.4341529188701202	0.9337783033405179
1.0000437169448759	0.5638910270894965	0.4356788789819138
0.9998992277750489	0.9323756480698910	0.4362610103952234

0.2385206051979026	0.0649346980161697	0.9369001001508092
0.7502397321961275	0.5646618554782823	0.0634951692474085
0.9882791785693469	0.4328150496612047	0.5642096666271396
0.7557677885476611	0.8636736646971174	0.1334646033085050
0.2324592620670663	0.3639058433929810	0.8657545684632305
0.0060520939535171	0.6337078251610416	0.3670106772192339
0.0058409541946663	0.8625190746226920	0.3676475887599045
0.2326063982837752	0.1348183656129815	0.8683379564466678
0.7561224999487911	0.6347861406601628	0.1317149329187880
0.9823163305643998	0.3629359996299081	0.6327402172349247
0.6009632879621369	0.5259735308463791	0.7645107990944106
0.3324029097047893	0.0637528097789193	0.5363940739473263
0.6463543235825747	0.0495848867917993	0.5817942770240840
0.4062662221156515	0.9327432645101525	0.0354015506362812
0.5826616679789688	0.4314731626320629	0.9671360388406454
0.6566848355023530	0.5608168809632378	0.4601788410825933
0.6564636331039315	0.9311067331285297	0.4666469588659946
0.5823000746907067	0.0661686997914614	0.9667651468370236
0.4048115854749904	0.5704700132501475	0.0259165408278037
0.3309030851773615	0.4339928515192451	0.5360416212112672
0.5926034044537121	0.9479503856142953	0.0822380787438970
0.3941523167346668	0.4528828350700854	0.9100920820158989
0.3416153403267966	0.5523532774405923	0.4207080648457440
0.3425348609727372	0.9453579217289908	0.4211842829328056
0.3960073080088405	0.0513861586182777	0.9204883291719000
0.5928830084994858	0.5507588117197209	0.0808678398641430
0.6462134932085914	0.4419421431373673	0.5743188447620622
0.8321714687394147	0.0648380703152839	0.5343457157571823

0.1458129925017756	0.0498767444788120	0.5813268860063799
0.9061376746967267	0.9323762891237842	0.0347923327192775
0.0834161438579585	0.4292993897704365	0.9694867415614855
0.1567461939182667	0.5628866846837131	0.4634554790547491
0.1561617930013961	0.9313712970399328	0.4662328405400591
0.0821228775946746	0.0655473617898215	0.9662114536746190
0.9064315014093565	0.5656057219504593	0.0331718798529308
0.8315113322493104	0.4341514934292556	0.5369676876793373
0.0923682329198481	0.9468800474474308	0.0811374211680326
0.8961438234141288	0.4465861781431165	0.9188298152888935
0.8421895013797053	0.5521504433673927	0.4211815505445289
0.8424989393702979	0.9462739014815403	0.4193406157386048
0.8958092279415228	0.0505116503587838	0.9192413049994229
0.0939594712139206	0.5475642275377209	0.0847273026899481
0.1461237307712127	0.4446255932401932	0.5788460110505093

6.3 CH_4 adsorbed within NH_2-MIL-47

V O N C H

1.00000000000000

13.4985622067023545	-0.0499106585101045	0.0004153708946451
-0.0603251698209909	16.3701571256556981	-0.0000748273775932
0.0002956204400902	-0.0002037468052315	13.9030928643390528

8 40 8 65 44

Direct

0.1082701253474209	0.7542881983870945	0.2337241777376844
0.2994101474218915	0.2537685236455631	0.7622670989975716
0.3583120713067098	0.7541998070924475	0.2674621481625296
0.5494023148251719	0.2537630724210425	0.7388522984669456
0.7993934940522801	0.2538165439087398	0.7621341644419415
0.6083050172591103	0.7542068906842532	0.2335681732653069
0.8582738725679803	0.7542141691123391	0.2675572353222324
0.0494151555317725	0.2536958653711075	0.7390984128370623
0.1338346093543039	0.6673465438588463	0.3312814294050010
0.1345923416590705	0.8442921814526698	0.3273990763277946
0.2730242730976294	0.3406749191096374	0.6654692202509320
0.2721427578886873	0.1637029893089010	0.6682943071939440
0.2251413287626605	0.7529072973310013	0.1954193837880318
0.3845902810047996	0.8446621896093780	0.1744312742357023
0.0498720134477939	0.8374506886779235	0.1479416925306974
0.0504242717962057	0.6681495608188027	0.1493225208256690
0.4339800741490694	0.2528521031575736	0.6960532953906234
0.5230329541609003	0.3405547742167961	0.8358067551503587
0.6055974174164284	0.1715838342087214	0.6497070138101481
0.5222564164686425	0.1636321110240977	0.8327494526038697

0.6839896979283331	0.2527123071362934	0.8049692458733696
0.7720998666319168	0.1642473937348273	0.6674183980319974
0.6054740324191000	0.3403749742437467	0.6544927626180552
0.6338115219336811	0.6674222302401841	0.3313326815227282
0.6344920003811492	0.8444124293116426	0.3269818359162643
0.7252002363371743	0.7527490928351815	0.1953579473941506
0.9751534205038138	0.7525669591506788	0.3057918680450175
0.4751915613869718	0.7525470966676748	0.3056683278578998
0.5500577948920038	0.8371463431339444	0.1474860424173430
0.5503936990868420	0.6680131273803640	0.1493327802371213
0.9340386619503660	0.2527351728747850	0.6961620079778461
0.8553607749551450	0.3401573319444353	0.8469361585726692
0.8553907303657513	0.1712510680026502	0.8509009102631773
0.7731744291047823	0.3409563275129351	0.6656325889411795
0.8003722333962386	0.6677510293952846	0.3513365575950025
0.7999567373205898	0.8369081850838211	0.3539833025479611
0.8838583881680644	0.6678952514915961	0.1692315533100111
0.8843647189841295	0.8448639029426140	0.1747941020048024
0.1840157235537688	0.2527530887232252	0.8052008990786702
0.0230455421391807	0.3407247075493096	0.8357024074679518
0.1056502355736391	0.1711233233932350	0.6505689031828422
0.0219551054619318	0.1639004778223306	0.8334250242681311
0.1053437973214403	0.3400662748058272	0.6542834404880252
0.3553268221175181	0.3402836873720908	0.8467886824601671
0.3558342191649425	0.1713745334067226	0.8508557426388863
0.3003963110637619	0.6676678562723074	0.3512786239062706
0.3001309468250608	0.8368794035190709	0.3540320380446891
0.3838090098303301	0.6678021148890646	0.1692145691393200

0.5190368897676573	0.0849300437471906	0.5105510999520451
0.7693892647350407	0.0861979065709728	-0.0079667171539885
0.5282875023105480	0.5431076766105011	0.3995746779346458
0.7780910295926819	0.5438728139542804	0.1007414430111383
0.0186137637817446	0.0834579955864432	0.5128511430947968
0.2680557471617365	0.0825405516401310	-0.0130853645689691
0.0282509611408400	0.5429874854262545	0.3994127400262222
0.2784205464454437	0.5431186462698442	0.1017175776813754
0.1965162466693845	0.4378519857591042	0.5646466585796218
0.1122947012686510	0.4594908107473525	0.5136196088365563
0.1127642054331576	0.5258483599036401	0.4483747988893624
0.2037316566259400	0.5703856412614275	0.4365569451603072
0.2876135707584526	0.5476319895461254	0.4907012689594776
0.2859124819173695	0.4822221111657089	0.5536186782343278
0.2135706899974010	0.6393298783381184	0.3692632652724800
0.2147882693361479	0.8681290801464682	0.3675786386191660
0.2082212989326027	0.9381525607631698	0.4356101397696661
0.1188229719140904	0.9788651908143214	0.4446535486753656
0.1911325346127878	0.3678524092645554	0.6329134096211413
0.1901782974390365	0.1391249946600846	0.6315292984219451
0.1924561893791761	0.0703057557937256	0.5634076309519157
0.2820463345947912	0.0272336976327385	0.5531821095481607
0.4647251727328542	0.8684521286619039	0.1340808366834492
0.4581609785150158	0.9384255271557663	0.0659676811596596
0.3685142979800731	0.9786296245560373	0.0561243710083719
0.4411673210209683	0.3679117212987774	0.8682337458275123
0.4466014103351963	0.4379779979386452	0.9363826546213432
0.3624135338106807	0.4595724360492727	0.9875047799926817

0.6901828230760843	0.1397988511768532	0.6304393632124458
0.6925528301156252	0.0712118506206218	0.5619272181906426
0.7821009160913386	0.0281447878283319	0.5517655983245977
0.4403095133846224	0.1392108188494062	0.8697367460951837
0.4425329172420288	0.0704606533506459	0.9379492696778253
0.3575080086544117	0.0453821110312844	0.9923948656570705
0.6912594753206660	0.3681510062541851	0.6331212360058571
0.6966131837000447	0.4381499076117423	0.5648855709287400
0.6123728347210063	0.4597023720520770	0.5138401549763643
0.6127944318789729	0.5260267846905714	0.4485579458010734
0.7037274143030646	0.5706028489002658	0.4367589604718225
0.7876300740050249	0.5479449102071619	0.4909279046575791
0.7859816369358620	0.4825619274258270	0.5538785010326984
0.7135413373929330	0.6394525237538037	0.3693629933518905
0.7146237466688499	0.8682737651279236	0.3672501055494548
0.7080730857070523	0.9385007653165266	0.4349435068610525
0.6187374948120193	0.9793095519245701	0.4438189678756364
0.4635541453131508	0.6397240699912594	0.1313217334973761
0.4537387274834656	0.5707305599129450	0.0641140757499757
0.3628554293170371	0.5260375927140226	0.0525915025482388
0.9411618027190504	0.3679649646841678	0.8682335521886794
0.9465795487114695	0.4380797658341120	0.9363243842580488
0.8622491204425532	0.4599949693522001	0.9870173708080631
0.9399517681564120	0.1394993204579197	0.8702960391423477
0.9422284755485273	0.0710450234485507	0.9389797414807284
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6.4 CO_2 adsorbed within NH_2-MIL-47

V O N C H

1.00000000000000

13.4985622067023545 -0.0499106585101045 0.0004153708946451

-0.0603251698209909 16.3701571256556981 -0.0000748273775932

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8 42 8 65 40

Direct

0.1029535633472480 0.7582858545684444 0.2347255338176447

0.2938701704339048 0.2579351666810518 0.7629820818351037

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